Full wwPDB X-ray Structure Validation Report (i)

Aug 4, 2026 – 12:10 PM EDT

PDB ID	:	2O01 / pdb_00002o01
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 (i) symbol.

The types of validation reports are described at
http://www.wwpdb.org/validation/2017/FAQs#types.

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

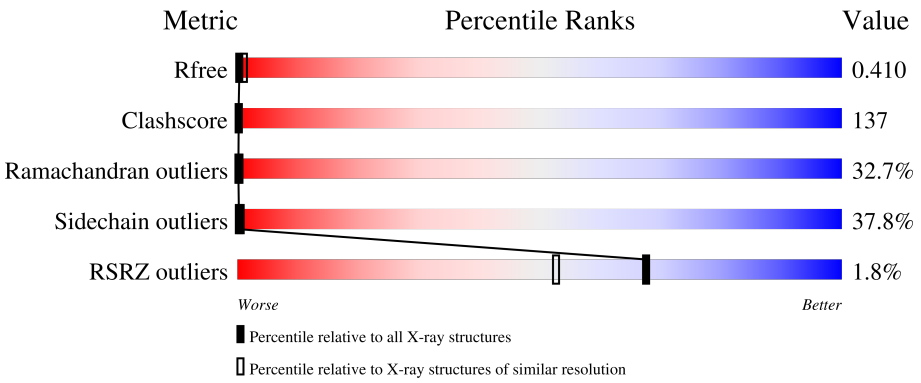
MolProbity	:	4-5-2 with Phenix2.0
Mogul	:	2022.3.0, CSD as543be (2022)
Xtriage (Phenix)	:	2.0
EDS	:	3.0
Buster-report	:	wwPDB partial adaption of 1.1.7 (2018)
Percentile statistics	:	20250101.v01 (using entries in the PDB archive January 1st 2025)
CCP4	:	9.0.015 (Gargrove)
Density-Fitness	:	1.0.12
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.50

1 Overall quality at a glance (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}	180053	1001 (3.44-3.36)
Clashscore	190562	1022 (3.44-3.36)
Ramachandran outliers	187476	1012 (3.44-3.36)
Sidechain outliers	187428	1012 (3.44-3.36)
RSRZ outliers	180081	1001 (3.44-3.36)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments of the lower bar indicate the fraction of residues that contain outliers for >=3, 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions <=5% 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	2% 5% 34% 41% 16% •
2	B	732	% 5% 40% 40% 15%
3	C	80	• 31% 40% 28%
4	D	138	2% 5% 31% 41% 23%
5	E	62	2% 6% 40% 34% 19%

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Mol	Chain	Length	Quality of chain
6	F	154	40% 38% 19%
7	G	95	2% 6% 33% 44% 17%
8	H	75	5% 37% 39% 19%
9	I	30	3% 43% 50% 7%
10	J	42	10% 48% 31% 12%
11	K	38	53% 45%
12	L	164	2% 6% 36% 40% 18%
13	N	85	44% 32% 24%
14	1	187	3% 14% 42% 31% 7% 6%
15	2	186	% 13% 37% 25% 15% 11%
16	3	165	% 8% 28% 27% 7% 30%
17	4	165	4% 12% 44% 32% 13%

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	4	1304	X	-	-	-
18	CLA	A	1103	-	-	X	-
18	CLA	A	1107	X	-	-	-
18	CLA	A	1119	X	-	-	-
18	CLA	A	1122	X	-	-	-
18	CLA	A	1123	X	-	X	-
18	CLA	A	1126	X	-	X	-
18	CLA	A	1128	X	-	-	-
18	CLA	A	1129	X	-	-	-
18	CLA	A	1136	X	-	X	-
18	CLA	A	1137	X	-	-	-
18	CLA	A	1140	X	-	X	-
18	CLA	A	9011	X	-	X	-
18	CLA	B	1138	X	-	X	-
18	CLA	B	1202	-	-	X	-
18	CLA	B	1205	X	-	-	-
18	CLA	B	1207	X	-	-	-

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Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
18	CLA	B	1208	X	-	-	-
18	CLA	B	1209	X	-	X	-
18	CLA	B	1212	X	-	-	-
18	CLA	B	1214	-	-	X	-
18	CLA	B	1215	-	-	X	-
18	CLA	B	1216	X	-	X	-
18	CLA	B	1218	-	-	X	-
18	CLA	B	1220	X	-	X	-
18	CLA	B	1222	X	-	-	-
18	CLA	B	1225	-	-	X	-
18	CLA	B	1228	X	-	X	-
18	CLA	B	1232	X	-	-	-
18	CLA	B	1234	-	-	X	-
18	CLA	B	1235	X	-	-	-
18	CLA	B	1238	-	-	X	-
18	CLA	B	1239	X	-	X	-
18	CLA	B	9010	-	-	X	-
18	CLA	B	9012	X	-	-	-
18	CLA	F	1302	X	-	-	-
18	CLA	H	1501	X	-	-	-
18	CLA	I	1204	X	-	-	-
18	CLA	J	2107	X	-	-	-
18	CLA	L	1503	-	-	X	-
18	CLA	L	1504	X	-	-	-
19	PQN	A	5001	X	-	X	-
19	PQN	B	5002	X	-	-	-
21	SF4	B	3101	-	-	X	-
21	SF4	C	3102	-	-	X	-
21	SF4	C	3103	-	-	X	-

2 Entry composition (i)

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
			Total	C	N	O	S			
1	A	728	5732	3758	975	981	18	0	0	0

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
			Total	C	N	O	S			
2	B	732	5844	3841	996	994	13	0	0	0

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
			Total	C	N	O	S			
3	C	80	611	379	107	114	11	0	0	0

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

- Molecule 14 is a protein called AT3g54890.

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

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

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

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

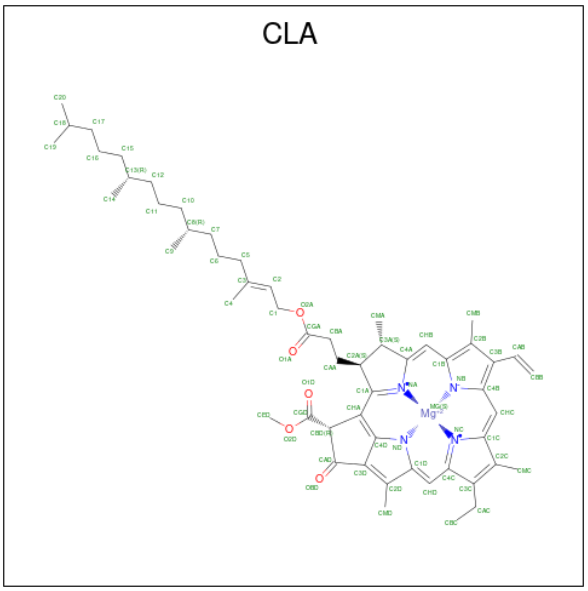
- Molecule 16 is a protein called PSI type III chlorophyll a/b-binding protein.

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

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

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

- Molecule 18 is CHLOROPHYLL A (CCD ID: CLA) (formula: $C_{55}H_{72}MgN_4O_5$).



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

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

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

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

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

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

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

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

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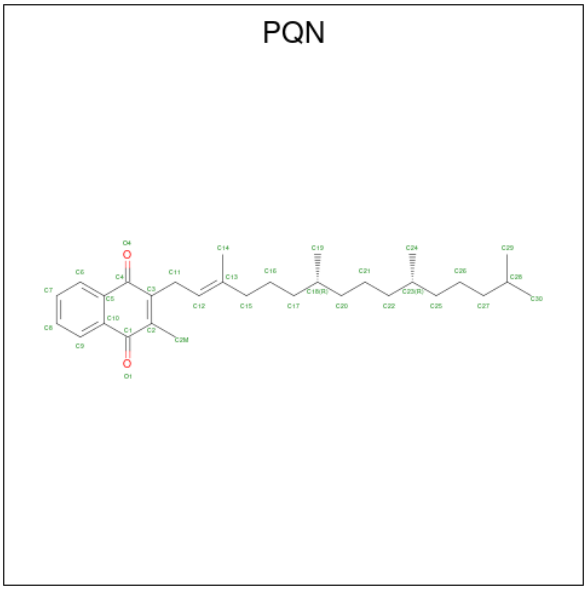
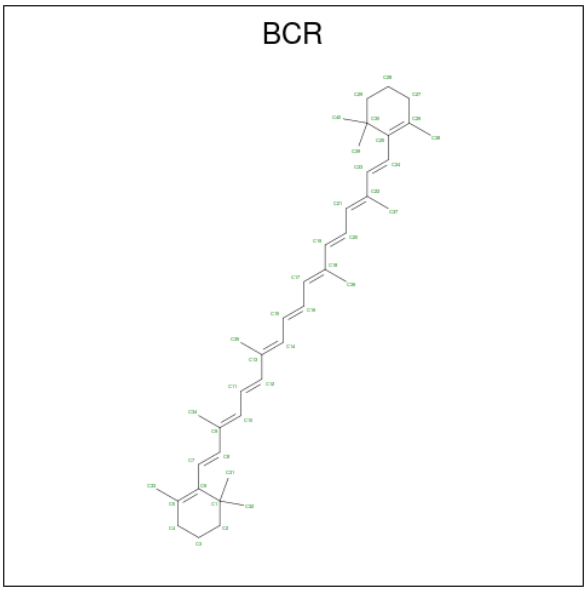
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
			Total	C	Mg	N		
18	4	1	25	20	1	4	0	0
			Total	C	Mg	N		
18	4	1	25	20	1	4	0	0
			Total	C	Mg	N		
18	4	1	25	20	1	4	0	0
			Total	C	Mg	N		
18	4	1	25	20	1	4	0	0
			Total	C	Mg	N		
18	4	1	25	20	1	4	0	0
			Total	C	Mg	N		
18	4	1	25	20	1	4	0	0
			Total	C	Mg	N		
18	4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

- Molecule 19 is PHYLLOQUINONE (CCD ID: PQN) (formula: $C_{31}H_{46}O_2$).



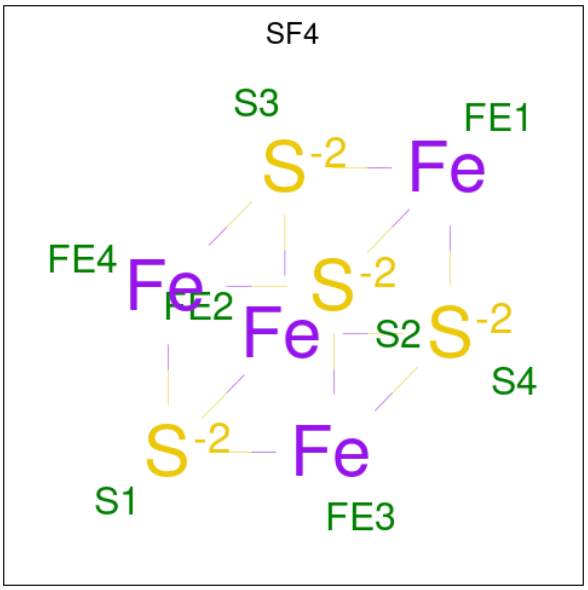
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
			Total	C	O		
19	A	1	33	31	2	0	0
			Total	C	O		
19	B	1	33	31	2	0	0

- Molecule 20 is BETA-CAROTENE (CCD ID: BCR) (formula: $C_{40}H_{56}$).



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

- Molecule 21 is IRON/SULFUR CLUSTER (CCD ID: SF4) (formula: Fe_4S_4).



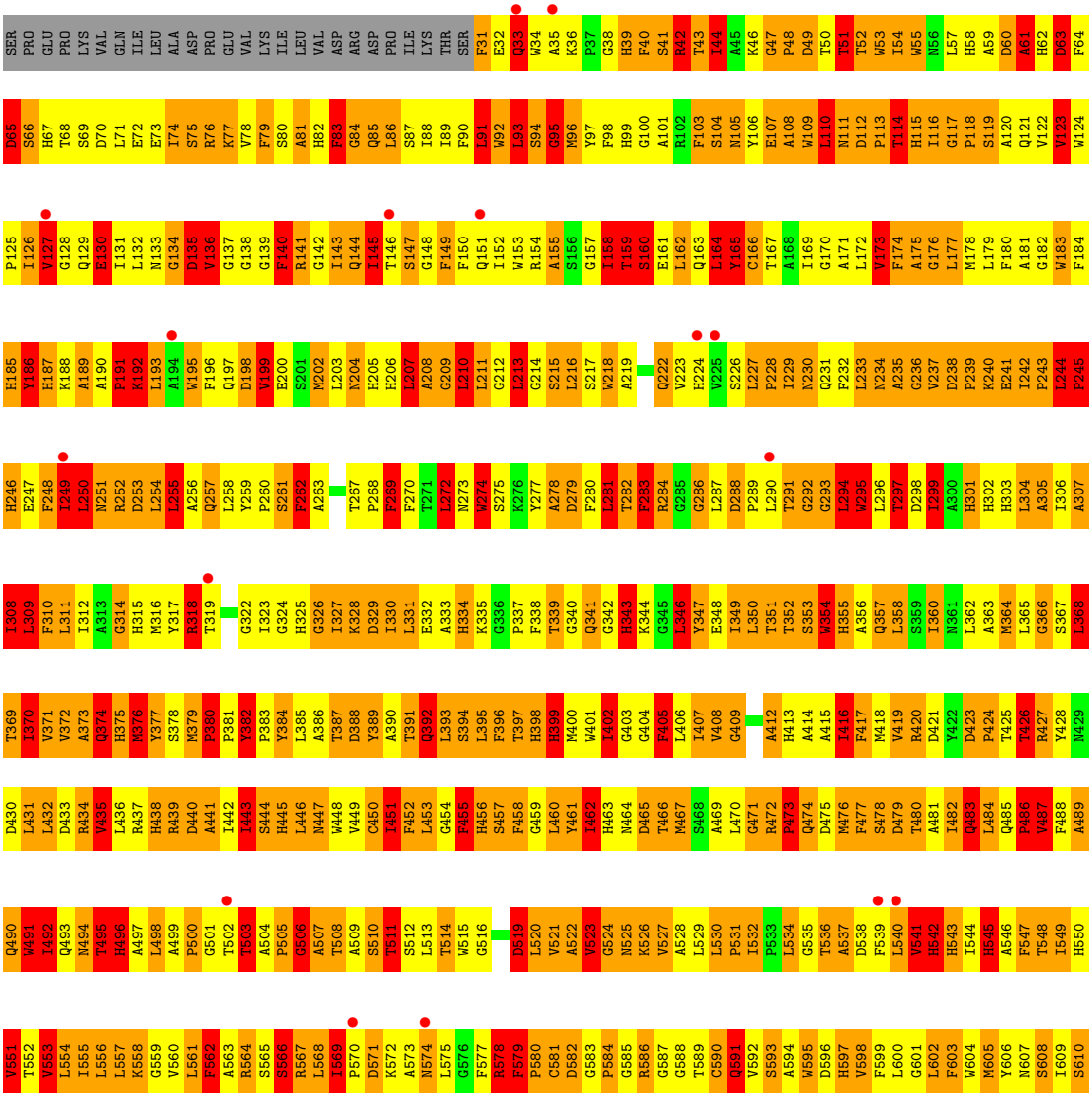
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
			Total	Fe	S		
21	B	1	8	4	4	0	0
			Total	Fe	S		
21	C	1	8	4	4	0	0
			Total	Fe	S		
21	C	1	8	4	4	0	0

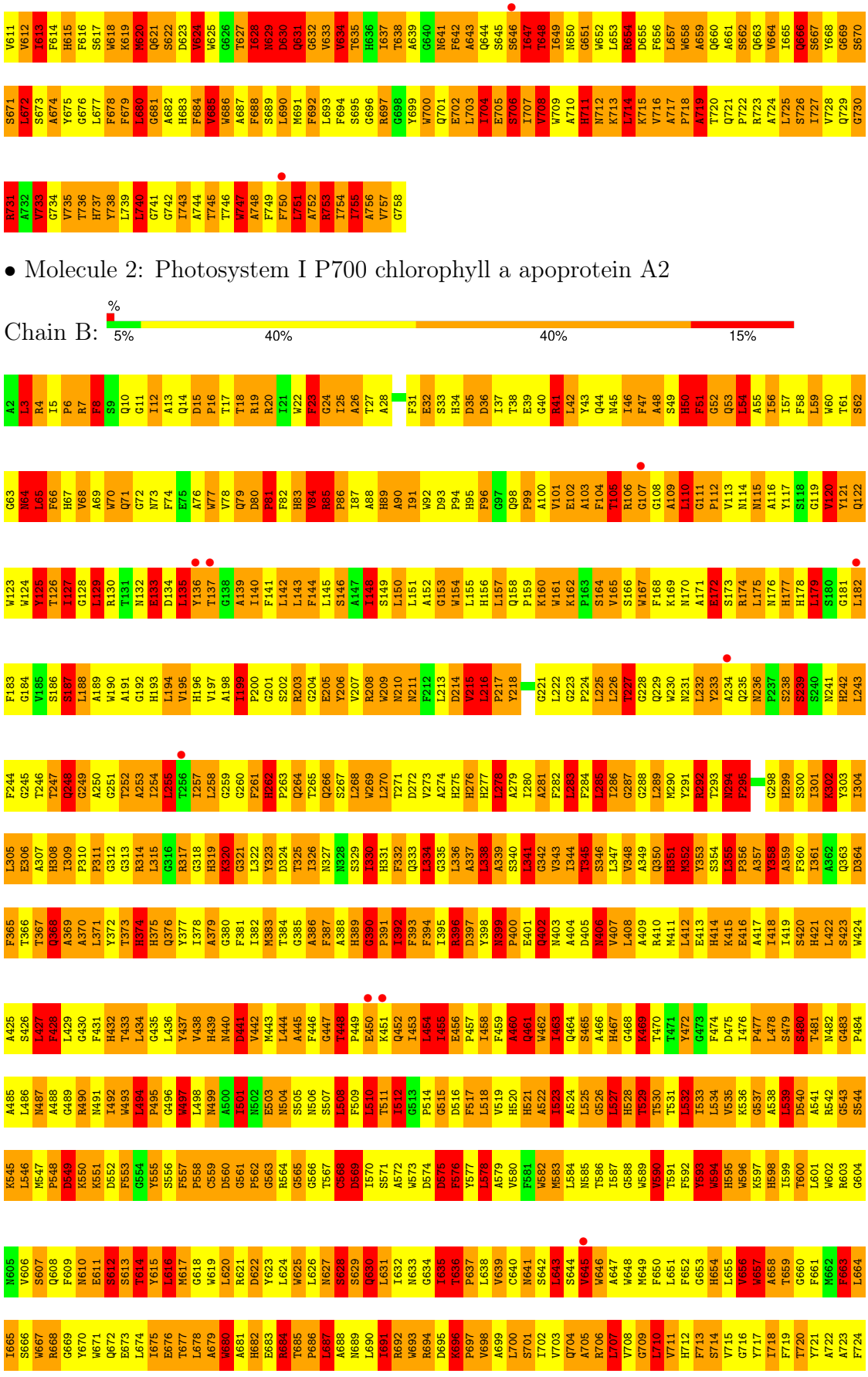
3 Residue-property plots (i)

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

Chain A:





• Molecule 2: Photosystem I P700 chlorophyll a apoprotein A2

Chain B: % 5% 40% 40% 15%

L725 I726 A727 S728 T729 S730 G731 K732 F733

• Molecule 3: Photosystem I iron-sulfur center

Chain C: 31% 40% 28%

S2 H3 S4 V5 K6 I7 Y8 D9 T10 C11 I12 G13 C14 T15 Q16 C17 V18 R19 A20 C21 P22 T23 D24 V25 L26 E27 M28 I29 P30 W31 G32 G33 C34 K35 A36 K37 Q38 I39 A40 S41 A42 P43 R44 T45 E46 D47 C48 V49 G50 C51 K52 R53 C54 E55 S56 A57 C58 P59 T60 D61

F62 L63 S64 V65 R66 V67 Y68 L69 W70 H71 E72 T73 T74 R75 S76 M77 G78 L79 A80 Y81

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

Chain D: 2% 5% 31% 41% 23%

E19 L20 D21 P22 N23 T24 P25 S26 P27 I28 F29 A30 G31 S32 T33 G34 G35 L36 L37 R38 K39 A40 Q41 V42 E43 E44 F45 Y46 V47 T48 T49 W50 E51 S52 P53 K54 E55 Q56 I57 F58 E59 N60 P61 T62 G63 G64 A65 A66 I67 M68 R69 E70 G71 P72 N73 L74 L75 K76 L77 A78

R79 K80 E81 Q82 C83 L84 A85 L86 G87 T88 R89 L90 R91 S92 K93 Y94 K95 I96 K97 Y98 Q99 F100 Y101 R102 V103 F104 P105 S106 G107 E108 V109 Q110 Y111 L112 H113 P114 K115 D116 G117 V118 Y119 P120 E121 K122 V123 N124 P125 G126 R127 Q128 G129 V130 G131 L132 N133 M134 R135 S136 I137 G138

K139 N140 V141 S142 P143 I144 E145 V146 K147 F148 T149 G150 K151 Q152 P153 Y154 D155 L156

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

Chain E: 2% 6% 40% 34% 19%

P30 K31 R32 G33 S34 K35 V36 K37 I38 L39 R40 R41 E42 S43 Y44 W45 F46 K47 N48 V49 G50 S51 V52 V53 A54 V55 D56 Q57 D58 P59 K60 T61 R62 Y63 P64 V65 V66 V67 R68 F69 A70 K71 V72 N73 Y74 A75 N76 I77 S78 T79 N80 N81 Y82 A83 L84 D85 E86 V87 E88 E89

V90 A91

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

Chain F: 40% 38% 19%

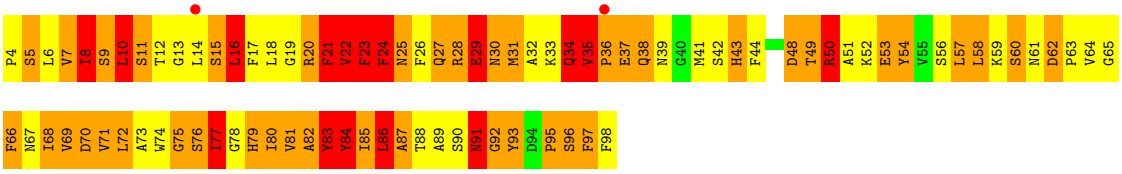
D1 I2 A3 G4 L5 T6 P7 C8 K9 E10 S11 K12 Q13 F14 A15 K16 R17 E18 K19 Q20 A21 L22 K23 K24 L25 Q26 A27 S28 L29 K30 L31 Y32 A33 D34 D35 S36 A37 P38 A39 L40 A41 I42 K43 A44 T45 M46 E47 K48 T49 K50 K51 R52 F53 D54 N55 Y56 G57 K58 Y59 G60

L61 L62 G63 G64 S65 D66 G67 L68 P69 H70 L71 I72 V73 S74 G75 D76 Q77 R78 H79 W80 G81 E82 R83 I84 T85 P86 G87 I88 L89 F90 L91 Y92 I93 A94 G95 W96 I97 G98 W99 V100 G101 R102 S103 Y104 L105 I106 A107 I108 R109 D110 E111 K112 K113 P114 I115 Q116 K117 E118 I119 I120

I121 D122 V123 P124 L125 A126 S127 S128 L129 L130 F131 R132 G133 F134 S135 W136 P137 V138 A139 A140 Y141 R142 E143 L144 L145 N146 G147 E148 L149 V150 D151 N152 N153 F154

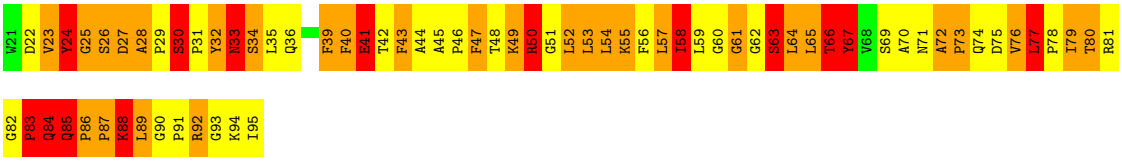
• Molecule 7: Photosystem I reaction center subunit V, chloroplast

Chain G: 2% 6% 33% 44% 17%



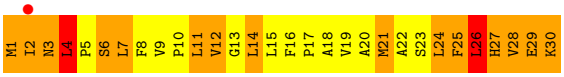
- Molecule 8: Photosystem I reaction center subunit VI, chloroplast

Chain H:



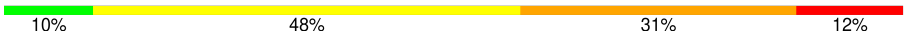
- Molecule 9: Photosystem I reaction center subunit VIII

Chain I:



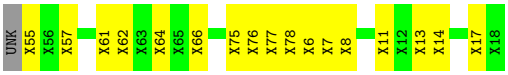
- Molecule 10: Photosystem I reaction center subunit IX

Chain J:



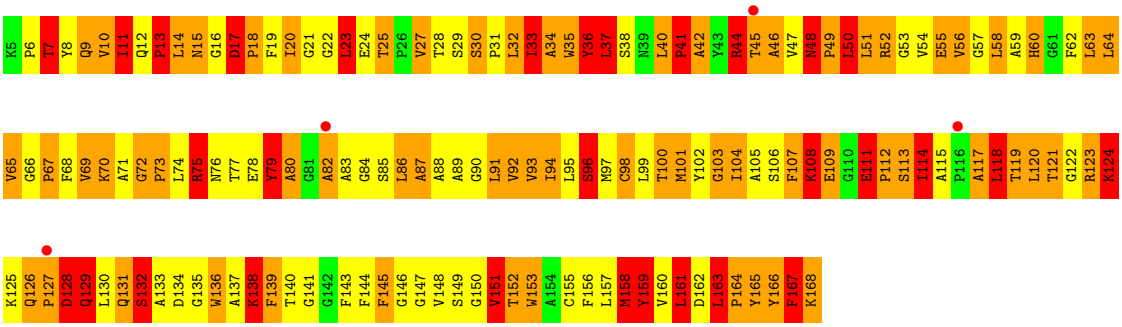
- Molecule 11: Photosystem I reaction center subunit psaK, chloroplast

Chain K:



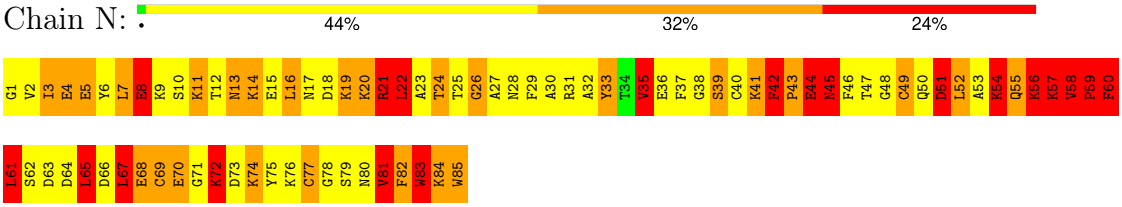
- Molecule 12: Photosystem I reaction center subunit XI, chloroplast

Chain L:



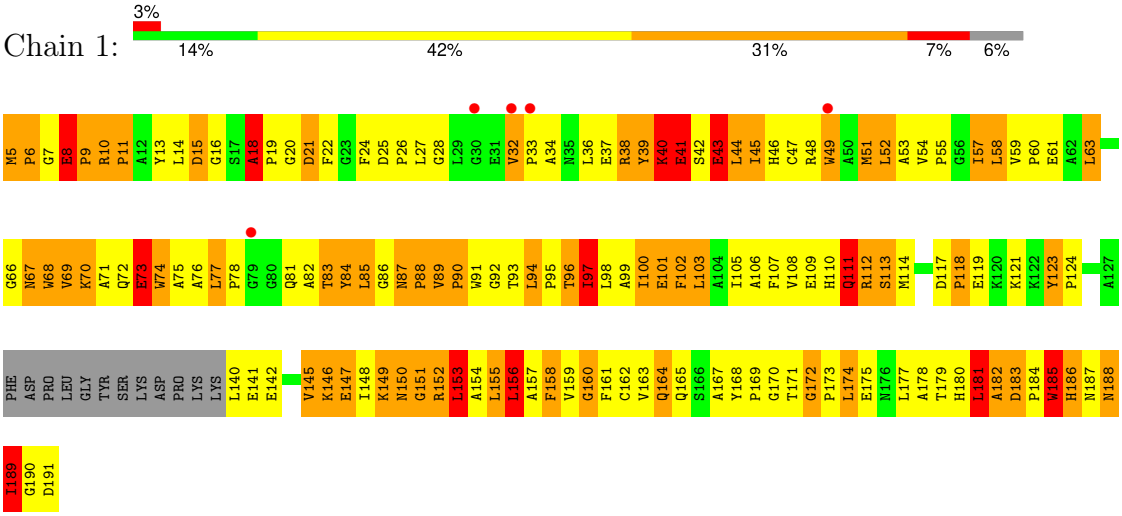
• Molecule 13: Photosystem I-N subunit

Chain N:



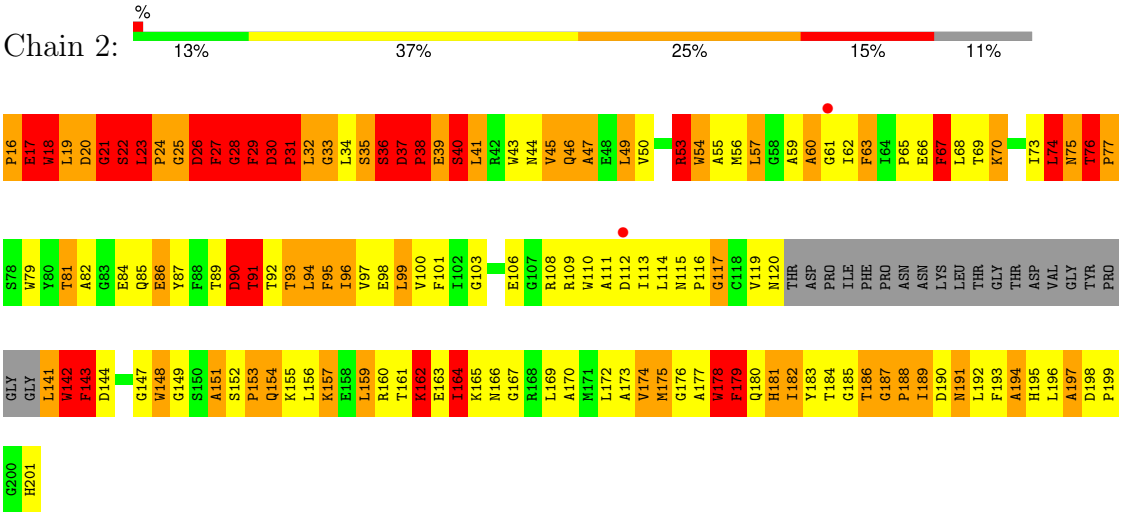
• Molecule 14: AT3g54890

Chain 1:



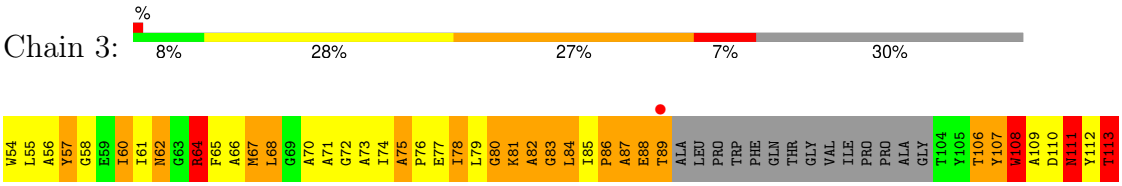
• Molecule 15: Type II chlorophyll a/b binding protein from photosystem I

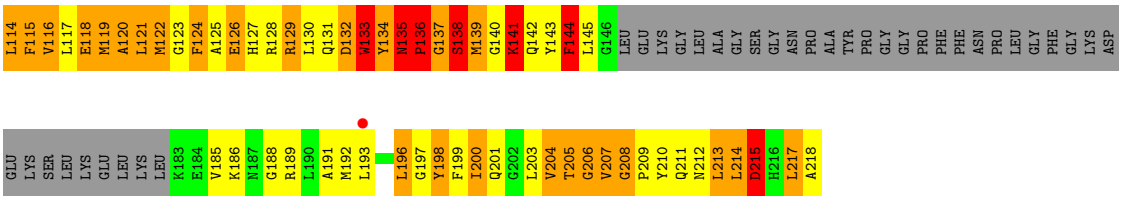
Chain 2:



• Molecule 16: PSI type III chlorophyll a/b-binding protein

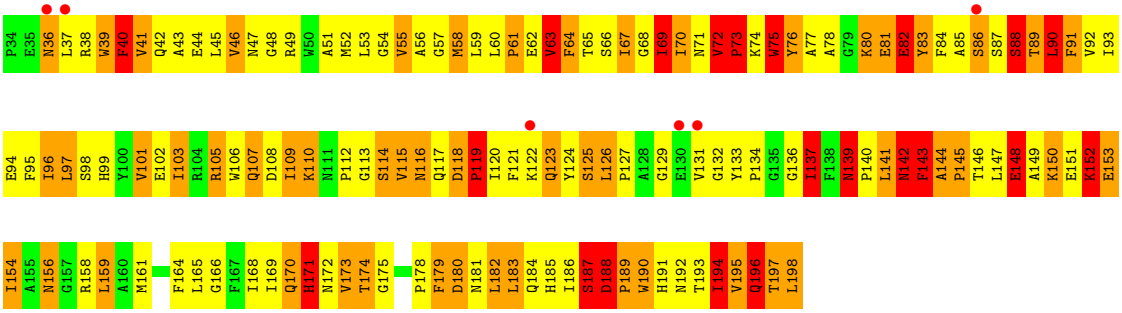
Chain 3:





- Molecule 17: PSI light-harvesting antenna chlorophyll a/b-binding protein

Chain 4:



4 Data and refinement statistics (i)

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 40.00 – 3.40	Depositor EDS
% Data completeness (in resolution range)	90.8 (40.00-3.40) 76.1 (40.00-3.40)	Depositor EDS
R_{merge}	0.14	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	2.32 (at 3.01Å)	Xtriage
Refinement program	REFMAC 5.2.0019	Depositor
R, R_{free}	0.348 , 0.409 0.353 , 0.410	Depositor DCC
R_{free} test set	3517 reflections (3.15%)	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)	0.38 , 976.7	EDS
L-test for twinning[2]	$< \|L\| > = 0.49$, $< L^2 > = 0.32$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o,F_c correlation	0.85	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.*

[1]Intensities estimated from amplitudes.

[2]Theoretical values of $< |L| >$, $< L^2 >$ for acentric reflections are 0.5, 0.333 respectively for untwinned datasets, and 0.375, 0.2 for perfectly twinned datasets.

5 Model quality (i)

5.1 Standard geometry (i)

Bond lengths and bond angles in the following residue types are not validated in this section: 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	0.98	6/5928 (0.1%)	1.46	90/8092 (1.1%)
2	B	0.98	7/6054 (0.1%)	1.45	98/8273 (1.2%)
3	C	1.26	5/624 (0.8%)	1.65	18/846 (2.1%)
4	D	1.10	3/1122 (0.3%)	1.59	24/1514 (1.6%)
5	E	0.90	0/513	1.46	14/694 (2.0%)
6	F	0.99	0/1250	1.50	25/1687 (1.5%)
7	G	0.93	1/764 (0.1%)	1.54	15/1035 (1.4%)
8	H	1.01	0/595	1.59	16/810 (2.0%)
9	I	1.04	0/235	1.44	2/320 (0.6%)
10	J	1.01	0/356	1.44	8/484 (1.7%)
12	L	0.99	1/1272 (0.1%)	1.56	39/1736 (2.2%)
13	N	0.74	0/699	1.43	9/936 (1.0%)
14	1	0.80	0/1215	1.28	16/1666 (1.0%)
15	2	0.93	3/1309 (0.2%)	1.60	21/1787 (1.2%)
16	3	0.76	0/879	1.25	9/1194 (0.8%)
17	4	0.87	1/1319 (0.1%)	1.21	11/1797 (0.6%)
All	All	0.96	27/24134 (0.1%)	1.46	415/32871 (1.3%)

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 (27) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
15	2	40	SER	C-N	-8.54	1.21	1.33
2	B	455	ILE	CA-CB	7.01	1.61	1.53
3	C	9	ASP	N-CA	6.86	1.55	1.45
2	B	89	HIS	CA-C	6.52	1.58	1.52
4	D	48	ILE	CA-CB	6.30	1.62	1.54
3	C	8	TYR	N-CA	6.26	1.54	1.46
2	B	164	SER	N-CA	6.23	1.50	1.46
7	G	85	ILE	CA-CB	6.21	1.61	1.54
4	D	49	THR	CA-CB	6.17	1.63	1.53
3	C	7	ILE	CA-C	6.02	1.60	1.52
1	A	664	VAL	CA-CB	5.94	1.61	1.54
1	A	391	THR	CA-CB	5.92	1.63	1.53
1	A	541	VAL	CA-CB	5.83	1.62	1.54
15	2	76	THR	CA-CB	5.81	1.62	1.53
2	B	137	THR	CA-CB	5.60	1.63	1.54
3	C	8	TYR	CA-C	5.56	1.60	1.52
15	2	76	THR	CA-C	5.52	1.59	1.52
4	D	49	THR	N-CA	5.44	1.52	1.46
2	B	523	ILE	CA-CB	5.30	1.61	1.54
1	A	435	VAL	CA-CB	5.25	1.60	1.54
12	L	33	ILE	CA-CB	5.23	1.61	1.54
3	C	7	ILE	CA-CB	5.21	1.61	1.54
2	B	710	LEU	CA-C	5.12	1.58	1.53
17	4	119	PRO	N-CD	5.11	1.54	1.47
2	B	345	THR	CA-C	5.10	1.59	1.52
1	A	489	ALA	CA-C	5.04	1.59	1.52
1	A	646	SER	N-CA	5.02	1.51	1.46

All (415) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
15	2	37	ASP	CA-C-N	22.23	147.63	119.84
15	2	37	ASP	C-N-CA	22.23	147.63	119.84
4	D	26	SER	C-N-CD	-17.32	82.50	120.60
15	2	40	SER	CA-C-N	-16.24	90.53	121.54
15	2	40	SER	C-N-CA	-16.24	90.53	121.54
13	N	42	PHE	CA-C-N	15.67	139.43	119.84
13	N	42	PHE	C-N-CA	15.67	139.43	119.84
7	G	58	LEU	N-CA-C	-14.25	94.23	112.90
6	F	72	ILE	N-CA-C	13.45	127.67	107.77
1	A	379	MET	CA-C-N	12.90	133.67	120.38
1	A	379	MET	C-N-CA	12.90	133.67	120.38
2	B	390	GLY	CA-C-N	-11.87	105.00	119.84
2	B	390	GLY	C-N-CA	-11.87	105.00	119.84
1	A	117	GLY	CA-C-N	11.35	134.02	119.84
1	A	117	GLY	C-N-CA	11.35	134.02	119.84
2	B	718	ILE	N-CA-C	-11.15	99.45	110.72
1	A	105	ASN	N-CA-C	-11.14	98.64	114.12
2	B	299	HIS	N-CA-C	10.99	126.00	110.50
1	A	686	TRP	N-CA-C	-10.94	100.42	113.88
4	D	115	LYS	N-CA-C	-10.76	98.81	112.90
2	B	89	HIS	N-CA-C	10.09	125.64	112.72
1	A	545	HIS	N-CA-C	-9.91	100.55	111.36
2	B	696	LYS	CA-C-N	9.52	131.74	119.84
2	B	696	LYS	C-N-CA	9.52	131.74	119.84
3	C	9	ASP	N-CA-C	9.37	121.80	110.19
7	G	80	ILE	N-CA-C	-9.34	103.93	112.90
1	A	412	ALA	N-CA-C	-9.28	101.50	112.92
12	L	95	LEU	N-CA-C	-9.20	101.97	113.01
1	A	213	LEU	N-CA-C	-9.15	101.22	112.38
2	B	239	SER	N-CA-C	9.00	123.77	108.02
2	B	636	THR	CA-C-N	8.88	130.94	119.84
2	B	636	THR	C-N-CA	8.88	130.94	119.84
6	F	25	LEU	N-CA-C	-8.84	101.56	111.82
17	4	133	TYR	CA-C-N	8.80	130.84	119.84
17	4	133	TYR	C-N-CA	8.80	130.84	119.84
12	L	17	ASP	CA-C-N	8.67	130.68	119.84
12	L	17	ASP	C-N-CA	8.67	130.68	119.84
1	A	747	TRP	N-CA-C	-8.65	103.57	114.56
2	B	314	ARG	N-CA-C	-8.64	101.18	112.41
2	B	341	LEU	N-CA-C	-8.63	101.46	113.37
1	A	244	LEU	CA-C-N	8.61	130.60	119.84
1	A	244	LEU	C-N-CA	8.61	130.60	119.84
2	B	561	GLY	CA-C-N	8.55	130.53	119.84

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	B	561	GLY	C-N-CA	8.55	130.53	119.84
12	L	48	ASN	CA-C-N	8.50	130.47	119.84
12	L	48	ASN	C-N-CA	8.50	130.47	119.84
1	A	211	LEU	N-CA-C	-8.49	99.99	111.96
15	2	30	ASP	CA-C-N	8.41	130.36	119.84
15	2	30	ASP	C-N-CA	8.41	130.36	119.84
2	B	406	ASN	N-CA-C	8.40	122.10	108.41
2	B	575	ASP	N-CA-C	-8.37	103.67	114.04
2	B	24	GLY	N-CA-C	-8.29	93.54	113.18
2	B	576	PHE	N-CA-C	-8.16	102.46	111.36
2	B	386	ALA	N-CA-C	-8.15	104.48	114.75
1	A	731	ARG	N-CA-C	-8.13	101.53	112.26
1	A	380	PRO	N-CA-C	8.12	120.61	110.70
1	A	124	TRP	CA-C-N	8.12	129.99	119.84
1	A	124	TRP	C-N-CA	8.12	129.99	119.84
1	A	270	PHE	N-CA-C	-8.12	102.43	111.28
1	A	218	TRP	N-CA-C	-8.09	104.29	114.56
1	A	309	LEU	N-CA-C	-8.05	97.76	109.59
2	B	10	GLN	N-CA-C	-8.00	102.16	111.03
2	B	269	TRP	N-CA-C	7.97	122.08	110.28
1	A	753	ARG	N-CA-C	-7.95	102.31	110.97
3	C	40	ALA	N-CA-C	7.82	121.12	108.76
16	3	205	THR	N-CA-C	7.82	120.49	107.20
12	L	141	GLY	N-CA-C	-7.75	105.04	114.66
2	B	709	GLY	N-CA-C	-7.64	103.56	112.73
17	4	80	LYS	CA-C-O	7.63	122.37	117.94
2	B	501	ILE	N-CA-C	7.62	125.19	109.34
2	B	129	LEU	N-CA-C	7.58	121.23	110.23
5	E	51	SER	N-CA-C	7.57	126.92	110.80
2	B	218	TYR	CA-C-N	7.54	127.08	119.24
2	B	218	TYR	C-N-CA	7.54	127.08	119.24
2	B	358	TYR	N-CA-C	7.52	118.48	107.88
12	L	30	SER	CA-C-N	7.50	129.22	119.84
12	L	30	SER	C-N-CA	7.50	129.22	119.84
13	N	44	GLU	CA-C-N	7.48	135.16	121.70
13	N	44	GLU	C-N-CA	7.48	135.16	121.70
6	F	132	ARG	N-CA-C	-7.46	104.70	113.88
1	A	477	PHE	N-CA-C	7.42	122.36	113.16
1	A	145	ILE	N-CA-C	7.41	118.56	107.75
12	L	46	ALA	N-CA-C	7.36	118.89	108.00
3	C	47	ASP	N-CA-C	-7.36	103.14	112.93
1	A	255	LEU	N-CA-C	-7.35	103.27	111.28

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
6	F	5	LEU	N-CA-C	-7.33	90.48	111.00
2	B	663	PHE	N-CA-C	-7.28	99.11	109.96
12	L	122	GLY	N-CA-C	-7.22	102.49	114.48
6	F	97	ILE	N-CA-C	-7.22	103.26	110.62
3	C	68	TYR	N-CA-C	7.21	126.17	110.80
15	2	31	PRO	N-CA-C	7.21	127.33	112.47
3	C	21	CYS	CA-C-N	7.20	128.84	119.84
3	C	21	CYS	C-N-CA	7.20	128.84	119.84
2	B	616	LEU	N-CA-C	7.14	121.74	112.89
8	H	30	SER	CA-C-N	7.14	128.76	119.84
8	H	30	SER	C-N-CA	7.14	128.76	119.84
6	F	6	THR	CA-C-N	7.13	128.75	119.84
6	F	6	THR	C-N-CA	7.13	128.75	119.84
1	A	491	TRP	CA-C-N	7.11	134.51	121.70
1	A	491	TRP	C-N-CA	7.11	134.51	121.70
12	L	139	PHE	N-CA-C	-7.11	102.94	111.69
1	A	66	SER	N-CA-C	-7.10	103.58	113.37
1	A	47	GLY	CA-C-N	7.09	128.71	119.84
1	A	47	GLY	C-N-CA	7.09	128.71	119.84
3	C	77	MET	N-CA-C	-7.08	104.77	113.19
12	L	96	SER	N-CA-C	-7.07	105.19	114.31
2	B	82	PHE	N-CA-C	7.06	125.84	110.80
1	A	735	VAL	CB-CA-C	-7.03	104.76	111.44
1	A	737	HIS	N-CA-C	7.02	118.72	111.14
6	F	68	LEU	CA-C-N	7.01	128.61	119.84
6	F	68	LEU	C-N-CA	7.01	128.61	119.84
6	F	2	ILE	N-CA-C	6.97	117.91	107.80
1	A	192	LYS	N-CA-C	6.95	125.61	110.80
2	B	351	HIS	N-CA-C	-6.94	99.76	110.10
1	A	520	LEU	N-CA-C	6.91	120.17	108.90
2	B	460	ALA	N-CA-C	-6.90	102.61	111.02
1	A	748	ALA	N-CA-C	-6.89	103.85	111.36
1	A	461	TYR	N-CA-C	-6.89	103.39	111.03
8	H	40	PHE	N-CA-C	6.89	121.76	112.88
7	G	92	GLY	N-CA-C	-6.88	96.87	113.18
14	1	177	LEU	N-CA-C	-6.88	103.78	112.93
4	D	100	PHE	N-CA-C	6.84	118.50	108.86
6	F	51	LYS	N-CA-C	-6.83	105.35	113.21
1	A	164	LEU	N-CA-C	-6.81	104.72	113.16
3	C	8	TYR	N-CA-C	6.81	125.30	110.80
10	J	2	ARG	CA-C-N	6.80	133.94	121.70
10	J	2	ARG	C-N-CA	6.80	133.94	121.70

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	B	289	LEU	N-CA-C	-6.75	101.65	111.30
10	J	39	PHE	N-CA-C	6.71	124.65	109.81
2	B	668	ARG	N-CA-C	6.71	121.82	111.56
4	D	23	ASN	N-CA-C	6.70	125.08	110.80
6	F	151	ASP	CA-C-N	6.70	133.75	121.70
6	F	151	ASP	C-N-CA	6.70	133.75	121.70
4	D	119	TYR	C-N-CD	-6.66	97.69	125.00
12	L	163	LEU	CA-C-N	6.66	128.17	119.84
12	L	163	LEU	C-N-CA	6.66	128.17	119.84
14	1	32	VAL	N-CA-C	6.65	123.25	108.88
13	N	16	LEU	N-CA-C	-6.64	105.58	113.21
15	2	57	LEU	N-CA-C	-6.63	104.05	111.28
15	2	25	GLY	N-CA-C	6.63	123.80	114.85
15	2	30	ASP	N-CA-C	6.61	124.42	109.81
5	E	81	ASN	N-CA-C	6.61	120.14	110.17
14	1	51	MET	N-CA-C	-6.58	102.99	111.02
7	G	91	ASN	N-CA-C	-6.56	103.95	112.68
14	1	123	TYR	CA-C-N	6.56	128.04	119.84
14	1	123	TYR	C-N-CA	6.56	128.04	119.84
6	F	109	ARG	N-CA-C	-6.55	106.50	114.75
4	D	95	LYS	N-CA-C	6.52	118.74	110.33
4	D	128	GLN	N-CA-C	6.52	118.28	110.19
15	2	111	ALA	N-CA-C	-6.52	100.59	110.70
4	D	41	GLN	N-CA-C	-6.51	105.16	113.23
12	L	25	THR	CA-C-N	-6.47	113.62	120.03
12	L	25	THR	C-N-CA	-6.47	113.62	120.03
12	L	165	TYR	N-CA-C	6.47	120.48	107.41
15	2	46	GLN	N-CA-C	-6.47	107.25	114.62
4	D	60	MET	CA-C-N	6.46	127.92	119.84
4	D	60	MET	C-N-CA	6.46	127.92	119.84
3	C	42	ALA	CA-C-N	6.42	127.86	119.84
3	C	42	ALA	C-N-CA	6.42	127.86	119.84
12	L	166	TYR	N-CA-C	6.41	120.42	112.03
2	B	133	GLU	N-CA-C	-6.37	105.47	113.18
12	L	56	VAL	N-CA-CB	6.37	117.56	110.62
12	L	72	GLY	C-N-CD	-6.37	98.90	125.00
1	A	360	ILE	N-CA-C	6.34	117.02	110.36
5	E	72	VAL	N-CA-C	6.34	119.09	108.81
2	B	35	ASP	N-CA-C	6.30	120.05	111.17
1	A	242	ILE	N-CA-C	6.29	114.38	108.15
2	B	292	ARG	N-CA-C	6.29	118.69	108.76
7	G	52	LYS	N-CA-C	6.28	119.78	110.48

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	B	295	PHE	N-CA-C	6.28	124.17	110.80
2	B	399	ASN	CB-CA-C	6.27	117.13	110.17
8	H	72	ALA	CA-C-N	6.25	127.66	119.84
8	H	72	ALA	C-N-CA	6.25	127.66	119.84
4	D	152	GLN	CA-C-N	6.25	127.65	119.84
4	D	152	GLN	C-N-CA	6.25	127.65	119.84
2	B	469	LYS	N-CA-C	6.25	118.77	109.59
17	4	40	PHE	N-CA-C	6.24	121.56	113.88
1	A	634	VAL	N-CA-C	6.24	119.80	111.44
1	A	672	LEU	N-CA-C	-6.23	105.77	113.19
2	B	125	TYR	N-CA-C	-6.19	97.61	110.80
7	G	97	PHE	N-CA-C	6.19	119.95	111.54
4	D	134	MET	N-CA-C	-6.17	105.46	112.87
16	3	135	ASN	CA-C-N	6.17	127.55	119.84
16	3	135	ASN	C-N-CA	6.17	127.55	119.84
4	D	97	LYS	N-CA-C	6.12	123.83	110.80
8	H	85	GLN	N-CA-C	-6.12	96.30	109.81
1	A	562	PHE	N-CA-C	-6.11	100.99	110.10
15	2	164	ILE	N-CA-C	-6.11	103.26	111.44
2	B	700	LEU	N-CA-C	6.09	118.34	108.41
2	B	179	LEU	N-CA-C	-6.09	102.25	111.56
2	B	287	GLY	N-CA-C	-6.07	106.87	115.43
2	B	338	LEU	N-CA-C	-6.06	106.53	114.04
5	E	39	LEU	N-CA-C	6.06	118.69	107.60
5	E	45	TRP	CA-C-N	6.06	132.60	121.70
5	E	45	TRP	C-N-CA	6.06	132.60	121.70
2	B	91	ILE	N-CA-C	6.05	115.07	106.53
9	I	2	ILE	N-CA-C	6.05	118.93	108.95
3	C	7	ILE	N-CA-C	6.04	121.91	109.34
7	G	75	GLY	N-CA-C	-6.03	102.20	112.51
1	A	242	ILE	CA-C-N	6.02	127.37	119.84
1	A	242	ILE	C-N-CA	6.02	127.37	119.84
2	B	70	TRP	CA-C-N	6.02	132.53	121.70
2	B	70	TRP	C-N-CA	6.02	132.53	121.70
1	A	175	ALA	N-CA-C	-6.01	104.36	111.03
12	L	118	LEU	CA-C-N	5.99	132.49	121.70
12	L	118	LEU	C-N-CA	5.99	132.49	121.70
2	B	494	LEU	N-CA-C	5.99	123.04	109.81
15	2	91	THR	N-CA-C	5.97	116.96	108.54
12	L	113	SER	CA-C-N	5.97	132.44	121.70
12	L	113	SER	C-N-CA	5.97	132.44	121.70
7	G	82	ALA	N-CA-C	5.96	123.51	110.80

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	506	GLY	N-CA-C	5.95	115.63	110.21
14	1	52	LEU	N-CA-C	5.95	120.56	112.88
2	B	48	ALA	N-CA-C	-5.94	103.98	111.11
12	L	159	TYR	N-CA-C	5.93	123.44	110.80
2	B	607	SER	N-CA-C	-5.92	105.36	113.30
5	E	60	LYS	N-CA-C	-5.92	100.06	108.23
7	G	84	TYR	N-CA-C	5.90	127.53	111.00
8	H	40	PHE	CA-C-N	5.87	132.27	121.70
8	H	40	PHE	C-N-CA	5.87	132.27	121.70
1	A	451	ILE	CB-CA-C	5.84	120.87	111.29
8	H	41	GLU	N-CA-C	5.84	127.35	111.00
2	B	625	TRP	N-CA-C	5.83	117.31	111.07
5	E	89	GLU	N-CA-C	5.82	117.07	108.86
2	B	85	ARG	CA-C-N	5.82	127.11	119.84
2	B	85	ARG	C-N-CA	5.82	127.11	119.84
2	B	456	GLU	CA-C-N	5.82	127.11	119.84
2	B	456	GLU	C-N-CA	5.82	127.11	119.84
17	4	197	THR	N-CA-C	5.81	118.32	109.95
2	B	203	ARG	N-CA-C	-5.79	105.89	113.12
1	A	498	LEU	CA-C-N	5.79	126.94	120.06
1	A	498	LEU	C-N-CA	5.79	126.94	120.06
2	B	81	PRO	N-CA-C	5.77	124.36	112.47
5	E	65	VAL	N-CA-C	5.77	114.92	106.55
4	D	93	LYS	N-CA-C	-5.76	105.88	114.64
6	F	143	GLU	N-CA-C	-5.76	104.97	112.23
17	4	132	GLY	N-CA-C	5.76	121.32	112.51
6	F	33	ALA	N-CA-C	5.75	120.16	113.20
2	B	80	ASP	CA-C-N	5.75	127.03	119.84
2	B	80	ASP	C-N-CA	5.75	127.03	119.84
4	D	48	ILE	N-CA-C	5.75	116.35	107.78
4	D	137	ILE	N-CA-C	5.75	121.30	109.34
14	1	8	GLU	CA-C-N	5.75	127.02	119.84
14	1	8	GLU	C-N-CA	5.75	127.02	119.84
1	A	140	PHE	N-CA-C	5.74	117.79	108.26
1	A	98	PHE	N-CA-C	-5.73	105.11	111.36
2	B	355	LEU	CA-C-N	5.73	127.00	119.84
2	B	355	LEU	C-N-CA	5.73	127.00	119.84
1	A	707	ILE	N-CA-C	-5.71	104.29	110.23
7	G	22	VAL	N-CA-C	-5.71	106.74	113.42
1	A	387	THR	N-CA-C	5.71	117.50	111.28
5	E	47	LYS	N-CA-C	-5.68	104.09	111.02
13	N	21	ARG	N-CA-C	-5.68	105.03	112.41

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
3	C	4	SER	N-CA-C	5.67	117.42	108.96
17	4	36	ASN	N-CA-C	5.67	122.88	110.80
3	C	61	ASP	N-CA-C	5.66	122.86	110.80
4	D	132	LEU	N-CA-C	5.66	122.86	110.80
2	B	302	LYS	N-CA-C	5.65	122.83	110.80
1	A	173	VAL	N-CA-C	-5.63	105.02	110.42
12	L	132	SER	N-CA-C	5.63	115.71	108.34
15	2	28	GLY	N-CA-C	5.62	119.50	110.90
10	J	27	ILE	CB-CA-C	-5.62	103.84	112.05
15	2	27	PHE	CA-C-N	-5.62	116.12	121.46
15	2	27	PHE	C-N-CA	-5.62	116.12	121.46
1	A	498	LEU	N-CA-C	-5.62	98.83	110.80
2	B	199	ILE	CA-C-N	5.62	125.32	119.82
2	B	199	ILE	C-N-CA	5.62	125.32	119.82
15	2	47	ALA	N-CA-C	-5.60	104.55	111.33
12	L	82	ALA	N-CA-C	-5.59	106.43	113.20
1	A	584	PRO	N-CA-C	-5.58	106.88	113.86
2	B	51	PHE	N-CA-C	-5.57	98.94	110.80
14	1	97	ILE	N-CA-C	-5.56	105.08	110.42
1	A	272	LEU	N-CA-C	5.56	120.01	113.23
6	F	37	ALA	N-CA-C	-5.54	97.56	109.81
12	L	129	GLN	N-CA-C	5.52	122.55	110.80
1	A	165	TYR	N-CA-C	-5.51	106.39	113.23
2	B	244	PHE	N-CA-C	5.51	118.22	109.96
2	B	402	GLN	N-CA-C	-5.51	106.51	113.18
1	A	486	PRO	N-CA-C	5.51	123.81	112.47
2	B	234	ALA	N-CA-C	-5.50	105.67	112.38
1	A	210	LEU	N-CA-C	5.46	118.74	112.57
3	C	20	ALA	N-CA-C	5.46	117.86	110.06
5	E	49	VAL	N-CA-C	5.45	117.17	108.89
1	A	297	THR	N-CA-C	-5.45	106.48	113.01
1	A	486	PRO	CA-C-N	5.44	131.49	121.70
1	A	486	PRO	C-N-CA	5.44	131.49	121.70
1	A	95	GLY	N-CA-C	-5.43	100.30	113.18
14	1	156	LEU	N-CA-C	5.43	117.96	111.71
1	A	510	SER	N-CA-C	5.43	119.07	111.90
12	L	167	PHE	CA-C-N	5.43	131.47	121.70
12	L	167	PHE	C-N-CA	5.43	131.47	121.70
16	3	138	SER	N-CA-C	5.43	121.45	114.56
4	D	21	ASP	CA-C-N	5.42	140.01	127.00
4	D	21	ASP	C-N-CA	5.42	140.01	127.00
1	A	751	LEU	N-CA-C	-5.41	99.27	110.80

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
8	H	81	ARG	N-CA-C	5.41	117.31	108.76
8	H	25	GLY	CA-C-N	5.41	131.44	121.70
8	H	25	GLY	C-N-CA	5.41	131.44	121.70
16	3	145	LEU	N-CA-C	5.41	117.33	109.71
2	B	262	HIS	CA-C-N	5.40	126.59	119.84
2	B	262	HIS	C-N-CA	5.40	126.59	119.84
8	H	63	SER	N-CA-C	-5.39	105.53	113.61
1	A	295	TRP	N-CA-C	5.38	118.12	110.10
4	D	86	LEU	N-CA-C	5.38	117.90	111.71
4	D	108	GLU	N-CA-C	5.38	122.26	110.80
10	J	5	LYS	CA-C-N	5.38	131.38	121.70
10	J	5	LYS	C-N-CA	5.38	131.38	121.70
2	B	557	PHE	CA-C-N	5.37	126.55	119.84
2	B	557	PHE	C-N-CA	5.37	126.55	119.84
1	A	61	ALA	N-CA-C	5.37	122.23	110.80
16	3	108	TRP	N-CA-C	5.36	122.22	110.80
4	D	71	GLY	N-CA-C	-5.36	101.41	112.34
1	A	738	TYR	N-CA-C	-5.35	102.59	111.37
2	B	483	GLY	CA-C-N	5.34	126.52	119.84
2	B	483	GLY	C-N-CA	5.34	126.52	119.84
2	B	319	HIS	N-CA-C	5.33	117.84	111.71
6	F	138	VAL	N-CA-C	5.33	120.44	109.34
1	A	186	TYR	N-CA-C	5.33	122.15	110.80
2	B	555	TYR	N-CA-C	-5.33	107.33	113.88
1	A	369	THR	CB-CA-C	5.32	120.74	111.86
12	L	111	GLU	CA-C-N	5.32	126.49	119.84
12	L	111	GLU	C-N-CA	5.32	126.49	119.84
12	L	145	PHE	N-CA-C	-5.32	104.73	111.11
1	A	406	LEU	N-CA-C	5.31	116.76	110.97
2	B	730	SER	N-CA-C	-5.31	99.49	110.80
1	A	299	ILE	N-CA-C	5.31	120.38	109.34
4	D	109	VAL	CB-CA-C	5.30	119.97	111.29
14	1	96	THR	N-CA-C	5.29	116.91	111.03
15	2	76	THR	CB-CA-C	5.29	120.59	110.17
5	E	55	VAL	N-CA-C	5.29	115.89	108.17
1	A	597	HIS	N-CA-C	-5.28	105.69	111.82
6	F	95	GLY	N-CA-C	5.27	125.67	113.18
2	B	368	GLN	N-CA-C	-5.26	99.59	110.80
8	H	70	ALA	N-CA-C	-5.26	104.29	111.56
10	J	10	VAL	CB-CA-C	5.26	119.92	111.29
2	B	617	MET	N-CA-C	-5.25	105.03	111.75
3	C	71	HIS	N-CA-C	-5.25	102.75	111.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	492	ILE	N-CA-CB	5.25	120.42	111.50
1	A	659	ALA	N-CA-C	-5.24	106.03	112.90
9	I	25	PHE	N-CA-C	5.24	119.39	112.89
2	B	643	LEU	N-CA-C	-5.24	105.97	114.09
17	4	118	ASP	CA-C-N	5.24	126.39	119.84
17	4	118	ASP	C-N-CA	5.24	126.39	119.84
14	1	111	GLN	N-CA-C	-5.23	105.75	111.82
15	2	40	SER	O-C-N	-5.22	115.64	122.59
6	F	113	LYS	N-CA-C	5.22	116.97	109.04
2	B	512	ILE	N-CA-C	5.20	120.16	109.34
1	A	353	SER	N-CA-C	5.20	116.51	107.93
3	C	56	SER	N-CA-C	-5.20	99.73	110.80
1	A	740	LEU	N-CA-C	-5.20	104.56	112.04
1	A	127	VAL	N-CA-C	5.19	120.14	109.34
1	A	595	TRP	N-CA-C	-5.19	105.05	111.33
1	A	248	PHE	N-CA-C	5.18	119.44	113.38
2	B	379	ALA	N-CA-C	-5.18	106.65	112.87
6	F	29	LEU	N-CA-C	-5.18	106.06	112.38
2	B	510	LEU	N-CA-C	5.18	121.83	110.80
6	F	6	THR	N-CA-C	5.17	121.24	109.81
5	E	59	PRO	N-CA-C	5.17	123.11	112.47
17	4	139	ASN	N-CA-C	5.16	121.22	109.81
2	B	247	THR	N-CA-C	-5.16	102.26	109.69
2	B	614	THR	N-CA-C	-5.15	99.83	110.80
1	A	114	THR	N-CA-C	5.15	121.77	110.80
16	3	196	LEU	CA-CB-CG	5.15	134.32	116.30
2	B	630	GLN	N-CA-C	-5.15	104.60	111.24
1	A	581	CYS	CA-C-O	5.14	120.92	117.94
2	B	710	LEU	N-CA-C	5.14	117.55	108.24
12	L	131	GLN	N-CA-C	5.14	117.31	110.53
3	C	48	CYS	CA-C-N	5.12	130.92	121.70
3	C	48	CYS	C-N-CA	5.12	130.92	121.70
13	N	43	PRO	CA-C-N	5.12	130.92	121.70
13	N	43	PRO	C-N-CA	5.12	130.92	121.70
6	F	113	LYS	CA-C-N	5.12	126.24	119.84
6	F	113	LYS	C-N-CA	5.12	126.24	119.84
2	B	96	PHE	CA-C-N	5.11	125.53	120.31
2	B	96	PHE	C-N-CA	5.11	125.53	120.31
14	1	59	VAL	N-CA-C	5.11	119.93	108.88
1	A	166	CYS	N-CA-C	-5.11	107.02	113.20
12	L	79	TYR	CA-C-N	5.09	130.87	121.70
12	L	79	TYR	C-N-CA	5.09	130.87	121.70

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	B	387	PHE	N-CA-C	-5.09	106.92	113.23
2	B	461	GLN	N-CA-C	5.09	121.64	110.80
8	H	33	ASN	N-CA-C	5.09	121.64	110.80
1	A	692	PHE	N-CA-C	-5.07	107.26	113.50
12	L	72	GLY	N-CA-C	5.07	122.68	112.34
1	A	391	THR	N-CA-CB	5.07	119.06	110.49
1	A	471	GLY	N-CA-C	5.07	125.19	113.18
1	A	629	ASN	N-CA-C	-5.07	100.00	110.80
14	1	5	MET	CA-C-N	5.06	126.17	119.84
14	1	5	MET	C-N-CA	5.06	126.17	119.84
5	E	82	TYR	N-CA-C	5.06	115.21	108.38
2	B	264	GLN	N-CA-C	5.06	117.19	111.02
12	L	41	PRO	CA-C-N	5.06	131.20	121.54
12	L	41	PRO	C-N-CA	5.06	131.20	121.54
14	1	73	GLU	N-CA-C	5.05	121.56	110.80
15	2	33	GLY	N-CA-C	-5.05	98.65	113.30
16	3	106	THR	N-CA-C	-5.05	105.96	112.68
1	A	123	VAL	N-CA-C	5.05	115.75	108.48
7	G	95	PRO	N-CA-C	-5.05	103.36	111.38
17	4	131	VAL	N-CA-C	5.05	119.84	109.34
1	A	326	GLY	N-CA-C	5.04	120.22	114.67
2	B	111	GLY	CA-C-N	5.04	126.14	119.84
2	B	111	GLY	C-N-CA	5.04	126.14	119.84
7	G	50	ARG	CA-C-N	5.04	130.78	121.70
7	G	50	ARG	C-N-CA	5.04	130.78	121.70
1	A	44	ILE	N-CA-C	-5.04	107.64	111.62
2	B	62	SER	N-CA-C	-5.04	105.30	111.75
13	N	31	ARG	N-CA-C	-5.04	107.68	113.88
6	F	119	ILE	N-CA-C	-5.04	107.48	111.81
10	J	15	SER	N-CA-C	-5.04	105.92	111.71
8	H	26	SER	N-CA-C	5.03	125.09	111.00
7	G	83	TYR	CA-C-N	5.03	130.75	121.70
7	G	83	TYR	C-N-CA	5.03	130.75	121.70
2	B	216	LEU	CA-C-N	5.01	126.10	119.84
2	B	216	LEU	C-N-CA	5.01	126.10	119.84
16	3	144	PHE	N-CA-C	5.00	121.45	110.80

All (7) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
13	N	59	PRO	CA
13	N	61	LEU	CA

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Mol	Chain	Res	Type	Atom
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
15	2	37	ASP	Peptide
15	2	38	PRO	Peptide
15	2	40	SER	Peptide,Mainchain
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

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Mol	Chain	Res	Type	Group
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
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

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Mol	Chain	Res	Type	Group
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
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

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Mol	Chain	Res	Type	Group
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
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

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Mol	Chain	Res	Type	Group
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	1916	0
2	B	5844	0	5659	2029	0
3	C	611	0	594	268	0
4	D	1095	0	1112	371	0
5	E	503	0	510	136	0
6	F	1221	0	1250	383	0
7	G	744	0	721	218	0
8	H	577	0	587	142	0
9	I	229	0	252	108	0
10	J	344	0	347	106	0
11	K	185	0	40	12	0
12	L	1235	0	1244	376	1
13	N	685	0	672	273	0
14	1	1187	0	1019	246	1
15	2	1268	0	1177	511	1
16	3	857	0	789	236	0
17	4	1282	0	1241	283	1
18	1	325	0	39	12	0
18	2	325	0	39	15	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
18	3	375	0	45	12	0
18	4	405	0	90	15	0
18	A	1601	0	870	342	0
18	B	2078	0	1535	681	0
18	F	224	0	94	41	0
18	G	76	0	43	12	0
18	H	80	0	51	12	0
18	I	55	0	48	9	0
18	J	111	0	66	8	0
18	K	75	0	9	5	0
18	L	227	0	162	101	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	17	0
20	F	40	0	54	13	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	7693	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 137.

All (7693) 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
2:B:289:LEU:C	18:B:1218:CLA:HBC1	1.22	1.59
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:CBC	1.31	1.56
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
15:2:21:GLY:HA2	15:2:25:GLY:C	1.36	1.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
15:2:21:GLY:C	15:2:25:GLY:HA2	1.41	1.43
2:B:287:GLY:N	18:B:1218:CLA:CMC	1.83	1.42
2:B:287:GLY:N	18:B:1218:CLA:HMC1	1.15	1.40
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
2:B:289:LEU:C	18:B:1218:CLA:CBC	1.97	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
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
15:2:17:GLU:HB3	15:2:18:TRP:CA	1.55	1.34
13:N:57:LYS:HD2	16:3:87:ALA:CB	1.55	1.34
18:A:1109:CLA:C4D	18:A:1109:CLA:C1A	2.05	1.33
1:A:141:ARG:HH11	1:A:141:ARG:CB	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:CBC	0.84	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
15:2:17:GLU:HB3	15:2:18:TRP:C	1.53	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
6:F:49:THR:HA	6:F:56:TYR:OH	1.25	1.28
15:2:21:GLY:CA	15:2:25:GLY:HA2	1.62	1.28
1:A:302:HIS:HD2	1:A:303:HIS:CE1	1.52	1.27
14:1:84:TYR:HB3	14:1:85:LEU:CA	1.64	1.27
7:G:60:SER:O	7:G:64:VAL:HG13	1.35	1.27

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:304:ILE:O	2:B:308:HIS:HB3	1.17	1.27
2:B:648:TRP:NE1	18:B:9022:CLA:H42	1.50	1.27
14:1:84:TYR:CB	14:1:85:LEU:HA	1.63	1.27
5:E:60:LYS:O	5:E:61:THR:HG22	1.33	1.26
6:F:126:ALA:H	6:F:130:LEU:CD1	1.48	1.26
1:A:96:MET:N	1:A:96:MET:SD	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
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
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
15:2:19:LEU:HA	15:2:20:ASP:CG	1.62	1.23
16:3:134:TYR:N	16:3:136:PRO:HD2	1.54	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
2:B:287:GLY:CA	18:B:1218:CLA:HMC1	1.69	1.21
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
3:C:55:GLU:CA	3:C:58:CYS:HB3	1.70	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
16:3:83:GLY:CA	16:3:86:PRO:HD2	1.67	1.21
1:A:290:LEU:O	1:A:291:THR:HG22	1.41	1.20
2:B:290:MET:N	18:B:1218:CLA:CBC	1.95	1.20
6:F:33:ALA:O	6:F:43:LYS:NZ	1.73	1.20
6:F:136:TRP:CG	6:F:137:PRO:HD3	1.74	1.20
18:F:1302:CLA:CMA	18:F:1302:CLA:H92	1.71	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
15:2:28:GLY:HA3	15:2:29:PHE:CD2	1.76	1.20
1:A:483:GLN:HG2	1:A:484:LEU:C	1.67	1.19
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
2:B:290:MET:CA	18:B:1218:CLA:CBC	1.92	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
2:B:336:LEU:HA	2:B:339:ALA:HB3	1.20	1.18
6:F:93:ILE:HA	6:F:96:TRP:CZ2	1.78	1.18
6:F:100:VAL:CG1	6:F:125:LEU:HD22	1.72	1.18
12:L:165:TYR:CD1	18:L:1503:CLA:OBD	1.95	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: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
18:F:1302:CLA:H92	18:F:1302:CLA:HMA3	1.19	1.17
2:B:37:ILE:O	4:D:148:PHE:CD1	1.98	1.17
2:B:547:MET:HB3	3:C:66:ARG:HH21	1.09	1.17
17:4:77:ALA:HB3	17:4:78:ALA:HA	1.19	1.17
3:C:12:ILE:HA	3:C:13:GLY:O	1.38	1.17
4:D:26:SER:HA	4:D:27:PRO:C	1.61	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
18:4:1304:CLA:HAA2	18:4:1304:CLA:C2	1.75	1.17
1:A:81:ALA:HB1	1:A:82:HIS:CB	1.75	1.17
1:A:621:GLN:O	1:A:623:ASP:N	1.78	1.17
10:J:11:ALA:CB	10:J:12:PRO:HD3	1.70	1.17
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
7:G:35:VAL:H	7:G:36:PRO:CD	1.58	1.16
12:L:65:VAL:CG2	12:L:84:GLY:HA2	1.74	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
2:B:304:ILE:O	2:B:308:HIS:CB	1.93	1.16
14:1:51:MET:O	14:1:55:PRO:HD3	1.43	1.16
1:A:450:CYS:HB3	1:A:551:VAL:HG12	1.21	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
13:N:48:GLY:HA2	13:N:50:GLN:H	1.11	1.15

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
1:A:606:TYR:O	1:A:610:SER:HB3	1.46	1.15
2:B:532:LEU:HD12	2:B:533:ILE:H	1.11	1.15
18:B:1224:CLA:CGA	18:B:1224:CLA:H3A	1.71	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
15:2:23:LEU:HD12	15:2:25:GLY:C	1.69	1.15
15:2:192:LEU:CA	15:2:195:HIS:CE1	2.28	1.15
1:A:141:ARG:HB2	1:A:141:ARG:NH1	1.60	1.15
7:G:35:VAL:N	7:G:36:PRO:HD3	1.54	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:397:THR:O	1:A:400:MET:N	1.80	1.15
2:B:672:GLN:HE22	2:B:698:VAL:HA	1.12	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
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
14:1:188:ASN:HA	14:1:189:ILE:CG1	1.77	1.14
17:4:41:VAL:HG23	17:4:42:GLN:H	0.99	1.14
18:A:1132:CLA:C2B	12:L:72:GLY:HA2	1.78	1.14
15:2:191:ASN:CA	15:2:192:LEU:HB2	1.77	1.14
15:2:24:PRO:HD2	15:2:27:PHE:CE2	1.81	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
15:2:24:PRO:CG	15:2:27:PHE:CE2	2.30	1.14
15:2:21:GLY:HA2	15:2:25:GLY:CA	1.78	1.14
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
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
20:A:6011:BCR:H321	20:A:6011:BCR:C8	1.77	1.13
2:B:20:ARG:HH22	9:I:28:VAL:HG13	1.02	1.13
1:A:483:GLN:CG	1:A:484:LEU:O	1.97	1.12
2:B:286:ILE:HD12	18:B:1218:CLA:HMC2	1.15	1.12
3:C:52:LYS:HE2	3:C:66:ARG:HA	1.24	1.13

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
17:4:115:VAL:HG12	17:4:116:ASN:H	1.02	1.13
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
15:2:21:GLY:CA	15:2:23:LEU:HD12	1.78	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
13:N:63:ASP:CB	13:N:64:ASP:HA	1.76	1.12
18:A:1136:CLA:H71	18:A:1137:CLA:HAC2	1.26	1.12
2:B:429:LEU:HD23	2:B:524:ALA:O	1.50	1.12
17:4:190:TRP:O	17:4:191:HIS:HD2	1.32	1.12
1:A:364:MET:HA	1:A:364:MET:HE3	1.29	1.12
18:A:1124:CLA:C3A	18:A:1135:CLA:CBB	2.27	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
20:I:6018:BCR:H383	20:L:6020:BCR:H341	1.25	1.12
1:A:238:ASP:HB3	1:A:239:PRO:HD3	1.29	1.11
18:L:1503:CLA:HHD	18:L:1503:CLA:CBC	1.78	1.11
1:A:521:VAL:HG13	1:A:522:ALA:H	1.01	1.11
18:B:1227:CLA:HMB2	18:B:1228:CLA:C4D	1.81	1.11
4:D:137:ILE:HG13	4:D:140:ASN:HD21	1.12	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
1:A:268:PRO:HB2	1:A:273:ASN:HB2	1.22	1.11
2:B:639:VAL:HG12	2:B:640:CYS:N	1.63	1.11
15:2:23:LEU:HB2	15:2:25:GLY:N	1.66	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:H	0.97	1.11
15:2:17:GLU:CG	15:2:18:TRP:CB	2.29	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
16:3:132:ASP:OD1	16:3:139:MET:HB2	1.51	1.10
16:3:212:ASN:HA	16:3:213:LEU:HB2	1.26	1.10
17:4:51:ALA:HB1	17:4:161:MET:HE1	1.10	1.10
1:A:64:PHE:HE1	18:A:1103:CLA:CMC	1.64	1.10
1:A:81:ALA:CB	1:A:83:PHE:N	2.15	1.10
1:A:629:ASN:HD21	1:A:633:VAL:CG2	1.64	1.10
2:B:527:LEU:HD23	2:B:586:THR:HG21	1.32	1.10

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
7:G:37:GLU:CG	7:G:43:HIS:HE1	1.64	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
15:2:28:GLY:C	15:2:29:PHE:CD2	2.29	1.10
2:B:74:PHE:HE2	2:B:130:ARG:HA	1.14	1.10
2:B:498:LEU:O	2:B:501:ILE:HG12	1.50	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
1:A:446:LEU:HD22	1:A:449:VAL:HG11	1.27	1.09
2:B:700:LEU:CD2	2:B:704:GLN:HE22	1.64	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: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
18:B:1138:CLA:HBB2	18:B:1138:CLA:H8	1.33	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
15:2:17:GLU:HG3	15:2:18:TRP:HB2	1.23	1.09
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
14:1:152:ARG:HD2	14:1:153:LEU:HD13	1.22	1.09
12:L:113:SER:H	12:L:114:ILE:HB	1.02	1.09
15:2:153:PRO:HB2	15:2:154:GLN:C	1.78	1.09
1:A:353:SER:HG	1:A:354:TRP:CD1	1.70	1.09
1:A:521:VAL:CG1	1:A:522:ALA:H	1.66	1.09
1:A:557:LEU:HA	1:A:560:VAL:HG22	1.10	1.09
1:A:663:GLN:O	1:A:667:SER:HB2	1.53	1.09
2:B:133:GLU:HA	2:B:136:TYR:CE1	1.87	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
15:2:21:GLY:HA2	15:2:23:LEU:HD12	1.13	1.09
16:3:83:GLY:HA2	16:3:86:PRO:CD	1.82	1.09

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:268:PRO:HD2	1:A:277:TYR:CE1	1.88	1.08
10:J:2:ARG:HB2	10:J:7:TYR:HE1	1.03	1.08
15:2:24:PRO:CD	15:2:27:PHE:CE2	2.36	1.08
15:2:28:GLY:C	15:2:29:PHE:CG	2.29	1.08
15:2:157:LYS:HA	15:2:160:ARG:HG2	1.21	1.08
1:A:64:PHE:HA	1:A:67:HIS:HB2	1.32	1.08
13:N:77:CYS:HB2	13:N:78:GLY:HA3	1.35	1.08
16:3:67:MET:HB2	18:3:3005:CLA:C3C	1.82	1.08
1:A:483:GLN:HA	1:A:484:LEU:CB	1.83	1.08
1:A:637:ILE:H	1:A:637:ILE:HD12	0.94	1.08
13:N:58:VAL:HG11	16:3:86:PRO:HA	1.35	1.08
14:1:162:CYS:HA	14:1:165:GLN:HB2	1.29	1.08
1:A:147:SER:N	1:A:391:THR:HG21	1.69	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
15:2:32:LEU:O	15:2:32:LEU:HD13	1.54	1.08
2:B:378:ILE:HG13	18:B:1225:CLA:HBB2	1.25	1.08
2:B:551:LYS:HB2	4:D:141:VAL:O	1.54	1.08
2:B:698:VAL:HG12	3:C:79:LEU:HD23	1.28	1.08
5:E:65:VAL:HG23	5:E:83:ALA:HB2	1.29	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
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
16:3:133:TRP:O	16:3:137:GLY:HA2	1.45	1.07
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
2:B:422:LEU:HB2	18:B:1236:CLA:HBB2	1.19	1.07
12:L:63:LEU:HD21	18:L:1502:CLA:HMB3	1.33	1.07
15:2:20:ASP:HB3	15:2:23:LEU:HD11	1.09	1.07
16:3:212:ASN:HB2	16:3:214:LEU:H	1.11	1.07
1:A:71:LEU:HD11	1:A:352:THR:HG22	1.36	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
2:B:74:PHE:CE2	2:B:130:ARG:HA	1.89	1.07
3:C:25:VAL:HG21	3:C:48:CYS:HB3	1.35	1.07
17:4:82:GLU:HG3	17:4:83:TYR:N	1.68	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:532:LEU:HD12	2:B:533:ILE:N	1.67	1.07

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
12:L:102:TYR:HE2	12:L:105:ALA:HB3	1.16	1.07
18:L:1503:CLA:HBD	18:L:1503:CLA:HAA2	1.37	1.07
20:L:6020:BCR:HC8	20:L:6020:BCR:H331	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: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
13:N:63:ASP:HB2	13:N:64:ASP:CA	1.85	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
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
17:4:59:LEU:HA	17:4:62:GLU:HB2	1.36	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
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
1:A:139:GLY:O	6:F:38:PRO:HB2	1.54	1.06
1:A:543:HIS:HA	1:A:546:ALA:HB3	1.16	1.06
4:D:47:VAL:HG23	4:D:103:VAL:HG11	1.38	1.06
13:N:44:GLU:N	13:N:45:ASN:HB2	1.70	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
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:658:TRP:CD1	2:B:625:TRP:NE1	2.24	1.06
2:B:646:TRP:HE3	2:B:723:ALA:CB	1.68	1.06
3:C:3:HIS:NE2	3:C:48:CYS:O	1.86	1.06
15:2:23:LEU:HD13	15:2:26:ASP:C	1.81	1.06
15:2:185:GLY:O	15:2:187:GLY:HA3	1.55	1.06
6:F:73:VAL:HG21	6:F:83:PHE:H	1.21	1.05
14:1:16:GLY:HA3	14:1:18:ALA:HA	1.11	1.05
15:2:22:SER:C	15:2:23:LEU:CG	2.30	1.05
15:2:23:LEU:HD13	15:2:26:ASP:CA	1.84	1.05
16:3:129:ARG:HD2	16:3:139:MET:SD	1.94	1.05
2:B:126:THR:HB	18:B:1215:CLA:HED1	1.37	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
14:1:103:LEU:HA	14:1:106:ALA:HB3	1.35	1.05
2:B:682:HIS:HB3	18:B:1237:CLA:HMA3	1.05	1.05
13:N:30:ALA:HA	13:N:33:TYR:HB2	1.34	1.05
15:2:21:GLY:CA	15:2:25:GLY:C	2.30	1.05
15:2:22:SER:C	15:2:23:LEU:HD23	1.81	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
2:B:287:GLY:H	18:B:1218:CLA:CMC	1.58	1.05
2:B:478:LEU:CD1	2:B:485:ALA:HB3	1.87	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
12:L:113:SER:N	12:L:114:ILE:HB	1.70	1.05
15:2:22:SER:C	15:2:23:LEU:CD2	2.29	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
15:2:22:SER:C	15:2:23:LEU:HG	1.81	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:35:ALA:HA	1:A:36:LYS:HB2	1.04	1.04
1:A:450:CYS:CB	1:A:551:VAL:HG12	1.88	1.04
6:F:5:LEU:HB3	6:F:62:LEU:HD23	1.07	1.04
13:N:79:SER:N	13:N:80:ASN:HA	1.72	1.04
15:2:17:GLU:CD	15:2:18:TRP:HB2	1.81	1.04
15:2:21:GLY:C	15:2:25:GLY:CA	2.30	1.04
2:B:83:HIS:N	2:B:84:VAL:HG23	1.73	1.04
2:B:658:ALA:O	2:B:661:PHE:HB2	1.56	1.04
2:B:58:PHE:CE2	18:B:1241:CLA:HHB	1.91	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
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
4:D:135:ARG:HG2	4:D:139:LYS:HD3	1.34	1.03
15:2:19:LEU:CA	15:2:20:ASP:CG	2.30	1.03
15:2:20:ASP:CB	15:2:23:LEU:HD11	1.88	1.03

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
15:2:21:GLY:H	15:2:22:SER:HB3	1.23	1.03
15:2:23:LEU:HD22	15:2:26:ASP:O	1.56	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
15:2:32:LEU:O	15:2:32:LEU:CD1	2.06	1.03
1:A:81:ALA:CB	1:A:83:PHE:H	1.70	1.03
1:A:268:PRO:HD2	1:A:277:TYR:HE1	1.22	1.03
15:2:22:SER:H	15:2:23:LEU:CA	1.71	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
15:2:17:GLU:CB	15:2:18:TRP:C	2.30	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
15:2:20:ASP:HB3	15:2:23:LEU:CD1	1.88	1.03
1:A:483:GLN:CA	1:A:484:LEU:HB2	1.89	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
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
1:A:492:ILE:H	1:A:493:GLN:CB	1.71	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
7:G:35:VAL:H	7:G:36:PRO:HD3	0.89	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
1:A:354:TRP:HB3	18:A:1103:CLA:HHD	1.42	1.02
1:A:489:ALA:HB1	1:A:490:GLN:O	1.56	1.02
2:B:627:ASN:HA	2:B:732:LYS:HE3	1.42	1.02
18:B:1202:CLA:HBB2	18:B:1203:CLA:HBA1	1.33	1.02
12:L:22:GLY:O	12:L:23:LEU:HB2	1.58	1.02
14:1:179:THR:HG21	17:4:88:SER:HB3	1.41	1.02
15:2:22:SER:H	15:2:25:GLY:H	1.05	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
7:G:35:VAL:HG13	7:G:36:PRO:CA	1.90	1.02

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
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:101:VAL:HG23	2:B:102:GLU:H	1.22	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
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
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: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
2:B:478:LEU:HD12	2:B:485:ALA:CB	1.89	1.01
2:B:485:ALA:HA	18:B:1232:CLA:CMA	1.90	1.01
13:N:77:CYS:HB2	13:N:78:GLY:CA	1.90	1.01
14:1:188:ASN:HA	14:1:189:ILE:HG12	1.05	1.01
1:A:452:PHE:HE2	18:A:1136:CLA:CBB	1.74	1.01
2:B:78:VAL:HG23	2:B:130:ARG:HD3	1.38	1.01
2:B:530:THR:HG21	2:B:583:MET:HB2	1.42	1.01
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
1:A:109:TRP:HE1	1:A:113:PRO:HA	1.21	1.01
2:B:174:ARG:HH11	2:B:174:ARG:CB	1.73	1.01
6:F:5:LEU:HB3	6:F:62:LEU:CD2	1.91	1.01
15:2:19:LEU:HG	15:2:20:ASP:CG	1.84	1.01
17:4:77:ALA:CB	17:4:78:ALA:HA	1.90	1.01
2:B:454:LEU:HD12	2:B:614:THR:HG21	1.42	1.01
12:L:36:TYR:O	12:L:38:SER:N	1.94	1.01
12:L:164:PRO:CG	18:L:1503:CLA:C2	2.39	1.01
1:A:147:SER:H	1:A:391:THR:HG21	1.25	1.00
2:B:334:LEU:CD1	2:B:389:HIS:HD2	1.74	1.00
4:D:94:TYR:HB2	4:D:95:LYS:HZ2	1.23	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
15:2:21:GLY:HA2	15:2:25:GLY:O	1.61	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
6:F:116:GLN:C	6:F:118:GLU:H	1.67	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
1:A:557:LEU:HA	1:A:560:VAL:CG2	1.90	1.00
1:A:588:GLY:HA3	2:B:668:ARG:HD2	1.42	1.00
1:A:637:ILE:HD12	1:A:637:ILE:N	1.74	1.00
2:B:422:LEU:HD21	2:B:531:THR:OG1	1.60	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
15:2:33:GLY:N	15:2:35:SER:N	2.08	1.00
15:2:189:ILE:HA	15:2:191:ASN:N	1.75	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
13:N:65:LEU:HD12	13:N:68:GLU:OE1	1.62	1.00
15:2:23:LEU:HB2	15:2:25:GLY:CA	1.92	1.00
1:A:147:SER:OG	18:A:1126:CLA:HMA2	1.62	1.00
6:F:5:LEU:CB	6:F:62:LEU:HD23	1.92	1.00
15:2:24:PRO:HG2	15:2:27:PHE:CE2	1.95	1.00
2:B:257:ILE:HA	2:B:272:ASP:OD1	1.62	1.00
2:B:694:ARG:HE	9:I:29:GLU:CD	1.68	1.00
4:D:153:PRO:O	4:D:154:TYR:HD2	1.45	1.00
2:B:378:ILE:CG1	18:B:1225:CLA:HBB2	1.91	1.00
14:1:10:ARG:H	17:4:110:LYS:HD2	1.26	1.00
1:A:347:TYR:HD2	1:A:348:GLU:N	1.58	0.99
9:I:4:LEU:HD22	9:I:5:PRO:HA	1.44	0.99
14:1:10:ARG:N	17:4:110:LYS:HD2	1.75	0.99
16:3:197:GLY:O	16:3:200:ILE:HG22	1.61	0.99
1:A:35:ALA:HA	1:A:36:LYS:CB	1.92	0.99
1:A:305:ALA:HB2	18:A:1115:CLA:HMA3	1.43	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
15:2:191:ASN:HA	15:2:192:LEU:HB2	1.00	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
12:L:66:GLY:C	18:L:1503:CLA:CAB	2.34	0.99

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
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
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
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
17:4:66:SER:O	17:4:67:ILE:HG23	1.63	0.99
2:B:73:ASN:HD22	2:B:108:GLY:HA3	1.28	0.99
2:B:574:ASP:HA	2:B:577:TYR:HB3	1.44	0.99
12:L:66:GLY:HA3	18:L:1503:CLA:C2B	1.88	0.99
3:C:5:VAL:HG13	3:C:6:LYS:H	1.26	0.98
16:3:212:ASN:HB2	16:3:214:LEU:N	1.76	0.98
9:I:25:PHE:H	9:I:26:LEU:CB	1.70	0.98
1:A:38:GLY:HA2	1:A:44:ILE:HB	1.45	0.98
18:A:1132:CLA:C2B	12:L:72:GLY:CA	2.40	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
15:2:194:ALA:CB	15:2:195:HIS:HA	1.92	0.98
2:B:174:ARG:HB2	2:B:174:ARG:HH11	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
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
15:2:18:TRP:HA	15:2:20:ASP:O	1.63	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
15:2:17:GLU:CB	15:2:18:TRP:CA	2.36	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
15:2:27:PHE:CD1	15:2:29:PHE:N	2.30	0.98
2:B:478:LEU:HD12	2:B:485:ALA:HB3	0.99	0.98
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
18:A:1124:CLA:HHC	18:A:1137:CLA:CGA	1.94	0.97
18:A:1132:CLA:C2B	12:L:72:GLY:N	2.26	0.97
2:B:101:VAL:HA	2:B:105:THR:OG1	1.64	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
18:A:1137:CLA:CMC	18:L:1130:CLA:HMC2	1.94	0.97
2:B:547:MET:HB3	3:C:66:ARG:NH2	1.77	0.97
1:A:207:LEU:C	1:A:310:PHE:O	2.07	0.97
1:A:654:ARG:NH1	1:A:655:ASP:HB3	1.78	0.97
13:N:58:VAL:CG1	16:3:86:PRO:CA	2.43	0.97
14:1:89:VAL:CG1	14:1:90:PRO:HD3	1.94	0.97
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
13:N:57:LYS:CB	16:3:87:ALA:HB2	1.94	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:1207:CLA:H61	8:H:65:LEU:HD22	1.44	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
15:2:20: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
15:2:84:GLU:OE2	17:4:186:ILE:HG13	1.65	0.97
1:A:618:TRP:CH2	1:A:646:SER:HB3	1.99	0.97
1:A:744:ALA:HB2	20:A:6011:BCR:C32	1.95	0.97
2:B:99:PRO:O	2:B:103:ALA:N	1.96	0.97
2:B:195:VAL:CG2	2:B:274:ALA:HB1	1.93	0.97
2:B:289:LEU:O	18:B:1218:CLA:CBC	2.01	0.97
2:B:345:THR:CG2	18:B:1225:CLA:HMC1	1.95	0.97
2:B:700:LEU:CD2	2:B:704:GLN:NE2	2.27	0.97
4:D:141:VAL:O	4:D:143:PRO:HD3	1.65	0.97
15:2:63:PHE:H	15:2:63:PHE:HD2	0.98	0.97

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
18:B:1217:CLA:HMA1	7:G:21:PHE:HD2	1.30	0.97
6:F:86:PRO:HG3	10:J:39:PHE:HB2	1.46	0.97
6:F:115:THR:O	6:F:117:LYS:C	2.08	0.97
12:L:44:ARG:HD2	12:L:46:ALA:HA	1.46	0.97
18:L:1503:CLA:CGA	18:L:1503:CLA:CGD	2.43	0.97
20:L:6020:BCR:HC8	20:L:6020:BCR:C33	1.91	0.97
1:A:475:ASP:OD2	12:L:75:ARG:HD3	1.64	0.96
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: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
1:A:431:LEU:HD12	18:A:1122:CLA:HMC3	1.46	0.96
1:A:450:CYS:HB3	1:A:551:VAL:CG1	1.95	0.96
18:A:1103:CLA:HBA1	18:A:1123:CLA:H43	1.45	0.96
6:F:127:SER:HA	6:F:131:PHE:HB2	1.43	0.96
14:1:152:ARG:CD	14:1:153:LEU:HD13	1.94	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
15:2:33:GLY:H	15:2:35:SER:CA	1.78	0.96
2:B:291:TYR:HA	2:B:299:HIS:N	1.80	0.96
6:F:49:THR:CA	6:F:56:TYR:OH	2.13	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
2:B:78:VAL:HA	2:B:130:ARG:CZ	1.96	0.96
18:B:1202:CLA:HBB2	18:B:1203:CLA:CBA	1.95	0.96
3:C:42:ALA:C	3:C:44:ARG:H	1.71	0.96
4:D:155:ASP:HB3	4:D:156:LEU:HA	1.44	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:126:ILE:HG22	1:A:129:GLN:CG	1.96	0.96
1:A:126:ILE:CD1	10:J:27:ILE:HG23	1.93	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:64:PHE:HE1	18:A:1103:CLA:HMC1	1.28	0.96
1:A:231:GLN:HA	1:A:234:ASN:ND2	1.81	0.96
1:A:277:TYR:CD2	18:A:1113:CLA:HBC1	2.01	0.96
1:A:725:LEU:HB3	19:A:5001:PQN:O4	1.66	0.96

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
20:A:6011:BCR:H321	20:A:6011:BCR:HC8	0.96	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
15:2:28:GLY:HA3	15:2:29:PHE:HD2	1.22	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
12:L:58:LEU:HD13	12:L:153:TRP:HZ3	1.31	0.96
1:A:84:GLY:O	1:A:88:ILE:N	1.97	0.95
1:A:543:HIS:HA	1:A:546:ALA:CB	1.94	0.95
15:2:18:TRP:CD1	15:2:21:GLY:CA	2.29	0.95
1:A:679:PHE:HA	1:A:682:ALA:CB	1.94	0.95
15:2:23:LEU:HA	15:2:25:GLY:N	1.80	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:379:ALA:O	2:B:383:MET:HB2	1.65	0.95
2:B:682:HIS:CE1	18:B:1238:CLA:HAC1	2.01	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
15:2:23:LEU:CA	15:2:25:GLY:N	2.30	0.95
15:2:24:PRO:HB3	15:2:32:LEU:CG	1.97	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
6:F:136:TRP:CD2	6:F:137:PRO:HD3	2.00	0.95
15:2:23:LEU:CD1	15:2:26:ASP:N	2.30	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:20:ARG:NH2	9:I:28:VAL:HG13	1.81	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
18:A:1123:CLA:HBC2	18:A:1123:CLA:HHD	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
13:N:63:ASP:HB2	13:N:64:ASP:CB	1.97	0.94
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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:64:PHE:CE1	18:A:1103:CLA:CMC	2.50	0.94
2:B:365:PHE:CD1	2:B:602:TRP:CD1	2.55	0.94
18:B:1209:CLA:H51	18:B:1209:CLA:O1A	1.66	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
1:A:347:TYR:HD2	1:A:348:GLU:H	1.01	0.94
1:A:453:LEU:HB2	18:A:1136:CLA:HBB2	1.47	0.94
20:I:6018:BCR:C38	20:L:6020:BCR:H341	1.95	0.94
14:1:16:GLY:CA	14:1:18:ALA:HA	1.98	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
15:2:157:LYS:HA	15:2:160:ARG:CG	1.97	0.94
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
2:B:649:MET:O	2:B:652:PHE:HB3	1.67	0.94
15:2:23:LEU:CB	15:2:26:ASP:N	2.30	0.94
1:A:620:MET:O	1:A:621:GLN:HB2	1.68	0.94
2:B:64:ASN:HA	2:B:67:HIS:HB2	1.49	0.94
2:B:100:ALA:HA	2:B:103:ALA:HB3	1.46	0.94
2:B:102:GLU:OE2	2:B:639:VAL:CG1	2.16	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
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
14:1:9:PRO:N	17:4:110:LYS:HZ3	1.63	0.94
15:2:23:LEU:CB	15:2:26:ASP:H	1.79	0.94
15:2:23:LEU:HD23	15:2:23:LEU:N	1.83	0.94
15:2:27:PHE:HD1	15:2:28:GLY:C	1.76	0.94
17:4:41:VAL:HG23	17:4:42:GLN:N	1.79	0.94
2:B:284:PHE:HE1	18:B:1216:CLA:HHC	1.28	0.94
18:B:1227:CLA:CHB	18:B:1228:CLA:OBD	2.15	0.94
13:N:58:VAL:HG12	16:3:86:PRO:CA	1.98	0.94
15:2:22:SER:N	15:2:23:LEU:CG	2.30	0.94
15:2:175:MET:O	15:2:179:PHE:HB3	1.66	0.94

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:414:ALA:O	1:A:417:PHE:HD2	1.49	0.94
18:A:1106:CLA:O2D	18:A:1106:CLA:H2A	1.68	0.94
2:B:351:HIS:O	2:B:352:MET:HB2	1.68	0.94
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
16:3:134:TYR:C	16:3:136:PRO:CD	2.41	0.93
2:B:299:HIS:CE1	18:B:1218:CLA:HED3	2.04	0.93
2:B:479:SER:C	2:B:481:THR:H	1.75	0.93
2:B:573:TRP:CZ3	2:B:574:ASP:HB3	2.02	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
8:H:54:LEU:HD13	8:H:55:LYS:N	1.83	0.93
17:4:116:ASN:HA	17:4:117:GLN:HG3	1.50	0.93
1:A:141:ARG:HH11	1:A:141:ARG:HB2	0.78	0.93
1:A:675:TYR:HB3	1:A:748:ALA:O	1.68	0.93
18:A:1123:CLA:H12	18:A:1123:CLA:C10	1.99	0.93
6:F:100:VAL:HG12	6:F:125:LEU:HD22	1.46	0.93
16:3:217:LEU:HA	16:3:218:ALA:HB3	1.48	0.93
7:G:35:VAL:HG13	7:G:36:PRO:CB	1.99	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
2:B:286:ILE:HD12	18:B:1218:CLA:CMC	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
1:A:139:GLY:O	6:F:38:PRO:CB	2.15	0.93
2:B:387:PHE:O	2:B:391:PRO:HD2	1.68	0.93
2:B:682:HIS:CB	18:B:1237:CLA:HMA3	1.98	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
16:3:55:LEU:HD13	16:3:58:GLY:HA3	1.48	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: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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
14:1:16:GLY:HA3	14:1:18:ALA:CA	1.97	0.93
1:A:119:SER:HA	1:A:145:ILE:CG2	1.97	0.93
2:B:415:LYS:NZ	2:B:540:ASP:HA	1.83	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
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
13:N:63:ASP:HB3	13:N:64:ASP:HA	1.50	0.92
15:2:178:TRP:C	15:2:180:GLN:H	1.76	0.92
17:4:82:GLU:HB3	17:4:84:PHE:CE1	2.05	0.92
1:A:64:PHE:CE1	18:A:1103:CLA:HMC1	2.02	0.92
1:A:442:ILE:HD11	1:A:561:LEU:HD21	1.52	0.92
6:F:100:VAL:HG12	6:F:125:LEU:CD2	1.98	0.92
15:2:154:GLN:HG2	15:2:155:LYS:N	1.85	0.92
1:A:89:ILE:O	1:A:92:TRP:HB3	1.69	0.92
1:A:454:GLY:O	1:A:456:HIS:N	2.03	0.92
1:A:476:MET:N	1:A:476:MET:SD	2.42	0.92
2:B:345:THR:HG23	18:B:1225:CLA:HMC1	1.49	0.92
2:B:526:GLY:HA2	2:B:582:TRP:HZ3	1.34	0.92
2:B:646:TRP:CD1	2:B:646:TRP:H	1.69	0.92
15:2:23:LEU:CB	15:2:25:GLY:N	2.29	0.92
1:A:665:ILE:HD13	2:B:625:TRP:CD1	2.05	0.92
18:A:1137:CLA:HMC2	18:L:1130:CLA:HMC2	1.49	0.92
2:B:589:TRP:HD1	2:B:592:PHE:HE2	1.14	0.92
18:B:1217:CLA:CMA	7:G:21:PHE:CD2	2.53	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
14:1:89:VAL:CB	14:1:90:PRO:HD3	1.99	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
14:1:102:PHE:O	14:1:105:ILE:HG22	1.70	0.92
1:A:97:TYR:HE2	1:A:153:TRP:CE3	1.88	0.92
1:A:569:ILE:O	1:A:569:ILE:HG22	1.69	0.92
2:B:355:LEU:HD21	18:B:1214:CLA:HED3	1.52	0.92
2:B:661:PHE:HB3	18:B:9023:CLA:HMC2	1.48	0.92
1:A:147:SER:H	1:A:391:THR:CG2	1.83	0.92
1:A:495:THR:C	1:A:497:ALA:H	1.74	0.92
2:B:523:ILE:HD12	2:B:590:VAL:HG21	1.48	0.92

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:D:155:ASP:HB3	4:D:156:LEU:C	1.93	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:347:TYR:HD2	1:A:349:ILE:H	1.17	0.92
16:3:134:TYR:CA	16:3:136:PRO:HD2	1.97	0.92
17:4:51:ALA:CB	17:4:161:MET:HE1	1.98	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
2:B:704:GLN:C	2:B:706:ARG:H	1.78	0.91
2:B:287:GLY:CA	18:B:1218:CLA:CMC	2.36	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
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
15:2:22:SER:CA	15:2:23:LEU:CG	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:14:LEU:HD22	12:L:23:LEU:H	1.32	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
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
1:A:228:PRO:C	1:A:230:ASN:H	1.75	0.91
2:B:71:GLN:NE2	2:B:89:HIS:O	2.03	0.91
2:B:311:PRO:HD2	18:B:1220:CLA:HMA1	1.53	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
4:D:26:SER:H	4:D:27:PRO:HB2	1.36	0.91
4:D:107:GLY:O	4:D:108:GLU:HB3	1.70	0.91
6:F:105:LEU:O	6:F:108:ILE:N	2.03	0.91
18:L:1503:CLA:CED	18:L:1503:CLA:H12	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
1:A:50:THR:HG21	1:A:723:ARG:NH1	1.85	0.91
1:A:317:TYR:HA	1:A:325:HIS:H	1.35	0.91
3:C:58:CYS:SG	21:C:3103:SF4:S3	2.69	0.91

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:N	13:N:60:PHE:HD2	1.69	0.91
16:3:132:ASP:CB	16:3:139:MET:CG	2.46	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
16:3:134:TYR:C	16:3:136:PRO:HD3	1.95	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
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
15:2:40:SER:CA	15:2:41:LEU:CB	2.45	0.90
15:2:194:ALA:HB1	15:2:195:HIS:HA	1.49	0.90
2:B:133:GLU:HA	2:B:136:TYR:HE1	1.30	0.90
18:B:1203:CLA:H2	18:B:1226:CLA:ND	1.86	0.90
6:F:81:GLY:O	6:F:86:PRO:CD	2.19	0.90
7:G:95:PRO:C	7:G:97:PHE:H	1.77	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
15:2:17:GLU:CD	15:2:18:TRP:N	2.29	0.90
1:A:452:PHE:CE2	18:A:1136:CLA:CBB	2.55	0.90
2:B:276:HIS:HD1	2:B:277:HIS:N	1.69	0.90
2:B:341:LEU:CD2	18:B:1202:CLA:HED2	2.01	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
16:3:132:ASP:HB3	16:3:139:MET:HG3	0.91	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
15:2:22:SER:CB	15:2:23:LEU:HG	2.01	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
1:A:557:LEU:CA	1:A:560:VAL:HG22	1.99	0.90
2:B:20:ARG:O	2:B:24:GLY:N	2.05	0.90

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
9:I:25:PHE:CD2	9:I:25:PHE:O	2.24	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
18:A:1113:CLA:HAA1	18:A:1113:CLA:HED2	1.52	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
15:2:21:GLY:N	15:2:23:LEU:CD1	2.35	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
15:2:41:LEU:C	15:2:45:VAL:HG11	1.96	0.90
14:1:183:ASP:H	14:1:184:PRO:CA	1.85	0.89
2:B:78:VAL:HA	2:B:130:ARG:NE	1.85	0.89
17:4:115:VAL:HG12	17:4:116:ASN:N	1.85	0.89
1:A:80:SER:N	1:A:81:ALA:HB2	1.87	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
15:2:63:PHE:HD2	15:2:63:PHE:N	1.70	0.89
15:2:154:GLN:HG2	15:2:155:LYS:H	1.36	0.89
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: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
15:2:106: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
14:1:76:ALA:C	14:1:78:PRO:HD3	1.98	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:H51	18:B:1205:CLA:CAB	2.03	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
7:G:85:ILE:HA	7:G:86:LEU:C	1.98	0.89
8:H:33:ASN:HD21	18:H:1501:CLA:HMD2	1.38	0.89
15:2:93:THR:HG22	15:2:94:LEU:HA	1.52	0.89
2:B:310:PRO:HA	2:B:312:GLY:N	1.87	0.89

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:621:GLN:HA	1:A:637:ILE:HD13	1.55	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
2:B:671:TRP:O	2:B:675:ILE:HG23	1.73	0.88
10:J:2:ARG:CB	10:J:7:TYR:HE1	1.86	0.88
1:A:223:VAL:HG23	1:A:224:HIS:CD2	2.08	0.88
18:B:1224:CLA:CGA	18:B:1224:CLA:C3A	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
17:4:115:VAL:CG1	17:4:116:ASN:H	1.86	0.88
2:B:593:TYR:CD1	2:B:594:TRP:N	2.42	0.88
3:C:12:ILE:HA	3:C:13:GLY:C	1.93	0.88
3:C:12:ILE:HG13	21:C:3103:SF4:S2	2.13	0.88
8:H:55:LYS:HA	8:H:58:ILE:HG13	1.55	0.88
15:2:86:GLU:O	15:2:89:THR:HB	1.74	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
9:I:26:LEU:HG	9:I:29:GLU:C	1.98	0.88
1:A:658:TRP:HD1	2:B:625:TRP:NE1	1.68	0.88
2:B:176:ASN:HB2	2:B:291:TYR:CD1	2.08	0.88
2:B:485:ALA:HA	18:B:1232:CLA:HMA2	1.54	0.88
1:A:349:ILE:HA	1:A:352:THR:OG1	1.74	0.88
2:B:98:GLN:HB2	8:H:78:PRO:HB3	1.55	0.88
2:B:259:GLY:HA3	2:B:269:TRP:HZ2	1.36	0.88
2:B:284:PHE:CE1	18:B:1216:CLA:HHC	2.08	0.88
4:D:90:LEU:O	4:D:91:ARG:HD3	1.72	0.88
8:H:92:ARG:N	8:H:93:GLY:HA3	1.89	0.88
17:4:147:LEU:O	17:4:148:GLU:HB2	1.71	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
14:1:180:HIS:O	18:1:1003:CLA:C2A	2.21	0.88
16:3:138:SER:H	16:3:139:MET:HB3	1.37	0.88
1:A:342:GLY:O	1:A:431:LEU:CD2	2.22	0.88
6:F:49:THR:HA	6:F:56:TYR:HH	1.34	0.88
6:F:105:LEU:HD21	18:F:1139:CLA:HED1	1.55	0.88
12:L:63:LEU:HD21	18:L:1502:CLA:CMB	2.03	0.88
12:L:66:GLY:HA2	18:L:1503:CLA:HMB3	1.53	0.88

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
12:L:92:VAL:HG13	12:L:93:VAL:N	1.89	0.88
2:B:649:MET:HE2	2:B:723:ALA:HB2	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
14:1:40:LYS:HG2	14:1:41:GLU:N	1.84	0.88
15:2:17:GLU:HB3	15:2:18:TRP:HB3	1.55	0.88
2:B:5:ILE:CG2	2:B:6:PRO:HA	2.04	0.88
18:B:1220:CLA:OBD	18:B:1221:CLA:CAB	2.21	0.88
12:L:70:LYS:HG2	12:L:75:ARG:HG3	1.53	0.88
17:4:172:ASN:O	17:4:173:VAL:HG23	1.72	0.88
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:76:ASP:O	6:F:77:GLN:O	1.91	0.87
6:F:126:ALA:N	6:F:130:LEU:CD1	2.32	0.87
7:G:8:ILE:CG1	7:G:9:SER:H	1.86	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
15:2:17:GLU:HG3	15:2:18:TRP:CB	1.96	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
17:4:58:MET:SD	17:4:58:MET:N	2.47	0.87
1:A:455:PHE:HD1	1:A:456:HIS:HB3	1.40	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
6:F:86:PRO:CG	10:J:39:PHE:HB2	2.04	0.87
14:1:27:LEU:CB	14:1:28:GLY:HA2	2.04	0.87
9:I:27:HIS:HA	9:I:30:LYS:HD3	1.52	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
17:4:82:GLU:HB3	17:4:84:PHE:CZ	2.09	0.87
1:A:268:PRO:HB2	1:A:273:ASN:HB3	1.53	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
17:4:63:VAL:HG12	17:4:67:ILE:H	1.38	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
2:B:302:LYS:HA	2:B:302:LYS:CE	2.05	0.87

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
18:B:1138:CLA:H8	18:B:1138:CLA:CBB	2.03	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
16:3:61:ILE:O	16:3:64:ARG:HB3	1.75	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
17:4:190:TRP:CE3	17:4:190:TRP:HA	2.07	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
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:64:ASN:HA	2:B:67:HIS:CB	2.05	0.86
2:B:553:PHE:CE2	3:C:66:ARG:HG3	2.09	0.86
3:C:81:TYR:CE1	4:D:37:LEU:O	2.27	0.86
13:N:81:VAL:C	13:N:83:TRP:HD1	1.82	0.86
13:N:82:PHE:CD2	13:N:82:PHE:N	2.36	0.86
17:4:51:ALA:HB1	17:4:161:MET:CE	2.03	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
18:B:1207:CLA:HED1	12:L:73:PRO:HG3	1.56	0.86
18:B:1224:CLA:H3A	18:B:1224:CLA:O1A	1.73	0.86
3:C:27:GLU:N	3:C:43:PRO:HG3	1.89	0.86
13:N:57:LYS:HB2	16:3:87:ALA:CB	2.01	0.86
2:B:63:GLY:O	2:B:66:PHE:N	2.09	0.86
18:L:1503:CLA:CHD	18:L:1503:CLA:CBC	2.37	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
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
12:L:97:MET:SD	12:L:98:CYS:N	2.48	0.86
18:L:1503:CLA:O1A	18:L:1503:CLA:HED3	1.75	0.86
1:A:101:ALA:HA	1:A:161:GLU:OE2	1.75	0.86

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
2:B:319:HIS:O	2:B:320:LYS:C	2.18	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
15:2:23:LEU:HB2	15:2:26:ASP:H	1.31	0.86
18:A:9011:CLA:HBB1	2:B:624:LEU:HD11	1.57	0.86
2:B:60:TRP:O	2:B:64:ASN:ND2	2.09	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
10:J:11:ALA:CB	10:J:12:PRO:CD	2.50	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:1209:CLA:HAA2	7:G:38:GLN:HA	1.57	0.86
18:B:1218:CLA:O1D	18:B:1218:CLA:H2A	1.76	0.86
3:C:44:ARG:O	3:C:45:THR:OG1	1.94	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
12:L:53:GLY:CA	12:L:139:PHE:CE1	2.58	0.86
2:B:458:ILE:H	18:B:1235:CLA:HMD1	1.38	0.86
15:2:86:GLU:OE1	17:4:187:SER:HB2	1.76	0.86
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
18:F:1302:CLA:CMA	18:F:1302:CLA:C9	2.54	0.85
15:2:23:LEU:HB2	15:2:25:GLY:C	1.99	0.85
2:B:411:MET:SD	18:B:1242:CLA:CMD	2.63	0.85
6:F:96:TRP:CD1	6:F:97:ILE:H	1.91	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:CG2	1:A:299:ILE:O	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
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:H13	18:J:2107:CLA:H91	1.58	0.85
2:B:307:ALA:O	2:B:310:PRO:HD2	1.76	0.85

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:HB2	12:L:44:ARG:NH1	1.91	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
15:2:28:GLY:O	15:2:29:PHE:CD1	2.30	0.85
2:B:92:TRP:HD1	9:I:9:VAL:HB	1.40	0.85
2:B:104:PHE:C	2:B:106:ARG:HD2	2.01	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:668:ARG:HH21	2:B:699:ALA:C	1.83	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
15:2:18:TRP:HD1	15:2:21:GLY:HA3	0.69	0.85
15:2:23:LEU:CD1	15:2:25:GLY:C	2.48	0.85
18:B:1138:CLA:CAD	18:B:1138:CLA:HED2	2.07	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
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
15:2:22: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
18:B:1212:CLA:HBC3	18:B:1212:CLA:HHD	1.59	0.84
13:N:63:ASP:HB2	13:N:64:ASP:HB2	1.58	0.84
15:2:18:TRP:CD1	15:2:21:GLY:O	2.30	0.84
1:A:90:PHE:HD1	1:A:175:ALA:HA	1.42	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
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
15:2:17: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: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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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: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:CGD	18:B:1203:CLA:HBA2	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
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
2:B:224:PRO:HB2	2:B:229:GLN:O	1.76	0.84
2:B:655:LEU:HB2	18:B:9022:CLA:HAA1	1.58	0.84
2:B:663:PHE:HD2	2:B:663:PHE:N	1.74	0.84
18:B:1205:CLA:CGA	18:B:1205:CLA:C1A	2.55	0.84
18:B:1220:CLA:C1B	18:B:1242:CLA:HBA1	2.07	0.84
15:2:21:GLY:CA	15:2:23:LEU:CD1	2.55	0.84
1:A:305:ALA:HB2	18:A:1115:CLA:CMA	2.06	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
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
2:B:346:SER:HB3	18:B:1222:CLA:O1D	1.78	0.84
6:F:116:GLN:C	6:F:118:GLU:N	2.34	0.84
6:F:124:PRO:CG	6:F:125:LEU:HG	2.05	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:455:PHE:CD1	1:A:456:HIS:HB3	2.12	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
15:2:28:GLY:O	15:2:29:PHE:CZ	2.31	0.84
1:A:63:ASP:OD1	1:A:66:SER:OG	1.94	0.84
1:A:64:PHE:HE1	18:A:1103:CLA:HMC2	1.41	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:718:PRO:HG3	1:A:722:PRO:HD3	1.60	0.84

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
14:1:7:GLY:HA2	14:1:9:PRO:N	1.93	0.84
2:B:458:ILE:HG12	6:F:74:SER:CB	2.07	0.84
2:B:537:GLY:HA3	2:B:575:ASP:HB3	1.59	0.84
4:D:144:ILE:HD12	4:D:144:ILE:N	1.93	0.84
15:2:28:GLY:O	15:2:29:PHE:CD2	2.30	0.84
15:2:32:LEU:HA	15:2:33:GLY:C	2.02	0.84
1:A:71:LEU:CD1	1:A:352:THR:HG22	2.07	0.83
1:A:688:PHE:O	1:A:688:PHE:CD1	2.31	0.83
1:A:712:ASN:O	1:A:715:LYS:N	2.09	0.83
2:B:564:ARG:O	2:B:564:ARG:HG2	1.76	0.83
2:B:663:PHE:N	2:B:663:PHE:CD2	2.45	0.83
18:B:1207:CLA:HBC3	20:I:6018:BCR:C21	2.03	0.83
14:1:89:VAL:HB	14:1:90:PRO:HD3	1.60	0.83
2:B:333:GLN:O	18:B:1202:CLA:HHD	1.78	0.83
14:1:85:LEU:C	14:1:87:ASN:HA	2.03	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
18:L:1503:CLA:HBC2	18:L:1503:CLA:HHD	0.87	0.83
15:2:96:ILE:O	15:2:100:VAL:HG13	1.78	0.83
15:2:178:TRP:HA	15:2:179:PHE:CD1	2.13	0.83
12:L:92:VAL:O	12:L:94:ILE:N	2.09	0.83
15:2:36:SER:HA	15:2:37:ASP:CB	2.08	0.83
1:A:489:ALA:HB1	1:A:490:GLN:C	2.03	0.83
1:A:658:TRP:HD1	2:B:625:TRP:CD1	1.96	0.83
2:B:700:LEU:O	2:B:701:SER:C	2.21	0.83
4:D:108:GLU:HG2	4:D:109:VAL:HG22	1.57	0.83
14:1:84:TYR:HB2	14:1:85:LEU:HG	1.60	0.83
1:A:77:LYS:HZ1	18:A:1109:CLA:C2B	1.91	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
18:A:9013:CLA:CHB	18:B:9012:CLA:HBB2	2.08	0.83
2:B:617:MET:O	2:B:621:ARG:N	2.09	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
15:2:32:LEU:HD13	15:2:32:LEU:C	2.04	0.83
15:2:197:ALA:H	15:2:198:ASP:CA	1.88	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
15:2:96:ILE:HG13	15:2:97:VAL:H	1.41	0.83
1:A:85:GLN:HE21	1:A:85:GLN:HA	1.44	0.83
1:A:398:HIS:HB2	18:A:1126:CLA:NB	1.93	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
14:1:54:VAL:HA	14:1:57:ILE:CG2	2.08	0.83
1:A:255:LEU:H	1:A:255:LEU:HD12	1.43	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
2:B:259:GLY:C	2:B:269:TRP:HE1	1.85	0.83
15:2:44:ASN:ND2	15:2:113:ILE:CB	2.41	0.83
1:A:472:ARG:O	1:A:474:GLN:N	2.11	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
18:B:1205:CLA:NA	18:B:1205:CLA:O2A	2.12	0.83
6:F:125:LEU:CA	6:F:130:LEU:HD11	2.09	0.83
17:4:72:VAL:H	17:4:73:PRO:HD2	1.44	0.83
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
17:4:102:GLU:O	17:4:105:ARG:HG3	1.79	0.82
17:4:106:TRP:CZ2	17:4:110:LYS:NZ	2.46	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:265:THR:HA	2:B:360:PHE:HE2	1.42	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:709:GLY:O	2:B:713:PHE:HB2	1.78	0.82

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
3:C:27:GLU:HB2	4:D:127:ARG:HD2	1.60	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:79:ARG:HE	4:D:81:GLU:CD	1.87	0.82
4:D:90:LEU:O	4:D:91:ARG:NH1	2.12	0.82
15:2:19:LEU:HD23	15:2:20:ASP:OD1	1.79	0.82
1:A:584:PRO:HD3	2:B:561:GLY:HA3	1.62	0.82
1:A:650:ASN:C	1:A:652:TRP:H	1.87	0.82
2:B:564:ARG:HH12	3:C:66:ARG:HH22	1.24	0.82
2:B:684:ARG:CZ	12:L:22:GLY:HA3	2.10	0.82
7:G:16:LEU:HD23	7:G:68:ILE:HG12	1.61	0.82
1:A:160:SER:O	1:A:163:GLN:HB3	1.80	0.82
1:A:402:ILE:H	1:A:402:ILE:HD12	1.41	0.82
2:B:262:HIS:CD2	2:B:264:GLN:HB3	2.13	0.82
2:B:593:TYR:CE1	18:B:1234:CLA:HAC2	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
15:2:194:ALA:HB3	15:2:195:HIS:CD2	2.14	0.82
2:B:450:GLU:HA	6:F:68:LEU:HD11	1.61	0.82
12:L:79:TYR:N	12:L:80:ALA:HB2	1.94	0.82
17:4:62:GLU:O	17:4:63:VAL:CG2	2.27	0.82
1:A:364:MET:HA	1:A:364:MET:CE	2.08	0.82
2:B:287:GLY:N	18:B:1218:CLA:HMC2	1.93	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:57:LYS:HD2	16:3:87:ALA:HB1	0.82	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:639:ALA:C	1:A:641:ASN:H	1.88	0.82
1:A:665:ILE:CD1	18:A:9011:CLA:HBC1	2.09	0.82
1:A:725:LEU:HD22	19:A:5001:PQN:C6	2.09	0.82
2:B:58:PHE:CZ	18:B:1241:CLA:HHB	2.14	0.82
2:B:424:TRP:HE1	18:B:1229:CLA:CED	1.91	0.82
2:B:443:MET:SD	2:B:451:LYS:HE3	2.18	0.82
1:A:735:VAL:HG13	1:A:736:THR:H	1.45	0.82
2:B:6:PRO:HD3	2:B:20:ARG:HE	1.45	0.82

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:20:ARG:NH2	9:I:28:VAL:HA	1.95	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:689:ASN:ND2	4:D:38:ARG:NH1	2.28	0.82
2:B:693:TRP:HB3	18:B:1238:CLA:HMD2	1.60	0.82
18:B:1216:CLA:CGA	18:B:1220:CLA:H11	2.09	0.82
4:D:133:ASN:OD1	4:D:135:ARG:HB2	1.79	0.82
13:N:67:LEU:HG	13:N:67:LEU:O	1.78	0.82
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
15:2:19:LEU:HG	15:2:20:ASP:OD1	1.79	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
18:A:1107:CLA:HAA2	18:A:1107:CLA:HBD	1.61	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
15:2:162: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
1:A:81:ALA:HB3	1:A:82:HIS:C	2.05	0.81
2:B:92:TRP:HD1	9:I:9:VAL:CB	1.93	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:311:PRO:HD2	18:B:1220:CLA:CMA	2.11	0.81
2:B:504:ASN:C	2:B:506:ASN:H	1.89	0.81
2:B:547:MET:CB	3:C:66:ARG:HH21	1.90	0.81
2:B:663:PHE:O	2:B:664:LEU:HB2	1.78	0.81
18:B:1212:CLA:HAA1	18:B:1212:CLA:C2	2.10	0.81
18:B:1216:CLA:HAA2	18:B:1221:CLA:HBB2	1.62	0.81
5:E:72:VAL:HG22	5:E:78:SER:HB3	1.62	0.81
7:G:35:VAL:CG1	7:G:36:PRO:CB	2.55	0.81
8:H:44:ALA:HB3	8:H:45:ALA:HA	1.60	0.81
15:2:23:LEU:HD13	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
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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:101:ALA:HA	1:A:161:GLU:CD	2.05	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:ND1	1:A:711:HIS:N	2.29	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
2:B:325:THR:O	2:B:329:SER:HB3	1.80	0.81
18:B:1202:CLA:HED3	18:B:1203:CLA:HMB3	1.60	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
1:A:358:LEU:HG	18:A:1103:CLA:HMD3	1.62	0.81
2:B:672:GLN:HE22	2:B:698:VAL:CA	1.93	0.81
8:H:47:PHE:CZ	12:L:50:LEU:HD11	2.14	0.81
10:J:2:ARG:HB3	10:J:3:ASP:CB	2.04	0.81
12:L:97:MET:SD	12:L:97:MET:C	2.64	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
2:B:485:ALA:HA	18:B:1232:CLA:HMA1	1.60	0.81
2:B:536:LYS:C	2:B:538:ALA:H	1.87	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
14:1:38:ARG:CA	14:1:39:TYR:CB	2.59	0.81
14:1:181:LEU:HA	14:1:182:ALA:O	1.80	0.81
15:2:24:PRO:CB	15:2:32:LEU:HG	2.09	0.81
1:A:245:PRO:HA	1:A:248:PHE:HE1	1.46	0.81
2:B:37:ILE:O	4:D:148:PHE:HD1	1.59	0.81
2:B:253:ALA:O	2:B:254:ILE:HG22	1.80	0.81
12:L:70:LYS:HG2	12:L:75:ARG:CG	2.10	0.81
1:A:238:ASP:CB	1:A:239:PRO:HD3	2.09	0.81
1:A:251:ASN:HD22	1:A:251:ASN:C	1.89	0.81
1:A:331:LEU:CD1	1:A:346:LEU:HB3	2.09	0.81
2:B:527:LEU:CD2	2:B:586:THR:HG21	2.09	0.81
2:B:536:LYS:C	2:B:538:ALA:N	2.36	0.81
18:B:1209:CLA:H3A	18:B:1209:CLA:CGA	2.10	0.81
6:F:130:LEU:O	6:F:133:GLY:N	2.13	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
12:L:107:PHE:HA	12:L:133:ALA:CB	2.10	0.81
14:1:10:ARG:O	17:4:110:LYS:HG3	1.80	0.81

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
15:2:40:SER:CB	15:2:41:LEU:CB	2.58	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
18:L:1503:CLA:CED	18:L:1503:CLA:H11	2.09	0.81
2:B:451:LYS:CD	10:J:35:ASP:OD1	2.29	0.81
2:B:684:ARG:CZ	12:L:22:GLY:CA	2.59	0.81
18:B:1218:CLA:OBD	18:B:1218:CLA:HED2	1.81	0.81
18:F:1302:CLA:H92	18:F:1302:CLA:HMA2	1.62	0.81
7:G:61:ASN:HA	7:G:64:VAL:HG22	1.61	0.81
8:H:33:ASN:HD21	18:H:1501:CLA:CMD	1.93	0.81
8:H:47:PHE:CE2	12:L:138:LYS:HB2	2.16	0.81
10:J:39:PHE:CZ	10:J:41:PHE:HB3	2.16	0.81
15:2:172:LEU:O	15:2:175:MET:SD	2.39	0.81
1:A:147:SER:HA	1:A:391:THR:HG21	1.61	0.80
18:A:1108:CLA:HBC2	18:A:1110:CLA:C2C	2.11	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
15:2:19:LEU:CD1	15:2:22:SER:OG	2.29	0.80
1:A:71:LEU:HD21	1:A:353:SER:HB2	1.63	0.80
2:B:83:HIS:HB3	2:B:84:VAL:HA	1.62	0.80
2:B:115:ASN:O	2:B:117:TYR:CD1	2.35	0.80
2:B:420:SER:HA	18:B:1138:CLA:HED1	1.63	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
8:H:33:ASN:ND2	18:H:1501:CLA:HMD2	1.95	0.80
9:I:4:LEU:CD2	9:I:5:PRO:HA	2.11	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
18:B:1217:CLA:HMA1	7:G:21:PHE:CD2	2.15	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
16:3:83:GLY:O	16:3:88:GLU:HA	1.81	0.80
1:A:555:ILE:H	1:A:556:LEU:HB2	0.65	0.80
2:B:84:VAL:HG12	2:B:85:ARG:N	1.95	0.80
14:1:34:ALA:HB3	14:1:37:GLU:HA	1.62	0.80
15:2:19:LEU:CD2	15:2:20:ASP:OD1	2.30	0.80
15:2:26:ASP:CG	15:2:27:PHE:HB3	2.05	0.80
6:F:127:SER:CA	6:F:131:PHE:HB2	2.12	0.80
14:1:91:TRP:N	14:1:92:GLY:HA2	1.96	0.80

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
15:2:22:SER:O	15:2:23:LEU:HD23	1.81	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:162:ASP:C	12:L:164:PRO:HD2	2.05	0.80
14:1:181:LEU:O	18:1:1003:CLA:CHA	2.30	0.80
15:2:19:LEU:CA	15:2:20:ASP:OD2	2.29	0.80
15:2:19:LEU:CG	15:2:20:ASP:OD1	2.30	0.80
17:4:42:GLN:HG2	17:4:46:VAL:HG23	1.63	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:CD1	4:D:45:PHE:C	2.56	0.80
4:D:45:PHE:O	4:D:78:ALA:HA	1.82	0.80
4:D:150:GLY:HA2	4:D:151:LYS:C	2.06	0.80
6:F:8:CYS:SG	6:F:63:CYS:HB3	2.22	0.80
1:A:699:TYR:HE1	2:B:536:LYS:HE3	1.47	0.80
2:B:119:GLY:HA3	2:B:371:LEU:CD1	2.11	0.80
2:B:174:ARG:NH2	18:B:1210:CLA:HHD	1.97	0.80
2:B:257:ILE:HG12	18:B:1214:CLA:HMB2	1.62	0.80
2:B:476:ILE:HB	2:B:477:PRO:CD	2.10	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
17:4:41:VAL:CG2	17:4:42:GLN:H	1.85	0.80
1:A:562:PHE:CZ	2:B:677:THR:HG21	2.17	0.80
2:B:117:TYR:CE2	2:B:366:THR:OG1	2.35	0.80
2:B:342:GLY:O	2:B:345:THR:OG1	2.00	0.80
2:B:621:ARG:O	2:B:625:TRP:HB3	1.82	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
15:2:32:LEU:HD22	15:2:33:GLY:O	1.81	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
2:B:287:GLY:HA2	18:B:1218:CLA:HMC1	1.61	0.80
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
14:1:187:ASN:O	14:1:188:ASN:HB2	1.81	0.80

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
15:2:20:ASP:OD2	15:2:22:SER:CB	2.30	0.80
1:A:527:VAL:HG13	1:A:528:ALA:H	1.45	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
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: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
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:CD2	2.30	0.79
1:A:295:TRP:HB2	1:A:298:ASP:HB2	1.64	0.79
1:A:458:PHE:C	1:A:458:PHE:CD2	2.60	0.79
2:B:86:PRO:O	2:B:116:ALA:N	2.15	0.79
18:B:1207:CLA:CBC	20:I:6018:BCR:H21C	2.04	0.79
6:F:136:TRP:CD1	6:F:136:TRP:H	1.99	0.79
7:G:83:TYR:CB	7:G:85:ILE:HG12	2.11	0.79
2:B:393:PHE:HD2	2:B:398:TYR:HB2	1.45	0.79
18:B:1235:CLA:CGA	18:B:1235:CLA:C1A	2.59	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:O	6:F:2:ILE:HG13	1.81	0.79
13:N:81:VAL:C	13:N:83:TRP:CD1	2.60	0.79
15:2:23:LEU:CD2	15:2:26:ASP:O	2.29	0.79
17:4:180:ASP:OD2	17:4:185:HIS:CD2	2.35	0.79
1:A:486:PRO:CD	1:A:487:VAL:HB	2.12	0.79
7:G:22:VAL:C	7:G:23:PHE:HD2	1.90	0.79
14:1:185:TRP:HA	14:1:185:TRP:CE3	2.18	0.79
15:2:59:ALA:O	15:2:63:PHE:HE2	1.63	0.79
16:3:132:ASP:CG	16:3:139:MET:HB2	2.08	0.79
17:4:42:GLN:HA	17:4:45:LEU:HB3	1.65	0.79
3:C:25:VAL:HG21	3:C:48:CYS:CB	2.13	0.79
18:L:1503:CLA:HAA2	18:L:1503:CLA:CBD	2.00	0.79
14:1:91:TRP:H	14:1:92:GLY:CA	1.95	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
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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
16:3:212:ASN:CB	16:3:213:LEU:HB2	2.13	0.79
1:A:198:ASP:CG	1:A:199:VAL:H	1.91	0.79
1:A:289:PRO:O	1:A:523:VAL:CG1	2.30	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:331:HIS:ND1	2:B:392:ILE:CG2	2.43	0.79
2:B:429:LEU:HD21	18:B:1235:CLA:HMB2	1.65	0.79
3:C:42:ALA:CB	3:C:45:THR:HG23	2.13	0.79
6:F:18:GLU:C	6:F:20:GLN:H	1.90	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
2:B:646:TRP:HB3	2:B:723:ALA:HB1	1.63	0.79
18:B:1239:CLA:HBD	19:B:5002:PQN:H262	1.64	0.79
6:F:130:LEU:HD12	6:F:130:LEU:H	1.48	0.79
13:N:58:VAL:HG23	13:N:59:PRO:N	1.97	0.79
15:2:18:TRP:CD1	15:2:21:GLY:C	2.60	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
13:N:83:TRP:O	13:N:84:LYS:HB3	1.80	0.79
14:1:52:LEU:HA	14:1:55:PRO:CD	2.12	0.79
1:A:638:THR:OG1	1:A:641:ASN:ND2	2.15	0.78
2:B:542:ARG:HD2	2:B:542:ARG:O	1.82	0.78
18:B:1220:CLA:HBC2	18:B:1220:CLA:CHD	2.11	0.78
14:1:94:LEU:CB	14:1:95:PRO:CD	2.61	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
2:B:176:ASN:HB2	2:B:291:TYR:HD1	1.45	0.78
2:B:286:ILE:CD1	18:B:1218:CLA:HMC2	2.08	0.78

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
4:D:102:ARG:HH11	4:D:110:GLN:HE22	1.31	0.78
14:1:103:LEU:O	14:1:107:PHE:HD1	1.66	0.78
15:2:56:MET:HB3	15:2:172:LEU:HD22	1.64	0.78
15:2:157:LYS:CA	15:2:160:ARG:HG2	2.10	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
15:2:153:PRO:HB2	15:2:154:GLN:O	1.82	0.78
15:2:187:GLY:C	15:2:189:ILE:H	1.91	0.78
16:3:106:THR:OG1	16:3:109:ALA:HA	1.83	0.78
2:B:294:ASN:CG	18:B:1209:CLA:HMA1	2.09	0.78
2:B:411:MET:SD	18:B:1242:CLA:HMD1	2.23	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
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
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:HHB	1.64	0.78
1:A:684:PHE:HE2	18:A:1140:CLA:HBB2	1.48	0.78
2:B:176:ASN:ND2	2:B:292:ARG:H	1.82	0.78
2:B:218:TYR:CE2	2:B:253:ALA:O	2.36	0.78
2:B:720:THR:O	2:B:723:ALA:N	2.15	0.78
18:B:1202:CLA:H41	18:B:1221:CLA:O1A	1.84	0.78
8:H:73:PRO:HB2	8:H:74:GLN:CA	2.14	0.78
1:A:330:ILE:O	1:A:333:ALA:HB2	1.84	0.78
1:A:404:GLY:O	1:A:405:PHE:C	2.27	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
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: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:290:MET:HA	18:B:1218:CLA:HBC2	0.81	0.78
2:B:330:ILE:CG2	18:B:1202:CLA:HAC1	2.13	0.78
2:B:348:VAL:HG21	18:B:1225:CLA:CMD	2.14	0.78

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
18:B:1227:CLA:HMB2	18:B:1228:CLA:C3D	2.13	0.78
6:F:52:ARG:HB3	6:F:56:TYR:CE1	2.18	0.78
17:4:82:GLU:CG	17:4:83:TYR:H	1.96	0.78
1:A:51:THR:OG1	1:A:52:THR:N	2.16	0.78
1:A:493:GLN:HG3	1:A:515:TRP:HB2	1.66	0.78
12:L:129:GLN:OE1	12:L:131:GLN:O	2.02	0.78
1:A:64:PHE:CE1	18:A:1103:CLA:HMC2	2.18	0.78
2:B:73:ASN:ND2	2:B:108:GLY:HA3	1.99	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
17:4:80:LYS:HD2	17:4:83:TYR:OH	1.84	0.78
2:B:115:ASN:O	2:B:117:TYR:CE1	2.37	0.77
2:B:396:ARG:O	2:B:397:ASP:OD2	2.01	0.77
18:B:1212:CLA:HAA1	18:B:1212:CLA:H2	1.63	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
15:2:23:LEU:CD1	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: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:493:GLN:C	1:A:496:HIS:HB2	2.09	0.77
1:A:687:ALA:HB1	18:A:9013:CLA:HBB2	1.65	0.77
17:4:110:LYS:O	17:4:112:PRO:HD3	1.83	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
15:2:179:PHE:CD1	15:2:179:PHE:C	2.62	0.77
1:A:71:LEU:HD21	1:A:353:SER:CB	2.14	0.77
1:A:495:THR:C	1:A:497:ALA:N	2.35	0.77
1:A:700:TRP:CZ2	19:A:5001:PQN:H2M3	2.18	0.77
1:A:705:GLU:O	1:A:707:ILE:N	2.17	0.77
2:B:170:ASN:ND2	18:B:1209:CLA:HED2	1.98	0.77
2:B:337:ALA:HB1	18:B:1202:CLA:OBD	1.85	0.77
12:L:86:LEU:C	12:L:88:ALA:H	1.92	0.77
1:A:81:ALA:HB1	1:A:82:HIS:CA	2.13	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
2:B:74:PHE:HB3	2:B:132:ASN:HD21	1.46	0.77
18:B:1209:CLA:CGA	18:B:1209:CLA:C3A	2.63	0.77

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:680:LEU:HB3	18:B:9012:CLA:C2	2.15	0.77
1:A:735:VAL:O	1:A:739:LEU:CB	2.32	0.77
2:B:20:ARG:O	2:B:23:PHE:C	2.27	0.77
6:F:71:LEU:HD11	10:J:38:THR:HG21	1.67	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
1:A:684:PHE:HD2	1:A:684:PHE:C	1.93	0.77
2:B:631:LEU:HA	2:B:643:LEU:HD12	1.66	0.77
18:B:1138:CLA:C3B	18:F:1139:CLA:HMD1	2.13	0.77
18:B:1207:CLA:HBB2	9:I:13:GLY:O	1.84	0.77
6:F:48:LYS:HE2	6:F:48:LYS:H	1.48	0.77
12:L:112:PRO:HB2	12:L:113:SER:HA	1.65	0.77
14:1:184:PRO:O	14:1:185:TRP:HB2	1.83	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
16:3:212:ASN:CB	16:3:214:LEU:H	1.96	0.77
1:A:687:ALA:C	1:A:689:SER:H	1.92	0.77
18:A:1123:CLA:HBC2	18:A:1123:CLA:CHD	2.13	0.77
2:B:58:PHE:HE2	18:B:1241:CLA:HHB	1.50	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
1:A:340:GLY:C	1:A:342:GLY:H	1.92	0.77
18:A:9011:CLA:HBB2	18:B:9010:CLA:C1D	2.14	0.77
2:B:287:GLY:H	18:B:1218:CLA:HMC1	0.83	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: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
2:B:705:ALA:HB1	19:B:5002:PQN:C8	2.14	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
1:A:75:SER:CA	1:A:354:TRP:HZ2	1.98	0.76
1:A:373:ALA:O	1:A:375:HIS:N	2.19	0.76

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:O	1:A:631:GLN:NE2	2.19	0.76
2:B:294:ASN:HA	7:G:37:GLU:OE1	1.85	0.76
2:B:348:VAL:CG2	18:B:1225:CLA:HMD2	2.14	0.76
2:B:717:TYR:HE2	18:B:9010:CLA:O1A	1.68	0.76
18:B:1207:CLA:H2A	18:B:1207:CLA:O2A	1.84	0.76
6:F:1:ASP:H2	6:F:62:LEU:HD13	1.48	0.76
6:F:122:ASP:H	10:J:9:SER:HB2	1.50	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:N	13:N:60:PHE:CD2	2.43	0.76
13:N:82:PHE:N	13:N:82:PHE:HD2	1.82	0.76
14:1:85:LEU:O	14:1:87:ASN:HA	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: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
2:B:104:PHE:HB2	2:B:112:PRO:C	2.11	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
17:4:114:SER:CB	17:4:120:ILE:HG12	2.14	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:12:ILE:HG12	3:C:28:MET:SD	2.26	0.76
3:C:20:ALA:O	3:C:22:PRO:HD2	1.85	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
1:A:705:GLU:HA	1:A:708:VAL:HB	1.66	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
2:B:203:ARG:NH1	2:B:252:THR:HB	2.00	0.76
4:D:149:THR:HB	4:D:152:GLN:C	2.10	0.76

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
12:L:143:PHE:O	12:L:147:GLY:N	2.19	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:547:PHE:HE1	1:A:551:VAL:CG1	1.98	0.76
1:A:548:THR:O	1:A:552:THR:OG1	2.04	0.76
1:A:751:LEU:HD13	1:A:752:ALA:H	1.51	0.76
2:B:192:GLY:O	2:B:195:VAL:HB	1.85	0.76
18:B:1202:CLA:HBD	18:B:1202:CLA:HBA1	1.67	0.76
7:G:20:ARG:HH11	7:G:20:ARG:CG	1.99	0.76
13:N:81:VAL:CB	13:N:82:PHE:CA	2.53	0.76
1:A:158:ILE:C	1:A:163:GLN:HE22	1.94	0.76
1:A:707:ILE:HG22	1:A:711:HIS:CE1	2.20	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:415:LYS:HZ1	2:B:540:ASP:HA	1.50	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
12:L:66:GLY:C	18:L:1503:CLA:HMB1	2.10	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
15:2:22:SER:N	15:2:23:LEU:HA	1.98	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
15:2:19:LEU:CG	15:2:20:ASP:OD2	2.30	0.76
15:2:21:GLY:N	15:2:23:LEU:HD12	1.99	0.76
1:A:71:LEU:HA	1:A:74:ILE:HG22	1.68	0.76
1:A:435:VAL:HG12	1:A:436:LEU:HD23	1.65	0.76
2:B:19:ARG:HA	2:B:22:TRP:CD1	2.21	0.76
4:D:111:TYR:N	4:D:111:TYR:HD1	1.82	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
15:2:26:ASP:HB3	15:2:27:PHE:CD2	2.21	0.76
3:C:55:GLU:HB3	3:C:65:VAL:CG2	2.15	0.75

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:D:122:LYS:HA	4:D:123:VAL:HG12	1.67	0.75
6:F:17:ARG:NH2	6:F:66:ASP:OD1	2.19	0.75
6:F:136:TRP:CD1	6:F:136:TRP:N	2.53	0.75
15:2:159:LEU:O	15:2:162:LYS:HB3	1.84	0.75
15:2:185:GLY:C	15:2:187:GLY:HA3	2.11	0.75
15:2:194:ALA:CB	15:2:195:HIS:CA	2.64	0.75
1:A:615:HIS:C	1:A:615:HIS:CD2	2.63	0.75
18:A:1124:CLA:HHC	18:A:1137:CLA:O1A	1.85	0.75
2:B:89:HIS:O	2:B:90:ALA:CB	2.34	0.75
2:B:174:ARG:NE	18:B:1210:CLA:HHD	2.00	0.75
18:B:1222:CLA:HBB2	18:B:1236:CLA:HHB	1.67	0.75
15:2:106:GLU:HG2	18:2:2012:CLA:C4C	2.16	0.75
15:2:188:PRO:HB2	15:2:193:PHE:CD2	2.20	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
1:A:590:CYS:O	1:A:591:GLN:C	2.28	0.75
3:C:72:GLU:OE2	3:C:77:MET:HG3	1.86	0.75
7:G:77:ILE:O	7:G:77:ILE:CG2	2.34	0.75
14:1:186:HIS:HB3	14:1:188:ASN:O	1.85	0.75
1:A:133:ASN:HB2	1:A:142:GLY:HA2	1.67	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
6:F:100:VAL:HG11	6:F:125:LEU:HD22	1.66	0.75
12:L:37:LEU:H	12:L:37:LEU:HD22	1.51	0.75
15:2:21:GLY:N	15:2:23:LEU:HD11	2.00	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
2:B:458:ILE:H	18:B:1235:CLA:CMD	1.98	0.75
18:B:1212:CLA:CGA	18:B:1212:CLA:H3A	2.16	0.75
3:C:16:GLN:NE2	3:C:16:GLN:O	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:C1	18:L:1503:CLA:O2D	2.34	0.75
15:2:17:GLU:HB3	15:2:19:LEU:N	2.00	0.75
15:2:86:GLU:OE2	17:4:187:SER:HB3	1.87	0.75
6:F:81:GLY:HA2	6:F:85:THR:H	1.50	0.75
6:F:124:PRO:HG2	6:F:125:LEU:CG	2.06	0.75
9:I:9:VAL:HA	9:I:12:VAL:HG12	1.68	0.75

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
13:N:45:ASN:HD22	13:N:46:PHE:N	1.84	0.75
1:A:223:VAL:HA	1:A:227:LEU:HD12	1.68	0.75
1:A:478:SER:CB	1:A:647:ILE:HD13	2.16	0.75
1:A:629:ASN:OD1	1:A:633:VAL:O	2.05	0.75
1:A:684:PHE:C	1:A:684:PHE:CD2	2.64	0.75
2:B:392:ILE:HG22	2:B:393:PHE:N	2.02	0.75
2:B:439:HIS:CD2	18:B:1230:CLA:NC	2.54	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
14:1:89:VAL:HB	14:1:90:PRO:CD	2.16	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
18:A:1105:CLA:C2B	18:A:1107:CLA:HED2	2.17	0.75
2:B:479:SER:C	2:B:481:THR:N	2.39	0.75
5:E:89:GLU:HG2	5:E:90:VAL:O	1.85	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
6:F:115:THR:CG2	6:F:116:GLN:H	1.95	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
14:1:74:TRP:CZ3	14:1:81:GLN:HG3	2.22	0.75
2:B:345:THR:HB	2:B:379:ALA:HB2	1.68	0.75
2:B:451:LYS:HD2	10:J:35:ASP:OD1	1.87	0.75
4:D:111:TYR:O	4:D:115:LYS:HD3	1.87	0.75
8:H:22:ASP:C	8:H:24:TYR:H	1.95	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
14:1:90:PRO:HG2	14:1:92:GLY:HA2	1.69	0.75
1:A:289:PRO:HD3	1:A:295:TRP:CH2	2.20	0.74
1:A:489:ALA:HA	1:A:490:GLN:HB2	1.67	0.74
2:B:428:PHE:CZ	18:B:1229:CLA:HMD1	2.22	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
4:D:50:TRP:CD1	4:D:51:GLU:C	2.65	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
15:2:17:GLU:C	15:2:17:GLU:OE2	2.30	0.74
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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
15:2:17:GLU:C	15:2:18:TRP:O	2.29	0.74
15:2:27:PHE:CD1	15:2:28:GLY:C	2.63	0.74
1:A:299:ILE:O	1:A:299:ILE:HG23	1.87	0.74
18:A:1119:CLA:HHD	18:A:1119:CLA:HBC2	1.69	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
18:H:1501:CLA:HMA1	12:L:58:LEU:HB3	1.68	0.74
15:2:161:THR:CG2	15:2:165:LYS:HG3	2.14	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
14:1:70:LYS:HB3	14:1:73:GLU:HG3	1.69	0.74
2:B:287:GLY:HA2	18:B:1218:CLA:CMC	2.14	0.74
2:B:344:ILE:CG1	18:B:1225:CLA:CAC	2.64	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
18:B:1227:CLA:H41	18:B:1228:CLA:H92	1.67	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
17:4:144:ALA:O	17:4:146:THR:N	2.20	0.74
1:A:112:ASP:O	1:A:112:ASP:CG	2.31	0.74
1:A:158:ILE:O	1:A:163:GLN:NE2	2.19	0.74
1:A:686:TRP:CE3	18:A:9011:CLA:HMA3	2.22	0.74
2:B:346:SER:OG	18:B:1222:CLA:OBD	2.04	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
4:D:50:TRP:HD1	4:D:51:GLU:C	1.93	0.74
13:N:8:GLU:CG	13:N:11:LYS:HB2	2.18	0.74
15:2:18:TRP:O	15:2:19:LEU:C	2.29	0.74
15:2:183:TYR:O	15:2:184:THR:HG22	1.87	0.74

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:367:SER:O	1:A:371:VAL:HG22	1.87	0.74
1:A:431:LEU:HD12	18:A:1122:CLA:CMC	2.17	0.74
1:A:588:GLY:CA	2:B:668:ARG:HD2	2.18	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
2:B:101:VAL:CG2	2:B:102:GLU:H	1.99	0.74
2:B:391:PRO:HD3	2:B:538:ALA:HB2	1.68	0.74
2:B:523:ILE:CD1	2:B:590:VAL:HG21	2.17	0.74
18:B:1202:CLA:CED	18:B:1203:CLA:HMB3	2.17	0.74
18:B:1239:CLA:H11	19:B:5002:PQN:H271	1.70	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
14:1:70:LYS:CB	14:1:73:GLU:HG3	2.16	0.74
14:1:164:GLN:HA	14:1:167:ALA:HB3	1.70	0.74
17:4:82:GLU:O	17:4:83:TYR:CD2	2.41	0.74
1:A:238:ASP:HB3	1:A:239:PRO:CD	2.12	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
18:A:1106:CLA:CBB	18:A:1126:CLA:H8	2.18	0.74
18:B:1217:CLA:HMB1	7:G:18:LEU:HD22	1.68	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
12:L:123:ARG:O	12:L:125:LYS:N	2.20	0.74
14:1:189:ILE:N	14:1:190:GLY:CA	2.51	0.74
15:2:23:LEU:HD12	15:2:26:ASP:N	1.99	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
13:N:58:VAL:CB	16:3:86:PRO:O	2.36	0.74
15:2:21:GLY:HA2	15:2:23:LEU:CD1	2.06	0.74
1:A:171:ALA:HA	1:A:174:PHE:HB3	1.69	0.74
1:A:373:ALA:C	1:A:375:HIS:H	1.92	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:348:VAL:HG21	18:B:1225:CLA:HMD2	1.70	0.74
2:B:428:PHE:CG	18:B:1229:CLA:OBD	2.41	0.74
4:D:111:TYR:HD1	4:D:111:TYR:H	1.33	0.74
17:4:120:ILE:HA	17:4:121:PHE:CD2	2.23	0.74
18:4:1304:CLA:C2	18:4:1304:CLA:CAA	2.64	0.74
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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:697:ARG:NH2	1:A:724:ALA:O	2.20	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
17:4:63:VAL:HG12	17:4:67:ILE:N	2.02	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
2:B:4:ARG:HH11	2:B:4:ARG:CG	2.01	0.73
2:B:589:TRP:CD1	2:B:592:PHE:HE2	2.02	0.73
6:F:55:ASN:O	6:F:56:TYR:C	2.31	0.73
17:4:113:GLY:O	17:4:114:SER:HB2	1.88	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
1:A:77:LYS:HZ2	18:A:1109:CLA:C2B	2.00	0.73
1:A:366:GLY:O	1:A:369:THR:N	2.20	0.73
1:A:397:THR:OG1	18:A:1126:CLA:HMB2	1.89	0.73
1:A:527:VAL:CG1	1:A:528:ALA:N	2.52	0.73
2:B:478:LEU:C	2:B:480:SER:H	1.94	0.73
2:B:569:ASP:CG	2:B:706:ARG:HH22	1.95	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
12:L:138:LYS:HZ2	12:L:138:LYS:HB3	1.51	0.73
14:1:150:ASN:HD22	14:1:153:LEU:HD23	1.52	0.73
1:A:64:PHE:CA	1:A:67:HIS:HB2	2.15	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:715:LYS:NZ	6:F:153:ASN:HD21	1.87	0.73
2:B:265:THR:HA	2:B:360:PHE:CE2	2.24	0.73
2:B:335:GLY:O	2:B:339:ALA:HB2	1.89	0.73
2:B:510:LEU:HD13	18:B:1234:CLA:HMD3	1.69	0.73
18:B:1216:CLA:HAA2	18:B:1221:CLA:CBB	2.17	0.73
3:C:27:GLU:OE1	3:C:43:PRO:HB3	1.88	0.73
6:F:89:LEU:O	6:F:93:ILE:N	2.20	0.73

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
18:L:1502:CLA:O1D	18:L:1502:CLA:H2A	1.87	0.73
15:2:22:SER:N	15:2:25:GLY:CA	2.51	0.73
17:4:55:VAL:O	17:4:59:LEU:HB2	1.88	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
2:B:542:ARG:HD2	2:B:542:ARG:C	2.13	0.73
4:D:112:LEU:CG	4:D:113:HIS:CE1	2.67	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:511:THR:HB	1:A:515:TRP:HZ2	1.54	0.73
2:B:174:ARG:HG3	18:B:1221:CLA:HMD3	1.69	0.73
2:B:573:TRP:CZ3	2:B:703:VAL:HG22	2.23	0.73
18:B:9023:CLA:HMA2	20:B:6017:BCR:H403	1.71	0.73
18:B:1220:CLA:OBD	18:B:1221:CLA:CBB	2.37	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
20:I:6018:BCR:H371	20:L:6020:BCR:C34	2.18	0.73
12:L:107:PHE:HD2	12:L:133:ALA:HB2	1.53	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
1:A:160:SER:O	1:A:163:GLN:CB	2.36	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
6:F:96:TRP:CD1	6:F:96:TRP:C	2.65	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:462:ILE:H	1:A:649:ILE:HD12	1.52	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
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
12:L:137:ALA:C	12:L:138:LYS:HZ2	1.97	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:355:LEU:HD21	18:B:1214:CLA:CED	2.19	0.72
3:C:41:SER:HG	4:D:132:LEU:HD21	1.51	0.72
4:D:83:CYS:O	4:D:84:LEU:C	2.31	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
16:3:67:MET:HB2	18:3:3005:CLA:C2C	2.19	0.72
16:3:133:TRP:O	16:3:137:GLY:N	2.22	0.72
1:A:526:LYS:HA	1:A:627:THR:CA	2.19	0.72
2:B:98:GLN:OE1	8:H:79:ILE:N	2.21	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
14:1:103:LEU:HA	14:1:106:ALA:CB	2.18	0.72
2:B:159:PRO:HA	2:B:162:LYS:HB3	1.70	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
2:B:284:PHE:O	2:B:288:GLY:N	2.23	0.72
4:D:72:PRO:HD2	4:D:73:ASN:CG	2.14	0.72
7:G:83:TYR:HA	7:G:85:ILE:H	1.51	0.72
8:H:58:ILE:HD12	8:H:58:ILE:C	2.14	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
2:B:235:GLN:C	2:B:236:ASN:HD22	1.98	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
18:B:1202:CLA:H2	18:B:1210:CLA:C4D	2.18	0.72
7:G:34:GLN:HE21	7:G:36:PRO:HG3	1.54	0.72
17:4:42:GLN:O	17:4:46:VAL:N	2.22	0.72
17:4:136:GLY:HA3	17:4:139:ASN:O	1.89	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:733:VAL:C	1:A:735:VAL:H	1.95	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
4:D:136:SER:N	4:D:139:LYS:HZ2	1.87	0.72

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
6:F:136:TRP:CG	6:F:137:PRO:CD	2.66	0.72
1:A:81:ALA:CB	1:A:82:HIS:CA	2.66	0.72
1:A:389:TYR:CE2	1:A:625:TRP:CD1	2.78	0.72
18:B:1222:CLA:HAA1	18:B:1236:CLA:HED1	1.72	0.72
3:C:11:CYS:C	3:C:12:ILE:O	2.32	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
18:F:1302:CLA:C9	18:F:1302:CLA:HMA2	2.19	0.72
1:A:250:LEU:HD23	1:A:251:ASN:N	2.05	0.72
2:B:74:PHE:HD1	2:B:121:TYR:CZ	2.07	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:682:HIS:HE1	18:B:1238:CLA:HAC1	1.54	0.72
4:D:111:TYR:N	4:D:111:TYR:CD1	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
15:2:178:TRP:C	15:2:180:GLN:N	2.47	0.72
15:2:179:PHE:CE1	15:2:180:GLN:HG2	2.25	0.72
1:A:31:PHE:C	1:A:31:PHE:CD2	2.67	0.72
1:A:347:TYR:HD2	1:A:349:ILE:N	1.88	0.72
1:A:437:ARG:O	4:D:32:SER:OG	2.08	0.72
2:B:63:GLY:O	2:B:65:LEU:C	2.32	0.72
2:B:176:ASN:CB	2:B:291:TYR:HD1	2.03	0.72
2:B:275:HIS:ND1	18:B:1214:CLA:HMB1	2.04	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
15:2:161:THR:HG23	15:2:165:LYS:CG	2.17	0.72
1:A:120:ALA:H	1:A:145:ILE:HG21	1.53	0.71
1:A:342:GLY:C	1:A:431:LEU:HD23	2.15	0.71
1:A:373:ALA:C	1:A:375:HIS:N	2.47	0.71
1:A:390:ALA:O	1:A:391:THR:HG23	1.90	0.71
18:A:1106:CLA:HBB2	18:A:1126:CLA:H8	1.72	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
18:B:1227:CLA:CMB	18:B:1228:CLA:C4D	2.65	0.71
7:G:37:GLU:CB	7:G:43:HIS:HE1	2.03	0.71
2:B:170:ASN:ND2	18:B:1209:CLA:CED	2.53	0.71

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:332:PHE:H	2:B:335:GLY:N	1.87	0.71
2:B:451:LYS:HD3	10:J:35:ASP:OD1	1.90	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
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
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
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:HH21	2:B:317:ARG:CG	2.00	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
13:N:81:VAL:C	13:N:82:PHE:HD2	1.97	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:39:HIS:N	1:A:44:ILE:HD13	2.05	0.71
1:A:64:PHE:O	1:A:420:ARG:NH2	2.23	0.71
1:A:65:ASP:C	1:A:67:HIS:H	1.99	0.71
1:A:493:GLN:CG	1:A:515:TRP:HB2	2.21	0.71
1:A:679:PHE:C	1:A:679:PHE:CD1	2.68	0.71
2:B:174:ARG:CZ	18:B:1210:CLA:HHD	2.20	0.71
2:B:276:HIS:C	2:B:276:HIS:ND1	2.48	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
15:2:19:LEU:CG	15:2:20:ASP:CG	2.60	0.71
1:A:49:ASP:O	1:A:721:GLN:HB2	1.89	0.71
1:A:387:THR:HA	1:A:527:VAL:O	1.91	0.71
1:A:688:PHE:CZ	18:A:1140:CLA:C2C	2.73	0.71
1:A:728:VAL:HA	1:A:731:ARG:HG3	1.71	0.71
18:A:1137:CLA:HBD	18:A:1137:CLA:HBA1	1.72	0.71
2:B:649:MET:HE3	2:B:719:PHE:CD1	2.26	0.71
12:L:165:TYR:HE1	18:L:1503:CLA:HBD	1.54	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
1:A:71:LEU:HD11	1:A:352:THR:CG2	2.18	0.71
1:A:553:VAL:CG1	1:A:556:LEU:HD12	2.21	0.71
1:A:709:TRP:CZ3	2:B:417:ALA:HA	2.25	0.71
2:B:117:TYR:HE2	2:B:366:THR:HG1	1.31	0.71
16:3:134:TYR:C	16:3:136:PRO:HD2	2.11	0.71

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
18:4:1304:CLA:HAA2	18:4:1304:CLA:H2	1.69	0.71
1:A:552:THR:O	1:A:556:LEU:HG	1.90	0.71
1:A:604:TRP:HE1	18:B:9023:CLA:CHD	2.03	0.71
2:B:57:ILE:O	2:B:60:TRP:HB3	1.91	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:591:THR:CG2	2:B:721:TYR:HE2	2.04	0.71
5:E:40:ARG:NH2	5:E:62:ARG:NH2	2.39	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
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
14:1:89: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:377:TYR:CD2	1:A:396:PHE:CE1	2.79	0.71
2:B:67:HIS:NE2	2:B:89:HIS:CB	2.54	0.71
2:B:330:ILE:HG21	18:B:1202:CLA:HAC1	1.72	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
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:40:PHE:CZ	1:A:61:ALA:HA	2.26	0.71
1:A:356:ALA:N	1:A:421:ASP:OD1	2.24	0.71
1:A:402:ILE:H	1:A:402:ILE:CD1	2.04	0.71
2:B:56:ILE:O	2:B:60:TRP:N	2.24	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
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
15:2:17:GLU:OE1	15:2:18:TRP:HB2	1.90	0.71
1:A:33:GLN:OE1	18:A:1109:CLA:CHC	2.38	0.70
1:A:81:ALA:CB	1:A:82:HIS:C	2.63	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
3:C:50:GLY:C	3:C:52:LYS:H	1.98	0.70
13:N:57:LYS:CB	13:N:58:VAL:HA	2.21	0.70
1:A:218:TRP:O	1:A:222:GLN:N	2.22	0.70
2:B:428:PHE:HB2	18:B:1229:CLA:O1D	1.91	0.70

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:64:PHE:O	1:A:66:SER:N	2.24	0.70
1:A:141:ARG:HH11	1:A:141:ARG:HB3	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
2:B:415:LYS:HZ2	2:B:540:ASP:HA	1.55	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
7:G:33:LYS:HD3	7:G:33:LYS:C	2.16	0.70
12:L:148:VAL:HA	12:L:151:VAL:HG23	1.71	0.70
16:3:107:TYR:H	16:3:108:TRP:C	1.98	0.70
1:A:54:ILE:O	1:A:54:ILE:HG22	1.91	0.70
1:A:196:PHE:C	1:A:196:PHE:CD2	2.69	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
2:B:415:LYS:HE3	2:B:540:ASP:HB2	1.73	0.70
2:B:439:HIS:HD2	18:B:1230:CLA:NC	1.89	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
3:C:5:VAL:C	3:C:6:LYS:HG2	2.15	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
15:2:33:GLY:HA2	15:2:34:LEU:C	2.15	0.70
1:A:385:LEU:O	1:A:388:ASP:N	2.24	0.70
1:A:397:THR:O	1:A:398:HIS:C	2.34	0.70
2:B:3:LEU:O	2:B:14:GLN:HA	1.92	0.70
2:B:276:HIS:HA	18:B:1214:CLA:C2B	2.21	0.70
2:B:304:ILE:CG2	2:B:305:LEU:N	2.54	0.70
18:B:1203:CLA:HMA3	18:B:1226:CLA:CHC	2.22	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
16:3:54:TRP:HB2	16:3:55:LEU:HA	0.79	0.70
17:4:62:GLU:C	17:4:63:VAL:CG2	2.65	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:98:GLN:HB2	8:H:78:PRO:CB	2.20	0.70
2:B:411:MET:HA	2:B:411:MET:HE3	1.73	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
9:I:25:PHE:HB3	9:I:26:LEU:HD13	1.71	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:126:ILE:HG22	1:A:129:GLN:HG3	1.72	0.70
18:A:1133:CLA:HHC	18:A:1134:CLA:C2B	2.21	0.70
2:B:530:THR:HG21	2:B:583:MET:CB	2.19	0.70
2:B:546:LEU:HD21	5:E:74:TYR:HE1	1.55	0.70
2:B:549:ASP:CA	2:B:551:LYS:HG2	2.21	0.70
2:B:652:PHE:CE1	2:B:656:VAL:CG2	2.74	0.70
4:D:32:SER:HA	12:L:23:LEU:HD21	1.73	0.70
4:D:45:PHE:C	4:D:45:PHE:HD1	1.98	0.70
16:3:133:TRP:CD1	16:3:139:MET:HE3	2.26	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
18:A:1132:CLA:CHB	12:L:72:GLY:HA2	2.21	0.70
2:B:51:PHE:O	2:B:53:GLN:N	2.24	0.70
2:B:259:GLY:C	2:B:269:TRP:NE1	2.49	0.70
2:B:428:PHE:HA	2:B:432:HIS:CD2	2.27	0.70
4:D:42:VAL:O	4:D:44:GLU:N	2.24	0.70
6:F:149:LEU:HA	6:F:151:ASP:CG	2.16	0.70
8:H:49:LYS:HD3	8:H:50:ARG:H	1.56	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
18:A:1103:CLA:O2D	18:A:1103:CLA:H2A	1.90	0.70
2:B:559:CYS:SG	2:B:702:ILE:HG12	2.31	0.70
18:B:1208:CLA:HED3	18:B:1208:CLA:H2A	1.72	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
14:1:181:LEU:HA	14:1:182:ALA:C	2.17	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
18:L:1502:CLA:C4	18:L:1504:CLA:HMA1	2.22	0.70
15:2:23:LEU:CB	15:2:26:ASP:O	2.40	0.70
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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:604:TRP:HE1	18:B:9023:CLA:C1D	2.04	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
3:C:52:LYS:HZ1	3:C:66:ARG:HH11	1.40	0.69
5:E:51:SER:HB2	5:E:69:PHE:HD2	1.56	0.69
6:F:153:ASN:CG	6:F:154:PHE:N	2.48	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
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: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:335:LYS:O	1:A:342:GLY:HA2	1.92	0.69
1:A:534:LEU:HD13	1:A:534:LEU:H	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
3:C:51:CYS:C	21:C:3102:SF4:S1	2.75	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
15:2:19: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
16:3:126:GLU:CD	16:3:127:HIS:H	1.98	0.69
17:4:156:ASN:N	17:4:156:ASN:ND2	2.39	0.69
2:B:77:TRP:NE1	2:B:81:PRO:HA	2.08	0.69
2:B:291:TYR:CD2	2:B:299:HIS:HB2	2.27	0.69
4:D:96:ILE:CG1	4:D:97:LYS:N	2.55	0.69
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:N	13:N:54:LYS:HD2	2.06	0.69
1:A:65:ASP:C	1:A:67:HIS:N	2.50	0.69
1:A:87:SER:O	1:A:91:LEU:HB2	1.92	0.69
1:A:250:LEU:HA	18:A:1113:CLA:O2D	1.91	0.69
2:B:59:LEU:O	2:B:59:LEU:CD2	2.40	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:HD12	2:B:463:ILE:N	2.06	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
17:4:96:ILE:HG23	17:4:97:LEU:N	2.07	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
1:A:679:PHE:HB2	1:A:745:THR:HG22	1.74	0.69
1:A:696:GLY:HA2	2:B:569:ASP:OD2	1.91	0.69
2:B:64:ASN:CA	2:B:67:HIS:HB2	2.22	0.69
18:B:1216:CLA:O2A	18:B:1220:CLA:C1	2.36	0.69
12:L:160:VAL:O	12:L:161:LEU:O	2.11	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:454:GLY:C	1:A:456:HIS:H	1.97	0.69
1:A:685:VAL:O	1:A:741:GLY:HA2	1.92	0.69
1:A:690:LEU:HD13	1:A:690:LEU:H	1.58	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
12:L:87:ALA:O	12:L:90:GLY:CA	2.40	0.69
18:L:1503:CLA:H11	18:L:1503:CLA:HED1	1.74	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
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
2:B:530:THR:HG22	2:B:530:THR:O	1.91	0.69
7:G:43:HIS:CD2	7:G:43:HIS:N	2.60	0.69
13:N:58:VAL:HG22	13:N:60:PHE:CD2	2.27	0.69
17:4:106:TRP:CE2	17:4:110:LYS:NZ	2.61	0.69
1:A:139:GLY:C	6:F:38:PRO:HB2	2.18	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:491:TRP:N	1:A:492:ILE:HG23	2.08	0.69
1:A:685:VAL:O	1:A:685:VAL:CG1	2.40	0.69
1:A:693:LEU:HD23	2:B:665:ILE:HG12	1.75	0.69
2:B:70:TRP:HB3	2:B:71:GLN:HB3	1.73	0.69
2:B:84:VAL:HG12	2:B:86:PRO:CD	2.23	0.69
2:B:84:VAL:HG13	2:B:85:ARG:H	1.57	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:392:ILE:O	2:B:393:PHE:C	2.35	0.69

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:395:ILE:HG23	2:B:551:LYS:O	1.91	0.69
2:B:458:ILE:HG12	6:F:74:SER:HB3	1.75	0.69
2:B:464:GLN:OE1	18:B:1234:CLA:HMD1	1.91	0.69
3:C:62:PHE:HE2	5:E:43:SER:O	1.75	0.69
4:D:27:PRO:C	4:D:28:ILE:HG13	2.13	0.69
6:F:12:LYS:CD	6:F:13:GLN:H	2.04	0.69
7:G:20:ARG:O	7:G:23:PHE:HB2	1.92	0.69
12:L:90:GLY:O	12:L:93:VAL:HG22	1.93	0.69
12:L:149:SER:O	12:L:153:TRP:HB3	1.93	0.69
14:1:11:PRO:N	17:4:107:GLN:HG3	2.07	0.69
16:3:75:ALA:HB3	16:3:76:PRO:HD3	1.75	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:1107:CLA:HAC1	2:B:446:PHE:CZ	2.27	0.69
18:A:9011:CLA:CBB	2:B:624:LEU:CD1	2.71	0.69
2:B:57:ILE:O	2:B:60:TRP:CB	2.41	0.69
2:B:456:GLU:HG3	2:B:514:PRO:CB	2.14	0.69
3:C:60:THR:CA	5:E:80:ASN:HD21	2.06	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
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
14:1:188:ASN:C	14:1:190:GLY:HA2	2.17	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
2:B:330:ILE:O	2:B:331:HIS:C	2.33	0.69
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
18:B:1209:CLA:O1A	18:B:1209:CLA:C5	2.39	0.69
3:C:42:ALA:C	3:C:44:ARG:N	2.39	0.69
4:D:30:ALA:HA	12:L:13:PRO:HD3	1.73	0.69
11:K:14:UNK:HA	18:K:1141:CLA:HHD	1.74	0.69
17:4:190:TRP:C	17:4:191:HIS:CD2	2.71	0.69
1:A:84:GLY:O	1:A:87:SER:N	2.26	0.68
18:A:1132:CLA:C1B	12:L:72:GLY:HA2	2.22	0.68
2:B:464:GLN:OE1	18:B:1234:CLA:CMD	2.41	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
12:L:64:LEU:C	12:L:66:GLY:H	2.01	0.68
12:L:87:ALA:O	12:L:91:LEU:N	2.25	0.68

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
15:2:84:GLU:OE2	17:4:186:ILE:CG1	2.41	0.68
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
17:4:190:TRP:HA	17:4:190:TRP:HE3	1.57	0.68
1:A:104:SER:HB2	1:A:161:GLU:CD	2.18	0.68
1:A:414:ALA:O	1:A:417:PHE:CD2	2.40	0.68
18:A:1119:CLA:C2	18:A:1123:CLA:HMB2	2.22	0.68
2:B:93:ASP:OD2	2:B:96:PHE:CE2	2.46	0.68
18:B:1242:CLA:HHD	18:B:1242:CLA:HBC3	1.74	0.68
3:C:27:GLU:OE2	3:C:29:ILE:HG23	1.93	0.68
15:2:17:GLU:CA	15:2:18:TRP:C	2.61	0.68
17:4:185:HIS:O	17:4:186:ILE:HG12	1.93	0.68
2:B:388:ALA:O	2:B:391:PRO:HD2	1.94	0.68
18:B:1208:CLA:H62	18:B:1209:CLA:C4	2.23	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
15:2:31:PRO:O	15:2:33:GLY:HA3	1.94	0.68
1:A:391:THR:HG22	1:A:394:SER:HB3	1.75	0.68
2:B:302:LYS:HE2	2:B:302:LYS:CA	2.21	0.68
2:B:355:LEU:O	2:B:355:LEU:HD22	1.94	0.68
2:B:440:ASN:O	2:B:615:TYR:HA	1.93	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:631:LEU:HA	2:B:643:LEU:CD1	2.23	0.68
4:D:31:GLY:HA2	12:L:13:PRO:HB3	1.72	0.68
6:F:141:TYR:CD2	6:F:142:ARG:N	2.60	0.68
12:L:27:VAL:HG13	18:L:1130:CLA:H12	1.74	0.68
18:L:1503:CLA:H11	18:L:1503:CLA:O2D	1.93	0.68
17:4:137:ILE:HG13	17:4:140:PRO:HD2	1.74	0.68
1:A:552:THR:HG22	1:A:604:TRP:HB3	1.74	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:37:LEU:C	12:L:42:ALA:CB	2.67	0.68
12:L:66:GLY:CA	18:L:1503:CLA:C1B	2.71	0.68
13:N:58:VAL:CG2	13:N:60:PHE:CG	2.76	0.68

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
13:N:58:VAL:N	13:N:60:PHE:CE2	2.61	0.68
15:2:19:LEU:CA	15:2:20:ASP:C	2.66	0.68
15:2:178:TRP:N	15:2:178:TRP:HE3	1.90	0.68
1:A:76:ARG:HD2	1:A:191:PRO:O	1.94	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:290:LEU:O	1:A:291:THR:CG2	2.32	0.68
1:A:568:LEU:HA	4:D:79:ARG:HH12	1.58	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:37:ILE:CA	2:B:41:ARG:HD2	2.23	0.68
2:B:85:ARG:NH1	2:B:115:ASN:OD1	2.26	0.68
2:B:143:LEU:C	2:B:145:LEU:N	2.51	0.68
2:B:415:LYS:HE3	2:B:540:ASP:CB	2.23	0.68
2:B:703:VAL:O	2:B:704:GLN:HB2	1.93	0.68
18:B:1222:CLA:O1A	18:B:1222:CLA:H2	1.94	0.68
6:F:73:VAL:HG21	6:F:83:PHE:N	2.02	0.68
6:F:122:ASP:N	10:J:9:SER:HB2	2.08	0.68
16:3:193:LEU:HA	16:3:196:LEU:HG	1.75	0.68
1:A:43:THR:HG22	1:A:46:LYS:CG	2.23	0.68
1:A:96:MET:CB	1:A:149:PHE:HE2	2.06	0.68
1:A:246:HIS:CE1	18:A:1147:CLA:C4A	2.76	0.68
1:A:620:MET:HB3	1:A:625:TRP:CZ2	2.29	0.68
2:B:42:LEU:HG	2:B:43:TYR:N	2.08	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:649:MET:CE	2:B:723:ALA:HB2	2.23	0.68
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
15:2:17:GLU:CB	15:2:18:TRP:HB3	2.15	0.68
15:2:70:LYS:H	15:2:70:LYS:HD2	1.58	0.68
15:2:188:PRO:C	15:2:192:LEU:HG	2.18	0.68
1:A:95:GLY:CA	1:A:96:MET:SD	2.82	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
18:A:1132:CLA:C2B	12:L:72:GLY:H	2.02	0.68
18:A:1140:CLA:C4	18:A:1140:CLA:C4C	2.72	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
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
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
2:B:120:VAL:CG2	18:B:1225:CLA:CBA	2.72	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
18:B:1203:CLA:HBA2	18:B:1203:CLA:O1D	1.94	0.68
18:B:1215:CLA:HBB2	18:B:1215:CLA:C6	2.23	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
17:4:40:PHE:O	17:4:41:VAL:C	2.37	0.68
17:4:181:ASN:C	17:4:183:LEU:H	2.02	0.68
1:A:612:VAL:O	1:A:613:ILE:C	2.34	0.68
1:A:715:LYS:HZ3	6:F:153:ASN:HD21	1.41	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
2:B:659:THR:C	2:B:661:PHE:H	2.02	0.68
18:B:1239:CLA:HBC1	20:B:6017:BCR:H392	1.75	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
13:N:65:LEU:HD12	13:N:68:GLU:CD	2.18	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
1:A:599:PHE:HZ	1:A:693:LEU:HD21	1.59	0.67
2:B:283:LEU:O	2:B:284:PHE:CD1	2.48	0.67
2:B:317:ARG:NH1	18:B:1227:CLA:CAD	2.57	0.67
2:B:687:LEU:HD11	12:L:40:LEU:HD12	1.75	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
10:J:4:PHE:HB2	10:J:5:LYS:O	1.94	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
15:2:192:LEU:HA	15:2:195:HIS:NE2	2.02	0.67

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
17:4:137:ILE:CG1	17:4:140:PRO:HD2	2.23	0.67
1:A:268:PRO:HD2	1:A:277:TYR:CD1	2.29	0.67
2:B:432:HIS:C	2:B:434:LEU:H	2.01	0.67
6:F:61:LEU:CD1	6:F:69:PRO:HB3	2.16	0.67
8:H:41:GLU:OE1	8:H:41:GLU:HA	1.94	0.67
1:A:398:HIS:HB2	18:A:1126:CLA:C4B	2.23	0.67
2:B:92:TRP:O	2:B:94:PRO:HD3	1.94	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
6:F:52:ARG:C	6:F:55:ASN:HB2	2.19	0.67
9:I:27:HIS:O	9:I:28:VAL:O	2.12	0.67
20:I:6018:BCR:C38	20:L:6020:BCR:C34	2.64	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
12:L:66:GLY:C	18:L:1503:CLA:CMB	2.66	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:72:GLU:HG3	1:A:76:ARG:NH1	2.08	0.67
1:A:441:ALA:C	1:A:445:HIS:CE1	2.73	0.67
1:A:604:TRP:O	1:A:608:SER:N	2.28	0.67
2:B:19:ARG:HA	2:B:22:TRP:HD1	1.58	0.67
2:B:104:PHE:HA	2:B:106:ARG:HD2	1.74	0.67
2:B:334:LEU:HD21	18:B:1226:CLA:C2B	2.25	0.67
2:B:561:GLY:N	21:B:3101:SF4:S4	2.68	0.67
2:B:678:LEU:HD22	2:B:678:LEU:C	2.18	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:C1	18:L:1503:CLA:HED1	2.24	0.67
1:A:92:TRP:O	1:A:94:SER:N	2.27	0.67
1:A:343:HIS:N	1:A:343:HIS:ND1	2.43	0.67
1:A:569:ILE:HG13	1:A:586:ARG:HH12	1.59	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
4:D:133:ASN:CG	4:D:135:ARG:HB2	2.20	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
14:1:84:TYR:CB	14:1:85:LEU:CA	2.42	0.67

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:57:LEU:HD23	1:A:57:LEU:C	2.20	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:277:TYR:CG	18:A:1113:CLA:HBC1	2.29	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:464:GLN:O	2:B:469:LYS:HB2	1.94	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
14:1:40:LYS:O	14:1:42:SER:N	2.28	0.67
15:2:21:GLY:H	15:2:23:LEU:HD11	1.59	0.67
16:3:200:ILE:C	16:3:204:VAL:HG22	2.19	0.67
1:A:452:PHE:CD2	1:A:453:LEU:N	2.63	0.67
1:A:590:CYS:H	2:B:669:GLY:H	1.43	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
2:B:684:ARG:NH2	12:L:22:GLY:HA3	2.09	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
12:L:59:ALA:HA	12:L:62:PHE:CE2	2.29	0.67
14:1:75:ALA:O	14:1:78:PRO:CD	2.43	0.67
15:2:19:LEU:N	15:2:20:ASP:C	2.53	0.67
15:2:63:PHE:N	15:2:63:PHE:CD2	2.42	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
16:3:207:VAL:O	16:3:208:GLY:C	2.37	0.67
1:A:86:LEU:HD11	1:A:90:PHE:CD1	2.30	0.67
1:A:690:LEU:HD13	1:A:690:LEU:N	2.10	0.67
18:A:1115:CLA:HBB2	18:K:1141:CLA:C3B	2.25	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
18:B:1205:CLA:O1A	18:B:1224:CLA:HAA1	1.94	0.67
18:B:1214:CLA:H43	18:B:1214:CLA:CHD	2.24	0.67
18:B:1217:CLA:HMA3	7:G:21:PHE:CD2	2.27	0.67

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
8:H:41:GLU:CD	12:L:50:LEU:HD13	2.20	0.67
12:L:86:LEU:C	12:L:88:ALA:N	2.51	0.67
1:A:64:PHE:C	1:A:67:HIS:H	2.03	0.67
1:A:548:THR:C	1:A:550:HIS:H	2.01	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
2:B:458:ILE:N	18:B:1235:CLA:HMD1	2.10	0.67
2:B:504:ASN:C	2:B:506:ASN:N	2.52	0.67
13:N:81:VAL:H	13:N:82:PHE:HD2	1.41	0.67
15:2:19:LEU:HA	15:2:21:GLY:N	2.10	0.67
15:2:86:GLU:HG2	17:4:184:GLN:CD	2.20	0.67
15:2:153:PRO:HB2	15:2:154:GLN:CA	2.24	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:686:TRP:CE3	18:A:9011:CLA:CMA	2.77	0.67
1:A:750:PHE:O	1:A:751:LEU:HB2	1.95	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
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
1:A:48:PRO:HB3	1:A:53:TRP:CZ3	2.30	0.66
1:A:353:SER:HG	1:A:354:TRP:CG	2.13	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
2:B:188:LEU:O	2:B:192:GLY:N	2.26	0.66
2:B:569:ASP:HB3	2:B:706:ARG:HH12	1.57	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
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
15:2:194:ALA:HB3	15:2:195:HIS:HA	1.78	0.66
1:A:441:ALA:C	1:A:445:HIS:HE1	2.03	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
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
1:A:308:ILE:HD12	1:A:311:LEU:CB	2.25	0.66
1:A:585:GLY:C	1:A:587:GLY:N	2.49	0.66
18:A:1136:CLA:O1D	18:A:1136:CLA:HAA1	1.95	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:92:TYR:CE2	6:F:96:TRP:HZ3	2.11	0.66
6:F:115:THR:O	6:F:117:LYS:N	2.28	0.66
7:G:8:ILE:O	7:G:10:LEU:N	2.28	0.66
16:3:108:TRP:CD1	16:3:108:TRP:H	2.13	0.66
16:3:132:ASP:HB3	16:3:139:MET:CB	2.26	0.66
1:A:75:SER:HA	1:A:354:TRP:CH2	2.30	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:545:HIS:HD1	1:A:612:VAL:HG22	1.55	0.66
1:A:658:TRP:CD1	2:B:625:TRP:CD1	2.81	0.66
2:B:187:SER:O	2:B:189:ALA:N	2.29	0.66
2:B:395:ILE:O	2:B:395:ILE:CG2	2.43	0.66
2:B:708:VAL:CG1	18:B:1239:CLA:O1D	2.43	0.66
6:F:55:ASN:O	6:F:58:LYS:HB2	1.95	0.66
6:F:127:SER:N	6:F:130:LEU:HD13	2.11	0.66
8:H:49:LYS:HG3	12:L:140:THR:HG21	1.77	0.66
12:L:111:GLU:OE1	12:L:134:ASP:O	2.14	0.66
13:N:38:GLY:N	13:N:39:SER:HA	2.08	0.66
1:A:81:ALA:HB3	1:A:83:PHE:H	0.85	0.66
1:A:340:GLY:C	1:A:342:GLY:N	2.53	0.66
1:A:370:ILE:HD13	18:A:1124:CLA:C3A	2.25	0.66
1:A:383:PRO:C	1:A:384:TYR:HD1	2.03	0.66
1:A:684:PHE:HA	1:A:687:ALA:HB3	1.77	0.66
2:B:463:ILE:HG23	2:B:467:HIS:ND1	2.10	0.66
2:B:680:TRP:C	2:B:680:TRP:HE3	2.03	0.66
18:B:1138:CLA:C4C	18:F:1139:CLA:HBC2	2.26	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
18:H:1501:CLA:HBB2	18:L:1502:CLA:CAA	2.22	0.66
9:I:24:LEU:HA	9:I:27:HIS:H	1.61	0.66
15:2:19:LEU:HA	15:2:22:SER:HB3	1.77	0.66

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
15:2:19:LEU:C	15:2:20:ASP:CG	2.64	0.66
16:3:85:ILE:N	16:3:86:PRO:CD	2.58	0.66
1:A:317:TYR:C	1:A:324:GLY:HA3	2.21	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:A:1129:CLA:CBB	18:L:1130:CLA:HBC3	2.25	0.66
2:B:58:PHE:CD1	2:B:145:LEU:HB3	2.30	0.66
2:B:280:ILE:HA	18:B:1214:CLA:HMC1	1.77	0.66
2:B:346:SER:O	2:B:350:GLN:OE1	2.13	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
18:B:1202:CLA:H2	18:B:1210:CLA:C3D	2.25	0.66
18:B:1208:CLA:C1	18:B:1209:CLA:H2	2.26	0.66
3:C:11:CYS:SG	3:C:59:PRO:HD2	2.36	0.66
3:C:27:GLU:HB3	3:C:43:PRO:CB	2.24	0.66
7:G:20:ARG:O	7:G:23:PHE:CB	2.43	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
14:1:84:TYR:OH	14:1:92:GLY:N	2.28	0.66
14:1:185:TRP:HA	14:1:185:TRP:HE3	1.56	0.66
17:4:93:ILE:HG13	17:4:94:GLU:H	1.60	0.66
17:4:126:LEU:C	17:4:153:GLU:OE2	2.39	0.66
1:A:579:PHE:O	1:A:580:PRO:O	2.12	0.66
1:A:653:LEU:HD21	18:B:9010:CLA:HBC2	1.75	0.66
1:A:696:GLY:CA	2:B:569:ASP:OD2	2.44	0.66
2:B:67:HIS:NE2	2:B:89:HIS:HB2	2.10	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
6:F:105:LEU:O	6:F:107:ALA:N	2.27	0.66
8:H:26:SER:HA	8:H:27:ASP:C	2.20	0.66
12:L:94:ILE:C	12:L:96:SER:H	2.04	0.66
15:2:23:LEU:CG	15:2:26:ASP:O	2.44	0.66
15:2:162:LYS:HZ2	15:2:163:GLU:H	1.42	0.66
17:4:185:HIS:C	17:4:186:ILE:HG12	2.20	0.66
1:A:80:SER:N	1:A:81:ALA:CB	2.57	0.66
1:A:185:HIS:CG	1:A:186:TYR:N	2.58	0.66
1:A:751:LEU:HD13	1:A:752:ALA:N	2.11	0.66

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
18:B:1202:CLA:HED3	18:B:1203:CLA:CMB	2.25	0.66
3:C:55:GLU:CB	3:C:65:VAL:CG2	2.73	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:415:LYS:O	2:B:417:ALA:N	2.27	0.66
2:B:678:LEU:O	2:B:682:HIS:HD2	1.78	0.66
4:D:47:VAL:HG23	4:D:103:VAL:CG1	2.21	0.66
4:D:112:LEU:HG	4:D:113:HIS:NE2	2.09	0.66
6:F:115:THR:O	6:F:118:GLU:HB2	1.95	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
1:A:613:ILE:O	1:A:616:PHE:HB3	1.96	0.66
2:B:261:PHE:O	2:B:262:HIS:ND1	2.29	0.66
2:B:375:HIS:CE1	18:B:1225:CLA:NA	2.64	0.66
2:B:463:ILE:C	2:B:465:SER:H	2.03	0.66
2:B:722:ALA:CB	18:B:1224:CLA:H42	2.23	0.66
18:B:1207:CLA:C6	8:H:65:LEU:HD22	2.25	0.66
3:C:25:VAL:O	3:C:25:VAL:HG12	1.96	0.66
10:J:2:ARG:HD3	10:J:7:TYR:HD1	1.60	0.66
17:4:96:ILE:CG2	17:4:97:LEU:H	2.08	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:473:PRO:O	1:A:474:GLN:C	2.37	0.65
1:A:582:ASP:HA	2:B:562:PRO:HG2	1.78	0.65
1:A:585:GLY:C	1:A:587:GLY:H	2.03	0.65
2:B:46:ILE:O	2:B:49:SER:OG	2.07	0.65
2:B:53:GLN:C	2:B:55:ALA:N	2.51	0.65
2:B:383:MET:O	2:B:386:ALA:HB3	1.96	0.65
2:B:569:ASP:CB	2:B:706:ARG:NH1	2.48	0.65
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
1:A:79:PHE:C	1:A:81:ALA:HB2	2.20	0.65
1:A:80:SER:H	1:A:81:ALA:HA	1.59	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
2:B:53:GLN:HE22	18:B:1202:CLA:H3A	1.61	0.65
2:B:126:THR:CG2	18:B:1215:CLA:HED1	2.26	0.65

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
6:F:153:ASN:CG	6:F:154:PHE:H	2.04	0.65
13:N:40:CYS:O	13:N:41:LYS:O	2.13	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
1:A:89:ILE:O	1:A:92:TRP:CB	2.43	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:439:ARG:C	1:A:441:ALA:H	2.04	0.65
2:B:78:VAL:HG23	2:B:130:ARG:CD	2.23	0.65
2:B:589:TRP:O	2:B:591:THR:N	2.27	0.65
18:F:1302:CLA:HMA3	18:F:1302:CLA:C9	2.13	0.65
12:L:66:GLY:HA2	18:L:1503:CLA:C1B	2.26	0.65
13:N:57:LYS:CB	16:3:87:ALA:CB	2.66	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
1:A:435:VAL:HG23	1:A:438:HIS:CE1	2.31	0.65
1:A:472:ARG:O	1:A:472:ARG:HG2	1.95	0.65
1:A:556:LEU:C	1:A:560:VAL:HG13	2.21	0.65
1:A:663:GLN:O	1:A:667:SER:CB	2.40	0.65
1:A:679:PHE:C	1:A:679:PHE:HD1	2.03	0.65
2:B:100:ALA:CA	2:B:103:ALA:HB3	2.24	0.65
2:B:284:PHE:C	2:B:286:ILE:H	2.05	0.65
2:B:458:ILE:HG22	6:F:72:ILE:HG21	1.78	0.65
2:B:636:THR:O	2:B:636:THR:HG23	1.95	0.65
12:L:63:LEU:HD11	18:L:1502:CLA:CHB	2.27	0.65
12:L:113:SER:CA	12:L:114:ILE:HB	2.26	0.65
13:N:36:GLU:O	13:N:40:CYS:HB3	1.95	0.65
17:4:105:ARG:O	17:4:108:ASP:HB3	1.95	0.65
17:4:190:TRP:CE3	17:4:190:TRP:CA	2.79	0.65
2:B:39:GLU:HA	2:B:39:GLU:OE2	1.96	0.65
2:B:432:HIS:C	2:B:434:LEU:N	2.51	0.65
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
18:B:1138:CLA:CBB	18:B:1138:CLA:H51	2.27	0.65
5:E:38:ILE:HB	5:E:46:PHE:O	1.97	0.65

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:E:40:ARG:HB3	5:E:42:GLU:HG3	1.79	0.65
6:F:26:GLN:C	6:F:28:SER:H	2.05	0.65
9:I:6:SER:O	9:I:7:LEU:C	2.39	0.65
15:2:33:GLY:CA	15:2:34:LEU:C	2.69	0.65
1:A:488:PHE:H	1:A:535:GLY:HA2	1.62	0.65
18:A:1131:CLA:CBC	18:A:1136:CLA:HAC1	2.26	0.65
2:B:117:TYR:HB3	2:B:370:ALA:HB2	1.79	0.65
2:B:197:VAL:HG21	18:B:1211:CLA:C2D	2.26	0.65
2:B:341:LEU:HA	2:B:344:ILE:CG2	2.26	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:CGD	18:L:1503:CLA:O1A	2.45	0.65
16:3:57:TYR:HE2	16:3:185:VAL:CB	2.10	0.65
16:3:82:ALA:HB1	16:3:83:GLY:C	2.22	0.65
1:A:58:HIS:HE1	18:A:1101:CLA:NC	1.94	0.65
1:A:665:ILE:CD1	2:B:625:TRP:CD1	2.79	0.65
1:A:750:PHE:CD1	1:A:750:PHE:C	2.74	0.65
2:B:348:VAL:HG23	18:B:1215:CLA:H42	1.77	0.65
2:B:646:TRP:CZ3	18:B:1205:CLA:HBC1	2.31	0.65
6:F:141:TYR:C	6:F:143:GLU:H	2.04	0.65
12:L:64:LEU:O	12:L:66:GLY:N	2.30	0.65
1:A:126:ILE:HG13	10:J:27:ILE:HG21	1.77	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:657:LEU:C	1:A:659:ALA:H	2.05	0.65
1:A:735:VAL:O	1:A:739:LEU:HB3	1.95	0.65
2:B:19:ARG:O	2:B:20:ARG:C	2.39	0.65
2:B:89:HIS:O	2:B:90:ALA:HB3	1.97	0.65
2:B:120:VAL:HG23	18:B:1225:CLA:CBA	2.27	0.65
2:B:365:PHE:HB3	2:B:602:TRP:CD2	2.32	0.65
2:B:424:TRP:HE1	18:B:1229:CLA:HED1	1.62	0.65
2:B:518:LEU:HD22	2:B:614:THR:HG22	1.79	0.65
2:B:568:CYS:SG	2:B:569:ASP:N	2.69	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
13:N:81:VAL:N	13:N:82:PHE:CD2	2.63	0.65
14:1:75:ALA:O	14:1:78:PRO:HD2	1.96	0.65
17:4:81:GLU:O	17:4:84:PHE:HE1	1.80	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:700:TRP:CH2	18:A:9013:CLA:O1D	2.50	0.65

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:193:HIS:HB2	18:B:1211:CLA:C1C	2.25	0.65
2:B:265:THR:O	2:B:360:PHE:HD2	1.80	0.65
2:B:414:HIS:CD2	18:B:1227:CLA:C4A	2.80	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
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
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:91:ILE:HD11	2:B:114:ASN:ND2	2.12	0.65
2:B:96:PHE:HZ	18:B:1206:CLA:C1D	2.10	0.65
2:B:478:LEU:O	2:B:480:SER:N	2.30	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
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:661:ALA:O	1:A:664:VAL:N	2.29	0.64
2:B:37:ILE:O	4:D:148:PHE:CG	2.50	0.64
2:B:187:SER:O	2:B:188:LEU:C	2.40	0.64
2:B:189:ALA:HB1	18:B:1211:CLA:C2C	2.28	0.64
2:B:631:LEU:HD13	2:B:632:ILE:N	2.11	0.64
3:C:63:LEU:HD13	3:C:63:LEU:C	2.21	0.64
6:F:82:GLU:O	10:J:38:THR:CG2	2.45	0.64
12:L:37:LEU:C	12:L:42:ALA:HB3	2.21	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
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: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:383:PRO:C	1:A:384:TYR:CD1	2.75	0.64
1:A:588:GLY:O	2:B:668:ARG:CD	2.44	0.64
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:310:PRO:HA	2:B:311:PRO:C	2.19	0.64
2:B:689:ASN:HD21	4:D:38:ARG:HH11	1.38	0.64

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
17:4:81:GLU:N	17:4:82:GLU:HA	2.12	0.64
1:A:198:ASP:CG	1:A:199:VAL:N	2.54	0.64
1:A:453:LEU:HD11	1:A:547:PHE:HA	1.80	0.64
1:A:582:ASP:CG	1:A:583:GLY:H	2.06	0.64
1:A:594:ALA:HA	1:A:597:HIS:CB	2.27	0.64
2:B:284:PHE:CE1	18:B:1216:CLA:CHC	2.80	0.64
2:B:290:MET:CB	18:B:1218:CLA:HBC2	2.18	0.64
2:B:325:THR:O	2:B:329:SER:CB	2.46	0.64
2:B:680:TRP:C	2:B:680:TRP:CE3	2.75	0.64
18:B:1222:CLA:CAD	18:B:1234:CLA:HBB2	2.28	0.64
18:G:1233:CLA:H52	18:G:1233:CLA:C4C	2.27	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: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:345:THR:CG2	18:B:1225:CLA:CMC	2.74	0.64
3:C:27:GLU:HB3	3:C:43:PRO:HG3	1.80	0.64
7:G:60:SER:C	7:G:64:VAL:HG13	2.21	0.64
12:L:126:GLN:O	12:L:127:PRO:C	2.40	0.64
13:N:12:THR:C	13:N:14:LYS:H	2.06	0.64
13:N:47:THR:OG1	13:N:50:GLN:HB2	1.98	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:736:THR:O	1:A:740:LEU:N	2.31	0.64
2:B:124:TRP:HZ3	2:B:135:LEU:HG	1.63	0.64
2:B:275:HIS:HE1	18:B:1214:CLA:CBB	2.10	0.64
2:B:287:GLY:HA2	2:B:290:MET:HE2	1.79	0.64
2:B:361:ILE:HG13	2:B:368:GLN:HE22	1.63	0.64
18:B:1222:CLA:CBD	18:B:1234:CLA:HBB2	2.28	0.64
9:I:4:LEU:HD22	9:I:5:PRO:CA	2.24	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:76:ARG:HH21	1:A:190:ALA:HB1	1.62	0.64
1:A:354:TRP:CB	18:A:1103:CLA:HHD	2.25	0.64
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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
18:A:1107:CLA:HAA2	18:A:1107:CLA:CBD	2.25	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: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
3:C:51:CYS:SG	3:C:51:CYS:O	2.55	0.64
7:G:61:ASN:HA	7:G:64:VAL:CG2	2.28	0.64
15:2:17:GLU:OE2	15:2:18:TRP:N	2.30	0.64
17:4:60:LEU:C	17:4:62:GLU:N	2.53	0.64
17:4:156:ASN:HD22	17:4:156:ASN:H	1.40	0.64
1:A:95:GLY:C	1:A:96:MET:SD	2.80	0.64
1:A:446:LEU:HD13	1:A:450:CYS:SG	2.37	0.64
1:A:456:HIS:C	1:A:456:HIS:CD2	2.76	0.64
18:A:1131:CLA:HBC1	18:A:1136:CLA:HAC1	1.80	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:48:ILE:O	4:D:73:ASN:O	2.16	0.64
4:D:64:GLY:O	4:D:65:ALA:CB	2.45	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
12:L:111:GLU:CD	12:L:138:LYS:HE3	2.22	0.64
14:1:91:TRP:HB2	14:1:92:GLY:O	1.97	0.64
1:A:143:ILE:HD13	1:A:144:GLN:O	1.98	0.64
1:A:203:LEU:HD21	18:A:1119:CLA:O2D	1.97	0.64
2:B:143:LEU:C	2:B:145:LEU:H	2.05	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
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:71:LEU:CD2	1:A:353:SER:HB2	2.27	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:606:TYR:HE1	1:A:742:GLY:O	1.81	0.64
2:B:153:GLY:O	2:B:154:TRP:C	2.41	0.64
2:B:596:TRP:O	2:B:597:LYS:HB2	1.96	0.64

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
18:B:1239:CLA:C2B	20:B:6017:BCR:H15C	2.27	0.64
18:B:1242:CLA:O1D	18:B:1242:CLA:HBA2	1.97	0.64
4:D:75:LEU:HD13	4:D:76:LYS:N	2.12	0.64
6:F:98:GLY:O	6:F:102:ARG:N	2.24	0.64
6:F:136:TRP:H	6:F:136:TRP:HD1	1.46	0.64
12:L:94:ILE:O	12:L:98:CYS:N	2.30	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
1:A:58:HIS:HE1	18:A:1101:CLA:C1C	2.10	0.64
1:A:301:HIS:C	1:A:301:HIS:CD2	2.76	0.64
1:A:441:ALA:O	1:A:445:HIS:HE1	1.81	0.64
2:B:5:ILE:CG2	2:B:6:PRO:CA	2.76	0.64
2:B:92:TRP:HD1	9:I:9:VAL:CG1	2.11	0.64
2:B:194:LEU:O	2:B:195:VAL:HG23	1.97	0.64
2:B:289:LEU:O	18:B:1218:CLA:HBC3	1.95	0.64
2:B:341:LEU:HD21	18:B:1202:CLA:HED2	1.80	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:705:ALA:HB1	19:B:5002:PQN:C7	2.28	0.64
18:B:1208:CLA:O2A	18:B:1209:CLA:H2	1.96	0.64
4:D:150:GLY:CA	4:D:151:LYS:C	2.70	0.64
12:L:18:PRO:HG2	12:L:19:PHE:CE1	2.33	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:120:ALA:N	1:A:145:ILE:HG21	2.13	0.63
1:A:246:HIS:HA	18:A:1147:CLA:C2D	2.28	0.63
1:A:397:THR:OG1	18:A:1126:CLA:CMB	2.46	0.63
1:A:479:ASP:C	1:A:481:ALA:H	2.05	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
2:B:432:HIS:HE1	18:B:1229:CLA:CHA	2.11	0.63
18:B:1235:CLA:HBB2	18:B:1236:CLA:HAC2	1.78	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
15:2:23:LEU:CD1	15:2:26:ASP:O	2.46	0.63
15:2:32:LEU:HD22	15:2:33:GLY:C	2.23	0.63
16:3:132:ASP:O	16:3:133:TRP:HD1	1.80	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
2:B:659:THR:HB	18:B:9023:CLA:C3B	2.28	0.63

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:703:VAL:HA	2:B:706:ARG:HG2	1.80	0.63
2:B:705:ALA:CB	19:B:5002:PQN:C7	2.76	0.63
3:C:4:SER:OG	3:C:68:TYR:C	2.41	0.63
4:D:109:VAL:CG2	4:D:110:GLN:HG3	2.28	0.63
14:1:54:VAL:HA	14:1:57:ILE:HG22	1.79	0.63
1:A:96:MET:HB3	1:A:149:PHE:CE2	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
18:A:1119:CLA:HBC2	18:A:1119:CLA:CHD	2.28	0.63
2:B:19:ARG:O	2:B:23:PHE:N	2.32	0.63
2:B:319:HIS:O	2:B:321:GLY:N	2.30	0.63
2:B:330:ILE:HG21	18:B:1202:CLA:CBC	2.27	0.63
2:B:446:PHE:O	2:B:447:GLY:C	2.40	0.63
2:B:672:GLN:CD	2:B:698:VAL:HB	2.23	0.63
7:G:83:TYR:CA	7:G:85:ILE:N	2.56	0.63
12:L:53:GLY:O	12:L:56:VAL:HG22	1.99	0.63
15:2:56:MET:HB3	15:2:172:LEU:CD2	2.28	0.63
15:2:178:TRP:N	15:2:178:TRP:CE3	2.66	0.63
1:A:126:ILE:HD13	1:A:127:VAL:HG13	1.79	0.63
1:A:214:GLY:O	1:A:215:SER:C	2.42	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: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
14:1:52:LEU:HD23	14:1:55:PRO:HG3	1.79	0.63
15:2:23:LEU:HD13	15:2:26:ASP:N	2.00	0.63
1:A:147:SER:OG	18:A:1126:CLA:HMA3	1.98	0.63
1:A:545:HIS:CE1	1:A:612:VAL:HG22	2.34	0.63
1:A:658:TRP:CG	1:A:658:TRP:O	2.51	0.63
18:A:1137:CLA:HBD	18:A:1137:CLA:HBA2	1.81	0.63
2:B:77:TRP:CZ3	2:B:130:ARG:NE	2.66	0.63
2:B:344:ILE:CG1	18:B:1225:CLA:CBC	2.69	0.63

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:441:ASP:CG	2:B:616:LEU:HD22	2.23	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
2:B:693:TRP:HA	18:B:1238:CLA:OBD	1.99	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
15:2:19: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
1:A:95:GLY:HA3	1:A:96:MET:CE	2.28	0.63
1:A:164:LEU:CD2	1:A:164:LEU:H	2.11	0.63
1:A:591:GLN:OE1	2:B:667:TRP:N	2.31	0.63
1:A:658:TRP:O	1:A:658:TRP:CD2	2.51	0.63
1:A:687:ALA:HB1	18:A:9013:CLA:HBB1	1.73	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
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
13:N:43:PRO:C	13:N:45:ASN:HB2	2.22	0.63
14:1:88:PRO:C	14:1:89:VAL:HG23	2.23	0.63
15:2:54:TRP:HA	15:2:54:TRP:HE3	1.63	0.63
17:4:59:LEU:O	17:4:62:GLU:CB	2.39	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: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
18:A:9011:CLA:H3A	18:B:9010:CLA:HMB2	1.81	0.63
2:B:239:SER:OG	2:B:249:GLY:O	2.17	0.63
2:B:243:LEU:HA	2:B:264:GLN:HE22	1.63	0.63
2:B:459:PHE:C	2:B:461:GLN:HB2	2.24	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
1:A:78:VAL:O	1:A:82:HIS:CD2	2.51	0.63
1:A:195:TRP:CZ3	18:A:1118:CLA:C1C	2.81	0.63
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
2:B:177:HIS:CE1	18:B:1209:CLA:C3C	2.81	0.63
2:B:337:ALA:HB3	18:B:1202:CLA:HMD2	1.81	0.63
2:B:533:ILE:HG21	2:B:579:ALA:N	2.14	0.63

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
18:B:1216:CLA:H2A	18:B:1216:CLA:O2D	1.98	0.63
4:D:23:ASN:HB2	12:L:17:ASP:OD2	1.99	0.63
8:H:47:PHE:HZ	12:L:50:LEU:HD11	1.61	0.63
14:1:94:LEU:CB	14:1:95:PRO:HD3	2.29	0.63
1:A:228:PRO:C	1:A:230:ASN:N	2.50	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:69:ALA:HB2	2:B:132:ASN:HB3	1.80	0.63
2:B:195:VAL:O	2:B:254:ILE:HD11	1.99	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
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: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
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: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:377:TYR:C	1:A:377:TYR:CD1	2.74	0.62
1:A:690:LEU:HG	1:A:694:PHE:CZ	2.34	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
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
6:F:97:ILE:HG23	18:F:1240:CLA:CHD	2.29	0.62
8:H:32:TYR:C	8:H:32:TYR:CD1	2.77	0.62
15:2:86:GLU:OE1	17:4:187:SER:CB	2.47	0.62
16:3:82:ALA:CA	16:3:83:GLY:C	2.72	0.62
17:4:56:ALA:C	17:4:59:LEU:HB3	2.24	0.62
1:A:90:PHE:CD1	1:A:175:ALA:HA	2.30	0.62
1:A:232:PHE:CD1	1:A:237:VAL:HG21	2.34	0.62
1:A:235:ALA:O	1:A:236:GLY:O	2.17	0.62
1:A:253:ASP:O	1:A:257:GLN:N	2.31	0.62
1:A:415:ALA:C	1:A:416:ILE:HG12	2.24	0.62
1:A:425:THR:HG21	1:A:428:TYR:HE2	1.64	0.62
1:A:455:PHE:HE1	18:A:1131:CLA:HMA1	1.63	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
2:B:149:SER:O	2:B:152:ALA:HB3	1.99	0.62
2:B:177:HIS:ND1	18:B:1217:CLA:HMD2	2.14	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:712:HIS:O	2:B:713:PHE:O	2.18	0.62
18:B:1212:CLA:H2	18:B:1212:CLA:CAA	2.29	0.62
7:G:35:VAL:HG12	7:G:36:PRO:HB3	1.79	0.62
12:L:83:ALA:HA	12:L:86:LEU:CD2	2.29	0.62
12:L:147:GLY:O	12:L:151:VAL:N	2.28	0.62
12:L:148:VAL:HA	12:L:151:VAL:HG22	1.80	0.62
12:L:166:TYR:N	12:L:167:PHE:C	2.56	0.62
13:N:57:LYS:CG	16:3:87:ALA:CB	2.73	0.62
14:1:89:VAL:HG12	14:1:90:PRO:CD	2.27	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:126:ILE:HG23	1:A:127:VAL:HG22	1.80	0.62
1:A:398:HIS:C	1:A:400:MET:H	2.07	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:O	3:C:49:VAL:HG13	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:83:PHE:O	6:F:87:GLY:HA3	1.99	0.62
6:F:125:LEU:HB3	6:F:130:LEU:HD21	1.79	0.62
12:L:66:GLY:C	12:L:68:PHE:H	2.08	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
17:4:62:GLU:C	17:4:63:VAL:HG22	2.23	0.62
1:A:150:PHE:HA	1:A:153:TRP:HE1	1.62	0.62
1:A:674:ALA:O	1:A:678:PHE:N	2.32	0.62
2:B:52:GLY:O	2:B:55:ALA:CB	2.47	0.62
2:B:77:TRP:O	2:B:130:ARG:NH2	2.33	0.62
2:B:374:HIS:C	2:B:376:GLN:N	2.57	0.62
2:B:416:GLU:HA	2:B:419:ILE:CD1	2.29	0.62
2:B:517:PHE:O	2:B:521:HIS:N	2.33	0.62
2:B:614:THR:O	2:B:615:TYR:HB3	1.99	0.62

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:697:PRO:HG2	18:B:1238:CLA:HBC2	1.81	0.62
6:F:80:TRP:HE1	18:F:1302:CLA:CBC	2.06	0.62
10:J:28:GLU:CD	10:J:31:ARG:HH11	2.07	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:8:PHE:N	2:B:8:PHE:CD1	2.67	0.62
2:B:65:LEU:HG	2:B:124:TRP:CH2	2.34	0.62
2:B:91:ILE:CD1	2:B:114:ASN:HD22	2.13	0.62
2:B:287:GLY:CA	2:B:290:MET:HE2	2.30	0.62
2:B:557:PHE:CZ	2:B:570:ILE:HG13	2.34	0.62
6:F:125:LEU:C	6:F:130:LEU:HD11	2.23	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
13:N:57:LYS:CD	16:3:87:ALA:CB	2.39	0.62
15:2:177:ALA:C	15:2:178:TRP:HE3	2.08	0.62
16:3:186:LYS:HA	18:3:3004:CLA:C2C	2.29	0.62
1:A:460:LEU:HD13	18:A:1132:CLA:C3C	2.30	0.62
1:A:750:PHE:CZ	18:A:1126:CLA:HMB3	2.35	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
18:B:1209:CLA:HMB3	18:B:1209:CLA:H91	1.82	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:21:PHE:C	7:G:23:PHE:HB3	2.24	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
12:L:64:LEU:C	12:L:66:GLY:N	2.56	0.62
13:N:47:THR:CA	13:N:49:CYS:SG	2.87	0.62
13:N:58:VAL:CB	16:3:86:PRO:HA	2.27	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
16:3:126:GLU:CD	16:3:127:HIS:N	2.57	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:681:GLY:CA	20:A:6011:BCR:H17C	2.30	0.62
1:A:714:LEU:HD23	6:F:149:LEU:HD22	1.80	0.62
1:A:740:LEU:O	1:A:743:ILE:HD13	2.00	0.62
18:A:1129:CLA:H3A	18:L:1130:CLA:OBD	2.00	0.62

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:311:PRO:HG2	18:B:1220:CLA:HMB3	1.81	0.62
2:B:374:HIS:O	2:B:376:GLN:N	2.33	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
12:L:73:PRO:HB2	12:L:74:LEU:HG	1.82	0.62
18:L:1503:CLA:CBD	18:L:1503:CLA:CAA	2.77	0.62
13:N:41:LYS:O	13:N:42:PHE:C	2.43	0.62
13:N:47:THR:N	13:N:49:CYS:SG	2.73	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:HD12	1.96	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: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
2:B:466:ALA:C	2:B:468:GLY:H	2.07	0.62
18:B:1207:CLA:HMA2	18:B:1207:CLA:H2	1.81	0.62
6:F:82:GLU:O	10:J:38:THR:HG21	1.99	0.62
6:F:136:TRP:N	6:F:136:TRP:HD1	1.97	0.62
14:1:44:LEU:HD22	14:1:44:LEU:H	1.64	0.62
15:2:59:ALA:C	15:2:61:GLY:H	2.07	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
2:B:31:PHE:HD2	2:B:34:HIS:HD1	1.46	0.62
2:B:121:TYR:C	2:B:122:GLN:HE21	2.07	0.62
2:B:215:VAL:CB	2:B:217:PRO:HD3	2.28	0.62
2:B:593:TYR:CZ	18:B:1234:CLA:HAC2	2.34	0.62
18:B:1208:CLA:H62	18:B:1209:CLA:H43	1.82	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
14:1:153:LEU:H	14:1:153:LEU:HD22	1.64	0.62
16:3:132:ASP:OD1	16:3:139:MET:CB	2.38	0.62
1:A:88:ILE:O	1:A:92:TRP:N	2.30	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
2:B:19:ARG:NH1	3:C:72:GLU:HB3	2.10	0.62
2:B:33:SER:O	2:B:34:HIS:CD2	2.52	0.62
2:B:207:VAL:HA	2:B:211:ASN:HD21	1.63	0.62

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:407:VAL:HB	18:B:1220:CLA:HMC2	1.80	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
5:E:37:LYS:HB2	5:E:89:GLU:HB2	1.80	0.62
15:2:26:ASP:HB2	15:2:27:PHE:CD2	2.35	0.62
15:2:32:LEU:CD1	15:2:32:LEU:C	2.69	0.62
15:2:178:TRP:CG	15:2:183:TYR:HH	2.17	0.62
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
2:B:52:GLY:O	2:B:55:ALA:HB3	2.00	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
18:B:1215:CLA:CBB	18:B:1215:CLA:H62	2.29	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
15:2:24:PRO:HB3	15:2:32:LEU:CB	2.30	0.61
17:4:158:ARG:HG2	17:4:158:ARG:HH11	1.65	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
4:D:58:PHE:HE2	4:D:90:LEU:CD2	2.13	0.61
18:G:1233:CLA:HHD	18:G:1233:CLA:HBC2	1.80	0.61
17:4:81:GLU:H	17:4:82:GLU:HA	1.66	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
1:A:567:ARG:HH22	4:D:37:LEU:CG	2.13	0.61
1:A:621:GLN:C	1:A:623:ASP:N	2.58	0.61
2:B:69:ALA:CB	2:B:132:ASN:HB3	2.31	0.61
2:B:135:LEU:C	2:B:137:THR:H	2.06	0.61
2:B:403:ASN:O	2:B:406:ASN:ND2	2.34	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:CG	5:E:45:TRP:O	2.51	0.61
10:J:13:VAL:O	10:J:17:LEU:HB2	2.00	0.61
14:1:173:PRO:C	14:1:175:GLU:N	2.56	0.61
1:A:95:GLY:N	1:A:96:MET:SD	2.73	0.61
1:A:311:LEU:HD11	18:A:1108:CLA:HAC1	1.82	0.61
1:A:330:ILE:O	1:A:333:ALA:HB3	2.00	0.61
1:A:369:THR:HB	18:A:1127:CLA:C3C	2.30	0.61
1:A:396:PHE:HD2	1:A:396:PHE:C	2.07	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:663:GLN:HE21	1:A:753:ARG:HH11	1.47	0.61
18:B:1218:CLA:O1D	18:B:1218:CLA:C2A	2.46	0.61
4:D:45:PHE:O	4:D:45:PHE:HD1	1.83	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:9:LYS:O	13:N:13:ASN:N	2.32	0.61
13:N:77:CYS:SG	13:N:81:VAL:O	2.57	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
1:A:464:ASN:CG	1:A:477:PHE:HB2	2.21	0.61
1:A:566:SER:C	1:A:568:LEU:H	2.09	0.61
18:A:1126:CLA:C4A	18:A:1126:CLA:HBA2	2.31	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
3:C:9:ASP:CG	3:C:10:THR:N	2.58	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
6:F:137:PRO:HA	6:F:141:TYR:HB3	0.73	0.61
8:H:76:VAL:O	8:H:77:LEU:O	2.18	0.61
8:H:85:GLN:O	8:H:86:PRO:C	2.42	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
13:N:59:PRO:HA	13:N:60:PHE:HB3	1.80	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
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:742:GLY:C	1:A:743:ILE:HD12	2.26	0.61
18:A:1133:CLA:CHC	18:A:1134:CLA:C2B	2.79	0.61
2:B:17:THR:C	2:B:19:ARG:H	2.09	0.61
2:B:35:ASP:HB3	4:D:154:TYR:HE1	1.66	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
5:E:79:THR:O	5:E:80:ASN:O	2.18	0.61
6:F:5:LEU:C	6:F:62:LEU:HG	2.26	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:33:ILE:O	12:L:34:ALA:C	2.43	0.61
12:L:53:GLY:N	12:L:139:PHE:HE1	1.98	0.61
12:L:107:PHE:HA	12:L:133:ALA:HB3	1.82	0.61
15:2:187:GLY:C	15:2:189:ILE:N	2.53	0.61
15:2:194:ALA:HB3	15:2:195:HIS:CA	2.29	0.61
1:A:222:GLN:O	1:A:222:GLN:NE2	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
1:A:718:PRO:HG2	1:A:722:PRO:HD3	1.80	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
2:B:71:GLN:CD	2:B:89:HIS:O	2.42	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
2:B:196:HIS:HE1	18:B:1211:CLA:C3C	2.12	0.61
2:B:287:GLY:CA	18:B:1218:CLA:HMC3	2.29	0.61
2:B:365:PHE:CD1	2:B:602:TRP:CG	2.89	0.61
2:B:593:TYR:O	2:B:594:TRP:HB2	2.01	0.61
2:B:708:VAL:HG12	18:B:1239:CLA:O1D	2.00	0.61
18:B:1238:CLA:O1A	9:I:21:MET:SD	2.58	0.61
4:D:96:ILE:HG12	4:D:97:LYS:H	1.63	0.61
16:3:143:TYR:O	16:3:144:PHE:HB2	2.00	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:O	1:A:688:PHE:CG	2.53	0.61
18:A:1105:CLA:C2B	18:A:1107:CLA:CED	2.78	0.61
2:B:4:ARG:HH11	2:B:4:ARG:HG3	1.66	0.61
2:B:19:ARG:HG3	2:B:19:ARG:HH11	1.65	0.61
2:B:191:ALA:HB1	2:B:277:HIS:C	2.25	0.61
2:B:273:VAL:HG22	18:B:1214:CLA:CMA	2.30	0.61
2:B:341:LEU:HD21	18:B:1202:CLA:CED	2.30	0.61
2:B:350:GLN:O	2:B:354:SER:N	2.28	0.61
18:B:1209:CLA:HBA2	7:G:38:GLN:HG2	1.82	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
13:N:72:LYS:CA	13:N:75:TYR:O	2.49	0.61
1:A:81:ALA:HB3	1:A:83:PHE:CA	2.24	0.61
1:A:434:ARG:HH21	1:A:438:HIS:CB	2.14	0.61
1:A:496:HIS:ND1	1:A:515:TRP:CD2	2.61	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
18:B:1215:CLA:HBC3	18:B:1215:CLA:HMC1	1.81	0.61
4:D:24:THR:O	4:D:24:THR:OG1	2.19	0.61
4:D:133:ASN:CG	4:D:135:ARG:H	2.08	0.61
5:E:75:ALA:O	5:E:76:ASN:HB2	2.00	0.61
6:F:122:ASP:O	6:F:123:VAL:C	2.43	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
14:1:164:GLN:OE1	14:1:181:LEU:HD11	2.00	0.61
1:A:654:ARG:HD2	1:A:655:ASP:OD2	2.01	0.61
2:B:175:LEU:HA	18:B:1221:CLA:HED1	1.83	0.61
2:B:286:ILE:C	18:B:1218:CLA:CMC	2.71	0.61
2:B:577:TYR:O	2:B:578:LEU:HB2	2.00	0.61
18:B:1209:CLA:HBA2	7:G:38:GLN:CG	2.31	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:39:ALA:C	6:F:41:ALA:H	2.09	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
6:F:100:VAL:HG12	6:F:125:LEU:HD21	1.82	0.61
11:K:55:UNK:O	11:K:57:UNK:N	2.34	0.61
15:2:17:GLU:CD	15:2:18:TRP:CB	2.66	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:32:GLU:HB2	1:A:33:GLN:CA	2.24	0.60
1:A:50:THR:CG2	1:A:723:ARG:NH1	2.53	0.60
1:A:364:MET:HG2	18:A:1123:CLA:C3A	2.31	0.60
1:A:369:THR:O	1:A:403:GLY:HA3	2.01	0.60
1:A:377:TYR:CD2	1:A:396:PHE:HE1	2.18	0.60
1:A:387:THR:OG1	1:A:526:LYS:HG3	2.01	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
18:B:1237:CLA:HAC1	18:B:1238:CLA:C4B	2.31	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
8:H:73:PRO:HA	8:H:75:ASP:OD2	2.01	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
14:1:21:ASP:N	14:1:22:PHE:C	2.59	0.60
14:1:185:TRP:O	14:1:186:HIS:HB2	2.00	0.60
17:4:37:LEU:O	17:4:39:TRP:N	2.28	0.60
17:4:194:ILE:O	17:4:196:GLN:HG2	1.99	0.60
1:A:41:SER:O	1:A:43:THR:N	2.33	0.60
1:A:199:VAL:O	1:A:199:VAL:CG2	2.36	0.60
1:A:458:PHE:CE1	18:B:9022:CLA:HMB1	2.36	0.60
1:A:505:PRO:HD3	18:A:1134:CLA:C4D	2.32	0.60
1:A:639:ALA:C	1:A:641:ASN:N	2.55	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:323:TYR:C	2:B:323:TYR:CD1	2.79	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
2:B:587:ILE:O	2:B:588:GLY:C	2.42	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
15:2:44:ASN:OD1	15:2:46:GLN:HB2	2.01	0.60
15:2:159:LEU:O	15:2:162:LYS:CG	2.49	0.60
1:A:396:PHE:CD2	1:A:396:PHE:C	2.77	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
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
18:B:1138:CLA:CAD	18:B:1138:CLA:CED	2.78	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
18:L:1502:CLA:C4	18:L:1504:CLA:CMA	2.78	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:224:HIS:HB3	1:A:248:PHE:CD2	2.36	0.60
1:A:472:ARG:O	1:A:473:PRO:C	2.44	0.60
1:A:496:HIS:HD1	1:A:515:TRP:CG	2.19	0.60
1:A:543:HIS:C	1:A:546:ALA:HB3	2.27	0.60
1:A:578:ARG:O	1:A:593:SER:OG	2.14	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:C:22:PRO:CD	3:C:51:CYS:SG	2.89	0.60
12:L:83:ALA:HA	12:L:86:LEU:HD21	1.84	0.60
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
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
1:A:603:PHE:CE2	1:A:735:VAL:HA	2.35	0.60
1:A:613:ILE:HG22	1:A:614:PHE:N	2.16	0.60
1:A:688:PHE:CZ	18:A:1140:CLA:C1C	2.84	0.60
1:A:707:ILE:HD13	18:B:1138:CLA:HMD2	1.83	0.60
2:B:90:ALA:C	2:B:91:ILE:HD12	2.27	0.60
2:B:257:ILE:CG1	18:B:1214:CLA:HMB2	2.32	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
2:B:564:ARG:O	2:B:565:GLY:C	2.44	0.60
5:E:40:ARG:HG3	5:E:85:ASP:O	2.02	0.60
7:G:22:VAL:C	7:G:23:PHE:CD2	2.76	0.60
9:I:16:PHE:CD1	9:I:16:PHE:C	2.79	0.60
16:3:134:TYR:CA	16:3:136:PRO:CD	2.75	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:317:ARG:HG2	2:B:317:ARG:NH2	2.04	0.60
2:B:332:PHE:C	2:B:335:GLY:H	2.10	0.60
2:B:593:TYR:OH	18:B:1234:CLA:CAC	2.50	0.60
2:B:606:VAL:HG22	2:B:610:ASN:ND2	2.17	0.60
2:B:713:PHE:O	2:B:714:SER:C	2.44	0.60
13:N:23:ALA:HB1	13:N:27:ALA:HB3	1.83	0.60
14:1:86:GLY:N	14:1:87:ASN:HA	2.15	0.60
15:2:162:LYS:NZ	15:2:163:GLU:HB2	2.16	0.60
15:2:178:TRP:HB3	15:2:183:TYR:CE2	2.37	0.60
15:2:180:GLN:O	15:2:182:ILE:N	2.32	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: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:311:LEU:HD21	18:A:1108:CLA:CMC	2.32	0.60
1:A:392:GLN:OE1	1:A:392:GLN:HA	2.00	0.60
1:A:462:ILE:HG22	1:A:463:HIS:N	2.15	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:472:ARG:C	1:A:474:GLN:N	2.56	0.60
2:B:351:HIS:NE2	18:B:1223:CLA:ND	2.49	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
12:L:36:TYR:C	12:L:38:SER:H	2.02	0.60
12:L:92:VAL:C	12:L:94:ILE:H	2.06	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
2:B:50:HIS:ND1	2:B:50:HIS:O	2.33	0.60
2:B:133:GLU:CA	2:B:136:TYR:HE1	2.11	0.60
2:B:410:ARG:HA	2:B:413:GLU:CD	2.27	0.60
2:B:558:PRO:HA	2:B:703:VAL:HG23	1.84	0.60
2:B:661:PHE:HB3	18:B:9023:CLA:CMC	2.27	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
15:2:180:GLN:C	15:2:182:ILE:N	2.59	0.60
16:3:133:TRP:NE1	16:3:139:MET:O	2.33	0.60
1:A:99:HIS:ND1	1:A:103:PHE:HZ	2.00	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
18:A:1107:CLA:HMB2	10:J:27:ILE:HG12	1.84	0.60
18:A:1137:CLA:HBA1	18:A:1137:CLA:CBD	2.32	0.60
2:B:520:HIS:NE2	18:B:1234:CLA:NC	2.50	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
7:G:16:LEU:CD2	7:G:68:ILE:HG12	2.32	0.60
13:N:36:GLU:HA	13:N:39:SER:HB3	1.83	0.60
15:2:18:TRP:C	15:2:20:ASP:O	2.44	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:87:SER:OG	1:A:179:LEU:HB2	2.02	0.60
1:A:109:TRP:O	1:A:111:ASN:OD1	2.20	0.60
1:A:208:ALA:O	1:A:209:GLY:C	2.45	0.60
1:A:347:TYR:HB3	1:A:350:LEU:HG	1.84	0.60
1:A:405:PHE:CE2	1:A:605:MET:HE1	2.37	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
2:B:260:GLY:N	2:B:269:TRP:CE2	2.70	0.60
2:B:374:HIS:C	2:B:376:GLN:H	2.08	0.60
2:B:399:ASN:C	2:B:401:GLU:H	2.09	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
15:2:85:GLN:C	15:2:86:GLU:HG3	2.27	0.60
15:2:93:THR:N	15:2:94:LEU:CB	2.61	0.60
1:A:135:ASP:H	1:A:136:VAL:HG22	1.65	0.59
1:A:197:GLN:OE1	1:A:351:THR:HB	2.02	0.59
1:A:642:PHE:O	1:A:643:ALA:C	2.45	0.59
2:B:216:LEU:N	2:B:217:PRO:HD3	2.17	0.59
2:B:311:PRO:HD3	18:B:1219:CLA:CBB	2.31	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
12:L:49:PRO:O	12:L:50:LEU:C	2.45	0.59
14:1:70:LYS:HZ3	18:1:1013:CLA:CHD	2.14	0.59
16:3:55:LEU:CD1	16:3:58:GLY:HA3	2.27	0.59
16:3:82:ALA:HA	16:3:83:GLY:C	2.26	0.59
1:A:232:PHE:CZ	1:A:243:PRO:HG2	2.37	0.59
1:A:465:ASP:C	1:A:467:MET:N	2.57	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
1:A:668:TYR:CG	2:B:445:ALA:HA	2.37	0.59
1:A:725:LEU:HG	1:A:729:GLN:CD	2.27	0.59
18:A:1129:CLA:HAA2	18:A:1129:CLA:HBD	1.84	0.59
2:B:20:ARG:HH21	9:I:28:VAL:HA	1.66	0.59
2:B:101:VAL:O	2:B:106:ARG:NH1	2.34	0.59
2:B:344:ILE:CD1	18:B:1225:CLA:CBC	1.81	0.59
2:B:346:SER:CB	18:B:1222:CLA:O1D	2.48	0.59
2:B:395:ILE:O	2:B:396:ARG:HB2	2.03	0.59
2:B:537:GLY:O	2:B:572:ALA:HB1	2.02	0.59
18:B:1235:CLA:O1A	18:B:1235:CLA:CHA	2.49	0.59
18:B:1239:CLA:H41	9:I:21:MET:HG3	1.83	0.59
4:D:102:ARG:O	4:D:108:GLU:C	2.45	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
9:I:18:ALA:O	9:I:22:ALA:HB2	2.02	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
1:A:230:ASN:O	1:A:234:ASN:CG	2.45	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:665:ILE:HD13	2:B:625:TRP:CG	2.36	0.59
1:A:709:TRP:CZ2	18:B:1228:CLA:HED1	2.37	0.59
19:A:5001:PQN:H171	18:F:1139:CLA:HBB2	1.84	0.59
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:242:HIS:HB2	2:B:249:GLY:C	2.28	0.59
2:B:291:TYR:C	2:B:292:ARG:HG3	2.27	0.59
2:B:330:ILE:HG21	18:B:1202:CLA:HAC2	1.78	0.59
2:B:439:HIS:HD2	18:B:1230:CLA:C1C	2.15	0.59
2:B:675:ILE:O	2:B:679:ALA:CB	2.50	0.59
18:B:1222:CLA:HBD	18:B:1234:CLA:HBB2	1.85	0.59
4:D:34:GLY:C	4:D:62:THR:HB	2.26	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
15:2:54: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: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:4:ARG:HD3	2:B:5:ILE:H	1.67	0.59
2:B:49:SER:HG	2:B:50:HIS:H	1.50	0.59
2:B:91:ILE:CD1	2:B:114:ASN:ND2	2.65	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
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
14:1:188:ASN:C	14:1:190:GLY:CA	2.75	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:58:HIS:CE1	18:A:1101:CLA:NC	2.70	0.59
1:A:83:PHE:HE1	1:A:182:GLY:HA2	1.68	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:92:TRP:O	1:A:94:SER:C	2.46	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:566:SER:O	1:A:568:LEU:N	2.34	0.59
2:B:49:SER:OG	2:B:50:HIS:N	2.35	0.59
2:B:676:GLU:C	2:B:678:LEU:H	2.10	0.59
3:C:12:ILE:C	3:C:38:GLN:HG3	2.28	0.59
3:C:23:THR:OG1	3:C:48:CYS:HA	2.02	0.59
3:C:31:TRP:O	3:C:37:LYS:HG2	2.02	0.59
7:G:68:ILE:C	7:G:68:ILE:HD12	2.27	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
14:1:152:ARG:HD3	14:1:153:LEU:N	2.16	0.59
15:2:24:PRO:HG3	15:2:27:PHE:CE2	2.34	0.59
15:2:166:ASN:OD1	18:2:2004:CLA:C4C	2.51	0.59
1:A:39:HIS:H	1:A:44:ILE:CD1	2.12	0.59
1:A:287:LEU:HA	1:A:294:LEU:HA	1.85	0.59
1:A:443:ILE:HG22	1:A:444:SER:N	2.16	0.59
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
2:B:497:TRP:O	2:B:501:ILE:HG23	2.02	0.59
2:B:546:LEU:CD2	5:E:74:TYR:CE1	2.85	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
18:B:1239:CLA:CBD	19:B:5002:PQN:H251	2.32	0.59
4:D:43:GLU:O	4:D:43:GLU:CG	2.46	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
6:F:73:VAL:HB	6:F:83:PHE:CD2	2.37	0.59
6:F:120:ILE:HG23	10:J:9:SER:HB3	1.85	0.59
9:I:26:LEU:C	9:I:28:VAL:N	2.61	0.59
16:3:138:SER:N	16:3:139:MET:HB3	2.13	0.59
17:4:75:TRP:CD1	17:4:75:TRP:H	2.18	0.59
1:A:130:GLU:N	1:A:130:GLU:CD	2.60	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:98:GLN:C	2:B:100:ALA:H	2.10	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:340:SER:C	2:B:342:GLY:N	2.57	0.59
2:B:341:LEU:HD11	18:B:1225:CLA:HMC2	1.84	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
18:B:1222:CLA:CHB	18:B:1236:CLA:HAA2	2.33	0.59
18:B:1229:CLA:ND	6:F:90:PHE:CZ	2.70	0.59
18:B:1239:CLA:C1	19:B:5002:PQN:H271	2.33	0.59
3:C:33:GLY:C	5:E:61:THR:HB	2.28	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
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: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
1:A:454:GLY:HA3	1:A:547:PHE:CD2	2.38	0.59
1:A:455:PHE:HB2	18:B:9023:CLA:CGA	2.33	0.59
1:A:599:PHE:CZ	1:A:693:LEU:HD11	2.37	0.59
18:A:1129:CLA:C3A	18:L:1130:CLA:OBD	2.50	0.59
2:B:41:ARG:HA	2:B:44:GLN:OE1	2.02	0.59
2:B:646:TRP:HB3	2:B:723:ALA:CB	2.33	0.59
10:J:5:LYS:NZ	15:2:120:ASN:O	2.22	0.59
12:L:27:VAL:O	12:L:27:VAL:HG12	2.02	0.59
13:N:50:GLN:C	13:N:52:LEU:HB2	2.26	0.59
14:1:52:LEU:C	14:1:55:PRO:HD2	2.28	0.59
14:1:86:GLY:N	14:1:87:ASN:CA	2.66	0.59
14:1:188:ASN:HA	14:1:189:ILE:CB	2.26	0.59
15:2:21:GLY:H	15:2:23:LEU:CD1	2.08	0.59
15:2:188:PRO:HA	15:2:192:LEU:CD1	2.32	0.59
1:A:133:ASN:O	1:A:134:GLY:O	2.21	0.59
1:A:258:LEU:O	1:A:259:TYR:C	2.46	0.59
1:A:401:TRP:CD1	18:A:1126:CLA:HHC	2.38	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:310:PRO:C	18:B:1219:CLA:HBB1	2.27	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
8:H:86:PRO:O	8:H:87:PRO:C	2.44	0.59
13:N:46:PHE:O	13:N:47:THR:CG2	2.46	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
16:3:119:MET:HG3	18:3:3010:CLA:C3D	2.32	0.59
1:A:86:LEU:HB2	18:A:1103:CLA:C2	2.33	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:542:HIS:C	1:A:544:ILE:H	2.11	0.59
1:A:654:ARG:HG2	2:B:633:ASN:OD1	2.03	0.59
2:B:53:GLN:O	2:B:55:ALA:N	2.36	0.59
2:B:103:ALA:CB	2:B:104:PHE:HD1	2.15	0.59
2:B:441:ASP:OD1	2:B:616:LEU:N	2.28	0.59
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:714:SER:O	2:B:718:ILE:HG13	2.03	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
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
16:3:56:ALA:C	16:3:58:GLY:H	2.11	0.59
17:4:116:ASN:HA	17:4:117:GLN:CG	2.30	0.59
1:A:299:ILE:O	1:A:299:ILE:HG22	2.03	0.58
1:A:649:ILE:HG22	1:A:650:ASN:N	2.17	0.58
2:B:368:GLN:HG2	2:B:594:TRP:HH2	1.68	0.58
2:B:527:LEU:C	2:B:529:THR:H	2.11	0.58
2:B:594:TRP:HA	2:B:598:HIS:ND1	2.17	0.58
2:B:652:PHE:CE1	18:B:1239:CLA:HMB1	2.39	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
4:D:146:VAL:O	4:D:149:THR:HG23	2.03	0.58
5:E:36:VAL:HG21	5:E:52:VAL:CG1	2.33	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
15:2:23:LEU:HD13	15:2:26:ASP:HA	1.83	0.58
1:A:358:LEU:HG	18:A:1103:CLA:CMD	2.32	0.58
1:A:397:THR:HB	1:A:613:ILE:CG1	2.31	0.58
1:A:461:TYR:HB3	1:A:649:ILE:N	2.17	0.58
1:A:536:THR:O	1:A:537:ALA:HB3	2.03	0.58
1:A:653:LEU:CD2	18:B:9010:CLA:HBC2	2.32	0.58
2:B:174:ARG:NH2	18:B:1210:CLA:CHD	2.66	0.58
2:B:241:ASN:O	2:B:242:HIS:C	2.46	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
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
14:1:90:PRO:HG2	14:1:92:GLY:CA	2.33	0.58
17:4:144:ALA:C	17:4:146:THR:H	2.10	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
1:A:608:SER:CA	1:A:611:VAL:HG12	2.28	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
18:B:1228:CLA:C2B	20:F:6016:BCR:C34	2.81	0.58
4:D:144:ILE:N	4:D:144:ILE:CD1	2.61	0.58
9:I:25:PHE:CD2	9:I:25:PHE:C	2.80	0.58
12:L:89:ALA:O	12:L:92:VAL:HG12	2.03	0.58
13:N:73:ASP:CG	13:N:76:LYS:HA	2.28	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
1:A:452:PHE:CE2	18:A:1136:CLA:HBB2	2.37	0.58
2:B:67:HIS:NE2	2:B:89:HIS:HB3	2.18	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:583:MET:SD	2:B:583:MET:C	2.86	0.58
2:B:652:PHE:CD1	2:B:656:VAL:HG21	2.37	0.58
2:B:700:LEU:HD22	2:B:704:GLN:HE22	1.36	0.58
18:B:1207:CLA:H2	18:B:1207:CLA:CMA	2.33	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:69:CYS:HB2	13:N:72:LYS:N	2.19	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:398:HIS:C	1:A:398:HIS:CD2	2.81	0.58
1:A:620:MET:HE3	1:A:624:VAL:HG11	1.86	0.58
1:A:679:PHE:HB3	1:A:748:ALA:HB3	1.85	0.58
1:A:722:PRO:HB2	18:F:1139:CLA:CMC	2.34	0.58
2:B:53:GLN:NE2	18:B:1202:CLA:H3A	2.18	0.58
2:B:73:ASN:HB2	2:B:76:ALA:HB3	1.84	0.58
2:B:104:PHE:HB2	2:B:112:PRO:O	2.03	0.58
2:B:174:ARG:O	18:B:1221:CLA:HMD3	2.03	0.58
2:B:646:TRP:HE3	2:B:723:ALA:CA	2.17	0.58
18:B:1138:CLA:C3B	18:F:1139:CLA:CMD	2.82	0.58
3:C:27:GLU:HB3	3:C:43:PRO:CG	2.34	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
15:2:180:GLN:C	15:2:182:ILE:H	2.11	0.58
16:3:133:TRP:NE1	16:3:139:MET:HE3	2.18	0.58
1:A:355:HIS:NE2	1:A:416:ILE:HD12	2.19	0.58
9:I:5:PRO:O	9:I:6:SER:C	2.47	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
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:95:GLY:HA3	1:A:96:MET:HE1	1.84	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
1:A:638:THR:HG1	1:A:641:ASN:HD21	1.47	0.58
1:A:645:SER:OG	2:B:637:PRO:CG	2.50	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
2:B:729:THR:HG23	2:B:733:PHE:HA	1.86	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:93:VAL:HA	12:L:96:SER:HB2	1.86	0.58
15:2:17:GLU:CA	15:2:18:TRP:O	2.51	0.58
15:2:26:ASP:HB2	15:2:27:PHE:HD2	1.67	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
16:3:212:ASN:CB	16:3:213:LEU:CB	2.82	0.58
1:A:344:LYS:C	1:A:344:LYS:HD3	2.29	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:621:ARG:HD3	2:B:622:ASP:HB2	1.85	0.58
4:D:69:ARG:HD2	4:D:70:GLU:H	1.67	0.58
4:D:119:TYR:HB3	4:D:121:GLU:O	2.03	0.58
13:N:78:GLY:C	13:N:80:ASN:HA	2.28	0.58
14:1:63:LEU:HD23	14:1:66:GLY:HA2	1.85	0.58
14:1:105:ILE:O	14:1:108:VAL:HG22	2.03	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:504:ALA:HB2	18:A:1134:CLA:CHB	2.33	0.58
1:A:504:ALA:O	1:A:505:PRO:C	2.46	0.58
1:A:567:ARG:HH22	4:D:37:LEU:HG	1.68	0.58
2:B:54:LEU:HA	2:B:57:ILE:HD12	1.86	0.58
2:B:135:LEU:HD22	2:B:136:TYR:N	2.19	0.58
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:456:GLU:CG	2:B:514:PRO:HB3	2.19	0.58
2:B:476:ILE:HB	2:B:477:PRO:HD2	1.86	0.58
2:B:675:ILE:O	2:B:679:ALA:HB3	2.04	0.58
4:D:75:LEU:HD11	12:L:19:PHE:CG	2.39	0.58
13:N:2:VAL:CB	13:N:4:GLU:HB2	2.34	0.58
15:2:109:ARG:CB	18:2:2011:CLA:C2C	2.81	0.58
1:A:31:PHE:C	1:A:31:PHE:HD2	2.12	0.58
1:A:83:PHE:CE1	1:A:182:GLY:HA2	2.39	0.58
1:A:431:LEU:O	1:A:432:LEU:C	2.45	0.58
1:A:484:LEU:CD2	1:A:539:PHE:CE2	2.87	0.58
1:A:566:SER:OG	2:B:673:GLU:OE2	2.14	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
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
18:B:1207:CLA:O2A	18:B:1207:CLA:C2A	2.51	0.58
4:D:112:LEU:C	4:D:113:HIS:CG	2.80	0.58
4:D:116:ASP:CG	4:D:118:VAL:HG13	2.28	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
13:N:58:VAL:HG12	16:3:86:PRO:C	2.29	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
13:N:71:GLY:HA3	13:N:75:TYR:CZ	2.39	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
17:4:89:THR:C	17:4:91:PHE:N	2.62	0.58
1:A:71:LEU:HA	1:A:74:ILE:HG23	1.85	0.57
1:A:223:VAL:HA	1:A:227:LEU:CD1	2.33	0.57
1:A:697:ARG:HD3	1:A:727:ILE:H	1.69	0.57
18:A:1123:CLA:HBD	18:A:1123:CLA:HBA1	1.84	0.57
2:B:57:ILE:HG23	18:B:1203:CLA:HMC3	1.84	0.57
2:B:144:PHE:CD2	2:B:145:LEU:HD22	2.39	0.57
2:B:254:ILE:HG21	18:B:1212:CLA:HBC1	1.85	0.57
2:B:259:GLY:CA	2:B:269:TRP:HZ2	2.10	0.57
2:B:364:ASP:O	2:B:365:PHE:C	2.44	0.57
2:B:493:TRP:HH2	18:B:1213:CLA:C3D	2.17	0.57
2:B:525:LEU:HD11	2:B:582:TRP:CH2	2.38	0.57
18:B:1217:CLA:CMB	7:G:18:LEU:HD22	2.32	0.57
18:B:1220:CLA:NB	18:B:1242:CLA:HBA1	2.19	0.57
3:C:42:ALA:O	3:C:44:ARG:N	2.37	0.57
3:C:81:TYR:CB	4:D:37:LEU:HD12	2.34	0.57
6:F:25:LEU:CD1	6:F:41:ALA:O	2.52	0.57
6:F:60:GLY:C	6:F:62:LEU:N	2.62	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
12:L:77:THR:O	12:L:80:ALA:HB1	2.03	0.57
13:N:64:ASP:CG	13:N:65:LEU:N	2.62	0.57
17:4:77:ALA:CB	17:4:78:ALA:CA	2.72	0.57
18:4:1304:CLA:H11	18:4:1304:CLA:HBD	1.86	0.57
1:A:51:THR:O	1:A:53:TRP:N	2.31	0.57
1:A:552:THR:CG2	1:A:604:TRP:HB3	2.33	0.57
1:A:590:CYS:H	2:B:669:GLY:N	2.01	0.57
2:B:103:ALA:HB1	2:B:104:PHE:CE1	2.38	0.57
12:L:24:GLU:HA	12:L:28:THR:HG21	1.86	0.57
14:1:10:ARG:O	17:4:110:LYS:CG	2.51	0.57
1:A:283:PHE:O	1:A:507:ALA:HA	2.04	0.57
1:A:286:GLY:O	1:A:287:LEU:HB3	2.04	0.57
1:A:367:SER:C	1:A:369:THR:N	2.62	0.57
1:A:455:PHE:CE1	18:A:1131:CLA:HMA1	2.39	0.57
1:A:605:MET:HA	1:A:608:SER:OG	2.04	0.57
1:A:652:TRP:N	1:A:652:TRP:CD1	2.71	0.57
2:B:325:THR:O	2:B:329:SER:N	2.35	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:340:SER:OG	18:B:1242:CLA:HBB1	2.03	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
4:D:58:PHE:CD1	4:D:58:PHE:C	2.83	0.57
5:E:62:ARG:O	5:E:83:ALA:HB3	2.04	0.57
6:F:102:ARG:HH21	6:F:148:GLU:CD	2.12	0.57
7:G:20:ARG:HH11	7:G:20:ARG:HG2	1.68	0.57
13:N:71:GLY:HA2	13:N:76:LYS:CB	2.34	0.57
15:2:54:TRP:HE3	15:2:57:LEU:HB2	1.68	0.57
17:4:63:VAL:HB	17:4:65:THR:O	2.05	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
1:A:251:ASN:C	1:A:251:ASN:ND2	2.56	0.57
1:A:302:HIS:C	1:A:303:HIS:ND1	2.62	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:4:ARG:HG2	2:B:5:ILE:N	2.19	0.57
2:B:166:SER:O	2:B:168:PHE:N	2.37	0.57
2:B:171:ALA:HB2	18:B:1221:CLA:HBC1	1.87	0.57
2:B:700:LEU:O	2:B:701:SER:O	2.21	0.57
3:C:6:LYS:C	3:C:8:TYR:CZ	2.82	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
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:52:THR:HA	1:A:55:TRP:HE1	1.69	0.57
1:A:63:ASP:CG	1:A:64:PHE:N	2.62	0.57
1:A:377:TYR:CG	1:A:378:SER:N	2.71	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
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
18:B:1220:CLA:CHB	18:B:1242:CLA:HBA1	2.35	0.57
3:C:46:GLU:OE2	3:C:46:GLU:HA	2.02	0.57
7:G:20:ARG:HG2	7:G:20:ARG:NH1	2.17	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
8:H:77:LEU:CD2	8:H:78:PRO:HD2	2.29	0.57
11:K:57:UNK:O	11:K:61:UNK:N	2.37	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:90:PHE:O	1:A:92:TRP:N	2.36	0.57
1:A:125:PRO:HA	1:A:130:GLU:CD	2.29	0.57
1:A:251:ASN:ND2	1:A:251:ASN:O	2.38	0.57
1:A:334:HIS:ND1	1:A:334:HIS:N	2.53	0.57
1:A:472:ARG:C	1:A:474:GLN:H	2.11	0.57
1:A:621:GLN:HA	1:A:637:ILE:HD11	1.85	0.57
2:B:65:LEU:O	2:B:67:HIS:N	2.37	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:646:TRP:CE3	2:B:723:ALA:HA	2.38	0.57
2:B:650:PHE:O	2:B:720:THR:HG22	2.04	0.57
7:G:61:ASN:C	7:G:64:VAL:HG22	2.29	0.57
14:1:188:ASN:HB3	14:1:190:GLY:C	2.29	0.57
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:HD13	1:A:534:LEU:N	2.20	0.57
1:A:743:ILE:HD12	1:A:743:ILE:N	2.20	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:421:HIS:NE2	18:B:1228:CLA:NB	2.53	0.57
2:B:713:PHE:O	2:B:715:VAL:N	2.38	0.57
2:B:717:TYR:O	2:B:717:TYR:CD1	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
1:A:80:SER:N	1:A:81:ALA:CA	2.67	0.57
1:A:243:PRO:O	1:A:244:LEU:C	2.48	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
18:A:1105:CLA:C2B	18:A:1107:CLA:H11	2.34	0.57
2:B:330:ILE:CG2	18:B:1202:CLA:CBC	2.82	0.57
2:B:594:TRP:O	2:B:595:HIS:C	2.45	0.57
2:B:686:PRO:HA	2:B:689:ASN:HB2	1.87	0.57
18:B:1238:CLA:HBA1	9:I:21:MET:HE1	1.87	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:C:48:CYS:HA	3:C:49:VAL:CG1	2.34	0.57
4:D:72:PRO:HB2	4:D:73:ASN:HA	0.72	0.57
4:D:111:TYR:CE2	4:D:115:LYS:HA	2.39	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
18:L:1502:CLA:H42	18:L:1504:CLA:CMA	2.35	0.57
15:2:86:GLU:HG2	17:4:184:GLN:NE2	2.20	0.57
15:2:159:LEU:O	15:2:162:LYS:CB	2.51	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
1:A:126:ILE:CG1	10:J:27:ILE:CG2	2.82	0.57
1:A:725:LEU:HD23	1:A:725:LEU:C	2.29	0.57
2:B:398:TYR:OH	2:B:409:ALA:HB2	2.05	0.57
18:B:1227:CLA:HMB2	18:B:1228:CLA:ND	2.20	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:C	4:D:58:PHE:HD1	2.12	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
17:4:59:LEU:C	17:4:62:GLU:CB	2.78	0.57
17:4:118:ASP:N	17:4:119:PRO:CD	2.67	0.57
1:A:569:ILE:HA	1:A:586:ARG:HH12	1.69	0.57
1:A:694:PHE:HE1	2:B:665:ILE:CD1	2.18	0.57
18:A:1115:CLA:HBB2	18:K:1141:CLA:C2B	2.34	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
2:B:551:LYS:HB2	4:D:141:VAL:C	2.29	0.57
2:B:646:TRP:O	2:B:650:PHE:HB3	2.05	0.57
2:B:678:LEU:C	2:B:678:LEU:CD2	2.77	0.57
18:B:9012:CLA:H41	18:B:9012:CLA:H72	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
7:G:20:ARG:C	7:G:23:PHE:HB3	2.29	0.57
9:I:6:SER:O	9:I:10:PRO:HD3	2.04	0.57
13:N:2:VAL:CG1	13:N:4:GLU:HB2	2.35	0.57
13:N:74:LYS:HG3	13:N:74:LYS:O	2.05	0.57
13:N:81:VAL:N	13:N:82:PHE:HD2	1.99	0.57
1:A:130:GLU:CD	1:A:130:GLU:H	2.12	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:415:ALA:O	1:A:416:ILE:HG12	2.05	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
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
2:B:450:GLU:CA	6:F:68:LEU:HD11	2.33	0.56
3:C:64:SER:C	3:C:65:VAL:HG22	2.29	0.56
4:D:57:ILE:HG13	4:D:67:ILE:CA	2.32	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
14:1:72:GLN:HE22	18:1:1013:CLA:C2D	2.16	0.56
15:2:20:ASP:CG	15:2:23:LEU:HD11	2.30	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: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:484:LEU:CD2	1:A:539:PHE:HE2	2.18	0.56
1:A:699:TYR:HE1	2:B:536:LYS:CE	2.17	0.56
2:B:487:ASN:C	2:B:489:GLY:H	2.13	0.56
3:C:12:ILE:CA	3:C:13:GLY:C	2.74	0.56
4:D:96:ILE:HG12	4:D:97:LYS:N	2.18	0.56
6:F:105:LEU:C	6:F:107:ALA:H	2.11	0.56
8:H:22:ASP:C	8:H:24:TYR:N	2.63	0.56
1:A:54:ILE:O	1:A:54:ILE:CG2	2.53	0.56
1:A:76:ARG:NH2	1:A:190:ALA:C	2.63	0.56
1:A:132:LEU:O	1:A:143:ILE:HB	2.05	0.56
1:A:370:ILE:HD13	18:A:1124:CLA:C2A	2.35	0.56
1:A:435:VAL:O	1:A:438:HIS:N	2.37	0.56
1:A:545:HIS:CD2	1:A:545:HIS:H	2.21	0.56
1:A:579:PHE:HE1	1:A:581:CYS:O	1.89	0.56
1:A:673:SER:OG	2:B:446:PHE:CE1	2.58	0.56
1:A:693:LEU:HD12	1:A:730:GLY:O	2.04	0.56
1:A:744:ALA:O	1:A:747:TRP:N	2.32	0.56
18:A:1140:CLA:H42	18:A:1140:CLA:C4C	2.34	0.56
2:B:50:HIS:HE1	18:B:1210:CLA:C3D	2.18	0.56
2:B:290:MET:CA	18:B:1218:CLA:HBC3	2.10	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:463:ILE:O	2:B:465:SER:N	2.38	0.56
2:B:506:ASN:C	2:B:508:LEU:H	2.12	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:530:THR:HG1	2:B:582:TRP:HB3	1.67	0.56
2:B:707:LEU:O	2:B:710:LEU:CA	2.53	0.56
3:C:17:CYS:HA	3:C:57:ALA:HA	1.88	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
6:F:110:ASP:C	6:F:112:LYS:H	2.12	0.56
6:F:144:LEU:HA	6:F:149:LEU:HD13	1.87	0.56
7:G:53:GLU:CD	7:G:53:GLU:H	2.13	0.56
12:L:124:LYS:O	12:L:124:LYS:HD3	2.05	0.56
14:1:108:VAL:O	14:1:109:GLU:OE2	2.24	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
1:A:80:SER:O	18:A:1109:CLA:C2A	2.53	0.56
1:A:197:GLN:NE2	1:A:352:THR:HG23	2.20	0.56
1:A:198:ASP:OD2	1:A:199:VAL:N	2.38	0.56
1:A:694:PHE:HE1	2:B:665:ILE:HD11	1.70	0.56
2:B:74:PHE:HB3	2:B:132:ASN:ND2	2.19	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
2:B:517:PHE:C	2:B:517:PHE:HD1	2.13	0.56
3:C:56:SER:O	3:C:57:ALA:HB3	2.04	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
14:1:15: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: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:458:PHE:CD1	18:B:9022:CLA:HMB2	2.41	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
2:B:53:GLN:O	2:B:56:ILE:N	2.38	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:442:VAL:O	2:B:443:MET:C	2.49	0.56
2:B:649:MET:HE3	2:B:719:PHE:CE1	2.41	0.56
2:B:672:GLN:NE2	3:C:79:LEU:HD22	2.20	0.56
18:B:1237:CLA:CGA	18:B:1237:CLA:C1A	2.84	0.56
3:C:48:CYS:CB	21:C:3102:SF4:S2	2.50	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:D:52:SER:CB	4:D:73:ASN:HD21	2.18	0.56
6:F:45:THR:C	6:F:47:GLU:N	2.62	0.56
6:F:81:GLY:CA	6:F:85:THR:H	2.18	0.56
6:F:130:LEU:O	6:F:132:ARG:N	2.38	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
14:1:40:LYS:NZ	14:1:41:GLU:HG3	2.19	0.56
1:A:71:LEU:HB2	1:A:193:LEU:HD22	1.88	0.56
1:A:152:ILE:O	1:A:155:ALA:HB3	2.06	0.56
1:A:551:VAL:HG23	1:A:551:VAL:O	2.06	0.56
1:A:690:LEU:N	1:A:690:LEU:CD1	2.68	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:304:ILE:CD1	18:B:1220:CLA:HED2	2.36	0.56
2:B:337:ALA:CB	18:B:1202:CLA:OBD	2.52	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:562:PRO:O	2:B:563:GLY:C	2.48	0.56
2:B:652:PHE:CZ	2:B:656:VAL:HG21	2.39	0.56
3:C:50:GLY:HA2	21:C:3102:SF4:S3	2.46	0.56
4:D:133:ASN:C	4:D:135:ARG:N	2.60	0.56
7:G:20:ARG:HH21	7:G:68:ILE:HG21	1.71	0.56
12:L:33:ILE:C	12:L:35:TRP:N	2.60	0.56
12:L:66:GLY:HA3	18:L:1503:CLA:C1B	2.32	0.56
16:3:200:ILE:O	16:3:204:VAL:N	2.35	0.56
17:4:81:GLU:O	17:4:84:PHE:CE1	2.59	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
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:603:PHE:CZ	1:A:735:VAL:HA	2.41	0.56
2:B:177:HIS:C	2:B:177:HIS:CD2	2.84	0.56
2:B:340:SER:C	2:B:342:GLY:H	2.14	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
5:E:40:ARG:C	5:E:42:GLU:H	2.13	0.56
7:G:91:ASN:N	7:G:93:TYR:H	2.04	0.56
12:L:53:GLY:C	12:L:55:GLU:N	2.59	0.56
14:1:180:HIS:O	14:1:181:LEU:C	2.48	0.56
1:A:51:THR:CG2	1:A:722:PRO:CA	2.63	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:O	2.18	0.56
2:B:83:HIS:CA	2:B:84:VAL:HG23	2.36	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
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
12:L:78:GLU:C	12:L:80:ALA:HA	2.31	0.56
1:A:78:VAL:O	1:A:82:HIS:HB2	2.06	0.56
1:A:161:GLU:O	1:A:163:GLN:N	2.35	0.56
1:A:210:LEU:HD22	18:A:1111:CLA:HHC	1.88	0.56
1:A:559:GLY:HA3	1:A:597:HIS:CD2	2.41	0.56
1:A:627:THR:OG1	1:A:635:THR:HB	2.06	0.56
1:A:692:PHE:CD2	19:A:5001:PQN:C1	2.89	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
18:B:1205:CLA:CAD	18:B:1224:CLA:HAA2	2.36	0.56
3:C:2:SER:O	3:C:3:HIS:ND1	2.39	0.56
3:C:73:THR:C	3:C:75:ARG:H	2.13	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
10:J:1:MET:C	10:J:2:ARG:HG3	2.30	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
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: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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:388:ALA:C	2:B:390:GLY:N	2.64	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:58:LEU:HD11	14:1:114:MET:HE3	1.88	0.56
15:2:19:LEU:HA	15:2:20:ASP:C	2.30	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:103:PHE:CB	1:A:140:PHE:HZ	2.19	0.55
1:A:204:ASN:CG	1:A:315:HIS:HA	2.31	0.55
1:A:305:ALA:CB	18:A:1115:CLA:HMA3	2.29	0.55
1:A:405:PHE:CD2	1:A:605:MET:HE1	2.41	0.55
1:A:658:TRP:HD1	2:B:625:TRP:CE2	2.13	0.55
2:B:37:ILE:HG23	2:B:41:ARG:HB3	1.89	0.55
2:B:53:GLN:C	2:B:55:ALA:H	2.14	0.55
2:B:65:LEU:O	2:B:66:PHE:C	2.48	0.55
2:B:620:LEU:O	2:B:625:TRP:N	2.31	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
13:N:16:LEU:HG	13:N:19:LYS:HZ1	1.70	0.55
13:N:22:LEU:C	13:N:24:THR:H	2.14	0.55
14:1:44:LEU:H	14:1:44:LEU:CD2	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:86:LEU:HD13	1:A:87:SER:N	2.21	0.55
1:A:90:PHE:O	1:A:92:TRP:C	2.49	0.55
1:A:113:PRO:HB3	1:A:384:TYR:CE2	2.41	0.55
1:A:360:ILE:HD11	18:A:1123:CLA:HMB3	1.88	0.55
1:A:458:PHE:CD1	18:B:9022:CLA:CMB	2.89	0.55
1:A:532:ILE:HG23	1:A:624:VAL:HG23	1.87	0.55
2:B:46:ILE:C	2:B:49:SER:HG	2.08	0.55
2:B:98:GLN:O	2:B:98:GLN:NE2	2.39	0.55
2:B:487:ASN:OD1	2:B:490:ARG:HG3	2.07	0.55
3:C:5:VAL:HG22	3:C:6:LYS:HG2	1.88	0.55
3:C:25:VAL:HA	3:C:44:ARG:HB2	1.87	0.55
13:N:81:VAL:HG23	13:N:82:PHE:CB	2.28	0.55
1:A:86:LEU:O	1:A:86:LEU:HD22	2.07	0.55
1:A:391:THR:HB	1:A:395:LEU:HD12	1.87	0.55
1:A:629:ASN:ND2	1:A:630:ASP:N	2.55	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:754:ILE:C	1:A:755:ILE:HG13	2.26	0.55
2:B:45:ASN:O	2:B:46:ILE:C	2.48	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
18:B:1215:CLA:HBB2	18:B:1215:CLA:H62	1.87	0.55
3:C:23:THR:O	3:C:25:VAL:HG23	2.06	0.55
6:F:108:ILE:O	6:F:108:ILE:HG22	2.06	0.55
18:I:1204:CLA:CBA	18:I:1204:CLA:CHA	2.81	0.55
18:4:1304:CLA:HBD	18:4:1304:CLA:CGA	2.37	0.55
1:A:195:TRP:CE3	18:A:1118:CLA:C3C	2.90	0.55
1:A:364:MET:C	1:A:366:GLY:N	2.62	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
1:A:567:ARG:HH12	4:D:37:LEU:HD21	1.70	0.55
1:A:733:VAL:C	1:A:735:VAL:N	2.61	0.55
2:B:64:ASN:O	2:B:68:VAL:HG12	2.05	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
18:B:1227:CLA:O1D	18:B:1227:CLA:OBD	2.23	0.55
18:B:1232:CLA:CMB	18:G:1233:CLA:C3B	2.83	0.55
5:E:62:ARG:HD3	5:E:63:TYR:CE1	2.41	0.55
12:L:36:TYR:C	12:L:38:SER:N	2.61	0.55
12:L:137:ALA:O	12:L:138:LYS:NZ	2.40	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: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
1:A:675:TYR:CZ	18:A:1106:CLA:HBC1	2.42	0.55
18:A:1106:CLA:O2D	18:A:1106:CLA:C2A	2.48	0.55
2:B:37:ILE:HG22	4:D:148:PHE:CE1	2.42	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
6:F:115:THR:C	6:F:117:LYS:N	2.65	0.55
7:G:95:PRO:C	7:G:97:PHE:N	2.49	0.55
8:H:41:GLU:OE1	8:H:41:GLU:CA	2.55	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
18:H:1501:CLA:HAA1	18:H:1505:CLA:C3C	2.36	0.55
15:2:190:ASP:C	15:2:192:LEU:HD23	2.32	0.55
1:A:578:ARG:HE	1:A:728:VAL:HG11	1.71	0.55
1:A:671:SER:C	1:A:673:SER:H	2.15	0.55
2:B:247:THR:O	2:B:248:GLN:O	2.25	0.55
2:B:532:LEU:CD1	2:B:533:ILE:N	2.55	0.55
2:B:593:TYR:HE1	18:B:1234:CLA:HAC2	1.67	0.55
2:B:659:THR:C	2:B:661:PHE:N	2.64	0.55
12:L:47:VAL:HG12	12:L:52:ARG:NH1	2.21	0.55
12:L:65:VAL:CG1	18:L:1503:CLA:HMA3	2.36	0.55
14:1:86:GLY:N	14:1:87:ASN:CB	2.69	0.55
15:2:23:LEU:HD12	15:2:25:GLY:O	2.02	0.55
1:A:205:HIS:O	1:A:209:GLY:CA	2.55	0.55
1:A:455:PHE:CD1	1:A:455:PHE:C	2.84	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:713:LYS:O	1:A:714:LEU:HB2	2.07	0.55
2:B:46:ILE:O	2:B:50:HIS:N	2.32	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:459:PHE:HB3	18:B:1234:CLA:H11	1.88	0.55
2:B:540:ASP:C	2:B:542:ARG:H	2.14	0.55
2:B:596:TRP:CD1	2:B:608:GLN:HE21	2.23	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
2:B:650:PHE:CD1	2:B:720:THR:HB	2.42	0.55
2:B:670:TYR:C	2:B:670:TYR:CD2	2.84	0.55
3:C:65:VAL:O	3:C:66:ARG:HG2	2.07	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
10:J:23:ALA:O	10:J:24:GLY:C	2.47	0.55
15:2:32:LEU:CA	15:2:33:GLY:C	2.67	0.55
16:3:109:ALA:O	16:3:111:ASN:N	2.40	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
2:B:117:TYR:HB3	2:B:370:ALA:CB	2.36	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:293:THR:HB	18:B:1209:CLA:HMA2	1.87	0.55
2:B:342:GLY:O	2:B:343:VAL:C	2.49	0.55
2:B:458:ILE:HG12	6:F:74:SER:HB2	1.85	0.55
2:B:478:LEU:HG	2:B:486:LEU:H	1.71	0.55
2:B:530:THR:O	2:B:530:THR:CG2	2.55	0.55
2:B:540:ASP:C	2:B:542:ARG:N	2.65	0.55
2:B:548:PRO:HG2	3:C:62:PHE:CG	2.42	0.55
2:B:652:PHE:HE1	18:B:1239:CLA:HMB1	1.69	0.55
2:B:672:GLN:HA	2:B:675:ILE:HG12	1.89	0.55
2:B:687:LEU:CD2	2:B:687:LEU:N	2.70	0.55
18:B:1208:CLA:H2	7:G:39:ASN:OD1	2.06	0.55
3:C:3:HIS:NE2	3:C:48:CYS:C	2.65	0.55
7:G:83:TYR:O	7:G:83:TYR:CG	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
15:2:185:GLY:O	15:2:186:THR:HB	2.06	0.55
17:4:61:PRO:HG3	17:4:71:ASN:OD1	2.06	0.55
17:4:105:ARG:HA	17:4:108:ASP:HB3	1.89	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:387:PHE:O	2:B:390:GLY:CA	2.55	0.55
2:B:388:ALA:C	2:B:390:GLY:H	2.14	0.55
2:B:411:MET:SD	18:B:1242:CLA:HMD2	2.47	0.55
2:B:433:THR:HG22	2:B:433:THR:O	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
18:B:1209:CLA:CHC	18:B:1217:CLA:HMD1	2.36	0.55
3:C:8:TYR:HA	4:D:132:LEU:HD13	1.88	0.55
5:E:83:ALA:O	5:E:84:LEU:HB2	2.07	0.55
6:F:148:GLU:C	6:F:149:LEU:HG	2.32	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
15:2:19:LEU:HA	15:2:20:ASP:CB	2.26	0.55
15:2:54:TRP:O	15:2:55:ALA:C	2.49	0.55
16:3:83:GLY:C	16:3:88:GLU:HA	2.31	0.55
1:A:88:ILE:HG22	1:A:89:ILE:N	2.21	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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: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
2:B:378:ILE:O	2:B:382:ILE:N	2.37	0.55
4:D:30:ALA:CA	12:L:13:PRO:HD3	2.36	0.55
7:G:81:VAL:CG1	7:G:83:TYR:CE1	2.89	0.55
7:G:83:TYR:CD2	7:G:83:TYR:C	2.84	0.55
9:I:25:PHE:N	9:I:26:LEU:CA	2.68	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
14:1:173:PRO:O	14:1:174:LEU:C	2.49	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: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
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
18:B:1218:CLA:HAA2	18:B:1218:CLA:HBD	1.88	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
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
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
17:4:137:ILE:CG2	17:4:141:LEU:HD23	2.35	0.54
18:4:1304:CLA:CAA	18:4:1304:CLA:H2	2.31	0.54
1:A:86:LEU:HD21	1:A:90:PHE:CD2	2.41	0.54
1:A:187:HIS:CE1	18:A:1109:CLA:C3C	2.90	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:146:SER:O	2:B:150:LEU:HD12	2.07	0.54
2:B:532:LEU:HD12	2:B:532:LEU:C	2.31	0.54
9:I:11:LEU:O	9:I:13:GLY:N	2.40	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
14:1:180:HIS:C	14:1:182:ALA:HB3	2.33	0.54
17:4:136:GLY:HA3	17:4:139:ASN:C	2.33	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:475:ASP:C	1:A:476:MET:SD	2.90	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
1:A:687:ALA:C	1:A:689:SER:N	2.60	0.54
2:B:304:ILE:O	2:B:308:HIS:HB2	2.02	0.54
2:B:517:PHE:C	2:B:517:PHE:CD1	2.83	0.54
2:B:593:TYR:CD1	2:B:593:TYR:C	2.86	0.54
18:B:1203:CLA:H2	18:B:1226:CLA:C4D	2.37	0.54
18:B:1209:CLA:CGA	18:B:1209:CLA:C5	2.85	0.54
18:B:1214:CLA:HBA1	18:B:1214:CLA:HBD	1.88	0.54
4:D:102:ARG:O	4:D:109:VAL:N	2.41	0.54
4:D:109:VAL:HB	4:D:110:GLN:CA	2.35	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
12:L:94:ILE:C	12:L:96:SER:N	2.63	0.54
13:N:71:GLY:CA	13:N:76:LYS:HB3	2.38	0.54
17:4:142:ASN:HD21	17:4:145:PRO:HG3	1.70	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:416:ILE:C	1:A:420:ARG:HB2	2.33	0.54
1:A:450:CYS:CB	1:A:551:VAL:CG1	2.69	0.54
1:A:668:TYR:CD1	2:B:445:ALA:HA	2.43	0.54
1:A:742:GLY:CA	18:A:9011:CLA:O1D	2.53	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
2:B:98:GLN:OE1	8:H:78:PRO:C	2.50	0.54
2:B:246:THR:HG22	2:B:247:THR:N	2.21	0.54
2:B:293:THR:HB	18:B:1209:CLA:CMA	2.38	0.54
2:B:439:HIS:CD2	18:B:1230:CLA:C1C	2.89	0.54
2:B:594:TRP:CE2	2:B:598:HIS:NE2	2.75	0.54
2:B:597:LYS:O	2:B:599:ILE:N	2.40	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:C:81:TYR:HB3	4:D:37:LEU:HD12	1.89	0.54
7:G:16:LEU:HB3	7:G:17:PHE:CE1	2.41	0.54
18:L:1502:CLA:H42	18:L:1504:CLA:HMA1	1.89	0.54
13:N:19:LYS:CD	13:N:20:LYS:N	2.69	0.54
13:N:71:GLY:HA2	13:N:76:LYS:HB2	1.90	0.54
13:N:72:LYS:HD2	13:N:72:LYS:O	2.07	0.54
13:N:76:LYS:O	13:N:77:CYS:SG	2.66	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:149:PHE:O	1:A:153:TRP:CD2	2.60	0.54
1:A:599:PHE:CZ	1:A:693:LEU:HD21	2.40	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:652:PHE:O	2:B:653:GLY:C	2.51	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
1:A:78:VAL:HG21	1:A:354:TRP:CE2	2.43	0.54
1:A:371:VAL:HG23	1:A:372:VAL:N	2.23	0.54
1:A:401:TRP:HH2	1:A:610:SER:HB2	1.72	0.54
1:A:451:ILE:O	1:A:455:PHE:HB3	2.07	0.54
2:B:141:PHE:C	2:B:143:LEU:H	2.14	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
4:D:46:TYR:CD2	4:D:80:LYS:HB3	2.43	0.54
6:F:26:GLN:C	6:F:28:SER:N	2.65	0.54
8:H:44:ALA:H	8:H:45:ALA:HB2	1.72	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
18:A:1106:CLA:CHC	18:A:1107:CLA:HMD2	2.38	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:125:TYR:CE1	2:B:359:ALA:HB2	2.41	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
6:F:127:SER:C	6:F:131:PHE:HB2	2.33	0.54
10:J:4:PHE:CB	10:J:5:LYS:O	2.56	0.54
10:J:26:LEU:O	10:J:29:ILE:CG2	2.56	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
13:N:69:CYS:HB3	13:N:72:LYS:CG	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
16:3:201:GLN:HA	16:3:204:VAL:HG22	1.90	0.54
17:4:60:LEU:O	17:4:61:PRO:C	2.50	0.54
1:A:427:ARG:O	1:A:430:ASP:N	2.37	0.54
18:A:1103:CLA:NB	18:A:1128:CLA:CMB	2.71	0.54
2:B:311:PRO:HG2	18:B:1220:CLA:HHB	1.89	0.54
2:B:374:HIS:C	2:B:374:HIS:ND1	2.66	0.54
2:B:388:ALA:O	2:B:391:PRO:CD	2.56	0.54
2:B:630:GLN:OE1	2:B:630:GLN:HA	2.07	0.54
6:F:42:ILE:CG1	6:F:43:LYS:H	2.13	0.54
8:H:64:LEU:O	8:H:65:LEU:C	2.50	0.54
14:1:110:HIS:NE2	18:1:1012:CLA:NB	2.56	0.54
15:2:44:ASN:C	15:2:46:GLN:H	2.16	0.54
17:4:158:ARG:NH2	17:4:161:MET:SD	2.79	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
1:A:615:HIS:C	1:A:615:HIS:HD2	2.13	0.54
2:B:518:LEU:HD21	2:B:614:THR:HG22	1.85	0.54
2:B:584:LEU:HD23	2:B:587:ILE:HD12	1.90	0.54
18:H:1501:CLA:CMA	12:L:58:LEU:HB3	2.35	0.54
20:I:6018:BCR:H383	20:L:6020:BCR:H342	1.85	0.54
15:2:191:ASN:N	15:2:192:LEU:HB2	2.19	0.54
16:3:67:MET:HE2	16:3:71:ALA:N	2.22	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
1:A:126:ILE:CG1	10:J:27:ILE:HG21	2.38	0.54
1:A:133:ASN:HA	1:A:143:ILE:N	2.23	0.54
1:A:386:ALA:HB1	1:A:528:ALA:HB1	1.90	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
1:A:737:HIS:CE1	18:A:1140:CLA:NA	2.76	0.54
2:B:91:ILE:HG12	2:B:114:ASN:ND2	2.23	0.54
2:B:93:ASP:OD2	18:B:1206:CLA:NA	2.41	0.54
2:B:286:ILE:C	18:B:1218:CLA:HMC2	2.32	0.54
2:B:391:PRO:HG2	2:B:555:TYR:CE1	2.43	0.54
2:B:457:PRO:HB3	18:B:1235:CLA:OBD	2.08	0.54
2:B:693:TRP:HD1	2:B:695:ASP:O	1.87	0.54
3:C:7:ILE:C	3:C:8:TYR:CG	2.86	0.54
6:F:49:THR:O	6:F:52:ARG:C	2.51	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
14:1:40:LYS:C	14:1:42:SER:H	2.13	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
17:4:59:LEU:C	17:4:62:GLU:HB3	2.28	0.54
1:A:109:TRP:HE1	1:A:113:PRO:CA	2.08	0.53
1:A:223:VAL:HG23	1:A:224:HIS:N	2.23	0.53
1:A:369:THR:CB	18:A:1127:CLA:C3C	2.86	0.53
1:A:408:VAL:O	1:A:408:VAL:HG12	2.08	0.53
1:A:492:ILE:H	1:A:493:GLN:HB2	1.66	0.53
2:B:284:PHE:C	2:B:286:ILE:N	2.67	0.53
2:B:304:ILE:CD1	18:B:1216:CLA:O1D	2.56	0.53
2:B:402:GLN:C	2:B:403:ASN:HD22	2.16	0.53
2:B:448:THR:CB	2:B:451:LYS:HE2	2.37	0.53
2:B:524:ALA:HB2	18:B:1235:CLA:HMA3	1.90	0.53
2:B:525:LEU:C	2:B:525:LEU:HD12	2.33	0.53
2:B:641:ASN:O	2:B:643:LEU:N	2.41	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
14:1:140:LEU:O	14:1:142:GLU:N	2.40	0.53
1:A:58:HIS:CE1	18:A:1101:CLA:C1C	2.90	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: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: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
2:B:650:PHE:CE1	2:B:720:THR:HB	2.43	0.53
2:B:674:LEU:O	2:B:678:LEU:CD1	2.56	0.53
18:B:1228:CLA:C2B	20:F:6016:BCR:H341	2.38	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
6:F:27:ALA:C	6:F:29:LEU:H	2.16	0.53
14:1:156:LEU:HD13	14:1:159:VAL:HB	1.91	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:283:PHE:CG	1:A:301:HIS:HE1	2.26	0.53
1:A:437:ARG:C	4:D:32:SER:OG	2.50	0.53
1:A:442:ILE:O	1:A:443:ILE:C	2.52	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:85:ALA:O	4:D:89:ARG:N	2.36	0.53
4:D:154:TYR:N	4:D:155:ASP:HA	2.22	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:N	8:H:43:PHE:CD1	2.72	0.53
8:H:45:ALA:O	8:H:47:PHE:HB2	2.08	0.53
9:I:1:MET:N	9:I:1:MET:HE3	2.24	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
15:2:92:THR:C	15:2:94:LEU:HB2	2.33	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:434:ARG:HH21	1:A:438:HIS:CG	2.26	0.53
1:A:525:ASN:C	1:A:627:THR:O	2.51	0.53
1:A:608:SER:O	1:A:611:VAL:O	2.27	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:547:MET:HE3	2:B:557:PHE:CE1	2.44	0.53
2:B:558:PRO:HG3	2:B:703:VAL:HB	1.90	0.53
18:B:9012:CLA:O2D	18:B:9012:CLA:OBD	2.24	0.53
18:B:1235:CLA:CGA	18:B:1235:CLA:CHA	2.86	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
12:L:27:VAL:O	12:L:27:VAL:CG1	2.55	0.53
14:1:15:ASP:O	14:1:18:ALA:HA	2.07	0.53
1:A:62:HIS:HB2	18:A:1128:CLA:HAA2	1.90	0.53
1:A:63:ASP:OD2	1:A:420:ARG:NH2	2.41	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
2:B:193:HIS:C	2:B:195:VAL:H	2.17	0.53
2:B:273:VAL:O	2:B:273:VAL:HG12	2.08	0.53
2:B:440:ASN:CB	2:B:614:THR:O	2.56	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:704:GLN:C	2:B:706:ARG:N	2.48	0.53
18:B:1202:CLA:HBB2	18:B:1203:CLA:CGA	2.37	0.53
3:C:55:GLU:CD	3:C:55:GLU:C	2.76	0.53
5:E:51:SER:C	5:E:53:VAL:H	2.16	0.53
6:F:49:THR:C	6:F:56:TYR:OH	2.51	0.53
6:F:105:LEU:C	6:F:107:ALA:N	2.67	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
13:N:47:THR:CB	13:N:50:GLN:HB2	2.38	0.53
14:1:15:ASP:O	14:1:18:ALA:CB	2.57	0.53
14:1:152:ARG:O	14:1:154:ALA:N	2.42	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
17:4:194:ILE:O	17:4:195:VAL:C	2.51	0.53
1:A:115:HIS:O	1:A:116:ILE:CB	2.57	0.53
1:A:120:ALA:HB3	18:A:1106:CLA:HED3	1.91	0.53
1:A:232:PHE:CD1	1:A:232:PHE:C	2.87	0.53
1:A:593:SER:O	1:A:597:HIS:N	2.39	0.53
1:A:668:TYR:HB3	2:B:445:ALA:HA	1.91	0.53
1:A:737:HIS:HE1	18:A:1140:CLA:NA	2.07	0.53
18:A:1137:CLA:CBA	18:A:1137:CLA:CBD	2.86	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
18:B:1227:CLA:CMB	18:B:1228:CLA:CHA	2.87	0.53
18:B:1232:CLA:HMB2	18:G:1233:CLA:C3B	2.38	0.53
18:B:1237:CLA:H42	20:L:6020:BCR:H361	1.90	0.53
18:H:1501:CLA:H62	18:H:1501:CLA:C1D	2.39	0.53
14:1:81:GLN:C	14:1:83:THR:HA	2.33	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
1:A:50:THR:O	1:A:51:THR:O	2.27	0.53
1:A:74:ILE:O	1:A:78:VAL:HG23	2.08	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:75:SER:CA	1:A:354:TRP:CZ2	2.73	0.53
1:A:80:SER:HA	1:A:83:PHE:CD1	2.43	0.53
1:A:405:PHE:N	1:A:605:MET:SD	2.82	0.53
1:A:714:LEU:CD2	6:F:149:LEU:HD22	2.39	0.53
2:B:186:SER:HB3	18:B:1215:CLA:HBC1	1.91	0.53
2:B:284:PHE:CE1	18:B:1216:CLA:CAB	2.91	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
6:F:111:GLU:O	6:F:111:GLU:CD	2.52	0.53
6:F:130:LEU:CD1	6:F:130:LEU:H	2.20	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
10:J:25:LEU:O	10:J:26:LEU:C	2.52	0.53
15:2:185:GLY:O	15:2:187:GLY:CA	2.44	0.53
1:A:106:TYR:CZ	1:A:153:TRP:CD1	2.96	0.53
1:A:196:PHE:C	1:A:196:PHE:HD2	2.17	0.53
2:B:26:ALA:O	2:B:28:ALA:N	2.41	0.53
2:B:672:GLN:CD	2:B:699:ALA:H	2.16	0.53
3:C:52:LYS:HZ3	3:C:66:ARG:HH11	1.55	0.53
3:C:60:THR:N	5:E:80:ASN:ND2	2.43	0.53
4:D:27:PRO:HG2	4:D:75:LEU:HB2	1.88	0.53
4:D:28:ILE:HA	12:L:19:PHE:CZ	2.43	0.53
4:D:67:ILE:HG12	4:D:68:MET:O	2.09	0.53
5:E:51:SER:CB	5:E:69:PHE:HD2	2.22	0.53
6:F:25:LEU:C	6:F:25:LEU:HD12	2.33	0.53
6:F:115:THR:C	6:F:118:GLU:HB2	2.33	0.53
10:J:33:PHE:O	10:J:35:ASP:O	2.26	0.53
14:1:57:ILE:O	14:1:57:ILE:HG13	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:347:TYR:HA	1:A:348:GLU:OE2	2.08	0.53
1:A:657:LEU:C	1:A:659:ALA:N	2.66	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
2:B:594:TRP:CD2	2:B:598:HIS:NE2	2.77	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
12:L:103:GLY:C	12:L:104:ILE:HG13	2.34	0.53
14:1:181:LEU:N	14:1:182:ALA:HB3	2.24	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
15:2:162:LYS:HZ1	15:2:163:GLU:HB2	1.74	0.53
16:3:54:TRP:HA	16:3:54:TRP:HE3	1.74	0.53
16:3:118:GLU:O	16:3:122:MET:HB2	2.09	0.53
17:4:99:HIS:HE1	17:4:103:ILE:HG13	1.74	0.53
1:A:228:PRO:HA	1:A:231:GLN:HB3	1.91	0.53
1:A:323:ILE:HG12	18:A:1108:CLA:HMA2	1.91	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
2:B:364:ASP:C	2:B:365:PHE:CG	2.86	0.53
2:B:423:SER:HG	2:B:424:TRP:H	1.56	0.53
2:B:557:PHE:H	2:B:557:PHE:HD2	1.57	0.53
2:B:627:ASN:OD1	2:B:732:LYS:HD2	2.09	0.53
3:C:70:TRP:O	3:C:71:HIS:C	2.51	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
12:L:136:TRP:C	12:L:136:TRP:CD1	2.86	0.53
13:N:74:LYS:CG	13:N:74:LYS:O	2.57	0.53
16:3:132:ASP:O	16:3:139:MET:HB3	2.09	0.53
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:602:LEU:HD21	18:A:1128:CLA:HBC1	1.91	0.52
1:A:664:VAL:HG21	1:A:675:TYR:O	2.09	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
2:B:702:ILE:HD12	2:B:702:ILE:C	2.32	0.52
18:B:1208:CLA:HAA1	18:B:1208:CLA:H12	1.91	0.52
3:C:22:PRO:HG3	3:C:53:ARG:HE	1.74	0.52
3:C:42:ALA:HB1	3:C:44:ARG:C	2.33	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
13:N:7:LEU:O	13:N:12:THR:OG1	2.27	0.52
13:N:29:PHE:CG	16:3:107:TYR:HE2	2.27	0.52
15:2:17:GLU:CD	15:2:17:GLU:C	2.76	0.52
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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
16:3:84:LEU:H	16:3:88:GLU:CD	2.17	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:497:ALA:CB	1:A:516:GLY:HA2	2.38	0.52
1:A:500:PRO:HD2	1:A:501:GLY:H	1.74	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: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:115:ASN:ND2	2:B:117:TYR:CZ	2.78	0.52
2:B:201:GLY:O	2:B:204:GLY:HA2	2.09	0.52
2:B:555:TYR:CD1	2:B:572:ALA:HB3	2.45	0.52
2:B:593:TYR:HD1	2:B:593:TYR:C	2.17	0.52
2:B:724:PHE:O	2:B:727:ALA:N	2.41	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
4:D:50:TRP:O	4:D:73:ASN:CG	2.52	0.52
4:D:76:LYS:C	4:D:77:LEU:HG	2.35	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
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:217:SER:O	18:A:1148:CLA:C2A	2.57	0.52
1:A:274:TRP:HE1	18:A:1115:CLA:CED	2.22	0.52
1:A:363:ALA:O	1:A:366:GLY:HA3	2.10	0.52
1:A:599:PHE:CD2	1:A:731:ARG:O	2.63	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
2:B:104:PHE:HA	2:B:106:ARG:HD3	1.91	0.52
2:B:186:SER:CB	18:B:1215:CLA:HBC1	2.38	0.52
2:B:311:PRO:O	18:B:1220:CLA:HMB3	2.09	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
2:B:663:PHE:HZ	18:B:1239:CLA:CHD	2.23	0.52
6:F:126:ALA:N	6:F:130:LEU:HD13	2.15	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:123:VAL:H	1:A:133:ASN:ND2	1.86	0.52
1:A:173:VAL:O	1:A:175:ALA:C	2.51	0.52
1:A:173:VAL:O	1:A:176:GLY:CA	2.54	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
2:B:194:LEU:CD1	18:B:1215:CLA:HED3	2.39	0.52
3:C:49:VAL:C	3:C:51:CYS:N	2.66	0.52
4:D:146:VAL:O	4:D:148:PHE:N	2.43	0.52
5:E:44:TYR:CZ	5:E:73:ASN:HA	2.45	0.52
5:E:45:TRP:O	5:E:45:TRP:CD2	2.62	0.52
6:F:79:HIS:C	6:F:81:GLY:N	2.61	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: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
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:118:LEU:C	12:L:120:LEU:HA	2.30	0.52
12:L:137:ALA:C	12:L:138:LYS:NZ	2.65	0.52
13:N:81:VAL:O	13:N:83:TRP:NE1	2.43	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
17:4:179:PHE:N	17:4:179:PHE:CD1	2.78	0.52
1:A:64:PHE:C	1:A:420:ARG:NH2	2.67	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:397:THR:O	1:A:399:HIS:C	2.51	0.52
1:A:540:LEU:O	1:A:541:VAL:C	2.50	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
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
7:G:21:PHE:N	7:G:23:PHE:HB3	2.21	0.52
12:L:33:ILE:HG23	12:L:35:TRP:CB	2.28	0.52
12:L:111:GLU:OE2	12:L:138:LYS:HE3	2.09	0.52
13:N:75:TYR:CD2	13:N:76:LYS:HG2	2.44	0.52
16:3:140:GLY:H	16:3:141:LYS:CB	2.22	0.52
1:A:326:GLY:O	1:A:328:LYS:N	2.42	0.52
1:A:349:ILE:HA	1:A:352:THR:HG1	1.72	0.52
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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
2:B:48:ALA:O	2:B:49:SER:C	2.53	0.52
2:B:61:THR:O	2:B:65:LEU:HB2	2.10	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
3:C:49:VAL:HA	3:C:76:SER:HB3	1.90	0.52
3:C:72:GLU:CD	3:C:77:MET:HG3	2.33	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
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
13:N:35:VAL:O	13:N:35:VAL:HG12	2.08	0.52
14:1:40:LYS:HZ2	14:1:41:GLU:HG3	1.73	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
17:4:40: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
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
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:586:ARG:HA	3:C:76:SER:O	2.09	0.52
1:A:691:MET:O	1:A:695:SER:HB2	2.09	0.52
2:B:35:ASP:HB3	4:D:154:TYR:CE1	2.44	0.52
2:B:68:VAL:C	2:B:71:GLN:O	2.52	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:392:ILE:CG2	2:B:393:PHE:N	2.72	0.52
2:B:411:MET:HE1	2:B:414:HIS:HE1	1.75	0.52
2:B:551:LYS:CB	4:D:141:VAL:O	2.44	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
2:B:717:TYR:CD1	2:B:717:TYR:C	2.87	0.52
18:B:1209:CLA:O2A	18:B:1209:CLA:C4A	2.58	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:F:130:LEU:CD1	6:F:130:LEU:N	2.69	0.52
7:G:62:ASP:N	7:G:63:PRO:HD2	2.25	0.52
13:N:58:VAL:CA	16:3:86:PRO:O	2.58	0.52
14:1:54:VAL:O	14:1:57:ILE:HG23	2.09	0.52
15:2:28:GLY:C	15:2:29:PHE:CD1	2.80	0.52
16:3:82:ALA:CB	16:3:83:GLY:C	2.82	0.52
1:A:110:LEU:O	1:A:113:PRO:CD	2.52	0.52
1:A:141:ARG:NH1	1:A:141:ARG:HB3	2.13	0.52
1:A:407:ILE:C	1:A:407:ILE:HD13	2.34	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
2:B:92:TRP:CD1	9:I:9:VAL:CG1	2.90	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
18:B:1221:CLA:HED3	18:B:1221:CLA:OBD	2.10	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
9:I:26:LEU:O	9:I:28:VAL:N	2.43	0.52
12:L:136:TRP:CD1	12:L:137:ALA:N	2.77	0.52
13:N:21:ARG:C	13:N:23:ALA:H	2.18	0.52
13:N:65:LEU:O	13:N:68:GLU:CG	2.55	0.52
14:1:63:LEU:HD11	14:1:68:TRP:NE1	2.24	0.52
1:A:229:ILE:HA	1:A:232:PHE:CZ	2.45	0.52
1:A:680:LEU:C	1:A:682:ALA:H	2.18	0.52
1:A:733:VAL:HG23	18:A:1140:CLA:O1D	2.10	0.52
18:A:1137:CLA:HBA1	18:A:1137:CLA:CHA	2.40	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
2:B:693:TRP:HB3	18:B:1238:CLA:CMD	2.36	0.52
7:G:78:GLY:O	7:G:79:HIS:O	2.28	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
16:3:138:SER:C	16:3:141:LYS:HB3	2.35	0.52
17:4:42:GLN:OE1	17:4:120:ILE:CG2	2.58	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
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
19:A:5001:PQN:H243	19:A:5001:PQN:C20	2.32	0.52
2:B:323:TYR:C	2:B:323:TYR:HD1	2.18	0.52
2:B:323:TYR:O	2:B:325:THR:N	2.43	0.52
2:B:536:LYS:O	2:B:537:GLY:C	2.53	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
7:G:68:ILE:HG13	7:G:69:VAL:HG13	1.91	0.52
18:G:1233:CLA:HBC2	18:G:1233:CLA:CHD	2.41	0.52
12:L:13:PRO:CG	12:L:18:PRO:HA	2.40	0.52
12:L:97:MET:O	12:L:100:THR:HG23	2.10	0.52
12:L:165:TYR:CE1	18:L:1503:CLA:CBD	2.89	0.52
14:1:146:LYS:HA	14:1:149:LYS:HG2	1.90	0.52
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
2:B:301:ILE:HG22	2:B:302:LYS:N	2.25	0.51
2:B:302:LYS:CE	2:B:302:LYS:CA	2.85	0.51
2:B:439:HIS:HB2	2:B:443:MET:HE2	1.92	0.51
2:B:485:ALA:CA	18:B:1232:CLA:HMA2	2.33	0.51
18:B:1209:CLA:H51	18:B:1209:CLA:CGA	2.36	0.51
3:C:3:HIS:CE1	3:C:48:CYS:O	2.58	0.51
3:C:12:ILE:CD1	21:C:3103:SF4:S4	2.98	0.51
4:D:72:PRO:CB	4:D:73:ASN:CA	2.51	0.51
6:F:29:LEU:O	6:F:31:LEU:O	2.27	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
13:N:29:PHE:O	13:N:33:TYR:N	2.43	0.51
14:1:8:GLU:C	17:4:110:LYS:HZ3	2.17	0.51
15:2:66:GLU:C	15:2:68:LEU:H	2.18	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:80:SER:H	1:A:81:ALA:CA	2.21	0.51
1:A:195:TRP:HZ3	18:A:1118:CLA:C2C	2.22	0.51
1:A:224:HIS:HB3	1:A:248:PHE:CE2	2.45	0.51
1:A:369:THR:CG2	1:A:402:ILE:O	2.58	0.51
1:A:382:TYR:CD1	1:A:382:TYR:N	2.76	0.51
1:A:689:SER:HB2	1:A:738:TYR:N	2.26	0.51
18:A:1119:CLA:H2	18:A:1123:CLA:HMB2	1.90	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
18:A:1126:CLA:H41	18:A:1126:CLA:H93	1.92	0.51
2:B:194:LEU:O	2:B:274:ALA:CB	2.58	0.51
2:B:330:ILE:HG22	18:B:1202:CLA:HBC1	1.91	0.51
2:B:587:ILE:C	2:B:589:TRP:N	2.66	0.51
18:B:1205:CLA:H51	18:B:1205:CLA:CBB	2.40	0.51
6:F:65:SER:O	6:F:66:ASP:CB	2.56	0.51
6:F:121:ILE:H	10:J:9:SER:CB	2.22	0.51
6:F:144:LEU:HD11	20:F:6016:BCR:H333	1.87	0.51
7:G:18:LEU:O	7:G:20:ARG:N	2.44	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:93:LEU:O	1:A:96:MET:SD	2.68	0.51
1:A:134:GLY:H	1:A:142:GLY:C	2.18	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
2:B:49:SER:HG	2:B:50:HIS:N	2.07	0.51
2:B:135:LEU:C	2:B:137:THR:N	2.68	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:521:HIS:O	2:B:522:ALA:C	2.53	0.51
18:B:1208:CLA:HAA1	18:B:1208:CLA:HBD	1.93	0.51
8:H:24:TYR:CB	8:H:25:GLY:CA	2.88	0.51
12:L:148:VAL:O	12:L:149:SER:CB	2.57	0.51
13:N:15:GLU:C	13:N:17:ASN:H	2.19	0.51
13:N:42:PHE:O	13:N:45:ASN:N	2.43	0.51
14:1:70:LYS:NZ	18:1:1013:CLA:CHD	2.73	0.51
14:1:90:PRO:CG	14:1:92:GLY:HA2	2.39	0.51
1:A:401:TRP:CZ2	1:A:610:SER:HB2	2.45	0.51
18:A:1110:CLA:C2D	18:A:1146:CLA:C3C	2.88	0.51
2:B:53:GLN:O	2:B:54:LEU:C	2.53	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:510:LEU:CD1	18:B:1234:CLA:HMD3	2.40	0.51
2:B:651:LEU:O	18:B:9022:CLA:HBA1	2.10	0.51
18:B:1216:CLA:CAA	18:B:1221:CLA:HBB2	2.37	0.51
18:B:1217:CLA:HMA3	7:G:21:PHE:HD2	1.63	0.51
8:H:65:LEU:O	8:H:66:THR:C	2.53	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
14:1:51:MET:SD	14:1:150:ASN:HB3	2.50	0.51
16:3:67:MET:CE	16:3:70:ALA:HB3	2.40	0.51
16:3:134:TYR:O	16:3:135:ASN:CB	2.59	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:504:ALA:HB2	18:A:1134:CLA:C1B	2.41	0.51
1:A:512:SER:O	1:A:512:SER:OG	2.26	0.51
1:A:558:LYS:NZ	1:A:597:HIS:CE1	2.78	0.51
1:A:562:PHE:CZ	2:B:677:THR:CG2	2.92	0.51
1:A:686:TRP:CZ3	18:A:9011:CLA:HMA3	2.45	0.51
1:A:750:PHE:O	1:A:750:PHE:CD1	2.63	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:687:LEU:N	2:B:687:LEU:HD22	2.26	0.51
18:B:1220:CLA:CHC	18:B:1242:CLA:HBD	2.40	0.51
4:D:102:ARG:HB3	4:D:110:GLN:HB2	1.92	0.51
18:F:1139:CLA:O2D	18:F:1139:CLA:OBD	2.27	0.51
12:L:99:LEU:HA	12:L:102:TYR:HB2	1.93	0.51
12:L:136:TRP:HD1	12:L:137:ALA:N	2.09	0.51
18:L:1503:CLA:CGA	18:L:1503:CLA:O2D	2.58	0.51
13:N:72:LYS:N	13:N:75:TYR:O	2.43	0.51
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:84:GLY:O	1:A:85:GLN:C	2.52	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
1:A:680:LEU:HD23	18:B:9012:CLA:H2	1.92	0.51
1:A:740:LEU:C	1:A:743:ILE:HD13	2.36	0.51
2:B:214:ASP:C	2:B:214:ASP:OD2	2.54	0.51
2:B:452:GLN:HG3	2:B:453:ILE:N	2.24	0.51
2:B:510:LEU:HD11	18:B:1234:CLA:HHD	1.92	0.51
2:B:680:TRP:CD1	4:D:37:LEU:HD11	2.46	0.51
6:F:88:ILE:O	6:F:89:LEU:C	2.53	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
13:N:69:CYS:SG	13:N:72:LYS:C	2.94	0.51
15:2:191:ASN:CA	15:2:192:LEU:CB	2.60	0.51
1:A:130:GLU:C	1:A:132:LEU:N	2.67	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:150:PHE:CD1	1:A:153:TRP:HZ2	2.28	0.51
1:A:311:LEU:HD21	18:A:1108:CLA:HMC3	1.92	0.51
1:A:393:LEU:HA	1:A:616:PHE:CZ	2.45	0.51
1:A:737:HIS:O	1:A:738:TYR:C	2.53	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
13:N:58:VAL:HG12	16:3:86:PRO:HB3	1.92	0.51
14:1:45:ILE:C	14:1:47:CYS:H	2.19	0.51
15:2:34:LEU:N	15:2:34:LEU:HD23	2.24	0.51
1:A:55:TRP:N	1:A:55:TRP:CD1	2.78	0.51
1:A:86:LEU:HD22	1:A:86:LEU:C	2.36	0.51
1:A:151:GLN:OE1	1:A:384:TYR:HB2	2.10	0.51
1:A:187:HIS:NE2	18:A:1109:CLA:C2C	2.74	0.51
1:A:301:HIS:C	1:A:301:HIS:HD2	2.19	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
2:B:98:GLN:O	2:B:100:ALA:N	2.44	0.51
2:B:257:ILE:HD13	18:B:1214:CLA:HMB3	1.92	0.51
2:B:393:PHE:CE2	2:B:398:TYR:CD1	2.98	0.51
2:B:571:SER:CB	2:B:574:ASP:H	2.20	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
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
16:3:81:LYS:HA	16:3:82:ALA:C	2.34	0.51
1:A:78:VAL:O	1:A:82:HIS:CG	2.64	0.51
1:A:112:ASP:O	1:A:112:ASP:OD2	2.29	0.51
1:A:210:LEU:HD13	18:A:1111:CLA:C3B	2.41	0.51
1:A:555:ILE:N	1:A:556:LEU:CB	2.30	0.51
2:B:192:GLY:C	2:B:195:VAL:HB	2.36	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
6:F:16:LYS:O	6:F:17:ARG:C	2.50	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
15:2:27:PHE:CD1	15:2:28:GLY:HA2	2.46	0.51
16:3:54:TRP:HA	16:3:54:TRP:CE3	2.45	0.51
16:3:61:ILE:C	16:3:64:ARG:HB3	2.36	0.51
17:4:114:SER:O	17:4:115:VAL:O	2.28	0.51
1:A:90:PHE:O	1:A:91:LEU:C	2.54	0.51
1:A:93:LEU:O	1:A:95:GLY:N	2.43	0.51
1:A:280:PHE:HD2	1:A:280:PHE:H	1.57	0.51
1:A:452:PHE:HD2	1:A:453:LEU:N	2.07	0.51
1:A:688:PHE:CD1	1:A:737:HIS:HD2	2.28	0.51
2:B:120:VAL:C	2:B:122:GLN:N	2.69	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:496:GLY:C	2:B:498:LEU:N	2.69	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
6:F:130:LEU:C	6:F:132:ARG:H	2.19	0.51
6:F:136:TRP:CB	6:F:137:PRO:HD3	2.37	0.51
6:F:141:TYR:C	6:F:143:GLU:N	2.69	0.51
7:G:78:GLY:C	7:G:79:HIS:O	2.53	0.51
7:G:85:ILE:CA	7:G:86:LEU:C	2.77	0.51
10:J:9:SER:HG	10:J:10:VAL:N	2.08	0.51
12:L:123:ARG:C	12:L:125:LYS:H	2.16	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:99:HIS:HD1	1:A:103:PHE:HZ	1.57	0.50
1:A:304:LEU:C	1:A:307:ALA:HB3	2.36	0.50
1:A:397:THR:HG21	1:A:750:PHE:CZ	2.46	0.50
1:A:434:ARG:CD	18:A:1129:CLA:OBD	2.59	0.50
1:A:558:LYS:HZ3	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
2:B:257:ILE:HA	2:B:272:ASP:CG	2.35	0.50
2:B:703:VAL:HA	2:B:706:ARG:CG	2.41	0.50
18:B:1203:CLA:HBA2	18:B:1203:CLA:HBD	1.93	0.50
18:B:1225:CLA:HAA2	18:B:1225:CLA:HBD	1.92	0.50
4:D:55:GLU:HB3	4:D:67:ILE:HG13	1.93	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:D:93:LYS:O	4:D:94:TYR:CD1	2.64	0.50
5:E:44:TYR:CE1	5:E:74:TYR:CE2	2.95	0.50
5:E:63:TYR:N	5:E:64:PRO:CD	2.74	0.50
9:I:12:VAL:CB	18:I:1204:CLA:O1A	2.59	0.50
12:L:65:VAL:HG23	12:L:84:GLY:HA2	0.80	0.50
12:L:109:GLU:N	12:L:133:ALA:O	2.31	0.50
17:4:143:PHE:O	17:4:144:ALA:HB2	2.10	0.50
17:4:170:GLN:HB3	17:4:174:THR:HG23	1.93	0.50
17:4:171:HIS:HA	17:4:175:GLY:HA2	1.92	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
1:A:542:HIS:C	1:A:544:ILE:N	2.67	0.50
1:A:547:PHE:CG	1:A:548:THR:N	2.79	0.50
18:A:9013:CLA:HMA3	18:A:9013:CLA:C1	2.41	0.50
2:B:98:GLN:C	2:B:100:ALA:N	2.69	0.50
2:B:166:SER:C	2:B:168:PHE:N	2.69	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:650:PHE:HZ	18:B:9010:CLA:C2D	2.24	0.50
2:B:722:ALA:O	2:B:726:ILE:HG13	2.11	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:46:MET:HB2	6:F:51:LYS:HZ2	1.76	0.50
7:G:87:ALA:HA	7:G:90:SER:HA	1.93	0.50
18:G:1233:CLA:H52	18:G:1233:CLA:NC	2.26	0.50
12:L:80:ALA:C	12:L:82:ALA:H	2.19	0.50
13:N:17:ASN:HA	13:N:20:LYS:HB2	1.92	0.50
16:3:133:TRP:O	16:3:133:TRP:CD1	2.64	0.50
1:A:470:LEU:CD2	2:B:96:PHE:CD2	2.94	0.50
1:A:565:SER:O	1:A:566:SER:C	2.53	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:254:ILE:O	2:B:255:LEU:C	2.54	0.50
2:B:303:TYR:O	2:B:305:LEU:O	2.28	0.50
2:B:439:HIS:CD2	18:B:1230:CLA:C4C	2.93	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
15:2:33:GLY:N	15:2:35:SER:H	2.02	0.50
15:2:147:GLY:O	15:2:148:TRP:HB2	2.10	0.50
16:3:85:ILE:H	16:3:86:PRO:HD3	1.75	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
1:A:328:LYS:O	1:A:331:LEU:N	2.44	0.50
1:A:331:LEU:C	1:A:333:ALA:H	2.18	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
1:A:671:SER:C	1:A:673:SER:N	2.70	0.50
2:B:187:SER:HA	2:B:190:TRP:HB3	1.92	0.50
2:B:294:ASN:ND2	18:B:1209:CLA:HMA1	2.25	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:459:PHE:O	2:B:460:ALA:C	2.55	0.50
2:B:492:ILE:HB	2:B:493:TRP:CE2	2.45	0.50
2:B:628:SER:C	2:B:630:GLN:H	2.09	0.50
18:B:1220:CLA:CHD	18:B:1220:CLA:CBC	2.80	0.50
4:D:29:PHE:O	4:D:30:ALA:HB3	2.12	0.50
4:D:103:VAL:H	4:D:108:GLU:H	1.60	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
7:G:20:ARG:CG	7:G:20:ARG:NH1	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
13:N:2:VAL:HA	13:N:3:ILE:HG13	1.93	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
17:4:91:PHE:O	17:4:95:PHE:CD2	2.64	0.50
1:A:548:THR:C	1:A:550:HIS:N	2.70	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:HA	1:A:663:GLN:OE1	2.12	0.50
1:A:726:SER:O	1:A:729:GLN:N	2.36	0.50
2:B:106:ARG:O	2:B:107:GLY:C	2.55	0.50
2:B:137:THR:O	2:B:141:PHE:N	2.43	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:144:PHE:HD2	2:B:145:LEU:CD2	2.24	0.50
2:B:343:VAL:O	2:B:344:ILE:C	2.53	0.50
2:B:428:PHE:O	2:B:429:LEU:HB2	2.11	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:560:ASP:O	3:C:52:LYS:HE3	2.10	0.50
2:B:618:GLY:CA	2:B:621:ARG:HG2	2.42	0.50
18:B:1215:CLA:HBB2	18:B:1215:CLA:H61	1.94	0.50
3:C:69:LEU:O	3:C:72:GLU:N	2.43	0.50
5:E:33:GLY:HA2	5:E:52:VAL:C	2.37	0.50
6:F:45:THR:O	6:F:46:MET:C	2.52	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
14:1:51:MET:HE1	14:1:150:ASN:HB3	1.91	0.50
15:2:157:LYS:HA	15:2:160:ARG:CB	2.41	0.50
1:A:50:THR:O	1:A:51:THR:C	2.52	0.50
1:A:484:LEU:HD21	1:A:539:PHE:CE2	2.47	0.50
2:B:92:TRP:CD1	9:I:9:VAL:HG11	2.47	0.50
2:B:368:GLN:O	2:B:369:ALA:HB3	2.12	0.50
2:B:375:HIS:NE2	18:B:1225:CLA:C4D	2.73	0.50
18:B:1221:CLA:CBB	18:B:1221:CLA:CHC	2.83	0.50
3:C:29:ILE:HG21	4:D:128:GLN:O	2.12	0.50
4:D:45:PHE:CE1	4:D:46:TYR:O	2.64	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
4:D:137:ILE:O	4:D:139:LYS:N	2.45	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
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
15:2:18:TRP:C	15:2:20:ASP:C	2.79	0.50
15:2:27:PHE:CE1	15:2:29:PHE:N	2.75	0.50
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
15:2:183:TYR:O	15:2:184:THR:CG2	2.59	0.50
16:3:212:ASN:HA	16:3:213:LEU:CB	2.18	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
17:4:45:LEU:O	17:4:46:VAL:C	2.55	0.50
17:4:94:GLU:O	17:4:95:PHE:CD1	2.64	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:721:GLN:HE22	5:E:72:VAL:H	1.58	0.50
1:A:723:ARG:HG3	1:A:724:ALA:H	1.77	0.50
18:A:1106:CLA:HHC	18:A:1107:CLA:HMD2	1.93	0.50
18:A:1137:CLA:HMC1	18:L:1130:CLA:HMC2	1.87	0.50
2:B:69:ALA:HA	2:B:132:ASN:HD22	1.76	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: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
3:C:48:CYS:SG	3:C:49:VAL:C	2.95	0.50
3:C:50:GLY:C	3:C:52:LYS:N	2.68	0.50
3:C:63:LEU:CD2	3:C:65:VAL:H	2.23	0.50
7:G:20:ARG:HH11	7:G:20:ARG:HG3	1.76	0.50
7:G:35:VAL:CG1	7:G:36:PRO:CD	2.89	0.50
12:L:108:LYS:HB2	12:L:132:SER:HB3	1.93	0.50
15:2:19:LEU:CB	15:2:20:ASP:CG	2.85	0.50
15:2:56:MET:SD	15:2:175:MET:CE	3.00	0.50
15:2:94:LEU:HD11	15:2:98:GLU:CD	2.37	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:369:THR:HG21	18:A:1127:CLA:C3C	2.42	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:A:1129:CLA:HMB2	18:L:1130:CLA:C1D	2.42	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
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
18:B:1209:CLA:CGA	18:B:1209:CLA:C4A	2.89	0.50
18:B:1215:CLA:H62	18:B:1215:CLA:CAB	2.41	0.50
18:B:1239:CLA:CBC	20:B:6017:BCR:H392	2.40	0.50
3:C:17:CYS:HB2	3:C:58:CYS:N	2.26	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:31:LEU:C	6:F:32:TYR:CD2	2.89	0.50
6:F:51:LYS:N	6:F:51:LYS:HD3	2.27	0.50
8:H:42:THR:O	8:H:42:THR:HG23	2.11	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
14:1:185:TRP:O	14:1:186:HIS:CB	2.60	0.50
15:2:33:GLY:N	15:2:34:LEU:C	2.70	0.50
17:4:106:TRP:O	17:4:110:LYS:HG2	2.11	0.50
1:A:86:LEU:O	1:A:90:PHE:N	2.32	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
1:A:448:TRP:CE3	18:L:1130:CLA:HBB2	2.47	0.50
1:A:560:VAL:HG23	1:A:561:LEU:HD12	1.94	0.50
2:B:31:PHE:HA	2:B:34:HIS:HB2	1.94	0.50
2:B:61:THR:C	2:B:63:GLY:N	2.66	0.50
2:B:176:ASN:CG	2:B:291:TYR:HD1	2.20	0.50
18:B:9023:CLA:HMA2	20:B:6017:BCR:C40	2.40	0.50
18:B:1225:CLA:HAA2	18:B:1225:CLA:CBD	2.42	0.50
3:C:49:VAL:N	3:C:76:SER:HB3	2.27	0.50
18:F:1302:CLA:HMC1	14:1:191:ASP:HB2	1.93	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
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
15:2:96:ILE:O	15:2:100:VAL:CG1	2.56	0.50
15:2:177:ALA:HA	15:2:178:TRP:CE3	2.47	0.50
16:3:86:PRO:HB2	16:3:87:ALA:CB	2.40	0.50
1:A:398:HIS:C	1:A:400:MET:N	2.70	0.49
1:A:465:ASP:C	1:A:467:MET:H	2.19	0.49
1:A:478:SER:C	1:A:481:ALA:HB3	2.37	0.49
1:A:541:VAL:HG21	1:A:615:HIS:ND1	2.26	0.49
1:A:564:ARG:HB2	1:A:564:ARG:CZ	2.42	0.49
1:A:662:SER:N	1:A:665:ILE:HD12	2.26	0.49
1:A:690:LEU:HB2	18:A:9013:CLA:HMC2	1.94	0.49
2:B:175:LEU:O	2:B:179:LEU:N	2.45	0.49
2:B:275:HIS:CE1	18:B:1214:CLA:CBB	2.92	0.49
2:B:411:MET:HA	2:B:411:MET:CE	2.40	0.49
4:D:113:HIS:CD2	4:D:113:HIS:N	2.78	0.49

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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	0.49
12:L:65:VAL:HG11	18:L:1503:CLA:HMA3	1.94	0.49
13:N:69:CYS:HB2	13:N:72:LYS:CA	2.42	0.49
15:2:50:VAL:HA	15:2:53:ARG:NE	2.27	0.49
15:2:186:THR:HB	15:2:187:GLY:CA	2.42	0.49
17:4:170:GLN:O	17:4:172:ASN:N	2.45	0.49
1:A:49:ASP:CG	1:A:50:THR:HG23	2.37	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:296:LEU:C	1:A:298:ASP:H	2.20	0.49
1:A:407:ILE:C	1:A:409:GLY:H	2.20	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:91:ILE:HD11	2:B:114:ASN:HD22	1.74	0.49
2:B:498:LEU:HA	2:B:501:ILE:CG2	2.42	0.49
2:B:626:LEU:HG	2:B:627:ASN:H	1.77	0.49
20:B:6017:BCR:H351	20:B:6017:BCR:C16	2.31	0.49
6:F:28:SER:HB3	6:F:42:ILE:HG22	1.90	0.49
6:F:115:THR:O	6:F:118:GLU:CB	2.58	0.49
7:G:35:VAL:CG1	7:G:36:PRO:CA	2.78	0.49
7:G:35:VAL:HG12	7:G:36:PRO:HD3	1.94	0.49
8:H:23:VAL:C	8:H:24:TYR:CG	2.91	0.49
12:L:63:LEU:CD2	18:L:1502:CLA:CMB	2.86	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
14:1:111:GLN:CD	14:1:111:GLN:C	2.80	0.49
15:2:56:MET:SD	15:2:175:MET:HE3	2.52	0.49
17:4:126:LEU:O	17:4:153:GLU:OE2	2.29	0.49
1:A:550:HIS:C	1:A:552:THR:H	2.21	0.49
1:A:556:LEU:O	1:A:560:VAL:HG13	2.11	0.49
1:A:661:ALA:HB3	1:A:665:ILE:HD11	1.93	0.49
2:B:7:ARG:HB3	2:B:8:PHE:CD1	2.47	0.49
2:B:18:THR:OG1	2:B:22:TRP:CZ2	2.63	0.49
2:B:98:GLN:NE2	8:H:80:THR:CG2	2.75	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
4:D:61:PRO:C	4:D:63:GLY:N	2.69	0.49
6:F:46:MET:O	6:F:50:LYS:N	2.45	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
12:L:47:VAL:HG12	12:L:52:ARG:HH12	1.77	0.49
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:79:PHE:HA	1:A:82:HIS:HB2	1.93	0.49
1:A:681:GLY:HA2	20:A:6011:BCR:H17C	1.94	0.49
18:A:1129:CLA:HMA2	12:L:25:THR:HG21	1.95	0.49
2:B:7:ARG:O	2:B:8:PHE:C	2.54	0.49
2:B:273:VAL:HG11	18:B:1215:CLA:CMA	2.42	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:378:ILE:C	2:B:380:GLY:N	2.71	0.49
2:B:464:GLN:OE1	18:B:1234:CLA:HMD2	2.13	0.49
2:B:489:GLY:O	2:B:492:ILE:HG12	2.12	0.49
2:B:549:ASP:C	2:B:551:LYS:N	2.65	0.49
18:B:1214:CLA:HBD	18:B:1223:CLA:C2B	2.43	0.49
3:C:14:CYS:C	3:C:16:GLN:H	2.20	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
14:1:152: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
15:2:27:PHE:CD1	15:2:28:GLY:CA	2.96	0.49
15:2:177:ALA:CA	15:2:178:TRP:HE3	2.25	0.49
16:3:132:ASP:CG	16:3:139:MET:CB	2.82	0.49
18:4:1304:CLA:O1D	18:4:1304:CLA:HBA1	2.13	0.49
1:A:446:LEU:C	1:A:449:VAL:HG12	2.32	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
2:B:57:ILE:O	2:B:60:TRP:HB2	2.13	0.49
2:B:433:THR:CG2	2:B:521:HIS:HB3	2.42	0.49
2:B:439:HIS:C	2:B:441:ASP:N	2.71	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
18:B:1138:CLA:H2A	18:B:1138:CLA:O1D	2.12	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
5:E:37:LYS:C	5:E:38:ILE:HD12	2.37	0.49
6:F:99:TRP:CZ2	6:F:143:GLU:HG2	2.47	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
7:G:35:VAL:HG12	7:G:36:PRO:CB	2.36	0.49
13:N:22:LEU:C	13:N:24:THR:N	2.70	0.49
13:N:51:ASP:CA	13:N:52:LEU:HB2	2.41	0.49
14:1:91:TRP:N	14:1:92:GLY:CA	2.62	0.49
14:1:155:LEU:HD13	14:1:158:PHE:CE1	2.48	0.49
15:2:36:SER:CA	15:2:37:ASP:CB	2.87	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: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: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:71:GLN:OE1	2:B:89:HIS:HA	2.13	0.49
2:B:120:VAL:O	2:B:122:GLN:N	2.46	0.49
2:B:141:PHE:C	2:B:143:LEU:N	2.71	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:332:PHE:CE1	2:B:393:PHE:CD1	3.00	0.49
2:B:371:LEU:HD21	18:B:1225:CLA:HMA1	1.94	0.49
4:D:102:ARG:HG2	4:D:109:VAL:HG23	1.94	0.49
6:F:127:SER:O	6:F:130:LEU:N	2.39	0.49
6:F:127:SER:H	6:F:130:LEU:HD13	1.77	0.49
7:G:86:LEU:O	7:G:87:ALA:CB	2.60	0.49
8:H:26:SER:CA	8:H:27:ASP:C	2.85	0.49
10:J:5:LYS:HE3	10:J:6:THR:OG1	2.11	0.49
12:L:70:LYS:HG2	12:L:75:ARG:HG2	1.92	0.49
12:L:108:LYS:O	12:L:109:GLU:HB2	2.10	0.49
13:N:59:PRO:C	13:N:60:PHE:HD2	2.20	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:90:PHE:C	1:A:92:TRP:N	2.70	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
2:B:70:TRP:N	2:B:71:GLN:O	2.44	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:408:LEU:HD22	18:B:1220:CLA:HAC2	1.95	0.49
2:B:510:LEU:CD2	18:B:1234:CLA:HHD	2.34	0.49
18:B:9010:CLA:HMB1	18:B:9022:CLA:HMD2	1.94	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
18:B:1229:CLA:C4D	6:F:90:PHE:CZ	2.96	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
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:92:TRP:O	1:A:93:LEU:C	2.56	0.49
1:A:567:ARG:HH12	2:B:680:TRP:HE1	1.60	0.49
1:A:678:PHE:CD1	1:A:747:TRP:CZ3	3.00	0.49
18:A:9013:CLA:C1	18:A:9013:CLA:CMA	2.91	0.49
2:B:96:PHE:CZ	18:B:1206:CLA:C1D	2.94	0.49
2:B:635:ILE:HG23	2:B:636:THR:N	2.20	0.49
18:B:1229:CLA:C1D	6:F:90:PHE:CE2	2.96	0.49
6:F:46:MET:HB2	6:F:51:LYS:NZ	2.28	0.49
6:F:49:THR:CA	6:F:56:TYR:HH	2.09	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
8:H:30:SER:HB2	12:L:35:TRP:HE1	1.78	0.49
12:L:138:LYS:HZ2	12:L:138:LYS:CB	2.23	0.49
14:1:159:VAL:O	14:1:160:GLY:C	2.56	0.49
15:2:175:MET:O	15:2:176:GLY:C	2.54	0.49
16:3:67:MET:HE2	16:3:67:MET:O	2.13	0.49
16:3:119:MET:O	16:3:120:ALA:C	2.55	0.49
1:A:130:GLU:O	1:A:132:LEU:N	2.46	0.49
1:A:147:SER:HG	18:A:1126:CLA:HMA2	1.75	0.49
1:A:149:PHE:CG	1:A:153:TRP:CZ3	3.01	0.49
1:A:151:GLN:CD	1:A:384:TYR:HB2	2.38	0.49
1:A:434:ARG:NE	18:A:1129:CLA:OBD	2.45	0.49
1:A:710:ALA:O	1:A:714:LEU:HB2	2.13	0.49
18:A:1123:CLA:HBA1	18:A:1123:CLA:CBD	2.42	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:171:ALA:CB	18:B:1221:CLA:HBC1	2.42	0.49
2:B:553:PHE:CE2	3:C:66:ARG:CG	2.92	0.49
2:B:588:GLY:HA2	2:B:717:TYR:HH	1.78	0.49
2:B:650:PHE:O	2:B:654:HIS:N	2.42	0.49
18:B:1138:CLA:C3C	18:F:1139:CLA:HBC2	2.43	0.49
18:B:1239:CLA:HBD	19:B:5002:PQN:C26	2.40	0.49
5:E:40:ARG:C	5:E:42:GLU:N	2.70	0.49
6:F:53:PHE:C	6:F:55:ASN:H	2.20	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
15:2:179: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
17:4:99:HIS:C	17:4:99:HIS:ND1	2.71	0.49
1:A:52:THR:CB	1:A:55:TRP:HE1	2.25	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:450:CYS:SG	1:A:550:HIS:HB3	2.53	0.49
1:A:490:GLN:HG3	1:A:494:ASN:CB	2.43	0.49
1:A:623:ASP:O	1:A:623:ASP:OD2	2.31	0.49
18:A:1126:CLA:NC	20:A:6011:BCR:HC42	2.28	0.49
18:A:1136:CLA:H91	18:L:1504:CLA:HMC3	1.95	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:27:GLU:CD	3:C:29:ILE:HG23	2.38	0.49
3:C:63:LEU:HD23	3:C:66:ARG:CG	2.42	0.49
3:C:76:SER:C	3:C:78:GLY:N	2.71	0.49
6:F:53:PHE:C	6:F:55:ASN:N	2.70	0.49
7:G:81:VAL:HG11	7:G:83:TYR:CE1	2.48	0.49
8:H:58:ILE:O	8:H:58:ILE:CD1	2.51	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
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:461:TYR:HB2	1:A:649:ILE:CD1	2.43	0.48
1:A:490:GLN:HA	1:A:491:TRP:O	2.12	0.48
1:A:567:ARG:HH22	4:D:37:LEU:CD2	2.26	0.48
1:A:581:CYS:HB3	1:A:590:CYS:SG	2.53	0.48
1:A:665:ILE:CG1	18:A:9011:CLA:HBC1	2.43	0.48
1:A:692:PHE:HD2	19:A:5001:PQN:C10	2.26	0.48
18:A:1123:CLA:CHD	18:A:1123:CLA:CBC	2.86	0.48
18:A:1140:CLA:HBC2	18:A:1140:CLA:CMC	2.43	0.48
2:B:4:ARG:HG3	2:B:4:ARG:NH1	2.28	0.48
2:B:42:LEU:HD21	2:B:43:TYR:CD2	2.48	0.48
2:B:66:PHE:CE1	18:I:1204:CLA:HAC1	2.47	0.48
2:B:402:GLN:HB3	2:B:403:ASN:HD22	1.77	0.48
2:B:510:LEU:N	2:B:510:LEU:CD1	2.76	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
18:B:1205:CLA:HMB2	18:I:1204:CLA:HMA2	1.95	0.48
4:D:133:ASN:HD22	4:D:134:MET:H	1.57	0.48
6:F:64:GLY:O	6:F:67:GLY:N	2.43	0.48
6:F:124:PRO:C	6:F:125:LEU:HD23	2.38	0.48
8:H:39:PHE:HA	8:H:43:PHE:HD2	1.78	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:8:GLU:HG2	13:N:11:LYS:CB	2.38	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
15:2:176:GLY:O	15:2:178:TRP:CZ3	2.65	0.48
17:4:63:VAL:O	17:4:64:PHE:C	2.55	0.48
1:A:354:TRP:CG	18:A:1103:CLA:HAC1	2.49	0.48
1:A:386:ALA:CB	1:A:528:ALA:HB1	2.43	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
2:B:209:TRP:CD1	2:B:209:TRP:C	2.91	0.48
2:B:496:GLY:C	2:B:498:LEU:H	2.22	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
15:2:59:ALA:C	15:2:61:GLY:N	2.71	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:491:TRP:HA	1:A:492:ILE:CG2	2.43	0.48
1:A:520:LEU:HD23	1:A:531:PRO:HD3	1.95	0.48
1:A:559:GLY:CA	1:A:597:HIS:CD2	2.97	0.48
1:A:570:PRO:O	1:A:571:ASP:HB3	2.13	0.48
1:A:681:GLY:O	20:A:6011:BCR:C15	2.62	0.48
18:A:1124:CLA:C4A	18:A:1135:CLA:HBB2	2.29	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
2:B:680:TRP:HE1	4:D:37:LEU:CD2	2.26	0.48
18:B:1207:CLA:H62	12:L:91:LEU:CD2	2.44	0.48
4:D:102:ARG:CA	4:D:103:VAL:CB	2.66	0.48
6:F:115:THR:O	6:F:117:LYS:CA	2.61	0.48
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
13:N:25:THR:O	13:N:26:GLY:C	2.55	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
17:4:60:LEU:C	17:4:62:GLU:H	2.20	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:462:ILE:CG2	1:A:463:HIS:N	2.75	0.48
1:A:615:HIS:CD2	1:A:615:HIS:O	2.66	0.48
1:A:619:LYS:HA	1:A:619:LYS:HD2	1.49	0.48
1:A:709:TRP:HZ2	18:B:1228:CLA:CED	2.25	0.48
2:B:20:ARG:HH22	9:I:28:VAL:HA	1.76	0.48
2:B:242:HIS:O	2:B:243:LEU:C	2.57	0.48
2:B:463:ILE:C	2:B:465:SER:N	2.71	0.48
2:B:649:MET:HG3	20:B:6017:BCR:HC41	1.94	0.48
6:F:45:THR:C	6:F:47:GLU:H	2.21	0.48
7:G:42:SER:H	7:G:43:HIS:CD2	2.27	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
15:2:19:LEU:C	15:2:20:ASP:OD1	2.57	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
16:3:206:GLY:O	16:3:207:VAL:C	2.56	0.48
16:3:209:PRO:HB2	16:3:210:TYR:HA	1.95	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
1:A:618:TRP:CD1	1:A:622:SER:HG	2.32	0.48
1:A:709:TRP:CE3	2:B:416:GLU:O	2.66	0.48
2:B:111:GLY:O	2:B:113:VAL:N	2.36	0.48
2:B:176:ASN:CB	2:B:291:TYR:CD1	2.85	0.48
4:D:58:PHE:O	4:D:58:PHE:HD1	1.96	0.48
6:F:50:LYS:HG2	6:F:53:PHE:CD1	2.49	0.48
6:F:100:VAL:HG22	6:F:130:LEU:HA	1.96	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
9:I:26:LEU:HA	9:I:29:GLU:C	2.39	0.48
12:L:97:MET:O	12:L:98:CYS:C	2.56	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
16:3:78:ILE:H	16:3:79:LEU:HA	1.79	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:590:CYS:H	2:B:669:GLY:CA	2.27	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:67:HIS:CD2	2:B:71:GLN:OE1	2.66	0.48
2:B:305:LEU:C	2:B:307:ALA:N	2.71	0.48
2:B:468:GLY:O	2:B:479:SER:OG	2.25	0.48
2:B:697:PRO:HG3	18:B:1238:CLA:C3C	2.44	0.48
2:B:720:THR:OG1	18:B:9010:CLA:CED	2.61	0.48
3:C:31:TRP:C	3:C:31:TRP:CD2	2.90	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: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
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:86:LEU:HD13	1:A:86:LEU:C	2.39	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:609:ILE:C	1:A:611:VAL:O	2.57	0.48
1:A:750:PHE:CZ	18:A:1126:CLA:CMB	2.96	0.48
2:B:120:VAL:C	2:B:122:GLN:H	2.22	0.48
2:B:177:HIS:CE1	18:B:1209:CLA:CHD	2.96	0.48
2:B:255:LEU:CD2	18:B:1212:CLA:HAC2	2.43	0.48
2:B:279:ALA:O	2:B:280:ILE:C	2.56	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:595:HIS:CE1	2:B:725:LEU:HA	2.48	0.48
18:B:1209:CLA:O1A	18:B:1209:CLA:H3A	2.12	0.48
4:D:108:GLU:HG2	4:D:109:VAL:H	1.74	0.48
4:D:122:LYS:C	4:D:127:ARG:HH22	2.12	0.48
6:F:137:PRO:HA	6:F:141:TYR:CA	2.38	0.48
6:F:137:PRO:CB	6:F:141:TYR:HB3	2.36	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
18:F:1302:CLA:O1D	18:F:1302:CLA:H2A	2.13	0.48
12:L:97:MET:O	12:L:100:THR:N	2.30	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:206:HIS:HD2	18:A:1123:CLA:OBD	1.96	0.48
1:A:493:GLN:O	1:A:494:ASN:C	2.56	0.48
1:A:613:ILE:O	1:A:614:PHE:C	2.57	0.48
1:A:747:TRP:HB2	18:A:1126:CLA:HBB2	1.95	0.48
2:B:32:GLU:O	2:B:32:GLU:HG2	2.13	0.48
2:B:84:VAL:HG12	2:B:86:PRO:N	2.27	0.48
2:B:160:LYS:C	2:B:162:LYS:H	2.22	0.48
2:B:273:VAL:HG11	18:B:1215:CLA:HMA3	1.96	0.48
2:B:585:ASN:CG	18:B:9012:CLA:HMC2	2.38	0.48
2:B:633:ASN:HA	2:B:636:THR:HB	1.96	0.48
19:B:5002:PQN:H192	19:B:5002:PQN:H161	1.58	0.48
4:D:107:GLY:O	4:D:108:GLU:CB	2.49	0.48
5:E:37:LYS:HB3	5:E:89:GLU:HB3	1.95	0.48
5:E:40:ARG:NH1	5:E:42:GLU:HG2	2.29	0.48
12:L:46:ALA:HB1	12:L:52:ARG:CZ	2.44	0.48
13:N:9:LYS:C	13:N:11:LYS:H	2.22	0.48
14:1:53:ALA:C	14:1:55:PRO:HD2	2.39	0.48
15:2:36:SER:OG	15:2:38:PRO:C	2.57	0.48
17:4:63:VAL:O	17:4:64:PHE:O	2.32	0.48
1:A:71:LEU:CD1	1:A:352:THR:CG2	2.85	0.48
1:A:253:ASP:C	1:A:256:ALA:HB3	2.38	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
18:A:9011:CLA:HBC2	18:A:9011:CLA:CMC	2.44	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
18:B:1220:CLA:C1B	18:B:1242:CLA:CBA	2.87	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
15:2:189:ILE:CB	15:2:190:ASP:HA	2.44	0.48
17:4:82:GLU:C	17:4:83:TYR:CG	2.91	0.48
17:4:97:LEU:O	17:4:101:VAL:HG13	2.14	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:228:PRO:HD2	1:A:229:ILE:H	1.79	0.48
1:A:287:LEU:HB2	1:A:294:LEU:HB3	1.96	0.48
1:A:308:ILE:C	1:A:311:LEU:H	2.22	0.48
1:A:366:GLY:O	1:A:367:SER:C	2.56	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
1:A:688:PHE:CE2	18:A:1140:CLA:HMC2	2.48	0.48
18:A:1136:CLA:H91	18:L:1504:CLA:CMC	2.44	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
2:B:675:ILE:HD11	2:B:698:VAL:C	2.39	0.48
2:B:720:THR:O	2:B:721:TYR:C	2.57	0.48
2:B:724:PHE:C	2:B:726:ILE:H	2.21	0.48
4:D:26:SER:H	4:D:27:PRO:CB	2.18	0.48
6:F:92:TYR:HA	6:F:136:TRP:HZ2	1.77	0.48
7:G:8:ILE:O	7:G:9:SER:C	2.57	0.48
7:G:92:GLY:C	7:G:93:TYR:O	2.56	0.48
14:1:82:ALA:H	14:1:83:THR:HA	1.75	0.48
15:2:81:THR:HG23	15:2:82:ALA:H	1.78	0.48
1:A:184:PHE:CD1	1:A:184:PHE:C	2.92	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:606:TYR:CE1	1:A:742:GLY:O	2.66	0.47
1:A:645:SER:CB	2:B:637:PRO:HG2	2.44	0.47
18:A:1106:CLA:HBB2	18:A:1126:CLA:C8	2.42	0.47
18:A:9013:CLA:HBB1	18:A:9013:CLA:HHC	1.95	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:58:PHE:CE2	18:B:1241:CLA:CHB	2.82	0.47
2:B:126:THR:O	2:B:127:ILE:C	2.55	0.47
2:B:284:PHE:CD1	18:B:1216:CLA:HMC3	2.49	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:591:THR:CG2	2:B:721:TYR:CE2	2.88	0.47
18:B:1218:CLA:OBD	18:B:1218:CLA:CED	2.56	0.47
18:B:1235:CLA:HBC1	6:F:83:PHE:CZ	2.49	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:D:61:PRO:O	4:D:63:GLY:N	2.47	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
12:L:25:THR:O	12:L:28:THR:OG1	2.28	0.47
14:1:77:LEU:N	14:1:78:PRO:HD3	2.27	0.47
14:1:82:ALA:C	14:1:84:TYR:H	2.22	0.47
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
1:A:160:SER:O	1:A:163:GLN:HB2	2.11	0.47
1:A:248:PHE:HB2	1:A:255:LEU:HD21	1.96	0.47
1:A:364:MET:SD	18:A:1123:CLA:HMB1	2.54	0.47
1:A:407:ILE:CG1	18:A:1124:CLA:C2D	2.90	0.47
1:A:457:SER:HA	1:A:460:LEU:CD2	2.42	0.47
1:A:686:TRP:CE3	18:A:9011:CLA:HMA1	2.49	0.47
2:B:22:TRP:CH2	18:B:1238:CLA:HMB3	2.49	0.47
2:B:56:ILE:O	2:B:57:ILE:C	2.58	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
18:B:1219:CLA:H42	18:B:1219:CLA:C4B	2.45	0.47
4:D:88:THR:O	4:D:89:ARG:C	2.55	0.47
6:F:73:VAL:CG2	6:F:83:PHE:H	2.08	0.47
18:F:1303:CLA:C3B	20:F:6016:BCR:H403	2.44	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
13:N:36:GLU:C	13:N:40:CYS:HA	2.38	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: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:396:PHE:CD1	1:A:616:PHE:CZ	3.02	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:570:PRO:O	1:A:571:ASP:CB	2.62	0.47
1:A:590:CYS:H	2:B:669:GLY:HA3	1.78	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
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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:531:THR:O	2:B:533:ILE:HG13	2.14	0.47
18:B:1227:CLA:H41	18:B:1228:CLA:C9	2.41	0.47
3:C:24:ASP:CG	4:D:112:LEU:HD21	2.39	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
12:L:55:GLU:C	18:L:1502:CLA:HED1	2.39	0.47
13:N:64:ASP:O	13:N:65:LEU:CB	2.62	0.47
14:1:19:PRO:N	14:1:20: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:80:SER:C	18:A:1109:CLA:C2A	2.87	0.47
1:A:327:ILE:O	1:A:330:ILE:HD11	2.15	0.47
1:A:409:GLY:CA	18:A:1128:CLA:HAC1	2.35	0.47
1:A:443:ILE:HD13	1:A:558:LYS:HA	1.97	0.47
1:A:688:PHE:HZ	18:A:1140:CLA:C3C	2.27	0.47
2:B:53:GLN:HG2	2:B:57:ILE:HD11	1.95	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:548:PRO:HG2	3:C:62:PHE:CD2	2.50	0.47
2:B:645:VAL:O	2:B:648:TRP:CA	2.62	0.47
18:B:1205:CLA:HBA1	18:B:1224:CLA:HBD	1.96	0.47
18:B:1239:CLA:C2B	20:B:6017:BCR:C15	2.91	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:45:THR:CG2	12:L:126:GLN:HE21	2.27	0.47
13:N:6:TYR:CD2	13:N:9:LYS:HE2	2.50	0.47
13:N:59:PRO:CA	13:N:60:PHE:HB3	2.45	0.47
17:4:85:ALA:HA	17:4:86:SER:HA	1.61	0.47
1:A:170:GLY:O	1:A:174:PHE:HB2	2.15	0.47
1:A:367:SER:C	1:A:369:THR:H	2.22	0.47
18:A:1124:CLA:HHB	18:A:1135:CLA:CBB	2.44	0.47
2:B:193:HIS:C	2:B:195:VAL:N	2.71	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:549:ASP:C	2:B:551:LYS:HG2	2.38	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:724:PHE:C	2:B:726:ILE:N	2.73	0.47
4:D:134:MET:O	4:D:134:MET:HG2	2.14	0.47
6:F:2:ILE:O	6:F:3:ALA:CB	2.61	0.47
6:F:13:GLN:C	6:F:67:GLY:HA3	2.39	0.47
7:G:21:PHE:C	7:G:23:PHE:CG	2.92	0.47
7:G:21:PHE:N	7:G:21:PHE:CD1	2.82	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
17:4:114:SER:O	17:4:115:VAL:C	2.57	0.47
1:A:57:LEU:C	1:A:57:LEU:CD2	2.88	0.47
1:A:82:HIS:CE1	18:A:1103:CLA:CHA	2.97	0.47
1:A:315:HIS:CD2	18:A:1108:CLA:NA	2.82	0.47
1:A:316:MET:O	1:A:324:GLY:HA2	2.15	0.47
1:A:416:ILE:HG22	1:A:420:ARG:HD2	1.96	0.47
1:A:586:ARG:NH2	3:C:53:ARG:HH22	2.13	0.47
1:A:744:ALA:O	1:A:745:THR:C	2.57	0.47
18:A:1140:CLA:H51	19:A:5001:PQN:H191	1.95	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:226:LEU:O	2:B:227:THR:C	2.57	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:388:ALA:C	2:B:391:PRO:HD2	2.39	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
6:F:115:THR:O	6:F:116:GLN:C	2.56	0.47
7:G:54:TYR:CD1	7:G:54:TYR:O	2.67	0.47
12:L:6:PRO:O	12:L:7:THR:C	2.57	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
14:1:189:ILE:O	14:1:189:ILE:HG13	2.13	0.47
15:2:18:TRP:CG	15:2:21:GLY:O	2.68	0.47
15:2:20:ASP:OD2	15:2:23:LEU:HD11	2.15	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
17:4:81:GLU:C	17:4:84:PHE:CE1	2.93	0.47
1:A:71:LEU:HD12	1:A:193:LEU:HD13	1.96	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:79:PHE:CG	1:A:79:PHE:O	2.67	0.47
1:A:133:ASN:HB2	1:A:142:GLY:CA	2.42	0.47
1:A:139:GLY:O	6:F:38:PRO:CG	2.63	0.47
1:A:395:LEU:C	1:A:397:THR:N	2.73	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:542:HIS:CA	1:A:545:HIS:HD2	2.27	0.47
1:A:543:HIS:NE2	18:A:1136:CLA:C4A	2.78	0.47
1:A:680:LEU:C	1:A:682:ALA:N	2.72	0.47
1:A:697:ARG:HH22	1:A:701:GLN:HB2	1.79	0.47
1:A:715:LYS:HZ3	6:F:109:ARG:HH12	1.62	0.47
2:B:16:PRO:HG3	3:C:74:THR:HG22	1.96	0.47
2:B:96:PHE:HZ	18:B:1206:CLA:C2D	2.27	0.47
2:B:209:TRP:CG	2:B:210:ASN:H	2.31	0.47
2:B:258:LEU:HD11	2:B:495:PRO:CD	2.44	0.47
2:B:301:ILE:CG2	2:B:304:ILE:HG21	2.40	0.47
2:B:372:TYR:CD2	2:B:372:TYR:C	2.93	0.47
2:B:527:LEU:O	2:B:529:THR:N	2.44	0.47
2:B:567:THR:O	2:B:568:CYS:CB	2.61	0.47
2:B:696:LYS:NZ	3:C:79:LEU:O	2.39	0.47
2:B:705:ALA:HB2	19:B:5002:PQN:C7	2.44	0.47
2:B:711:VAL:CG1	18:B:1239:CLA:HED3	2.43	0.47
18:B:1216:CLA:HAA2	18:B:1221:CLA:CAB	2.45	0.47
18:B:1218:CLA:C6	18:1:1012:CLA:C2A	2.93	0.47
4:D:135:ARG:HA	4:D:139:LYS:NZ	2.29	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
6:F:18:GLU:C	6:F:20:GLN:N	2.58	0.47
6:F:56:TYR:O	6:F:58:LYS:HB3	2.12	0.47
6:F:73:VAL:O	6:F:83:PHE:CE2	2.68	0.47
6:F:133:GLY:O	6:F:136:TRP:NE1	2.47	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:15:ASN:ND2	12:L:16:GLY:N	2.63	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
13:N:76:LYS:O	13:N:77:CYS:CB	2.62	0.47
15:2:59:ALA:O	15:2:61:GLY:N	2.46	0.47
15:2:94:LEU:C	15:2:96:ILE:N	2.71	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
15:2:167:GLY:O	15:2:170:ALA:HB3	2.14	0.47
16:3:67:MET:HE2	16:3:70:ALA:HB3	1.95	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
17:4:124:TYR:HD2	17:4:125:SER:HB3	1.79	0.47
17:4:192:ASN:ND2	17:4:196:GLN:HE22	2.12	0.47
1:A:31:PHE:HB2	1:A:32:GLU:HA	1.97	0.47
1:A:57:LEU:C	1:A:59:ALA:H	2.22	0.47
1:A:69:SER:O	1:A:71:LEU:N	2.48	0.47
1:A:95:GLY:HA3	1:A:96:MET:SD	2.55	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:664:VAL:HG23	1:A:675:TYR:C	2.40	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
2:B:69:ALA:N	2:B:71:GLN:O	2.48	0.47
2:B:545:LYS:CA	2:B:548:PRO:HG3	2.41	0.47
2:B:580:VAL:O	2:B:580:VAL:HG12	2.13	0.47
2:B:616:LEU:HD23	2:B:616:LEU:C	2.39	0.47
18:B:1227:CLA:HBD	18:B:1227:CLA:HAA1	1.96	0.47
3:C:23:THR:OG1	3:C:49:VAL:CG1	2.63	0.47
3:C:69:LEU:O	3:C:70:TRP:C	2.57	0.47
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
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:CBB	18:A:9013:CLA:HHC	2.44	0.47
2:B:4:ARG:CG	2:B:5:ILE:N	2.77	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:520:HIS:O	2:B:521:HIS:C	2.58	0.47
2:B:533:ILE:CG2	2:B:575:ASP:O	2.63	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:3:ASP:CB	10:J:5:LYS:HG3	2.45	0.47
10:J:37:LEU:O	10:J:38:THR:HG23	2.15	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
13:N:14:LYS:HG3	13:N:14:LYS:O	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:82:HIS:CE1	18:A:1103:CLA:C1A	2.98	0.47
1:A:188:LYS:NZ	16:3:54:TRP:HH2	2.11	0.47
1:A:216:LEU:C	1:A:218:TRP:H	2.22	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
18:A:1137:CLA:HMC1	18:A:1137:CLA:HBC3	1.97	0.47
2:B:46:ILE:O	2:B:47:PHE:C	2.58	0.47
2:B:79:GLN:CD	2:B:80:ASP:OD1	2.58	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
7:G:18:LEU:C	7:G:20:ARG:H	2.23	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:59:PRO:HD2	16:3:86:PRO:O	2.15	0.47
13:N:70:GLU:OE2	13:N:76:LYS:HD2	2.14	0.47
15:2:190:ASP:O	15:2:191:ASN:C	2.57	0.47
17:4:105:ARG:O	17:4:109:ILE:N	2.39	0.47
1:A:51:THR:HB	18:F:1139:CLA:C3B	2.45	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
1:A:566:SER:C	1:A:568:LEU:N	2.73	0.46
1:A:618:TRP:HB2	1:A:656:PHE:CE1	2.49	0.46
20:A:6011:BCR:H392	20:A:6011:BCR:C23	2.45	0.46
2:B:73:ASN:ND2	2:B:108:GLY:CA	2.74	0.46
2:B:91:ILE:O	2:B:91:ILE:HG22	2.14	0.46
2:B:98:GLN:NE2	8:H:80:THR:HG22	2.30	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:520:HIS:NE2	18:B:1234:CLA:C1C	2.78	0.46
2:B:680:TRP:CE3	2:B:680:TRP:O	2.68	0.46
2:B:708:VAL:HG11	18:B:1239:CLA:O1D	2.14	0.46
18:B:1203:CLA:HBA2	18:B:1203:CLA:CBD	2.44	0.46
18:B:1205:CLA:CGA	18:B:1205:CLA:CHA	2.92	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:D:50:TRP:HH2	4:D:58:PHE:HZ	1.63	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
12:L:38:SER:C	12:L:44:ARG:HH12	2.16	0.46
17:4:114:SER:HB3	17:4:120:ILE:HG12	1.96	0.46
1:A:53:TRP:C	1:A:55:TRP:H	2.23	0.46
1:A:80:SER:CA	1:A:81:ALA:HB2	2.44	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:451:ILE:O	1:A:452:PHE:C	2.57	0.46
1:A:464:ASN:ND2	1:A:477:PHE:CB	2.31	0.46
1:A:479:ASP:C	1:A:481:ALA:N	2.71	0.46
1:A:493:GLN:CA	1:A:496:HIS:HB2	2.45	0.46
1:A:587:GLY:O	2:B:668:ARG:NH1	2.49	0.46
1:A:697:ARG:HD2	1:A:727:ILE:H	1.81	0.46
18:A:1107:CLA:H91	18:A:1107:CLA:H111	1.66	0.46
2:B:74:PHE:CE1	2:B:77:TRP:CZ3	3.03	0.46
2:B:459:PHE:HB2	18:B:1235:CLA:CAD	2.45	0.46
6:F:36:SER:O	6:F:37:ALA:HB3	2.15	0.46
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:109:ARG:HH12	6:F:153:ASN:HD21	1.63	0.46
7:G:6:LEU:HD13	7:G:8:ILE:HG21	1.97	0.46
7:G:43:HIS:N	7:G:43:HIS:HD2	2.10	0.46
7:G:64:VAL:O	7:G:68:ILE:HG22	2.15	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:59:ALA:HA	12:L:62:PHE:HE2	1.75	0.46
12:L:165:TYR:CE1	18:L:1503:CLA:HBD	2.42	0.46
14:1:153:LEU:O	14:1:157:ALA:HB2	2.15	0.46
15:2:92:THR:C	15:2:94:LEU:CB	2.88	0.46
1:A:33:GLN:HE21	1:A:33:GLN:HB2	1.59	0.46
1:A:71:LEU:HD21	1:A:353:SER:HB3	1.94	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:439:ARG:C	1:A:441:ALA:N	2.73	0.46
1:A:679:PHE:HB2	1:A:745:THR:HA	1.94	0.46
19:A:5001:PQN:H171	18:F:1139:CLA:CBB	2.45	0.46
2:B:38:THR:H	2:B:41:ARG:CD	2.28	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:41:ARG:O	2:B:45:ASN:ND2	2.48	0.46
2:B:51:PHE:CE2	2:B:152:ALA:HB1	2.50	0.46
2:B:279:ALA:CB	18:B:1214:CLA:HHC	2.45	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:596:TRP:CD1	2:B:608:GLN:NE2	2.83	0.46
18:B:1138:CLA:C4B	18:F:1139:CLA:HMD1	2.46	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:51:ASP:H	13:N:52:LEU:C	2.23	0.46
13:N:59:PRO:CA	13:N:60:PHE:CB	2.93	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
17:4:74:LYS:O	17:4:75:TRP:C	2.59	0.46
1:A:84:GLY:HA2	1:A:87:SER:CB	2.38	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:376:MET:HE2	1:A:376:MET:HB2	1.77	0.46
1:A:437:ARG:HB3	4:D:32:SER:HB3	1.98	0.46
1:A:570:PRO:C	1:A:571:ASP:CG	2.82	0.46
1:A:608:SER:O	1:A:611:VAL:HG12	2.15	0.46
2:B:25:ILE:O	2:B:26:ALA:O	2.32	0.46
2:B:104:PHE:C	2:B:106:ARG:N	2.72	0.46
2:B:216:LEU:H	2:B:217:PRO:HD3	1.80	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:466:ALA:C	2:B:468:GLY:N	2.70	0.46
2:B:596:TRP:CE2	2:B:608:GLN:O	2.69	0.46
2:B:596:TRP:CH2	2:B:618:GLY:C	2.93	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
18:B:1138:CLA:HMC3	18:F:1139:CLA:C1D	2.46	0.46
18:B:1237:CLA:HAC1	18:B:1238:CLA:C1C	2.45	0.46
4:D:26:SER:OG	4:D:67:ILE:O	2.23	0.46
4:D:43:GLU:O	4:D:44:GLU:CB	2.62	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
13:N:42:PHE:CD2	13:N:43:PRO:HA	2.50	0.46
1:A:105:ASN:HB3	1:A:150:PHE:CZ	2.50	0.46
1:A:338:PHE:O	1:A:339:THR:OG1	2.23	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
1:A:706:SER:OG	1:A:707:ILE:N	2.48	0.46
18:A:1140:CLA:H41	19:A:5001:PQN:H192	1.97	0.46
2:B:265:THR:O	2:B:360:PHE:CD2	2.66	0.46
2:B:301:ILE:C	2:B:304:ILE:HB	2.41	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
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
7:G:37:GLU:CD	7:G:43:HIS:CE1	2.93	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
11:K:62:UNK:C	11:K:64:UNK:N	2.79	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:104:SER:O	1:A:140:PHE:CE1	2.69	0.46
1:A:113:PRO:CG	1:A:384:TYR:CE2	2.98	0.46
1:A:132:LEU:HD11	2:B:446:PHE:HZ	1.80	0.46
1:A:158:ILE:C	1:A:163:GLN:NE2	2.66	0.46
1:A:213:LEU:HD13	1:A:213:LEU:C	2.41	0.46
1:A:352:THR:HG1	1:A:352:THR:H	1.54	0.46
1:A:371:VAL:O	1:A:375:HIS:ND1	2.48	0.46
1:A:393:LEU:HD13	1:A:617:SER:OG	2.16	0.46
1:A:439:ARG:HH11	4:D:62:THR:C	2.23	0.46
1:A:452:PHE:CD2	1:A:452:PHE:C	2.94	0.46
1:A:524:GLY:O	1:A:526:LYS:N	2.48	0.46
1:A:570:PRO:HD3	4:D:79:ARG:NH2	2.31	0.46
1:A:582:ASP:CG	1:A:583:GLY:N	2.72	0.46
1:A:743:ILE:O	1:A:744:ALA:C	2.57	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
18:B:1222:CLA:HHD	18:B:1222:CLA:HBC2	1.97	0.46
3:C:7:ILE:N	3:C:8:TYR:CE2	2.84	0.46
3:C:26:LEU:HD23	4:D:120:PRO:HB2	1.98	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:C:55:GLU:HB2	3:C:65:VAL:HG22	1.96	0.46
4:D:123:VAL:N	4:D:127:ARG:NH1	2.57	0.46
5:E:60:LYS:C	5:E:61:THR:HG22	2.30	0.46
6:F:1:ASP:CA	6:F:62:LEU:CD1	2.92	0.46
6:F:50:LYS:C	6:F:52:ARG:H	2.23	0.46
6:F:77:GLN:O	6:F:80:TRP:CD2	2.69	0.46
7:G:37:GLU:CD	7:G:43:HIS:HE1	2.22	0.46
8:H:49:LYS:CG	12:L:140:THR:HG21	2.44	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
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
14:1:172:GLY:C	14:1:174:LEU:H	2.22	0.46
15:2:66:GLU:O	15:2:68:LEU:N	2.48	0.46
15:2:179:PHE:C	15:2:179:PHE:HD1	2.19	0.46
17:4:169:ILE:HG13	17:4:170:GLN:N	2.30	0.46
1:A:146:THR:O	1:A:147:SER:CB	2.63	0.46
1:A:236:GLY:O	1:A:237:VAL:C	2.58	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
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:343:VAL:HG22	2:B:383:MET:HE3	1.97	0.46
2:B:373:THR:O	2:B:374:HIS:C	2.59	0.46
2:B:459:PHE:N	2:B:461:GLN:HG3	2.31	0.46
2:B:460:ALA:HB1	18:B:1234:CLA:HAA2	1.96	0.46
2:B:527:LEU:CD2	2:B:586:THR:CG2	2.90	0.46
18:B:1209:CLA:HBA1	7:G:39:ASN:ND2	2.31	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
13:N:51:ASP:CG	13:N:52:LEU:HG	2.40	0.46
14:1:60:PRO:HD3	18:1:1006:CLA:C4D	2.46	0.46
15:2:85:GLN:HA	15:2:89:THR:HG21	1.97	0.46
15:2:192:LEU:CB	15:2:193:PHE:HA	2.46	0.46
16:3:132:ASP:O	16:3:133:TRP:O	2.34	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
2:B:109:ALA:HB1	2:B:111:GLY:H	1.80	0.46
2:B:334:LEU:HD21	18:B:1226:CLA:C3B	2.46	0.46
2:B:334:LEU:HD23	18:B:1202:CLA:C1D	2.45	0.46
2:B:410:ARG:O	2:B:411:MET:C	2.59	0.46
2:B:479:SER:O	2:B:480:SER:C	2.59	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
18:B:1220:CLA:OBD	18:B:1221:CLA:HBB2	2.11	0.46
18:B:1237:CLA:HBB1	18:B:1238:CLA:CAD	2.45	0.46
18:B:1239:CLA:HBA2	19:B:5002:PQN:H252	1.96	0.46
20:F:6016:BCR:C33	20:F:6016:BCR:C8	2.91	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
14:1:63:LEU:HD13	14:1:68:TRP:HE1	1.80	0.46
14:1:84:TYR:OH	14:1:91:TRP:C	2.58	0.46
15:2:189:ILE:CG1	15:2:190:ASP:HA	2.46	0.46
16:3:131:GLN:C	16:3:133:TRP:N	2.73	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
17:4:114:SER:HB3	17:4:120:ILE:CG1	2.46	0.46
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
1:A:602:LEU:O	1:A:603:PHE:C	2.59	0.46
1:A:722:PRO:HB2	18:F:1139:CLA:HMC3	1.97	0.46
2:B:16:PRO:O	2:B:696:LYS:CG	2.64	0.46
2:B:209:TRP:CD1	2:B:210:ASN:N	2.83	0.46
2:B:257:ILE:CD1	18:B:1214:CLA:HMB2	2.45	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
6:F:85:THR:HB	10:J:39:PHE:CE2	2.49	0.46
6:F:90:PHE:O	6:F:91:LEU:C	2.59	0.46
7:G:54:TYR:O	7:G:54:TYR:CG	2.69	0.46
12:L:58:LEU:O	12:L:62:PHE:HE2	1.99	0.46
16:3:132:ASP:CB	16:3:139:MET:CB	2.91	0.46
17:4:52:MET:HE1	18:4:4001:CLA:HHC	1.97	0.46
17:4:82:GLU:HG2	17:4:84:PHE:CE2	2.51	0.46
17:4:141:LEU:O	17:4:142:ASN:CB	2.60	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
17:4:152:LYS:HB3	17:4:153:GLU:H	1.48	0.46
1:A:287:LEU:CB	1:A:294:LEU:HB3	2.46	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:451:ILE:C	1:A:455:PHE:HB3	2.41	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:144:PHE:C	2:B:145:LEU:HD22	2.41	0.46
2:B:257:ILE:HD13	18:B:1214:CLA:CMB	2.45	0.46
2:B:311:PRO:CD	18:B:1219:CLA:CBB	2.94	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
18:B:1220:CLA:H62	18:B:1220:CLA:H101	1.63	0.46
4:D:87:GLY:HA2	4:D:90:LEU:HD12	1.98	0.46
6:F:7:PRO:CA	6:F:62:LEU:HD12	2.46	0.46
6:F:31:LEU:C	6:F:32:TYR:HD2	2.24	0.46
6:F:150:VAL:HA	6:F:151:ASP:HB2	1.98	0.46
18:L:1503:CLA:O2D	18:L:1503:CLA:O2A	2.34	0.46
15:2:17:GLU:CD	15:2:18:TRP:H	2.18	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
17:4:186:ILE:C	17:4:187:SER:OG	2.59	0.46
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
1:A:312:ILE:HA	1:A:315:HIS:CE1	2.50	0.45
1:A:470:LEU:HD23	2:B:96:PHE:CE2	2.51	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:718:PRO:O	1:A:719:ALA:HB2	2.15	0.45
2:B:47:PHE:O	2:B:48:ALA:C	2.58	0.45
2:B:158:GLN:OE1	2:B:159:PRO:O	2.33	0.45
2:B:340:SER:OG	18:B:1242:CLA:CBB	2.64	0.45
2:B:399:ASN:OD1	2:B:402:GLN:N	2.48	0.45
2:B:534:LEU:O	2:B:538:ALA:CB	2.64	0.45
2:B:645:VAL:O	2:B:648:TRP:HB3	2.16	0.45
2:B:720:THR:HG1	18:B:9010:CLA:HED2	1.80	0.45
18:B:1209:CLA:HBB2	18:B:1217:CLA:C1D	2.46	0.45
18:B:1218:CLA:C2A	18:B:1218:CLA:CGD	2.94	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
18:B:1220:CLA:HMC3	18:B:1242:CLA:HMD2	1.97	0.45
4:D:77:LEU:HD13	4:D:83:CYS:SG	2.57	0.45
4:D:104:PHE:CD1	4:D:108:GLU:OE2	2.68	0.45
6:F:60:GLY:C	6:F:62:LEU:H	2.23	0.45
8:H:58:ILE:C	8:H:58:ILE:CD1	2.82	0.45
8:H:85:GLN:CD	8:H:86:PRO:HD2	2.41	0.45
9:I:5:PRO:C	9:I:7:LEU:N	2.74	0.45
12:L:16:GLY:O	12:L:17:ASP:C	2.58	0.45
14:1:173:PRO:C	14:1:175:GLU:H	2.23	0.45
16:3:61:ILE:O	16:3:64:ARG:CB	2.57	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:205:HIS:O	1:A:208:ALA:C	2.60	0.45
1:A:302:HIS:CG	1:A:303:HIS:CE1	2.98	0.45
1:A:393:LEU:HD23	1:A:754:ILE:HD13	1.99	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
2:B:39:GLU:HA	4:D:148:PHE:CE2	2.51	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:50:TRP:NE1	4:D:73:ASN:ND2	2.64	0.45
4:D:104:PHE:CD2	4:D:105:PRO:HD2	2.51	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
15:2:157:LYS:C	15:2:160:ARG:H	2.24	0.45
16:3:111:ASN:O	16:3:112:TYR:CD1	2.68	0.45
1:A:60:ASP:O	1:A:62:HIS:N	2.49	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:553:VAL:CG1	1:A:556:LEU:CD1	2.92	0.45
1:A:621:GLN:N	1:A:624:VAL:HG12	2.31	0.45
1:A:725:LEU:CD2	19:A:5001:PQN:C6	2.88	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:391:PRO:CB	2:B:538:ALA:HA	2.47	0.45
2:B:399:ASN:CG	2:B:402:GLN:HB2	2.42	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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: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
7:G:35:VAL:HG13	7:G:36:PRO:N	2.21	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
12:L:66:GLY:C	12:L:68:PHE:N	2.73	0.45
13:N:65:LEU:HB3	13:N:68:GLU:OE2	2.16	0.45
14:1:155:LEU:HD13	14:1:158:PHE:HE1	1.80	0.45
15:2:32:LEU:HD22	15:2:34:LEU:N	2.30	0.45
17:4:96:ILE:CG2	17:4:97:LEU:N	2.72	0.45
17:4:180:ASP:O	17:4:185:HIS:CG	2.69	0.45
17:4:181:ASN:C	17:4:183:LEU:N	2.72	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: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
2:B:7:ARG:HB3	2:B:8:PHE:H	1.50	0.45
2:B:64:ASN:HA	2:B:67:HIS:HB3	1.91	0.45
2:B:98:GLN:OE1	8:H:78:PRO:HB2	2.17	0.45
2:B:148:ILE:HG22	2:B:149:SER:N	2.31	0.45
2:B:384:THR:HG21	2:B:583:MET:HE3	1.99	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:539:LEU:C	2:B:539:LEU:HD12	2.40	0.45
2:B:547:MET:CE	2:B:557:PHE:CE1	3.00	0.45
18:B:1138:CLA:H8	18:B:1138:CLA:H51	1.75	0.45
18:B:1202:CLA:CBB	18:B:1203:CLA:HBA1	2.25	0.45
18:B:1227:CLA:HHD	18:B:1242:CLA:HMD1	1.99	0.45
4:D:23:ASN:ND2	4:D:25:PRO:HD3	2.31	0.45
4:D:146:VAL:O	4:D:147:LYS:C	2.59	0.45
5:E:61:THR:CG2	5:E:62:ARG:H	2.26	0.45
6:F:1:ASP:CA	6:F:62:LEU:HD13	2.43	0.45
6:F:29:LEU:C	6:F:31:LEU:N	2.75	0.45
6:F:42:ILE:HD13	6:F:42:ILE:H	1.80	0.45
7:G:34:GLN:OE1	7:G:35:VAL:HG12	2.16	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
7:G:96:SER:C	7:G:98:PHE:C	2.84	0.45
10:J:2:ARG:CZ	15:2:119:VAL:CB	2.95	0.45
12:L:155:CYS:O	12:L:156:PHE:C	2.59	0.45
15:2:22:SER:HB3	15:2:23:LEU:CG	2.46	0.45
15:2:193:PHE:O	15:2:194:ALA:HB2	2.16	0.45
1:A:57:LEU:C	1:A:59:ALA:N	2.75	0.45
1:A:65:ASP:N	1:A:67:HIS:H	2.15	0.45
1:A:104:SER:O	1:A:140:PHE:CD1	2.70	0.45
1:A:132:LEU:HG	2:B:446:PHE:CZ	2.52	0.45
1:A:460:LEU:HD12	1:A:460:LEU:HA	1.81	0.45
1:A:467:MET:HG3	1:A:471:GLY:HA3	1.98	0.45
1:A:599:PHE:CE2	1:A:735:VAL:HB	2.51	0.45
1:A:602:LEU:O	1:A:605:MET:N	2.48	0.45
1:A:721:GLN:OE1	5:E:71:LYS:HG2	2.16	0.45
2:B:4:ARG:HH11	2:B:4:ARG:HG2	1.79	0.45
2:B:77:TRP:O	2:B:77:TRP:CG	2.70	0.45
2:B:558:PRO:HA	2:B:702:ILE:HD11	1.97	0.45
2:B:613:SER:O	2:B:614:THR:HG23	2.16	0.45
2:B:696:LYS:HE3	2:B:696:LYS:HB2	1.41	0.45
18:B:1219:CLA:H3A	18:B:1219:CLA:HBA2	1.30	0.45
18:B:1239:CLA:C4B	20:B:6017:BCR:H17C	2.46	0.45
20:B:6017:BCR:H311	20:B:6017:BCR:HC8	1.99	0.45
3:C:8:TYR:CE1	4:D:137:ILE:HG12	2.52	0.45
3:C:23:THR:OG1	3:C:49:VAL:HG12	2.16	0.45
4:D:61:PRO:O	4:D:62:THR:C	2.59	0.45
4:D:109:VAL:HG21	4:D:110:GLN:HG3	1.98	0.45
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:65:SER:C	6:F:67:GLY:H	2.23	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
14:1:9:PRO:C	17:4:110:LYS:HD2	2.39	0.45
14:1:57:ILE:O	14:1:58:LEU:C	2.60	0.45
14:1:103:LEU:HD22	14:1:103:LEU:H	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
16:3:67:MET:HE2	16:3:71:ALA:H	1.81	0.45
17:4:54:GLY:O	17:4:57:GLY:N	2.39	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:81:ALA:CA	1:A:83:PHE:H	2.28	0.45
1:A:86:LEU:C	1:A:88:ILE:N	2.74	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:218:TRP:CZ3	18:A:1148:CLA:C4D	2.97	0.45
1:A:287:LEU:HB2	1:A:294:LEU:CA	2.46	0.45
1:A:465:ASP:OD2	1:A:648:THR:HG23	2.17	0.45
1:A:527:VAL:HG21	1:A:634:VAL:HG11	1.99	0.45
1:A:600:LEU:O	1:A:601:GLY:C	2.60	0.45
1:A:611:VAL:HG22	1:A:612:VAL:N	2.32	0.45
1:A:678:PHE:O	1:A:682:ALA:N	2.50	0.45
2:B:16:PRO:HG2	3:C:74:THR:HB	1.98	0.45
2:B:190:TRP:CH2	18:B:1215:CLA:CAD	2.99	0.45
2:B:282:PHE:HA	2:B:285:LEU:HB2	1.99	0.45
2:B:342:GLY:CA	2:B:383:MET:HG3	2.47	0.45
2:B:592:PHE:C	2:B:593:TYR:O	2.59	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
18:B:1227:CLA:HHD	18:B:1242:CLA:OBD	2.16	0.45
3:C:12:ILE:HD12	21:C:3103:SF4:S4	2.57	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:25:LEU:HG	6:F:26:GLN:N	2.31	0.45
6:F:94:ALA:HA	6:F:97:ILE:CD1	2.47	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
7:G:43:HIS:O	7:G:48:ASP:CG	2.60	0.45
9:I:20:ALA:C	9:I:22:ALA:H	2.24	0.45
12:L:78:GLU:HG3	12:L:79:TYR:N	2.31	0.45
12:L:127:PRO:O	12:L:128:ASP:CB	2.62	0.45
13:N:8:GLU:OE2	13:N:11:LYS:HB3	2.16	0.45
14:1:11:PRO:N	17:4:107:GLN:CG	2.77	0.45
15:2:33:GLY:CA	15:2:35:SER:N	2.78	0.45
15:2:86:GLU:OE2	15:2:86:GLU:N	2.50	0.45
16:3:57:TYR:CE2	16:3:185:VAL:CB	2.97	0.45
17:4:60:LEU:O	17:4:62:GLU:N	2.49	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:A:1119:CLA:H2	18:A:1123:CLA:CMB	2.46	0.45
18:A:1129:CLA:HBB2	18:L:1130:CLA:HBC3	1.98	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
18:A:1137:CLA:HMC2	18:L:1130:CLA:CMC	2.33	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:506:ASN:C	2:B:508:LEU:N	2.74	0.45
2:B:536:LYS:NZ	2:B:536:LYS:HB3	2.32	0.45
2:B:576:PHE:C	2:B:576:PHE:CD2	2.94	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
2:B:684:ARG:NH1	12:L:22:GLY:CA	2.80	0.45
18:B:9010:CLA:C1	18:B:9012:CLA:CHD	2.87	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
3:C:49:VAL:HG13	3:C:51:CYS:CB	2.46	0.45
4:D:36:LEU:HD23	12:L:19:PHE:O	2.17	0.45
8:H:43:PHE:HA	8:H:44:ALA:HA	1.80	0.45
12:L:48:ASN:OD1	12:L:48:ASN:C	2.58	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
15:2:63: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
17:4:106:TRP:NE1	17:4:110:LYS:HZ1	2.15	0.45
17:4:158:ARG:HG2	17:4:158:ARG:NH1	2.30	0.45
1:A:323:ILE:CG2	18:A:1108:CLA:HAA2	2.47	0.45
1:A:547:PHE:CE1	1:A:551:VAL:CG1	2.90	0.45
20:A:6011:BCR:H23C	20:A:6011:BCR:H392	1.99	0.45
2:B:88:ALA:CA	2:B:116:ALA:HB2	2.47	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:462:TRP:C	2:B:463:ILE:O	2.59	0.45
2:B:593:TYR:O	2:B:594:TRP:CB	2.61	0.45
2:B:697:PRO:HB3	18:B:1238:CLA:C1C	2.46	0.45
18:B:1215:CLA:C7	18:B:1215:CLA:C2	2.95	0.45
4:D:151:LYS:O	4:D:152:GLN:O	2.35	0.45
5:E:39:LEU:HD13	5:E:88:GLU:OE2	2.17	0.45
5:E:45:TRP:CE3	5:E:45:TRP:C	2.95	0.45
7:G:73:ALA:HA	7:G:77:ILE:O	2.17	0.45
8:H:66:THR:O	8:H:67:TYR:C	2.58	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
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:76:ARG:H	1:A:76:ARG:HG2	1.60	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:494:ASN:O	1:A:495:THR:CB	2.63	0.45
1:A:594:ALA:O	1:A:595:TRP:C	2.59	0.45
1:A:621:GLN:HB2	1:A:621:GLN:HE21	1.42	0.45
2:B:192:GLY:O	2:B:195:VAL:CB	2.61	0.45
2:B:439:HIS:C	2:B:441:ASP:H	2.24	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
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
15:2:33:GLY:N	15:2:35:SER:HB3	2.32	0.45
15:2:159:LEU:HB3	15:2:160:ARG:HH21	1.82	0.45
16:3:196:LEU:CD2	18:3:3005:CLA:C3B	2.95	0.45
1:A:76:ARG:HH21	1:A:190:ALA:CB	2.29	0.45
1:A:85:GLN:HA	1:A:85:GLN:NE2	2.23	0.45
1:A:212:GLY:C	1:A:214:GLY:N	2.68	0.45
1:A:331:LEU:O	1:A:334:HIS:CE1	2.70	0.45
1:A:389:TYR:CE2	1:A:625:TRP:CG	3.05	0.45
1:A:462:ILE:HD11	18:B:9022:CLA:O1A	2.17	0.45
1:A:482:ILE:HD13	1:A:482:ILE:HA	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: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
18:A:1140:CLA:H51	19:A:5001:PQN:H192	1.97	0.45
2:B:345:THR:HG23	18:B:1225:CLA:HAC1	1.99	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:689:ASN:ND2	4:D:38:ARG:HH11	2.06	0.45
18:B:1215:CLA:HMC1	18:B:1215:CLA:CBC	2.47	0.45
3:C:12:ILE:HG21	3:C:28:MET:HE3	1.99	0.45
4:D:79:ARG:CB	4:D:81:GLU:HG3	2.42	0.45
4:D:108:GLU:CD	4:D:109:VAL:HG22	2.42	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
6:F:6:THR:C	6:F:8:CYS:H	2.25	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
12:L:165:TYR:C	12:L:167:PHE:O	2.60	0.45
16:3:74:ILE:HD11	16:3:199:PHE:HA	1.99	0.45
16:3:138:SER:O	16:3:141:LYS:CB	2.65	0.45
1:A:58:HIS:O	18:A:1128:CLA:C2	2.65	0.44
1:A:121:GLN:NE2	18:A:1107:CLA:HED3	2.32	0.44
1:A:128:GLY:O	2:B:446:PHE:CD2	2.69	0.44
1:A:244:LEU:O	1:A:246:HIS:HB2	2.16	0.44
1:A:441:ALA:O	1:A:445:HIS:CE1	2.67	0.44
1:A:618:TRP:CE3	1:A:656:PHE:HD1	2.35	0.44
1:A:684:PHE:CE1	18:A:9013:CLA:HMB1	2.52	0.44
18:A:1136:CLA:O1D	18:A:1136:CLA:CAA	2.64	0.44
18:A:9011:CLA:CBB	18:B:9010:CLA:ND	2.63	0.44
2:B:60:TRP:O	2:B:64:ASN:CG	2.59	0.44
2:B:77:TRP:HE1	2:B:81:PRO:HA	1.80	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:170:ASN:CG	2:B:170:ASN:O	2.60	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:596:TRP:HE1	2:B:608:GLN:CD	2.25	0.44
2:B:721:TYR:HD1	18:B:9010:CLA:OBD	1.99	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
3:C:51:CYS:C	3:C:53:ARG:N	2.73	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:73:VAL:HG13	6:F:80:TRP:HA	1.99	0.44
6:F:75:GLY:O	18:F:1302:CLA:CHD	2.64	0.44
6:F:124:PRO:O	6:F:125:LEU:HD23	2.17	0.44
12:L:37:LEU:C	12:L:42:ALA:HB1	2.40	0.44
13:N:7:LEU:O	13:N:7:LEU:HG	2.16	0.44
13:N:73:ASP:OD1	13:N:76:LYS:HA	2.17	0.44
15:2:66:GLU:C	15:2:68:LEU:N	2.75	0.44
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:130:GLU:O	1:A:131:ILE:C	2.59	0.44
1:A:173:VAL:C	1:A:175:ALA:N	2.75	0.44
1:A:260:PRO:O	1:A:261:SER:HB3	2.17	0.44
1:A:444:SER:HB3	2:B:677:THR:O	2.17	0.44
1:A:458:PHE:C	1:A:460:LEU:N	2.74	0.44
1:A:588:GLY:C	2:B:668:ARG:HD2	2.42	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:248:GLN:C	2:B:250:ALA:H	2.26	0.44
2:B:291:TYR:O	2:B:292:ARG:HG3	2.18	0.44
2:B:311:PRO:N	18:B:1219:CLA:CBB	2.80	0.44
2:B:353:TYR:CD2	2:B:353:TYR:C	2.95	0.44
2:B:388:ALA:CA	2:B:391:PRO:HD2	2.47	0.44
2:B:492:ILE:C	2:B:493:TRP:CG	2.94	0.44
2:B:598:HIS:O	2:B:599:ILE:C	2.60	0.44
2:B:725:LEU:H	2:B:725:LEU:HD23	1.82	0.44
18:B:1239:CLA:C4D	19:B:5002:PQN:H251	2.46	0.44
6:F:7:PRO:O	6:F:8:CYS:HB2	2.18	0.44
7:G:28:ARG:O	7:G:29:GLU:CD	2.60	0.44
9:I:24:LEU:C	9:I:26:LEU:C	2.85	0.44
12:L:33:ILE:CG2	12:L:33:ILE:O	2.65	0.44
12:L:108:LYS:C	12:L:109:GLU:OE2	2.60	0.44
13:N:8:GLU:HG2	13:N:8:GLU:O	2.16	0.44
15:2:16:PRO:N	15:2:19:LEU:O	2.49	0.44
15:2:69:THR:O	15:2:70:LYS:C	2.61	0.44
16:3:67:MET:SD	16:3:71:ALA:HB2	2.58	0.44
17:4:89:THR:OG1	17:4:91:PHE:HB2	2.17	0.44
17:4:137:ILE:N	17:4:141:LEU:HD23	2.32	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:52:THR:CA	1:A:55:TRP:HE1	2.29	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:668:TYR:CD1	2:B:445:ALA:CB	3.01	0.44
18:A:9013:CLA:C1D	2:B:582:TRP:HD1	2.30	0.44
2:B:85:ARG:HB3	2:B:85:ARG:HH11	1.82	0.44
2:B:91:ILE:HD13	2:B:113:VAL:HA	1.98	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:319:HIS:HA	2:B:406:ASN:HB3	1.98	0.44
2:B:334:LEU:HD23	18:B:1202:CLA:C4C	2.47	0.44
2:B:357:ALA:C	2:B:358:TYR:CG	2.93	0.44
2:B:463:ILE:HG22	2:B:464:GLN:H	1.79	0.44
2:B:527:LEU:C	2:B:529:THR:N	2.76	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:14:LEU:CD2	12:L:23:LEU:H	2.16	0.44
12:L:87:ALA:O	12:L:89:ALA:C	2.58	0.44
15:2:17:GLU:CB	15:2:19:LEU:N	2.72	0.44
15:2:110:TRP:C	15:2:112:ASP:N	2.73	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
16:3:75:ALA:CB	16:3:76:PRO:HD3	2.46	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
1:A:481:ALA:C	1:A:483:GLN:N	2.75	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
18:A:9013:CLA:C1D	2:B:582:TRP:CD1	3.01	0.44
19:A:5001:PQN:H221	19:A:5001:PQN:H261	1.66	0.44
2:B:37:ILE:CG2	4:D:148:PHE:CE1	3.00	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
2:B:458:ILE:C	2:B:461:GLN:HG3	2.41	0.44
18:B:1138:CLA:H91	18:B:1229:CLA:H2	1.98	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
18:B:9022:CLA:HAC2	18:B:9023:CLA:HBC3	1.99	0.44
18:B:1207:CLA:HBB2	9:I:13:GLY:C	2.43	0.44
18:B:1208:CLA:H12	18:B:1208:CLA:CAA	2.48	0.44
18:B:1227:CLA:CMB	18:B:1228:CLA:C3D	2.90	0.44
3:C:30:PRO:O	3:C:31:TRP:O	2.35	0.44
5:E:45:TRP:CA	5:E:46:PHE:CB	2.96	0.44
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:CD1	12:L:167:PHE:N	2.74	0.44
13:N:58:VAL:HG11	16:3:86:PRO:CA	2.22	0.44
13:N:72:LYS:C	13:N:75:TYR:O	2.60	0.44
15:2:23:LEU:HA	15:2:24:PRO:C	2.41	0.44
1:A:164:LEU:H	1:A:164:LEU:HD23	1.81	0.44
1:A:239:PRO:HG2	1:A:240:LYS:HE3	2.00	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:493:GLN:HG2	1:A:515:TRP:HB2	2.00	0.44
1:A:668:TYR:O	1:A:669:GLY:C	2.60	0.44
1:A:711:HIS:HB3	1:A:716:VAL:HB	2.00	0.44
1:A:725:LEU:O	19:A:5001:PQN:H6	2.18	0.44
18:A:1131:CLA:HBC3	18:A:1136:CLA:HAC1	1.95	0.44
2:B:38:THR:H	2:B:41:ARG:HD2	1.83	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:456:GLU:CD	6:F:70:HIS:HD2	2.26	0.44
2:B:594:TRP:CD2	2:B:598:HIS:CD2	3.06	0.44
18:B:1235:CLA:HBB1	18:B:1235:CLA:H92	2.00	0.44
3:C:51:CYS:O	21:C:3102:SF4:S1	2.76	0.44
3:C:52:LYS:HZ3	3:C:66:ARG:NH1	2.13	0.44
6:F:75:GLY:C	6:F:80:TRP:HD1	2.26	0.44
6:F:150:VAL:HB	6:F:151:ASP:C	2.43	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
14:1:84:TYR:CD2	14:1:88:PRO:O	2.71	0.44
1:A:126:ILE:O	1:A:128:GLY:N	2.50	0.44
1:A:650:ASN:HB2	2:B:651:LEU:HD13	2.00	0.44
1:A:747:TRP:CZ2	18:A:1126:CLA:O2A	2.71	0.44
18:A:1107:CLA:O1A	18:A:1107:CLA:H43	2.17	0.44
2:B:12:ILE:H	2:B:12:ILE:HG13	1.55	0.44
2:B:37:ILE:O	4:D:148:PHE:HB3	2.18	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:393:PHE:CD2	2:B:393:PHE:C	2.95	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
2:B:657:TRP:CH2	2:B:713:PHE:CZ	3.05	0.44
18:B:1218:CLA:CBD	18:B:1218:CLA:CAA	2.96	0.44
18:B:1219:CLA:O2D	18:B:1219:CLA:H2A	2.17	0.44
18:B:1231:CLA:HBA2	18:B:1231:CLA:H3A	1.57	0.44
3:C:73:THR:C	3:C:75:ARG:N	2.75	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
4:D:102:ARG:CB	4:D:110:GLN:HB2	2.48	0.44
6:F:116:GLN:C	6:F:119:ILE:H	2.23	0.44
7:G:35:VAL:HG12	7:G:36:PRO:CG	2.47	0.44
8:H:43:PHE:N	8:H:43:PHE:HD1	2.15	0.44
9:I:9:VAL:C	9:I:11:LEU:H	2.24	0.44
10:J:3:ASP:O	10:J:5:LYS:N	2.50	0.44
10:J:16:THR:O	10:J:18:TRP:N	2.50	0.44
18:L:1502:CLA:HBC2	18:L:1502:CLA:HHD	2.00	0.44
13:N:70:GLU:CD	13:N:76:LYS:HD2	2.42	0.44
15:2:90:ASP:HB3	15:2:91:THR:OG1	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
18:A:1107:CLA:HED3	18:A:1107:CLA:OBD	2.18	0.44
2:B:196:HIS:CE1	18:B:1211:CLA:C3C	2.99	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
2:B:548:PRO:C	2:B:549:ASP:CG	2.86	0.44
18:B:1235:CLA:OBD	18:B:1235:CLA:O2D	2.35	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:96:TRP:CD1	6:F:96:TRP:H	2.35	0.44
6:F:96:TRP:CD1	6:F:96:TRP:N	2.83	0.44
18:F:1302:CLA:H71	18:F:1302:CLA:H2	1.98	0.44
9:I:16:PHE:CE1	20:I:6018:BCR:H341	2.52	0.44
12:L:97:MET:SD	12:L:98:CYS:HA	2.58	0.44
14:1:10:ARG:CB	14:1:11:PRO:CB	2.95	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
14:1:183:ASP:HA	17:4:87:SER:HA	2.00	0.44
15:2:110:TRP:C	15:2:112:ASP:H	2.25	0.44
16:3:64:ARG:O	16:3:68:LEU:HB2	2.17	0.44
1:A:110:LEU:O	1:A:111:ASN:C	2.59	0.44
1:A:331:LEU:O	1:A:334:HIS:ND1	2.50	0.44
1:A:692:PHE:CE2	19:A:5001:PQN:C2	3.00	0.44
18:A:1107:CLA:HAC1	2:B:446:PHE:HZ	1.76	0.44
18:A:9011:CLA:H62	18:A:9011:CLA:H41	1.76	0.44
2:B:103:ALA:O	2:B:106:ARG:NH1	2.51	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
18:B:1212:CLA:H2	18:B:1212:CLA:CBA	2.48	0.44
3:C:49:VAL:CA	3:C:76:SER:HB3	2.47	0.44
4:D:137:ILE:O	4:D:138:GLY:C	2.60	0.44
6:F:44:ALA:O	6:F:46:MET:N	2.51	0.44
18:F:1139:CLA:HAA1	18:F:1139:CLA:HBD	2.00	0.44
8:H:88:LYS:C	8:H:90:GLY:N	2.73	0.44
10:J:24:GLY:O	10:J:25:LEU:C	2.61	0.44
12:L:69:VAL:HG22	12:L:83:ALA:CB	2.47	0.44
12:L:159:TYR:HD1	12:L:159:TYR:HA	1.55	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
17:4:51:ALA:CB	17:4:161:MET:CE	2.79	0.44
1:A:82:HIS:CE1	18:A:1103:CLA:C4D	3.01	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
18:A:1115:CLA:H12	18:K:1141:CLA:C3B	2.48	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:337:ALA:O	18:B:1202:CLA:O1D	2.36	0.44
2:B:392:ILE:O	2:B:394:PHE:N	2.51	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:53:PHE:HB3	6:F:54:ASP:H	1.30	0.44
6:F:128:SER:O	6:F:132:ARG:HB2	2.17	0.44
7:G:65:GLY:O	7:G:66:PHE:C	2.61	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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: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
14:1:15:ASP:C	14:1:18:ALA:HA	2.43	0.44
16:3:140:GLY:N	16:3:141:LYS:HB3	2.31	0.44
17:4:118:ASP:HB2	17:4:119:PRO:HD3	2.00	0.44
17:4:178:PRO:C	17:4:179:PHE:HD1	2.25	0.44
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:331:LEU:C	1:A:333:ALA:N	2.76	0.43
1:A:453:LEU:HD23	18:A:1136:CLA:CBB	2.47	0.43
1:A:520:LEU:CD2	1:A:530:LEU:CB	2.95	0.43
1:A:700:TRP:CZ2	19:A:5001:PQN:C2M	2.97	0.43
1:A:733:VAL:O	1:A:737:HIS:N	2.33	0.43
18:A:1113:CLA:HAA1	18:A:1113:CLA:CED	2.36	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
2:B:681:ALA:C	2:B:683:GLU:H	2.25	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:3:ASP:O	10:J:4:PHE:C	2.60	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
13:N:37:PHE:C	13:N:39:SER:HA	2.43	0.43
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
16:3:83:GLY:CA	16:3:84:LEU:C	2.91	0.43
16:3:114:LEU:O	16:3:115:PHE:HD1	2.01	0.43
17:4:94:GLU:C	17:4:95:PHE:CG	2.96	0.43
17:4:166:GLY:O	17:4:169:ILE:HG12	2.18	0.43
1:A:154:ARG:CZ	1:A:384:TYR:CE1	3.01	0.43
1:A:204:ASN:ND2	1:A:317:TYR:HD1	2.16	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:272:LEU:HD23	1:A:274:TRP:CE3	2.40	0.43
1:A:416:ILE:O	1:A:417:PHE:C	2.61	0.43
1:A:490:GLN:HA	1:A:491:TRP:C	2.43	0.43
2:B:88:ALA:HB3	2:B:114:ASN:CB	2.48	0.43
2:B:205:GLU:O	2:B:207:VAL:HG12	2.18	0.43
2:B:233:TYR:C	2:B:235:GLN:N	2.75	0.43
2:B:276:HIS:HB2	18:B:1214:CLA:C1B	2.47	0.43
2:B:303:TYR:HB3	18:B:1219:CLA:HED3	2.00	0.43
2:B:399:ASN:CB	4:D:144:ILE:HD13	2.49	0.43
2:B:444:LEU:HG	2:B:615:TYR:CZ	2.53	0.43
2:B:586:THR:O	2:B:586:THR:HG22	2.17	0.43
2:B:680:TRP:NE1	4:D:37:LEU:CD2	2.81	0.43
18:B:1238:CLA:HBC3	18:B:1238:CLA:HHD	1.99	0.43
3:C:70:TRP:HA	3:C:70:TRP:CE3	2.52	0.43
4:D:90:LEU:HG	4:D:90:LEU:H	1.69	0.43
5:E:51:SER:C	5:E:53:VAL:N	2.76	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
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
13:N:70:GLU:OE1	13:N:70:GLU:HA	2.17	0.43
14:1:5:MET:O	14:1:9:PRO:O	2.36	0.43
14:1:34:ALA:C	14:1:36:LEU:H	2.25	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:63:ASP:O	1:A:67:HIS:ND1	2.51	0.43
1:A:64:PHE:C	1:A:67:HIS:N	2.74	0.43
1:A:83:PHE:HB3	1:A:84:GLY:H	1.46	0.43
1:A:130:GLU:OE1	1:A:130:GLU:N	2.51	0.43
1:A:158:ILE:CA	1:A:163:GLN:HE22	2.31	0.43
1:A:548:THR:C	1:A:552:THR:OG1	2.60	0.43
1:A:613:ILE:CG2	1:A:614:PHE:N	2.81	0.43
1:A:701:GLN:C	1:A:703:LEU:N	2.76	0.43
1:A:707:ILE:CD1	18:B:1138:CLA:HMD2	2.47	0.43
1:A:715:LYS:NZ	6:F:153:ASN:ND2	2.62	0.43
19:A:5001:PQN:H191	19:A:5001:PQN:H23	2.00	0.43
2:B:19:ARG:HH11	2:B:19:ARG:CG	2.31	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:120:VAL:O	2:B:124:TRP:HD1	2.01	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:353:TYR:CE2	2:B:354:SER:HA	2.53	0.43
2:B:420:SER:CB	18:B:1138:CLA:CED	2.96	0.43
2:B:532:LEU:O	2:B:533:ILE:C	2.62	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
2:B:652:PHE:C	2:B:654:HIS:N	2.75	0.43
18:B:9010:CLA:HMB3	18:B:9022:CLA:HMD3	2.00	0.43
18:B:1208:CLA:HAA1	18:B:1208:CLA:CBD	2.46	0.43
4:D:23:ASN:ND2	12:L:17:ASP:HA	2.33	0.43
4:D:115:LYS:NZ	4:D:116:ASP:OD1	2.39	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
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
2:B:56:ILE:H	2:B:56:ILE:HG13	1.68	0.43
2:B:468:GLY:CA	2:B:498:LEU:CD2	2.96	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
18:B:1227:CLA:HBC3	18:B:1242:CLA:HMD3	2.00	0.43
6:F:50:LYS:C	6:F:52:ARG:N	2.76	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
9:I:20:ALA:C	9:I:22:ALA:N	2.76	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
12:L:56:VAL:HG23	12:L:57:GLY:N	2.33	0.43
14:1:145:VAL:O	14:1:146:LYS:C	2.61	0.43
15:2:56:MET:O	15:2:60:ALA:N	2.49	0.43
15:2:166:ASN:HD21	18:2:2004:CLA:C1C	2.31	0.43
17:4:136:GLY:HA2	17:4:141:LEU:HD21	2.00	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:365:LEU:HD22	18:A:1123:CLA:O1A	2.18	0.43
1:A:377:TYR:O	1:A:380:PRO:HD3	2.19	0.43
1:A:389:TYR:C	1:A:391:THR:H	2.27	0.43
1:A:415:ALA:O	1:A:417:PHE:HB3	2.19	0.43
18:A:1115:CLA:CBB	18:K:1141:CLA:C2B	2.96	0.43
2:B:57:ILE:HA	2:B:60:TRP:HB2	2.01	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:74:PHE:HE2	2:B:130:ARG:CA	2.05	0.43
2:B:326:ILE:HG12	18:B:1221:CLA:C2C	2.48	0.43
2:B:387:PHE:CE2	18:B:1242:CLA:CMC	3.01	0.43
2:B:467:HIS:CD2	2:B:467:HIS:N	2.86	0.43
18:B:1202:CLA:O2A	18:B:1210:CLA:CHA	2.66	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
6:F:121:ILE:N	10:J:9:SER:HB2	2.33	0.43
7:G:34:GLN:CD	7:G:35:VAL:HG12	2.44	0.43
7:G:50:ARG:HD3	7:G:51:ALA:HB2	2.01	0.43
7:G:63:PRO:HG3	18:G:1248:CLA:C3C	2.47	0.43
13:N:41:LYS:C	13:N:42:PHE:O	2.62	0.43
15:2:56:MET:HA	15:2:59:ALA:H	1.83	0.43
15:2:151:ALA:O	15:2:153:PRO:O	2.36	0.43
17:4:59:LEU:C	17:4:62:GLU:HB2	2.41	0.43
17:4:142:ASN:HD22	17:4:145:PRO:CD	2.30	0.43
1:A:92:TRP:HB3	1:A:93:LEU:H	1.54	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:436:LEU:O	4:D:62:THR:O	2.37	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:622:SER:H	1:A:637:ILE:HD13	1.83	0.43
1:A:632:GLY:N	1:A:633:VAL:HG22	2.33	0.43
1:A:679:PHE:HD1	1:A:679:PHE:O	2.01	0.43
2:B:5:ILE:HG22	2:B:6:PRO:N	2.34	0.43
2:B:135:LEU:CD2	2:B:136:TYR:N	2.81	0.43
2:B:199:ILE:HA	2:B:199:ILE:HD13	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:283:LEU:HG	18:B:1216:CLA:CMC	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:585:ASN:ND2	18:B:9012:CLA:HMC2	2.34	0.43
2:B:657:TRP:CZ3	2:B:661:PHE:CE1	2.87	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
13:N:25:THR:HB	15:2:201:HIS:HB2	1.98	0.43
15:2:22:SER:OG	15:2:22:SER:O	2.30	0.43
15:2:53:ARG:C	15:2:57:LEU:HG	2.43	0.43
16:3:198:TYR:HD1	16:3:198:TYR:HA	1.62	0.43
17:4:89:THR:O	17:4:90:LEU:C	2.61	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: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
1:A:356:ALA:HA	1:A:417:PHE:CD1	2.54	0.43
1:A:393:LEU:HA	1:A:616:PHE:HZ	1.82	0.43
1:A:455:PHE:HA	18:B:9023:CLA:O1A	2.18	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:23:PHE:N	2:B:23:PHE:CD2	2.87	0.43
2:B:64:ASN:N	2:B:67:HIS:HB2	2.33	0.43
2:B:222:LEU:HA	2:B:222:LEU:HD12	1.80	0.43
2:B:280:ILE:HG22	18:B:1214:CLA:C3C	2.49	0.43
2:B:283:LEU:O	18:B:1216:CLA:HMC3	2.19	0.43
2:B:294:ASN:ND2	18:B:1209:CLA:CMA	2.82	0.43
2:B:366:THR:C	2:B:369:ALA:HB3	2.44	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:534:LEU:C	2:B:536:LYS:H	2.26	0.43
2:B:536:LYS:O	2:B:541:ALA:CB	2.66	0.43
18:B:9010:CLA:O2A	18:B:9012:CLA:HMD2	2.19	0.43
18:B:1209:CLA:HBA2	7:G:38:GLN:HG3	2.00	0.43
18:B:1209:CLA:C1C	18:B:1217:CLA:HMD1	2.49	0.43
18:B:1242:CLA:HBA2	18:B:1242:CLA:CGD	2.48	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
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
6:F:113:LYS:HA	6:F:114:PRO:HD3	1.81	0.43
7:G:86:LEU:HD13	7:G:86:LEU:H	1.84	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
15:2:86:GLU:CD	17:4:187:SER:CB	2.92	0.43
1:A:80:SER:O	1:A:83:PHE:HD1	2.02	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:296:LEU:C	1:A:298:ASP:N	2.75	0.43
1:A:445:HIS:CD2	18:A:1129:CLA:HMB1	2.54	0.43
1:A:461:TYR:O	1:A:462:ILE:C	2.62	0.43
1:A:572:LYS:HD2	1:A:579:PHE:HE2	1.83	0.43
1:A:674:ALA:C	1:A:677:LEU:H	2.26	0.43
18:A:9011:CLA:CBB	2:B:624:LEU:HD11	2.36	0.43
2:B:12:ILE:O	2:B:20:ARG:HG3	2.19	0.43
2:B:68:VAL:HG23	2:B:69:ALA:H	1.84	0.43
2:B:101:VAL:C	2:B:105:THR:HG1	2.26	0.43
2:B:238:SER:HA	2:B:251:GLY:H	1.84	0.43
2:B:290:MET:HB3	2:B:291:TYR:CD1	2.54	0.43
2:B:646:TRP:C	2:B:648:TRP:N	2.72	0.43
2:B:650:PHE:CE2	2:B:654:HIS:CE1	3.07	0.43
2:B:653:GLY:CA	2:B:720:THR:CG2	2.88	0.43
2:B:676:GLU:C	2:B:678:LEU:N	2.76	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
3:C:60:THR:CA	5:E:80:ASN:ND2	2.73	0.43
3:C:76:SER:C	3:C:78:GLY:H	2.26	0.43
4:D:80:LYS:HE3	4:D:100:PHE:CE2	2.53	0.43
5:E:62:ARG:NH2	5:E:83:ALA:O	2.50	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:29:PHE:HE1	15:2:201:HIS:CD2	2.37	0.43
13:N:36:GLU:HA	13:N:39:SER:HB2	2.00	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
14:1:162:CYS:CA	14:1:165:GLN:HB2	2.21	0.43
16:3:131:GLN:HB3	16:3:134:TYR:CE1	2.54	0.43
17:4:49:ARG:C	17:4:51:ALA:H	2.26	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
1:A:427:ARG:O	1:A:428:TYR:C	2.62	0.43
1:A:557:LEU:O	1:A:558:LYS:C	2.62	0.43
18:A:1123:CLA:HHD	18:A:1123:CLA:CBC	2.31	0.43
2:B:155:LEU:O	2:B:158:GLN:N	2.51	0.43
2:B:533:ILE:HG21	2:B:579:ALA:CA	2.49	0.43
2:B:534:LEU:O	2:B:538:ALA:HB3	2.19	0.43
2:B:536:LYS:HB3	2:B:536:LYS:HZ2	1.84	0.43
18:B:1205:CLA:HMD3	18:B:1224:CLA:O1A	2.19	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
18:B:1207:CLA:H41	12:L:91:LEU:HD21	2.01	0.43
18:B:1227:CLA:CBC	18:B:1242:CLA:HMD3	2.49	0.43
3:C:8:TYR:CD1	4:D:137:ILE:HB	2.53	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
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
12:L:128:ASP:HB3	12:L:129:GLN:H	1.67	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
14:1:43: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
1:A:253:ASP:CA	1:A:256:ALA:HB3	2.49	0.43
1:A:360:ILE:C	1:A:362:LEU:H	2.26	0.43
1:A:401:TRP:HB3	18:A:1126:CLA:HMC2	2.01	0.43
1:A:646:SER:HB2	1:A:652:TRP:CZ2	2.54	0.43
1:A:725:LEU:HD12	18:A:1140:CLA:HMD2	2.01	0.43
1:A:733:VAL:O	1:A:735:VAL:N	2.51	0.43
18:A:1124:CLA:CHC	18:A:1137:CLA:CGA	2.81	0.43
2:B:166:SER:C	2:B:168:PHE:H	2.27	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: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
2:B:705:ALA:CB	19:B:5002:PQN:C8	2.93	0.43
18:B:1217:CLA:O1A	18:B:1217:CLA:C4A	2.67	0.43
18:B:1224:CLA:CBC	18:B:1225:CLA:HBB1	2.49	0.43
4:D:46:TYR:CG	4:D:80:LYS:HB3	2.54	0.43
5:E:38:ILE:HD12	5:E:38:ILE:N	2.34	0.43
6:F:33:ALA:HA	6:F:42:ILE:HD11	2.01	0.43
8:H:60:GLY:O	8:H:61:GLY:C	2.62	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:N	2.76	0.43
14:1:160:GLY:HA2	18:1:1003:CLA:C2C	2.49	0.43
15:2:193:PHE:C	15:2:195:HIS:NE2	2.77	0.43
16:3:78:ILE:HB	16:3:79:LEU:O	2.19	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:63:ASP:N	18:A:1128:CLA:HAA2	2.16	0.42
1:A:71:LEU:C	1:A:73:GLU:N	2.77	0.42
1:A:78:VAL:HG21	1:A:354:TRP:CD2	2.53	0.42
1:A:149:PHE:O	1:A:153:TRP:CG	2.72	0.42
1:A:750:PHE:HZ	18:A:1126:CLA:CMB	2.32	0.42
18:A:1140:CLA:H3A	18:A:1140:CLA:HBA2	1.54	0.42
2:B:42:LEU:O	2:B:45:ASN:HB2	2.19	0.42
2:B:65:LEU:HG	2:B:124:TRP:CZ3	2.54	0.42
2:B:90:ALA:H	2:B:91:ILE:HD12	1.84	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:558:PRO:CA	2:B:702:ILE:HD11	2.49	0.42
2:B:710:LEU:HD12	2:B:710:LEU:HA	1.84	0.42
18:B:1217:CLA:HBA1	18:B:1217:CLA:CHA	2.48	0.42
18:B:1236:CLA:O1D	18:B:1236:CLA:OBD	2.35	0.42
4:D:53:PRO:CB	4:D:95:LYS:HD2	2.49	0.42
5:E:79:THR:O	5:E:80:ASN:C	2.61	0.42
6:F:73:VAL:HG21	6:F:82:GLU:N	2.33	0.42
9:I:14:LEU:HD22	9:I:14:LEU:HA	1.85	0.42
9:I:15:LEU:O	9:I:16:PHE:C	2.60	0.42
10:J:33:PHE:O	10:J:34:PRO:C	2.62	0.42
12:L:41:PRO:O	12:L:42:ALA:C	2.62	0.42
12:L:138:LYS:N	12:L:138:LYS:HD2	2.34	0.42
18:L:1502:CLA:O2D	18:L:1502:CLA:OBD	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
15:2:86:GLU:OE1	17:4:184:GLN:HB3	2.19	0.42
15:2:117:GLY:C	15:2:119:VAL:N	2.75	0.42
18:3:3002:CLA:C3B	18:3:3007:CLA:C3C	2.97	0.42
17:4:41:VAL:CG2	17:4:42:GLN:N	2.53	0.42
17:4:144:ALA:N	17:4:145:PRO:CD	2.71	0.42
1:A:71:LEU:HD23	1:A:74:ILE:HG23	2.01	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:418:MET:C	1:A:420:ARG:H	2.27	0.42
1:A:433:ASP:O	1:A:434:ARG:C	2.62	0.42
1:A:567:ARG:O	4:D:79:ARG:NH1	2.51	0.42
1:A:595:TRP:C	1:A:595:TRP:CE3	2.98	0.42
1:A:692:PHE:HA	19:A:5001:PQN:H9	2.01	0.42
2:B:81:PRO:HB3	2:B:130:ARG:HH22	1.84	0.42
2:B:88:ALA:N	2:B:116:ALA:HB2	2.35	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:254:ILE:CG2	18:B:1212:CLA:HBC1	2.50	0.42
2:B:456:GLU:HB2	6:F:70:HIS:HB3	2.01	0.42
2:B:550:LYS:NZ	2:B:570:ILE:O	2.52	0.42
6:F:5:LEU:O	6:F:63:CYS:O	2.37	0.42
6:F:76:ASP:C	6:F:77:GLN:O	2.59	0.42
12:L:118:LEU:HB3	12:L:119:THR:HA	2.00	0.42
14:1:173:PRO:O	14:1:175:GLU:N	2.52	0.42
15:2:86:GLU:HG2	17:4:184:GLN:OE1	2.18	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
1:A:144:GLN:HE21	1:A:144:GLN:HB3	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
18:A:1107:CLA:HMB1	10:J:27:ILE:HD11	2.00	0.42
2:B:119:GLY:O	2:B:121:TYR:N	2.52	0.42
2:B:155:LEU:C	2:B:157:LEU:N	2.77	0.42
2:B:209:TRP:O	2:B:210:ASN:C	2.62	0.42
2:B:323:TYR:C	2:B:325:THR:N	2.77	0.42
2:B:344:ILE:O	2:B:348:VAL:N	2.53	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
2:B:599:ILE:O	2:B:600:THR:C	2.63	0.42
18:B:1205:CLA:CMD	18:B:1224:CLA:O1A	2.68	0.42
18:B:1237:CLA:H52	18:B:1237:CLA:H11	1.70	0.42
3:C:72:GLU:OE2	3:C:77:MET:CG	2.64	0.42
4:D:52:SER:CB	4:D:68:MET:HB2	2.48	0.42
4:D:102:ARG:HH11	4:D:110:GLN:HE21	1.52	0.42
6:F:83:PHE:O	6:F:86:PRO:C	2.61	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:54:LEU:O	8:H:55:LYS:C	2.62	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
13:N:81:VAL:CG1	13:N:83:TRP:HA	2.48	0.42
14:1:72:GLN:C	14:1:73:GLU:OE1	2.61	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
15:2:20:ASP:OD2	15:2:23:LEU:HD21	2.19	0.42
15:2:174:VAL:HG12	15:2:175:MET:N	2.34	0.42
16:3:83:GLY:HA2	16:3:84:LEU:C	2.43	0.42
17:4:109:ILE:O	17:4:110:LYS:C	2.62	0.42
1:A:46:LYS:HB3	5:E:76:ASN:HD21	1.84	0.42
1:A:62:HIS:CG	18:A:1128:CLA:O1A	2.73	0.42
1:A:81:ALA:HB1	1:A:82:HIS:C	2.40	0.42
1:A:219:ALA:O	1:A:223:VAL:HG22	2.19	0.42
1:A:273:ASN:O	1:A:274:TRP:C	2.62	0.42
1:A:367:SER:HA	1:A:370:ILE:CG2	2.45	0.42
1:A:447:ASN:OD1	2:B:674:LEU:HD21	2.19	0.42
1:A:503:THR:O	1:A:504:ALA:HB3	2.19	0.42
1:A:751:LEU:HD12	1:A:752:ALA:H	1.82	0.42
18:A:1132:CLA:HHB	12:L:72:GLY:O	2.18	0.42
2:B:91:ILE:CG1	2:B:114:ASN:ND2	2.81	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: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
2:B:714:SER:O	2:B:717:TYR:N	2.53	0.42
18:B:1239:CLA:H11	19:B:5002:PQN:C27	2.47	0.42
4:D:58:PHE:CE1	4:D:66:ALA:HB3	2.54	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
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
12:L:87:ALA:C	12:L:90:GLY:N	2.75	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
16:3:84:LEU:HA	16:3:85:ILE:C	2.44	0.42
17:4:60:LEU:HD11	17:4:76:TYR:OH	2.19	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:379:MET:HE3	1:A:379:MET:HB2	1.85	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:465:ASP:O	1:A:467:MET:N	2.52	0.42
1:A:654:ARG:CG	2:B:633:ASN:OD1	2.67	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:92:TRP:HD1	9:I:9:VAL:HG11	1.80	0.42
2:B:287:GLY:HA2	18:B:1218:CLA:HMC3	1.95	0.42
2:B:687:LEU:HD11	12:L:40:LEU:CD1	2.47	0.42
3:C:2:SER:C	3:C:3:HIS:ND1	2.77	0.42
3:C:30:PRO:HD2	3:C:31:TRP:H	1.83	0.42
3:C:49:VAL:HG13	3:C:51:CYS:HB2	2.02	0.42
6:F:60:GLY:C	6:F:61:LEU:HG	2.44	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
18:L:1502:CLA:H42	18:L:1504:CLA:HMA2	2.01	0.42
13:N:48:GLY:HA3	13:N:50:GLN:H	1.73	0.42
14:1:75:ALA:C	14:1:77:LEU:N	2.76	0.42
16:3:56:ALA:C	16:3:58:GLY:N	2.77	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
16:3:212:ASN:HB2	16:3:213:LEU:C	2.40	0.42
1:A:205:HIS:CD2	18:A:1108:CLA:HMD2	2.54	0.42
1:A:239:PRO:HB2	1:A:240:LYS:H	1.43	0.42
1:A:262:PHE:HD2	1:A:262:PHE:HA	1.71	0.42
1:A:293:GLY:O	1:A:380:PRO:HB2	2.20	0.42
1:A:401:TRP:CE3	1:A:609:ILE:HG21	2.54	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:520:LEU:HD22	1:A:520:LEU:C	2.44	0.42
18:A:1129:CLA:HMA1	18:L:1130:CLA:OBD	2.18	0.42
2:B:31:PHE:C	2:B:33:SER:H	2.28	0.42
2:B:181:GLY:O	2:B:182:LEU:C	2.63	0.42
2:B:232:LEU:HA	2:B:235:GLN:NE2	2.34	0.42
2:B:303:TYR:O	2:B:304:ILE:C	2.60	0.42
2:B:375:HIS:HE1	18:B:1225:CLA:C4A	2.32	0.42
2:B:439:HIS:CB	2:B:443:MET:HE2	2.49	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:627:ASN:OD1	2:B:732:LYS:CD	2.67	0.42
2:B:643:LEU:HD21	2:B:727:ALA:HA	2.01	0.42
2:B:648:TRP:CZ3	20:B:6017:BCR:HC21	2.36	0.42
3:C:12:ILE:O	3:C:38:GLN:HG3	2.19	0.42
6:F:28:SER:C	6:F:30:LYS:N	2.75	0.42
6:F:43:LYS:HG3	6:F:44:ALA:N	2.31	0.42
6:F:61:LEU:O	6:F:62:LEU:C	2.63	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:30:SER:H	12:L:34:ALA:HB2	1.85	0.42
13:N:58:VAL:HA	16:3:86:PRO:O	2.19	0.42
13:N:74:LYS:O	13:N:85:TRP:NE1	2.43	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
17:4:48:GLY:CA	17:4:158:ARG:HH22	2.32	0.42
17:4:194:ILE:HB	17:4:195:VAL:H	1.60	0.42
1:A:83:PHE:O	1:A:84:GLY:C	2.62	0.42
1:A:161:GLU:C	1:A:163:GLN:N	2.75	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:A:1140:CLA:HAC1	19:A:5001:PQN:H152	2.02	0.42
2:B:80:ASP:HA	2:B:81:PRO:HD3	1.70	0.42
2:B:189:ALA:C	18:B:1211:CLA:C2C	2.93	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:O	2:B:580:VAL:CG1	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
18:B:9012:CLA:H3A	18:B:9012:CLA:HBA1	1.68	0.42
3:C:63:LEU:C	3:C:63:LEU:CD1	2.89	0.42
4:D:90:LEU:C	4:D:91:ARG:HD3	2.44	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
14:1:67:ASN:HB3	14:1:68:TRP:H	1.49	0.42
15:2:22:SER:O	15:2:23:LEU:HD21	2.17	0.42
1:A:55:TRP:CH2	18:F:1139:CLA:HBB2	2.55	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:249:ILE:HB	1:A:250:LEU:H	1.42	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:346:LEU:HG	18:A:1122:CLA:HMD3	2.00	0.42
1:A:395:LEU:O	1:A:396:PHE:C	2.62	0.42
1:A:470:LEU:HD23	2:B:96:PHE:CD2	2.55	0.42
1:A:547:PHE:CD1	1:A:548:THR:N	2.88	0.42
1:A:574:ASN:C	1:A:575:LEU:HD22	2.44	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:A:1122:CLA:HBA1	18:A:1122:CLA:H3A	1.91	0.42
2:B:188:LEU:C	2:B:188:LEU:HD23	2.44	0.42
2:B:251:GLY:O	2:B:252:THR:O	2.38	0.42
2:B:465:SER:O	2:B:468:GLY:C	2.63	0.42
2:B:655:LEU:HB2	18:B:9022:CLA:CGA	2.50	0.42
2:B:672:GLN:HE22	2:B:698:VAL:CB	2.33	0.42
2:B:700:LEU:HD12	19:B:5002:PQN:C4	2.49	0.42
18:B:1212:CLA:CHD	18:B:1212:CLA:CBC	2.86	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
8:H:26:SER:CB	8:H:29:PRO:HB3	2.50	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
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
17:4:49: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
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
1:A:48:PRO:HB3	1:A:53:TRP:HZ3	1.81	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:547:PHE:O	1:A:548:THR:C	2.63	0.42
1:A:599:PHE:O	1:A:599:PHE:CD1	2.73	0.42
1:A:658:TRP:CD1	2:B:625:TRP:HE1	2.28	0.42
1:A:675:TYR:CE1	1:A:751:LEU:HD11	2.54	0.42
1:A:751:LEU:HD22	1:A:751:LEU:HA	1.86	0.42
2:B:176:ASN:OD1	2:B:291:TYR:HD1	2.02	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
18:B:1209:CLA:H61	18:B:1209:CLA:H41	1.70	0.42
18:B:1212:CLA:HED3	18:B:1212:CLA:C4D	2.50	0.42
3:C:6:LYS:C	3:C:7:ILE:HG12	2.45	0.42
3:C:32:GLY:O	5:E:60:LYS:HD3	2.19	0.42
6:F:5:LEU:HB3	6:F:62:LEU:CG	2.48	0.42
6:F:38:PRO:O	6:F:39:ALA:CB	2.68	0.42
6:F:92:TYR:CE1	6:F:96:TRP:CZ3	3.08	0.42
6:F:111:GLU:O	6:F:111:GLU:OE1	2.38	0.42
9:I:24:LEU:C	9:I:26:LEU:CB	2.88	0.42
13:N:72:LYS:C	13:N:74:LYS:H	2.26	0.42
14:1:9:PRO:HA	17:4:110:LYS:CD	2.50	0.42
14:1:24:PHE:O	14:1:25:ASP:C	2.63	0.42
14:1:60:PRO:HD3	18:1:1006:CLA:C3D	2.49	0.42
15:2:86:GLU:CD	17:4:187:SER:HB3	2.43	0.42
15:2:180:GLN:HB3	15:2:182:ILE:HG12	2.00	0.42
17:4:91:PHE:HB3	17:4:92:VAL:H	1.64	0.42
17:4:166:GLY:O	17:4:170:GLN:NE2	2.53	0.42
1:A:84:GLY:O	1:A:86:LEU:C	2.63	0.42
1:A:163:GLN:C	1:A:166:CYS:H	2.27	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: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:218:TYR:HE2	2:B:253:ALA:HA	1.85	0.42
2:B:355:LEU:CD2	18:B:1214:CLA:CED	2.96	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:569:ASP:CG	2:B:706:ARG:NH2	2.71	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
3:C:31:TRP:C	3:C:31:TRP:CE3	2.98	0.42
4:D:41:GLN:H	4:D:41:GLN:HG3	1.64	0.42
4:D:125:PRO:HB2	4:D:126:GLY:H	1.56	0.42
5:E:40:ARG:O	5:E:42:GLU:N	2.53	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:F:110:ASP:C	6:F:112:LYS:N	2.77	0.42
7:G:61:ASN:O	7:G:64:VAL:N	2.53	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
14:1:13:TYR:CB	17:4:107:GLN:NE2	2.82	0.42
14:1:150:ASN:O	14:1:152:ARG:N	2.53	0.42
14:1:158:PHE:CD2	14:1:158:PHE:C	2.97	0.42
15:2:23:LEU:CB	15:2:25:GLY:CA	2.80	0.42
15:2:97:VAL:O	15:2:101:PHE:CD1	2.73	0.42
15:2:177:ALA:C	15:2:178:TRP:CE3	2.92	0.42
1:A:196:PHE:CD2	1:A:196:PHE:O	2.73	0.41
1:A:461:TYR:O	1:A:464:ASN:N	2.53	0.41
18:A:1129:CLA:HMA2	18:L:1130:CLA:OBD	2.18	0.41
2:B:319:HIS:C	2:B:321:GLY:N	2.77	0.41
2:B:332:PHE:CA	2:B:335:GLY:HA3	2.49	0.41
2:B:334:LEU:O	2:B:389:HIS:CB	2.68	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:559:CYS:HA	2:B:570:ILE:HG22	2.02	0.41
2:B:616:LEU:C	2:B:618:GLY:N	2.74	0.41
2:B:722:ALA:HB2	18:B:1224:CLA:HBB2	2.01	0.41
6:F:13:GLN:O	6:F:14:PHE:HB2	2.15	0.41
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
7:G:22:VAL:CA	7:G:23:PHE:HD2	2.32	0.41
8:H:62:GLY:C	9:I:15:LEU:HD12	2.45	0.41
8:H:88:LYS:C	8:H:90:GLY:H	2.27	0.41
12:L:168:LYS:C	12:L:168:LYS:HE2	2.45	0.41
13:N:35:VAL:O	13:N:35:VAL:CG1	2.68	0.41
15:2:94:LEU:O	15:2:96:ILE:HG13	2.20	0.41
16:3:132:ASP:C	16:3:133:TRP:HD1	2.27	0.41
17:4:181:ASN:O	17:4:183:LEU:N	2.45	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: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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:571:SER:HB2	2:B:574:ASP:CG	2.45	0.41
2:B:595:HIS:HB3	2:B:623:TYR:CE1	2.55	0.41
2:B:656:VAL:HA	18:B:1239:CLA:CBB	2.49	0.41
2:B:682:HIS:CB	18:B:1237:CLA:CMA	2.76	0.41
18:B:1235:CLA:HBB2	18:B:1235:CLA:H72	2.02	0.41
3:C:28:MET:O	4:D:123:VAL:HA	2.19	0.41
4:D:102:ARG:NE	4:D:108:GLU:OE2	2.53	0.41
7:G:76:SER:HB2	7:G:77:ILE:H	1.72	0.41
9:I:1:MET:HE3	9:I:1:MET:H3	1.84	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
15:2:94:LEU:O	15:2:95:PHE:C	2.63	0.41
16:3:217:LEU:N	16:3:218:ALA:HB3	2.34	0.41
1:A:57:LEU:HD23	1:A:57:LEU:O	2.20	0.41
1:A:200:GLU:CG	1:A:327:ILE:HG12	2.51	0.41
1:A:290:LEU:C	1:A:291:THR:HG22	2.32	0.41
1:A:325:HIS:CE1	18:A:1120:CLA:CHA	3.03	0.41
1:A:349:ILE:HD12	1:A:352:THR:CB	2.48	0.41
1:A:454:GLY:C	1:A:456:HIS:N	2.65	0.41
1:A:473:PRO:O	1:A:476:MET:SD	2.78	0.41
1:A:627:THR:O	1:A:628:ILE:HB	2.19	0.41
1:A:700:TRP:CH2	19:A:5001:PQN:H2M3	2.54	0.41
1:A:707:ILE:HG12	18:B:1138:CLA:HED3	2.02	0.41
1:A:751:LEU:O	1:A:754:ILE:HG22	2.19	0.41
18:A:1129:CLA:HBB1	18:L:1130:CLA:HBC3	2.00	0.41
2:B:16:PRO:O	2:B:696:LYS:HG3	2.20	0.41
2:B:74:PHE:HD2	2:B:132:ASN:OD1	2.02	0.41
2:B:122:GLN:HE21	2:B:122:GLN:N	2.18	0.41
2:B:195:VAL:HG13	2:B:254:ILE:CD1	2.48	0.41
2:B:322:LEU:HD12	2:B:322:LEU:HA	1.74	0.41
2:B:330:ILE:HD13	18:B:1202:CLA:HAC2	2.01	0.41
2:B:382:ILE:O	2:B:383:MET:C	2.64	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
18:B:1224:CLA:H11	18:B:1224:CLA:H51	1.76	0.41
4:D:52:SER:OG	4:D:72:PRO:CD	2.69	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
6:F:16:LYS:C	6:F:18:GLU:N	2.74	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:F:77:GLN:HA	6:F:80:TRP:CZ2	2.56	0.41
6:F:150:VAL:HA	6:F:151:ASP:CG	2.45	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
13:N:51:ASP:H	13:N:52:LEU:HB2	1.73	0.41
14:1:70:LYS:C	14:1:73:GLU:OE2	2.63	0.41
14:1:109:GLU:C	14:1:110:HIS:CG	2.98	0.41
15:2:85:GLN:C	15:2:86:GLU:CG	2.92	0.41
16:3:119:MET:HE2	18:3:3010:CLA:CHA	2.50	0.41
16:3:199:PHE:CD1	16:3:199:PHE:C	2.99	0.41
1:A:97:TYR:CE2	1:A:153:TRP:CZ3	3.05	0.41
1:A:395:LEU:C	1:A:397:THR:H	2.28	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
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
2:B:59:LEU:O	2:B:59:LEU:HD23	2.19	0.41
2:B:103:ALA:CB	2:B:104:PHE:CD1	2.90	0.41
2:B:193:HIS:NE2	2:B:197:VAL:O	2.53	0.41
2:B:311:PRO:HA	18:B:1301:CLA:HHD	2.03	0.41
2:B:391:PRO:HD3	2:B:538:ALA:HB1	1.97	0.41
2:B:534:LEU:HD13	2:B:534:LEU:HA	1.64	0.41
2:B:582:TRP:HZ2	18:B:9012:CLA:CBB	2.33	0.41
3:C:71:HIS:N	3:C:71:HIS:ND1	2.48	0.41
6:F:12:LYS:HD2	6:F:12:LYS:C	2.41	0.41
9:I:4:LEU:HB2	9:I:5:PRO:HA	2.02	0.41
12:L:70:LYS:CG	12:L:75:ARG:HG3	2.38	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
14:1:9:PRO:HA	17:4:110:LYS:HD2	2.02	0.41
14:1:84:TYR:CZ	14:1:90:PRO:HD2	2.55	0.41
14:1:97:ILE:C	14:1:99:ALA:H	2.28	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:HHB	2.50	0.41
1:A:50:THR:HA	1:A:721:GLN:N	2.35	0.41
1:A:127:VAL:HG12	10:J:30:ASN:ND2	2.36	0.41
1:A:242:ILE:O	1:A:242:ILE:HG23	2.21	0.41
1:A:292:GLY:O	1:A:294:LEU:N	2.54	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:428:TYR:CZ	4:D:57:ILE:HG21	2.56	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:84:VAL:O	2:B:85:ARG:CZ	2.68	0.41
2:B:348:VAL:CG2	18:B:1225:CLA:CMD	2.84	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:691:ILE:HG22	12:L:102:TYR:HE1	1.84	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
4:D:88:THR:O	4:D:91:ARG:CB	2.68	0.41
6:F:27:ALA:C	6:F:29:LEU:N	2.78	0.41
7:G:83:TYR:HA	7:G:84:TYR:C	2.39	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
12:L:53:GLY:HA2	12:L:56:VAL:HG13	2.01	0.41
20:L:6020:BCR:H371	20:L:6020:BCR:H24C	1.78	0.41
13:N:36:GLU:CB	13:N:37:PHE:CA	2.74	0.41
14:1:47:CYS:O	14:1:151:GLY:HA2	2.21	0.41
14:1:150:ASN:HA	14:1:153:LEU:HD23	2.03	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
17:4:60:LEU:CD1	17:4:76:TYR:OH	2.69	0.41
17:4:126:LEU:HD12	17:4:126:LEU:N	2.36	0.41
1:A:35:ALA:HB1	1:A:36:LYS:O	2.20	0.41
1:A:308:ILE:HA	1:A:311:LEU:CB	2.49	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:675:TYR:CZ	1:A:751:LEU:HD11	2.54	0.41
1:A:718:PRO:O	1:A:719:ALA:CB	2.68	0.41
2:B:55:ALA:O	2:B:58:PHE:HB2	2.20	0.41
2:B:65:LEU:C	2:B:67:HIS:N	2.78	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
2:B:141:PHE:C	2:B:141:PHE:CD2	2.99	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:518:LEU:HD23	2:B:614:THR:HG22	1.97	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:558:PRO:O	2:B:559:CYS:C	2.64	0.41
2:B:594:TRP:N	2:B:596:TRP:O	2.54	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
12:L:17:ASP:HA	12:L:18:PRO:HD2	1.57	0.41
12:L:125:LYS:O	12:L:125:LYS:HG2	2.19	0.41
14:1:75:ALA:C	14:1:77:LEU:H	2.27	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
1:A:108:ALA:HB1	1:A:138:GLY:O	2.20	0.41
1:A:663:GLN:OE1	1:A:663:GLN:CA	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
18:A:1132:CLA:C3A	18:B:1207:CLA:HMD3	2.51	0.41
2:B:20:ARG:HH22	9:I:28:VAL:CB	2.32	0.41
2:B:51:PHE:HB2	2:B:52:GLY:H	1.60	0.41
2:B:91:ILE:HG12	2:B:114:ASN:HD21	1.85	0.41
2:B:391:PRO:CG	2:B:538:ALA:HA	2.50	0.41
2:B:415:LYS:HZ2	2:B:540:ASP:CA	2.29	0.41
2:B:423:SER:OG	2:B:424:TRP:N	2.47	0.41
2:B:455:ILE:O	2:B:455:ILE:HG13	2.20	0.41
2:B:517:PHE:O	2:B:521:HIS:HB2	2.20	0.41
2:B:577:TYR:CE1	2:B:706:ARG:HB2	2.56	0.41
2:B:697:PRO:HB3	18:B:1238:CLA:CMC	2.51	0.41
2:B:729:THR:O	2:B:730:SER:HB2	2.21	0.41
18:B:1222:CLA:HBB2	18:B:1236:CLA:HMB1	2.01	0.41
18:B:1228:CLA:C1B	20:F:6016:BCR:H341	2.50	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
6:F:78:ARG:HE	6:F:78:ARG:HB2	1.58	0.41
13:N:69:CYS:HB2	13:N:71:GLY:C	2.45	0.41
14:1:181:LEU:CA	14:1:182:ALA:C	2.91	0.41
15:2:94:LEU:O	15:2:96:ILE:N	2.54	0.41
15:2:178:TRP:CB	15:2:183:TYR:HH	2.32	0.41
17:4:56:ALA:HA	17:4:59:LEU:HD13	2.01	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
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:568:LEU:HD22	4:D:79:ARG:CZ	2.51	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
18:A:1135:CLA:HBA1	18:A:1135:CLA:H3A	1.63	0.41
2:B:103:ALA:C	2:B:104:PHE:CD1	2.99	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:547:MET:HE2	3:C:66:ARG:HE	1.84	0.41
2:B:666:SER:O	19:B:5002:PQN:C9	2.68	0.41
2:B:666:SER:O	2:B:666:SER:OG	2.39	0.41
4:D:37:LEU:O	4:D:38:ARG:C	2.63	0.41
4:D:84:LEU:O	4:D:85:ALA:C	2.63	0.41
7:G:34:GLN:HB3	7:G:36:PRO:CD	2.51	0.41
12:L:40:LEU:C	12:L:42:ALA:H	2.28	0.41
12:L:89:ALA:O	12:L:90:GLY:C	2.63	0.41
13:N:32:ALA:O	13:N:35:VAL:HB	2.21	0.41
17:4:105:ARG:HG3	17:4:105:ARG:H	1.72	0.41
17:4:136:GLY:C	17:4:141:LEU:HD21	2.45	0.41
1:A:33:GLN:CD	18:A:1109:CLA:HHC	2.46	0.41
1:A:121:GLN:HE21	18:A:1107:CLA:CED	2.34	0.41
1:A:158:ILE:O	1:A:159:THR:HG23	2.21	0.41
1:A:171:ALA:C	1:A:174:PHE:HB3	2.46	0.41
1:A:204:ASN:ND2	1:A:314:GLY:C	2.78	0.41
1:A:204:ASN:HD21	1:A:316:MET:H	1.69	0.41
1:A:241:GLU:H	1:A:241:GLU:HG3	1.73	0.41
1:A:302:HIS:C	1:A:303:HIS:HD1	2.20	0.41
1:A:492:ILE:H	1:A:493:GLN:CA	2.32	0.41
1:A:502:THR:OG1	1:A:503:THR:N	2.54	0.41
1:A:715:LYS:O	6:F:106:ILE:HD11	2.20	0.41
1:A:725:LEU:HD22	19:A:5001:PQN:C5	2.48	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
18:A:1129:CLA:HAA2	18:A:1129:CLA:CBD	2.45	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
18:A:1131:CLA:HED3	18:A:1131:CLA:OBD	2.21	0.41
2:B:42:LEU:HA	2:B:45:ASN:HD22	1.86	0.41
2:B:65:LEU:O	2:B:68:VAL:N	2.54	0.41
2:B:78:VAL:HB	2:B:130:ARG:HG2	2.02	0.41
2:B:89:HIS:O	2:B:90:ALA:HB2	2.18	0.41
2:B:142:LEU:HD13	2:B:142:LEU:HA	1.50	0.41
2:B:192:GLY:C	2:B:196:HIS:CE1	2.99	0.41
2:B:216:LEU:H	2:B:217:PRO:CD	2.34	0.41
2:B:273:VAL:HG22	18:B:1214:CLA:HMA2	2.01	0.41
2:B:294:ASN:OD1	18:B:1209:CLA:HMA1	2.20	0.41
2:B:373:THR:O	2:B:377:TYR:N	2.52	0.41
2:B:421:HIS:N	2:B:423:SER:OG	2.54	0.41
2:B:440:ASN:C	2:B:615:TYR:HB2	2.45	0.41
2:B:453:ILE:O	2:B:455:ILE:N	2.54	0.41
2:B:591:THR:O	2:B:721:TYR:OH	2.36	0.41
2:B:616:LEU:O	2:B:617:MET:C	2.64	0.41
2:B:628:SER:C	2:B:630:GLN:N	2.70	0.41
2:B:632:ILE:HD12	2:B:647:ALA:HA	2.03	0.41
18:B:1235:CLA:HBC3	18:B:1235:CLA:HHD	2.03	0.41
3:C:42:ALA:HB1	3:C:45:THR:HG23	1.98	0.41
3:C:63:LEU:HD22	3:C:63:LEU:C	2.45	0.41
4:D:47:VAL:HG12	4:D:48:ILE:N	2.36	0.41
4:D:136:SER:N	4:D:139:LYS:NZ	2.60	0.41
5:E:32:ARG:NH2	5:E:54:ALA:HB2	2.36	0.41
5:E:52:VAL:O	5:E:53:VAL:C	2.64	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:26:SER:HG	8:H:27:ASP:C	2.24	0.41
9:I:25:PHE:O	9:I:25:PHE:HD2	1.95	0.41
9:I:28:VAL:HB	9:I:29:GLU:H	1.47	0.41
9:I:28:VAL:C	9:I:30:LYS:H	2.29	0.41
10:J:24:GLY:O	10:J:26:LEU:N	2.54	0.41
10:J:26:LEU:CA	10:J:29:ILE:HG22	2.51	0.41
18:J:2107:CLA:H91	18:J:2107:CLA:HBA2	2.03	0.41
12:L:10:VAL:O	12:L:11:ILE:O	2.37	0.41
12:L:31:PRO:C	12:L:33:ILE:N	2.79	0.41
18:L:1504:CLA:H12	18:L:1504:CLA:H52	1.94	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
14:1:52:LEU:HA	14:1:55:PRO:HG3	2.01	0.41
14:1:54:VAL:N	14:1:55:PRO:HD2	2.35	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
14:1:94:LEU:CB	14:1:95:PRO:HD2	2.46	0.41
14:1:97:ILE:HG23	14:1:98:LEU:N	2.36	0.41
14:1:112:ARG:HD2	14:1:112:ARG:C	2.46	0.41
15:2:33:GLY:H	15:2:35:SER:CB	2.31	0.41
15:2:44:ASN:C	15:2:46:GLN:N	2.79	0.41
15:2:62:ILE:HG13	18:2:2006:CLA:C2B	2.50	0.41
15:2:192:LEU:N	15:2:195:HIS:CE1	2.86	0.41
16:3:84:LEU:HG	16:3:85:ILE:CA	2.43	0.41
16:3:121:LEU:O	16:3:125:ALA:HB2	2.21	0.41
17:4:75:TRP:C	17:4:76:TYR:CG	2.98	0.41
17:4:190:TRP:HB3	17:4:191:HIS:H	1.59	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:202:MET:SD	18:A:1123:CLA:HMD2	2.60	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:341:GLN:CD	1:A:344:LYS:HD2	2.46	0.41
1:A:675:TYR:CE2	18:A:1106:CLA:CBC	3.01	0.41
1:A:736:THR:O	1:A:739:LEU:C	2.63	0.41
2:B:273:VAL:HG22	18:B:1214:CLA:HMA3	2.02	0.41
2:B:359:ALA:C	2:B:360:PHE:CG	2.99	0.41
2:B:460:ALA:CB	18:B:1234:CLA:HAA2	2.51	0.41
2:B:548:PRO:HD2	3:C:63:LEU:H	1.86	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
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
4:D:87:GLY:O	4:D:90:LEU:HB2	2.20	0.41
6:F:83:PHE:O	6:F:87:GLY:N	2.54	0.41
6:F:89:LEU:O	6:F:90:PHE:C	2.64	0.41
6:F:105:LEU:HD12	6:F:105:LEU:HA	1.65	0.41
8:H:91:PRO:HA	8:H:92:ARG:HA	1.90	0.41
12:L:44:ARG:O	12:L:45:THR:CB	2.69	0.41
12:L:97:MET:HE1	12:L:98:CYS:HA	2.03	0.41
13:N:58:VAL:HB	16:3:86:PRO:HA	2.01	0.41
13:N:58:VAL:HB	16:3:86:PRO:C	2.43	0.41
13:N:81:VAL:HB	13:N:83:TRP:CA	2.19	0.41
14:1:155:LEU:O	14:1:158:PHE:N	2.50	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
15:2:189:ILE:HG13	15:2:190:ASP:N	2.34	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
16:3:62:ASN:OD1	16:3:62:ASN:N	2.42	0.41
17:4:90:LEU:HD23	17:4:94:GLU:OE1	2.21	0.41
17:4:117:GLN:O	17:4:121:PHE:C	2.64	0.41
1:A:84:GLY:C	1:A:86:LEU:N	2.78	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:570:PRO:HD3	4:D:79:ARG:HH22	1.85	0.40
1:A:621:GLN:NE2	1:A:625:TRP:CZ3	2.89	0.40
18:A:1107:CLA:H43	18:A:1107:CLA:CGA	2.51	0.40
18:A:1129:CLA:H12	18:A:1129:CLA:H51	1.82	0.40
18:A:1131:CLA:HMB2	18:A:1132:CLA:CHC	2.51	0.40
2:B:99:PRO:HB3	2:B:102:GLU:HB3	2.03	0.40
2:B:115:ASN:HB3	2:B:117:TYR:CE1	2.55	0.40
2:B:207:VAL:C	2:B:208:ARG:HG3	2.46	0.40
2:B:317:ARG:HA	2:B:410:ARG:CZ	2.51	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:561:GLY:HA2	21:B:3101:SF4:S2	2.60	0.40
4:D:119:TYR:C	4:D:121:GLU:N	2.77	0.40
5:E:45:TRP:HZ3	5:E:82:TYR:OH	2.04	0.40
5:E:46:PHE:O	5:E:47:LYS:C	2.64	0.40
14:1:54:VAL:N	14:1:55:PRO:CD	2.84	0.40
15:2:17:GLU:OE2	15:2:17:GLU:CA	2.69	0.40
1:A:83:PHE:HD2	1:A:83:PHE:HA	1.77	0.40
1:A:97:TYR:C	1:A:100:GLY:H	2.30	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:701:GLN:O	1:A:703:LEU:N	2.54	0.40
1:A:711:HIS:O	1:A:714:LEU:C	2.64	0.40
2:B:78:VAL:HA	2:B:130:ARG:NH2	2.33	0.40
2:B:79:GLN:HG2	2:B:80:ASP:CG	2.46	0.40
2:B:525:LEU:CG	2:B:526:GLY:N	2.83	0.40
2:B:672:GLN:HE21	3:C:79:LEU:HD22	1.86	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
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
4:D:54:LYS:O	4:D:68:MET:HG3	2.21	0.40
4:D:72:PRO:HD2	4:D:73:ASN:OD1	2.21	0.40
4:D:104:PHE:CD1	4:D:104:PHE:C	2.99	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:D:104:PHE:CE1	4:D:106:SER:C	3.00	0.40
6:F:2:ILE:N	6:F:62:LEU:HD22	2.35	0.40
6:F:59:TYR:N	6:F:59:TYR:HD1	2.19	0.40
7:G:63:PRO:CG	18:G:1248:CLA:C3C	2.99	0.40
12:L:67:PRO:HA	12:L:71:ALA:HB3	2.03	0.40
12:L:158:MET:O	12:L:159:TYR:CG	2.74	0.40
14:1:5:MET:O	14:1:6:PRO:C	2.63	0.40
14:1:188:ASN:CB	14:1:190:GLY:N	2.81	0.40
15:2:163:GLU:HG2	15:2:166:ASN:HB3	2.02	0.40
17:4:158:ARG:NE	17:4:158:ARG:HA	2.36	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:604:TRP:O	1:A:605:MET:C	2.63	0.40
1:A:650:ASN:C	1:A:650:ASN:OD1	2.65	0.40
1:A:697:ARG:NE	1:A:725:LEU:O	2.53	0.40
18:A:1136:CLA:H71	18:A:1137:CLA:CAC	2.20	0.40
2:B:20:ARG:NH2	9:I:28:VAL:CA	2.78	0.40
2:B:85:ARG:NH1	2:B:85:ARG:HA	2.37	0.40
2:B:98:GLN:HE22	8:H:80:THR:CG2	2.35	0.40
2:B:392:ILE:HD13	2:B:392:ILE:HA	1.55	0.40
2:B:422:LEU:N	18:B:1236:CLA:HBB2	2.37	0.40
2:B:453:ILE:HD12	2:B:453:ILE:HA	1.96	0.40
2:B:561:GLY:O	2:B:563:GLY:N	2.54	0.40
2:B:594:TRP:C	2:B:596:TRP:O	2.64	0.40
2:B:596:TRP:CE2	2:B:623:TYR:HB2	2.56	0.40
2:B:596:TRP:HH2	2:B:612:SER:HB2	1.87	0.40
2:B:654:HIS:O	18:B:9022:CLA:HAA2	2.22	0.40
18:B:1214:CLA:CBA	18:B:1223:CLA:C3B	2.99	0.40
18:B:1218:CLA:H52	18:B:1218:CLA:H11	1.90	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
6:F:137:PRO:C	6:F:139:ALA:H	2.18	0.40
7:G:27:GLN:C	7:G:28:ARG:HG2	2.47	0.40
8:H:30:SER:HB2	12:L:35:TRP:CZ2	2.57	0.40
18:I:1204:CLA:H2A	18:I:1204:CLA:O1D	2.22	0.40
12:L:136:TRP:C	12:L:138:LYS:HD2	2.46	0.40
13:N:8:GLU:CG	13:N:11:LYS:CB	2.94	0.40
13:N:58:VAL:CG1	16:3:86:PRO:C	2.91	0.40
15:2:53:ARG:O	15:2:54:TRP:C	2.63	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
17:4:110:LYS:C	17:4:112:PRO:HD3	2.44	0.40
1:A:52:THR:HA	1:A:55:TRP:NE1	2.36	0.40
1:A:63:ASP:HB2	18:A:1128:CLA:HAA1	2.04	0.40
1:A:80:SER:O	1:A:83:PHE:CD1	2.75	0.40
1:A:233:LEU:C	1:A:235:ALA:H	2.29	0.40
1:A:341:GLN:NE2	1:A:344:LYS:CD	2.84	0.40
1:A:458:PHE:CD1	18:B:9022:CLA:HMB1	2.54	0.40
1:A:502:THR:O	1:A:505:PRO:O	2.39	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
18:A:1108:CLA:CBC	18:A:1110:CLA:C2C	2.92	0.40
2:B:36:ASP:O	2:B:41:ARG:CD	2.69	0.40
2:B:74:PHE:CD1	2:B:121:TYR:CZ	2.98	0.40
2:B:283:LEU:HG	18:B:1216:CLA:HMC2	2.03	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:H161	19:B:5002:PQN:H141	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
7:G:8:ILE:O	7:G:10:LEU:C	2.64	0.40
7:G:18:LEU:C	7:G:20:ARG:N	2.80	0.40
7:G:57:LEU:H	7:G:57:LEU:HD23	1.87	0.40
13:N:12:THR:C	13:N:14:LYS:N	2.74	0.40
13:N:71:GLY:HA3	13:N:76:LYS:HB3	2.03	0.40
14:1:52:LEU:HA	14:1:55:PRO:HD3	1.98	0.40
15:2:17:GLU:N	15:2:18:TRP:C	2.79	0.40
16:3:64:ARG:HD3	16:3:65:PHE:CE2	2.56	0.40
16:3:138:SER:N	16:3:139:MET:C	2.80	0.40
17:4:40:PHE:HD1	17:4:40:PHE:HA	1.66	0.40
1:A:42:ARG:HG2	1:A:43:THR:N	2.35	0.40
1:A:177:LEU:HA	1:A:180:PHE:HB3	2.03	0.40
1:A:204:ASN:HD22	1:A:204:ASN:HA	1.57	0.40
1:A:258:LEU:CG	1:A:259:TYR:H	2.35	0.40
1:A:394:SER:O	1:A:395:LEU:C	2.65	0.40
1:A:526:LYS:N	1:A:627:THR:O	2.55	0.40
1:A:571:ASP:O	1:A:572:LYS:C	2.63	0.40
18:A:1103:CLA:HHC	18:A:1103:CLA:HMC3	1.86	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:421:HIS:NE2	18:B:1228:CLA:C1B	2.85	0.40
2:B:641:ASN:C	2:B:643:LEU:H	2.29	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
6:F:14:PHE:CG	6:F:15:ALA:N	2.89	0.40
6:F:76:ASP:C	6:F:80:TRP:CD1	3.00	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
13:N:36:GLU:HB3	13:N:37:PHE:CB	2.50	0.40
15:2:47:ALA:HA	15:2:50:VAL:HG12	2.02	0.40
16:3:112:TYR:C	16:3:113:THR:HG23	2.46	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 (i)

5.3.1 Protein backbone (i)

In the following table, the Percentiles column shows the percent Ramachandran outliers of the chain as a percentile score with respect to all X-ray entries followed by that with respect to entries of similar resolution.

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	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

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
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
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

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Mol	Chain	Res	Type
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
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

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Mol	Chain	Res	Type
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
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

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Mol	Chain	Res	Type
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
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

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Mol	Chain	Res	Type
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
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

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Mol	Chain	Res	Type
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
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

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Mol	Chain	Res	Type
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
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

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Mol	Chain	Res	Type
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
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

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Mol	Chain	Res	Type
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
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

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Mol	Chain	Res	Type
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
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

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Mol	Chain	Res	Type
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
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

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Mol	Chain	Res	Type
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
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

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Mol	Chain	Res	Type
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
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

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Mol	Chain	Res	Type
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
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

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Mol	Chain	Res	Type
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
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

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Mol	Chain	Res	Type
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
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

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Mol	Chain	Res	Type
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
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

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Mol	Chain	Res	Type
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
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

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Mol	Chain	Res	Type
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
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

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Mol	Chain	Res	Type
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
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

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Mol	Chain	Res	Type
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
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

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Mol	Chain	Res	Type
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
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

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Mol	Chain	Res	Type
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
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

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Mol	Chain	Res	Type
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
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 (i)

In the following table, the Percentiles column shows the percent sidechain outliers of the chain as a percentile score with respect to all X-ray entries followed by that with respect to entries of similar resolution.

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
1	A	588/613 (96%)	341 (58%)	247 (42%)	0 0
2	B	598/598 (100%)	387 (65%)	211 (35%)	0 0
3	C	69/69 (100%)	39 (56%)	30 (44%)	0 0
4	D	118/118 (100%)	79 (67%)	39 (33%)	0 0
5	E	55/55 (100%)	38 (69%)	17 (31%)	0 0

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
6	F	127/127 (100%)	83 (65%)	44 (35%)	0	0
7	G	80/80 (100%)	44 (55%)	36 (45%)	0	0
8	H	62/62 (100%)	37 (60%)	25 (40%)	0	0
9	I	26/26 (100%)	17 (65%)	9 (35%)	0	0
10	J	37/37 (100%)	28 (76%)	9 (24%)	1	2
12	L	127/127 (100%)	77 (61%)	50 (39%)	0	0
13	N	74/74 (100%)	45 (61%)	29 (39%)	0	0
14	1	92/147 (63%)	58 (63%)	34 (37%)	0	0
15	2	122/151 (81%)	80 (66%)	42 (34%)	0	0
16	3	74/123 (60%)	44 (60%)	30 (40%)	0	0
17	4	130/139 (94%)	83 (64%)	47 (36%)	0	0
All	All	2379/2546 (93%)	1480 (62%)	899 (38%)	0	0

All (899) 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	51	THR
1	A	53	TRP
1	A	55	TRP
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

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Mol	Chain	Res	Type
1	A	96	MET
1	A	103	PHE
1	A	107	GLU
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
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	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	172	LEU
1	A	173	VAL
1	A	177	LEU
1	A	178	MET
1	A	183	TRP
1	A	192	LYS
1	A	193	LEU
1	A	195	TRP
1	A	199	VAL
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

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Mol	Chain	Res	Type
1	A	230	ASN
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
1	A	257	GLN
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	279	ASP
1	A	281	LEU
1	A	282	THR
1	A	283	PHE
1	A	284	ARG
1	A	288	ASP
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	309	LEU
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

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Mol	Chain	Res	Type
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	368	LEU
1	A	370	ILE
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	397	THR
1	A	399	HIS
1	A	402	ILE
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	435	VAL
1	A	438	HIS
1	A	440	ASP
1	A	443	ILE
1	A	445	HIS
1	A	446	LEU
1	A	447	ASN
1	A	451	ILE
1	A	453	LEU
1	A	455	PHE
1	A	456	HIS
1	A	458	PHE

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Mol	Chain	Res	Type
1	A	462	ILE
1	A	465	ASP
1	A	467	MET
1	A	473	PRO
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	487	VAL
1	A	490	GLN
1	A	495	THR
1	A	496	HIS
1	A	503	THR
1	A	508	THR
1	A	511	THR
1	A	514	THR
1	A	519	ASP
1	A	521	VAL
1	A	523	VAL
1	A	527	VAL
1	A	530	LEU
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	557	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

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Mol	Chain	Res	Type
1	A	578	ARG
1	A	579	PHE
1	A	590	CYS
1	A	591	GLN
1	A	598	VAL
1	A	605	MET
1	A	608	SER
1	A	613	ILE
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	634	VAL
1	A	637	ILE
1	A	638	THR
1	A	644	GLN
1	A	647	ILE
1	A	648	THR
1	A	649	ILE
1	A	654	ARG
1	A	657	LEU
1	A	662	SER
1	A	666	GLN
1	A	671	SER
1	A	672	LEU
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	697	ARG
1	A	702	GLU
1	A	703	LEU
1	A	704	ILE
1	A	706	SER
1	A	708	VAL
1	A	711	HIS

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Mol	Chain	Res	Type
1	A	713	LYS
1	A	714	LEU
1	A	720	THR
1	A	731	ARG
1	A	733	VAL
1	A	736	THR
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	755	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
2	B	15	ASP
2	B	23	PHE
2	B	41	ARG
2	B	42	LEU
2	B	46	ILE
2	B	50	HIS
2	B	53	GLN
2	B	54	LEU
2	B	56	ILE
2	B	59	LEU
2	B	64	ASN
2	B	65	LEU
2	B	68	VAL
2	B	77	TRP
2	B	79	GLN
2	B	84	VAL
2	B	85	ARG
2	B	87	ILE
2	B	102	GLU
2	B	104	PHE
2	B	105	THR
2	B	106	ARG

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Mol	Chain	Res	Type
2	B	110	LEU
2	B	115	ASN
2	B	120	VAL
2	B	122	GLN
2	B	126	THR
2	B	127	ILE
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	161	TRP
2	B	162	LYS
2	B	172	GLU
2	B	174	ARG
2	B	177	HIS
2	B	179	LEU
2	B	182	LEU
2	B	187	SER
2	B	199	ILE
2	B	205	GLU
2	B	209	TRP
2	B	213	LEU
2	B	214	ASP
2	B	215	VAL
2	B	217	PRO
2	B	225	LEU
2	B	227	THR
2	B	232	LEU
2	B	236	ASN
2	B	239	SER
2	B	243	LEU
2	B	248	GLN
2	B	255	LEU
2	B	258	LEU
2	B	266	GLN
2	B	268	LEU
2	B	270	LEU

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Mol	Chain	Res	Type
2	B	276	HIS
2	B	278	LEU
2	B	283	LEU
2	B	286	ILE
2	B	302	LYS
2	B	304	ILE
2	B	308	HIS
2	B	309	ILE
2	B	315	LEU
2	B	317	ARG
2	B	320	LYS
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
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	373	THR
2	B	374	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	412	LEU

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Mol	Chain	Res	Type
2	B	414	HIS
2	B	415	LYS
2	B	418	ILE
2	B	420	SER
2	B	422	LEU
2	B	427	LEU
2	B	432	HIS
2	B	434	LEU
2	B	438	VAL
2	B	439	HIS
2	B	441	ASP
2	B	444	LEU
2	B	448	THR
2	B	452	GLN
2	B	453	ILE
2	B	454	LEU
2	B	455	ILE
2	B	458	ILE
2	B	462	TRP
2	B	463	ILE
2	B	465	SER
2	B	467	HIS
2	B	469	LYS
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
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	517	PHE
2	B	518	LEU
2	B	523	ILE
2	B	525	LEU

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Mol	Chain	Res	Type
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	546	LEU
2	B	549	ASP
2	B	550	LYS
2	B	551	LYS
2	B	560	ASP
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	590	VAL
2	B	593	TYR
2	B	594	TRP
2	B	595	HIS
2	B	596	TRP
2	B	607	SER
2	B	611	GLU
2	B	612	SER
2	B	614	THR
2	B	616	LEU
2	B	620	LEU
2	B	628	SER
2	B	630	GLN
2	B	631	LEU
2	B	643	LEU
2	B	645	VAL
2	B	646	TRP
2	B	654	HIS
2	B	656	VAL
2	B	657	TRP
2	B	659	THR
2	B	663	PHE
2	B	665	ILE
2	B	675	ILE
2	B	676	GLU

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Mol	Chain	Res	Type
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	691	ILE
2	B	692	ARG
2	B	694	ARG
2	B	696	LYS
2	B	698	VAL
2	B	706	ARG
2	B	707	LEU
2	B	710	LEU
2	B	725	LEU
3	C	4	SER
3	C	6	LYS
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	37	LYS
3	C	38	GLN
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

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Mol	Chain	Res	Type
3	C	71	HIS
3	C	72	GLU
3	C	75	ARG
3	C	79	LEU
4	D	20	LEU
4	D	21	ASP
4	D	23	ASN
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	54	LYS
4	D	58	PHE
4	D	60	MET
4	D	62	THR
4	D	67	ILE
4	D	69	ARG
4	D	74	LEU
4	D	75	LEU
4	D	76	LYS
4	D	77	LEU
4	D	84	LEU
4	D	89	ARG
4	D	90	LEU
4	D	91	ARG
4	D	96	ILE
4	D	102	ARG
4	D	104	PHE
4	D	108	GLU
4	D	109	VAL
4	D	111	TYR
4	D	113	HIS
4	D	123	VAL
4	D	128	GLN
4	D	130	VAL
4	D	134	MET
4	D	139	LYS
4	D	144	ILE
4	D	146	VAL
4	D	153	PRO

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Mol	Chain	Res	Type
4	D	156	LEU
5	E	39	LEU
5	E	45	TRP
5	E	53	VAL
5	E	56	ASP
5	E	59	PRO
5	E	62	ARG
5	E	65	VAL
5	E	66	VAL
5	E	72	VAL
5	E	73	ASN
5	E	74	TYR
5	E	76	ASN
5	E	77	ILE
5	E	84	LEU
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	23	LYS
6	F	24	LYS
6	F	25	LEU
6	F	32	TYR
6	F	35	ASP
6	F	42	ILE
6	F	45	THR
6	F	46	MET
6	F	48	LYS
6	F	49	THR
6	F	54	ASP
6	F	59	TYR
6	F	61	LEU
6	F	63	CYS
6	F	68	LEU
6	F	72	ILE
6	F	78	ARG

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Mol	Chain	Res	Type
6	F	80	TRP
6	F	84	ILE
6	F	88	ILE
6	F	93	ILE
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	119	ILE
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
7	G	5	SER
7	G	7	VAL
7	G	8	ILE
7	G	10	LEU
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	41	MET
7	G	43	HIS
7	G	49	THR
7	G	50	ARG
7	G	53	GLU

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Mol	Chain	Res	Type
7	G	56	SER
7	G	60	SER
7	G	62	ASP
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	80	ILE
7	G	83	TYR
7	G	86	LEU
7	G	91	ASN
8	H	24	TYR
8	H	32	TYR
8	H	33	ASN
8	H	41	GLU
8	H	43	PHE
8	H	49	LYS
8	H	50	ARG
8	H	52	LEU
8	H	53	LEU
8	H	54	LEU
8	H	57	LEU
8	H	58	ILE
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	83	PRO
8	H	84	GLN
8	H	85	GLN
8	H	88	LYS
8	H	89	LEU
8	H	92	ARG
8	H	95	ILE
9	I	1	MET
9	I	2	ILE
9	I	4	LEU

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Mol	Chain	Res	Type
9	I	11	LEU
9	I	14	LEU
9	I	21	MET
9	I	24	LEU
9	I	29	GLU
9	I	30	LYS
10	J	5	LYS
10	J	8	LEU
10	J	10	VAL
10	J	13	VAL
10	J	19	PHE
10	J	22	LEU
10	J	25	LEU
10	J	26	LEU
10	J	38	THR
12	L	7	THR
12	L	9	GLN
12	L	10	VAL
12	L	11	ILE
12	L	15	ASN
12	L	20	ILE
12	L	23	LEU
12	L	27	VAL
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	91	LEU
12	L	94	ILE
12	L	96	SER
12	L	100	THR

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Mol	Chain	Res	Type
12	L	101	MET
12	L	107	PHE
12	L	108	LYS
12	L	111	GLU
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	130	LEU
12	L	132	SER
12	L	136	TRP
12	L	138	LYS
12	L	151	VAL
12	L	152	THR
12	L	153	TRP
12	L	157	LEU
12	L	161	LEU
12	L	167	PHE
12	L	168	LYS
13	N	5	GLU
13	N	8	GLU
13	N	11	LYS
13	N	18	ASP
13	N	19	LYS
13	N	21	ARG
13	N	22	LEU
13	N	24	THR
13	N	28	ASN
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

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Mol	Chain	Res	Type
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	58	LEU
14	1	61	GLU
14	1	67	ASN
14	1	69	VAL
14	1	73	GLU
14	1	87	ASN
14	1	96	THR
14	1	97	ILE
14	1	100	ILE
14	1	101	GLU
14	1	103	LEU
14	1	111	GLN
14	1	112	ARG
14	1	113	SER
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	181	LEU

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Mol	Chain	Res	Type
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	32	LEU
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
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

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Mol	Chain	Res	Type
15	2	182	ILE
15	2	189	ILE
16	3	57	TYR
16	3	60	ILE
16	3	62	ASN
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	113	THR
16	3	115	PHE
16	3	116	VAL
16	3	118	GLU
16	3	119	MET
16	3	121	LEU
16	3	122	MET
16	3	124	PHE
16	3	126	GLU
16	3	129	ARG
16	3	138	SER
16	3	139	MET
16	3	141	LYS
16	3	142	GLN
16	3	144	PHE
16	3	200	ILE
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

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Mol	Chain	Res	Type
17	4	82	GLU
17	4	86	SER
17	4	88	SER
17	4	89	THR
17	4	90	LEU
17	4	101	VAL
17	4	103	ILE
17	4	105	ARG
17	4	107	GLN
17	4	116	ASN
17	4	123	GLN
17	4	126	LEU
17	4	137	ILE
17	4	141	LEU
17	4	142	ASN
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	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
17	4	183	LEU
17	4	187	SER
17	4	190	TRP
17	4	194	ILE
17	4	196	GLN
17	4	198	LEU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (110) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	33	GLN

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Mol	Chain	Res	Type
1	A	56	ASN
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	485	GLN
1	A	494	ASN
1	A	525	ASN
1	A	597	HIS
1	A	607	ASN
1	A	621	GLN
1	A	629	ASN
1	A	631	GLN
1	A	650	ASN
1	A	663	GLN
1	A	729	GLN
1	A	737	HIS
2	B	14	GLN
2	B	45	ASN
2	B	53	GLN
2	B	73	ASN
2	B	114	ASN
2	B	122	GLN
2	B	132	ASN
2	B	158	GLN
2	B	170	ASN

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Mol	Chain	Res	Type
2	B	193	HIS
2	B	196	HIS
2	B	211	ASN
2	B	235	GLN
2	B	236	ASN
2	B	248	GLN
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	504	ASN
2	B	521	HIS
2	B	585	ASN
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	128	GLN
4	D	133	ASN
5	E	80	ASN
6	F	152	ASN
6	F	153	ASN
7	G	27	GLN
7	G	30	ASN
7	G	38	GLN
7	G	39	ASN
7	G	43	HIS
7	G	61	ASN
7	G	91	ASN
8	H	33	ASN
8	H	36	GLN

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Mol	Chain	Res	Type
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	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	195	HIS
16	3	127	HIS
17	4	47	ASN
17	4	99	HIS
17	4	111	ASN
17	4	123	GLN
17	4	142	ASN
17	4	156	ASN
17	4	170	GLN
17	4	172	ASN
17	4	191	HIS
17	4	196	GLN

5.3.3 RNA (i)

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates (i)

There are no oligosaccharides in this entry.

5.6 Ligand geometry (i)

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	2	2015	-	24,32,73	2.34	8 (33%)	31,54,113	2.76	17 (54%)
18	CLA	K	1153	-	24,32,73	2.27	8 (33%)	31,54,113	2.72	19 (61%)
18	CLA	2	2003	-	24,32,73	2.33	10 (41%)	31,54,113	2.99	19 (61%)
18	CLA	A	1101	1	24,32,73	2.35	8 (33%)	31,54,113	2.96	19 (61%)
18	CLA	3	3009	-	24,32,73	2.40	9 (37%)	31,54,113	2.80	19 (61%)
18	CLA	A	1113	-	54,58,73	2.44	15 (27%)	64,95,113	3.14	28 (43%)
18	CLA	2	2002	-	24,32,73	2.34	8 (33%)	31,54,113	2.77	18 (58%)
18	CLA	A	1309	-	24,32,73	2.31	8 (33%)	31,54,113	2.77	17 (54%)
18	CLA	4	4001	-	24,32,73	2.37	8 (33%)	31,54,113	2.82	18 (58%)
18	CLA	B	1238	-	58,62,73	2.42	15 (25%)	68,99,113	2.96	30 (44%)
18	CLA	4	4007	-	24,32,73	2.40	8 (33%)	31,54,113	2.83	18 (58%)
18	CLA	A	1123	-	59,63,73	2.42	17 (28%)	70,101,113	2.81	25 (35%)
18	CLA	B	1223	2	24,32,73	2.39	9 (37%)	31,54,113	2.83	17 (54%)
18	CLA	A	1103	1	51,55,73	2.51	15 (29%)	60,91,113	3.10	23 (38%)
18	CLA	B	1222	-	69,73,73	2.12	13 (18%)	82,113,113	2.49	29 (35%)
18	CLA	1	1001	-	24,32,73	2.40	8 (33%)	31,54,113	2.73	18 (58%)
18	CLA	4	4011	-	24,32,73	2.32	8 (33%)	31,54,113	2.75	17 (54%)
18	CLA	B	1226	18	24,32,73	2.37	8 (33%)	31,54,113	2.78	19 (61%)
18	CLA	I	1204	-	59,63,73	2.36	16 (27%)	70,101,113	2.67	26 (37%)
20	BCR	L	6020	-	41,41,41	1.66	3 (7%)	56,56,56	4.94	25 (44%)
18	CLA	A	1122	-	59,63,73	2.41	17 (28%)	70,101,113	2.82	27 (38%)
18	CLA	A	9013	-	50,54,73	2.51	16 (32%)	59,90,113	2.80	25 (42%)
18	CLA	A	1105	1	24,32,73	2.30	8 (33%)	31,54,113	2.81	18 (58%)
18	CLA	A	1106	-	45,49,73	2.46	14 (31%)	54,84,113	3.47	26 (48%)
18	CLA	A	1140	1	59,63,73	2.39	15 (25%)	70,101,113	2.91	27 (38%)
18	CLA	3	3006	16	24,32,73	2.33	8 (33%)	31,54,113	2.79	19 (61%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\| > 2$	Counts	RMSZ	$\#\|Z\| > 2$
18	CLA	1	1013	-	24,32,73	2.37	8 (33%)	31,54,113	2.77	18 (58%)
18	CLA	F	1139	-	47,52,73	2.49	12 (25%)	55,87,113	3.02	24 (43%)
18	CLA	1	1006	-	24,32,73	2.33	8 (33%)	31,54,113	2.80	17 (54%)
18	CLA	4	4013	-	24,32,73	2.36	8 (33%)	31,54,113	2.85	18 (58%)
18	CLA	B	1205	2	59,63,73	2.31	15 (25%)	70,101,113	3.00	26 (37%)
18	CLA	4	1009	-	24,32,73	2.40	7 (29%)	31,54,113	2.73	17 (54%)
18	CLA	B	1230	-	24,32,73	2.34	8 (33%)	31,54,113	2.71	17 (54%)
18	CLA	A	1115	-	51,55,73	2.50	17 (33%)	60,91,113	3.00	26 (43%)
18	CLA	4	1304	-	59,63,73	2.32	14 (23%)	70,101,113	2.69	27 (38%)
18	CLA	2	2001	-	24,32,73	2.36	8 (33%)	31,54,113	2.77	17 (54%)
18	CLA	B	1235	-	59,63,73	2.38	16 (27%)	70,101,113	2.78	23 (32%)
18	CLA	B	1212	-	64,68,73	2.25	15 (23%)	76,107,113	2.69	26 (34%)
18	CLA	F	1305	-	24,32,73	2.31	8 (33%)	31,54,113	2.81	18 (58%)
18	CLA	B	1242	-	51,55,73	2.57	17 (33%)	60,91,113	3.03	21 (35%)
18	CLA	3	3004	-	24,32,73	2.37	9 (37%)	31,54,113	2.84	19 (61%)
18	CLA	A	1144	-	24,32,73	2.30	8 (33%)	31,54,113	2.87	18 (58%)
18	CLA	F	4015	-	24,32,73	2.33	8 (33%)	31,54,113	2.89	19 (61%)
18	CLA	A	1152	-	24,32,73	2.33	8 (33%)	31,54,113	2.76	17 (54%)
18	CLA	1	1010	-	24,32,73	2.36	8 (33%)	31,54,113	2.79	19 (61%)
18	CLA	A	1135	-	49,53,73	2.52	16 (32%)	58,89,113	3.02	21 (36%)
18	CLA	A	9011	1	59,63,73	2.28	16 (27%)	70,101,113	2.91	29 (41%)
18	CLA	K	1141	-	24,32,73	2.33	8 (33%)	31,54,113	2.71	17 (54%)
18	CLA	4	4002	-	24,32,73	2.29	8 (33%)	31,54,113	2.83	19 (61%)
18	CLA	B	9022	-	58,62,73	2.41	16 (27%)	68,99,113	3.39	30 (44%)
18	CLA	2	2006	-	24,32,73	2.32	8 (33%)	31,54,113	2.79	18 (58%)
18	CLA	3	3001	-	24,32,73	2.40	8 (33%)	31,54,113	2.85	18 (58%)
18	CLA	A	1127	1	24,32,73	2.35	10 (41%)	31,54,113	2.78	19 (61%)
18	CLA	A	1102	-	24,32,73	2.37	8 (33%)	31,54,113	2.79	18 (58%)
18	CLA	A	1108	1	54,58,73	2.40	15 (27%)	64,95,113	3.01	25 (39%)
18	CLA	B	1221	-	52,56,73	2.45	14 (26%)	61,92,113	2.90	27 (44%)
20	BCR	I	6018	-	41,41,41	1.56	4 (9%)	56,56,56	4.92	32 (57%)
18	CLA	A	1128	-	59,63,73	2.36	17 (28%)	70,101,113	2.61	26 (37%)
21	SF4	C	3103	3	0,12,12	-	-	-		
18	CLA	B	1203	18	50,56,73	2.32	12 (24%)	58,92,113	2.76	26 (44%)
18	CLA	A	1142	-	24,32,73	2.35	8 (33%)	31,54,113	2.76	18 (58%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\| > 2$	Counts	RMSZ	$\#\|Z\| > 2$
18	CLA	F	1303	-	24,32,73	2.37	8 (33%)	31,54,113	2.81	17 (54%)
18	CLA	A	1137	-	59,63,73	2.37	16 (27%)	70,101,113	2.75	27 (38%)
18	CLA	1	1011	14	24,32,73	2.36	8 (33%)	31,54,113	2.82	18 (58%)
20	BCR	B	6017	-	41,41,41	1.38	4 (9%)	56,56,56	4.38	25 (44%)
18	CLA	B	1217	-	54,58,73	2.49	18 (33%)	64,95,113	3.00	24 (37%)
18	CLA	B	1301	-	24,32,73	2.44	8 (33%)	31,54,113	2.76	19 (61%)
18	CLA	A	1117	-	24,32,73	2.32	8 (33%)	31,54,113	2.77	18 (58%)
18	CLA	A	1124	-	24,32,73	2.39	7 (29%)	31,54,113	2.93	18 (58%)
18	CLA	4	4003	-	24,32,73	2.36	8 (33%)	31,54,113	2.73	19 (61%)
18	CLA	J	2107	10	65,69,73	2.24	15 (23%)	77,108,113	2.67	25 (32%)
18	CLA	1	1012	14	24,32,73	2.32	8 (33%)	31,54,113	2.97	19 (61%)
18	CLA	4	4012	-	24,32,73	2.49	9 (37%)	31,54,113	2.94	19 (61%)
18	CLA	B	1210	-	24,32,73	2.36	8 (33%)	31,54,113	2.77	19 (61%)
18	CLA	A	1111	-	24,32,73	2.43	8 (33%)	31,54,113	2.78	18 (58%)
18	CLA	4	4004	-	24,32,73	2.36	10 (41%)	31,54,113	2.76	17 (54%)
18	CLA	A	1134	1	24,32,73	2.31	8 (33%)	31,54,113	2.89	20 (64%)
18	CLA	B	1241	-	24,32,73	2.40	8 (33%)	31,54,113	2.76	18 (58%)
18	CLA	G	1248	-	24,32,73	2.33	10 (41%)	31,54,113	2.98	19 (61%)
20	BCR	F	6016	-	41,41,41	1.28	2 (4%)	56,56,56	4.95	32 (57%)
18	CLA	A	1119	-	59,63,73	2.39	14 (23%)	70,101,113	2.73	25 (35%)
18	CLA	A	1118	-	24,32,73	2.38	9 (37%)	31,54,113	2.88	19 (61%)
19	PQN	A	5001	-	34,34,34	1.78	2 (5%)	43,45,45	1.43	5 (11%)
18	CLA	2	2010	-	24,32,73	2.35	8 (33%)	31,54,113	2.86	18 (58%)
18	CLA	A	1133	-	24,32,73	2.41	9 (37%)	31,54,113	2.73	18 (58%)
18	CLA	B	1225	2	49,53,73	2.60	16 (32%)	58,89,113	3.50	30 (51%)
18	CLA	A	1126	1	59,63,73	2.41	18 (30%)	70,101,113	3.05	32 (45%)
18	CLA	B	1227	2	54,58,73	2.42	16 (29%)	64,95,113	2.98	27 (42%)
18	CLA	B	1228	2	59,63,73	2.37	18 (30%)	70,101,113	3.15	28 (40%)
18	CLA	1	1007	-	24,32,73	2.37	8 (33%)	31,54,113	2.75	19 (61%)
18	CLA	3	3012	-	24,32,73	2.34	10 (41%)	31,54,113	2.72	18 (58%)
18	CLA	4	4009	-	24,32,73	2.33	8 (33%)	31,54,113	2.84	17 (54%)
18	CLA	A	1147	1	24,32,73	2.35	9 (37%)	31,54,113	2.80	18 (58%)
18	CLA	F	1302	-	59,63,73	2.29	14 (23%)	70,101,113	2.74	26 (37%)
18	CLA	B	9012	-	59,63,73	2.44	16 (27%)	70,101,113	2.87	33 (47%)
18	CLA	A	1129	-	59,63,73	2.40	16 (27%)	70,101,113	2.88	29 (41%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\| > 2$	Counts	RMSZ	$\#\|Z\| > 2$
18	CLA	B	1239	2	59,63,73	2.35	15 (25%)	70,101,113	2.75	26 (37%)
18	CLA	A	1131	-	48,52,73	2.71	14 (29%)	59,88,113	2.83	26 (44%)
18	CLA	B	1236	-	50,54,73	2.54	15 (30%)	59,90,113	3.21	23 (38%)
18	CLA	2	2004	-	24,32,73	2.39	8 (33%)	31,54,113	2.84	20 (64%)
18	CLA	L	1130	-	54,58,73	2.46	16 (29%)	64,95,113	2.74	27 (42%)
18	CLA	B	1206	2	24,32,73	2.36	9 (37%)	31,54,113	2.86	20 (64%)
18	CLA	B	1224	-	55,59,73	2.35	17 (30%)	64,96,113	2.63	27 (42%)
18	CLA	L	1125	-	24,32,73	2.37	8 (33%)	31,54,113	2.75	17 (54%)
18	CLA	B	1209	-	59,63,73	2.35	16 (27%)	70,101,113	2.80	26 (37%)
18	CLA	A	1132	-	24,32,73	2.37	9 (37%)	31,54,113	2.80	19 (61%)
18	CLA	H	1505	8	24,32,73	2.32	9 (37%)	31,54,113	2.84	18 (58%)
18	CLA	A	1107	1	61,65,73	2.42	17 (27%)	72,103,113	3.03	31 (43%)
18	CLA	1	1008	14	24,32,73	2.37	8 (33%)	31,54,113	2.80	18 (58%)
18	CLA	3	2009	-	24,32,73	2.34	8 (33%)	31,54,113	2.83	18 (58%)
18	CLA	L	1504	-	59,63,73	2.29	15 (25%)	70,101,113	2.78	23 (32%)
18	CLA	3	3003	16	24,32,73	2.37	8 (33%)	31,54,113	2.70	17 (54%)
18	CLA	A	1104	1	24,32,73	2.30	8 (33%)	31,54,113	2.62	16 (51%)
18	CLA	B	1201	-	24,32,73	2.42	8 (33%)	31,54,113	2.91	19 (61%)
18	CLA	B	1232	-	59,63,73	2.34	14 (23%)	70,101,113	2.78	22 (31%)
18	CLA	3	3010	-	24,32,73	2.32	8 (33%)	31,54,113	2.74	17 (54%)
18	CLA	J	1307	-	24,32,73	2.40	8 (33%)	31,54,113	2.77	19 (61%)
18	CLA	3	3015	-	24,32,73	2.33	8 (33%)	31,54,113	2.75	19 (61%)
18	CLA	L	1502	12	55,59,73	2.46	15 (27%)	64,96,113	2.77	25 (39%)
18	CLA	4	4010	-	24,32,73	2.36	8 (33%)	31,54,113	2.78	18 (58%)
21	SF4	C	3102	3	0,12,12	-	-	-		
18	CLA	2	2008	-	24,32,73	2.32	8 (33%)	31,54,113	2.86	19 (61%)
21	SF4	B	3101	2,1	0,12,12	-	-	-		
18	CLA	B	9023	-	51,55,73	2.47	18 (35%)	60,91,113	3.00	26 (43%)
20	BCR	A	6011	-	41,41,41	1.42	3 (7%)	56,56,56	4.59	17 (30%)
18	CLA	B	1219	2	55,59,73	2.44	13 (23%)	64,96,113	2.90	25 (39%)
18	CLA	B	1213	2	24,32,73	2.32	8 (33%)	31,54,113	2.79	18 (58%)
18	CLA	4	4008	-	24,32,73	2.35	8 (33%)	31,54,113	2.78	18 (58%)
18	CLA	L	1503	-	50,54,73	2.95	24 (48%)	61,90,113	3.74	31 (50%)
18	CLA	2	2011	-	24,32,73	2.35	8 (33%)	31,54,113	2.81	19 (61%)
18	CLA	3	3013	-	24,32,73	2.35	8 (33%)	31,54,113	2.80	19 (61%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\| > 2$	Counts	RMSZ	$\#\|Z\| > 2$
18	CLA	1	1003	-	24,32,73	2.31	8 (33%)	31,54,113	2.75	17 (54%)
18	CLA	2	2005	-	24,32,73	2.42	8 (33%)	31,54,113	2.77	18 (58%)
18	CLA	A	1110	-	24,32,73	2.34	8 (33%)	31,54,113	2.93	19 (61%)
18	CLA	K	1150	-	24,32,73	2.34	8 (33%)	31,54,113	2.83	19 (61%)
18	CLA	A	1136	1	59,63,73	2.31	15 (25%)	70,101,113	3.04	29 (41%)
18	CLA	G	1233	-	55,59,73	2.49	16 (29%)	64,96,113	2.81	21 (32%)
18	CLA	3	3005	-	24,32,73	2.33	9 (37%)	31,54,113	2.94	19 (61%)
18	CLA	3	3008	-	24,32,73	2.36	8 (33%)	31,54,113	2.91	17 (54%)
18	CLA	1	1004	-	24,32,73	2.38	8 (33%)	31,54,113	2.74	19 (61%)
18	CLA	F	1240	-	24,32,73	2.38	8 (33%)	31,54,113	2.98	20 (64%)
18	CLA	B	1215	2	56,60,73	2.40	16 (28%)	65,97,113	2.95	34 (52%)
18	CLA	3	3002	-	24,32,73	2.36	8 (33%)	31,54,113	2.81	18 (58%)
18	CLA	A	1146	-	24,32,73	2.41	8 (33%)	31,54,113	2.72	18 (58%)
18	CLA	1	1002	-	24,32,73	2.34	8 (33%)	31,54,113	2.81	17 (54%)
18	CLA	4	4006	-	24,32,73	2.45	8 (33%)	31,54,113	2.85	19 (61%)
18	CLA	B	9010	2	51,55,73	2.52	17 (33%)	60,91,113	3.13	30 (50%)
18	CLA	A	1148	-	24,32,73	2.34	8 (33%)	31,54,113	2.89	18 (58%)
18	CLA	B	1216	-	60,64,73	2.37	14 (23%)	71,102,113	2.72	26 (36%)
18	CLA	B	1218	-	55,59,73	2.77	23 (41%)	64,96,113	3.03	27 (42%)
18	CLA	B	1220	-	64,68,73	2.19	16 (25%)	76,107,113	2.99	28 (36%)
18	CLA	2	2012	-	24,32,73	2.39	10 (41%)	31,54,113	2.79	19 (61%)
18	CLA	2	2007	-	24,32,73	2.31	8 (33%)	31,54,113	2.89	19 (61%)
18	CLA	1	1005	-	24,32,73	2.41	8 (33%)	31,54,113	2.82	18 (58%)
18	CLA	A	1116	-	24,32,73	2.36	9 (37%)	31,54,113	2.85	18 (58%)
18	CLA	A	1151	-	24,32,73	2.36	8 (33%)	31,54,113	2.76	18 (58%)
18	CLA	B	1138	-	60,64,73	2.38	17 (28%)	71,102,113	2.63	29 (40%)
18	CLA	H	1501	-	59,63,73	2.35	15 (25%)	70,101,113	2.83	30 (42%)
18	CLA	3	3007	-	24,32,73	2.28	8 (33%)	31,54,113	2.94	17 (54%)
18	CLA	B	1211	2	24,32,73	2.30	8 (33%)	31,54,113	2.91	19 (61%)
18	CLA	F	1306	-	24,32,73	2.42	8 (33%)	31,54,113	2.81	19 (61%)
18	CLA	A	1120	-	24,32,73	2.38	8 (33%)	31,54,113	2.90	18 (58%)
18	CLA	J	1308	-	24,32,73	2.36	8 (33%)	31,54,113	2.90	17 (54%)
18	CLA	A	1143	-	24,32,73	2.38	8 (33%)	31,54,113	2.78	19 (61%)
18	CLA	B	1202	-	54,58,73	2.52	16 (29%)	64,95,113	3.40	28 (43%)
18	CLA	B	1208	-	59,63,73	2.40	17 (28%)	70,101,113	3.10	35 (50%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\| > 2$	Counts	RMSZ	$\#\|Z\| > 2$
18	CLA	B	1214	-	53,57,73	2.52	17 (32%)	61,93,113	2.85	27 (44%)
18	CLA	B	1231	2	50,54,73	2.59	15 (30%)	59,90,113	2.99	22 (37%)
18	CLA	B	1234	2	54,58,73	2.45	15 (27%)	64,95,113	2.83	25 (39%)
18	CLA	B	1229	-	53,57,73	2.67	17 (32%)	65,94,113	3.19	24 (36%)
18	CLA	4	4005	-	24,32,73	2.39	8 (33%)	31,54,113	2.96	20 (64%)
19	PQN	B	5002	-	34,34,34	1.81	2 (5%)	43,45,45	1.62	8 (18%)
18	CLA	3	3011	-	24,32,73	2.36	8 (33%)	31,54,113	2.72	17 (54%)
18	CLA	B	1237	-	55,59,73	2.42	14 (25%)	64,96,113	3.26	28 (43%)
18	CLA	1	1014	-	24,32,73	2.34	8 (33%)	31,54,113	2.86	19 (61%)
18	CLA	A	1109	-	24,30,73	2.98	10 (41%)	28,49,113	2.94	14 (50%)
18	CLA	2	2013	-	24,32,73	2.37	8 (33%)	31,54,113	2.77	18 (58%)
18	CLA	B	1207	2	59,63,73	2.28	17 (28%)	70,101,113	3.12	30 (42%)

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	B	1219	2	-	13/23/99/115	-
18	CLA	B	1212	-	1/1/14/20	20/33/109/115	-
18	CLA	L	1503	-	-	6/16/92/115	-
18	CLA	B	1236	-	-	5/17/93/115	-
18	CLA	B	1242	-	-	12/18/94/115	-
18	CLA	A	1135	-	-	8/15/91/115	-
20	BCR	F	6016	-	-	13/29/63/63	0/2/2/2
18	CLA	A	1113	-	-	6/21/97/115	-
18	CLA	A	1119	-	1/1/13/20	14/27/103/115	-
18	CLA	A	9011	1	1/1/13/20	12/27/103/115	-
18	CLA	A	1136	1	1/1/13/20	12/27/103/115	-
19	PQN	A	5001	-	1/1/8/9	11/23/43/43	0/2/2/2
18	CLA	G	1233	-	-	10/23/99/115	-
18	CLA	B	1225	2	-	6/15/91/115	-
18	CLA	B	9022	-	-	13/26/102/115	-
18	CLA	A	1126	1	1/1/13/20	13/27/103/115	-
18	CLA	B	1227	2	-	10/21/97/115	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
18	CLA	B	1228	2	1/1/13/20	10/27/103/115	-
18	CLA	A	1108	1	-	6/21/97/115	-
18	CLA	B	1215	2	-	13/24/100/115	-
18	CLA	B	1221	-	-	13/19/95/115	-
18	CLA	A	1128	-	1/1/13/20	10/27/103/115	-
21	SF4	C	3103	3	-	-	0/6/5/5
18	CLA	F	1302	-	1/1/13/20	7/27/103/115	-
18	CLA	B	1203	18	-	11/19/95/115	-
18	CLA	B	1238	-	-	11/26/102/115	-
18	CLA	B	9012	-	1/1/13/20	16/27/103/115	-
18	CLA	A	1129	-	1/1/13/20	10/27/103/115	-
18	CLA	B	1239	2	1/1/13/20	6/27/103/115	-
18	CLA	B	9010	2	-	7/18/94/115	-
18	CLA	A	1123	-	1/1/13/20	15/27/103/115	-
18	CLA	A	1131	-	-	6/13/89/115	-
18	CLA	B	1216	-	1/1/13/20	11/29/105/115	-
18	CLA	B	1222	-	1/1/15/20	19/39/115/115	-
18	CLA	A	1103	1	-	11/18/94/115	-
18	CLA	B	1218	-	-	11/23/99/115	-
18	CLA	B	1224	-	-	5/23/99/115	-
18	CLA	A	1137	-	1/1/13/20	14/27/103/115	-
18	CLA	B	1220	-	1/1/14/20	18/33/109/115	-
18	CLA	B	1209	-	1/1/13/20	13/27/103/115	-
18	CLA	L	1130	-	-	4/21/97/115	-
20	BCR	B	6017	-	-	19/29/63/63	0/2/2/2
18	CLA	B	1217	-	-	7/21/97/115	-
18	CLA	I	1204	-	1/1/13/20	17/27/103/115	-
20	BCR	L	6020	-	-	16/29/63/63	0/2/2/2
18	CLA	A	1107	1	1/1/13/20	19/30/106/115	-
18	CLA	B	1138	-	1/1/13/20	13/29/105/115	-
18	CLA	A	1122	-	1/1/13/20	8/27/103/115	-
18	CLA	H	1501	-	1/1/13/20	10/27/103/115	-
18	CLA	A	9013	-	-	4/17/93/115	-
18	CLA	L	1504	-	1/1/13/20	10/27/103/115	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
18	CLA	A	1140	1	1/1/13/20	13/27/103/115	-
18	CLA	A	1106	-	-	3/10/86/115	-
18	CLA	B	1232	-	1/1/13/20	11/27/103/115	-
18	CLA	F	1139	-	-	8/14/90/115	-
18	CLA	B	1205	2	1/1/13/20	13/27/103/115	-
18	CLA	B	1202	-	-	7/21/97/115	-
18	CLA	B	1208	-	1/1/13/20	13/27/103/115	-
18	CLA	J	2107	10	1/1/14/20	14/35/111/115	-
18	CLA	B	1214	-	-	7/20/96/115	-
18	CLA	L	1502	12	-	9/23/99/115	-
18	CLA	B	1231	2	-	9/17/93/115	-
21	SF4	B	3101	2,1	-	-	0/6/5/5
18	CLA	B	1234	2	-	9/21/97/115	-
18	CLA	B	1229	-	-	8/19/95/115	-
21	SF4	C	3102	3	-	-	0/6/5/5
19	PQN	B	5002	-	1/1/8/9	9/23/43/43	0/2/2/2
20	BCR	A	6011	-	-	15/29/63/63	0/2/2/2
18	CLA	4	1304	-	1/1/13/20	10/27/103/115	-
18	CLA	A	1115	-	-	8/18/94/115	-
18	CLA	B	1237	-	-	10/23/99/115	-
20	BCR	I	6018	-	-	11/29/63/63	0/2/2/2
18	CLA	B	9023	-	-	6/18/94/115	-
18	CLA	B	1207	2	1/1/13/20	12/27/103/115	-
18	CLA	B	1235	-	1/1/13/20	11/27/103/115	-

All (1896) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
19	B	5002	PQN	C3-C2	8.64	1.50	1.35
19	A	5001	PQN	C3-C2	8.33	1.50	1.35
18	B	1229	CLA	CAB-C3B	-7.87	1.34	1.50
18	A	1131	CLA	CAB-C3B	-7.79	1.34	1.50
20	L	6020	BCR	C11-C10	-7.61	1.19	1.43
18	A	1109	CLA	C4D-C3D	-7.14	1.39	1.49
18	G	1233	CLA	CHC-C1C	7.08	1.52	1.38
18	L	1503	CLA	CAB-C3B	-7.02	1.36	1.50
18	B	1208	CLA	CHC-C1C	7.02	1.52	1.38

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
18	B	9022	CLA	CHD-C1D	6.81	1.51	1.38
18	2	2005	CLA	CHC-C1C	6.81	1.51	1.38
18	A	1109	CLA	CHC-C1C	6.80	1.51	1.38
18	B	1301	CLA	CHC-C1C	6.77	1.51	1.38
18	A	1119	CLA	CHC-C1C	6.74	1.52	1.38
18	4	4012	CLA	CHC-C1C	6.73	1.51	1.38
18	B	1219	CLA	CHC-C1C	6.63	1.51	1.38
18	B	1229	CLA	CHC-C1C	6.63	1.51	1.38
18	4	4006	CLA	CHC-C1C	6.62	1.51	1.38
18	B	1231	CLA	CHD-C1D	6.62	1.51	1.38
18	B	1218	CLA	CHC-C1C	6.60	1.51	1.38
18	B	1236	CLA	CHC-C1C	6.59	1.51	1.38
18	F	1306	CLA	CHC-C1C	6.58	1.51	1.38
18	B	1237	CLA	CHD-C1D	6.55	1.51	1.38
18	B	1210	CLA	CHC-C1C	6.55	1.51	1.38
18	B	1219	CLA	CHD-C1D	6.54	1.51	1.38
18	B	1242	CLA	CHC-C1C	6.53	1.51	1.38
18	A	1146	CLA	CHC-C1C	6.52	1.51	1.38
18	3	3003	CLA	CHC-C1C	6.52	1.51	1.38
18	A	1103	CLA	CHD-C1D	6.50	1.51	1.38
18	A	9013	CLA	CHD-C4C	6.49	1.54	1.39
18	L	1125	CLA	CHC-C1C	6.49	1.51	1.38
18	A	1129	CLA	CHC-C1C	6.48	1.51	1.38
18	3	3009	CLA	CHC-C1C	6.48	1.51	1.38
18	A	1117	CLA	CHC-C1C	6.48	1.51	1.38
18	L	1502	CLA	CHC-C1C	6.45	1.51	1.38
18	B	1216	CLA	CHC-C1C	6.45	1.51	1.38
18	A	1143	CLA	CHC-C1C	6.44	1.51	1.38
18	L	1130	CLA	CHC-C1C	6.44	1.51	1.38
18	B	1235	CLA	CHD-C1D	6.43	1.51	1.38
18	B	1215	CLA	O2D-CGD	6.43	1.49	1.33
18	1	1014	CLA	CHC-C1C	6.43	1.51	1.38
18	A	9013	CLA	CHD-C1D	6.42	1.51	1.38
18	1	1004	CLA	CHC-C1C	6.42	1.51	1.38
18	B	1214	CLA	CHC-C1C	6.41	1.51	1.38
18	1	1010	CLA	CHC-C1C	6.41	1.51	1.38
18	B	1202	CLA	CHD-C1D	6.41	1.51	1.38
18	3	3001	CLA	CHC-C1C	6.40	1.51	1.38
18	A	1107	CLA	CHD-C1D	6.39	1.50	1.38
18	F	1139	CLA	O2D-CGD	6.39	1.48	1.33
18	4	4007	CLA	CHC-C1C	6.38	1.51	1.38
18	A	9011	CLA	O2D-CGD	6.37	1.48	1.33

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
18	B	1217	CLA	CHD-C1D	6.36	1.50	1.38
18	B	1224	CLA	CHC-C1C	6.36	1.51	1.38
18	A	1151	CLA	CHC-C1C	6.36	1.51	1.38
18	B	1228	CLA	CHD-C1D	6.35	1.50	1.38
18	4	4005	CLA	CHC-C1C	6.34	1.51	1.38
18	K	1150	CLA	CHC-C1C	6.34	1.51	1.38
18	1	1005	CLA	CHC-C1C	6.33	1.50	1.38
18	B	1219	CLA	CHD-C4C	6.33	1.53	1.39
18	4	4013	CLA	CHC-C1C	6.33	1.50	1.38
18	B	1239	CLA	CHD-C1D	6.32	1.50	1.38
18	B	1205	CLA	CHC-C1C	6.31	1.51	1.38
18	4	1304	CLA	CHC-C1C	6.31	1.51	1.38
18	J	1307	CLA	CHC-C1C	6.31	1.50	1.38
18	A	1142	CLA	CHC-C1C	6.31	1.50	1.38
18	A	1129	CLA	CHD-C1D	6.31	1.50	1.38
18	4	4001	CLA	CHC-C1C	6.30	1.50	1.38
18	B	9012	CLA	O2D-CGD	6.30	1.48	1.33
18	1	1001	CLA	CHC-C1C	6.30	1.50	1.38
18	4	1009	CLA	CHC-C1C	6.29	1.50	1.38
18	1	1013	CLA	CHC-C1C	6.29	1.50	1.38
18	B	9012	CLA	CHC-C1C	6.28	1.51	1.38
18	K	1141	CLA	CHC-C1C	6.28	1.50	1.38
18	B	1230	CLA	CHC-C1C	6.27	1.50	1.38
18	B	1138	CLA	CHD-C1D	6.26	1.50	1.38
18	2	2001	CLA	CHC-C1C	6.26	1.50	1.38
18	F	1302	CLA	CHC-C1C	6.26	1.51	1.38
18	A	1111	CLA	CHC-C1C	6.25	1.50	1.38
18	I	1204	CLA	CHC-C1C	6.25	1.51	1.38
18	L	1503	CLA	C3D-C4D	-6.25	1.30	1.44
18	3	3012	CLA	CHC-C1C	6.24	1.50	1.38
18	F	1303	CLA	CHC-C1C	6.24	1.50	1.38
18	B	1227	CLA	O2D-CGD	6.24	1.48	1.33
18	A	1152	CLA	CHC-C1C	6.24	1.50	1.38
18	B	1213	CLA	CHC-C1C	6.24	1.50	1.38
18	1	1012	CLA	CHC-C1C	6.24	1.50	1.38
18	4	4008	CLA	CHC-C1C	6.24	1.50	1.38
18	4	4003	CLA	CHC-C1C	6.23	1.50	1.38
18	B	1235	CLA	CHD-C4C	6.23	1.53	1.39
18	H	1505	CLA	CHC-C1C	6.22	1.50	1.38
18	B	1218	CLA	O2D-CGD	6.22	1.48	1.33
18	B	1222	CLA	CHC-C1C	6.21	1.50	1.38
18	B	1212	CLA	CHC-C1C	6.21	1.50	1.38

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
18	2	2013	CLA	CHC-C1C	6.21	1.50	1.38
18	B	1232	CLA	CHC-C1C	6.20	1.50	1.38
18	B	1201	CLA	CHC-C1C	6.20	1.50	1.38
18	B	9022	CLA	CHC-C1C	6.20	1.50	1.38
18	2	2012	CLA	CHC-C1C	6.20	1.50	1.38
18	A	1102	CLA	CHC-C1C	6.20	1.50	1.38
18	2	2015	CLA	CHC-C1C	6.18	1.50	1.38
18	1	1007	CLA	CHC-C1C	6.18	1.50	1.38
18	A	1118	CLA	CHC-C1C	6.18	1.50	1.38
18	2	2004	CLA	CHC-C1C	6.16	1.50	1.38
18	B	1218	CLA	C3D-C4D	-6.16	1.30	1.44
18	4	4009	CLA	CHC-C1C	6.15	1.50	1.38
18	A	1131	CLA	CHD-C4C	6.15	1.53	1.39
18	B	1241	CLA	CHC-C1C	6.15	1.50	1.38
18	A	1101	CLA	CHC-C1C	6.15	1.50	1.38
18	3	3011	CLA	CHC-C1C	6.15	1.50	1.38
18	A	1124	CLA	CHC-C1C	6.14	1.50	1.38
18	A	1131	CLA	CHD-C1D	6.13	1.50	1.38
18	3	3002	CLA	CHC-C1C	6.13	1.50	1.38
18	3	2009	CLA	CHC-C1C	6.13	1.50	1.38
18	2	2010	CLA	CHC-C1C	6.12	1.50	1.38
18	A	1126	CLA	CHC-C1C	6.12	1.50	1.38
18	2	2011	CLA	CHC-C1C	6.11	1.50	1.38
18	2	2007	CLA	CHC-C1C	6.11	1.50	1.38
18	1	1002	CLA	CHC-C1C	6.10	1.50	1.38
18	A	1110	CLA	CHC-C1C	6.10	1.50	1.38
18	A	1120	CLA	CHC-C1C	6.10	1.50	1.38
18	A	1148	CLA	CHC-C1C	6.10	1.50	1.38
18	1	1011	CLA	CHC-C1C	6.09	1.50	1.38
18	A	1132	CLA	CHC-C1C	6.09	1.50	1.38
18	3	3006	CLA	CHC-C1C	6.09	1.50	1.38
18	3	3008	CLA	CHC-C1C	6.08	1.50	1.38
18	A	1113	CLA	O2D-CGD	6.08	1.48	1.33
18	A	1309	CLA	CHC-C1C	6.08	1.50	1.38
18	A	1137	CLA	CHC-C1C	6.07	1.50	1.38
18	3	3010	CLA	CHC-C1C	6.07	1.50	1.38
18	B	1223	CLA	CHC-C1C	6.06	1.50	1.38
18	B	9010	CLA	CHD-C1D	6.06	1.50	1.38
18	A	1126	CLA	CHD-C1D	6.06	1.50	1.38
18	J	2107	CLA	CHC-C1C	6.06	1.50	1.38
18	A	1147	CLA	CHC-C1C	6.06	1.50	1.38
18	F	1240	CLA	CHC-C1C	6.06	1.50	1.38

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
18	3	3004	CLA	CHC-C1C	6.05	1.50	1.38
18	B	1237	CLA	CHD-C4C	6.04	1.52	1.39
18	1	1003	CLA	CHC-C1C	6.03	1.50	1.38
18	4	4002	CLA	CHC-C1C	6.03	1.50	1.38
18	A	1133	CLA	CHC-C1C	6.03	1.50	1.38
20	F	6016	BCR	C11-C10	-6.03	1.24	1.43
18	2	2003	CLA	CHC-C1C	6.02	1.50	1.38
18	H	1501	CLA	CHC-C1C	6.02	1.50	1.38
18	4	1304	CLA	CHD-C1D	6.01	1.50	1.38
18	F	1305	CLA	CHC-C1C	6.01	1.50	1.38
18	3	3015	CLA	CHC-C1C	6.01	1.50	1.38
18	B	1211	CLA	CHC-C1C	6.01	1.50	1.38
20	I	6018	BCR	C11-C10	-6.01	1.24	1.43
18	B	1238	CLA	CHC-C1C	6.00	1.50	1.38
18	4	4010	CLA	CHC-C1C	5.99	1.50	1.38
18	B	9023	CLA	CHC-C1C	5.99	1.50	1.38
18	A	1140	CLA	CHD-C1D	5.98	1.50	1.38
18	A	1128	CLA	CHC-C1C	5.98	1.50	1.38
18	A	1115	CLA	CHD-C1D	5.98	1.50	1.38
18	B	1209	CLA	CHC-C1C	5.98	1.50	1.38
18	A	1129	CLA	CHD-C4C	5.97	1.52	1.39
18	A	1137	CLA	CHD-C1D	5.97	1.50	1.38
18	1	1006	CLA	CHC-C1C	5.97	1.50	1.38
18	J	2107	CLA	CHD-C1D	5.96	1.50	1.38
18	4	4004	CLA	CHC-C1C	5.96	1.50	1.38
18	B	9012	CLA	CHD-C1D	5.96	1.50	1.38
18	G	1248	CLA	CHC-C1C	5.96	1.50	1.38
18	L	1504	CLA	CHC-C1C	5.96	1.50	1.38
18	B	1231	CLA	CHD-C4C	5.96	1.52	1.39
18	A	1116	CLA	CHC-C1C	5.96	1.50	1.38
18	B	1225	CLA	CHD-C4C	5.95	1.52	1.39
18	B	1226	CLA	CHC-C1C	5.95	1.50	1.38
18	3	3005	CLA	CHC-C1C	5.94	1.50	1.38
18	1	1008	CLA	CHC-C1C	5.93	1.50	1.38
18	B	1138	CLA	CHD-C4C	5.92	1.52	1.39
18	F	4015	CLA	CHC-C1C	5.92	1.50	1.38
18	A	1127	CLA	CHC-C1C	5.92	1.50	1.38
18	L	1502	CLA	CHD-C1D	5.91	1.50	1.38
18	3	3013	CLA	CHC-C1C	5.91	1.50	1.38
18	4	4011	CLA	CHC-C1C	5.91	1.50	1.38
18	2	2002	CLA	CHC-C1C	5.90	1.50	1.38
18	2	2006	CLA	CHC-C1C	5.90	1.50	1.38

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
18	A	1126	CLA	CHD-C4C	5.89	1.52	1.39
18	2	2008	CLA	CHC-C1C	5.89	1.50	1.38
18	B	1215	CLA	CHD-C4C	5.88	1.52	1.39
18	L	1502	CLA	CHD-C4C	5.87	1.52	1.39
18	A	1123	CLA	CHD-C4C	5.87	1.52	1.39
18	B	1202	CLA	CHD-C4C	5.86	1.52	1.39
18	J	1308	CLA	CHC-C1C	5.86	1.50	1.38
18	B	1208	CLA	O2D-CGD	5.86	1.47	1.33
18	A	1104	CLA	CHC-C1C	5.84	1.50	1.38
18	A	1134	CLA	CHC-C1C	5.84	1.50	1.38
18	A	1122	CLA	CHC-C1C	5.84	1.50	1.38
18	I	1204	CLA	CHD-C1D	5.84	1.49	1.38
18	A	1108	CLA	CHC-C1C	5.84	1.50	1.38
18	B	1231	CLA	CHC-C1C	5.83	1.50	1.38
18	A	1144	CLA	CHC-C1C	5.82	1.49	1.38
18	H	1501	CLA	O2D-CGD	5.82	1.47	1.33
18	B	1202	CLA	CHC-C1C	5.82	1.50	1.38
18	B	1138	CLA	CHC-C1C	5.81	1.50	1.38
18	B	1217	CLA	CHD-C4C	5.81	1.52	1.39
18	B	1236	CLA	CHD-C1D	5.80	1.49	1.38
18	B	1217	CLA	CHC-C1C	5.80	1.50	1.38
18	A	1105	CLA	CHC-C1C	5.80	1.49	1.38
18	B	1232	CLA	CHD-C1D	5.79	1.49	1.38
18	B	1238	CLA	O2D-CGD	5.78	1.47	1.33
18	B	1234	CLA	CHC-C1C	5.78	1.50	1.38
18	B	1202	CLA	C3D-C4D	-5.78	1.31	1.44
18	F	1302	CLA	CHD-C1D	5.77	1.49	1.38
18	A	1103	CLA	CHD-C4C	5.77	1.52	1.39
18	L	1130	CLA	CHD-C1D	5.76	1.49	1.38
18	L	1503	CLA	C1B-NB	-5.76	1.30	1.37
18	B	1221	CLA	CHD-C1D	5.76	1.49	1.38
18	A	1123	CLA	CHD-C1D	5.76	1.49	1.38
18	B	1227	CLA	CHD-C1D	5.75	1.49	1.38
18	A	1140	CLA	O2D-CGD	5.75	1.47	1.33
18	B	1216	CLA	O2D-CGD	5.74	1.47	1.33
18	B	1203	CLA	CHD-C4C	5.74	1.52	1.39
18	A	1140	CLA	CHD-C4C	5.73	1.52	1.39
18	A	1123	CLA	CHC-C1C	5.73	1.50	1.38
18	L	1503	CLA	O2D-CGD	5.73	1.47	1.33
18	B	1225	CLA	CHC-C1C	5.73	1.50	1.38
18	F	1139	CLA	CHC-C1C	5.72	1.50	1.38
18	B	1222	CLA	CHD-C1D	5.72	1.49	1.38

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
18	B	1239	CLA	CHD-C4C	5.72	1.52	1.39
18	B	1228	CLA	CHC-C1C	5.72	1.49	1.38
18	F	1139	CLA	CHD-C1D	5.72	1.49	1.38
18	I	1204	CLA	O2D-CGD	5.72	1.47	1.33
18	B	1238	CLA	CHD-C1D	5.71	1.49	1.38
18	B	1237	CLA	CHC-C1C	5.71	1.49	1.38
18	A	1122	CLA	CHD-C1D	5.70	1.49	1.38
18	B	1225	CLA	CHD-C1D	5.70	1.49	1.38
18	A	1107	CLA	CHD-C4C	5.70	1.52	1.39
18	B	9022	CLA	C3D-C4D	-5.69	1.31	1.44
18	K	1153	CLA	CHC-C1C	5.69	1.49	1.38
18	L	1503	CLA	CHC-C1C	5.69	1.49	1.38
18	A	1115	CLA	CHC-C1C	5.69	1.49	1.38
18	A	9011	CLA	CHD-C4C	5.69	1.52	1.39
18	B	1220	CLA	CHC-C1C	5.69	1.49	1.38
18	A	1108	CLA	O2D-CGD	5.68	1.47	1.33
18	F	1302	CLA	CHD-C4C	5.68	1.52	1.39
18	B	9023	CLA	O2D-CGD	5.68	1.47	1.33
18	J	2107	CLA	O2D-CGD	5.67	1.47	1.33
18	A	1122	CLA	CHD-C4C	5.67	1.52	1.39
18	B	1208	CLA	CHD-C1D	5.67	1.49	1.38
18	B	1203	CLA	O2D-CGD	5.67	1.47	1.33
18	B	1207	CLA	CHC-C1C	5.66	1.49	1.38
18	B	1208	CLA	CHD-C4C	5.66	1.52	1.39
18	H	1501	CLA	CHD-C1D	5.65	1.49	1.38
18	B	1238	CLA	CHD-C4C	5.65	1.52	1.39
18	B	1209	CLA	O2D-CGD	5.64	1.47	1.33
18	B	1232	CLA	CHD-C4C	5.63	1.52	1.39
18	B	1207	CLA	CHD-C1D	5.63	1.49	1.38
18	J	2107	CLA	CHD-C4C	5.63	1.52	1.39
18	A	1128	CLA	CHD-C4C	5.61	1.52	1.39
18	B	1203	CLA	CHC-C1C	5.61	1.49	1.38
18	I	1204	CLA	CHD-C4C	5.61	1.52	1.39
18	B	1228	CLA	CHD-C4C	5.61	1.52	1.39
18	3	3007	CLA	CHC-C1C	5.60	1.49	1.38
18	G	1233	CLA	O2D-CGD	5.60	1.47	1.33
18	A	1137	CLA	CHD-C4C	5.60	1.51	1.39
18	B	1222	CLA	CHD-C4C	5.59	1.51	1.39
18	B	1221	CLA	O2D-CGD	5.59	1.47	1.33
18	A	1128	CLA	CHD-C1D	5.59	1.49	1.38
18	B	1234	CLA	CHD-C1D	5.59	1.49	1.38
18	A	1107	CLA	C3D-C4D	-5.59	1.31	1.44

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
18	L	1503	CLA	C4C-C3C	-5.59	1.35	1.45
18	A	1135	CLA	CHC-C1C	5.58	1.49	1.38
18	B	9023	CLA	CHD-C1D	5.57	1.49	1.38
20	B	6017	BCR	C11-C10	-5.57	1.25	1.43
18	L	1130	CLA	CHD-C4C	5.56	1.51	1.39
18	B	1206	CLA	CHC-C1C	5.56	1.49	1.38
18	B	1209	CLA	CHD-C4C	5.56	1.51	1.39
18	A	1103	CLA	CHC-C1C	5.56	1.49	1.38
18	B	1207	CLA	CHD-C4C	5.55	1.51	1.39
18	B	1212	CLA	O2D-CGD	5.55	1.46	1.33
18	A	1136	CLA	CHC-C1C	5.54	1.49	1.38
18	B	1209	CLA	CHD-C1D	5.54	1.49	1.38
18	L	1504	CLA	CHD-C1D	5.54	1.49	1.38
18	B	1205	CLA	CHD-C1D	5.54	1.49	1.38
18	B	1208	CLA	O2A-CGA	5.54	1.49	1.33
18	4	1304	CLA	CHD-C4C	5.54	1.51	1.39
18	B	1217	CLA	C3D-C4D	-5.53	1.31	1.44
18	B	9012	CLA	CHD-C4C	5.53	1.51	1.39
18	B	1227	CLA	C3D-C4D	-5.53	1.31	1.44
18	A	1131	CLA	CHC-C1C	5.52	1.49	1.38
18	A	1129	CLA	C3D-C4D	-5.52	1.31	1.44
18	A	1119	CLA	O2D-CGD	5.50	1.46	1.33
18	A	1107	CLA	CHC-C1C	5.50	1.49	1.38
18	A	1119	CLA	CHD-C4C	5.50	1.51	1.39
18	B	1236	CLA	CHD-C4C	5.50	1.51	1.39
18	B	1205	CLA	CHD-C4C	5.49	1.51	1.39
18	B	1220	CLA	CHD-C4C	5.49	1.51	1.39
18	G	1233	CLA	CHC-C4B	5.49	1.51	1.39
18	B	9010	CLA	O2D-CGD	5.49	1.46	1.33
18	B	1234	CLA	C3D-C4D	-5.48	1.31	1.44
18	L	1130	CLA	C3D-C4D	-5.48	1.31	1.44
18	B	1234	CLA	CHD-C4C	5.47	1.51	1.39
18	H	1501	CLA	CHD-C4C	5.46	1.51	1.39
18	B	1236	CLA	C3D-C4D	-5.46	1.31	1.44
18	B	1208	CLA	CHC-C4B	5.45	1.51	1.39
18	A	1136	CLA	CHD-C1D	5.45	1.49	1.38
18	A	1123	CLA	O2D-CGD	5.45	1.46	1.33
18	B	9022	CLA	CHD-C4C	5.45	1.51	1.39
18	B	1209	CLA	C3D-C4D	-5.45	1.31	1.44
18	A	9011	CLA	CHD-C1D	5.43	1.49	1.38
18	B	1218	CLA	CHD-C1D	5.43	1.49	1.38
18	B	1229	CLA	O2D-CGD	5.43	1.46	1.33

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
18	J	2107	CLA	C3D-C4D	-5.41	1.32	1.44
18	B	9012	CLA	CAB-C3B	-5.40	1.33	1.47
18	A	1106	CLA	CAB-C3B	-5.40	1.33	1.47
18	B	1216	CLA	CHD-C4C	5.40	1.51	1.39
18	B	1228	CLA	O2A-CGA	5.39	1.49	1.33
18	B	1224	CLA	O2D-CGD	5.39	1.46	1.33
18	A	1126	CLA	C3D-C4D	-5.39	1.32	1.44
18	A	1113	CLA	CHC-C1C	5.39	1.49	1.38
18	A	1136	CLA	O2D-CGD	5.39	1.46	1.33
18	A	1135	CLA	CHD-C1D	5.38	1.48	1.38
18	A	1106	CLA	CHC-C1C	5.38	1.49	1.38
18	G	1233	CLA	CHD-C4C	5.38	1.51	1.39
18	A	1128	CLA	C3D-C4D	-5.38	1.32	1.44
18	B	1229	CLA	CHC-C4B	5.38	1.51	1.39
18	A	1129	CLA	CHC-C4B	5.38	1.51	1.39
18	4	1304	CLA	O2D-CGD	5.37	1.46	1.33
18	B	1202	CLA	O2D-CGD	5.37	1.46	1.33
18	B	1232	CLA	O2D-CGD	5.37	1.46	1.33
18	A	1128	CLA	O2D-CGD	5.37	1.46	1.33
18	A	9013	CLA	O2D-CGD	5.37	1.46	1.33
18	B	1214	CLA	CHD-C1D	5.36	1.48	1.38
18	L	1504	CLA	CHD-C4C	5.36	1.51	1.39
18	B	1234	CLA	O2D-CGD	5.36	1.46	1.33
18	B	1242	CLA	O2D-CGD	5.36	1.46	1.33
18	B	1237	CLA	O2D-CGD	5.35	1.46	1.33
18	B	9010	CLA	CHD-C4C	5.35	1.51	1.39
18	B	1225	CLA	O2D-CGD	5.35	1.46	1.33
18	F	1139	CLA	C3D-C4D	-5.34	1.32	1.44
18	B	1221	CLA	CHD-C4C	5.34	1.51	1.39
18	B	1239	CLA	CHC-C1C	5.32	1.49	1.38
18	B	1242	CLA	C3D-C4D	-5.32	1.32	1.44
18	B	1242	CLA	CHD-C1D	5.32	1.48	1.38
18	A	1103	CLA	O2D-CGD	5.32	1.46	1.33
18	B	1138	CLA	O2D-CGD	5.32	1.46	1.33
18	B	1217	CLA	CAB-C3B	-5.32	1.33	1.47
18	L	1502	CLA	C3D-C4D	-5.31	1.32	1.44
18	A	1135	CLA	CHD-C4C	5.31	1.51	1.39
18	A	1107	CLA	CAB-C3B	-5.30	1.33	1.47
18	A	1140	CLA	C3D-C4D	-5.30	1.32	1.44
18	A	1122	CLA	O2D-CGD	5.29	1.46	1.33
18	A	1115	CLA	CHD-C4C	5.29	1.51	1.39
18	B	1214	CLA	CHD-C4C	5.29	1.51	1.39

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
18	B	1222	CLA	O2D-CGD	5.29	1.46	1.33
18	1	1005	CLA	CHD-C1D	5.28	1.51	1.38
18	B	1220	CLA	O2D-CGD	5.28	1.46	1.33
18	B	1242	CLA	CAB-C3B	-5.27	1.33	1.47
18	A	1108	CLA	CHD-C1D	5.27	1.48	1.38
18	A	1113	CLA	CHD-C4C	5.27	1.51	1.39
18	B	1225	CLA	C3D-C4D	-5.27	1.32	1.44
18	A	1119	CLA	CHC-C4B	5.25	1.51	1.39
18	B	1239	CLA	O2A-CGA	5.25	1.48	1.33
18	B	1227	CLA	CHD-C4C	5.25	1.51	1.39
18	L	1504	CLA	C3D-C4D	-5.25	1.32	1.44
18	B	1216	CLA	CHD-C1D	5.25	1.48	1.38
18	B	1212	CLA	O2A-CGA	5.25	1.48	1.33
18	A	9011	CLA	CHC-C1C	5.25	1.49	1.38
18	B	1218	CLA	C4C-C3C	-5.25	1.36	1.45
18	B	1226	CLA	CHD-C1D	5.24	1.51	1.38
18	A	1106	CLA	CHD-C4C	5.24	1.51	1.39
18	B	1301	CLA	CHD-C1D	5.24	1.51	1.38
18	A	1126	CLA	O2A-CGA	5.24	1.48	1.33
18	B	1214	CLA	O2D-CGD	5.23	1.46	1.33
18	A	1119	CLA	CHD-C1D	5.23	1.48	1.38
18	B	1234	CLA	CHC-C4B	5.23	1.51	1.39
18	B	1212	CLA	CHD-C4C	5.22	1.51	1.39
18	A	1140	CLA	O2A-CGA	5.22	1.48	1.33
18	A	1135	CLA	O2D-CGD	5.22	1.46	1.33
18	B	1242	CLA	CHC-C4B	5.21	1.51	1.39
18	A	1140	CLA	CHC-C1C	5.20	1.48	1.38
18	L	1502	CLA	CHC-C4B	5.20	1.51	1.39
18	J	1308	CLA	CHD-C1D	5.20	1.51	1.38
18	B	1237	CLA	O2A-CGA	5.20	1.48	1.33
18	B	1206	CLA	CHD-C1D	5.20	1.51	1.38
18	B	1235	CLA	CHC-C1C	5.20	1.48	1.38
18	J	1307	CLA	CHD-C1D	5.19	1.51	1.38
18	A	1137	CLA	CAB-C3B	-5.19	1.33	1.47
20	A	6011	BCR	C11-C10	-5.18	1.27	1.43
18	B	1224	CLA	CHD-C4C	5.17	1.51	1.39
18	B	1238	CLA	CAB-C3B	-5.17	1.33	1.47
18	A	1122	CLA	C3D-C4D	-5.16	1.32	1.44
18	A	1113	CLA	CHD-C1D	5.15	1.48	1.38
18	A	1107	CLA	O2A-CGA	5.15	1.48	1.33
18	B	1216	CLA	C3D-C4D	-5.15	1.32	1.44
18	A	1113	CLA	C3D-C4D	-5.14	1.32	1.44

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
18	B	1205	CLA	O2D-CGD	5.14	1.45	1.33
18	A	1108	CLA	CHD-C4C	5.14	1.50	1.39
18	A	1137	CLA	CHC-C4B	5.13	1.50	1.39
18	A	1115	CLA	O2D-CGD	5.13	1.45	1.33
18	B	1214	CLA	CHC-C4B	5.13	1.50	1.39
18	A	1111	CLA	CHD-C1D	5.12	1.50	1.38
18	L	1130	CLA	O2A-CGA	5.11	1.48	1.33
18	B	1239	CLA	CAB-C3B	-5.11	1.33	1.47
18	B	1237	CLA	C3D-C4D	-5.11	1.32	1.44
18	B	9012	CLA	C3D-C4D	-5.11	1.32	1.44
18	B	1215	CLA	CAB-C3B	-5.11	1.33	1.47
18	A	1133	CLA	CHD-C1D	5.10	1.50	1.38
18	B	1224	CLA	CHD-C1D	5.10	1.48	1.38
18	B	1138	CLA	C3D-C4D	-5.10	1.32	1.44
18	F	1302	CLA	O2D-CGD	5.10	1.45	1.33
18	B	1202	CLA	CAB-C3B	-5.09	1.33	1.47
18	L	1504	CLA	O2D-CGD	5.09	1.45	1.33
18	A	1115	CLA	O2A-CGA	5.09	1.48	1.33
18	B	1220	CLA	CAB-C3B	-5.08	1.33	1.47
18	B	1231	CLA	C3D-C4D	-5.08	1.32	1.44
18	1	1001	CLA	CHD-C1D	5.08	1.50	1.38
18	B	1218	CLA	CHC-C4B	5.08	1.50	1.39
18	A	1106	CLA	O2D-CGD	5.07	1.45	1.33
18	B	1220	CLA	O2A-CGA	5.07	1.48	1.33
18	A	1108	CLA	O2A-CGA	5.07	1.48	1.33
18	B	1214	CLA	C3D-C4D	-5.06	1.32	1.44
18	B	1138	CLA	O2A-CGA	5.06	1.48	1.33
18	B	1221	CLA	C3D-C4D	-5.05	1.32	1.44
18	1	1007	CLA	CHD-C1D	5.05	1.50	1.38
18	4	4006	CLA	CHD-C1D	5.05	1.50	1.38
18	B	9023	CLA	CHD-C4C	5.05	1.50	1.39
18	A	1109	CLA	MG-NA	-5.05	1.94	2.06
18	A	1129	CLA	O2D-CGD	5.05	1.45	1.33
18	2	2006	CLA	CHD-C1D	5.05	1.50	1.38
18	B	1225	CLA	CAB-C3B	-5.05	1.33	1.47
18	A	1122	CLA	CHC-C4B	5.04	1.50	1.39
18	B	1236	CLA	CHC-C4B	5.04	1.50	1.39
18	3	3011	CLA	CHD-C1D	5.04	1.50	1.38
18	A	1103	CLA	C3D-C4D	-5.04	1.32	1.44
18	A	1102	CLA	CHD-C1D	5.03	1.50	1.38
18	A	1137	CLA	O2D-CGD	5.03	1.45	1.33
18	B	1242	CLA	CHD-C4C	5.03	1.50	1.39

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
18	B	1215	CLA	CHD-C1D	5.03	1.48	1.38
18	B	1201	CLA	CHD-C1D	5.03	1.50	1.38
18	B	1203	CLA	CHD-C1D	5.03	1.50	1.38
18	I	1204	CLA	O2A-CGA	5.03	1.48	1.33
18	4	4001	CLA	CHD-C1D	5.02	1.50	1.38
18	F	1306	CLA	CHD-C1D	5.02	1.50	1.38
18	B	1222	CLA	CHC-C4B	5.01	1.50	1.39
18	F	1139	CLA	CHD-C4C	5.01	1.50	1.39
18	B	9010	CLA	CHC-C1C	5.01	1.48	1.38
18	G	1233	CLA	CHD-C1D	5.01	1.48	1.38
18	L	1502	CLA	CAB-C3B	-5.01	1.34	1.47
18	B	1229	CLA	C3D-C4D	-5.00	1.32	1.44
18	B	1212	CLA	CHD-C1D	5.00	1.48	1.38
18	B	1216	CLA	O2A-CGA	5.00	1.47	1.33
18	L	1130	CLA	CHC-C4B	4.99	1.50	1.39
18	A	1126	CLA	CAB-C3B	-4.99	1.34	1.47
18	A	1119	CLA	C3D-C4D	-4.99	1.33	1.44
18	2	2001	CLA	CHD-C1D	4.99	1.50	1.38
18	A	1106	CLA	CHD-C1D	4.99	1.48	1.38
18	L	1502	CLA	O2D-CGD	4.99	1.45	1.33
18	4	4012	CLA	CHD-C1D	4.98	1.50	1.38
18	A	1123	CLA	CAB-C3B	-4.98	1.34	1.47
18	B	1224	CLA	CHC-C4B	4.98	1.50	1.39
18	J	2107	CLA	CHC-C4B	4.97	1.50	1.39
18	B	1232	CLA	C3D-C4D	-4.97	1.33	1.44
18	A	1116	CLA	CHD-C1D	4.96	1.50	1.38
18	3	3009	CLA	CHD-C1D	4.96	1.50	1.38
18	H	1501	CLA	C3D-C4D	-4.96	1.33	1.44
18	A	1119	CLA	O2A-CGA	4.96	1.47	1.33
18	A	1146	CLA	CHD-C1D	4.96	1.50	1.38
18	F	1139	CLA	CAB-C3B	-4.96	1.34	1.47
18	B	1219	CLA	O2D-CGD	4.95	1.45	1.33
18	B	1239	CLA	C3D-C4D	-4.95	1.33	1.44
18	B	1238	CLA	C3D-C4D	-4.95	1.33	1.44
18	2	2004	CLA	CHD-C1D	4.95	1.50	1.38
18	A	1127	CLA	CHD-C1D	4.95	1.50	1.38
18	B	1216	CLA	CHC-C4B	4.95	1.50	1.39
18	B	1237	CLA	CAB-C3B	-4.94	1.34	1.47
18	B	1221	CLA	O2A-CGA	4.94	1.47	1.33
18	A	1122	CLA	CAB-C3B	-4.94	1.34	1.47
18	A	1135	CLA	CHC-C4B	4.94	1.50	1.39
18	B	1214	CLA	O2A-CGA	4.93	1.47	1.33

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
18	B	1236	CLA	O2D-CGD	4.93	1.45	1.33
18	B	9022	CLA	CAB-C3B	-4.93	1.34	1.47
18	4	1009	CLA	CHD-C1D	4.93	1.50	1.38
18	G	1233	CLA	C3D-C4D	-4.93	1.33	1.44
18	A	1101	CLA	CHD-C1D	4.93	1.50	1.38
18	A	1136	CLA	C4C-C3C	-4.92	1.36	1.45
18	L	1130	CLA	O2D-CGD	4.92	1.45	1.33
18	1	1008	CLA	CHD-C1D	4.92	1.50	1.38
18	G	1233	CLA	CAB-C3B	-4.92	1.34	1.47
18	B	9010	CLA	C3D-C4D	-4.92	1.33	1.44
18	B	1220	CLA	C3D-C4D	-4.92	1.33	1.44
18	F	1303	CLA	CHD-C1D	4.92	1.50	1.38
18	B	1241	CLA	CHD-C1D	4.92	1.50	1.38
18	B	1232	CLA	CAB-C3B	-4.91	1.34	1.47
18	L	1125	CLA	CHD-C1D	4.91	1.50	1.38
18	A	1122	CLA	O2A-CGA	4.91	1.47	1.33
18	3	3001	CLA	CHD-C1D	4.91	1.50	1.38
18	B	1218	CLA	CAB-C3B	-4.91	1.34	1.47
18	2	2011	CLA	CHD-C1D	4.90	1.50	1.38
18	B	1231	CLA	CAB-C3B	-4.90	1.34	1.47
18	4	1304	CLA	CHC-C4B	4.90	1.50	1.39
18	2	2005	CLA	CHD-C1D	4.90	1.50	1.38
18	B	1207	CLA	CHC-C4B	4.90	1.50	1.39
18	B	1223	CLA	CHD-C1D	4.90	1.50	1.38
18	J	2107	CLA	CAB-C3B	-4.90	1.34	1.47
18	2	2015	CLA	CHD-C1D	4.90	1.50	1.38
18	A	1120	CLA	CHD-C1D	4.90	1.50	1.38
18	3	3015	CLA	CHD-C1D	4.89	1.50	1.38
18	A	1123	CLA	CHC-C4B	4.89	1.50	1.39
18	F	4015	CLA	CHD-C1D	4.89	1.50	1.38
18	B	1220	CLA	CHD-C1D	4.89	1.48	1.38
18	B	1207	CLA	C3D-C4D	-4.89	1.33	1.44
18	4	4003	CLA	CHD-C1D	4.89	1.50	1.38
18	B	1212	CLA	CHC-C4B	4.89	1.50	1.39
18	2	2010	CLA	CHD-C1D	4.88	1.50	1.38
18	A	1126	CLA	CHC-C4B	4.88	1.50	1.39
18	A	1105	CLA	CHD-C1D	4.88	1.50	1.38
18	B	9023	CLA	CHC-C4B	4.87	1.50	1.39
18	B	1235	CLA	CAB-C3B	-4.87	1.34	1.47
18	A	1104	CLA	CHD-C1D	4.87	1.50	1.38
18	3	3003	CLA	CHD-C1D	4.87	1.50	1.38
18	3	3013	CLA	CHD-C1D	4.87	1.50	1.38

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
18	H	1501	CLA	O2A-CGA	4.86	1.47	1.33
18	K	1150	CLA	CHD-C1D	4.86	1.50	1.38
18	F	1240	CLA	CHD-C1D	4.86	1.50	1.38
18	3	3002	CLA	CHD-C1D	4.86	1.50	1.38
18	B	1219	CLA	CAB-C3B	-4.86	1.34	1.47
18	A	1143	CLA	CHD-C1D	4.85	1.50	1.38
18	B	1232	CLA	CHC-C4B	4.85	1.50	1.39
18	B	1205	CLA	C3D-C4D	-4.84	1.33	1.44
18	2	2013	CLA	CHD-C1D	4.84	1.50	1.38
18	A	1103	CLA	CAB-C3B	-4.84	1.34	1.47
18	A	1118	CLA	CHD-C1D	4.83	1.50	1.38
18	3	3006	CLA	CHD-C1D	4.83	1.50	1.38
18	A	1115	CLA	C3D-C4D	-4.83	1.33	1.44
18	L	1503	CLA	O2A-CGA	4.83	1.47	1.33
18	A	1108	CLA	C3D-C4D	-4.83	1.33	1.44
18	B	1208	CLA	C3D-C4D	-4.83	1.33	1.44
18	2	2012	CLA	CHD-C1D	4.82	1.50	1.38
18	F	1302	CLA	CHC-C4B	4.82	1.50	1.39
18	B	1220	CLA	CHC-C4B	4.82	1.50	1.39
18	B	9012	CLA	O2A-CGA	4.81	1.47	1.33
18	A	1117	CLA	CHD-C1D	4.81	1.50	1.38
18	B	1219	CLA	CHC-C4B	4.81	1.50	1.39
18	B	1227	CLA	CHC-C1C	4.81	1.48	1.38
18	B	9012	CLA	CHC-C4B	4.81	1.50	1.39
18	1	1002	CLA	CHD-C1D	4.81	1.50	1.38
18	B	1229	CLA	CHD-C1D	4.80	1.47	1.38
18	2	2002	CLA	CHD-C1D	4.80	1.50	1.38
18	B	1238	CLA	O2A-CGA	4.80	1.47	1.33
18	4	1304	CLA	C3D-C4D	-4.80	1.33	1.44
18	A	9013	CLA	CAB-C3B	-4.80	1.34	1.47
18	4	4005	CLA	CHD-C1D	4.80	1.50	1.38
18	A	1147	CLA	CHD-C1D	4.80	1.50	1.38
18	A	1136	CLA	CAB-C3B	-4.79	1.34	1.47
18	4	4010	CLA	CHD-C1D	4.79	1.50	1.38
18	1	1004	CLA	CHD-C1D	4.79	1.50	1.38
18	B	1214	CLA	CAB-C3B	-4.79	1.34	1.47
18	3	3008	CLA	CHD-C1D	4.79	1.50	1.38
18	F	1305	CLA	CHD-C1D	4.78	1.50	1.38
18	A	1137	CLA	C3D-C4D	-4.78	1.33	1.44
18	B	1218	CLA	CHD-C4C	4.78	1.50	1.39
18	A	1135	CLA	CAB-C3B	-4.77	1.34	1.47
18	B	9023	CLA	O2A-CGA	4.77	1.47	1.33

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
18	B	1235	CLA	C3D-C4D	-4.77	1.33	1.44
18	A	1123	CLA	C3D-C4D	-4.77	1.33	1.44
18	B	9010	CLA	CHC-C4B	4.77	1.50	1.39
18	3	3012	CLA	CHD-C1D	4.77	1.50	1.38
18	B	1238	CLA	CHC-C4B	4.77	1.50	1.39
18	B	1230	CLA	CHD-C1D	4.76	1.50	1.38
18	A	1134	CLA	CHD-C1D	4.76	1.50	1.38
18	3	3004	CLA	CHD-C1D	4.76	1.50	1.38
18	4	4008	CLA	CHD-C1D	4.76	1.50	1.38
18	H	1501	CLA	CAB-C3B	-4.76	1.34	1.47
18	B	9010	CLA	CAB-C3B	-4.76	1.34	1.47
18	1	1013	CLA	CHD-C1D	4.75	1.50	1.38
18	A	1124	CLA	CHD-C1D	4.75	1.50	1.38
18	B	1222	CLA	C3D-C4D	-4.75	1.33	1.44
18	4	4004	CLA	CHD-C1D	4.75	1.50	1.38
18	B	1209	CLA	CAB-C3B	-4.75	1.34	1.47
18	B	1237	CLA	CHC-C4B	4.74	1.50	1.39
18	B	9010	CLA	O2A-CGA	4.74	1.47	1.33
18	B	1228	CLA	O2D-CGD	4.73	1.44	1.33
18	B	1212	CLA	C3D-C4D	-4.73	1.33	1.44
18	A	1123	CLA	C1B-NB	-4.73	1.31	1.37
18	A	1309	CLA	CHD-C1D	4.73	1.50	1.38
18	B	1229	CLA	CHD-C4C	4.73	1.50	1.39
18	1	1011	CLA	CHD-C1D	4.73	1.50	1.38
18	3	3005	CLA	CHD-C1D	4.73	1.49	1.38
18	B	9023	CLA	CAB-C3B	-4.73	1.34	1.47
18	4	4007	CLA	CHD-C1D	4.72	1.49	1.38
18	B	1231	CLA	CHC-C4B	4.72	1.50	1.39
18	A	1135	CLA	C3D-C4D	-4.72	1.33	1.44
18	A	1129	CLA	O2A-CGA	4.72	1.47	1.33
18	A	1144	CLA	CHD-C1D	4.72	1.49	1.38
18	1	1012	CLA	CHD-C1D	4.72	1.49	1.38
18	A	1113	CLA	O2A-CGA	4.72	1.47	1.33
18	A	1109	CLA	CHD-C1D	4.72	1.49	1.38
18	A	1131	CLA	O2D-CGD	4.71	1.44	1.33
18	3	3010	CLA	CHD-C1D	4.71	1.49	1.38
18	K	1141	CLA	CHD-C1D	4.71	1.49	1.38
18	4	4009	CLA	CHD-C1D	4.70	1.49	1.38
18	2	2008	CLA	CHD-C1D	4.70	1.49	1.38
18	H	1501	CLA	CHC-C4B	4.70	1.50	1.39
18	A	1136	CLA	CHD-C4C	4.70	1.49	1.39
18	A	1148	CLA	CHD-C1D	4.69	1.49	1.38

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
18	A	1131	CLA	O2A-CGA	4.69	1.46	1.30
18	B	1216	CLA	CAB-C3B	-4.69	1.34	1.47
18	L	1503	CLA	MG-NA	-4.69	1.95	2.06
18	B	1218	CLA	O2A-CGA	4.68	1.47	1.33
18	A	1113	CLA	C4C-C3C	-4.68	1.37	1.45
18	B	1211	CLA	CHD-C1D	4.68	1.49	1.38
18	B	1228	CLA	C3D-C4D	-4.67	1.33	1.44
18	B	1207	CLA	O2A-CGA	4.67	1.47	1.33
18	A	1122	CLA	OBD-CAD	4.67	1.30	1.22
18	F	1302	CLA	C3D-C4D	-4.67	1.33	1.44
18	A	1151	CLA	CHD-C1D	4.67	1.49	1.38
18	A	1107	CLA	O2D-CGD	4.67	1.44	1.33
18	4	4011	CLA	CHD-C1D	4.66	1.49	1.38
18	B	1221	CLA	CHC-C1C	4.66	1.47	1.38
18	B	1219	CLA	C3D-C4D	-4.66	1.33	1.44
18	2	2003	CLA	CHD-C1D	4.66	1.49	1.38
18	B	1235	CLA	O2A-CGA	4.66	1.46	1.33
18	B	1239	CLA	O2D-CGD	4.66	1.44	1.33
18	1	1010	CLA	CHD-C1D	4.66	1.49	1.38
18	A	9013	CLA	C3D-C4D	-4.66	1.33	1.44
18	K	1153	CLA	CHD-C1D	4.65	1.49	1.38
19	B	5002	PQN	C10-C5	4.65	1.48	1.40
18	B	1222	CLA	CAB-C3B	-4.65	1.35	1.47
18	1	1003	CLA	CHD-C1D	4.64	1.49	1.38
18	1	1014	CLA	CHD-C1D	4.64	1.49	1.38
18	B	1228	CLA	CHC-C4B	4.64	1.49	1.39
18	B	1205	CLA	CHC-C4B	4.64	1.49	1.39
18	B	1203	CLA	CAB-C3B	-4.63	1.35	1.47
18	L	1504	CLA	CHC-C4B	4.62	1.49	1.39
18	4	4002	CLA	CHD-C1D	4.62	1.49	1.38
18	B	1217	CLA	O2D-CGD	4.62	1.44	1.33
18	F	1139	CLA	OBD-CAD	4.62	1.30	1.22
18	B	1213	CLA	CHD-C1D	4.62	1.49	1.38
18	B	9022	CLA	O2D-CGD	4.62	1.44	1.33
18	A	1128	CLA	C1B-NB	-4.61	1.31	1.37
18	L	1502	CLA	O2A-CGA	4.61	1.46	1.33
18	I	1204	CLA	CHC-C4B	4.61	1.49	1.39
18	A	1128	CLA	CHC-C4B	4.61	1.49	1.39
18	B	1215	CLA	CHC-C1C	4.60	1.47	1.38
18	B	1212	CLA	C4C-C3C	-4.60	1.37	1.45
18	A	1136	CLA	CHC-C4B	4.60	1.49	1.39
18	A	1142	CLA	CHD-C1D	4.60	1.49	1.38

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
18	B	1225	CLA	CHC-C4B	4.60	1.49	1.39
18	B	1231	CLA	O2D-CGD	4.60	1.44	1.33
18	F	1302	CLA	CAB-C3B	-4.60	1.35	1.47
18	A	9011	CLA	O2A-CGA	4.60	1.46	1.33
18	B	1229	CLA	C4C-C3C	-4.60	1.37	1.45
18	L	1504	CLA	O2A-CGA	4.60	1.46	1.33
18	4	4013	CLA	CHD-C1D	4.59	1.49	1.38
18	3	2009	CLA	CHD-C1D	4.59	1.49	1.38
18	B	9022	CLA	O2A-CGA	4.59	1.46	1.33
18	L	1503	CLA	CHD-C4C	4.59	1.49	1.39
18	A	1137	CLA	O2A-CGA	4.59	1.46	1.33
18	A	9013	CLA	CHC-C1C	4.59	1.47	1.38
18	A	1108	CLA	CHC-C4B	4.59	1.49	1.39
18	G	1233	CLA	O2A-CGA	4.59	1.46	1.33
18	B	1222	CLA	O2A-CGA	4.58	1.46	1.33
18	B	1215	CLA	C3D-C4D	-4.58	1.33	1.44
18	A	1108	CLA	CAB-C3B	-4.57	1.35	1.47
18	A	1115	CLA	CAB-C3B	-4.56	1.35	1.47
18	3	3007	CLA	CHD-C1D	4.56	1.49	1.38
18	L	1503	CLA	CHD-C1D	4.56	1.47	1.38
18	A	1123	CLA	O2A-CGA	4.55	1.46	1.33
18	A	1140	CLA	CHB-C1B	4.55	1.49	1.39
18	B	9023	CLA	C3D-C4D	-4.55	1.34	1.44
18	A	1107	CLA	CHC-C4B	4.55	1.49	1.39
18	I	1204	CLA	C3D-C4D	-4.55	1.34	1.44
18	B	1234	CLA	CAB-C3B	-4.55	1.35	1.47
18	A	1119	CLA	OBD-CAD	4.55	1.30	1.22
18	L	1504	CLA	CAB-C3B	-4.54	1.35	1.47
18	B	1236	CLA	CAB-C3B	-4.54	1.35	1.47
18	A	9011	CLA	CAB-C3B	-4.53	1.35	1.47
18	A	1136	CLA	O2A-CGA	4.52	1.46	1.33
18	A	1123	CLA	OBD-CAD	4.52	1.30	1.22
18	A	1131	CLA	C3D-C4D	-4.52	1.34	1.44
18	A	1132	CLA	CHD-C1D	4.51	1.49	1.38
18	B	1217	CLA	CHC-C4B	4.51	1.49	1.39
18	A	1152	CLA	CHD-C1D	4.50	1.49	1.38
18	A	1110	CLA	CHD-C1D	4.50	1.49	1.38
18	A	1136	CLA	C3D-C4D	-4.50	1.34	1.44
18	A	1129	CLA	CAB-C3B	-4.50	1.35	1.47
18	B	1209	CLA	O2A-CGA	4.50	1.46	1.33
18	B	9022	CLA	CHC-C4B	4.49	1.49	1.39
18	A	1140	CLA	CAB-C3B	-4.49	1.35	1.47

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
18	H	1505	CLA	CHD-C1D	4.49	1.49	1.38
18	G	1248	CLA	CHD-C1D	4.49	1.49	1.38
18	A	9011	CLA	C3D-C4D	-4.48	1.34	1.44
18	B	1207	CLA	O2D-CGD	4.48	1.44	1.33
18	B	1227	CLA	O2A-CGA	4.48	1.46	1.33
18	B	1242	CLA	O2A-CGA	4.47	1.46	1.33
18	B	1231	CLA	O2A-CGA	4.47	1.46	1.33
18	B	1221	CLA	CAB-C3B	-4.47	1.35	1.47
18	B	1209	CLA	CHC-C4B	4.46	1.49	1.39
18	A	1103	CLA	O2A-CGA	4.45	1.46	1.33
18	B	1217	CLA	O2A-CGA	4.45	1.46	1.33
18	A	1107	CLA	CHB-C1B	4.45	1.49	1.39
18	B	1236	CLA	O2A-CGA	4.44	1.46	1.33
18	A	1137	CLA	OBD-CAD	4.43	1.30	1.22
18	I	1204	CLA	CAB-C3B	-4.43	1.35	1.47
18	B	1239	CLA	CHC-C4B	4.43	1.49	1.39
18	B	1216	CLA	OBD-CAD	4.43	1.30	1.22
18	B	1234	CLA	O2A-CGA	4.42	1.46	1.33
18	A	1135	CLA	OBD-CAD	4.42	1.30	1.22
18	B	1219	CLA	OBD-CAD	4.42	1.30	1.22
18	B	1231	CLA	OBD-CAD	4.41	1.30	1.22
18	B	1202	CLA	CHC-C4B	4.41	1.49	1.39
18	4	1304	CLA	CAB-C3B	-4.40	1.35	1.47
18	B	1215	CLA	C1C-C2C	-4.39	1.35	1.44
18	A	1113	CLA	CAB-C3B	-4.39	1.35	1.47
18	F	1139	CLA	CHC-C4B	4.39	1.49	1.39
18	L	1503	CLA	CHC-C4B	4.38	1.49	1.39
18	4	1304	CLA	O2A-CGA	4.38	1.46	1.33
18	B	1235	CLA	CHC-C4B	4.37	1.49	1.39
18	B	1218	CLA	OBD-CAD	4.37	1.30	1.22
18	A	1119	CLA	CAB-C3B	-4.37	1.35	1.47
18	A	1131	CLA	CHC-C4B	4.35	1.49	1.39
18	A	1140	CLA	OBD-CAD	4.35	1.30	1.22
18	B	1229	CLA	O2A-CGA	4.35	1.46	1.33
18	B	1215	CLA	CHC-C4B	4.34	1.49	1.39
18	B	1202	CLA	O2A-CGA	4.34	1.46	1.33
18	B	1232	CLA	O2A-CGA	4.34	1.46	1.33
18	2	2007	CLA	CHD-C1D	4.34	1.49	1.38
18	B	1235	CLA	C1B-NB	-4.34	1.32	1.37
18	B	1224	CLA	O2A-CGA	4.34	1.46	1.33
20	I	6018	BCR	C10-C9	-4.33	1.25	1.35
18	B	1219	CLA	O2A-CGA	4.32	1.45	1.33

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
18	A	1140	CLA	CHC-C4B	4.30	1.49	1.39
18	A	1131	CLA	OBD-CAD	4.28	1.29	1.22
18	B	1228	CLA	CAB-C3B	-4.28	1.36	1.47
18	B	1301	CLA	CHC-C4B	4.28	1.51	1.39
18	A	1128	CLA	CAB-C3B	-4.28	1.36	1.47
18	1	1006	CLA	CHD-C1D	4.27	1.48	1.38
18	A	9013	CLA	O2A-CGA	4.26	1.46	1.33
18	B	1203	CLA	C3D-C4D	-4.26	1.32	1.44
18	B	1210	CLA	CHD-C1D	4.25	1.48	1.38
18	4	1009	CLA	CHC-C4B	4.24	1.51	1.39
18	F	1306	CLA	CHC-C4B	4.23	1.51	1.39
18	A	1106	CLA	CHC-C4B	4.23	1.48	1.39
18	2	2005	CLA	CHC-C4B	4.23	1.51	1.39
18	B	1224	CLA	C3D-C4D	-4.22	1.34	1.44
18	B	1207	CLA	CAB-C3B	-4.21	1.36	1.47
18	A	1135	CLA	O2A-CGA	4.21	1.44	1.30
18	B	1222	CLA	OBD-CAD	4.20	1.29	1.22
18	B	1224	CLA	C4C-C3C	-4.19	1.37	1.45
18	A	1113	CLA	CHC-C4B	4.19	1.48	1.39
18	B	1225	CLA	C4C-C3C	-4.19	1.37	1.45
18	F	1302	CLA	O2A-CGA	4.18	1.45	1.33
18	J	2107	CLA	O2A-CGA	4.18	1.45	1.33
18	B	1138	CLA	CHC-C4B	4.17	1.48	1.39
18	B	1203	CLA	O2A-CGA	4.17	1.45	1.33
18	B	1220	CLA	CHB-C1B	4.17	1.48	1.39
18	B	1228	CLA	C4C-C3C	-4.17	1.38	1.45
18	A	1132	CLA	CHC-C4B	4.16	1.51	1.39
18	A	1107	CLA	OBD-CAD	4.16	1.29	1.22
18	1	1005	CLA	CHC-C4B	4.16	1.51	1.39
18	1	1001	CLA	CHC-C4B	4.16	1.51	1.39
18	B	1215	CLA	CHB-C1B	4.16	1.48	1.39
18	B	1227	CLA	CAB-C3B	-4.15	1.36	1.47
18	4	4006	CLA	CHC-C4B	4.15	1.50	1.39
18	B	1225	CLA	O2A-CGA	4.15	1.44	1.30
18	A	9011	CLA	OBD-CAD	4.15	1.29	1.22
18	B	1210	CLA	CHC-C4B	4.14	1.50	1.39
18	4	4012	CLA	CHC-C4B	4.14	1.50	1.39
18	A	1103	CLA	C1C-C2C	-4.13	1.36	1.44
18	F	1303	CLA	CHC-C4B	4.13	1.50	1.39
18	I	1204	CLA	OBD-CAD	4.13	1.29	1.22
18	A	1106	CLA	C3D-C4D	-4.13	1.34	1.44
18	J	1307	CLA	CHC-C4B	4.12	1.50	1.39

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
18	3	3001	CLA	CHC-C4B	4.12	1.50	1.39
18	A	1143	CLA	CHC-C4B	4.11	1.50	1.39
18	J	2107	CLA	OBD-CAD	4.11	1.29	1.22
18	B	1234	CLA	CHB-C1B	4.11	1.48	1.39
18	A	1146	CLA	CHC-C4B	4.11	1.50	1.39
18	B	1232	CLA	OBD-CAD	4.11	1.29	1.22
18	L	1502	CLA	OBD-CAD	4.11	1.29	1.22
18	A	9011	CLA	CHC-C4B	4.11	1.48	1.39
18	B	1202	CLA	OBD-CAD	4.10	1.29	1.22
18	1	1004	CLA	CHC-C4B	4.10	1.50	1.39
18	A	1142	CLA	CHC-C4B	4.09	1.50	1.39
18	B	1203	CLA	CHC-C4B	4.09	1.48	1.39
18	B	1205	CLA	C4C-C3C	-4.09	1.38	1.45
18	A	1109	CLA	CHC-C4B	4.09	1.50	1.39
18	B	1205	CLA	O2A-CGA	4.08	1.45	1.33
18	1	1010	CLA	CHC-C4B	4.08	1.50	1.39
18	2	2004	CLA	CHC-C4B	4.08	1.50	1.39
18	B	1238	CLA	OBD-CAD	4.07	1.29	1.22
18	B	1229	CLA	CHB-C1B	4.07	1.48	1.39
18	B	1235	CLA	OBD-CAD	4.07	1.29	1.22
18	1	1014	CLA	CHC-C4B	4.07	1.50	1.39
18	B	1221	CLA	CHC-C4B	4.06	1.48	1.39
18	A	1106	CLA	C3A-C2A	-4.06	1.50	1.54
18	4	4007	CLA	CHC-C4B	4.06	1.50	1.39
18	B	1205	CLA	CHB-C1B	4.05	1.48	1.39
18	B	1138	CLA	CAB-C3B	-4.05	1.36	1.47
18	B	1230	CLA	CHC-C4B	4.04	1.50	1.39
18	B	1235	CLA	C4B-NB	-4.04	1.32	1.37
18	A	1103	CLA	CHC-C4B	4.03	1.48	1.39
18	4	4003	CLA	CHC-C4B	4.03	1.50	1.39
18	A	1106	CLA	OBD-CAD	4.02	1.29	1.22
18	B	1224	CLA	CAB-C3B	-4.01	1.36	1.47
18	A	1152	CLA	CHC-C4B	4.01	1.50	1.39
18	G	1233	CLA	C4C-C3C	-4.01	1.38	1.45
18	4	4005	CLA	CHC-C4B	4.01	1.50	1.39
18	A	1104	CLA	CHC-C4B	4.00	1.50	1.39
18	F	1305	CLA	CHC-C4B	4.00	1.50	1.39
18	1	1006	CLA	CHC-C4B	4.00	1.50	1.39
18	B	1235	CLA	O2D-CGD	3.99	1.43	1.33
18	B	1241	CLA	CHC-C4B	3.99	1.50	1.39
18	2	2013	CLA	CHC-C4B	3.99	1.50	1.39
18	4	4010	CLA	CHC-C4B	3.99	1.50	1.39

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
18	F	4015	CLA	CHC-C4B	3.99	1.50	1.39
18	A	1134	CLA	CHC-C4B	3.99	1.50	1.39
18	B	1205	CLA	CAB-C3B	-3.99	1.36	1.47
18	A	1115	CLA	CHC-C4B	3.99	1.48	1.39
18	2	2011	CLA	CHC-C4B	3.98	1.50	1.39
18	4	4001	CLA	CHC-C4B	3.98	1.50	1.39
18	A	1120	CLA	CHC-C4B	3.98	1.50	1.39
18	F	1240	CLA	CHC-C4B	3.98	1.50	1.39
18	B	1227	CLA	CHB-C1B	3.97	1.48	1.39
18	4	1304	CLA	OBD-CAD	3.96	1.29	1.22
18	B	1232	CLA	C1B-NB	-3.96	1.32	1.37
18	B	1203	CLA	OBD-CAD	3.96	1.29	1.22
18	A	1124	CLA	CHC-C4B	3.95	1.50	1.39
18	A	1116	CLA	CHC-C4B	3.95	1.50	1.39
18	1	1013	CLA	CHC-C4B	3.95	1.50	1.39
18	3	3011	CLA	CHC-C4B	3.95	1.50	1.39
18	A	1111	CLA	CHC-C4B	3.94	1.50	1.39
18	K	1141	CLA	CHC-C4B	3.94	1.50	1.39
18	A	1118	CLA	CHC-C4B	3.94	1.50	1.39
20	L	6020	BCR	C10-C9	-3.94	1.26	1.35
18	A	1108	CLA	C4C-C3C	-3.93	1.38	1.45
18	A	1133	CLA	CHC-C4B	3.93	1.50	1.39
18	A	1102	CLA	CHC-C4B	3.93	1.50	1.39
18	3	3010	CLA	CHC-C4B	3.92	1.50	1.39
18	K	1150	CLA	CHC-C4B	3.92	1.50	1.39
18	3	3015	CLA	CHC-C4B	3.92	1.50	1.39
18	A	1151	CLA	CHC-C4B	3.92	1.50	1.39
18	B	1206	CLA	CHC-C4B	3.92	1.50	1.39
18	1	1011	CLA	CHC-C4B	3.92	1.50	1.39
20	F	6016	BCR	C10-C9	-3.92	1.26	1.35
18	A	1101	CLA	CHC-C4B	3.92	1.50	1.39
18	L	1125	CLA	CHC-C4B	3.92	1.50	1.39
18	2	2007	CLA	CHC-C4B	3.92	1.50	1.39
18	3	3013	CLA	CHC-C4B	3.91	1.50	1.39
18	4	4002	CLA	CHC-C4B	3.91	1.50	1.39
18	3	3004	CLA	CHC-C4B	3.91	1.50	1.39
18	L	1504	CLA	OBD-CAD	3.91	1.29	1.22
18	1	1008	CLA	CHC-C4B	3.90	1.50	1.39
18	3	3012	CLA	CHC-C4B	3.90	1.50	1.39
18	B	1223	CLA	CHC-C4B	3.90	1.50	1.39
18	B	1225	CLA	C1C-C2C	-3.89	1.36	1.44
18	L	1130	CLA	CAB-C3B	-3.89	1.37	1.47

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
18	B	1222	CLA	CHB-C1B	3.89	1.48	1.39
18	2	2015	CLA	CHC-C4B	3.89	1.50	1.39
18	A	1126	CLA	C1B-NB	-3.89	1.32	1.37
18	A	1128	CLA	CHB-C1B	3.88	1.48	1.39
18	2	2012	CLA	CHC-C4B	3.88	1.50	1.39
18	B	9023	CLA	C4C-C3C	-3.88	1.38	1.45
18	B	1221	CLA	OBD-CAD	3.88	1.29	1.22
18	3	3006	CLA	CHC-C4B	3.88	1.50	1.39
18	3	3003	CLA	CHC-C4B	3.88	1.50	1.39
18	B	1214	CLA	OBD-CAD	3.88	1.29	1.22
18	2	2010	CLA	CHC-C4B	3.88	1.50	1.39
18	B	1205	CLA	OBD-CAD	3.87	1.29	1.22
18	3	2009	CLA	CHC-C4B	3.87	1.50	1.39
18	B	1227	CLA	CHC-C4B	3.87	1.48	1.39
18	4	4004	CLA	CHC-C4B	3.87	1.50	1.39
18	3	3009	CLA	CHC-C4B	3.87	1.50	1.39
18	B	9010	CLA	C1C-C2C	-3.87	1.36	1.44
18	A	1148	CLA	CHC-C4B	3.87	1.50	1.39
18	A	1117	CLA	CHC-C4B	3.86	1.50	1.39
18	3	3002	CLA	CHC-C4B	3.86	1.50	1.39
18	1	1003	CLA	CHC-C4B	3.85	1.50	1.39
18	J	1308	CLA	CHC-C4B	3.85	1.50	1.39
18	A	1110	CLA	CHC-C4B	3.85	1.50	1.39
18	B	1208	CLA	CAB-C3B	-3.85	1.37	1.47
18	A	1136	CLA	OBD-CAD	3.85	1.29	1.22
18	4	4013	CLA	CHC-C4B	3.84	1.50	1.39
18	B	1201	CLA	CHC-C4B	3.84	1.50	1.39
18	B	1215	CLA	O2A-CGA	3.83	1.44	1.33
18	2	2003	CLA	CHC-C4B	3.82	1.50	1.39
18	2	2001	CLA	CHC-C4B	3.82	1.50	1.39
18	A	1147	CLA	CHC-C4B	3.82	1.50	1.39
18	1	1002	CLA	CHC-C4B	3.81	1.50	1.39
18	B	1213	CLA	CHC-C4B	3.81	1.50	1.39
18	1	1007	CLA	CHC-C4B	3.81	1.50	1.39
20	L	6020	BCR	C11-C12	-3.81	1.24	1.34
18	A	1107	CLA	C4C-C3C	-3.80	1.38	1.45
18	A	1113	CLA	OBD-CAD	3.80	1.29	1.22
18	2	2002	CLA	CHC-C4B	3.80	1.50	1.39
18	A	1309	CLA	CHC-C4B	3.80	1.50	1.39
18	3	3008	CLA	CHC-C4B	3.79	1.50	1.39
18	F	1139	CLA	CHB-C1B	3.79	1.47	1.39
18	4	4008	CLA	CHC-C4B	3.79	1.50	1.39

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
18	B	1203	CLA	CHB-C1B	3.78	1.47	1.39
18	A	1144	CLA	CHC-C4B	3.77	1.49	1.39
18	B	1212	CLA	OBD-CAD	3.77	1.29	1.22
18	A	1105	CLA	CHC-C4B	3.76	1.49	1.39
19	A	5001	PQN	C10-C5	3.76	1.46	1.40
18	2	2006	CLA	CHC-C4B	3.76	1.49	1.39
18	H	1505	CLA	CHC-C4B	3.75	1.49	1.39
18	K	1153	CLA	CHC-C4B	3.74	1.49	1.39
18	B	1239	CLA	OBD-CAD	3.74	1.28	1.22
18	4	4009	CLA	CHC-C4B	3.73	1.49	1.39
18	1	1012	CLA	CHC-C4B	3.73	1.49	1.39
18	B	1201	CLA	MG-NA	-3.73	1.97	2.06
18	A	1131	CLA	C1B-NB	-3.73	1.33	1.37
18	4	4011	CLA	CHC-C4B	3.73	1.49	1.39
18	B	1221	CLA	CHB-C1B	3.72	1.47	1.39
18	3	3005	CLA	CHC-C4B	3.72	1.49	1.39
18	G	1233	CLA	OBD-CAD	3.72	1.28	1.22
18	B	1234	CLA	OBD-CAD	3.72	1.28	1.22
18	A	1113	CLA	CHB-C1B	3.72	1.47	1.39
18	A	1103	CLA	OBD-CAD	3.72	1.28	1.22
18	A	1124	CLA	MG-NA	-3.71	1.97	2.06
18	A	9013	CLA	CHC-C4B	3.71	1.47	1.39
18	B	1212	CLA	CAB-C3B	-3.70	1.37	1.47
18	A	9013	CLA	OBD-CAD	3.70	1.28	1.22
18	B	9010	CLA	C1B-NB	-3.70	1.33	1.37
18	J	2107	CLA	CHB-C1B	3.70	1.47	1.39
18	2	2008	CLA	CHC-C4B	3.69	1.49	1.39
18	B	1227	CLA	C1B-NB	-3.69	1.33	1.37
18	A	1127	CLA	CHC-C4B	3.69	1.49	1.39
18	B	1209	CLA	C1B-NB	-3.68	1.33	1.37
18	B	9010	CLA	C4C-C3C	-3.68	1.38	1.45
18	A	1135	CLA	C1B-NB	-3.67	1.33	1.37
18	A	1126	CLA	OBD-CAD	3.67	1.28	1.22
18	B	1218	CLA	C1C-C2C	-3.66	1.37	1.44
18	B	1226	CLA	CHC-C4B	3.66	1.49	1.39
18	G	1233	CLA	C1B-NB	-3.65	1.33	1.37
18	L	1504	CLA	CHB-C1B	3.65	1.47	1.39
18	A	1108	CLA	CHB-C1B	3.64	1.47	1.39
18	G	1248	CLA	CHC-C4B	3.64	1.49	1.39
18	3	3007	CLA	CHC-C4B	3.63	1.49	1.39
18	4	4006	CLA	MG-NA	-3.63	1.97	2.06
18	B	1239	CLA	CHB-C1B	3.63	1.47	1.39

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
18	B	1212	CLA	CHB-C1B	3.62	1.47	1.39
18	L	1130	CLA	CHB-C1B	3.62	1.47	1.39
18	A	1120	CLA	MG-NA	-3.61	1.97	2.06
18	B	1231	CLA	CHB-C1B	3.61	1.47	1.39
18	A	1135	CLA	C4C-C3C	-3.61	1.38	1.45
18	4	4012	CLA	MG-NA	-3.60	1.97	2.06
18	A	1119	CLA	C4C-C3C	-3.60	1.38	1.45
18	A	1126	CLA	O2D-CGD	3.60	1.42	1.33
18	B	1219	CLA	CHB-C1B	3.60	1.47	1.39
18	A	1103	CLA	C1B-NB	-3.59	1.33	1.37
18	B	1236	CLA	C4C-C3C	-3.59	1.38	1.45
18	B	1214	CLA	C4C-C3C	-3.59	1.38	1.45
18	H	1501	CLA	OBD-CAD	3.59	1.28	1.22
18	F	1302	CLA	OBD-CAD	3.58	1.28	1.22
18	A	1136	CLA	CHB-C1B	3.56	1.47	1.39
18	B	1242	CLA	C4C-C3C	-3.56	1.39	1.45
18	B	1214	CLA	C1B-NB	-3.56	1.33	1.37
18	B	1242	CLA	OBD-CAD	3.55	1.28	1.22
18	A	1106	CLA	CHB-C1B	3.55	1.47	1.39
18	A	1115	CLA	OBD-CAD	3.54	1.28	1.22
18	B	1202	CLA	CHB-C1B	3.54	1.47	1.39
18	I	1204	CLA	CHB-C1B	3.54	1.47	1.39
18	B	1223	CLA	MG-NA	-3.54	1.97	2.06
18	A	1111	CLA	CHD-C4C	3.53	1.52	1.40
18	B	1220	CLA	C4C-C3C	-3.53	1.39	1.45
18	2	2012	CLA	MG-NA	-3.52	1.97	2.06
18	B	1236	CLA	OBD-CAD	3.52	1.28	1.22
18	A	1107	CLA	C1C-C2C	-3.51	1.37	1.44
18	A	1128	CLA	O2A-CGA	3.51	1.43	1.33
18	B	1207	CLA	C4C-C3C	-3.48	1.39	1.45
18	B	1238	CLA	C1B-NB	-3.48	1.33	1.37
18	G	1233	CLA	CHB-C1B	3.48	1.47	1.39
18	A	1123	CLA	C4C-C3C	-3.48	1.39	1.45
18	A	1135	CLA	CHB-C1B	3.47	1.47	1.39
18	A	1115	CLA	C1B-NB	-3.47	1.33	1.37
18	A	1129	CLA	OBD-CAD	3.47	1.28	1.22
18	B	1217	CLA	C1B-NB	-3.47	1.33	1.37
18	4	1304	CLA	CHB-C1B	3.47	1.47	1.39
18	F	1302	CLA	CHB-C1B	3.46	1.47	1.39
18	1	1007	CLA	CHD-C4C	3.46	1.52	1.40
18	B	1235	CLA	C1C-C2C	-3.46	1.37	1.44
18	B	1138	CLA	CHB-C1B	3.46	1.47	1.39

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
18	B	9012	CLA	OBD-CAD	3.45	1.28	1.22
18	B	1218	CLA	MG-NA	-3.45	1.98	2.06
18	H	1501	CLA	C4C-C3C	-3.44	1.39	1.45
18	A	1108	CLA	OBD-CAD	3.44	1.28	1.22
18	A	9011	CLA	CHB-C1B	3.44	1.47	1.39
18	A	1101	CLA	CHD-C4C	3.43	1.52	1.40
18	B	1224	CLA	OBD-CAD	3.43	1.28	1.22
18	B	1208	CLA	OBD-CAD	3.42	1.28	1.22
18	L	1502	CLA	CHB-C1B	3.42	1.47	1.39
18	G	1248	CLA	MG-NA	-3.41	1.98	2.06
18	B	9012	CLA	C4C-C3C	-3.41	1.39	1.45
18	1	1014	CLA	MG-NA	-3.40	1.98	2.06
18	A	1133	CLA	CHD-C4C	3.40	1.51	1.40
18	3	3013	CLA	MG-NA	-3.40	1.98	2.06
18	B	9022	CLA	OBD-CAD	3.40	1.28	1.22
18	2	2007	CLA	MG-NA	-3.40	1.98	2.06
18	B	1231	CLA	C1B-NB	-3.39	1.33	1.37
18	J	1308	CLA	CHD-C4C	3.38	1.51	1.40
18	A	1129	CLA	C1B-NB	-3.38	1.33	1.37
18	B	1205	CLA	C1C-C2C	-3.38	1.37	1.44
20	I	6018	BCR	C1-C6	-3.37	1.49	1.53
18	B	1225	CLA	CHB-C1B	3.37	1.47	1.39
18	4	4005	CLA	MG-NA	-3.37	1.98	2.06
18	B	1224	CLA	CHB-C1B	3.36	1.46	1.39
18	B	1211	CLA	CHC-C4B	3.35	1.48	1.39
18	B	1239	CLA	C1C-C2C	-3.35	1.37	1.44
18	3	3008	CLA	MG-NA	-3.35	1.98	2.06
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	2	2001	CLA	CHD-C4C	3.34	1.51	1.40
18	2	2003	CLA	MG-NA	-3.34	1.98	2.06
18	A	1128	CLA	C4C-C3C	-3.34	1.39	1.45
18	A	1120	CLA	CHD-C4C	3.34	1.51	1.40
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	3	3008	CLA	CHD-C4C	3.33	1.51	1.40
18	L	1502	CLA	C4C-C3C	-3.33	1.39	1.45
18	B	1242	CLA	C1B-NB	-3.33	1.33	1.37
18	B	1215	CLA	OBD-CAD	3.33	1.28	1.22
18	2	2005	CLA	CHD-C4C	3.32	1.51	1.40
18	3	3004	CLA	MG-NA	-3.32	1.98	2.06

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
18	J	1308	CLA	MG-NA	-3.32	1.98	2.06
18	3	3001	CLA	MG-NA	-3.32	1.98	2.06
18	L	1130	CLA	C4C-C3C	-3.32	1.39	1.45
18	B	1221	CLA	C1B-NB	-3.32	1.33	1.37
18	2	2008	CLA	CHD-C4C	3.31	1.51	1.40
18	B	1218	CLA	C1B-NB	-3.31	1.33	1.37
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	B	1201	CLA	CHD-C4C	3.30	1.51	1.40
18	F	1240	CLA	CHD-C4C	3.30	1.51	1.40
18	A	1129	CLA	CHB-C1B	3.30	1.46	1.39
18	A	1102	CLA	CHD-C4C	3.30	1.51	1.40
18	B	1234	CLA	C4C-C3C	-3.30	1.39	1.45
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	F	1302	CLA	C4C-C3C	-3.29	1.39	1.45
18	1	1013	CLA	CHD-C4C	3.29	1.51	1.40
18	A	9013	CLA	C4B-NB	-3.29	1.33	1.37
18	1	1006	CLA	MG-NA	-3.29	1.98	2.06
18	B	1229	CLA	OBD-CAD	3.29	1.28	1.22
18	L	1130	CLA	OBD-CAD	3.29	1.28	1.22
18	B	1217	CLA	OBD-CAD	3.29	1.28	1.22
18	4	4012	CLA	CHD-C4C	3.28	1.51	1.40
18	B	1211	CLA	MG-NA	-3.28	1.98	2.06
18	2	2015	CLA	CHD-C4C	3.28	1.51	1.40
18	B	1210	CLA	MG-NA	-3.28	1.98	2.06
18	B	1209	CLA	OBD-CAD	3.28	1.28	1.22
18	2	2006	CLA	CHD-C4C	3.28	1.51	1.40
18	4	1304	CLA	C1B-NB	-3.28	1.33	1.37
18	B	1221	CLA	C1C-C2C	-3.28	1.37	1.44
18	1	1007	CLA	MG-NA	-3.28	1.98	2.06
18	B	1226	CLA	CHD-C4C	3.28	1.51	1.40
18	4	4009	CLA	MG-NA	-3.28	1.98	2.06
18	A	9013	CLA	C1C-C2C	-3.28	1.37	1.44
18	1	1008	CLA	CHD-C4C	3.28	1.51	1.40
18	4	4003	CLA	CHD-C4C	3.28	1.51	1.40
18	B	1237	CLA	C4C-C3C	-3.28	1.39	1.45
18	B	1215	CLA	C1D-ND	-3.27	1.33	1.37
18	B	1216	CLA	C1B-NB	-3.27	1.33	1.37
18	3	3007	CLA	MG-NA	-3.27	1.98	2.06
18	B	1227	CLA	OBD-CAD	3.27	1.28	1.22
18	A	1119	CLA	CHB-C1B	3.26	1.46	1.39

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
18	B	9012	CLA	C1B-NB	-3.26	1.33	1.37
18	I	1204	CLA	C1B-NB	-3.26	1.33	1.37
18	A	1118	CLA	MG-NA	-3.26	1.98	2.06
18	4	4008	CLA	CHD-C4C	3.26	1.51	1.40
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
18	A	1118	CLA	CHD-C4C	3.25	1.51	1.40
18	L	1503	CLA	C1C-C2C	-3.25	1.37	1.44
18	4	4007	CLA	MG-NA	-3.25	1.98	2.06
18	F	1305	CLA	CHD-C4C	3.24	1.51	1.40
18	B	1237	CLA	C1C-C2C	-3.24	1.37	1.44
18	4	4010	CLA	CHD-C4C	3.24	1.51	1.40
18	1	1014	CLA	CHD-C4C	3.24	1.51	1.40
18	1	1005	CLA	MG-NA	-3.24	1.98	2.06
18	B	1242	CLA	CHB-C1B	3.23	1.46	1.39
18	1	1011	CLA	MG-NA	-3.23	1.98	2.06
18	2	2002	CLA	MG-NA	-3.23	1.98	2.06
18	A	1104	CLA	CHA-C1A	3.23	1.50	1.41
18	1	1012	CLA	MG-NA	-3.23	1.98	2.06
18	B	1138	CLA	C4B-NB	-3.22	1.33	1.37
18	2	2010	CLA	CHD-C4C	3.22	1.51	1.40
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	B	1225	CLA	OBD-CAD	3.21	1.28	1.22
18	B	1207	CLA	OBD-CAD	3.21	1.28	1.22
18	B	9010	CLA	OBD-CAD	3.21	1.28	1.22
18	4	4009	CLA	CHD-C4C	3.21	1.51	1.40
18	3	3015	CLA	CHD-C4C	3.21	1.51	1.40
18	A	1144	CLA	CHD-C4C	3.21	1.51	1.40
18	1	1013	CLA	MG-NA	-3.21	1.98	2.06
18	A	1116	CLA	CHD-C4C	3.20	1.51	1.40
18	K	1153	CLA	CHD-C4C	3.20	1.51	1.40
18	A	1127	CLA	CHD-C4C	3.20	1.51	1.40
18	B	9022	CLA	CHB-C1B	3.20	1.46	1.39
18	3	3002	CLA	CHD-C4C	3.20	1.51	1.40
18	A	1137	CLA	C1B-NB	-3.20	1.33	1.37
18	4	4001	CLA	CHD-C4C	3.20	1.51	1.40
18	3	3004	CLA	CHD-C4C	3.20	1.51	1.40
18	4	4006	CLA	CHD-C4C	3.19	1.51	1.40
18	3	3005	CLA	CHD-C4C	3.19	1.51	1.40
18	A	1309	CLA	CHD-C4C	3.19	1.51	1.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
18	1	1008	CLA	MG-NA	-3.19	1.98	2.06
18	2	2013	CLA	CHD-C4C	3.19	1.51	1.40
18	H	1501	CLA	C1B-NB	-3.19	1.33	1.37
18	A	1122	CLA	CHB-C1B	3.19	1.46	1.39
18	F	1303	CLA	CHD-C4C	3.19	1.51	1.40
18	B	9022	CLA	C4C-C3C	-3.18	1.39	1.45
18	J	1307	CLA	CHD-C4C	3.18	1.51	1.40
18	A	1111	CLA	MG-NA	-3.18	1.98	2.06
18	H	1501	CLA	CHB-C1B	3.18	1.46	1.39
18	A	1131	CLA	C1C-C2C	-3.17	1.38	1.44
18	4	4011	CLA	MG-NA	-3.17	1.98	2.06
18	A	1148	CLA	CHD-C4C	3.17	1.51	1.40
18	2	2004	CLA	MG-NA	-3.17	1.98	2.06
18	1	1011	CLA	CHD-C4C	3.17	1.51	1.40
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	B	1241	CLA	MG-NA	-3.16	1.98	2.06
18	3	3001	CLA	CHD-C4C	3.16	1.51	1.40
18	3	3006	CLA	MG-NA	-3.16	1.98	2.06
18	B	1223	CLA	CHD-C4C	3.16	1.51	1.40
18	2	2004	CLA	CHD-C4C	3.16	1.51	1.40
18	K	1150	CLA	CHD-C4C	3.16	1.51	1.40
18	4	4013	CLA	MG-NA	-3.16	1.98	2.06
18	A	1143	CLA	MG-NA	-3.16	1.98	2.06
18	2	2011	CLA	CHD-C4C	3.16	1.51	1.40
18	4	4007	CLA	CHD-C4C	3.16	1.51	1.40
18	1	1002	CLA	CHD-C4C	3.15	1.51	1.40
18	4	4005	CLA	CHD-C4C	3.15	1.51	1.40
18	B	1206	CLA	MG-NA	-3.15	1.98	2.06
18	1	1001	CLA	CHD-C4C	3.15	1.51	1.40
18	4	1304	CLA	C4C-C3C	-3.15	1.39	1.45
18	B	1216	CLA	C4C-C3C	-3.15	1.39	1.45
18	3	3011	CLA	CHD-C4C	3.15	1.51	1.40
18	B	1206	CLA	CHD-C4C	3.15	1.51	1.40
18	B	1232	CLA	CHB-C1B	3.14	1.46	1.39
18	A	1122	CLA	C4C-C3C	-3.14	1.39	1.45
18	B	1301	CLA	CHD-C4C	3.14	1.51	1.40
18	B	9012	CLA	CHB-C1B	3.14	1.46	1.39
18	B	1218	CLA	C4B-NB	-3.14	1.33	1.37
18	F	1306	CLA	CHD-C4C	3.14	1.51	1.40
18	1	1010	CLA	CHD-C4C	3.14	1.51	1.40
18	L	1125	CLA	CHD-C4C	3.14	1.51	1.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
18	A	1309	CLA	MG-NA	-3.14	1.98	2.06
18	F	1306	CLA	MG-NA	-3.13	1.98	2.06
18	A	1115	CLA	C4B-NB	-3.13	1.33	1.37
18	3	3013	CLA	CHD-C4C	3.13	1.51	1.40
18	B	1138	CLA	OBD-CAD	3.13	1.27	1.22
18	2	2002	CLA	CHD-C4C	3.13	1.51	1.40
18	B	1301	CLA	MG-NA	-3.13	1.98	2.06
18	A	1109	CLA	CHD-C4C	3.13	1.51	1.40
18	A	1105	CLA	CHD-C4C	3.13	1.51	1.40
18	A	1146	CLA	CHD-C4C	3.13	1.51	1.40
18	A	9013	CLA	CHB-C1B	3.13	1.46	1.39
18	B	1221	CLA	C4B-NB	-3.12	1.33	1.37
18	B	9023	CLA	C1B-NB	-3.12	1.33	1.37
18	A	1128	CLA	C1D-ND	-3.12	1.33	1.37
18	F	4015	CLA	CHD-C4C	3.12	1.50	1.40
18	3	3007	CLA	CHD-C4C	3.12	1.50	1.40
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	1003	CLA	CHD-C4C	3.12	1.50	1.40
18	B	1209	CLA	CHB-C1B	3.11	1.46	1.39
18	A	1132	CLA	CHD-C4C	3.11	1.50	1.40
18	A	1105	CLA	MG-NA	-3.11	1.98	2.06
18	B	1216	CLA	CHB-C1B	3.11	1.46	1.39
18	B	1218	CLA	C1C-NC	-3.11	1.33	1.37
18	A	1109	CLA	C1D-ND	-3.11	1.33	1.37
18	B	1215	CLA	C1B-NB	-3.10	1.33	1.37
18	3	3009	CLA	CHD-C4C	3.10	1.50	1.40
18	B	1230	CLA	CHD-C4C	3.10	1.50	1.40
18	1	1005	CLA	CHD-C4C	3.10	1.50	1.40
18	A	1142	CLA	MG-NA	-3.09	1.98	2.06
18	A	1134	CLA	CHD-C4C	3.09	1.50	1.40
18	3	3010	CLA	CHD-C4C	3.09	1.50	1.40
18	A	1115	CLA	C4C-C3C	-3.09	1.39	1.45
18	B	1214	CLA	CHB-C1B	3.09	1.46	1.39
18	4	4004	CLA	CHD-C4C	3.09	1.50	1.40
18	2	2012	CLA	CHD-C4C	3.08	1.50	1.40
18	B	1241	CLA	CHD-C4C	3.08	1.50	1.40
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	1143	CLA	CHD-C4C	3.08	1.50	1.40
18	B	1210	CLA	CHD-C4C	3.07	1.50	1.40
18	B	1221	CLA	C4C-C3C	-3.07	1.39	1.45

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
18	B	1228	CLA	C4B-NB	-3.07	1.33	1.37
18	B	1227	CLA	C4C-C3C	-3.07	1.39	1.45
18	3	3003	CLA	CHD-C4C	3.07	1.50	1.40
18	2	2013	CLA	MG-NA	-3.07	1.99	2.06
18	B	1213	CLA	CHD-C4C	3.06	1.50	1.40
18	3	2009	CLA	CHD-C4C	3.06	1.50	1.40
18	4	4001	CLA	MG-NA	-3.06	1.99	2.06
18	H	1505	CLA	MG-NA	-3.06	1.99	2.06
18	A	1102	CLA	MG-NA	-3.06	1.99	2.06
18	4	4002	CLA	CHD-C4C	3.06	1.50	1.40
18	B	1238	CLA	C1C-C2C	-3.06	1.38	1.44
18	4	4011	CLA	CHD-C4C	3.05	1.50	1.40
18	A	1101	CLA	MG-NA	-3.05	1.99	2.06
18	B	1202	CLA	C1C-C2C	-3.05	1.38	1.44
18	L	1503	CLA	CHB-C1B	3.05	1.46	1.39
18	B	9022	CLA	C1C-C2C	-3.05	1.38	1.44
18	K	1141	CLA	CHD-C4C	3.05	1.50	1.40
18	B	1231	CLA	C4B-NB	-3.04	1.33	1.37
18	1	1012	CLA	CHD-C4C	3.04	1.50	1.40
18	B	1222	CLA	C4C-C3C	-3.04	1.39	1.45
18	B	1226	CLA	CHB-C1B	3.04	1.48	1.39
18	B	1239	CLA	C4C-C3C	-3.04	1.39	1.45
18	A	1134	CLA	CHB-C1B	3.04	1.48	1.39
18	2	2003	CLA	CHD-C4C	3.03	1.50	1.40
18	A	1136	CLA	C1B-NB	-3.03	1.33	1.37
18	3	3002	CLA	CHB-C1B	3.03	1.48	1.39
18	B	1202	CLA	C4C-C3C	-3.03	1.39	1.45
18	K	1150	CLA	MG-NA	-3.03	1.99	2.06
18	B	1138	CLA	C1B-NB	-3.02	1.33	1.37
18	A	1142	CLA	CHD-C4C	3.02	1.50	1.40
18	A	1140	CLA	C4C-C3C	-3.02	1.39	1.45
18	B	1231	CLA	C4C-C3C	-3.02	1.39	1.45
18	B	1232	CLA	C4C-C3C	-3.02	1.39	1.45
18	F	1302	CLA	C1B-NB	-3.02	1.33	1.37
18	B	1211	CLA	CHD-C4C	3.01	1.50	1.40
18	B	1201	CLA	CHA-C1A	3.01	1.49	1.41
18	A	1117	CLA	CHD-C4C	3.01	1.50	1.40
18	B	9010	CLA	CHB-C1B	3.01	1.46	1.39
18	4	4008	CLA	MG-NA	-3.01	1.99	2.06
18	B	1223	CLA	CHB-C1B	3.00	1.47	1.39
18	B	1301	CLA	CHB-C1B	3.00	1.47	1.39
18	4	4011	CLA	CHB-C1B	3.00	1.47	1.39

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
18	B	1237	CLA	CHB-C1B	3.00	1.46	1.39
18	B	1235	CLA	CHB-C1B	3.00	1.46	1.39
18	B	1238	CLA	C4C-C3C	-2.99	1.40	1.45
18	1	1012	CLA	CHB-C1B	2.99	1.47	1.39
18	A	1119	CLA	C1B-NB	-2.99	1.33	1.37
18	A	1110	CLA	CHD-C4C	2.99	1.50	1.40
18	H	1505	CLA	CHD-C4C	2.99	1.50	1.40
18	B	1228	CLA	CHB-C1B	2.99	1.46	1.39
18	3	3009	CLA	MG-NA	-2.99	1.99	2.06
18	A	1122	CLA	C1C-C2C	-2.99	1.38	1.44
18	A	1104	CLA	CHD-C4C	2.99	1.50	1.40
20	B	6017	BCR	C10-C9	-2.99	1.28	1.35
18	2	2011	CLA	MG-NA	-2.99	1.99	2.06
18	B	1138	CLA	C1C-C2C	-2.99	1.38	1.44
18	A	1152	CLA	CHD-C4C	2.98	1.50	1.40
18	A	1124	CLA	C3D-C4D	-2.98	1.36	1.44
18	3	3006	CLA	CHD-C4C	2.98	1.50	1.40
18	L	1504	CLA	C4C-C3C	-2.98	1.40	1.45
18	G	1248	CLA	CHD-C4C	2.98	1.50	1.40
18	1	1010	CLA	MG-NA	-2.98	1.99	2.06
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	4	1009	CLA	CHB-C1B	2.97	1.47	1.39
18	A	1147	CLA	CHD-C4C	2.97	1.50	1.40
18	B	1238	CLA	CHB-C1B	2.97	1.46	1.39
18	A	1151	CLA	CHD-C4C	2.97	1.50	1.40
18	4	4013	CLA	CHD-C4C	2.97	1.50	1.40
18	B	9023	CLA	OBD-CAD	2.96	1.27	1.22
18	A	1110	CLA	MG-NA	-2.96	1.99	2.06
18	B	1239	CLA	C1B-NB	-2.96	1.34	1.37
18	3	3012	CLA	CHD-C4C	2.96	1.50	1.40
18	A	1126	CLA	CHB-C1B	2.96	1.46	1.39
18	A	1134	CLA	CHA-C1A	2.95	1.49	1.41
18	A	1133	CLA	C3D-C4D	-2.95	1.36	1.44
18	1	1004	CLA	MG-NA	-2.95	1.99	2.06
18	2	2006	CLA	MG-NA	-2.95	1.99	2.06
18	L	1125	CLA	CHB-C1B	2.94	1.47	1.39
18	A	1128	CLA	OBD-CAD	2.94	1.27	1.22
18	2	2005	CLA	CHA-C1A	2.94	1.49	1.41
18	A	1115	CLA	MG-NA	-2.94	1.99	2.06
18	B	9022	CLA	C3D-CAD	-2.93	1.35	1.45
18	B	1230	CLA	CHB-C1B	2.93	1.47	1.39

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
18	B	1217	CLA	C1B-C2B	-2.92	1.36	1.43
18	A	1137	CLA	C4C-C3C	-2.92	1.40	1.45
18	2	2006	CLA	CHB-C1B	2.92	1.47	1.39
18	K	1141	CLA	CHB-C1B	2.92	1.47	1.39
18	B	1227	CLA	C1C-C2C	-2.92	1.38	1.44
18	3	3007	CLA	CHB-C1B	2.92	1.47	1.39
18	B	1236	CLA	C1B-NB	-2.92	1.34	1.37
18	1	1006	CLA	CHD-C4C	2.92	1.50	1.40
18	2	2001	CLA	MG-NA	-2.91	1.99	2.06
18	A	1131	CLA	CHB-C1B	2.91	1.45	1.39
18	2	2007	CLA	CHD-C4C	2.91	1.50	1.40
18	K	1153	CLA	CHB-C1B	2.90	1.47	1.39
18	3	3012	CLA	CHB-C1B	2.90	1.47	1.39
18	3	3002	CLA	MG-NA	-2.90	1.99	2.06
18	A	9013	CLA	C1C-NC	-2.90	1.33	1.37
18	B	9022	CLA	C1B-NB	-2.90	1.34	1.37
18	A	1113	CLA	C1C-C2C	-2.90	1.38	1.44
18	A	1133	CLA	MG-NA	-2.90	1.99	2.06
18	A	1151	CLA	CHB-C1B	2.89	1.47	1.39
18	L	1130	CLA	C1B-NB	-2.89	1.34	1.37
18	B	1211	CLA	CHB-C1B	2.89	1.47	1.39
18	1	1013	CLA	CHB-C1B	2.89	1.47	1.39
18	A	1103	CLA	C4C-C3C	-2.89	1.40	1.45
18	B	1209	CLA	C4B-NB	-2.88	1.34	1.37
18	K	1141	CLA	MG-NA	-2.88	1.99	2.06
18	B	1213	CLA	CHB-C1B	2.88	1.47	1.39
18	4	1009	CLA	CHD-C4C	2.88	1.50	1.40
18	B	1208	CLA	C4C-C3C	-2.88	1.40	1.45
18	A	1131	CLA	MG-NA	-2.88	1.99	2.06
18	F	1139	CLA	C4C-C3C	-2.88	1.40	1.45
18	4	4001	CLA	CHB-C1B	2.87	1.47	1.39
18	1	1004	CLA	CHD-C4C	2.87	1.50	1.40
18	A	1146	CLA	MG-NA	-2.87	1.99	2.06
18	B	1216	CLA	MG-NA	-2.87	1.99	2.06
18	J	1307	CLA	MG-NA	-2.87	1.99	2.06
18	B	1216	CLA	C1C-C2C	-2.86	1.38	1.44
18	G	1248	CLA	CHB-C1B	2.86	1.47	1.39
18	L	1503	CLA	C4D-CHA	-2.86	1.28	1.38
18	2	2015	CLA	MG-NA	-2.86	1.99	2.06
18	B	1217	CLA	CHB-C1B	2.86	1.45	1.39
18	I	1204	CLA	C4C-C3C	-2.86	1.40	1.45
18	A	1118	CLA	CHB-C1B	2.86	1.47	1.39

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
18	3	3011	CLA	CHB-C1B	2.86	1.47	1.39
18	B	1218	CLA	CHB-C1B	2.85	1.45	1.39
18	L	1504	CLA	C1B-NB	-2.85	1.34	1.37
18	B	1231	CLA	C1C-C2C	-2.85	1.38	1.44
18	K	1153	CLA	CHA-C1A	2.84	1.49	1.41
18	A	1126	CLA	C1B-C2B	-2.84	1.36	1.43
18	1	1011	CLA	CHA-C1A	2.84	1.49	1.41
18	1	1006	CLA	CHB-C1B	2.84	1.47	1.39
18	A	1117	CLA	CHB-C1B	2.84	1.47	1.39
18	I	1204	CLA	C4B-NB	-2.84	1.34	1.37
18	B	1212	CLA	C1B-NB	-2.84	1.34	1.37
18	B	1236	CLA	C1B-C2B	-2.84	1.36	1.43
18	2	2011	CLA	CHB-C1B	2.84	1.47	1.39
18	1	1004	CLA	CHB-C1B	2.84	1.47	1.39
18	A	1113	CLA	MG-NA	-2.83	1.99	2.06
18	B	1232	CLA	C1B-C2B	-2.83	1.36	1.43
18	F	1305	CLA	CHA-C1A	2.83	1.49	1.41
18	A	1106	CLA	C4B-NB	-2.83	1.34	1.37
18	A	1102	CLA	CHB-C1B	2.83	1.47	1.39
18	B	1226	CLA	MG-NA	-2.83	1.99	2.06
18	A	1124	CLA	CHD-C4C	2.83	1.49	1.40
18	B	1237	CLA	OBD-CAD	2.82	1.27	1.22
18	J	1307	CLA	CHB-C1B	2.82	1.47	1.39
18	B	1236	CLA	CHB-C1B	2.82	1.45	1.39
18	2	2001	CLA	CHB-C1B	2.82	1.47	1.39
18	B	1206	CLA	CHB-C1B	2.82	1.47	1.39
18	A	1103	CLA	CHB-C1B	2.82	1.45	1.39
18	B	1138	CLA	C4C-C3C	-2.81	1.40	1.45
18	3	3004	CLA	CHA-C1A	2.81	1.49	1.41
18	A	1142	CLA	CHB-C1B	2.81	1.47	1.39
18	F	1305	CLA	CHB-C1B	2.81	1.47	1.39
18	B	1208	CLA	C1B-C2B	-2.81	1.36	1.43
18	B	1217	CLA	C4C-C3C	-2.81	1.40	1.45
18	3	3010	CLA	CHB-C1B	2.80	1.47	1.39
18	B	1214	CLA	C1D-ND	-2.80	1.34	1.37
18	B	1235	CLA	C1C-NC	-2.80	1.33	1.37
18	B	9023	CLA	CHB-C1B	2.80	1.45	1.39
18	A	1135	CLA	C1C-C2C	-2.80	1.38	1.44
18	3	3006	CLA	CHB-C1B	2.80	1.47	1.39
18	B	1212	CLA	CBB-CAB	2.80	1.43	1.30
18	4	4003	CLA	CHB-C1B	2.80	1.47	1.39
18	B	1219	CLA	C4C-C3C	-2.80	1.40	1.45

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
18	3	3009	CLA	CHA-C1A	2.79	1.49	1.41
18	A	9011	CLA	C1C-C2C	-2.79	1.38	1.44
18	B	1215	CLA	C4C-C3C	-2.79	1.40	1.45
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	1230	CLA	MG-NA	-2.79	1.99	2.06
18	1	1005	CLA	CHB-C1B	2.79	1.47	1.39
18	F	1240	CLA	CHA-C1A	2.78	1.49	1.41
18	A	1147	CLA	CHB-C1B	2.78	1.47	1.39
18	L	1503	CLA	MG-ND	-2.78	2.00	2.05
18	1	1008	CLA	CHB-C1B	2.78	1.47	1.39
18	A	1152	CLA	CHA-C1A	2.78	1.49	1.41
18	B	1227	CLA	C4B-NB	-2.78	1.34	1.37
18	A	1137	CLA	MG-NA	-2.77	1.99	2.06
18	F	1303	CLA	CHB-C1B	2.77	1.47	1.39
18	A	1128	CLA	C1C-C2C	-2.77	1.38	1.44
18	2	2015	CLA	CHB-C1B	2.77	1.47	1.39
18	1	1006	CLA	CHA-C1A	2.77	1.49	1.41
18	A	1151	CLA	CHA-C1A	2.76	1.49	1.41
18	A	1133	CLA	CHB-C1B	2.76	1.47	1.39
18	4	4009	CLA	CHB-C1B	2.76	1.47	1.39
18	3	3009	CLA	CHB-C1B	2.76	1.47	1.39
18	A	1137	CLA	CHB-C1B	2.76	1.45	1.39
18	B	1229	CLA	C4B-NB	-2.76	1.34	1.37
18	4	4005	CLA	CHB-C1B	2.76	1.47	1.39
18	1	1011	CLA	CHB-C1B	2.76	1.47	1.39
18	B	1202	CLA	C4B-NB	-2.76	1.34	1.37
18	A	1110	CLA	CHA-C1A	2.75	1.49	1.41
18	A	1132	CLA	MG-NA	-2.75	1.99	2.06
18	A	1110	CLA	CHB-C1B	2.75	1.47	1.39
18	3	3015	CLA	MG-NA	-2.75	1.99	2.06
18	A	1122	CLA	C4B-NB	-2.74	1.34	1.37
18	A	1111	CLA	CHA-C1A	2.74	1.49	1.41
18	A	1115	CLA	C1C-C2C	-2.74	1.39	1.44
18	A	1107	CLA	C1D-ND	-2.74	1.34	1.37
18	B	1208	CLA	CHB-C1B	2.74	1.45	1.39
18	4	4003	CLA	MG-NA	-2.74	1.99	2.06
18	4	4007	CLA	CHB-C1B	2.74	1.47	1.39
18	4	4008	CLA	CHB-C1B	2.73	1.47	1.39
18	A	1101	CLA	CHB-C1B	2.73	1.47	1.39
18	B	1228	CLA	OBD-CAD	2.73	1.27	1.22
18	4	4002	CLA	CHB-C1B	2.73	1.47	1.39

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
18	2	2004	CLA	CHB-C1B	2.73	1.47	1.39
18	L	1130	CLA	C1C-C2C	-2.73	1.39	1.44
18	3	3008	CLA	CHA-C1A	2.72	1.49	1.41
18	3	3004	CLA	CHB-C1B	2.72	1.47	1.39
18	4	4006	CLA	CHB-C1B	2.72	1.47	1.39
18	F	1305	CLA	MG-NA	-2.72	1.99	2.06
18	3	3011	CLA	MG-NA	-2.72	1.99	2.06
18	3	3003	CLA	MG-NA	-2.72	1.99	2.06
18	A	1126	CLA	C4B-NB	-2.71	1.34	1.37
18	2	2005	CLA	CHB-C1B	2.71	1.47	1.39
18	4	4004	CLA	CHB-C1B	2.71	1.47	1.39
18	A	1110	CLA	C3D-C4D	-2.70	1.37	1.44
18	A	1122	CLA	C1B-NB	-2.70	1.34	1.37
18	A	1127	CLA	CHB-C1B	2.70	1.47	1.39
18	1	1010	CLA	CHA-C1A	2.70	1.49	1.41
18	3	3012	CLA	CHA-C1A	2.70	1.49	1.41
18	2	2002	CLA	CHB-C1B	2.70	1.47	1.39
18	4	4008	CLA	C3D-C4D	-2.70	1.37	1.44
18	L	1503	CLA	C1D-ND	-2.70	1.34	1.37
18	2	2008	CLA	CHB-C1B	2.70	1.47	1.39
18	B	1226	CLA	CHA-C1A	2.70	1.49	1.41
18	B	1207	CLA	C4B-NB	-2.70	1.34	1.37
18	3	2009	CLA	CHB-C1B	2.70	1.47	1.39
18	2	2004	CLA	C3D-C4D	-2.69	1.37	1.44
18	B	1208	CLA	C1B-NB	-2.69	1.34	1.37
18	B	1219	CLA	C1B-NB	-2.69	1.34	1.37
18	1	1014	CLA	CHB-C1B	2.69	1.47	1.39
18	1	1010	CLA	CHB-C1B	2.69	1.47	1.39
18	B	1217	CLA	C1C-C2C	-2.69	1.39	1.44
18	A	9013	CLA	C1B-NB	-2.69	1.34	1.37
18	B	1242	CLA	C1C-C2C	-2.68	1.39	1.44
18	A	1140	CLA	MG-NA	-2.68	1.99	2.06
18	B	1218	CLA	C1D-ND	-2.68	1.34	1.37
18	3	3015	CLA	CHB-C1B	2.68	1.47	1.39
18	G	1233	CLA	C1B-C2B	-2.68	1.36	1.43
18	3	3012	CLA	MG-NA	-2.68	1.99	2.06
18	A	1129	CLA	C4C-C3C	-2.67	1.40	1.45
18	4	4003	CLA	CHA-C1A	2.67	1.48	1.41
18	2	2013	CLA	CHB-C1B	2.67	1.47	1.39
18	B	1241	CLA	C3D-C4D	-2.67	1.37	1.44
18	B	1206	CLA	CHA-C1A	2.67	1.48	1.41
18	B	1224	CLA	C1C-C2C	-2.67	1.39	1.44

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
18	4	4004	CLA	CHA-C1A	2.67	1.48	1.41
18	B	1228	CLA	C1C-C2C	-2.67	1.39	1.44
18	H	1501	CLA	C1C-C2C	-2.67	1.39	1.44
18	A	1126	CLA	C4C-C3C	-2.66	1.40	1.45
18	2	2012	CLA	CHB-C1B	2.66	1.47	1.39
18	4	4013	CLA	CHB-C1B	2.66	1.47	1.39
18	A	1132	CLA	CHB-C1B	2.66	1.47	1.39
18	H	1505	CLA	CHB-C1B	2.66	1.47	1.39
18	3	3010	CLA	MG-NA	-2.66	2.00	2.06
18	A	9011	CLA	C4C-C3C	-2.66	1.40	1.45
18	B	1210	CLA	CHB-C1B	2.66	1.47	1.39
18	3	3006	CLA	C3D-C4D	-2.66	1.37	1.44
18	3	3001	CLA	CHB-C1B	2.66	1.47	1.39
18	A	1105	CLA	CHB-C1B	2.66	1.47	1.39
18	A	1104	CLA	CHB-C1B	2.65	1.47	1.39
18	1	1007	CLA	CHB-C1B	2.65	1.47	1.39
18	2	2003	CLA	CHB-C1B	2.65	1.46	1.39
20	B	6017	BCR	C8-C9	2.65	1.51	1.46
18	B	1202	CLA	C1B-NB	-2.65	1.34	1.37
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	2	2012	CLA	CHA-C1A	2.64	1.48	1.41
18	B	1207	CLA	CHB-C1B	2.64	1.45	1.39
20	A	6011	BCR	C10-C9	-2.64	1.29	1.35
18	A	1106	CLA	C1C-C2C	-2.64	1.39	1.44
18	A	1144	CLA	CHB-C1B	2.64	1.46	1.39
18	B	1224	CLA	C1B-NB	-2.64	1.34	1.37
18	3	3015	CLA	CHA-C1A	2.64	1.48	1.41
18	4	4002	CLA	CHA-C1A	2.64	1.48	1.41
18	3	3005	CLA	CHB-C1B	2.63	1.46	1.39
18	F	1240	CLA	C3D-C4D	-2.63	1.37	1.44
18	J	1308	CLA	CHB-C1B	2.63	1.46	1.39
18	A	1134	CLA	MG-NA	-2.63	2.00	2.06
18	4	1304	CLA	C1C-C2C	-2.63	1.39	1.44
18	J	2107	CLA	C1B-NB	-2.63	1.34	1.37
18	B	1207	CLA	MG-NA	-2.63	2.00	2.06
18	A	1147	CLA	CHA-C1A	2.63	1.48	1.41
18	1	1002	CLA	CHB-C1B	2.63	1.46	1.39
18	A	1115	CLA	CHB-C1B	2.63	1.45	1.39
18	1	1001	CLA	CHA-C1A	2.63	1.48	1.41
18	H	1505	CLA	CHA-C1A	2.63	1.48	1.41
18	A	1108	CLA	C4B-NB	-2.63	1.34	1.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
18	3	3010	CLA	CHA-C1A	2.63	1.48	1.41
18	3	3003	CLA	CHB-C1B	2.62	1.46	1.39
18	2	2007	CLA	CHA-C1A	2.62	1.48	1.41
18	3	3013	CLA	C3D-C4D	-2.62	1.37	1.44
18	J	1307	CLA	CHA-C1A	2.62	1.48	1.41
18	2	2013	CLA	CHA-C1A	2.62	1.48	1.41
18	4	4010	CLA	CHA-C1A	2.62	1.48	1.41
18	2	2010	CLA	CHB-C1B	2.61	1.46	1.39
18	B	1234	CLA	C1B-NB	-2.61	1.34	1.37
18	A	1142	CLA	CHA-C1A	2.61	1.48	1.41
18	A	1119	CLA	MG-NA	-2.61	2.00	2.06
18	B	1229	CLA	C1D-C2D	-2.61	1.40	1.45
18	3	3005	CLA	CHA-C1A	2.61	1.48	1.41
18	A	1148	CLA	CHB-C1B	2.61	1.46	1.39
18	A	1127	CLA	CHA-C1A	2.61	1.48	1.41
18	4	4008	CLA	CHA-C1A	2.61	1.48	1.41
18	A	1118	CLA	CHA-C1A	2.61	1.48	1.41
18	A	1309	CLA	CHB-C1B	2.61	1.46	1.39
18	1	1002	CLA	CHA-C1A	2.61	1.48	1.41
18	2	2008	CLA	C3D-C4D	-2.60	1.37	1.44
18	1	1003	CLA	CHB-C1B	2.60	1.46	1.39
18	B	9023	CLA	MG-NA	-2.60	2.00	2.06
18	1	1008	CLA	CHA-C1A	2.60	1.48	1.41
18	A	1109	CLA	CHB-C1B	2.60	1.46	1.39
18	B	1235	CLA	C1B-C2B	-2.60	1.37	1.43
18	2	2005	CLA	MG-NA	-2.60	2.00	2.06
18	B	1211	CLA	C3D-C4D	-2.60	1.37	1.44
18	2	2002	CLA	CHA-C1A	2.60	1.48	1.41
18	4	4010	CLA	CHB-C1B	2.60	1.46	1.39
18	A	1143	CLA	CHA-C1A	2.60	1.48	1.41
18	B	9012	CLA	MG-NA	-2.59	2.00	2.06
18	A	1101	CLA	CHA-C1A	2.59	1.48	1.41
18	A	1116	CLA	CHB-C1B	2.59	1.46	1.39
18	A	1146	CLA	CHA-C1A	2.59	1.48	1.41
18	A	1143	CLA	CHB-C1B	2.59	1.46	1.39
18	4	4007	CLA	CHA-C1A	2.59	1.48	1.41
18	3	3002	CLA	CHA-C1A	2.58	1.48	1.41
18	A	1120	CLA	CHB-C1B	2.58	1.46	1.39
18	J	2107	CLA	C1C-C2C	-2.58	1.39	1.44
18	4	4013	CLA	CHA-C1A	2.58	1.48	1.41
18	2	2015	CLA	CHA-C1A	2.58	1.48	1.41
18	A	1123	CLA	C1C-C2C	-2.58	1.39	1.44

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
18	A	1117	CLA	CHA-C1A	2.58	1.48	1.41
18	1	1013	CLA	CHA-C1A	2.58	1.48	1.41
18	3	3003	CLA	CHA-C1A	2.58	1.48	1.41
18	A	1111	CLA	CHB-C1B	2.58	1.46	1.39
18	3	3013	CLA	CHB-C1B	2.58	1.46	1.39
18	B	1202	CLA	MG-NA	-2.57	2.00	2.06
18	A	1107	CLA	C1C-NC	-2.57	1.33	1.37
18	B	1237	CLA	C1B-NB	-2.57	1.34	1.37
18	A	1137	CLA	C1C-C2C	-2.57	1.39	1.44
18	3	3013	CLA	CHA-C1A	2.57	1.48	1.41
18	2	2011	CLA	CHA-C1A	2.57	1.48	1.41
18	4	4009	CLA	CHA-C1A	2.57	1.48	1.41
18	A	1132	CLA	C3D-C4D	-2.57	1.37	1.44
18	A	9013	CLA	C4C-C3C	-2.57	1.40	1.45
18	L	1504	CLA	C1C-C2C	-2.57	1.39	1.44
18	1	1007	CLA	CHA-C1A	2.57	1.48	1.41
18	1	1001	CLA	C3D-C4D	-2.56	1.37	1.44
18	2	2006	CLA	CHA-C1A	2.56	1.48	1.41
18	B	1207	CLA	C1B-NB	-2.56	1.34	1.37
18	A	1144	CLA	CHA-C1A	2.56	1.48	1.41
18	A	1123	CLA	C1B-C2B	-2.56	1.37	1.43
18	A	1123	CLA	MG-NA	-2.55	2.00	2.06
18	B	1226	CLA	C3D-C4D	-2.55	1.37	1.44
18	4	4005	CLA	C3D-C4D	-2.55	1.37	1.44
18	2	2001	CLA	CHA-C1A	2.55	1.48	1.41
18	B	1212	CLA	C1C-C2C	-2.55	1.39	1.44
18	A	1309	CLA	CHA-C1A	2.55	1.48	1.41
18	4	4003	CLA	C3D-C4D	-2.55	1.37	1.44
18	G	1248	CLA	CHA-C1A	2.55	1.48	1.41
18	B	1231	CLA	C1B-C2B	-2.54	1.37	1.43
18	A	1123	CLA	CHB-C1B	2.54	1.45	1.39
18	2	2010	CLA	CHA-C1A	2.54	1.48	1.41
18	4	4005	CLA	CHA-C1A	2.54	1.48	1.41
18	B	1222	CLA	C1B-NB	-2.54	1.34	1.37
18	J	1307	CLA	C3D-C4D	-2.54	1.37	1.44
18	F	1240	CLA	CHB-C1B	2.54	1.46	1.39
18	A	1123	CLA	CHB-C4A	-2.54	1.31	1.37
18	K	1150	CLA	CHB-C1B	2.54	1.46	1.39
18	A	1116	CLA	CHA-C1A	2.53	1.48	1.41
18	B	1212	CLA	MG-NA	-2.53	2.00	2.06
18	3	3015	CLA	C3D-C4D	-2.53	1.37	1.44
18	B	1207	CLA	C1D-C2D	-2.53	1.40	1.45

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
18	A	1148	CLA	C3D-C4D	-2.53	1.37	1.44
18	3	3011	CLA	CHA-C1A	2.53	1.48	1.41
18	4	1009	CLA	C3D-C4D	-2.53	1.37	1.44
18	A	1146	CLA	CHB-C1B	2.53	1.46	1.39
18	A	1131	CLA	C4C-C3C	-2.53	1.40	1.45
18	B	1232	CLA	C1C-C2C	-2.52	1.39	1.44
18	B	1218	CLA	C1D-C2D	-2.52	1.40	1.45
18	F	1306	CLA	CHB-C1B	2.52	1.46	1.39
18	J	2107	CLA	C4C-C3C	-2.52	1.40	1.45
18	B	1220	CLA	C1C-C2C	-2.52	1.39	1.44
18	B	1230	CLA	CHA-C1A	2.52	1.48	1.41
18	B	1218	CLA	C1B-C2B	-2.52	1.37	1.43
18	F	4015	CLA	CHB-C1B	2.52	1.46	1.39
18	A	1117	CLA	MG-NA	-2.51	2.00	2.06
18	B	1229	CLA	C1C-C2C	-2.51	1.39	1.44
18	B	1210	CLA	CHA-C1A	2.51	1.48	1.41
18	1	1004	CLA	C3D-C4D	-2.51	1.37	1.44
18	B	1228	CLA	C1B-C2B	-2.51	1.37	1.43
18	A	1108	CLA	C1B-NB	-2.51	1.34	1.37
18	A	1146	CLA	C3D-C4D	-2.51	1.37	1.44
18	A	1111	CLA	C3D-C4D	-2.51	1.37	1.44
18	1	1005	CLA	C3D-C4D	-2.51	1.37	1.44
18	B	9023	CLA	C1C-C2C	-2.50	1.39	1.44
18	A	1151	CLA	C3D-C4D	-2.50	1.38	1.44
18	A	1102	CLA	CHA-C1A	2.50	1.48	1.41
18	F	1306	CLA	CHA-C1A	2.50	1.48	1.41
18	B	1205	CLA	MG-NA	-2.50	2.00	2.06
18	1	1001	CLA	CHB-C1B	2.50	1.46	1.39
18	3	2009	CLA	CHA-C1A	2.50	1.48	1.41
18	H	1501	CLA	MG-NA	-2.50	2.00	2.06
18	B	1202	CLA	C3D-CAD	-2.50	1.36	1.45
18	L	1503	CLA	C3D-CAD	-2.50	1.36	1.45
18	J	2107	CLA	C4B-NB	-2.50	1.34	1.37
18	3	3008	CLA	CHB-C1B	2.49	1.46	1.39
18	B	1213	CLA	C3D-C4D	-2.49	1.38	1.44
18	L	1502	CLA	C1B-NB	-2.49	1.34	1.37
18	B	1213	CLA	CHA-C1A	2.49	1.48	1.41
18	4	4010	CLA	C3D-C4D	-2.48	1.38	1.44
18	1	1008	CLA	C3D-C4D	-2.48	1.38	1.44
18	2	2003	CLA	CHA-C1A	2.48	1.48	1.41
18	A	1152	CLA	CHB-C1B	2.48	1.46	1.39
18	A	1105	CLA	CHA-C1A	2.48	1.48	1.41

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
18	B	1217	CLA	C4B-NB	-2.48	1.34	1.37
18	K	1150	CLA	CHA-C1A	2.48	1.48	1.41
18	A	1140	CLA	C1D-C2D	-2.47	1.40	1.45
18	F	1303	CLA	CHA-C1A	2.47	1.48	1.41
18	J	1308	CLA	CHA-C1A	2.47	1.48	1.41
18	4	4013	CLA	C3D-C4D	-2.46	1.38	1.44
18	B	1211	CLA	CHA-C1A	2.46	1.48	1.41
18	K	1141	CLA	CHA-C1A	2.46	1.48	1.41
18	B	1227	CLA	C1D-ND	-2.46	1.34	1.37
18	3	3010	CLA	C3D-C4D	-2.46	1.38	1.44
18	L	1504	CLA	C4B-NB	-2.46	1.34	1.37
18	4	4001	CLA	C3D-C4D	-2.46	1.38	1.44
20	I	6018	BCR	C23-C22	2.46	1.51	1.46
18	F	4015	CLA	CHA-C1A	2.46	1.48	1.41
18	B	1207	CLA	C1C-C2C	-2.45	1.39	1.44
18	A	1148	CLA	CHA-C1A	2.45	1.48	1.41
18	3	3001	CLA	C3D-C4D	-2.45	1.38	1.44
18	2	2007	CLA	CHB-C1B	2.45	1.46	1.39
18	B	1205	CLA	C1B-NB	-2.45	1.34	1.37
18	A	1140	CLA	C1C-C2C	-2.45	1.39	1.44
18	A	1133	CLA	CHA-C1A	2.45	1.48	1.41
18	L	1125	CLA	CHA-C1A	2.45	1.48	1.41
18	A	9011	CLA	C1D-ND	-2.45	1.34	1.37
18	K	1141	CLA	C3D-C4D	-2.45	1.38	1.44
18	B	1228	CLA	C1B-NB	-2.44	1.34	1.37
18	B	1238	CLA	C1B-C2B	-2.44	1.37	1.43
18	B	1223	CLA	CHA-C1A	2.44	1.48	1.41
18	4	4011	CLA	CHA-C1A	2.44	1.48	1.41
18	3	3001	CLA	CHA-C1A	2.44	1.48	1.41
18	3	3007	CLA	C3D-C4D	-2.44	1.38	1.44
18	2	2001	CLA	C3D-C4D	-2.44	1.38	1.44
18	2	2013	CLA	C3D-C4D	-2.43	1.38	1.44
18	A	1143	CLA	C3D-C4D	-2.43	1.38	1.44
18	B	1218	CLA	C4D-CHA	-2.43	1.30	1.38
18	4	4012	CLA	CHA-C1A	2.43	1.48	1.41
18	B	1220	CLA	OBD-CAD	2.43	1.26	1.22
18	B	1234	CLA	C1C-C2C	-2.43	1.39	1.44
18	3	3008	CLA	C3D-C4D	-2.43	1.38	1.44
18	A	1144	CLA	C3D-C4D	-2.43	1.38	1.44
18	B	1242	CLA	C1B-C2B	-2.42	1.37	1.43
18	1	1014	CLA	CHA-C1A	2.42	1.48	1.41
18	A	1123	CLA	C4B-NB	-2.42	1.34	1.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
18	A	1108	CLA	C1C-C2C	-2.42	1.39	1.44
20	A	6011	BCR	C27-C26	2.41	1.55	1.51
18	B	1214	CLA	C1B-C2B	-2.41	1.37	1.43
18	B	1239	CLA	MG-NA	-2.41	2.00	2.06
18	A	1107	CLA	C4B-NB	-2.41	1.34	1.37
18	F	1306	CLA	C3D-C4D	-2.40	1.38	1.44
18	3	3002	CLA	C3D-C4D	-2.40	1.38	1.44
18	B	1206	CLA	C3D-C4D	-2.40	1.38	1.44
18	A	1124	CLA	CHB-C1B	2.40	1.46	1.39
18	B	1201	CLA	CHB-C1B	2.40	1.46	1.39
18	B	1210	CLA	C3D-C4D	-2.40	1.38	1.44
18	4	4001	CLA	CHA-C1A	2.40	1.48	1.41
18	4	4006	CLA	C3D-C4D	-2.39	1.38	1.44
18	A	9011	CLA	C1D-C2D	-2.39	1.40	1.45
18	G	1248	CLA	C3C-C4C	-2.39	1.37	1.43
18	B	1218	CLA	C2-C3	2.39	1.38	1.33
18	J	1308	CLA	C3D-C4D	-2.39	1.38	1.44
18	2	2010	CLA	C3D-C4D	-2.39	1.38	1.44
18	3	3009	CLA	C3D-C4D	-2.39	1.38	1.44
18	L	1502	CLA	C1B-C2B	-2.39	1.37	1.43
18	4	4012	CLA	C3D-C4D	-2.38	1.38	1.44
18	3	3004	CLA	C3D-C4D	-2.38	1.38	1.44
18	A	1115	CLA	C1B-C2B	-2.38	1.37	1.43
18	B	1218	CLA	CHB-C4A	-2.38	1.31	1.37
18	A	1109	CLA	C3C-C4C	-2.38	1.37	1.43
18	A	1120	CLA	CHA-C1A	2.38	1.48	1.41
18	B	1201	CLA	C3D-C4D	-2.38	1.38	1.44
18	B	1217	CLA	MG-NA	-2.38	2.00	2.06
18	A	9011	CLA	C4B-NB	-2.38	1.34	1.37
18	A	1126	CLA	MG-NA	-2.38	2.00	2.06
18	4	1304	CLA	C4B-NB	-2.37	1.34	1.37
18	B	1229	CLA	C1C-NC	-2.37	1.34	1.37
18	A	1136	CLA	C4B-NB	-2.37	1.34	1.37
18	B	9022	CLA	C1B-C2B	-2.37	1.37	1.43
18	B	1228	CLA	C1C-NC	-2.36	1.34	1.37
18	A	1120	CLA	C3D-C4D	-2.36	1.38	1.44
18	B	1301	CLA	C3D-C4D	-2.36	1.38	1.44
18	A	1102	CLA	C3D-C4D	-2.36	1.38	1.44
18	1	1005	CLA	CHA-C1A	2.36	1.48	1.41
18	3	3005	CLA	C3D-C4D	-2.36	1.38	1.44
18	A	1136	CLA	MG-NA	-2.36	2.00	2.06
18	4	4012	CLA	CHB-C1B	2.36	1.46	1.39

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
18	1	1006	CLA	C3D-C4D	-2.36	1.38	1.44
18	3	3011	CLA	C3D-C4D	-2.36	1.38	1.44
18	A	1117	CLA	C3D-C4D	-2.36	1.38	1.44
18	A	1116	CLA	C3D-C4D	-2.35	1.38	1.44
18	B	1225	CLA	C1C-NC	-2.35	1.34	1.37
18	2	2008	CLA	CHA-C1A	2.35	1.48	1.41
18	2	2002	CLA	C3D-C4D	-2.35	1.38	1.44
18	3	3006	CLA	CHA-C1A	2.35	1.48	1.41
18	F	1302	CLA	C1C-C2C	-2.35	1.39	1.44
18	2	2011	CLA	C3D-C4D	-2.35	1.38	1.44
18	I	1204	CLA	C1C-C2C	-2.35	1.39	1.44
18	B	1217	CLA	CHB-C4A	-2.35	1.31	1.37
18	H	1505	CLA	C3D-C4D	-2.35	1.38	1.44
18	4	4011	CLA	C3D-C4D	-2.35	1.38	1.44
18	B	9010	CLA	MG-NA	-2.35	2.00	2.06
18	A	1122	CLA	C1C-NC	-2.34	1.34	1.37
18	3	3003	CLA	C3D-C4D	-2.34	1.38	1.44
18	1	1013	CLA	C3D-C4D	-2.33	1.38	1.44
18	2	2003	CLA	C3D-C4D	-2.33	1.38	1.44
18	B	1224	CLA	C1B-C2B	-2.33	1.37	1.43
18	L	1125	CLA	C3D-C4D	-2.33	1.38	1.44
18	4	4006	CLA	CHA-C1A	2.33	1.47	1.41
18	L	1503	CLA	OBD-CAD	2.33	1.26	1.22
18	F	1303	CLA	C3D-C4D	-2.32	1.38	1.44
18	G	1248	CLA	C2C-C1C	-2.32	1.37	1.43
18	B	1242	CLA	MG-NA	-2.32	2.00	2.06
18	B	1241	CLA	CHB-C1B	2.32	1.46	1.39
18	2	2015	CLA	C3D-C4D	-2.32	1.38	1.44
18	1	1004	CLA	CHA-C1A	2.32	1.47	1.41
18	A	1129	CLA	C4B-NB	-2.32	1.34	1.37
18	B	1138	CLA	MG-NA	-2.31	2.00	2.06
18	4	4002	CLA	C3D-C4D	-2.31	1.38	1.44
18	A	1105	CLA	C3D-C4D	-2.31	1.38	1.44
18	A	1147	CLA	C3D-C4D	-2.31	1.38	1.44
18	K	1153	CLA	MG-NA	-2.31	2.00	2.06
18	A	1136	CLA	C1C-C2C	-2.31	1.39	1.44
18	A	1107	CLA	C1B-NB	-2.31	1.34	1.37
18	L	1503	CLA	C1B-C2B	-2.30	1.37	1.43
18	B	9012	CLA	C1D-ND	-2.30	1.34	1.37
18	A	1135	CLA	C1C-NC	-2.30	1.34	1.37
18	B	1220	CLA	C1D-C2D	-2.30	1.40	1.45
18	3	3012	CLA	C3D-C4D	-2.29	1.38	1.44

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
18	A	1104	CLA	MG-NA	-2.29	2.00	2.06
18	4	4007	CLA	C3D-C4D	-2.29	1.38	1.44
18	2	2007	CLA	C3D-C4D	-2.29	1.38	1.44
18	B	1214	CLA	MG-NA	-2.29	2.00	2.06
18	2	2004	CLA	CHA-C1A	2.29	1.47	1.41
18	3	2009	CLA	C3D-C4D	-2.29	1.38	1.44
18	B	1214	CLA	C1C-C2C	-2.28	1.39	1.44
18	B	1208	CLA	C1C-C2C	-2.28	1.39	1.44
18	B	1203	CLA	C1C-C2C	-2.28	1.39	1.44
18	B	1301	CLA	CHA-C1A	2.28	1.47	1.41
18	A	1118	CLA	C3D-C4D	-2.28	1.38	1.44
18	L	1502	CLA	C1C-C2C	-2.28	1.39	1.44
18	2	2006	CLA	C3D-C4D	-2.27	1.38	1.44
18	B	1237	CLA	MG-NA	-2.27	2.00	2.06
18	3	3007	CLA	CHA-C1A	2.27	1.47	1.41
18	F	4015	CLA	C3D-C4D	-2.27	1.38	1.44
18	B	1236	CLA	C1C-C2C	-2.27	1.39	1.44
18	B	1203	CLA	MG-NA	-2.27	2.00	2.06
18	1	1012	CLA	CHA-C1A	2.27	1.47	1.41
18	B	1228	CLA	MG-NA	-2.27	2.00	2.06
18	B	1209	CLA	C1C-C2C	-2.26	1.39	1.44
18	1	1003	CLA	CHA-C1A	2.26	1.47	1.41
18	B	1205	CLA	C1D-C2D	-2.26	1.40	1.45
18	A	9011	CLA	MG-NA	-2.26	2.00	2.06
18	4	4012	CLA	C3C-C4C	-2.26	1.37	1.43
18	A	1109	CLA	C2C-C1C	-2.26	1.37	1.43
18	A	1309	CLA	C3D-C4D	-2.26	1.38	1.44
18	A	1122	CLA	C1D-ND	-2.26	1.34	1.37
18	B	9022	CLA	C1A-CHA	2.26	1.52	1.43
18	K	1153	CLA	C3D-C4D	-2.25	1.38	1.44
18	A	1142	CLA	C3D-C4D	-2.25	1.38	1.44
18	A	1106	CLA	C4C-C3C	-2.25	1.41	1.45
18	A	1140	CLA	C1B-NB	-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	A	1113	CLA	C1B-NB	-2.24	1.34	1.37
18	A	9013	CLA	C3B-C4B	-2.24	1.36	1.42
18	B	1138	CLA	C3A-C2A	-2.24	1.48	1.54
18	B	1242	CLA	C4B-NB	-2.24	1.34	1.37
18	B	1215	CLA	MG-NA	-2.24	2.01	2.06
18	B	1236	CLA	C3D-CAD	-2.24	1.37	1.45
18	2	2012	CLA	C3D-C4D	-2.24	1.38	1.44

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
18	B	1241	CLA	CHA-C1A	2.24	1.47	1.41
18	B	1208	CLA	MG-NA	-2.23	2.01	2.06
18	A	1129	CLA	C1C-C2C	-2.23	1.40	1.44
18	A	1152	CLA	C3D-C4D	-2.23	1.38	1.44
18	B	1218	CLA	C1-C2	2.23	1.55	1.49
18	B	1222	CLA	C1C-C2C	-2.23	1.40	1.44
18	B	1209	CLA	C1B-C2B	-2.22	1.37	1.43
18	A	1101	CLA	C3D-C4D	-2.22	1.38	1.44
18	A	1119	CLA	C1D-ND	-2.22	1.34	1.37
18	A	1137	CLA	C1B-C2B	-2.22	1.37	1.43
18	L	1504	CLA	C1D-ND	-2.22	1.34	1.37
18	L	1503	CLA	C2A-C1A	-2.22	1.47	1.52
18	A	1129	CLA	C1B-C2B	-2.21	1.37	1.43
18	B	9012	CLA	C1C-C2C	-2.21	1.40	1.44
18	B	1219	CLA	C1B-C2B	-2.21	1.37	1.43
18	I	1204	CLA	C1B-C2B	-2.21	1.37	1.43
18	B	9010	CLA	C3D-CAD	-2.21	1.37	1.45
18	A	1113	CLA	C1D-C2D	-2.21	1.41	1.45
18	A	1127	CLA	C3D-C4D	-2.20	1.38	1.44
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	4	4009	CLA	C3D-C4D	-2.20	1.38	1.44
18	L	1130	CLA	C4B-NB	-2.20	1.35	1.37
18	1	1002	CLA	C3D-C4D	-2.20	1.38	1.44
18	A	1107	CLA	C3B-C2B	-2.20	1.33	1.41
18	A	1106	CLA	C1B-NB	-2.19	1.35	1.37
18	1	1003	CLA	C3D-C4D	-2.19	1.38	1.44
18	A	1115	CLA	CHB-C4A	-2.19	1.32	1.37
18	A	1122	CLA	C1B-C2B	-2.19	1.38	1.43
18	1	1010	CLA	C3D-C4D	-2.19	1.38	1.44
18	L	1503	CLA	CHB-C4A	-2.19	1.32	1.37
18	A	1103	CLA	C1B-C2B	-2.19	1.38	1.43
18	A	1137	CLA	C1C-NC	-2.19	1.34	1.37
18	A	1132	CLA	C3D-C2D	2.19	1.40	1.35
18	1	1012	CLA	C3D-C4D	-2.19	1.38	1.44
18	F	1139	CLA	C1D-ND	-2.18	1.35	1.37
18	L	1130	CLA	MG-NA	-2.18	2.01	2.06
18	B	1242	CLA	C1D-C2D	-2.18	1.41	1.45
18	F	1305	CLA	C3D-C4D	-2.18	1.38	1.44
18	B	1214	CLA	CHB-C4A	-2.18	1.32	1.37
18	B	1138	CLA	C1B-C2B	-2.18	1.38	1.43
18	1	1011	CLA	C3D-C4D	-2.17	1.38	1.44

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
18	B	1225	CLA	C1B-NB	-2.17	1.35	1.37
18	A	1128	CLA	MG-NA	-2.17	2.01	2.06
18	A	1128	CLA	C1B-C2B	-2.17	1.38	1.43
18	A	1127	CLA	C2C-C1C	-2.17	1.37	1.43
18	L	1503	CLA	C1D-C2D	-2.16	1.41	1.45
18	A	1126	CLA	C1C-C2C	-2.16	1.40	1.44
18	3	3004	CLA	C3C-C4C	-2.15	1.38	1.43
18	B	1209	CLA	C4C-C3C	-2.15	1.41	1.45
18	L	1502	CLA	MG-NA	-2.15	2.01	2.06
18	B	9010	CLA	C1A-CHA	2.15	1.52	1.43
18	B	1229	CLA	C3D-CAD	-2.15	1.38	1.45
18	B	9023	CLA	CHB-C4A	-2.15	1.32	1.37
18	B	1229	CLA	C1D-ND	-2.15	1.35	1.37
18	B	1206	CLA	C2C-C1C	-2.14	1.38	1.43
18	1	1014	CLA	C3D-C4D	-2.14	1.38	1.44
18	4	4004	CLA	C3C-C4C	-2.14	1.38	1.43
18	B	1234	CLA	C1D-ND	-2.14	1.35	1.37
18	B	1209	CLA	CHB-C4A	-2.13	1.32	1.37
18	J	2107	CLA	C1D-ND	-2.13	1.35	1.37
18	2	2005	CLA	C3D-C4D	-2.13	1.38	1.44
18	2	2003	CLA	C3C-C4C	-2.13	1.38	1.43
18	K	1150	CLA	C3D-C4D	-2.13	1.38	1.44
18	G	1248	CLA	C3D-C4D	-2.13	1.38	1.44
18	2	2012	CLA	C3C-C4C	-2.12	1.38	1.43
18	4	4004	CLA	C2C-C1C	-2.12	1.38	1.43
18	2	2003	CLA	C2C-C1C	-2.12	1.38	1.43
18	B	1224	CLA	C4B-NB	-2.12	1.35	1.37
18	B	1207	CLA	C1C-NC	-2.12	1.34	1.37
18	4	4004	CLA	C3D-C4D	-2.12	1.38	1.44
18	L	1130	CLA	CBB-CAB	2.12	1.40	1.30
18	B	1227	CLA	MG-NA	-2.12	2.01	2.06
18	B	1234	CLA	MG-NA	-2.12	2.01	2.06
18	I	1204	CLA	MG-NA	-2.12	2.01	2.06
18	F	1139	CLA	C4D-CHA	-2.11	1.31	1.38
18	H	1501	CLA	C4B-NB	-2.10	1.35	1.37
18	B	1223	CLA	C2C-C1C	-2.10	1.38	1.43
18	B	1217	CLA	C1D-ND	-2.09	1.35	1.37
18	B	9010	CLA	C1C-NC	-2.09	1.34	1.37
18	B	9023	CLA	C1B-C2B	-2.09	1.38	1.43
18	G	1233	CLA	MG-NA	-2.09	2.01	2.06
18	L	1503	CLA	C3B-C2B	-2.09	1.36	1.44
18	A	1127	CLA	C3C-C4C	-2.09	1.38	1.43

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
18	B	1239	CLA	C4B-NB	-2.09	1.35	1.37
18	B	9023	CLA	C1D-ND	-2.08	1.35	1.37
20	B	6017	BCR	C7-C6	2.08	1.52	1.45
18	3	3012	CLA	C3C-C4C	-2.08	1.38	1.43
18	B	1230	CLA	C3D-C4D	-2.08	1.39	1.44
18	B	1220	CLA	C3D-CAD	-2.07	1.38	1.45
18	G	1233	CLA	C1C-C2C	-2.07	1.40	1.44
18	A	1132	CLA	CHA-C1A	2.06	1.47	1.41
18	B	9012	CLA	C1B-C2B	-2.06	1.38	1.43
18	B	9023	CLA	C4B-NB	-2.05	1.35	1.37
18	B	1224	CLA	CBB-CAB	2.05	1.40	1.30
18	B	1228	CLA	C3A-C2A	-2.04	1.48	1.54
18	B	1220	CLA	C1D-ND	-2.04	1.35	1.37
18	B	1208	CLA	C1D-ND	-2.04	1.35	1.37
18	B	1220	CLA	C1B-NB	-2.04	1.35	1.37
18	B	1225	CLA	C3D-CAD	-2.04	1.38	1.45
18	A	1128	CLA	C4B-NB	-2.03	1.35	1.37
18	3	3005	CLA	C2C-C1C	-2.03	1.38	1.43
18	A	1126	CLA	C2-C3	2.03	1.37	1.33
18	G	1233	CLA	C1D-C2D	-2.03	1.41	1.45
18	A	1133	CLA	C2D-C1D	-2.03	1.39	1.44
18	A	1135	CLA	C1B-C2B	-2.03	1.38	1.43
18	3	3009	CLA	C3C-C4C	-2.03	1.38	1.43
18	A	1108	CLA	MG-NA	-2.03	2.01	2.06
18	B	1208	CLA	C2-C3	2.03	1.37	1.33
18	A	1134	CLA	C3D-C2D	2.02	1.39	1.35
18	A	1116	CLA	C2C-C1C	-2.02	1.38	1.43
18	2	2012	CLA	C2C-C1C	-2.02	1.38	1.43
18	A	1104	CLA	C3D-C4D	-2.01	1.39	1.44
18	A	1126	CLA	C1D-ND	-2.01	1.35	1.37
18	B	1223	CLA	C3D-C4D	-2.01	1.39	1.44
18	A	1118	CLA	C2C-C1C	-2.01	1.38	1.43
18	L	1503	CLA	CBD-CGD	-2.01	1.46	1.52
18	1	1007	CLA	C3D-C4D	-2.01	1.39	1.44
18	H	1505	CLA	C3C-C4C	-2.01	1.38	1.43
18	F	1302	CLA	MG-NA	-2.00	2.01	2.06
18	B	1215	CLA	C3B-C4B	-2.00	1.37	1.42
18	3	3012	CLA	C2C-C1C	-2.00	1.38	1.43
18	A	1147	CLA	C3C-C4C	-2.00	1.38	1.43

All (3757) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
20	A	6011	BCR	C11-C10-C9	29.52	168.68	127.28
20	L	6020	BCR	C11-C10-C9	27.37	165.66	127.28
20	F	6016	BCR	C11-C10-C9	27.31	165.58	127.28
20	B	6017	BCR	C11-C10-C9	24.78	162.03	127.28
20	I	6018	BCR	C11-C10-C9	20.82	156.47	127.28
20	I	6018	BCR	C7-C8-C9	-17.42	100.47	126.23
20	L	6020	BCR	C10-C11-C12	15.89	169.25	123.20
18	B	9022	CLA	OBD-CAD-C3D	-14.69	94.09	128.42
20	I	6018	BCR	C10-C11-C12	12.52	159.48	123.20
20	F	6016	BCR	C10-C11-C12	12.17	158.47	123.20
18	B	1207	CLA	OBD-CAD-C3D	-12.01	100.34	128.42
18	B	1229	CLA	OBD-CAD-C3D	-11.88	100.64	128.42
20	B	6017	BCR	C10-C11-C12	11.76	157.27	123.20
18	B	1236	CLA	OBD-CAD-C3D	-11.72	101.02	128.42
18	B	1202	CLA	OBD-CAD-C3D	-11.08	102.51	128.42
20	A	6011	BCR	C10-C11-C12	10.71	154.22	123.20
18	B	1237	CLA	OBD-CAD-C3D	-10.58	103.68	128.42
18	B	1217	CLA	OBD-CAD-C3D	-10.57	103.71	128.42
18	B	1227	CLA	OBD-CAD-C3D	-10.53	103.81	128.42
18	B	1220	CLA	OBD-CAD-C3D	-10.52	103.83	128.42
18	A	1129	CLA	OBD-CAD-C3D	-10.37	104.18	128.42
18	J	2107	CLA	OBD-CAD-C3D	-10.30	104.34	128.42
18	B	1242	CLA	CBB-CAB-C3B	10.28	178.89	127.53
18	B	1205	CLA	OBD-CAD-C3D	-10.19	104.59	128.42
18	A	1103	CLA	OBD-CAD-C3D	-10.19	104.60	128.42
18	B	1231	CLA	CBB-CAB-C3B	10.15	178.24	127.53
18	A	1140	CLA	OBD-CAD-C3D	-10.12	104.75	128.42
18	B	1225	CLA	OBD-CAD-C3D	-10.10	104.80	128.42
18	B	1237	CLA	CBB-CAB-C3B	10.08	177.88	127.53
18	J	2107	CLA	CBB-CAB-C3B	10.00	177.48	127.53
18	L	1503	CLA	OBD-CAD-C3D	-9.99	105.08	128.42
18	L	1504	CLA	CBB-CAB-C3B	9.95	177.25	127.53
18	A	1106	CLA	CBB-CAB-C3B	9.95	177.21	127.53
18	A	1126	CLA	CBB-CAB-C3B	9.91	177.05	127.53
18	B	1242	CLA	OBD-CAD-C3D	-9.88	105.32	128.42
18	A	1113	CLA	OBD-CAD-C3D	-9.88	105.32	128.42
18	B	1231	CLA	OBD-CAD-C3D	-9.83	105.43	128.42
18	B	1214	CLA	CBB-CAB-C3B	9.83	176.63	127.53
18	B	1232	CLA	CBB-CAB-C3B	9.78	176.38	127.53
18	B	1239	CLA	CBB-CAB-C3B	9.77	176.32	127.53
18	A	1108	CLA	CBB-CAB-C3B	9.65	175.75	127.53
18	B	1219	CLA	CBB-CAB-C3B	9.63	175.65	127.53
18	B	1228	CLA	O2D-CGD-CBD	9.63	128.07	111.23

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
18	B	1229	CLA	CAB-C3B-C4B	-9.57	110.85	125.42
18	H	1501	CLA	OBD-CAD-C3D	-9.54	106.11	128.42
18	B	1218	CLA	CBB-CAB-C3B	9.51	175.04	127.53
18	B	1209	CLA	CBB-CAB-C3B	9.48	174.91	127.53
18	L	1504	CLA	OBD-CAD-C3D	-9.33	106.61	128.42
18	A	1107	CLA	CBB-CAB-C3B	9.30	173.99	127.53
18	L	1503	CLA	CAB-C3B-C2B	-9.25	98.95	123.53
18	A	9011	CLA	CBB-CAB-C3B	9.23	173.66	127.53
18	B	1234	CLA	O2D-CGD-CBD	9.23	127.37	111.23
18	B	1225	CLA	CBB-CAB-C3B	9.23	173.65	127.53
18	A	1123	CLA	OBD-CAD-C3D	-9.23	106.84	128.42
18	F	1139	CLA	CBB-CAB-C3B	9.16	173.28	127.53
18	B	1220	CLA	CBB-CAB-C3B	9.14	173.18	127.53
18	A	1103	CLA	CBB-CAB-C3B	9.09	172.97	127.53
18	B	1232	CLA	OBD-CAD-C3D	-9.09	107.16	128.42
18	B	1228	CLA	OBD-CAD-C3D	-9.09	107.17	128.42
18	A	1108	CLA	OBD-CAD-C3D	-9.08	107.19	128.42
18	A	1136	CLA	O2D-CGD-CBD	9.06	127.08	111.23
18	G	1233	CLA	OBD-CAD-C3D	-9.04	107.29	128.42
18	B	1202	CLA	CMD-C2D-C1D	9.03	140.63	124.73
18	A	1107	CLA	OBD-CAD-C3D	-9.00	107.38	128.42
18	L	1502	CLA	CBB-CAB-C3B	8.92	172.10	127.53
18	A	1137	CLA	CBB-CAB-C3B	8.90	171.99	127.53
18	B	1205	CLA	CBB-CAB-C3B	8.89	171.96	127.53
18	I	1204	CLA	CBB-CAB-C3B	8.88	171.91	127.53
18	B	1216	CLA	OBD-CAD-C3D	-8.85	107.74	128.42
18	F	1302	CLA	CBB-CAB-C3B	8.84	171.70	127.53
18	B	1203	CLA	CBB-CAB-C3B	8.81	171.53	127.53
18	A	1119	CLA	CBB-CAB-C3B	8.81	171.52	127.53
18	A	1123	CLA	CBB-CAB-C3B	8.77	171.33	127.53
18	A	1115	CLA	CBB-CAB-C3B	8.71	171.06	127.53
18	A	1106	CLA	OBD-CAD-C3D	-8.69	108.11	128.42
18	A	1115	CLA	OBD-CAD-C3D	-8.68	108.13	128.42
18	B	1202	CLA	CBB-CAB-C3B	8.63	170.65	127.53
18	B	1238	CLA	OBD-CAD-C3D	-8.61	108.30	128.42
18	B	1238	CLA	CBB-CAB-C3B	8.58	170.37	127.53
18	A	1135	CLA	OBD-CAD-C3D	-8.57	108.39	128.42
18	B	9023	CLA	CBB-CAB-C3B	8.52	170.11	127.53
18	B	9012	CLA	CBB-CAB-C3B	8.51	170.03	127.53
18	B	1215	CLA	CBB-CAB-C3B	8.47	169.87	127.53
18	A	1135	CLA	CBB-CAB-C3B	8.47	169.87	127.53
18	A	1126	CLA	OBD-CAD-C3D	-8.39	108.81	128.42

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
18	B	9010	CLA	CBB-CAB-C3B	8.32	169.12	127.53
18	G	1233	CLA	CBB-CAB-C3B	8.32	169.12	127.53
18	I	1204	CLA	OBD-CAD-C3D	-8.27	109.09	128.42
18	A	1122	CLA	CBB-CAB-C3B	8.24	168.71	127.53
18	B	1222	CLA	CBB-CAB-C3B	8.18	168.38	127.53
20	I	6018	BCR	C16-C15-C14	-8.17	106.81	123.52
18	B	1228	CLA	CBB-CAB-C3B	8.16	168.30	127.53
18	L	1130	CLA	OBD-CAD-C3D	-8.15	109.38	128.42
18	A	1129	CLA	CBB-CAB-C3B	8.14	168.18	127.53
18	B	1227	CLA	CBB-CAB-C3B	8.11	168.07	127.53
18	4	1304	CLA	CBB-CAB-C3B	8.08	167.89	127.53
18	A	1131	CLA	CAB-C3B-C4B	-8.07	113.14	125.42
18	4	1304	CLA	OBD-CAD-C3D	-8.06	109.58	128.42
18	B	1212	CLA	OBD-CAD-C3D	-8.00	109.72	128.42
18	B	1208	CLA	CBB-CAB-C3B	7.99	167.44	127.53
18	A	1119	CLA	OBD-CAD-C3D	-7.95	109.83	128.42
18	A	1140	CLA	CBB-CAB-C3B	7.91	167.05	127.53
18	B	9023	CLA	OBD-CAD-C3D	-7.88	109.99	128.42
18	B	1138	CLA	OBD-CAD-C3D	-7.88	110.00	128.42
18	H	1501	CLA	CBB-CAB-C3B	7.86	166.78	127.53
18	B	1239	CLA	OBD-CAD-C3D	-7.85	110.06	128.42
18	B	1218	CLA	OBD-CAD-C3D	-7.84	110.09	128.42
18	B	1208	CLA	OBD-CAD-C3D	-7.82	110.14	128.42
20	I	6018	BCR	C30-C25-C26	-7.79	111.99	122.64
18	F	1302	CLA	OBD-CAD-C3D	-7.76	110.28	128.42
18	B	9010	CLA	OBD-CAD-C3D	-7.76	110.28	128.42
18	A	1135	CLA	O2D-CGD-CBD	7.74	124.77	111.23
18	B	1235	CLA	CAC-C3C-C4C	7.74	134.87	124.79
18	L	1503	CLA	CMD-C2D-C1D	7.74	138.36	124.73
18	B	1217	CLA	CMD-C2D-C1D	7.69	138.26	124.73
18	B	1209	CLA	OBD-CAD-C3D	-7.68	110.46	128.42
18	L	1503	CLA	C4D-C3D-CAD	7.68	116.45	108.11
18	A	1128	CLA	CBB-CAB-C3B	7.66	165.79	127.53
18	A	9011	CLA	OBD-CAD-C3D	-7.65	110.54	128.42
18	B	9022	CLA	CBB-CAB-C3B	7.63	165.66	127.53
18	A	1109	CLA	C3D-C4D-ND	7.61	106.53	101.67
18	B	1235	CLA	CBB-CAB-C3B	7.51	165.05	127.53
18	B	1221	CLA	CBB-CAB-C3B	7.46	164.78	127.53
18	B	1235	CLA	O2D-CGD-CBD	7.44	124.24	111.23
18	B	1216	CLA	CBB-CAB-C3B	7.39	164.46	127.53
18	B	1218	CLA	O2D-CGD-CBD	7.38	124.13	111.23
18	B	1217	CLA	CBB-CAB-C3B	7.36	164.31	127.53

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
18	L	1503	CLA	CHD-C4C-NC	7.36	135.64	124.23
18	A	1128	CLA	OBD-CAD-C3D	-7.35	111.23	128.42
18	A	1136	CLA	CBB-CAB-C3B	7.31	164.06	127.53
18	B	1225	CLA	CMD-C2D-C1D	7.31	137.59	124.73
18	A	1136	CLA	OBD-CAD-C3D	-7.28	111.41	128.42
18	B	1234	CLA	CBB-CAB-C3B	7.25	163.73	127.53
18	B	1238	CLA	CMD-C2D-C1D	7.18	137.38	124.73
18	A	1122	CLA	OBD-CAD-C3D	-7.17	111.66	128.42
18	B	1208	CLA	CMD-C2D-C1D	7.16	137.34	124.73
18	L	1503	CLA	C1D-CHD-C4C	-7.16	110.81	126.02
18	B	1219	CLA	C1-C2-C3	-7.15	114.48	126.20
18	A	1136	CLA	C4D-C3D-CAD	7.14	115.86	108.11
18	B	1224	CLA	CBB-CAB-C3B	7.12	163.08	127.53
18	L	1502	CLA	OBD-CAD-C3D	-7.10	111.82	128.42
18	L	1503	CLA	CAB-C3B-C4B	-7.06	114.67	125.42
18	A	1106	CLA	CMD-C2D-C1D	7.05	137.14	124.73
18	B	1207	CLA	CBB-CAB-C3B	7.04	162.71	127.53
18	B	1236	CLA	C4D-C3D-CAD	7.02	115.73	108.11
20	L	6020	BCR	C24-C23-C22	-7.02	115.86	126.23
18	J	2107	CLA	O2D-CGD-CBD	7.00	123.47	111.23
18	F	1139	CLA	CMD-C2D-C1D	7.00	137.06	124.73
18	B	9010	CLA	C4A-NA-C1A	6.97	109.86	106.68
18	B	1212	CLA	CMD-C2D-C1D	6.96	136.99	124.73
18	L	1130	CLA	O2D-CGD-CBD	6.94	123.37	111.23
18	B	1236	CLA	CMD-C2D-C1D	6.94	136.95	124.73
18	A	9013	CLA	CBB-CAB-C3B	6.92	162.09	127.53
18	A	1137	CLA	CMD-C2D-C1D	6.87	136.83	124.73
18	B	1224	CLA	O2D-CGD-CBD	6.85	123.21	111.23
18	B	1232	CLA	O2D-CGD-CBD	6.83	123.18	111.23
18	A	1129	CLA	CMD-C2D-C1D	6.81	136.72	124.73
18	B	9022	CLA	CMD-C2D-C1D	6.79	136.68	124.73
18	B	1234	CLA	OBD-CAD-C3D	-6.79	112.55	128.42
18	B	1231	CLA	CMD-C2D-C1D	6.78	136.66	124.73
18	B	1229	CLA	C1D-CHD-C4C	-6.78	111.62	126.02
18	A	1119	CLA	CMD-C2D-C1D	6.76	136.64	124.73
18	B	1218	CLA	C1D-CHD-C4C	-6.74	111.70	126.02
18	B	1237	CLA	CMD-C2D-C1D	6.69	136.51	124.73
18	A	1131	CLA	CMD-C2D-C1D	6.68	136.49	124.73
20	L	6020	BCR	C7-C8-C9	6.65	136.08	126.23
18	A	1123	CLA	CMD-C2D-C1D	6.64	136.42	124.73
18	B	1235	CLA	OBD-CAD-C3D	-6.60	112.99	128.42
18	A	1107	CLA	CMD-C2D-C1D	6.57	136.30	124.73

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
18	A	9013	CLA	CMD-C2D-C1D	6.57	136.30	124.73
18	B	1225	CLA	C4D-C3D-CAD	6.57	115.24	108.11
18	F	1302	CLA	C4D-C3D-CAD	6.56	115.23	108.11
18	B	1205	CLA	CMD-C2D-C1D	6.55	136.26	124.73
18	B	1236	CLA	CBB-CAB-C3B	6.54	160.21	127.53
18	A	1126	CLA	O2D-CGD-CBD	6.52	122.63	111.23
18	B	1202	CLA	C4D-C3D-CAD	6.52	115.18	108.11
18	A	1106	CLA	CMB-C2B-C1B	6.50	135.32	125.42
18	B	1220	CLA	C4D-C3D-CAD	6.50	115.16	108.11
18	B	1212	CLA	C4D-C3D-CAD	6.49	115.15	108.11
18	A	1122	CLA	C3B-C2B-C1B	-6.48	99.53	107.17
18	B	1217	CLA	C4D-C3D-CAD	6.46	115.12	108.11
18	B	1208	CLA	C4D-C3D-CAD	6.45	115.11	108.11
18	A	1113	CLA	C1D-CHD-C4C	-6.44	112.33	126.02
18	B	1221	CLA	O2D-CGD-CBD	6.41	122.44	111.23
18	B	1229	CLA	C4D-C3D-CAD	6.39	115.05	108.11
18	A	1107	CLA	C4D-C3D-CAD	6.39	115.04	108.11
18	F	1139	CLA	C4D-C3D-CAD	6.39	115.04	108.11
18	L	1502	CLA	O2D-CGD-CBD	6.38	122.38	111.23
18	A	1123	CLA	C4D-C3D-CAD	6.36	115.01	108.11
18	B	1234	CLA	CMD-C2D-C1D	6.35	135.90	124.73
18	B	1222	CLA	CMD-C2D-C1D	6.34	135.90	124.73
18	A	1106	CLA	C3B-C2B-C1B	-6.32	99.72	107.17
18	B	1222	CLA	O2D-CGD-CBD	6.32	122.28	111.23
18	B	1214	CLA	CMD-C2D-C1D	6.30	135.82	124.73
18	B	1219	CLA	CMD-C2D-C1D	6.29	135.81	124.73
18	B	1242	CLA	C1D-CHD-C4C	-6.28	112.67	126.02
18	B	1209	CLA	CMD-C2D-C1D	6.28	135.78	124.73
18	A	1113	CLA	CHD-C4C-NC	6.28	133.96	124.23
18	B	1205	CLA	O2D-CGD-CBD	6.27	122.19	111.23
18	B	1221	CLA	C1D-CHD-C4C	-6.25	112.73	126.02
18	L	1504	CLA	CMD-C2D-C1D	6.25	135.73	124.73
18	A	1126	CLA	CMD-C2D-C1D	6.24	135.72	124.73
18	B	9022	CLA	O2D-CGD-CBD	6.24	122.13	111.23
18	B	1228	CLA	C4D-C3D-CAD	6.23	114.87	108.11
18	B	1220	CLA	C1D-CHD-C4C	-6.22	112.80	126.02
18	F	1302	CLA	CMD-C2D-C1D	6.22	135.68	124.73
18	A	1128	CLA	C4D-C3D-CAD	6.21	114.85	108.11
18	A	1108	CLA	C4D-C3D-CAD	6.19	114.83	108.11
18	B	9010	CLA	O2D-CGD-CBD	6.18	122.03	111.23
18	A	1108	CLA	CMD-C2D-C1D	6.17	135.59	124.73
18	4	1304	CLA	CMD-C2D-C1D	6.16	135.58	124.73

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
18	B	1225	CLA	O2D-CGD-CBD	6.16	122.00	111.23
18	A	1126	CLA	C4D-C3D-CAD	6.14	114.78	108.11
18	A	1136	CLA	CHD-C4C-C3C	-6.14	115.82	124.77
20	F	6016	BCR	C19-C18-C17	-6.13	109.36	119.01
18	B	1202	CLA	C1D-CHD-C4C	-6.13	112.99	126.02
18	B	9012	CLA	O2D-CGD-CBD	6.13	121.95	111.23
18	4	4012	CLA	C4A-NA-C1A	6.13	109.47	106.68
18	4	1304	CLA	C4D-C3D-CAD	6.12	114.75	108.11
18	A	1126	CLA	O2D-CGD-O1D	-6.10	111.97	123.85
18	A	1136	CLA	C1D-CHD-C4C	-6.10	113.05	126.02
18	L	1503	CLA	CHD-C4C-C3C	-6.09	115.89	124.77
20	B	6017	BCR	C20-C21-C22	-6.09	118.74	127.28
18	A	1136	CLA	CMD-C2D-C1D	6.09	135.45	124.73
18	A	1113	CLA	CBB-CAB-C3B	6.08	157.91	127.53
18	A	9011	CLA	C4D-C3D-CAD	6.07	114.70	108.11
18	A	1103	CLA	CMD-C2D-C1D	6.07	135.41	124.73
18	A	1106	CLA	C4D-C3D-CAD	6.07	114.69	108.11
18	B	9022	CLA	C4D-C3D-CAD	6.06	114.69	108.11
18	B	1228	CLA	C1D-CHD-C4C	-6.06	113.13	126.02
18	A	1140	CLA	C4D-C3D-CAD	6.06	114.68	108.11
18	B	1225	CLA	C1D-CHD-C4C	-6.05	113.15	126.02
18	A	1122	CLA	C4D-C3D-CAD	6.05	114.67	108.11
18	B	1221	CLA	CMD-C2D-C1D	6.04	135.36	124.73
18	B	9023	CLA	C4D-C3D-CAD	6.03	114.66	108.11
18	B	1205	CLA	C1D-CHD-C4C	-6.03	113.20	126.02
20	F	6016	BCR	C23-C22-C21	-6.03	109.53	119.01
18	A	1108	CLA	C1D-CHD-C4C	-6.01	113.24	126.02
18	B	1212	CLA	CHD-C4C-NC	6.00	133.53	124.23
18	B	1215	CLA	O2D-CGD-CBD	5.98	121.69	111.23
18	B	1202	CLA	CMD-C2D-C3D	-5.97	114.00	127.69
18	B	1220	CLA	CMD-C2D-C1D	5.97	135.24	124.73
20	F	6016	BCR	C24-C23-C22	-5.97	117.41	126.23
18	A	1103	CLA	CHC-C1C-NC	5.96	133.29	124.31
18	B	9022	CLA	C1D-CHD-C4C	-5.96	113.36	126.02
18	A	1131	CLA	C4D-C3D-CAD	5.94	114.56	108.11
18	B	1138	CLA	C4D-C3D-CAD	5.94	114.56	108.11
20	L	6020	BCR	C8-C7-C6	-5.94	111.13	127.00
18	B	1202	CLA	O2D-CGD-CBD	5.94	121.61	111.23
18	A	1140	CLA	CMD-C2D-C1D	5.94	135.19	124.73
18	L	1504	CLA	O2D-CGD-CBD	5.94	121.61	111.23
18	A	1135	CLA	C1D-CHD-C4C	-5.93	113.41	126.02
18	B	1212	CLA	C1D-CHD-C4C	-5.91	113.45	126.02

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
18	B	1216	CLA	C1D-CHD-C4C	-5.90	113.48	126.02
18	B	9012	CLA	OBD-CAD-C3D	-5.89	114.65	128.42
18	B	1237	CLA	C4-C3-C5	5.88	123.05	116.13
18	G	1233	CLA	C1D-CHD-C4C	-5.88	113.53	126.02
18	B	1239	CLA	C1D-CHD-C4C	-5.88	113.53	126.02
18	L	1502	CLA	C1D-CHD-C4C	-5.87	113.54	126.02
18	B	1239	CLA	CMD-C2D-C1D	5.87	135.06	124.73
18	L	1130	CLA	CMD-C2D-C1D	5.87	135.06	124.73
18	G	1233	CLA	CMD-C2D-C1D	5.86	135.06	124.73
18	A	1135	CLA	CMD-C2D-C1D	5.86	135.04	124.73
18	B	1242	CLA	O2D-CGD-CBD	5.85	121.45	111.23
18	A	1119	CLA	C4D-C3D-CAD	5.84	114.45	108.11
18	B	1207	CLA	C4D-C3D-CAD	5.84	114.45	108.11
18	B	1215	CLA	C4A-NA-C1A	5.84	109.34	106.68
18	B	1222	CLA	OBD-CAD-C3D	-5.84	114.78	128.42
18	B	1138	CLA	CBB-CAB-C3B	5.82	156.60	127.53
18	B	1205	CLA	C4D-C3D-CAD	5.82	114.43	108.11
20	F	6016	BCR	C21-C20-C19	-5.82	106.34	123.20
18	A	1113	CLA	O2D-CGD-CBD	5.80	121.38	111.23
18	H	1501	CLA	CMD-C2D-C1D	5.79	134.93	124.73
18	B	1219	CLA	C4D-C3D-CAD	5.79	114.40	108.11
18	B	1237	CLA	C1D-CHD-C4C	-5.79	113.72	126.02
18	B	1238	CLA	O2D-CGD-CBD	5.78	121.34	111.23
18	A	1131	CLA	C4A-NA-C1A	5.78	109.32	106.68
18	A	1129	CLA	C4D-C3D-CAD	5.77	114.38	108.11
18	B	1225	CLA	CHD-C4C-NC	5.77	133.18	124.23
18	A	1107	CLA	CMB-C2B-C1B	5.76	134.18	125.42
18	B	1232	CLA	CMD-C2D-C1D	5.75	134.85	124.73
18	B	1208	CLA	C1-O2A-CGA	5.75	130.56	116.65
18	B	1222	CLA	C4D-C3D-CAD	5.73	114.33	108.11
18	A	1122	CLA	C2B-C1B-NB	5.73	116.27	110.33
18	H	1501	CLA	C4D-C3D-CAD	5.73	114.33	108.11
18	L	1130	CLA	CBB-CAB-C3B	5.73	156.13	127.53
19	B	5002	PQN	C11-C12-C13	-5.72	116.97	126.83
18	B	1229	CLA	CHD-C4C-C3C	-5.72	116.43	124.77
18	A	1113	CLA	C4D-C3D-CAD	5.70	114.30	108.11
18	B	1224	CLA	CMD-C2D-C1D	5.70	134.76	124.73
18	B	1237	CLA	C4D-C3D-CAD	5.69	114.29	108.11
18	B	1138	CLA	CMD-C2D-C1D	5.69	134.75	124.73
18	A	1119	CLA	C1D-CHD-C4C	-5.68	113.94	126.02
20	F	6016	BCR	C11-C12-C13	-5.67	110.81	126.36
18	B	1208	CLA	C2B-C1B-NB	5.67	116.21	110.33

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
18	B	1242	CLA	C4D-C3D-CAD	5.67	114.27	108.11
18	A	1132	CLA	C3A-C4A-CHB	-5.67	116.97	123.91
18	A	9011	CLA	C3B-C2B-C1B	-5.67	100.49	107.17
20	B	6017	BCR	C21-C20-C19	-5.66	106.81	123.20
18	B	1207	CLA	CMD-C2D-C1D	5.65	134.67	124.73
18	B	1217	CLA	CMD-C2D-C3D	-5.64	114.75	127.69
18	L	1504	CLA	C1D-CHD-C4C	-5.64	114.03	126.02
18	F	1302	CLA	C1D-CHD-C4C	-5.62	114.07	126.02
18	B	1228	CLA	C2B-C1B-NB	5.62	116.15	110.33
18	A	1131	CLA	C1D-CHD-C4C	-5.61	114.09	126.02
18	B	1207	CLA	CAA-C2A-C3A	-5.61	97.83	113.00
18	B	1216	CLA	C4D-C3D-CAD	5.61	114.20	108.11
18	L	1502	CLA	CMD-C2D-C1D	5.60	134.59	124.73
18	B	1229	CLA	CMD-C2D-C1D	5.60	134.59	124.73
18	H	1501	CLA	C1D-CHD-C4C	-5.60	114.12	126.02
18	A	1137	CLA	O2D-CGD-CBD	5.60	121.01	111.23
18	A	1136	CLA	CHD-C4C-NC	5.59	132.91	124.23
18	B	1214	CLA	C4D-C3D-CAD	5.59	114.18	108.11
18	B	1232	CLA	C1D-CHD-C4C	-5.59	114.15	126.02
18	L	1130	CLA	C1D-CHD-C4C	-5.58	114.16	126.02
18	B	9010	CLA	CMD-C2D-C1D	5.58	134.55	124.73
18	B	1239	CLA	O2D-CGD-CBD	5.58	120.98	111.23
18	A	1122	CLA	O2D-CGD-CBD	5.57	120.96	111.23
20	A	6011	BCR	C38-C26-C25	-5.56	118.41	124.48
18	A	1128	CLA	O2D-CGD-CBD	5.56	120.96	111.23
18	B	1236	CLA	C1D-CHD-C4C	-5.56	114.19	126.02
18	A	1113	CLA	CHD-C4C-C3C	-5.56	116.66	124.77
18	A	1115	CLA	C1D-CHD-C4C	-5.56	114.20	126.02
18	B	1236	CLA	O2D-CGD-CBD	5.56	120.95	111.23
18	A	1119	CLA	O2D-CGD-CBD	5.55	120.94	111.23
18	B	9012	CLA	C4D-C3D-CAD	5.55	114.14	108.11
18	B	1212	CLA	CHD-C4C-C3C	-5.55	116.68	124.77
18	B	1231	CLA	O2D-CGD-CBD	5.55	120.93	111.23
18	A	1136	CLA	O1D-CGD-CBD	-5.55	113.58	124.52
18	B	1203	CLA	C1-C2-C3	-5.54	117.79	126.76
18	B	1208	CLA	CAC-C3C-C4C	5.54	132.00	124.79
18	B	1224	CLA	C1D-CHD-C4C	-5.54	114.25	126.02
18	B	1221	CLA	OBD-CAD-C3D	-5.53	115.48	128.42
18	B	1219	CLA	OBD-CAD-C3D	-5.53	115.48	128.42
18	A	1128	CLA	CMD-C2D-C1D	5.53	134.47	124.73
18	A	1129	CLA	C1D-CHD-C4C	-5.51	114.30	126.02
18	B	1227	CLA	CMD-C2D-C1D	5.51	134.44	124.73

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
18	I	1204	CLA	CMD-C2D-C1D	5.51	134.43	124.73
18	A	1115	CLA	C4D-C3D-CAD	5.51	114.09	108.11
18	B	1212	CLA	CBB-CAB-C3B	5.51	155.06	127.53
18	B	1227	CLA	C4D-C3D-CAD	5.51	114.09	108.11
18	B	1207	CLA	C1D-CHD-C4C	-5.51	114.32	126.02
18	4	1304	CLA	C1D-CHD-C4C	-5.51	114.32	126.02
18	G	1248	CLA	CHD-C4C-NC	5.50	132.60	124.24
18	B	1237	CLA	C3B-C2B-C1B	-5.49	100.69	107.17
18	B	9023	CLA	C1D-CHD-C4C	-5.49	114.35	126.02
18	4	1304	CLA	O2D-CGD-CBD	5.49	120.82	111.23
18	B	1235	CLA	C4D-C3D-CAD	5.48	114.06	108.11
18	B	1209	CLA	C4D-C3D-CAD	5.47	114.05	108.11
18	B	1223	CLA	CHC-C1C-NC	5.45	132.34	124.33
18	B	1227	CLA	C4B-CHC-C1C	-5.45	113.44	126.25
18	B	1138	CLA	C1D-CHD-C4C	-5.45	114.45	126.02
18	B	1234	CLA	O2D-CGD-O1D	-5.44	113.27	123.85
18	B	1216	CLA	CMD-C2D-C1D	5.43	134.29	124.73
18	1	1006	CLA	C3A-C4A-CHB	-5.43	117.27	123.91
18	L	1503	CLA	CHC-C1C-NC	5.42	132.48	124.31
18	B	9010	CLA	C1D-CHD-C4C	-5.40	114.55	126.02
18	A	1113	CLA	CMD-C2D-C1D	5.39	134.22	124.73
18	B	1227	CLA	CHC-C4B-NB	5.39	132.14	124.05
18	L	1503	CLA	CMD-C2D-C3D	-5.39	115.33	127.69
18	B	1234	CLA	C1D-CHD-C4C	-5.39	114.57	126.02
18	I	1204	CLA	C1D-CHD-C4C	-5.38	114.58	126.02
18	B	1215	CLA	CMD-C2D-C1D	5.38	134.20	124.73
18	A	1116	CLA	C3A-C4A-CHB	-5.38	117.32	123.91
18	G	1233	CLA	CHD-C4C-NC	5.38	132.57	124.23
18	A	1103	CLA	O2D-CGD-CBD	5.37	120.62	111.23
18	A	1113	CLA	C3B-C2B-C1B	-5.36	100.85	107.17
18	B	1238	CLA	CAA-C2A-C1A	-5.35	94.44	111.97
18	B	1225	CLA	C3B-C2B-C1B	-5.35	100.86	107.17
18	B	1218	CLA	CED-O2D-CGD	5.35	128.04	115.92
18	A	1120	CLA	C3A-C4A-CHB	-5.34	117.37	123.91
18	B	1227	CLA	C1D-CHD-C4C	-5.34	114.67	126.02
18	B	1215	CLA	C4B-CHC-C1C	-5.34	113.69	126.25
18	B	1209	CLA	CGD-CBD-CAD	-5.34	93.57	110.85
18	B	1217	CLA	C1D-CHD-C4C	-5.33	114.68	126.02
18	B	1227	CLA	CMB-C2B-C1B	5.32	133.52	125.42
18	G	1233	CLA	CHD-C4C-C3C	-5.32	117.01	124.77
18	A	1109	CLA	CHD-C4C-NC	5.32	132.32	124.24
18	B	1220	CLA	C3B-C2B-C1B	-5.31	100.91	107.17

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
18	L	1503	CLA	C4B-CHC-C1C	-5.31	113.76	126.25
18	B	1208	CLA	C3B-C2B-C1B	-5.30	100.93	107.17
18	A	1123	CLA	C1D-CHD-C4C	-5.29	114.77	126.02
18	A	1134	CLA	C3A-C4A-CHB	-5.29	117.43	123.91
18	A	1108	CLA	CHD-C4C-NC	5.29	132.44	124.23
18	A	1104	CLA	C3A-C4A-CHB	-5.29	117.44	123.91
18	B	1216	CLA	O2D-CGD-CBD	5.29	120.47	111.23
18	B	9010	CLA	C4D-C3D-CAD	5.28	113.85	108.11
18	B	1207	CLA	C4A-NA-C1A	5.28	109.09	106.68
18	A	1119	CLA	CHD-C4C-NC	5.27	132.40	124.23
18	G	1233	CLA	O2D-CGD-CBD	5.26	120.43	111.23
20	F	6016	BCR	C33-C5-C6	-5.26	118.74	124.48
18	B	1242	CLA	CMD-C2D-C1D	5.26	133.99	124.73
18	L	1503	CLA	O2D-CGD-CBD	5.26	120.42	111.23
18	B	1229	CLA	CHD-C4C-NC	5.26	132.38	124.23
18	B	1232	CLA	C4D-C3D-CAD	5.25	113.81	108.11
18	B	1209	CLA	C1D-CHD-C4C	-5.25	114.85	126.02
18	B	1219	CLA	O2D-CGD-CBD	5.25	120.41	111.23
18	B	9022	CLA	O2D-CGD-O1D	-5.25	113.64	123.85
18	B	1217	CLA	O2D-CGD-CBD	5.24	120.40	111.23
18	A	1124	CLA	C2A-C1A-CHA	-5.24	113.69	122.63
18	B	9012	CLA	CMD-C2D-C1D	5.24	133.96	124.73
18	B	1207	CLA	C2B-C1B-NB	5.24	115.76	110.33
18	A	1137	CLA	OBD-CAD-C3D	-5.23	116.19	128.42
18	B	1214	CLA	C1D-CHD-C4C	-5.23	114.91	126.02
18	A	1115	CLA	C2B-C1B-NB	5.23	115.75	110.33
18	A	9013	CLA	C4D-C3D-CAD	5.22	113.78	108.11
18	I	1204	CLA	C4D-C3D-CAD	5.22	113.77	108.11
18	1	1012	CLA	C4A-NA-C1A	5.21	109.06	106.68
18	1	1010	CLA	C3A-C4A-CHB	-5.21	117.53	123.91
18	A	1118	CLA	C4A-NA-C1A	5.21	109.06	106.68
18	A	9013	CLA	C3B-C2B-C1B	-5.21	101.03	107.17
18	A	1140	CLA	C1D-CHD-C4C	-5.21	114.95	126.02
18	A	1122	CLA	C1D-CHD-C4C	-5.20	114.96	126.02
18	A	1103	CLA	C4A-NA-C1A	5.20	109.05	106.68
18	A	9013	CLA	CHC-C4B-NB	5.20	131.85	124.05
18	B	1229	CLA	C1B-C2B-C3B	-5.20	102.14	107.03
18	B	1207	CLA	C3B-C2B-C1B	-5.20	101.04	107.17
18	A	1122	CLA	CMD-C2D-C1D	5.19	133.87	124.73
18	B	1222	CLA	C1D-CHD-C4C	-5.19	114.99	126.02
18	A	1137	CLA	C4D-C3D-CAD	5.19	113.74	108.11
18	A	9011	CLA	C1D-CHD-C4C	-5.18	115.01	126.02

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
18	J	2107	CLA	C1D-CHD-C4C	-5.18	115.02	126.02
18	B	1215	CLA	CHC-C1C-NC	5.17	132.10	124.31
18	A	1148	CLA	C3A-C4A-CHB	-5.17	117.58	123.91
18	L	1502	CLA	CHD-C4C-NC	5.17	132.24	124.23
18	A	1115	CLA	CMD-C2D-C1D	5.16	133.82	124.73
18	B	1209	CLA	C2B-C1B-NB	5.16	115.68	110.33
18	A	1103	CLA	C1D-CHD-C4C	-5.16	115.06	126.02
18	B	1218	CLA	CHD-C4C-NC	5.16	132.23	124.23
18	B	1220	CLA	CHD-C4C-NC	5.16	132.23	124.23
18	B	1201	CLA	C3A-C4A-CHB	-5.16	117.60	123.91
18	B	1218	CLA	C4D-C3D-CAD	5.15	113.70	108.11
18	A	9011	CLA	CHC-C4B-NB	5.14	131.76	124.05
18	4	4009	CLA	C3A-C4A-CHB	-5.14	117.61	123.91
18	G	1248	CLA	CHC-C1C-NC	5.14	131.88	124.33
20	L	6020	BCR	C23-C22-C21	5.14	127.09	119.01
18	A	1123	CLA	CHD-C4C-NC	5.12	132.17	124.23
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
18	2	2003	CLA	CHD-C4C-NC	5.11	132.01	124.24
18	A	1115	CLA	CHC-C1C-NC	5.10	132.00	124.31
18	B	1223	CLA	CHD-C4C-NC	5.10	131.99	124.24
18	B	1225	CLA	CAA-C2A-C1A	-5.10	95.27	111.97
18	B	9012	CLA	C4A-NA-C1A	5.09	109.00	106.68
18	F	1139	CLA	C1D-CHD-C4C	-5.09	115.20	126.02
18	1	1013	CLA	C3A-C4A-CHB	-5.09	117.68	123.91
18	I	1204	CLA	O2D-CGD-CBD	5.09	120.12	111.23
18	2	2015	CLA	C3A-C4A-CHB	-5.08	117.69	123.91
18	A	1101	CLA	C4A-NA-C1A	5.08	109.00	106.68
18	B	9023	CLA	C4A-NA-C1A	5.07	108.99	106.68
20	F	6016	BCR	C23-C24-C25	-5.05	113.50	127.00
18	A	1135	CLA	CHD-C4C-NC	5.05	132.06	124.23
18	A	1135	CLA	C4D-C3D-CAD	5.05	113.59	108.11
18	1	1012	CLA	C2A-C1A-CHA	-5.04	114.03	122.63
18	B	1202	CLA	CAA-C2A-C3A	-5.03	99.40	113.00
18	B	1203	CLA	C4A-NA-C1A	5.03	108.97	106.68
18	B	1235	CLA	O2D-CGD-O1D	-5.03	114.06	123.85
18	A	1108	CLA	O2D-CGD-CBD	5.03	120.02	111.23
18	J	2107	CLA	CMD-C2D-C1D	5.03	133.58	124.73
18	3	3001	CLA	C3A-C4A-CHB	-5.02	117.76	123.91
18	A	1131	CLA	CAB-C3B-C2B	-5.02	110.21	123.53
18	A	1136	CLA	C4A-NA-C1A	5.02	108.97	106.68
18	2	2005	CLA	C3A-C4A-CHB	-5.01	117.77	123.91

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
18	2	2003	CLA	C4A-NA-C1A	5.01	108.97	106.68
18	A	1126	CLA	C1D-CHD-C4C	-5.01	115.37	126.02
18	J	1307	CLA	C3A-C4A-CHB	-5.01	117.78	123.91
18	A	1123	CLA	C2B-C1B-NB	5.00	115.52	110.33
18	A	1107	CLA	C3B-C2B-C1B	-5.00	101.28	107.17
18	B	1224	CLA	CHD-C4C-NC	5.00	131.98	124.23
18	B	1239	CLA	C4D-C3D-CAD	4.99	113.53	108.11
18	A	9013	CLA	C1D-CHD-C4C	-4.99	115.41	126.02
18	3	3007	CLA	C3A-C4A-CHB	-4.99	117.81	123.91
18	A	1135	CLA	CHD-C4C-C3C	-4.98	117.51	124.77
18	B	1231	CLA	C4D-C3D-CAD	4.98	113.51	108.11
18	L	1502	CLA	C4D-C3D-CAD	4.98	113.51	108.11
18	B	1229	CLA	CAB-C3B-C2B	-4.97	110.33	123.53
20	B	6017	BCR	C15-C16-C17	-4.97	113.35	123.52
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	A	1129	CLA	O2D-CGD-CBD	4.96	119.89	111.23
18	B	1228	CLA	C3B-C2B-C1B	-4.95	101.33	107.17
18	B	1235	CLA	C2B-C1B-NB	4.95	115.46	110.33
18	A	1119	CLA	CHD-C4C-C3C	-4.95	117.55	124.77
18	B	9012	CLA	C1-C2-C3	4.95	134.31	126.20
18	1	1008	CLA	C3A-C4A-CHB	-4.95	117.85	123.91
18	3	2009	CLA	CHD-C4C-NC	4.95	131.76	124.24
18	B	1220	CLA	CHD-C4C-C3C	-4.95	117.56	124.77
18	F	1240	CLA	C3A-C4A-CHB	-4.94	117.86	123.91
18	A	9011	CLA	C4A-NA-C1A	4.94	108.93	106.68
18	B	1205	CLA	CHD-C4C-NC	4.94	131.89	124.23
18	A	1124	CLA	C4C-CHD-C1D	-4.94	111.90	125.98
18	B	1203	CLA	O2D-CGD-O1D	-4.94	114.23	123.85
20	L	6020	BCR	C37-C22-C21	-4.94	114.81	122.82
18	3	2009	CLA	C3A-C4A-CHB	-4.94	117.87	123.91
18	B	1242	CLA	CHD-C4C-C3C	-4.93	117.58	124.77
18	B	9010	CLA	C3B-C2B-C1B	-4.93	101.36	107.17
18	G	1233	CLA	C4D-C3D-CAD	4.93	113.46	108.11
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	L	1504	CLA	C4D-C3D-CAD	4.92	113.45	108.11
18	B	1239	CLA	CHC-C1C-NC	4.92	131.72	124.31
18	A	1108	CLA	CHD-C4C-C3C	-4.92	117.60	124.77
18	L	1503	CLA	CAA-C2A-C3A	4.92	126.30	113.00
18	B	1221	CLA	CHC-C4B-NB	4.92	131.43	124.05
18	B	1220	CLA	O2D-CGD-CBD	4.92	119.83	111.23

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
18	3	3008	CLA	C3A-C4A-CHB	-4.92	117.89	123.91
18	1	1003	CLA	C3A-C4A-CHB	-4.91	117.89	123.91
18	A	1106	CLA	C1D-CHD-C4C	-4.91	115.58	126.02
18	F	1240	CLA	C2A-C1A-CHA	-4.91	114.27	122.63
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	A	1137	CLA	C2B-C1B-NB	4.90	115.41	110.33
18	B	1236	CLA	CHD-C4C-NC	4.90	131.83	124.23
18	B	1207	CLA	CHD-C4C-C3C	-4.90	117.63	124.77
18	3	3008	CLA	C4A-NA-C1A	4.89	108.91	106.68
18	B	1216	CLA	C2B-C1B-NB	4.89	115.40	110.33
18	A	1152	CLA	C3A-C4A-CHB	-4.89	117.92	123.91
18	A	1146	CLA	C3A-C4A-CHB	-4.88	117.93	123.91
18	A	1142	CLA	CHD-C4C-NC	4.88	131.66	124.24
18	A	1135	CLA	O2D-CGD-O1D	-4.88	114.35	123.85
18	B	1213	CLA	C3A-C4A-CHB	-4.87	117.94	123.91
18	B	1205	CLA	C4A-NA-C1A	4.87	108.90	106.68
18	4	4005	CLA	C2A-C1A-CHA	-4.87	114.33	122.63
18	B	1216	CLA	CHD-C4C-NC	4.87	131.78	124.23
18	4	4004	CLA	C3A-C4A-CHB	-4.87	117.95	123.91
18	A	1103	CLA	C4D-C3D-CAD	4.87	113.39	108.11
18	A	9011	CLA	CMD-C2D-C1D	4.87	133.30	124.73
18	B	1238	CLA	CHD-C4C-NC	4.87	131.78	124.23
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	A	1101	CLA	C2A-C1A-CHA	-4.86	114.34	122.63
18	A	1126	CLA	CGD-CBD-CAD	-4.86	95.10	110.85
18	1	1011	CLA	C3A-C4A-CHB	-4.86	117.95	123.91
18	L	1503	CLA	C4A-NA-C1A	4.86	108.90	106.68
18	B	1242	CLA	CHD-C4C-NC	4.86	131.77	124.23
18	L	1130	CLA	C4D-C3D-CAD	4.86	113.39	108.11
18	F	4015	CLA	C3A-C4A-CHB	-4.86	117.96	123.91
18	B	9022	CLA	C4B-CHC-C1C	-4.86	114.82	126.25
18	K	1150	CLA	C3A-C4A-CHB	-4.86	117.96	123.91
18	A	1127	CLA	CHD-C4C-NC	4.86	131.62	124.24
18	A	1102	CLA	C2A-C1A-CHA	-4.86	114.35	122.63
18	H	1505	CLA	C4A-NA-C1A	4.86	108.89	106.68
18	A	1109	CLA	CHC-C1C-NC	4.85	131.46	124.33
18	B	1201	CLA	C4A-NA-C1A	4.85	108.89	106.68
18	B	9023	CLA	CHD-C4C-NC	4.85	131.75	124.23
18	2	2004	CLA	C2A-C1A-CHA	-4.85	114.36	122.63
18	A	1101	CLA	CHD-C4C-NC	4.85	131.61	124.24

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
18	A	1106	CLA	CAA-C2A-C3A	-4.84	105.13	116.23
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	1219	CLA	C4B-CHC-C1C	-4.83	114.88	126.25
18	A	1128	CLA	C1D-CHD-C4C	-4.83	115.75	126.02
18	B	1229	CLA	CAA-CBA-CGA	-4.83	99.49	113.21
18	B	1208	CLA	C1D-CHD-C4C	-4.83	115.75	126.02
20	I	6018	BCR	C15-C16-C17	4.83	133.41	123.52
18	4	4010	CLA	C3A-C4A-CHB	-4.83	118.00	123.91
18	A	1147	CLA	CHD-C4C-NC	4.83	131.57	124.24
18	3	3012	CLA	CHD-C4C-NC	4.83	131.57	124.24
18	F	1139	CLA	O2D-CGD-CBD	4.82	119.67	111.23
18	2	2001	CLA	CHD-C4C-NC	4.82	131.57	124.24
18	3	3005	CLA	C3A-C4A-CHB	-4.82	118.00	123.91
18	B	1202	CLA	CHC-C1C-NC	4.82	131.57	124.31
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	G	1248	CLA	C4A-NA-C1A	4.82	108.88	106.68
18	B	1228	CLA	CMD-C2D-C1D	4.82	133.22	124.73
18	A	1151	CLA	CHD-C4C-NC	4.82	131.56	124.24
18	B	1202	CLA	CHD-C4C-NC	4.81	131.69	124.23
18	B	1225	CLA	C2B-C1B-NB	4.81	115.31	110.33
18	B	9023	CLA	C2B-C1B-NB	4.81	115.31	110.33
18	B	1207	CLA	O2D-CGD-O1D	-4.81	114.49	123.85
18	A	1108	CLA	C4A-NA-C1A	4.80	108.87	106.68
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	B	1234	CLA	C4D-C3D-CAD	4.80	113.31	108.11
18	4	4005	CLA	CHD-C4C-NC	4.79	131.53	124.24
18	3	3004	CLA	C4A-NA-C1A	4.79	108.86	106.68
20	L	6020	BCR	C15-C14-C13	-4.79	120.57	127.28
18	K	1150	CLA	C2A-C1A-CHA	-4.78	114.48	122.63
18	2	2007	CLA	CHD-C4C-NC	4.77	131.49	124.24
18	B	9012	CLA	C1D-CHD-C4C	-4.77	115.88	126.02
18	2	2006	CLA	C2A-C1A-CHA	-4.77	114.50	122.63
18	4	4013	CLA	CHD-C4C-NC	4.77	131.48	124.24
18	B	1228	CLA	CHD-C4C-NC	4.76	131.62	124.23
18	B	1232	CLA	CHD-C4C-NC	4.76	131.61	124.23
18	A	1140	CLA	O2A-CGA-CBA	4.76	126.35	111.83
18	F	1302	CLA	CHD-C4C-NC	4.76	131.61	124.23
18	A	1105	CLA	C3A-C4A-CHB	-4.76	118.08	123.91
18	L	1130	CLA	CHD-C4C-NC	4.75	131.60	124.23

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
18	3	3005	CLA	CHD-C4C-NC	4.75	131.46	124.24
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	A	1106	CLA	CMD-C2D-C3D	-4.75	116.80	127.69
18	A	1113	CLA	C4B-CHC-C1C	-4.74	115.09	126.25
18	4	1009	CLA	C1C-NC-C4C	-4.74	104.52	106.68
18	3	3006	CLA	C2A-C1A-CHA	-4.74	114.55	122.63
18	B	9012	CLA	C2B-C1B-NB	4.74	115.24	110.33
18	3	3009	CLA	CHD-C4C-NC	4.74	131.45	124.24
18	A	1124	CLA	CHA-C4D-ND	4.74	131.54	124.84
18	B	1207	CLA	CHB-C4A-NA	4.74	131.24	124.40
18	A	1137	CLA	C1D-CHD-C4C	-4.74	115.94	126.02
18	A	1123	CLA	O2D-CGD-CBD	4.74	119.52	111.23
18	B	1238	CLA	C4B-CHC-C1C	-4.74	115.10	126.25
18	F	1139	CLA	CMD-C2D-C3D	-4.74	116.82	127.69
18	A	1309	CLA	C3A-C4A-CHB	-4.74	118.11	123.91
18	1	1008	CLA	CHD-C4C-NC	4.74	131.44	124.24
20	I	6018	BCR	C27-C26-C25	-4.73	116.31	122.70
18	F	1139	CLA	C4B-CHC-C1C	-4.73	115.11	126.25
18	2	2007	CLA	C3A-C4A-CHB	-4.73	118.12	123.91
18	B	1235	CLA	C1D-CHD-C4C	-4.73	115.96	126.02
18	A	1137	CLA	C4-C3-C5	4.73	123.44	115.23
18	B	9023	CLA	CMD-C2D-C1D	4.73	133.05	124.73
18	3	3015	CLA	C3A-C4A-CHB	-4.73	118.12	123.91
18	B	9010	CLA	C4B-CHC-C1C	-4.72	115.14	126.25
18	A	1101	CLA	CHC-C1C-NC	4.72	131.27	124.33
18	B	1202	CLA	O2D-CGD-O1D	-4.72	114.65	123.85
18	1	1005	CLA	C2A-C1A-CHA	-4.72	114.58	122.63
18	B	1225	CLA	CMD-C2D-C3D	-4.72	116.86	127.69
18	B	9010	CLA	CHD-C4C-C3C	-4.72	117.89	124.77
18	A	1144	CLA	CHD-C4C-NC	4.72	131.41	124.24
18	K	1153	CLA	C3A-C4A-CHB	-4.72	118.13	123.91
18	3	3002	CLA	C3A-C4A-CHB	-4.72	118.13	123.91
18	B	1214	CLA	CHD-C4C-NC	4.72	131.55	124.23
18	B	1215	CLA	CMB-C2B-C1B	4.72	132.61	125.42
18	2	2010	CLA	C3A-C4A-CHB	-4.72	118.13	123.91
18	B	1208	CLA	CMD-C2D-C3D	-4.72	116.88	127.69
18	4	4006	CLA	C3A-C4A-CHB	-4.71	118.14	123.91
18	1	1011	CLA	CHD-C4C-NC	4.71	131.40	124.24
18	2	2002	CLA	C3A-C4A-CHB	-4.71	118.14	123.91
18	4	4012	CLA	CHD-C4C-NC	4.71	131.40	124.24
18	4	4005	CLA	C2D-C3D-C4D	-4.71	101.63	107.35

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
18	B	1238	CLA	C1D-CHD-C4C	-4.71	116.01	126.02
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	3	3003	CLA	C3A-C4A-CHB	-4.70	118.15	123.91
18	A	1147	CLA	C3A-C4A-CHB	-4.70	118.15	123.91
18	4	4001	CLA	C2A-C1A-CHA	-4.70	114.62	122.63
18	3	3007	CLA	CHD-C4C-NC	4.70	131.38	124.24
18	A	1118	CLA	C3A-C4A-CHB	-4.70	118.16	123.91
18	4	4002	CLA	CHD-C4C-NC	4.70	131.38	124.24
20	I	6018	BCR	C20-C19-C18	-4.70	113.48	126.36
18	3	3002	CLA	CHD-C4C-NC	4.70	131.38	124.24
18	2	2003	CLA	CHC-C1C-NC	4.69	131.23	124.33
18	B	1211	CLA	CHD-C4C-NC	4.69	131.37	124.24
18	F	1305	CLA	CHD-C4C-NC	4.69	131.37	124.24
18	2	2010	CLA	CHD-C4C-NC	4.69	131.37	124.24
18	4	4007	CLA	CHD-C4C-NC	4.69	131.37	124.24
18	B	1238	CLA	C2B-C1B-NB	4.69	115.19	110.33
18	A	1113	CLA	C4A-NA-C1A	4.69	108.82	106.68
18	A	1123	CLA	CHD-C4C-C3C	-4.69	117.94	124.77
18	A	1126	CLA	C2B-C1B-NB	4.69	115.19	110.33
18	A	9013	CLA	C4B-CHC-C1C	-4.69	115.23	126.25
18	3	3007	CLA	C2A-C1A-CHA	-4.68	114.65	122.63
18	A	1137	CLA	CHD-C4C-C3C	-4.68	117.95	124.77
18	B	1237	CLA	O2D-CGD-CBD	4.68	119.40	111.23
18	A	1106	CLA	CHC-C4B-NB	4.67	131.06	124.05
18	3	3011	CLA	C3A-C4A-CHB	-4.67	118.19	123.91
18	A	1131	CLA	CMD-C2D-C3D	-4.67	116.98	127.69
18	A	1147	CLA	C4A-NA-C1A	4.67	108.81	106.68
18	B	9010	CLA	CHD-C4C-NC	4.67	131.47	124.23
18	L	1125	CLA	C2A-C1A-CHA	-4.66	114.68	122.63
18	F	1303	CLA	C2A-C1A-CHA	-4.66	114.68	122.63
18	1	1006	CLA	CHD-C4C-NC	4.66	131.32	124.24
18	A	1115	CLA	O2D-CGD-CBD	4.66	119.37	111.23
18	B	9023	CLA	C4B-CHC-C1C	-4.66	115.30	126.25
18	B	1235	CLA	CMD-C2D-C1D	4.65	132.93	124.73
18	A	1140	CLA	O2D-CGD-CBD	4.65	119.36	111.23
18	B	1225	CLA	CHD-C4C-C3C	-4.65	117.99	124.77
18	2	2008	CLA	C2A-C1A-CHA	-4.65	114.70	122.63
18	B	1218	CLA	CHD-C4C-C3C	-4.65	118.00	124.77
18	A	1134	CLA	C3B-C2B-C1B	-4.65	101.64	106.81
18	A	1110	CLA	C3A-C4A-CHB	-4.65	118.22	123.91
18	4	1009	CLA	CHA-C4D-ND	4.65	131.40	124.84

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
18	A	1143	CLA	C3A-C4A-CHB	-4.65	118.22	123.91
18	3	3007	CLA	C4A-NA-C1A	4.64	108.80	106.68
18	B	1214	CLA	OBD-CAD-C3D	-4.64	117.56	128.42
18	A	1148	CLA	CHD-C4C-NC	4.64	131.29	124.24
18	1	1002	CLA	CHD-C4C-NC	4.64	131.29	124.24
18	B	1218	CLA	C1-C2-C3	-4.64	118.59	126.20
18	B	1224	CLA	CHD-C4C-C3C	-4.64	118.01	124.77
18	3	3008	CLA	C2A-C1A-CHA	-4.64	114.72	122.63
18	B	1234	CLA	CHD-C4C-NC	4.63	131.41	124.23
18	A	1131	CLA	CHC-C1C-NC	4.63	131.29	124.31
18	A	1120	CLA	C2A-C1A-CHA	-4.63	114.74	122.63
18	B	1236	CLA	CHD-C4C-C3C	-4.63	118.02	124.77
18	A	9013	CLA	OBD-CAD-C3D	-4.63	117.60	128.42
18	B	9023	CLA	CHB-C4A-NA	4.63	131.08	124.40
18	H	1501	CLA	CHD-C4C-NC	4.63	131.40	124.23
18	F	1139	CLA	CHC-C4B-NB	4.63	130.99	124.05
18	J	1308	CLA	C2A-C1A-CHA	-4.62	114.75	122.63
18	B	1231	CLA	C1D-CHD-C4C	-4.62	116.20	126.02
18	3	3008	CLA	CHD-C4C-NC	4.62	131.26	124.24
18	H	1505	CLA	CHD-C4C-NC	4.62	131.26	124.24
18	B	1215	CLA	CHC-C4B-NB	4.62	130.98	124.05
18	3	3005	CLA	C3B-C2B-C1B	-4.62	101.67	106.81
20	I	6018	BCR	C38-C26-C27	4.61	123.43	113.60
18	B	1236	CLA	CMD-C2D-C3D	-4.61	117.11	127.69
18	L	1503	CLA	C2A-C1A-CHA	-4.61	115.87	123.87
18	A	1111	CLA	CHD-C4C-NC	4.61	131.25	124.24
18	B	1237	CLA	C2B-C1B-NB	4.61	115.10	110.33
18	1	1007	CLA	C3A-C4A-CHB	-4.61	118.27	123.91
18	B	1214	CLA	O2D-CGD-CBD	4.60	119.28	111.23
18	A	1140	CLA	C4B-CHC-C1C	-4.60	115.42	126.25
18	3	2009	CLA	CHC-C1C-NC	4.60	131.09	124.33
18	B	9022	CLA	CHC-C1C-NC	4.60	131.23	124.31
20	B	6017	BCR	C28-C27-C26	-4.60	105.86	114.06
18	A	1127	CLA	CHC-C1C-NC	4.59	131.08	124.33
18	2	2003	CLA	C2A-C1A-CHA	-4.59	114.81	122.63
18	A	1103	CLA	C2B-C1B-NB	4.59	115.08	110.33
18	B	1215	CLA	CHD-C4C-NC	4.58	131.34	124.23
18	A	1109	CLA	C4C-CHD-C1D	-4.58	112.92	125.98
18	F	1306	CLA	C2A-C1A-CHA	-4.58	114.82	122.63
18	G	1233	CLA	C2B-C1B-NB	4.58	115.08	110.33
18	A	1143	CLA	C2A-C1A-CHA	-4.58	114.82	122.63
18	A	1103	CLA	C4B-CHC-C1C	-4.58	115.48	126.25

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
18	B	1216	CLA	CHD-C4C-C3C	-4.58	118.10	124.77
18	A	1116	CLA	CHD-C4C-NC	4.57	131.19	124.24
18	3	3008	CLA	CHC-C1C-NC	4.57	131.05	124.33
18	1	1012	CLA	CHC-C1C-NC	4.57	131.05	124.33
18	A	1151	CLA	C3A-C4A-CHB	-4.57	118.31	123.91
18	B	1203	CLA	C1D-CHD-C4C	-4.57	113.64	125.03
18	3	3004	CLA	CHC-C1C-NC	4.57	131.05	124.33
18	A	9013	CLA	CMD-C2D-C3D	-4.57	117.22	127.69
18	2	2011	CLA	C3A-C4A-CHB	-4.56	118.32	123.91
18	A	1118	CLA	CHC-C1C-NC	4.56	131.04	124.33
18	J	2107	CLA	C4D-C3D-CAD	4.56	113.05	108.11
18	3	3004	CLA	CHD-C4C-NC	4.56	131.16	124.24
18	B	1212	CLA	O2D-CGD-CBD	4.56	119.19	111.23
18	4	4013	CLA	CHC-C1C-NC	4.55	131.02	124.33
18	1	1012	CLA	CHD-C4C-NC	4.55	131.16	124.24
18	1	1001	CLA	C3A-C4A-CHB	-4.55	118.34	123.91
18	A	1110	CLA	C2A-C1A-CHA	-4.55	114.88	122.63
18	4	1304	CLA	CHD-C4C-NC	4.55	131.28	124.23
18	B	1237	CLA	CMD-C2D-C3D	-4.55	117.27	127.69
18	2	2001	CLA	CHC-C1C-NC	4.54	131.01	124.33
18	B	1211	CLA	C2A-C1A-CHA	-4.54	114.89	122.63
18	B	1234	CLA	CHD-C4C-C3C	-4.54	118.15	124.77
18	H	1501	CLA	C3B-C2B-C1B	-4.54	101.82	107.17
18	A	1118	CLA	CHD-C4C-NC	4.53	131.13	124.24
18	B	1222	CLA	CHD-C4C-NC	4.53	131.26	124.23
18	H	1501	CLA	C4A-NA-C1A	4.53	108.75	106.68
18	F	4015	CLA	CHD-C4C-NC	4.53	131.13	124.24
18	A	1110	CLA	C3B-C2B-C1B	-4.53	101.77	106.81
18	B	1225	CLA	CHC-C1C-NC	4.53	131.13	124.31
18	K	1141	CLA	C2A-C1A-CHA	-4.53	114.91	122.63
18	4	4004	CLA	CHD-C4C-NC	4.53	131.12	124.24
18	B	1206	CLA	C2D-C3D-C4D	-4.53	101.85	107.35
18	4	4010	CLA	CHD-C4C-NC	4.53	131.12	124.24
18	A	1107	CLA	C1D-CHD-C4C	-4.52	116.40	126.02
18	A	1128	CLA	CHD-C4C-NC	4.52	131.24	124.23
18	B	1219	CLA	C1D-CHD-C4C	-4.52	116.41	126.02
18	A	1144	CLA	CHC-C1C-NC	4.52	130.97	124.33
18	A	1107	CLA	C4B-CHC-C1C	-4.52	115.62	126.25
18	A	1128	CLA	C4B-CHC-C1C	-4.52	115.62	126.25
18	B	1241	CLA	C3A-C4A-CHB	-4.52	118.38	123.91
18	L	1504	CLA	CHD-C4C-NC	4.52	131.23	124.23
18	B	1214	CLA	CHD-C4C-C3C	-4.52	118.19	124.77

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
18	B	1216	CLA	CHC-C1C-NC	4.52	131.11	124.31
18	A	1131	CLA	OBD-CAD-C3D	-4.52	117.86	128.42
18	3	3001	CLA	C2A-C1A-CHA	-4.51	114.94	122.63
20	A	6011	BCR	C1-C6-C5	-4.51	116.47	122.64
18	1	1001	CLA	C2A-C1A-CHA	-4.51	114.94	122.63
18	A	1116	CLA	C4A-NA-C1A	4.51	108.74	106.68
18	A	1133	CLA	C3B-C2B-C1B	-4.51	101.79	106.81
18	G	1248	CLA	C4C-CHD-C1D	-4.51	113.14	125.98
18	B	1138	CLA	C4B-CHC-C1C	-4.51	115.65	126.25
18	F	1306	CLA	C3A-C4A-CHB	-4.50	118.39	123.91
18	2	2010	CLA	C2A-C1A-CHA	-4.50	114.95	122.63
18	B	9012	CLA	C3B-C2B-C1B	-4.50	101.86	107.17
18	A	1129	CLA	CMD-C2D-C3D	-4.50	117.36	127.69
18	A	1127	CLA	C2A-C1A-CHA	-4.50	114.96	122.63
18	F	1303	CLA	C4A-NA-C1A	4.50	108.73	106.68
18	B	1211	CLA	C1B-NB-C4B	-4.50	103.16	106.31
18	4	4012	CLA	C2A-C1A-CHA	-4.50	114.96	122.63
18	B	1228	CLA	C4A-NA-C1A	4.50	108.73	106.68
18	B	1228	CLA	O2D-CGD-O1D	-4.50	115.10	123.85
18	B	1225	CLA	C4A-NA-C1A	4.50	108.73	106.68
18	4	4002	CLA	C3A-C4A-CHB	-4.49	118.41	123.91
18	A	1144	CLA	C3A-C4A-CHB	-4.49	118.41	123.91
18	B	1223	CLA	C1B-NB-C4B	-4.49	103.16	106.31
18	A	1144	CLA	C2A-C1A-CHA	-4.49	114.97	122.63
18	A	1101	CLA	C3A-C4A-CHB	-4.49	118.41	123.91
18	F	1303	CLA	C3A-C4A-CHB	-4.49	118.41	123.91
18	4	4001	CLA	C3A-C4A-CHB	-4.49	118.41	123.91
18	4	4009	CLA	CHD-C4C-NC	4.49	131.06	124.24
19	A	5001	PQN	O4-C4-C5	-4.49	114.39	121.57
18	1	1014	CLA	C4A-NA-C1A	4.48	108.72	106.68
18	2	2007	CLA	CHC-C1C-NC	4.48	130.92	124.33
18	A	1152	CLA	CHD-C4C-NC	4.48	131.05	124.24
18	A	1118	CLA	C2A-C1A-CHA	-4.48	114.99	122.63
18	H	1505	CLA	CHC-C1C-NC	4.48	130.91	124.33
18	1	1012	CLA	C3A-C4A-CHB	-4.48	118.42	123.91
18	B	1208	CLA	C3B-C4B-NB	-4.48	106.53	110.53
18	3	3002	CLA	CHC-C1C-NC	4.48	130.91	124.33
18	2	2007	CLA	C4A-NA-C1A	4.48	108.72	106.68
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	1238	CLA	CHC-C1C-NC	4.47	131.04	124.31
18	A	1140	CLA	CMB-C2B-C1B	4.47	132.23	125.42

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
18	A	1129	CLA	CHD-C4C-NC	4.47	131.16	124.23
18	B	9010	CLA	CHC-C4B-NB	4.47	130.75	124.05
18	2	2013	CLA	CHD-C4C-NC	4.47	131.03	124.24
18	B	1210	CLA	CHD-C4C-NC	4.46	131.02	124.24
18	K	1150	CLA	CHD-C4C-NC	4.46	131.02	124.24
18	B	1203	CLA	O2D-CGD-CBD	4.46	119.03	111.23
18	3	3010	CLA	CHD-C4C-NC	4.46	131.02	124.24
18	B	1221	CLA	CHD-C4C-NC	4.46	131.15	124.23
18	B	9012	CLA	C4B-CHC-C1C	-4.46	115.76	126.25
18	F	4015	CLA	C2A-C1A-CHA	-4.46	115.03	122.63
18	B	1202	CLA	C4B-CHC-C1C	-4.46	115.77	126.25
18	B	1241	CLA	C2A-C1A-CHA	-4.46	115.03	122.63
18	2	2011	CLA	CHC-C1C-NC	4.45	130.88	124.33
18	B	1201	CLA	CHD-C4C-NC	4.45	131.01	124.24
18	1	1004	CLA	C2A-C1A-CHA	-4.45	115.04	122.63
18	3	3003	CLA	CHD-C4C-NC	4.45	131.01	124.24
18	B	1220	CLA	CHC-C4B-NB	4.45	130.73	124.05
18	B	1223	CLA	C1C-CHC-C4B	-4.45	114.30	126.04
18	B	1201	CLA	C1B-NB-C4B	-4.45	103.19	106.31
18	B	1211	CLA	CHC-C1C-NC	4.45	130.87	124.33
18	4	4008	CLA	C3A-C4A-CHB	-4.45	118.46	123.91
18	B	1227	CLA	CHC-C1C-NC	4.45	131.01	124.31
18	B	1213	CLA	C2A-C1A-CHA	-4.45	115.05	122.63
18	4	4012	CLA	C1B-NB-C4B	-4.45	103.19	106.31
18	A	1142	CLA	CHC-C1C-NC	4.45	130.87	124.33
18	B	1212	CLA	C1-O2A-CGA	4.44	127.41	116.65
18	2	2008	CLA	CHD-C4C-NC	4.44	130.99	124.24
18	B	1211	CLA	C4A-NA-C1A	4.44	108.70	106.68
18	B	1218	CLA	CMD-C2D-C1D	4.44	132.55	124.73
18	3	3007	CLA	CHC-C1C-NC	4.44	130.85	124.33
18	2	2004	CLA	C3A-C4A-CHB	-4.43	118.48	123.91
18	A	1106	CLA	C4B-C3B-C2B	4.43	112.82	107.30
18	2	2010	CLA	CHC-C1C-NC	4.43	130.85	124.33
18	B	1228	CLA	CHB-C4A-NA	4.43	130.80	124.40
18	B	1237	CLA	CHD-C4C-NC	4.43	131.10	124.23
18	4	4013	CLA	C2A-C1A-CHA	-4.43	115.07	122.63
18	B	1217	CLA	CHD-C4C-NC	4.43	131.10	124.23
18	A	1109	CLA	C1C-NC-C4C	4.43	108.70	106.68
18	1	1002	CLA	CHC-C1C-NC	4.43	130.84	124.33
18	I	1204	CLA	CHD-C4C-NC	4.43	131.10	124.23
18	B	1238	CLA	O2D-CGD-O1D	-4.43	115.23	123.85
18	B	1223	CLA	C3A-C4A-CHB	-4.43	118.49	123.91

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
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	A	1137	CLA	CHD-C4C-NC	4.42	131.09	124.23
18	A	1102	CLA	C4A-NA-C1A	4.42	108.70	106.68
18	3	3009	CLA	C3A-C4A-CHB	-4.42	118.50	123.91
18	B	9022	CLA	CHC-C4B-NB	4.42	130.68	124.05
18	B	1221	CLA	C4A-NA-C1A	4.42	108.69	106.68
18	A	1128	CLA	O2D-CGD-O1D	-4.42	115.25	123.85
18	A	1105	CLA	C2A-C1A-CHA	-4.41	115.10	122.63
18	4	4009	CLA	C4A-NA-C1A	4.41	108.69	106.68
18	B	1205	CLA	O2A-CGA-CBA	4.41	125.29	111.83
18	B	1215	CLA	C1D-CHD-C4C	-4.41	116.64	126.02
18	4	1304	CLA	C2B-C1B-NB	4.41	114.90	110.33
20	B	6017	BCR	C1-C6-C5	-4.41	116.61	122.64
18	F	1240	CLA	C2D-C3D-C4D	-4.41	101.99	107.35
18	F	1139	CLA	CED-O2D-CGD	4.40	125.90	115.92
18	A	1111	CLA	C4A-NA-C1A	4.40	108.69	106.68
18	L	1502	CLA	CHD-C4C-C3C	-4.40	118.36	124.77
18	A	1105	CLA	CHD-C4C-NC	4.40	130.93	124.24
18	2	2002	CLA	CHD-C4C-NC	4.40	130.93	124.24
18	2	2011	CLA	CHD-C4C-NC	4.40	130.93	124.24
18	B	1236	CLA	C3B-C2B-C1B	-4.40	101.99	107.17
18	A	1113	CLA	CHC-C4B-NB	4.40	130.64	124.05
18	A	1147	CLA	CHC-C1C-NC	4.40	130.79	124.33
18	B	1238	CLA	C4D-C3D-CAD	4.39	112.88	108.11
18	F	1240	CLA	C3B-C2B-C1B	-4.39	101.92	106.81
18	F	1302	CLA	C2B-C1B-NB	4.39	114.88	110.33
18	B	1227	CLA	O2D-CGD-CBD	4.39	118.90	111.23
18	F	4015	CLA	C3B-C2B-C1B	-4.39	101.93	106.81
18	A	1117	CLA	C2A-C1A-CHA	-4.38	115.16	122.63
18	2	2013	CLA	C2A-C1A-CHA	-4.38	115.16	122.63
18	B	9010	CLA	CHC-C1C-NC	4.38	130.91	124.31
18	F	1305	CLA	CHC-C1C-NC	4.38	130.77	124.33
18	B	1201	CLA	C2A-C1A-CHA	-4.38	115.16	122.63
18	A	1126	CLA	CMD-C2D-C3D	-4.38	117.65	127.69
18	A	1119	CLA	CMD-C2D-C3D	-4.38	117.65	127.69
18	B	1208	CLA	CHC-C1C-NC	4.38	130.91	124.31
18	K	1141	CLA	C3A-C4A-CHB	-4.38	118.55	123.91
18	I	1204	CLA	CHD-C4C-C3C	-4.38	118.39	124.77
18	2	2002	CLA	C2A-C1A-CHA	-4.37	115.18	122.63
18	B	1208	CLA	C4B-CHC-C1C	-4.37	115.97	126.25
18	1	1003	CLA	CHD-C4C-NC	4.37	130.88	124.24

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
18	4	4005	CLA	C4C-CHD-C1D	-4.37	113.54	125.98
18	2	2015	CLA	CHD-C4C-NC	4.37	130.88	124.24
18	B	1226	CLA	CHD-C4C-NC	4.36	130.87	124.24
18	A	1119	CLA	C2B-C1B-NB	4.36	114.85	110.33
18	H	1501	CLA	C2B-C1B-NB	4.36	114.85	110.33
18	3	3012	CLA	C3A-C4A-CHB	-4.36	118.57	123.91
18	G	1248	CLA	C1B-NB-C4B	-4.36	103.25	106.31
18	B	1221	CLA	CMD-C2D-C3D	-4.36	117.69	127.69
18	B	1209	CLA	C3B-C2B-C1B	-4.36	102.03	107.17
18	A	1148	CLA	C2A-C1A-CHA	-4.36	115.20	122.63
18	4	4003	CLA	C3A-C4A-CHB	-4.36	118.57	123.91
20	A	6011	BCR	C31-C1-C6	-4.36	103.41	110.24
18	B	1239	CLA	CHD-C4C-NC	4.36	130.99	124.23
18	1	1014	CLA	CHC-C1C-NC	4.36	130.73	124.33
18	4	4003	CLA	C2A-C1A-CHA	-4.36	115.21	122.63
18	F	1303	CLA	CHD-C4C-NC	4.36	130.86	124.24
18	A	1115	CLA	CHD-C4C-NC	4.35	130.98	124.23
18	2	2012	CLA	CHD-C4C-NC	4.35	130.85	124.24
18	B	1301	CLA	C3A-C4A-CHB	-4.35	118.58	123.91
18	A	1104	CLA	C3B-C2B-C1B	-4.35	101.97	106.81
18	1	1008	CLA	C4C-CHD-C1D	-4.35	113.59	125.98
18	A	1140	CLA	CHC-C4B-NB	4.35	130.57	124.05
18	A	1309	CLA	C2A-C1A-CHA	-4.35	115.22	122.63
18	A	1137	CLA	CMD-C2D-C3D	-4.35	117.72	127.69
20	I	6018	BCR	C11-C12-C13	-4.34	114.45	126.36
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	3005	CLA	CHC-C1C-NC	4.34	130.71	124.33
18	B	1208	CLA	O2D-CGD-CBD	4.34	118.81	111.23
18	4	4009	CLA	C2A-C1A-CHA	-4.34	115.23	122.63
18	2	2004	CLA	CHD-C4C-NC	4.34	130.83	124.24
18	4	4010	CLA	C2A-C1A-CHA	-4.34	115.24	122.63
18	B	1239	CLA	C4B-CHC-C1C	-4.33	116.05	126.25
18	K	1150	CLA	C4A-NA-C1A	4.33	108.66	106.68
18	1	1010	CLA	C4A-NA-C1A	4.33	108.66	106.68
18	A	1131	CLA	CHD-C4C-NC	4.33	130.95	124.23
18	2	2012	CLA	CHC-C1C-NC	4.33	130.70	124.33
18	2	2006	CLA	C3A-C4A-CHB	-4.33	118.61	123.91
18	A	1140	CLA	C3B-C2B-C1B	-4.33	102.06	107.17
18	3	3005	CLA	C2A-C1A-CHA	-4.33	115.25	122.63
18	B	1232	CLA	C4B-CHC-C1C	-4.33	116.07	126.25

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
18	B	1236	CLA	C3B-C4B-NB	-4.33	106.67	110.53
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	2	2008	CLA	C4A-NA-C1A	4.32	108.65	106.68
18	B	1207	CLA	CHD-C4C-NC	4.32	130.93	124.23
18	3	3007	CLA	C1C-CHC-C4B	-4.32	114.65	126.04
18	B	1227	CLA	CHD-C4C-NC	4.32	130.93	124.23
18	B	1235	CLA	CAC-C3C-C2C	-4.32	119.62	127.56
18	B	1217	CLA	C4B-CHC-C1C	-4.32	116.09	126.25
18	A	1134	CLA	CHD-C4C-NC	4.32	130.80	124.24
18	3	3011	CLA	CHD-C4C-NC	4.32	130.80	124.24
18	G	1248	CLA	C2A-C1A-CHA	-4.32	115.27	122.63
18	1	1013	CLA	CHD-C4C-NC	4.32	130.80	124.24
18	J	1308	CLA	CHD-C4C-NC	4.31	130.79	124.24
18	2	2007	CLA	C2A-C1A-CHA	-4.31	115.28	122.63
18	A	1122	CLA	CHD-C4C-C3C	-4.31	118.49	124.77
18	A	1107	CLA	CHC-C1C-NC	4.31	130.81	124.31
18	A	1127	CLA	C4A-NA-C1A	4.31	108.65	106.68
18	B	1221	CLA	C4B-CHC-C1C	-4.31	116.11	126.25
18	4	4007	CLA	C2A-C1A-CHA	-4.31	115.28	122.63
18	2	2013	CLA	C3A-C4A-CHB	-4.31	118.63	123.91
18	B	1202	CLA	C2B-C1B-NB	4.31	114.80	110.33
18	3	3004	CLA	C2A-C1A-CHA	-4.31	115.29	122.63
18	4	4005	CLA	CHC-C1C-NC	4.31	130.66	124.33
18	B	1212	CLA	C2B-C1B-NB	4.31	114.79	110.33
18	2	2008	CLA	C3A-C4A-CHB	-4.30	118.64	123.91
18	4	4004	CLA	C4A-NA-C1A	4.30	108.64	106.68
18	1	1010	CLA	CHD-C4C-NC	4.30	130.78	124.24
18	A	1117	CLA	C3A-C4A-CHB	-4.30	118.64	123.91
18	B	1224	CLA	C2B-C1B-NB	4.30	114.79	110.33
18	3	3009	CLA	CHC-C1C-NC	4.30	130.65	124.33
18	A	9011	CLA	CED-O2D-CGD	4.30	125.67	115.92
18	A	1124	CLA	C3B-C2B-C1B	-4.30	102.03	106.81
18	J	1307	CLA	C2A-C1A-CHA	-4.30	115.31	122.63
18	B	1210	CLA	CHC-C1C-NC	4.30	130.65	124.33
18	1	1005	CLA	C4A-NA-C1A	4.30	108.64	106.68
18	B	9012	CLA	CHD-C4C-NC	4.30	130.89	124.23
18	B	1225	CLA	C4B-CHC-C1C	-4.29	116.15	126.25
18	3	3010	CLA	CHC-C1C-NC	4.29	130.64	124.33
18	1	1004	CLA	C3A-C4A-CHB	-4.29	118.66	123.91
18	3	3010	CLA	C3A-C4A-CHB	-4.29	118.66	123.91
18	3	3009	CLA	C2A-C1A-CHA	-4.29	115.32	122.63

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
18	A	1151	CLA	C4C-CHD-C1D	-4.29	113.76	125.98
18	2	2005	CLA	CHD-C4C-NC	4.29	130.76	124.24
18	3	3013	CLA	CHD-C4C-NC	4.29	130.75	124.24
18	A	1134	CLA	C2A-C1A-CHA	-4.29	115.33	122.63
18	A	1148	CLA	C4C-CHD-C1D	-4.28	113.78	125.98
18	3	3006	CLA	C3A-C4A-CHB	-4.28	118.67	123.91
18	I	1204	CLA	O2A-CGA-CBA	4.28	124.89	111.83
18	B	1206	CLA	C4A-NA-C1A	4.28	108.63	106.68
20	F	6016	BCR	C36-C18-C19	4.28	124.62	118.09
18	L	1125	CLA	CHC-C1C-NC	4.28	130.62	124.33
18	4	4006	CLA	CHC-C1C-NC	4.28	130.62	124.33
18	2	2008	CLA	CHC-C1C-NC	4.28	130.62	124.33
18	F	1240	CLA	CHD-C4C-NC	4.28	130.74	124.24
18	1	1014	CLA	CHD-C4C-NC	4.28	130.74	124.24
18	F	1139	CLA	CHD-C4C-C3C	-4.28	118.54	124.77
18	2	2015	CLA	C4A-NA-C1A	4.28	108.63	106.68
18	3	2009	CLA	C4A-NA-C1A	4.28	108.63	106.68
18	3	2009	CLA	C4C-CHD-C1D	-4.27	113.80	125.98
18	4	4002	CLA	CHC-C1C-NC	4.27	130.61	124.33
18	1	1002	CLA	C2A-C1A-CHA	-4.27	115.34	122.63
18	2	2011	CLA	C2A-C1A-CHA	-4.27	115.35	122.63
18	A	1124	CLA	CHD-C4C-NC	4.27	130.73	124.24
18	B	1237	CLA	CHC-C4B-NB	4.27	130.45	124.05
18	L	1125	CLA	C3A-C4A-CHB	-4.27	118.69	123.91
18	B	1230	CLA	CHD-C4C-NC	4.27	130.72	124.24
18	3	3012	CLA	CHC-C1C-NC	4.26	130.60	124.33
18	A	1126	CLA	CHD-C4C-NC	4.26	130.84	124.23
18	B	1209	CLA	CHD-C4C-NC	4.26	130.84	124.23
18	J	1308	CLA	C4A-NA-C1A	4.26	108.62	106.68
18	2	2005	CLA	CHC-C1C-NC	4.26	130.59	124.33
18	1	1007	CLA	C2A-C1A-CHA	-4.26	115.37	122.63
18	B	1220	CLA	CAA-C2A-C3A	-4.26	101.49	113.00
18	3	3001	CLA	C4A-NA-C1A	4.26	108.62	106.68
18	F	1139	CLA	CHD-C4C-NC	4.26	130.83	124.23
18	B	1221	CLA	CHC-C1C-NC	4.26	130.72	124.31
18	1	1004	CLA	CHD-C4C-NC	4.26	130.71	124.24
18	B	1236	CLA	C2B-C1B-NB	4.26	114.74	110.33
18	1	1008	CLA	CHC-C1C-NC	4.26	130.59	124.33
18	A	1102	CLA	CHD-C4C-NC	4.26	130.71	124.24
18	A	1151	CLA	CHC-C1C-NC	4.26	130.58	124.33
18	A	1115	CLA	C4B-CHC-C1C	-4.25	116.24	126.25
18	A	1107	CLA	CMD-C2D-C3D	-4.25	117.94	127.69

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
18	F	1302	CLA	CHD-C4C-C3C	-4.25	118.57	124.77
18	A	1122	CLA	CHD-C4C-NC	4.25	130.82	124.23
18	B	9022	CLA	CMD-C2D-C3D	-4.25	117.95	127.69
18	1	1007	CLA	CHD-C4C-NC	4.25	130.69	124.24
18	A	1124	CLA	C3D-C4D-CHA	-4.25	115.72	125.20
18	B	1219	CLA	CMD-C2D-C3D	-4.24	117.95	127.69
18	G	1248	CLA	C3A-C4A-CHB	-4.24	118.71	123.91
18	B	1230	CLA	CHC-C1C-NC	4.24	130.57	124.33
18	B	1220	CLA	O2A-CGA-CBA	4.24	124.77	111.83
18	K	1153	CLA	C1C-CHC-C4B	-4.24	114.86	126.04
18	3	3001	CLA	CHD-C4C-NC	4.24	130.69	124.24
18	A	1110	CLA	C2D-C3D-C4D	-4.24	102.20	107.35
18	4	1304	CLA	CHD-C4C-C3C	-4.24	118.59	124.77
18	3	3012	CLA	C4C-CHD-C1D	-4.24	113.90	125.98
18	F	1302	CLA	C4B-CHC-C1C	-4.24	116.28	126.25
18	B	1209	CLA	CMD-C2D-C3D	-4.24	117.97	127.69
18	A	1106	CLA	C4B-CHC-C1C	-4.24	116.29	126.25
18	B	1210	CLA	C2A-C1A-CHA	-4.23	115.41	122.63
18	2	2012	CLA	C2A-C1A-CHA	-4.23	115.41	122.63
18	A	1117	CLA	CHA-C4D-ND	4.23	130.82	124.84
18	4	4013	CLA	C4C-CHD-C1D	-4.23	113.92	125.98
18	A	1151	CLA	C2A-C1A-CHA	-4.23	115.42	122.63
18	B	1212	CLA	C4B-CHC-C1C	-4.23	116.30	126.25
18	1	1011	CLA	C2A-C1A-CHA	-4.23	115.42	122.63
18	A	1107	CLA	O2D-CGD-CBD	4.23	118.62	111.23
18	A	1147	CLA	C4C-CHD-C1D	-4.23	113.93	125.98
18	4	4002	CLA	C4C-CHD-C1D	-4.23	113.93	125.98
18	B	1138	CLA	CHC-C1C-NC	4.23	130.68	124.31
20	I	6018	BCR	C8-C9-C10	4.23	125.66	119.01
18	3	3006	CLA	CHD-C4C-NC	4.23	130.66	124.24
18	B	1212	CLA	C4A-NA-C1A	4.23	108.61	106.68
18	A	1132	CLA	CHA-C4D-ND	4.23	130.81	124.84
18	A	1142	CLA	C4C-CHD-C1D	-4.23	113.94	125.98
18	B	1226	CLA	C3A-C4A-CHB	-4.22	118.74	123.91
18	A	1108	CLA	C2B-C1B-NB	4.22	114.71	110.33
18	B	9023	CLA	CHD-C4C-C3C	-4.22	118.61	124.77
18	A	1132	CLA	C3B-C2B-C1B	-4.22	102.11	106.81
18	B	9012	CLA	CHD-C4C-C3C	-4.22	118.62	124.77
18	A	1123	CLA	CMD-C2D-C3D	-4.22	118.01	127.69
18	A	1127	CLA	C3A-C4A-CHB	-4.22	118.74	123.91
18	B	1231	CLA	CMD-C2D-C3D	-4.22	118.01	127.69
18	4	4007	CLA	C4C-CHD-C1D	-4.22	113.96	125.98

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
18	2	2013	CLA	CHC-C1C-NC	4.22	130.53	124.33
18	4	4002	CLA	C2A-C1A-CHA	-4.22	115.44	122.63
18	B	9010	CLA	C2B-C1B-NB	4.21	114.69	110.33
18	4	4013	CLA	C4A-NA-C1A	4.21	108.60	106.68
18	3	3002	CLA	C4C-CHD-C1D	-4.21	113.98	125.98
19	A	5001	PQN	C11-C3-C4	4.21	123.02	118.58
18	4	4007	CLA	CHC-C1C-NC	4.21	130.51	124.33
18	3	3005	CLA	C4C-CHD-C1D	-4.21	113.99	125.98
18	B	1138	CLA	CHD-C4C-NC	4.21	130.75	124.23
18	A	1144	CLA	C4A-NA-C1A	4.21	108.60	106.68
18	3	3008	CLA	C1C-CHC-C4B	-4.21	114.95	126.04
18	A	1309	CLA	CHD-C4C-NC	4.20	130.63	124.24
18	B	1237	CLA	C4B-CHC-C1C	-4.20	116.36	126.25
18	A	1113	CLA	C2B-C1B-NB	4.20	114.68	110.33
18	3	3010	CLA	C2A-C1A-CHA	-4.20	115.47	122.63
18	4	4009	CLA	CHC-C1C-NC	4.20	130.50	124.33
18	4	4012	CLA	CHC-C1C-NC	4.20	130.50	124.33
18	2	2001	CLA	C4C-CHD-C1D	-4.19	114.04	125.98
18	4	4011	CLA	C1C-CHC-C4B	-4.19	115.00	126.04
18	1	1011	CLA	CHC-C1C-NC	4.19	130.48	124.33
18	3	3013	CLA	C2A-C1A-CHA	-4.19	115.49	122.63
18	B	1205	CLA	CHC-C1C-NC	4.19	130.62	124.31
18	K	1153	CLA	CHC-C4B-NB	4.19	130.13	124.08
18	2	2006	CLA	CHC-C1C-NC	4.18	130.48	124.33
18	A	1101	CLA	C1B-NB-C4B	-4.18	103.38	106.31
18	B	9023	CLA	C3B-C2B-C1B	-4.18	102.24	107.17
18	B	1210	CLA	C1C-CHC-C4B	-4.18	115.02	126.04
18	H	1505	CLA	C2A-C1A-CHA	-4.18	115.50	122.63
18	1	1014	CLA	C1C-CHC-C4B	-4.18	115.02	126.04
18	F	1302	CLA	C1-O2A-CGA	4.18	126.76	116.65
18	A	1143	CLA	CHD-C4C-NC	4.18	130.59	124.24
18	A	1127	CLA	C1B-NB-C4B	-4.18	103.38	106.31
18	4	4011	CLA	C2A-C1A-CHA	-4.18	115.51	122.63
18	B	1213	CLA	C4A-NA-C1A	4.18	108.58	106.68
18	1	1001	CLA	C3B-C2B-C1B	-4.17	102.16	106.81
18	A	9011	CLA	C4B-CHC-C1C	-4.17	116.43	126.25
18	H	1501	CLA	CHD-C4C-C3C	-4.17	118.69	124.77
18	A	1134	CLA	C1B-NB-C4B	-4.17	103.39	106.31
18	A	1116	CLA	C2A-C1A-CHA	-4.17	115.52	122.63
18	4	4011	CLA	CHD-C4C-NC	4.17	130.57	124.24
18	2	2010	CLA	C1C-CHC-C4B	-4.17	115.05	126.04
18	3	3002	CLA	C1C-CHC-C4B	-4.17	115.05	126.04

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
18	4	4001	CLA	CHC-C1C-NC	4.16	130.45	124.33
18	A	1110	CLA	CHD-C4C-NC	4.16	130.57	124.24
18	3	3011	CLA	C2A-C1A-CHA	-4.16	115.54	122.63
18	A	1110	CLA	C1C-CHC-C4B	-4.16	115.07	126.04
18	A	1110	CLA	CHC-C1C-NC	4.16	130.44	124.33
18	3	3002	CLA	C2A-C1A-CHA	-4.16	115.54	122.63
18	F	1306	CLA	CHD-C4C-NC	4.16	130.56	124.24
18	1	1002	CLA	C4C-CHD-C1D	-4.16	114.14	125.98
18	2	2003	CLA	C4C-CHD-C1D	-4.16	114.14	125.98
18	4	4010	CLA	CHC-C1C-NC	4.16	130.44	124.33
18	A	1120	CLA	CHD-C4C-NC	4.15	130.55	124.24
18	B	9022	CLA	C4A-NA-C1A	4.15	108.57	106.68
18	B	1205	CLA	O2A-CGA-O1A	-4.15	113.24	123.63
18	B	1231	CLA	O2D-CGD-O1D	-4.15	115.77	123.85
18	3	3010	CLA	C4A-NA-C1A	4.15	108.57	106.68
18	B	1202	CLA	CMB-C2B-C1B	4.15	131.73	125.42
18	B	1205	CLA	CMD-C2D-C3D	-4.15	118.18	127.69
18	A	1105	CLA	CHC-C1C-NC	4.15	130.42	124.33
18	B	1229	CLA	C4A-NA-C1A	4.14	108.57	106.68
18	L	1125	CLA	C1C-CHC-C4B	-4.14	115.11	126.04
18	F	1302	CLA	CHC-C1C-NC	4.14	130.55	124.31
18	1	1006	CLA	C4A-NA-C1A	4.14	108.57	106.68
18	1	1007	CLA	CHC-C1C-NC	4.14	130.42	124.33
18	4	4006	CLA	CHD-C4C-NC	4.14	130.53	124.24
18	B	1238	CLA	CMD-C2D-C3D	-4.14	118.19	127.69
18	A	1144	CLA	C1C-CHC-C4B	-4.14	115.12	126.04
18	B	1208	CLA	CHD-C4C-NC	4.14	130.65	124.23
18	A	1136	CLA	C4B-CHC-C1C	-4.14	116.51	126.25
18	L	1130	CLA	CHD-C4C-C3C	-4.14	118.74	124.77
18	B	1241	CLA	C1C-CHC-C4B	-4.14	115.13	126.04
18	B	1205	CLA	CHD-C4C-C3C	-4.14	118.74	124.77
18	A	1107	CLA	CHD-C4C-NC	4.14	130.65	124.23
18	L	1504	CLA	CHD-C4C-C3C	-4.14	118.74	124.77
18	B	1222	CLA	CHD-C4C-C3C	-4.14	118.74	124.77
18	1	1011	CLA	C4C-CHD-C1D	-4.14	114.20	125.98
18	1	1011	CLA	C4A-NA-C1A	4.13	108.56	106.68
18	B	1241	CLA	CHC-C4B-NB	4.13	130.05	124.08
18	F	4015	CLA	CHC-C1C-NC	4.13	130.40	124.33
18	K	1150	CLA	CHC-C1C-NC	4.13	130.40	124.33
18	1	1013	CLA	C2A-C1A-CHA	-4.13	115.59	122.63
18	4	4008	CLA	CHD-C4C-NC	4.13	130.51	124.24
18	B	1231	CLA	C4B-CHC-C1C	-4.13	116.54	126.25

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
18	3	2009	CLA	C2A-C1A-CHA	-4.12	115.60	122.63
18	A	1152	CLA	CHC-C1C-NC	4.12	130.39	124.33
18	A	1111	CLA	C4C-CHD-C1D	-4.12	114.23	125.98
18	B	1229	CLA	C2B-C1B-NB	4.12	114.60	110.33
18	3	3006	CLA	CHC-C1C-NC	4.12	130.38	124.33
18	2	2011	CLA	C1C-CHC-C4B	-4.12	115.18	126.04
18	A	1148	CLA	C4A-NA-C1A	4.12	108.56	106.68
18	B	9023	CLA	CHC-C1C-NC	4.12	130.51	124.31
18	B	1207	CLA	CHC-C4B-NB	4.12	130.23	124.05
18	A	1140	CLA	CHD-C4C-NC	4.12	130.62	124.23
18	B	1205	CLA	C4B-CHC-C1C	-4.12	116.56	126.25
18	B	1203	CLA	C3B-C2B-C1B	-4.12	102.32	107.17
20	I	6018	BCR	C30-C25-C24	4.11	126.81	115.65
18	B	1214	CLA	CAA-CBA-CGA	4.11	124.89	113.21
18	A	1102	CLA	CHC-C1C-NC	4.11	130.38	124.33
18	A	9013	CLA	O2D-CGD-CBD	4.11	118.42	111.23
18	1	1006	CLA	CHC-C1C-NC	4.11	130.38	124.33
18	L	1130	CLA	C4B-CHC-C1C	-4.11	116.58	126.25
18	F	4015	CLA	C1C-CHC-C4B	-4.11	115.20	126.04
18	A	1116	CLA	C1B-NB-C4B	-4.11	103.43	106.31
18	F	1139	CLA	OBD-CAD-C3D	-4.11	118.82	128.42
18	B	1214	CLA	CMD-C2D-C3D	-4.11	118.27	127.69
18	3	3009	CLA	C4C-CHD-C1D	-4.11	114.28	125.98
18	A	1123	CLA	C4B-CHC-C1C	-4.10	116.59	126.25
18	B	1215	CLA	OBD-CAD-C3D	-4.10	118.82	128.42
18	3	3015	CLA	C2A-C1A-CHA	-4.10	115.63	122.63
18	F	1305	CLA	C1C-CHC-C4B	-4.10	115.22	126.04
18	4	4001	CLA	CHD-C4C-NC	4.10	130.47	124.24
18	B	1220	CLA	C4B-CHC-C1C	-4.10	116.60	126.25
18	1	1004	CLA	C4C-CHD-C1D	-4.10	114.29	125.98
18	1	1003	CLA	C2A-C1A-CHA	-4.10	115.64	122.63
18	J	1307	CLA	C3B-C2B-C1B	-4.10	102.25	106.81
18	B	1214	CLA	C2B-C1B-NB	4.10	114.58	110.33
18	1	1002	CLA	C1C-CHC-C4B	-4.10	115.23	126.04
18	A	1127	CLA	C1C-CHC-C4B	-4.10	115.23	126.04
18	B	1211	CLA	CHA-C4D-ND	4.10	130.63	124.84
18	F	1139	CLA	C3B-C2B-C1B	-4.10	102.34	107.17
18	B	1138	CLA	C2B-C1B-NB	4.10	114.57	110.33
18	B	1230	CLA	C3A-C4A-CHB	-4.10	118.89	123.91
18	4	1009	CLA	C4C-CHD-C1D	-4.09	114.32	125.98
18	A	1107	CLA	CHD-C4C-C3C	-4.09	118.81	124.77
18	4	4010	CLA	C4C-CHD-C1D	-4.09	114.32	125.98

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
18	A	1152	CLA	C4C-CHD-C1D	-4.09	114.32	125.98
18	B	1232	CLA	CHD-C4C-C3C	-4.09	118.81	124.77
18	A	1136	CLA	C2B-C1B-NB	4.09	114.57	110.33
18	B	1217	CLA	C2B-C1B-NB	4.09	114.57	110.33
18	A	1147	CLA	C2A-C1A-CHA	-4.09	115.66	122.63
18	1	1007	CLA	C4A-NA-C1A	4.09	108.54	106.68
18	A	1146	CLA	C4C-CHD-C1D	-4.08	114.34	125.98
18	4	4004	CLA	CHC-C1C-NC	4.08	130.33	124.33
18	4	4011	CLA	C3B-C2B-C1B	-4.08	102.27	106.81
18	B	1213	CLA	CHD-C4C-NC	4.08	130.44	124.24
18	2	2008	CLA	C1C-CHC-C4B	-4.08	115.28	126.04
18	4	4005	CLA	C1B-NB-C4B	-4.08	103.45	106.31
18	2	2013	CLA	C1C-CHC-C4B	-4.08	115.28	126.04
18	K	1150	CLA	C4C-CHD-C1D	-4.08	114.36	125.98
18	4	4001	CLA	C3B-C2B-C1B	-4.08	102.27	106.81
18	F	1306	CLA	CHC-C1C-NC	4.08	130.32	124.33
20	I	6018	BCR	C38-C26-C25	-4.08	120.04	124.48
18	B	1221	CLA	CHD-C4C-C3C	-4.08	118.83	124.77
18	3	3003	CLA	C4C-CHD-C1D	-4.07	114.37	125.98
18	B	1236	CLA	C4B-CHC-C1C	-4.07	116.67	126.25
18	A	1142	CLA	C2A-C1A-CHA	-4.07	115.69	122.63
18	L	1125	CLA	CHD-C4C-NC	4.07	130.43	124.24
18	2	2001	CLA	C2A-C1A-CHA	-4.07	115.69	122.63
18	B	1207	CLA	C1-O2A-CGA	4.07	126.51	116.65
18	B	1212	CLA	CMD-C2D-C3D	-4.07	118.35	127.69
18	2	2006	CLA	C1C-CHC-C4B	-4.07	115.30	126.04
18	B	1215	CLA	CHC-C1C-C2C	-4.07	115.37	126.95
18	B	1221	CLA	C4D-C3D-CAD	4.07	112.53	108.11
18	A	1105	CLA	C4C-CHD-C1D	-4.07	114.38	125.98
18	B	1223	CLA	C4C-CHD-C1D	-4.07	114.38	125.98
18	1	1006	CLA	C2A-C1A-CHA	-4.07	115.69	122.63
18	B	1202	CLA	C3B-C2B-C1B	-4.07	102.37	107.17
18	L	1130	CLA	O2D-CGD-O1D	-4.07	115.93	123.85
18	A	9011	CLA	CHB-C4A-NA	4.07	130.27	124.40
18	A	1146	CLA	C2A-C1A-CHA	-4.07	115.69	122.63
18	A	1142	CLA	C1C-CHC-C4B	-4.07	115.31	126.04
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	A	1116	CLA	C3B-C2B-C1B	-4.06	102.29	106.81
18	A	1129	CLA	O2A-CGA-CBA	4.06	124.23	111.83
18	B	1215	CLA	CHD-C4C-C3C	-4.06	118.85	124.77

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
18	B	1211	CLA	C1C-CHC-C4B	-4.06	115.33	126.04
18	4	4004	CLA	C4C-CHD-C1D	-4.06	114.41	125.98
18	B	1301	CLA	CHD-C4C-NC	4.06	130.41	124.24
18	4	4003	CLA	CHD-C4C-NC	4.06	130.40	124.24
18	B	1203	CLA	CHC-C1C-NC	4.05	130.42	124.31
18	2	2006	CLA	CHD-C4C-NC	4.05	130.40	124.24
18	A	1118	CLA	C1B-NB-C4B	-4.05	103.47	106.31
18	A	1152	CLA	C1C-CHC-C4B	-4.05	115.35	126.04
18	F	1305	CLA	C2A-C1A-CHA	-4.05	115.72	122.63
18	A	1116	CLA	CHC-C1C-NC	4.05	130.29	124.33
18	B	1222	CLA	CMD-C2D-C3D	-4.05	118.39	127.69
18	1	1010	CLA	C3B-C2B-C1B	-4.05	102.30	106.81
18	A	1146	CLA	CHD-C4C-NC	4.05	130.40	124.24
18	J	1308	CLA	CHC-C1C-NC	4.05	130.28	124.33
18	B	1242	CLA	C2B-C1B-NB	4.05	114.53	110.33
18	B	1210	CLA	C3B-C2B-C1B	-4.05	102.30	106.81
18	3	3003	CLA	CHC-C1C-NC	4.05	130.28	124.33
18	1	1001	CLA	CHD-C4C-NC	4.05	130.39	124.24
18	A	1102	CLA	C3A-C4A-CHB	-4.05	118.95	123.91
18	A	1140	CLA	CHD-C4C-C3C	-4.05	118.87	124.77
18	B	1230	CLA	C1C-CHC-C4B	-4.05	115.37	126.04
18	A	1132	CLA	C4C-CHD-C1D	-4.05	114.45	125.98
18	A	1107	CLA	C1-O2A-CGA	4.05	126.44	116.65
18	2	2002	CLA	C4C-CHD-C1D	-4.04	114.46	125.98
18	A	1120	CLA	C1B-NB-C4B	-4.04	103.47	106.31
18	A	1101	CLA	C1C-CHC-C4B	-4.04	115.38	126.04
18	K	1141	CLA	C4A-NA-C1A	4.04	108.52	106.68
18	4	4007	CLA	C4A-NA-C1A	4.04	108.52	106.68
18	B	1138	CLA	C3B-C2B-C1B	-4.04	102.41	107.17
18	2	2012	CLA	C1C-CHC-C4B	-4.04	115.39	126.04
18	B	9022	CLA	CHD-C4C-NC	4.04	130.49	124.23
18	A	1107	CLA	C4B-C3B-C2B	4.04	112.32	107.30
18	G	1248	CLA	C1C-CHC-C4B	-4.04	115.40	126.04
18	A	1134	CLA	CHC-C1C-NC	4.04	130.26	124.33
18	2	2012	CLA	C1B-NB-C4B	-4.03	103.48	106.31
18	A	1148	CLA	CHC-C1C-NC	4.03	130.26	124.33
18	1	1012	CLA	C1C-CHC-C4B	-4.03	115.41	126.04
18	A	1124	CLA	C1B-NB-C4B	-4.03	103.48	106.31
18	B	1222	CLA	C4B-CHC-C1C	-4.03	116.77	126.25
18	J	2107	CLA	C2B-C1B-NB	4.03	114.50	110.33
18	4	4001	CLA	C1C-CHC-C4B	-4.03	115.42	126.04
18	F	1305	CLA	C4A-NA-C1A	4.03	108.52	106.68

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
18	2	2001	CLA	C1C-CHC-C4B	-4.03	115.42	126.04
18	A	9013	CLA	CHD-C4C-NC	4.03	130.47	124.23
18	A	1103	CLA	CMD-C2D-C3D	-4.03	118.46	127.69
18	B	1234	CLA	CMD-C2D-C3D	-4.03	118.46	127.69
18	2	2005	CLA	C1C-CHC-C4B	-4.02	115.43	126.04
18	2	2006	CLA	C4A-NA-C1A	4.02	108.52	106.68
18	A	1132	CLA	C2A-C1A-CHA	-4.02	115.77	122.63
18	B	1241	CLA	CHA-C4D-ND	4.02	130.53	124.84
18	F	4015	CLA	CHC-C4B-NB	4.02	129.89	124.08
18	1	1007	CLA	C1C-CHC-C4B	-4.02	115.43	126.04
18	1	1010	CLA	CHC-C1C-NC	4.02	130.24	124.33
18	B	1218	CLA	CHC-C1C-NC	4.02	130.37	124.31
18	2	2003	CLA	C1C-CHC-C4B	-4.02	115.44	126.04
18	B	1224	CLA	C4D-C3D-CAD	4.02	112.47	108.11
18	B	1210	CLA	C4A-NA-C1A	4.02	108.51	106.68
18	F	1240	CLA	C4A-NA-C1A	4.02	108.51	106.68
18	A	1136	CLA	CGD-CBD-CAD	4.02	123.85	110.85
18	B	1219	CLA	CHD-C4C-NC	4.02	130.46	124.23
18	4	4005	CLA	C3D-C4D-CHA	-4.02	116.23	125.20
18	3	3012	CLA	C2A-C1A-CHA	-4.01	115.79	122.63
18	B	1237	CLA	CHC-C1C-NC	4.01	130.36	124.31
18	F	1303	CLA	CHC-C1C-NC	4.01	130.23	124.33
18	2	2007	CLA	C1C-CHC-C4B	-4.01	115.46	126.04
18	4	4008	CLA	C4A-NA-C1A	4.01	108.51	106.68
18	B	1226	CLA	CHC-C1C-NC	4.01	130.22	124.33
18	A	1106	CLA	C4A-NA-C1A	4.01	108.51	106.68
18	F	1306	CLA	C1B-NB-C4B	-4.01	103.50	106.31
18	4	4013	CLA	C1C-CHC-C4B	-4.01	115.48	126.04
18	A	1140	CLA	CHC-C1C-NC	4.00	130.34	124.31
18	3	3010	CLA	C1C-CHC-C4B	-4.00	115.48	126.04
18	1	1013	CLA	CHC-C1C-NC	4.00	130.21	124.33
18	A	1133	CLA	C3A-C4A-CHB	-4.00	119.01	123.91
18	3	3005	CLA	C1C-CHC-C4B	-4.00	115.49	126.04
18	A	1103	CLA	CHD-C4C-NC	4.00	130.43	124.23
18	B	1207	CLA	C4B-CHC-C1C	-4.00	116.84	126.25
18	F	4015	CLA	C4C-CHD-C1D	-4.00	114.59	125.98
18	2	2004	CLA	CHC-C1C-NC	3.99	130.20	124.33
18	J	1307	CLA	CHA-C4D-ND	3.99	130.48	124.84
18	1	1011	CLA	C3B-C2B-C1B	-3.99	102.37	106.81
18	K	1153	CLA	CHA-C4D-ND	3.99	130.48	124.84
18	A	1120	CLA	C3B-C2B-C1B	-3.99	102.37	106.81
18	B	1241	CLA	CHD-C4C-NC	3.99	130.30	124.24

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
18	A	1122	CLA	C3B-C4B-NB	-3.99	106.97	110.53
18	B	1201	CLA	CHC-C1C-NC	3.99	130.19	124.33
18	B	1235	CLA	CHC-C1C-NC	3.98	130.31	124.31
18	H	1505	CLA	C1C-CHC-C4B	-3.98	115.53	126.04
18	2	2015	CLA	CHC-C1C-NC	3.98	130.19	124.33
18	B	9022	CLA	CHB-C4A-NA	3.98	130.15	124.40
18	3	3006	CLA	C1C-CHC-C4B	-3.98	115.53	126.04
18	J	1308	CLA	C3B-C2B-C1B	-3.98	102.38	106.81
18	4	1009	CLA	C3A-C4A-CHB	-3.98	119.03	123.91
18	3	3011	CLA	CHC-C1C-NC	3.98	130.18	124.33
18	3	3004	CLA	C1C-CHC-C4B	-3.98	115.54	126.04
18	B	1221	CLA	O2D-CGD-O1D	-3.98	116.10	123.85
18	K	1153	CLA	CHD-C4C-NC	3.98	130.29	124.24
18	B	1235	CLA	C6-C5-C3	-3.98	103.78	113.47
18	1	1010	CLA	C2A-C1A-CHA	-3.98	115.85	122.63
18	L	1125	CLA	C4A-NA-C1A	3.98	108.49	106.68
18	3	3011	CLA	C4C-CHD-C1D	-3.98	114.65	125.98
18	1	1013	CLA	C4C-CHD-C1D	-3.98	114.66	125.98
18	B	1215	CLA	CHB-C1B-NB	-3.97	118.09	124.05
18	4	4011	CLA	CHC-C1C-NC	3.97	130.17	124.33
18	B	1213	CLA	C4C-CHD-C1D	-3.97	114.66	125.98
18	4	4011	CLA	CHC-C4B-NB	3.97	129.82	124.08
18	A	1120	CLA	C2D-C3D-C4D	-3.97	102.52	107.35
18	2	2003	CLA	C1B-NB-C4B	-3.97	103.53	106.31
18	H	1501	CLA	C4B-CHC-C1C	-3.97	116.91	126.25
18	A	1113	CLA	CHC-C1C-NC	3.97	130.29	124.31
18	2	2002	CLA	C4A-NA-C1A	3.97	108.49	106.68
18	B	1211	CLA	C3D-C4D-CHA	-3.97	116.34	125.20
18	4	4006	CLA	C1C-CHC-C4B	-3.97	115.57	126.04
18	A	1110	CLA	C4C-CHD-C1D	-3.97	114.68	125.98
18	3	3013	CLA	C3B-C2B-C1B	-3.97	102.39	106.81
18	B	1236	CLA	O2D-CGD-O1D	-3.96	116.13	123.85
18	B	1241	CLA	C3B-C2B-C1B	-3.96	102.40	106.81
18	2	2004	CLA	C4C-CHD-C1D	-3.96	114.69	125.98
18	A	1117	CLA	CHD-C4C-NC	3.96	130.26	124.24
18	A	1152	CLA	C2A-C1A-CHA	-3.96	115.88	122.63
18	4	1009	CLA	C3D-C4D-CHA	-3.96	116.35	125.20
18	3	3013	CLA	C4C-CHD-C1D	-3.96	114.69	125.98
18	B	1228	CLA	O2A-CGA-CBA	3.96	123.91	111.83
18	A	1110	CLA	CHA-C4D-ND	3.96	130.44	124.84
18	B	1220	CLA	C1-C2-C3	-3.96	119.71	126.20
18	2	2010	CLA	C4C-CHD-C1D	-3.96	114.70	125.98

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
18	A	1113	CLA	CED-O2D-CGD	3.96	124.90	115.92
18	B	1203	CLA	CAC-C3C-C4C	3.96	131.22	125.03
18	F	1240	CLA	C3D-C4D-CHA	-3.96	116.36	125.20
18	1	1014	CLA	C1B-NB-C4B	-3.96	103.53	106.31
18	1	1010	CLA	C1B-NB-C4B	-3.96	103.54	106.31
18	B	1209	CLA	C4B-CHC-C1C	-3.96	116.94	126.25
18	A	1136	CLA	C3B-C2B-C1B	-3.96	102.51	107.17
18	A	1105	CLA	C2D-C3D-C4D	-3.96	102.54	107.35
18	B	1221	CLA	C1-O2A-CGA	3.95	126.22	116.65
20	F	6016	BCR	C33-C5-C4	3.95	122.02	113.60
18	2	2007	CLA	C4C-CHD-C1D	-3.95	114.73	125.98
18	F	1240	CLA	CHC-C1C-NC	3.95	130.13	124.33
18	4	4008	CLA	C4C-CHD-C1D	-3.95	114.73	125.98
18	H	1501	CLA	O2D-CGD-CBD	3.95	118.13	111.23
18	4	4012	CLA	C4C-CHD-C1D	-3.95	114.74	125.98
18	B	1223	CLA	C2A-C1A-CHA	-3.94	115.91	122.63
18	A	1117	CLA	C4C-CHD-C1D	-3.94	114.75	125.98
18	A	1143	CLA	C4A-NA-C1A	3.94	108.48	106.68
18	B	1216	CLA	C4A-NA-C1A	3.94	108.48	106.68
18	1	1008	CLA	C2A-C1A-CHA	-3.94	115.91	122.63
18	1	1003	CLA	C4C-CHD-C1D	-3.94	114.75	125.98
18	B	9022	CLA	O2A-CGA-O1A	-3.94	113.77	123.63
18	4	4010	CLA	C4A-NA-C1A	3.94	108.48	106.68
18	3	3015	CLA	CHD-C4C-NC	3.94	130.23	124.24
18	A	1108	CLA	C4B-CHC-C1C	-3.94	116.99	126.25
18	A	1107	CLA	C6-C5-C3	-3.94	103.88	113.47
18	2	2011	CLA	C3B-C2B-C1B	-3.94	102.43	106.81
18	B	1228	CLA	CHD-C4C-C3C	-3.93	119.04	124.77
18	A	1143	CLA	CHC-C1C-NC	3.93	130.11	124.33
18	4	4002	CLA	C2D-C3D-C4D	-3.93	102.57	107.35
18	A	9011	CLA	CMB-C2B-C1B	3.93	131.40	125.42
18	3	3003	CLA	C2A-C1A-CHA	-3.93	115.93	122.63
18	F	4015	CLA	C4A-NA-C1A	3.93	108.47	106.68
18	1	1007	CLA	C1B-NB-C4B	-3.93	103.56	106.31
18	4	4006	CLA	C1B-NB-C4B	-3.93	103.56	106.31
18	B	1241	CLA	C4C-CHD-C1D	-3.93	114.79	125.98
18	F	1303	CLA	C3B-C2B-C1B	-3.93	102.44	106.81
18	2	2008	CLA	C4C-CHD-C1D	-3.93	114.79	125.98
18	H	1505	CLA	C4C-CHD-C1D	-3.93	114.80	125.98
18	A	1148	CLA	C3B-C2B-C1B	-3.93	102.44	106.81
18	F	1240	CLA	C4C-CHD-C1D	-3.93	114.80	125.98
18	A	1133	CLA	CHD-C4C-NC	3.93	130.21	124.24

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
18	B	1217	CLA	CHC-C1C-NC	3.93	130.22	124.31
18	B	1203	CLA	C4B-CHC-C1C	-3.93	117.02	126.25
18	2	2004	CLA	C2D-C3D-C4D	-3.92	102.58	107.35
18	I	1204	CLA	C4B-CHC-C1C	-3.92	117.02	126.25
18	2	2015	CLA	C2A-C1A-CHA	-3.92	115.94	122.63
18	2	2012	CLA	C4A-NA-C1A	3.92	108.47	106.68
18	A	1122	CLA	C4B-C3B-C2B	3.92	112.18	107.30
18	1	1013	CLA	C1B-NB-C4B	-3.92	103.56	106.31
18	A	1106	CLA	C2B-C1B-NB	3.92	114.39	110.33
18	3	3009	CLA	C4A-NA-C1A	3.92	108.47	106.68
18	B	1210	CLA	C1B-NB-C4B	-3.92	103.56	106.31
18	A	1107	CLA	O2D-CGD-O1D	-3.92	116.22	123.85
18	4	4003	CLA	C4C-CHD-C1D	-3.92	114.82	125.98
18	B	1211	CLA	C4C-CHD-C1D	-3.91	114.83	125.98
18	F	1303	CLA	C4C-CHD-C1D	-3.91	114.83	125.98
18	F	1302	CLA	CMD-C2D-C3D	-3.91	118.71	127.69
18	1	1001	CLA	C1C-CHC-C4B	-3.91	115.72	126.04
18	3	2009	CLA	C1C-CHC-C4B	-3.91	115.72	126.04
18	A	1140	CLA	C4A-NA-C1A	3.91	108.46	106.68
18	3	3009	CLA	C1B-NB-C4B	-3.91	103.57	106.31
18	A	1133	CLA	C4C-CHD-C1D	-3.91	114.84	125.98
18	A	1135	CLA	C4B-CHC-C1C	-3.91	117.05	126.25
18	A	1111	CLA	CHC-C1C-NC	3.91	130.07	124.33
18	B	9022	CLA	CMB-C2B-C1B	3.91	131.37	125.42
18	A	1106	CLA	CHD-C4C-NC	3.91	130.29	124.23
18	2	2002	CLA	C1B-NB-C4B	-3.91	103.57	106.31
18	A	1124	CLA	C3A-C4A-CHB	-3.91	119.13	123.91
18	4	4012	CLA	C3B-C2B-C1B	-3.91	102.46	106.81
18	1	1003	CLA	CHC-C1C-NC	3.91	130.07	124.33
18	L	1130	CLA	CHC-C1C-NC	3.91	130.19	124.31
18	A	1136	CLA	CHC-C4B-NB	3.90	129.91	124.05
18	I	1204	CLA	CHC-C1C-NC	3.90	130.19	124.31
18	A	1309	CLA	C1C-CHC-C4B	-3.90	115.75	126.04
18	B	1232	CLA	CHC-C1C-NC	3.90	130.19	124.31
18	B	1227	CLA	CMD-C2D-C3D	-3.90	118.74	127.69
18	A	1104	CLA	CHD-C4C-NC	3.90	130.17	124.24
18	3	3006	CLA	CHA-C4D-ND	3.90	130.35	124.84
18	A	1102	CLA	C1C-CHC-C4B	-3.90	115.75	126.04
18	4	4003	CLA	C1C-CHC-C4B	-3.90	115.76	126.04
18	1	1006	CLA	C3B-C2B-C1B	-3.90	102.47	106.81
18	A	1108	CLA	C1-O2A-CGA	3.90	126.09	116.65
18	2	2011	CLA	C4C-CHD-C1D	-3.90	114.87	125.98

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
18	4	4009	CLA	C3B-C2B-C1B	-3.90	102.47	106.81
18	A	1105	CLA	C1C-CHC-C4B	-3.90	115.76	126.04
18	J	1308	CLA	C1C-CHC-C4B	-3.90	115.76	126.04
18	B	1209	CLA	CHC-C1C-NC	3.90	130.18	124.31
18	B	1226	CLA	C4C-CHD-C1D	-3.90	114.88	125.98
18	3	3007	CLA	C3B-C2B-C1B	-3.90	102.47	106.81
18	A	1101	CLA	C4C-CHD-C1D	-3.89	114.88	125.98
18	3	3001	CLA	CHC-C1C-NC	3.89	130.06	124.33
18	B	1228	CLA	O1D-CGD-CBD	-3.89	116.84	124.52
18	A	9011	CLA	CMD-C2D-C3D	-3.89	118.76	127.69
18	B	1201	CLA	C4C-CHD-C1D	-3.89	114.89	125.98
18	F	1306	CLA	C1C-CHC-C4B	-3.89	115.78	126.04
18	B	1301	CLA	C1B-NB-C4B	-3.89	103.58	106.31
18	G	1233	CLA	C4B-CHC-C1C	-3.89	117.10	126.25
18	L	1504	CLA	CMD-C2D-C3D	-3.89	118.77	127.69
18	A	1107	CLA	C2A-C1A-CHA	-3.89	117.12	123.87
18	A	1151	CLA	C4A-NA-C1A	3.89	108.45	106.68
18	A	1123	CLA	C3B-C2B-C1B	-3.89	102.59	107.17
18	2	2004	CLA	C3D-C4D-CHA	-3.89	116.52	125.20
18	K	1141	CLA	CHD-C4C-NC	3.89	130.14	124.24
18	2	2013	CLA	C4A-NA-C1A	3.88	108.45	106.68
18	A	1116	CLA	C4C-CHD-C1D	-3.88	114.92	125.98
18	2	2015	CLA	C4C-CHD-C1D	-3.88	114.92	125.98
18	2	2004	CLA	C1C-CHC-C4B	-3.88	115.80	126.04
20	B	6017	BCR	C16-C17-C18	-3.88	121.83	127.28
18	A	1152	CLA	CHC-C4B-NB	3.88	129.69	124.08
18	4	4002	CLA	C1C-CHC-C4B	-3.88	115.81	126.04
18	1	1006	CLA	C1B-NB-C4B	-3.88	103.59	106.31
18	1	1006	CLA	C4C-CHD-C1D	-3.88	114.94	125.98
18	A	1110	CLA	C3D-C4D-CHA	-3.87	116.55	125.20
18	A	1118	CLA	C4C-CHD-C1D	-3.87	114.94	125.98
18	B	9022	CLA	CHD-C4C-C3C	-3.87	119.12	124.77
18	B	1219	CLA	CHC-C4B-NB	3.87	129.86	124.05
18	B	1205	CLA	C2B-C1B-NB	3.87	114.34	110.33
18	A	1137	CLA	C4B-CHC-C1C	-3.87	117.14	126.25
18	1	1008	CLA	C4A-NA-C1A	3.87	108.44	106.68
18	4	4010	CLA	C3B-C2B-C1B	-3.87	102.50	106.81
18	A	1309	CLA	CHC-C1C-NC	3.87	130.02	124.33
18	A	1110	CLA	CHC-C4B-NB	3.87	129.67	124.08
18	3	3006	CLA	C4C-CHD-C1D	-3.87	114.96	125.98
18	A	1106	CLA	CHD-C4C-C3C	-3.87	119.14	124.77
20	F	6016	BCR	C37-C22-C21	3.87	129.08	122.82

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
18	2	2013	CLA	C4C-CHD-C1D	-3.87	114.96	125.98
18	A	1309	CLA	C4C-CHD-C1D	-3.87	114.96	125.98
18	B	1202	CLA	C5-C3-C4	3.87	123.49	114.59
18	B	1203	CLA	CHD-C4C-NC	3.86	130.22	124.23
18	A	1103	CLA	CHC-C1C-C2C	-3.86	115.97	126.95
18	3	3010	CLA	C4C-CHD-C1D	-3.86	114.97	125.98
18	1	1003	CLA	C1C-CHC-C4B	-3.86	115.85	126.04
18	A	1129	CLA	C2B-C1B-NB	3.86	114.33	110.33
18	K	1153	CLA	CHC-C1C-NC	3.86	130.01	124.33
18	1	1008	CLA	C1C-CHC-C4B	-3.86	115.85	126.04
18	3	3012	CLA	C1C-CHC-C4B	-3.86	115.85	126.04
18	A	1120	CLA	C4C-CHD-C1D	-3.86	114.98	125.98
18	3	3013	CLA	CHC-C1C-NC	3.86	130.00	124.33
18	4	4011	CLA	C4A-NA-C1A	3.86	108.44	106.68
18	B	1231	CLA	CHD-C4C-NC	3.86	130.21	124.23
18	3	3003	CLA	C1C-CHC-C4B	-3.86	115.87	126.04
18	B	1226	CLA	C4A-NA-C1A	3.86	108.44	106.68
18	4	4009	CLA	C4C-CHD-C1D	-3.86	114.99	125.98
18	1	1004	CLA	CHA-C4D-ND	3.86	130.29	124.84
18	F	1305	CLA	C4C-CHD-C1D	-3.86	115.00	125.98
18	B	1209	CLA	CHD-C4C-C3C	-3.85	119.15	124.77
18	3	3001	CLA	C4C-CHD-C1D	-3.85	115.00	125.98
18	A	1115	CLA	C3B-C2B-C1B	-3.85	102.63	107.17
18	B	1231	CLA	C2B-C1B-NB	3.85	114.32	110.33
18	4	4007	CLA	C1B-NB-C4B	-3.85	103.61	106.31
18	2	2003	CLA	C2D-C3D-C4D	-3.85	102.67	107.35
18	2	2007	CLA	C3B-C2B-C1B	-3.85	102.53	106.81
18	J	1308	CLA	C4C-CHD-C1D	-3.85	115.01	125.98
18	A	1134	CLA	C4C-CHD-C1D	-3.85	115.01	125.98
18	3	3004	CLA	C3B-C2B-C1B	-3.85	102.53	106.81
18	A	1117	CLA	C3B-C2B-C1B	-3.85	102.53	106.81
18	3	3015	CLA	C3B-C2B-C1B	-3.85	102.53	106.81
18	A	1131	CLA	C2B-C1B-NB	3.85	114.32	110.33
18	3	3015	CLA	C4C-CHD-C1D	-3.85	115.02	125.98
18	A	1144	CLA	C4C-CHD-C1D	-3.85	115.02	125.98
18	3	3001	CLA	C3B-C2B-C1B	-3.85	102.53	106.81
18	H	1501	CLA	CHC-C1C-NC	3.85	130.10	124.31
18	3	3001	CLA	C1B-NB-C4B	-3.85	103.61	106.31
18	A	1143	CLA	C4C-CHD-C1D	-3.84	115.03	125.98
18	4	4009	CLA	C1C-CHC-C4B	-3.84	115.91	126.04
18	B	1241	CLA	CHC-C1C-NC	3.84	129.98	124.33
18	3	3007	CLA	CHC-C4B-NB	3.84	129.63	124.08

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
18	B	1222	CLA	C2B-C1B-NB	3.84	114.31	110.33
18	2	2012	CLA	C3B-C2B-C1B	-3.84	102.54	106.81
18	B	9023	CLA	CHC-C4B-NB	3.84	129.81	124.05
18	B	1212	CLA	CHC-C1C-NC	3.84	130.09	124.31
18	B	1219	CLA	CHD-C4C-C3C	-3.84	119.18	124.77
18	4	4008	CLA	C3D-C4D-CHA	-3.84	116.63	125.20
18	B	1205	CLA	C3B-C2B-C1B	-3.83	102.65	107.17
18	A	1118	CLA	C1C-CHC-C4B	-3.83	115.93	126.04
18	2	2005	CLA	C1B-NB-C4B	-3.83	103.62	106.31
18	B	9010	CLA	CHB-C4A-NA	3.83	129.93	124.40
18	3	3007	CLA	C4C-CHD-C1D	-3.83	115.07	125.98
18	A	1120	CLA	CHC-C1C-NC	3.83	129.96	124.33
18	J	1307	CLA	C4C-CHD-C1D	-3.83	115.07	125.98
18	3	3005	CLA	C4A-NA-C1A	3.83	108.42	106.68
18	4	4003	CLA	CHC-C1C-NC	3.83	129.96	124.33
18	F	1240	CLA	C1B-NB-C4B	-3.83	103.63	106.31
18	2	2001	CLA	C1B-NB-C4B	-3.82	103.63	106.31
18	B	1201	CLA	C2D-C3D-C4D	-3.82	102.71	107.35
18	B	1218	CLA	C2B-C1B-NB	3.82	114.29	110.33
18	2	2006	CLA	C2D-C3D-C4D	-3.82	102.71	107.35
18	1	1005	CLA	C3B-C2B-C1B	-3.82	102.56	106.81
18	B	1219	CLA	C2B-C1B-NB	3.82	114.29	110.33
18	4	4008	CLA	CHA-C4D-ND	3.82	130.24	124.84
18	1	1003	CLA	C3B-C2B-C1B	-3.82	102.56	106.81
18	3	3009	CLA	C3B-C2B-C1B	-3.82	102.56	106.81
18	4	4003	CLA	CHA-C4D-ND	3.82	130.23	124.84
18	A	1129	CLA	CHD-C4C-C3C	-3.82	119.21	124.77
18	B	1224	CLA	OBD-CAD-C3D	-3.81	119.50	128.42
18	H	1505	CLA	C3B-C2B-C1B	-3.81	102.56	106.81
18	L	1130	CLA	CMD-C2D-C3D	-3.81	118.94	127.69
18	B	1242	CLA	C4A-NA-C1A	3.81	108.42	106.68
18	A	1147	CLA	C1B-NB-C4B	-3.81	103.64	106.31
18	B	1138	CLA	O2D-CGD-CBD	3.81	117.89	111.23
18	A	1127	CLA	C4C-CHD-C1D	-3.81	115.12	125.98
18	3	3008	CLA	C4C-CHD-C1D	-3.81	115.12	125.98
18	B	1216	CLA	C1-O2A-CGA	3.81	125.87	116.65
18	A	1103	CLA	CHB-C4A-NA	3.81	129.90	124.40
18	3	3015	CLA	C1C-CHC-C4B	-3.81	116.00	126.04
18	B	1230	CLA	C4C-CHD-C1D	-3.81	115.13	125.98
18	1	1005	CLA	C1C-CHC-C4B	-3.81	116.00	126.04
18	2	2007	CLA	C1B-NB-C4B	-3.81	103.64	106.31
18	2	2005	CLA	C2A-C1A-CHA	-3.81	116.14	122.63

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
18	3	3011	CLA	C1C-CHC-C4B	-3.81	116.00	126.04
18	F	1139	CLA	CHC-C1C-NC	3.80	130.04	124.31
18	B	1208	CLA	C1-C2-C3	3.80	132.43	126.20
18	F	1306	CLA	C4A-NA-C1A	3.80	108.41	106.68
18	J	2107	CLA	CAC-C3C-C4C	3.80	129.74	124.79
18	B	1138	CLA	CMD-C2D-C3D	-3.80	118.97	127.69
18	B	1242	CLA	CHC-C1C-NC	3.80	130.04	124.31
18	1	1012	CLA	C4C-CHD-C1D	-3.80	115.15	125.98
18	1	1010	CLA	C1C-CHC-C4B	-3.80	116.02	126.04
18	F	1303	CLA	C1C-CHC-C4B	-3.80	116.03	126.04
18	4	4002	CLA	C4A-NA-C1A	3.80	108.41	106.68
18	3	3015	CLA	CHA-C4D-ND	3.80	130.20	124.84
18	B	1228	CLA	CHC-C1C-NC	3.79	130.03	124.31
18	L	1502	CLA	C4B-CHC-C1C	-3.79	117.33	126.25
18	1	1004	CLA	CHC-C1C-NC	3.79	129.91	124.33
18	J	1308	CLA	C2D-C3D-C4D	-3.79	102.74	107.35
18	B	9012	CLA	CHB-C4A-NA	3.79	129.87	124.40
18	A	9011	CLA	O2A-CGA-CBA	3.79	123.40	111.83
18	1	1011	CLA	C1C-CHC-C4B	-3.79	116.05	126.04
18	1	1001	CLA	CHC-C4B-NB	3.79	129.55	124.08
18	A	1104	CLA	CHC-C4B-NB	3.78	129.55	124.08
18	3	3004	CLA	C1B-NB-C4B	-3.78	103.66	106.31
18	B	1238	CLA	C3B-C2B-C1B	-3.78	102.71	107.17
18	3	3013	CLA	C1C-CHC-C4B	-3.78	116.06	126.04
18	B	1206	CLA	C4C-CHD-C1D	-3.78	115.21	125.98
18	A	1108	CLA	CMD-C2D-C3D	-3.78	119.02	127.69
18	2	2015	CLA	C1C-CHC-C4B	-3.78	116.07	126.04
18	1	1005	CLA	CHD-C4C-NC	3.78	129.98	124.24
20	F	6016	BCR	C15-C16-C17	-3.78	115.78	123.52
18	4	4006	CLA	C4A-NA-C1A	3.78	108.40	106.68
18	A	1146	CLA	CHC-C1C-NC	3.78	129.88	124.33
18	I	1204	CLA	C2B-C1B-NB	3.78	114.24	110.33
18	B	1215	CLA	CMD-C2D-C3D	-3.78	119.03	127.69
18	3	3015	CLA	CHC-C1C-NC	3.78	129.88	124.33
18	3	3002	CLA	CHC-C4B-NB	3.78	129.54	124.08
18	B	1211	CLA	C3A-C4A-CHB	-3.77	119.29	123.91
18	A	1124	CLA	C4A-NA-C1A	3.77	108.40	106.68
18	B	1237	CLA	C1-C2-C3	-3.77	120.01	126.20
18	1	1011	CLA	C1B-NB-C4B	-3.77	103.67	106.31
18	4	4006	CLA	C3B-C2B-C1B	-3.77	102.61	106.81
18	A	1135	CLA	CHC-C1C-NC	3.77	129.99	124.31
18	A	1120	CLA	C1C-CHC-C4B	-3.77	116.10	126.04

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
18	4	1009	CLA	CHD-C4C-NC	3.76	129.96	124.24
18	A	1108	CLA	C3B-C2B-C1B	-3.76	102.73	107.17
18	B	1209	CLA	O2A-CGA-CBA	3.76	123.31	111.83
20	L	6020	BCR	C40-C30-C25	-3.76	104.34	110.24
18	A	1309	CLA	C4A-NA-C1A	3.76	108.39	106.68
18	B	1212	CLA	C3B-C2B-C1B	-3.76	102.74	107.17
18	A	1128	CLA	CHD-C4C-C3C	-3.76	119.29	124.77
18	A	1113	CLA	CBC-CAC-C3C	-3.76	102.22	112.42
18	A	1140	CLA	CMD-C2D-C3D	-3.76	119.07	127.69
18	A	1131	CLA	CHB-C4A-NA	3.75	129.82	124.40
18	1	1012	CLA	C1B-NB-C4B	-3.75	103.68	106.31
18	J	1307	CLA	C3D-C4D-CHA	-3.75	116.82	125.20
18	B	1214	CLA	C4B-CHC-C1C	-3.75	117.43	126.25
18	A	9011	CLA	C2B-C1B-NB	3.75	114.22	110.33
18	B	1235	CLA	C3B-C2B-C1B	-3.75	102.75	107.17
18	3	3008	CLA	C1B-NB-C4B	-3.75	103.68	106.31
18	1	1005	CLA	CHA-C4D-ND	3.75	130.14	124.84
18	2	2004	CLA	CHA-C4D-ND	3.75	130.14	124.84
18	2	2010	CLA	C1B-NB-C4B	-3.75	103.68	106.31
18	A	1146	CLA	CHA-C4D-ND	3.75	130.14	124.84
18	3	3009	CLA	C1C-CHC-C4B	-3.75	116.16	126.04
18	4	4001	CLA	C4C-CHD-C1D	-3.75	115.30	125.98
18	A	1134	CLA	C1C-CHC-C4B	-3.75	116.16	126.04
18	4	1304	CLA	C4B-CHC-C1C	-3.75	117.44	126.25
18	A	1152	CLA	C3B-C2B-C1B	-3.74	102.64	106.81
18	3	3006	CLA	C3D-C4D-CHA	-3.74	116.84	125.20
18	A	1111	CLA	C1B-NB-C4B	-3.74	103.69	106.31
18	2	2008	CLA	C2D-C3D-C4D	-3.74	102.80	107.35
18	1	1005	CLA	C3D-C4D-CHA	-3.74	116.85	125.20
18	2	2005	CLA	C4C-CHD-C1D	-3.74	115.33	125.98
18	A	1122	CLA	C4-C3-C5	3.74	121.72	115.23
18	2	2002	CLA	CHC-C1C-NC	3.74	129.82	124.33
18	B	1301	CLA	C1C-CHC-C4B	-3.74	116.18	126.04
18	K	1141	CLA	CHC-C1C-NC	3.74	129.82	124.33
18	2	2003	CLA	C3B-C2B-C1B	-3.74	102.65	106.81
18	1	1012	CLA	C3B-C2B-C1B	-3.73	102.66	106.81
18	3	3001	CLA	C2D-C3D-C4D	-3.73	102.82	107.35
18	B	1231	CLA	CHC-C1C-NC	3.73	129.93	124.31
18	B	1234	CLA	C4B-CHC-C1C	-3.73	117.48	126.25
18	B	1215	CLA	C1D-ND-C4D	-3.73	103.70	106.31
18	B	1301	CLA	CHC-C1C-NC	3.73	129.81	124.33
18	B	9022	CLA	C1-O2A-CGA	3.73	125.67	116.65

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
18	A	1143	CLA	C1C-CHC-C4B	-3.73	116.21	126.04
18	A	1104	CLA	C4C-CHD-C1D	-3.73	115.36	125.98
18	B	1220	CLA	CMD-C2D-C3D	-3.73	119.15	127.69
18	L	1503	CLA	O2A-CGA-CBA	3.72	123.19	111.83
18	B	1206	CLA	C3D-C4D-CHA	-3.72	116.88	125.20
18	B	1203	CLA	CED-O2D-CGD	3.72	124.36	115.92
18	B	1226	CLA	C1C-CHC-C4B	-3.72	116.22	126.04
18	F	1306	CLA	C4C-CHD-C1D	-3.72	115.38	125.98
18	K	1150	CLA	C1B-NB-C4B	-3.72	103.70	106.31
18	B	1301	CLA	C3B-C2B-C1B	-3.72	102.67	106.81
18	3	3006	CLA	C4A-NA-C1A	3.72	108.38	106.68
18	4	1304	CLA	CHC-C1C-NC	3.72	129.91	124.31
18	2	2008	CLA	CHA-C4D-ND	3.72	130.09	124.84
18	B	1213	CLA	C1C-CHC-C4B	-3.72	116.24	126.04
18	4	4003	CLA	C3D-C4D-CHA	-3.71	116.91	125.20
18	A	1132	CLA	C3D-C4D-CHA	-3.71	116.91	125.20
18	4	4001	CLA	C3D-C4D-CHA	-3.71	116.91	125.20
18	B	1224	CLA	C4B-CHC-C1C	-3.71	117.52	126.25
18	A	1309	CLA	CHC-C4B-NB	3.71	129.44	124.08
18	L	1504	CLA	CHC-C1C-NC	3.71	129.90	124.31
18	1	1004	CLA	C3D-C4D-CHA	-3.71	116.92	125.20
18	A	1148	CLA	C1B-NB-C4B	-3.71	103.71	106.31
18	F	1305	CLA	C3B-C2B-C1B	-3.71	102.69	106.81
18	4	1304	CLA	CMD-C2D-C3D	-3.71	119.19	127.69
18	B	1224	CLA	CHC-C1C-NC	3.71	129.89	124.31
18	2	2008	CLA	C3D-C4D-CHA	-3.70	116.93	125.20
18	A	1102	CLA	C4C-CHD-C1D	-3.70	115.43	125.98
18	4	4010	CLA	C1B-NB-C4B	-3.70	103.71	106.31
18	4	4009	CLA	C1B-NB-C4B	-3.70	103.72	106.31
18	K	1153	CLA	C4C-CHD-C1D	-3.70	115.44	125.98
18	B	1241	CLA	C3D-C4D-CHA	-3.70	116.94	125.20
18	A	1144	CLA	C2D-C3D-C4D	-3.70	102.85	107.35
18	A	1102	CLA	C1B-NB-C4B	-3.70	103.72	106.31
18	2	2006	CLA	C3D-C4D-CHA	-3.70	116.94	125.20
18	4	4003	CLA	CHC-C4B-NB	3.69	129.42	124.08
18	1	1013	CLA	C1C-CHC-C4B	-3.69	116.30	126.04
18	2	2015	CLA	C3B-C2B-C1B	-3.69	102.70	106.81
18	1	1006	CLA	C1C-CHC-C4B	-3.69	116.30	126.04
18	B	1235	CLA	C4B-CHC-C1C	-3.69	117.56	126.25
18	A	1147	CLA	C1C-CHC-C4B	-3.69	116.30	126.04
18	B	1238	CLA	CHC-C4B-NB	3.69	129.59	124.05
18	1	1001	CLA	CHC-C1C-NC	3.69	129.76	124.33

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
18	A	1142	CLA	C4A-NA-C1A	3.69	108.36	106.68
18	B	1218	CLA	C2A-C1A-CHA	-3.69	117.47	123.87
18	F	1306	CLA	C3D-C4D-CHA	-3.69	116.97	125.20
18	A	1148	CLA	C1C-CHC-C4B	-3.69	116.32	126.04
18	A	1117	CLA	C3D-C4D-CHA	-3.69	116.97	125.20
18	J	1308	CLA	C3D-C4D-CHA	-3.68	116.97	125.20
18	B	1213	CLA	CHC-C1C-NC	3.68	129.74	124.33
18	A	1126	CLA	O2A-CGA-CBA	3.68	123.06	111.83
18	4	4013	CLA	CHA-C4D-ND	3.68	130.04	124.84
18	4	4008	CLA	CHC-C1C-NC	3.68	129.74	124.33
18	B	1224	CLA	O2D-CGD-O1D	-3.68	116.68	123.85
18	3	3013	CLA	C3D-C4D-CHA	-3.68	116.98	125.20
18	A	1108	CLA	CHC-C1C-NC	3.68	129.85	124.31
18	1	1007	CLA	C4C-CHD-C1D	-3.68	115.49	125.98
18	A	1132	CLA	CHD-C4C-NC	3.68	129.83	124.24
18	1	1001	CLA	C2D-C3D-C4D	-3.68	102.88	107.35
18	3	3005	CLA	C2D-C3D-C4D	-3.68	102.88	107.35
18	B	1138	CLA	CHC-C4B-NB	3.68	129.56	124.05
18	F	1305	CLA	CHC-C4B-NB	3.68	129.39	124.08
18	B	1212	CLA	O2A-CGA-CBA	3.68	123.04	111.83
18	B	1224	CLA	C4A-NA-C1A	3.68	108.36	106.68
18	B	1226	CLA	CHA-C4D-ND	3.68	130.03	124.84
18	1	1010	CLA	C4C-CHD-C1D	-3.68	115.51	125.98
18	4	4006	CLA	C2D-C3D-C4D	-3.67	102.89	107.35
18	4	4008	CLA	C1C-CHC-C4B	-3.67	116.35	126.04
18	4	4001	CLA	C2D-C3D-C4D	-3.67	102.89	107.35
18	A	1117	CLA	C1C-CHC-C4B	-3.67	116.36	126.04
18	3	3001	CLA	C1C-CHC-C4B	-3.67	116.36	126.04
18	L	1503	CLA	O1D-CGD-CBD	-3.67	117.28	124.52
18	A	1106	CLA	O2D-CGD-O1D	-3.67	116.70	123.85
18	1	1005	CLA	CHC-C1C-NC	3.67	129.73	124.33
18	K	1141	CLA	C1C-CHC-C4B	-3.67	116.36	126.04
18	A	1151	CLA	C1C-CHC-C4B	-3.67	116.36	126.04
18	L	1504	CLA	C4B-CHC-C1C	-3.67	117.62	126.25
18	A	1101	CLA	C2D-C3D-C4D	-3.67	102.89	107.35
18	F	4015	CLA	CHA-C4D-ND	3.67	130.03	124.84
18	4	4001	CLA	CHA-C4D-ND	3.67	130.02	124.84
18	4	4005	CLA	C1C-CHC-C4B	-3.67	116.37	126.04
20	I	6018	BCR	C23-C24-C25	-3.67	117.20	127.00
18	A	1137	CLA	C3B-C2B-C1B	-3.67	102.85	107.17
18	2	2005	CLA	C3B-C2B-C1B	-3.67	102.73	106.81
18	A	1128	CLA	CMD-C2D-C3D	-3.66	119.29	127.69

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
18	A	1102	CLA	CHA-C4D-ND	3.66	130.02	124.84
18	A	1143	CLA	C3B-C2B-C1B	-3.66	102.73	106.81
18	3	3005	CLA	CHC-C4B-NB	3.66	129.37	124.08
18	3	3015	CLA	C3D-C4D-CHA	-3.66	117.03	125.20
18	A	1144	CLA	C1B-NB-C4B	-3.66	103.75	106.31
18	A	1134	CLA	C2D-C3D-C4D	-3.66	102.91	107.35
18	K	1141	CLA	C3B-C2B-C1B	-3.66	102.74	106.81
18	1	1014	CLA	C4C-CHD-C1D	-3.66	115.56	125.98
18	B	1226	CLA	C3D-C4D-CHA	-3.65	117.04	125.20
18	B	1228	CLA	CAA-C2A-C3A	-3.65	103.12	113.00
18	B	9023	CLA	CBC-CAC-C3C	-3.65	102.51	112.42
18	F	1306	CLA	C2D-C3D-C4D	-3.65	102.91	107.35
18	B	1239	CLA	C1-O2A-CGA	3.65	125.49	116.65
18	F	1240	CLA	C1C-CHC-C4B	-3.65	116.41	126.04
18	A	9013	CLA	CHC-C1C-NC	3.65	129.81	124.31
18	A	1133	CLA	C3D-C4D-CHA	-3.65	117.05	125.20
18	B	1232	CLA	CMD-C2D-C3D	-3.65	119.32	127.69
18	1	1012	CLA	C3D-C4D-CHA	-3.65	117.05	125.20
18	A	9013	CLA	O1D-CGD-CBD	-3.65	117.33	124.52
18	1	1005	CLA	C1B-NB-C4B	-3.65	103.75	106.31
18	A	1122	CLA	C4B-CHC-C1C	-3.65	117.67	126.25
18	B	1211	CLA	C3B-C2B-C1B	-3.65	102.75	106.81
18	A	1126	CLA	CAA-C2A-C3A	-3.65	103.15	113.00
18	4	4008	CLA	C1B-NB-C4B	-3.64	103.76	106.31
18	A	9013	CLA	CHC-C1C-C2C	-3.64	116.60	126.95
18	3	3007	CLA	CHA-C4D-ND	3.64	129.99	124.84
18	A	1120	CLA	C4A-NA-C1A	3.64	108.34	106.68
18	A	1143	CLA	C1B-NB-C4B	-3.64	103.76	106.31
18	1	1002	CLA	CHC-C4B-NB	3.64	129.34	124.08
18	F	1306	CLA	C3B-C2B-C1B	-3.64	102.76	106.81
18	4	4004	CLA	C1C-CHC-C4B	-3.64	116.45	126.04
18	1	1004	CLA	C1C-CHC-C4B	-3.64	116.45	126.04
18	J	1308	CLA	C1B-NB-C4B	-3.64	103.76	106.31
18	4	4003	CLA	C2D-C3D-C4D	-3.63	102.93	107.35
18	4	4007	CLA	C1C-CHC-C4B	-3.63	116.46	126.04
18	2	2011	CLA	CHC-C4B-NB	3.63	129.33	124.08
18	A	1126	CLA	C4B-CHC-C1C	-3.63	117.71	126.25
18	F	1139	CLA	C4A-NA-C1A	3.63	108.34	106.68
18	A	1120	CLA	C3D-C4D-CHA	-3.63	117.09	125.20
18	B	1239	CLA	CHC-C4B-NB	3.63	129.50	124.05
18	3	3004	CLA	C4C-CHD-C1D	-3.63	115.64	125.98
18	A	1101	CLA	C3D-C4D-CHA	-3.63	117.10	125.20

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
18	4	4013	CLA	C3D-C4D-CHA	-3.63	117.10	125.20
18	2	2006	CLA	CHA-C4D-ND	3.63	129.97	124.84
18	B	1236	CLA	CHC-C1C-NC	3.63	129.77	124.31
18	B	1209	CLA	O2D-CGD-CBD	3.63	117.57	111.23
18	B	1239	CLA	CMD-C2D-C3D	-3.62	119.38	127.69
18	A	1106	CLA	CHB-C4A-NA	3.62	129.63	124.40
18	A	1104	CLA	C1C-CHC-C4B	-3.62	116.49	126.04
18	2	2013	CLA	C1B-NB-C4B	-3.62	103.77	106.31
18	B	1301	CLA	C4C-CHD-C1D	-3.62	115.67	125.98
18	A	1143	CLA	CHA-C4D-ND	3.62	129.95	124.84
18	A	1132	CLA	C1B-NB-C4B	-3.62	103.77	106.31
18	3	3013	CLA	C1B-NB-C4B	-3.62	103.77	106.31
18	B	1207	CLA	CMD-C2D-C3D	-3.62	119.39	127.69
18	2	2010	CLA	C4A-NA-C1A	3.62	108.33	106.68
18	B	1227	CLA	CHD-C4C-C3C	-3.61	119.50	124.77
18	1	1001	CLA	C4C-CHD-C1D	-3.61	115.68	125.98
18	2	2010	CLA	C3B-C2B-C1B	-3.61	102.79	106.81
18	B	1213	CLA	CHA-C4D-ND	3.61	129.94	124.84
18	2	2001	CLA	C4A-NA-C1A	3.61	108.33	106.68
18	A	1105	CLA	C3D-C4D-CHA	-3.61	117.14	125.20
18	B	9012	CLA	CHC-C1C-NC	3.61	129.75	124.31
18	1	1013	CLA	C3B-C2B-C1B	-3.61	102.79	106.81
18	A	1146	CLA	C3D-C4D-CHA	-3.61	117.14	125.20
18	H	1501	CLA	CMD-C2D-C3D	-3.61	119.41	127.69
18	A	1105	CLA	C3B-C2B-C1B	-3.61	102.79	106.81
18	K	1150	CLA	C3B-C2B-C1B	-3.61	102.79	106.81
18	3	3013	CLA	C4A-NA-C1A	3.61	108.33	106.68
18	L	1125	CLA	C4C-CHD-C1D	-3.61	115.70	125.98
18	3	3013	CLA	CHA-C4D-ND	3.61	129.94	124.84
20	F	6016	BCR	C8-C7-C6	-3.61	117.37	127.00
18	L	1130	CLA	O2A-CGA-CBA	3.60	122.83	111.83
18	B	1223	CLA	C4A-NA-C1A	3.60	108.32	106.68
18	3	3015	CLA	CHC-C4B-NB	3.60	129.29	124.08
20	L	6020	BCR	C1-C6-C5	-3.60	117.71	122.64
18	A	1124	CLA	CHD-C1D-ND	3.60	129.93	124.84
18	B	1226	CLA	C1B-NB-C4B	-3.60	103.78	106.31
18	L	1125	CLA	CHC-C4B-NB	3.60	129.28	124.08
18	3	3002	CLA	CHA-C4D-ND	3.60	129.93	124.84
18	A	1135	CLA	O2A-CGA-O1A	-3.60	114.08	123.33
18	B	1221	CLA	O2A-CGA-CBA	3.60	122.81	111.83
18	2	2010	CLA	C2D-C3D-C4D	-3.60	102.98	107.35
18	4	4010	CLA	C1C-CHC-C4B	-3.60	116.55	126.04

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
18	4	4002	CLA	C3D-C4D-CHA	-3.60	117.17	125.20
18	B	1301	CLA	C3D-C4D-CHA	-3.60	117.17	125.20
18	B	1213	CLA	CHC-C4B-NB	3.60	129.28	124.08
18	1	1013	CLA	C4A-NA-C1A	3.59	108.32	106.68
18	B	1237	CLA	O2A-CGA-CBA	3.59	122.80	111.83
18	1	1003	CLA	C2D-C3D-C4D	-3.59	102.98	107.35
18	B	9022	CLA	C3B-C2B-C1B	-3.59	102.93	107.17
18	4	4006	CLA	C4C-CHD-C1D	-3.59	115.74	125.98
18	2	2006	CLA	C4C-CHD-C1D	-3.59	115.75	125.98
18	A	1111	CLA	C1C-CHC-C4B	-3.59	116.57	126.04
18	B	1228	CLA	C4B-CHC-C1C	-3.59	117.81	126.25
18	A	1117	CLA	CHC-C1C-NC	3.59	129.60	124.33
18	3	3011	CLA	C3B-C2B-C1B	-3.59	102.82	106.81
18	J	2107	CLA	CHD-C4C-NC	3.59	129.79	124.23
18	2	2013	CLA	C3D-C4D-CHA	-3.59	117.19	125.20
18	1	1008	CLA	CHC-C4B-NB	3.59	129.26	124.08
18	3	3010	CLA	CHA-C4D-ND	3.59	129.91	124.84
18	3	3005	CLA	C3D-C4D-CHA	-3.59	117.19	125.20
18	J	1308	CLA	CHC-C4B-NB	3.58	129.26	124.08
18	B	1201	CLA	C1C-CHC-C4B	-3.58	116.59	126.04
18	2	2003	CLA	C3D-C4D-CHA	-3.58	117.20	125.20
18	A	1116	CLA	C1C-CHC-C4B	-3.58	116.60	126.04
18	1	1003	CLA	CHC-C4B-NB	3.58	129.25	124.08
18	F	1302	CLA	O2D-CGD-CBD	3.58	117.49	111.23
18	A	9011	CLA	CMA-C3A-C4A	-3.58	102.15	111.77
18	B	9023	CLA	CMB-C2B-C1B	3.58	130.87	125.42
18	B	1219	CLA	CHC-C1C-NC	3.58	129.70	124.31
18	B	1213	CLA	C3D-C4D-CHA	-3.58	117.21	125.20
18	2	2013	CLA	CHA-C4D-ND	3.58	129.89	124.84
18	A	1107	CLA	CHC-C4B-NB	3.57	129.41	124.05
18	J	1307	CLA	CHC-C4B-NB	3.57	129.24	124.08
18	B	1220	CLA	C2B-C1B-NB	3.57	114.03	110.33
18	G	1233	CLA	C3B-C2B-C1B	-3.57	102.96	107.17
18	K	1150	CLA	C1C-CHC-C4B	-3.57	116.62	126.04
18	A	1146	CLA	C1C-CHC-C4B	-3.57	116.63	126.04
18	B	1206	CLA	CHD-C4C-NC	3.57	129.66	124.24
18	J	1307	CLA	CHD-C4C-NC	3.57	129.66	124.24
18	J	1307	CLA	C1C-CHC-C4B	-3.56	116.64	126.04
18	2	2007	CLA	C2D-C3D-C4D	-3.56	103.02	107.35
18	2	2011	CLA	C4A-NA-C1A	3.56	108.31	106.68
18	B	1238	CLA	CHD-C4C-C3C	-3.56	119.58	124.77
18	A	1146	CLA	C3B-C2B-C1B	-3.56	102.84	106.81

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
18	A	1102	CLA	C3D-C4D-CHA	-3.56	117.24	125.20
18	2	2012	CLA	C4C-CHD-C1D	-3.56	115.83	125.98
18	B	1221	CLA	CHC-C1C-C2C	-3.56	116.82	126.95
18	A	1131	CLA	C4B-CHC-C1C	-3.56	117.87	126.25
18	B	1214	CLA	C1-O2A-CGA	3.56	125.27	116.65
18	A	1148	CLA	C3D-C4D-CHA	-3.56	117.25	125.20
18	A	1309	CLA	C3B-C2B-C1B	-3.56	102.85	106.81
20	F	6016	BCR	C1-C6-C7	3.56	125.31	115.65
18	3	3001	CLA	C3D-C4D-CHA	-3.56	117.25	125.20
18	3	3003	CLA	C1B-NB-C4B	-3.56	103.82	106.31
18	L	1502	CLA	CMD-C2D-C3D	-3.56	119.53	127.69
18	A	1144	CLA	C3D-C4D-CHA	-3.56	117.26	125.20
18	A	1109	CLA	C3B-C2B-C1B	-3.55	102.86	106.81
18	4	4007	CLA	C3B-C2B-C1B	-3.55	102.86	106.81
18	A	1129	CLA	O2D-CGD-O1D	-3.55	116.94	123.85
18	B	1301	CLA	C4A-NA-C1A	3.55	108.30	106.68
18	4	4004	CLA	C3B-C2B-C1B	-3.55	102.86	106.81
18	K	1141	CLA	C4C-CHD-C1D	-3.55	115.86	125.98
18	1	1007	CLA	CHC-C4B-NB	3.55	129.21	124.08
18	1	1002	CLA	C4A-NA-C1A	3.55	108.30	106.68
18	B	1234	CLA	CHC-C4B-NB	3.55	129.37	124.05
18	4	4008	CLA	C2D-C3D-C4D	-3.55	103.04	107.35
18	2	2010	CLA	CHC-C4B-NB	3.54	129.20	124.08
18	3	3011	CLA	C4A-NA-C1A	3.54	108.30	106.68
18	4	4011	CLA	CHA-C4D-ND	3.54	129.84	124.84
18	2	2005	CLA	C2D-C3D-C4D	-3.54	103.05	107.35
18	3	3007	CLA	C3D-C4D-CHA	-3.54	117.30	125.20
18	3	3011	CLA	CHA-C4D-ND	3.54	129.84	124.84
18	3	3008	CLA	CHC-C4B-NB	3.54	129.19	124.08
18	B	1242	CLA	C4B-CHC-C1C	-3.54	117.93	126.25
18	A	1147	CLA	CHA-C4D-ND	3.53	129.84	124.84
18	1	1012	CLA	CHA-C4D-ND	3.53	129.84	124.84
18	A	1142	CLA	C1B-NB-C4B	-3.53	103.83	106.31
18	B	1230	CLA	CHC-C4B-NB	3.53	129.19	124.08
18	A	1133	CLA	C1B-NB-C4B	-3.53	103.83	106.31
18	A	1119	CLA	C4B-CHC-C1C	-3.53	117.94	126.25
18	3	3005	CLA	C1B-NB-C4B	-3.53	103.83	106.31
18	B	1208	CLA	CHD-C4C-C3C	-3.53	119.62	124.77
18	F	1302	CLA	CAA-C2A-C1A	3.53	123.54	111.97
18	A	1133	CLA	C4A-NA-C1A	3.53	108.29	106.68
18	A	1117	CLA	CHC-C4B-NB	3.53	129.18	124.08
18	4	4005	CLA	C3B-C2B-C1B	-3.53	102.89	106.81

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
18	B	9010	CLA	CHC-C1C-C2C	-3.53	116.93	126.95
18	2	2006	CLA	C1B-NB-C4B	-3.53	103.84	106.31
18	2	2008	CLA	C1B-NB-C4B	-3.53	103.84	106.31
18	2	2002	CLA	C3B-C2B-C1B	-3.52	102.89	106.81
18	3	3010	CLA	CHC-C4B-NB	3.52	129.17	124.08
18	A	1115	CLA	CMD-C2D-C3D	-3.52	119.61	127.69
18	A	9013	CLA	CHD-C4C-C3C	-3.52	119.64	124.77
18	A	1143	CLA	C3D-C4D-CHA	-3.52	117.33	125.20
18	A	1140	CLA	C1-O2A-CGA	3.52	125.18	116.65
18	A	1133	CLA	CHC-C1C-NC	3.52	129.51	124.33
18	B	1201	CLA	C3D-C4D-CHA	-3.52	117.33	125.20
18	B	1230	CLA	CHA-C4D-ND	3.52	129.82	124.84
18	2	2010	CLA	C3D-C4D-CHA	-3.52	117.33	125.20
18	4	1304	CLA	O2A-CGA-CBA	3.52	122.57	111.83
18	A	1107	CLA	C4A-NA-C1A	3.52	108.28	106.68
18	1	1002	CLA	C3B-C2B-C1B	-3.52	102.89	106.81
18	1	1014	CLA	C3D-C4D-CHA	-3.52	117.34	125.20
18	3	3012	CLA	CHC-C4B-NB	3.52	129.16	124.08
18	3	3006	CLA	CHC-C4B-NB	3.52	129.16	124.08
18	2	2015	CLA	C1B-NB-C4B	-3.52	103.84	106.31
20	I	6018	BCR	C24-C23-C22	3.51	131.44	126.23
18	A	1133	CLA	CHA-C4D-ND	3.51	129.81	124.84
18	A	1137	CLA	CAA-C2A-C1A	3.51	123.49	111.97
18	A	1111	CLA	C3B-C2B-C1B	-3.51	102.90	106.81
18	2	2004	CLA	C3B-C2B-C1B	-3.51	102.90	106.81
18	B	1239	CLA	CHD-C4C-C3C	-3.51	119.65	124.77
18	K	1153	CLA	C4A-NA-C1A	3.51	108.28	106.68
18	L	1502	CLA	O2D-CGD-O1D	-3.51	117.01	123.85
18	A	1136	CLA	CMD-C2D-C3D	-3.51	119.64	127.69
18	B	1217	CLA	CHC-C4B-NB	3.51	129.31	124.05
18	K	1141	CLA	C3D-C4D-CHA	-3.51	117.36	125.20
18	1	1005	CLA	C4C-CHD-C1D	-3.51	115.98	125.98
18	3	3013	CLA	C2D-C3D-C4D	-3.51	103.09	107.35
18	3	3008	CLA	C2D-C3D-C4D	-3.51	103.09	107.35
18	F	1305	CLA	C1B-NB-C4B	-3.51	103.85	106.31
18	A	9011	CLA	CHD-C4C-NC	3.51	129.67	124.23
18	3	3005	CLA	CHA-C4D-ND	3.50	129.79	124.84
18	A	1118	CLA	C2D-C3D-C4D	-3.50	103.09	107.35
18	B	1230	CLA	C2D-C3D-C4D	-3.50	103.09	107.35
18	B	1205	CLA	O1D-CGD-CBD	-3.50	117.61	124.52
18	2	2015	CLA	CHC-C4B-NB	3.50	129.14	124.08
18	A	1128	CLA	CHC-C1C-NC	3.50	129.58	124.31

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
18	A	1148	CLA	C2D-C3D-C4D	-3.50	103.10	107.35
18	B	1230	CLA	C3D-C4D-CHA	-3.50	117.39	125.20
18	H	1505	CLA	C1B-NB-C4B	-3.49	103.86	106.31
18	4	4011	CLA	C4C-CHD-C1D	-3.49	116.02	125.98
18	H	1501	CLA	CHC-C4B-NB	3.49	129.29	124.05
18	B	1211	CLA	C2D-C3D-C4D	-3.49	103.11	107.35
18	2	2011	CLA	C3D-C4D-CHA	-3.49	117.40	125.20
18	A	1142	CLA	CHC-C4B-NB	3.49	129.13	124.08
18	L	1125	CLA	C3D-C4D-CHA	-3.49	117.41	125.20
18	B	1214	CLA	CAA-C2A-C3A	-3.49	103.57	113.00
18	1	1004	CLA	C1B-NB-C4B	-3.49	103.86	106.31
18	A	1309	CLA	CHA-C4D-ND	3.49	129.77	124.84
18	3	3013	CLA	CHC-C4B-NB	3.49	129.12	124.08
18	2	2006	CLA	CHC-C4B-NB	3.49	129.12	124.08
18	2	2013	CLA	CHC-C4B-NB	3.49	129.12	124.08
18	A	1151	CLA	C1B-NB-C4B	-3.49	103.87	106.31
18	A	1106	CLA	O2D-CGD-CBD	3.49	117.32	111.23
18	F	1303	CLA	CHC-C4B-NB	3.49	129.12	124.08
18	1	1008	CLA	C3B-C2B-C1B	-3.49	102.93	106.81
18	4	4008	CLA	C3B-C2B-C1B	-3.49	102.93	106.81
18	A	1115	CLA	CHD-C4C-C3C	-3.49	119.69	124.77
18	4	4004	CLA	C1B-NB-C4B	-3.48	103.87	106.31
18	L	1130	CLA	C2B-C1B-NB	3.48	113.94	110.33
18	4	4001	CLA	C1B-NB-C4B	-3.48	103.87	106.31
18	A	1113	CLA	O1D-CGD-CBD	-3.48	117.65	124.52
18	4	4002	CLA	CHA-C4D-ND	3.48	129.76	124.84
18	1	1003	CLA	C1B-NB-C4B	-3.48	103.87	106.31
18	B	1227	CLA	CED-O2D-CGD	3.48	123.81	115.92
18	A	1148	CLA	CHA-C4D-ND	3.48	129.76	124.84
18	3	3012	CLA	CHA-C4D-ND	3.48	129.76	124.84
18	1	1002	CLA	C1B-NB-C4B	-3.48	103.87	106.31
18	2	2011	CLA	CHA-C4D-ND	3.48	129.76	124.84
18	B	1219	CLA	CAA-C2A-C3A	-3.48	103.60	113.00
18	J	2107	CLA	C3B-C2B-C1B	-3.48	103.07	107.17
18	B	1237	CLA	C4B-C3B-C2B	3.48	111.63	107.30
18	L	1502	CLA	CHC-C1C-NC	3.48	129.55	124.31
18	1	1001	CLA	C3D-C4D-CHA	-3.47	117.44	125.20
18	1	1012	CLA	C2D-C3D-C4D	-3.47	103.13	107.35
18	K	1141	CLA	CHA-C4D-ND	3.47	129.75	124.84
18	B	1237	CLA	CHD-C4C-C3C	-3.47	119.71	124.77
18	A	1135	CLA	CMD-C2D-C3D	-3.47	119.73	127.69
18	A	1142	CLA	CHA-C4D-ND	3.47	129.75	124.84

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
18	1	1011	CLA	CHA-C4D-ND	3.47	129.75	124.84
18	3	3003	CLA	C3B-C2B-C1B	-3.47	102.95	106.81
18	3	3002	CLA	C3D-C4D-CHA	-3.47	117.45	125.20
18	1	1008	CLA	CHA-C4D-ND	3.47	129.74	124.84
18	A	1129	CLA	C4B-CHC-C1C	-3.47	118.09	126.25
18	F	4015	CLA	C3D-C4D-CHA	-3.47	117.46	125.20
18	B	1203	CLA	CHC-C4B-NB	3.47	129.25	124.05
18	B	1206	CLA	CHA-C4D-ND	3.47	129.74	124.84
18	1	1005	CLA	C2D-C3D-C4D	-3.47	103.14	107.35
18	2	2008	CLA	CHC-C4B-NB	3.47	129.09	124.08
18	L	1503	CLA	C1D-ND-C4D	-3.46	103.88	106.31
18	A	1137	CLA	CBC-CAC-C3C	3.46	121.81	112.42
18	2	2011	CLA	C2D-C3D-C4D	-3.46	103.14	107.35
18	F	1303	CLA	CHA-C4D-ND	3.46	129.73	124.84
18	A	1144	CLA	CHC-C4B-NB	3.46	129.08	124.08
18	A	1144	CLA	C3B-C2B-C1B	-3.46	102.96	106.81
18	3	3015	CLA	C2D-C3D-C4D	-3.46	103.15	107.35
18	3	2009	CLA	C1B-NB-C4B	-3.46	103.89	106.31
18	H	1505	CLA	CHA-C4D-ND	3.46	129.72	124.84
18	B	1239	CLA	CHC-C1C-C2C	-3.46	117.13	126.95
18	A	9011	CLA	O2D-CGD-CBD	3.46	117.27	111.23
18	G	1233	CLA	O2A-CGA-CBA	3.45	122.37	111.83
18	F	1303	CLA	C3D-C4D-CHA	-3.45	117.49	125.20
18	A	1117	CLA	C4A-NA-C1A	3.45	108.25	106.68
18	A	1309	CLA	C3D-C4D-CHA	-3.45	117.49	125.20
18	3	3008	CLA	C3D-C4D-CHA	-3.45	117.49	125.20
18	3	3011	CLA	CHC-C4B-NB	3.45	129.07	124.08
18	3	2009	CLA	CHA-C4D-ND	3.45	129.72	124.84
18	B	1232	CLA	C2B-C1B-NB	3.45	113.90	110.33
18	3	3012	CLA	C4A-NA-C1A	3.45	108.25	106.68
18	1	1014	CLA	C2D-C3D-C4D	-3.45	103.16	107.35
18	B	1224	CLA	CHB-C4A-NA	3.45	129.38	124.40
20	L	6020	BCR	C30-C25-C26	-3.45	117.92	122.64
18	J	2107	CLA	CHD-C4C-C3C	-3.45	119.75	124.77
18	2	2002	CLA	C3D-C4D-CHA	-3.45	117.50	125.20
18	B	9012	CLA	CHC-C4B-NB	3.45	129.22	124.05
20	B	6017	BCR	C30-C25-C24	3.44	124.99	115.65
18	J	1308	CLA	CHA-C4D-ND	3.44	129.71	124.84
18	2	2001	CLA	C3D-C4D-CHA	-3.44	117.51	125.20
18	J	2107	CLA	C4B-CHC-C1C	-3.44	118.15	126.25
18	B	1203	CLA	O2A-CGA-CBA	3.44	122.33	111.83
18	B	1202	CLA	CHC-C4B-NB	3.44	129.21	124.05

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
18	B	1210	CLA	CHC-C4B-NB	3.44	129.05	124.08
18	B	9022	CLA	O2A-CGA-CBA	3.44	122.32	111.83
18	B	1213	CLA	C2D-C3D-C4D	-3.44	103.17	107.35
18	A	9013	CLA	C2C-C1C-NC	3.44	113.59	109.98
18	B	1206	CLA	C1B-NB-C4B	-3.44	103.90	106.31
18	A	1105	CLA	CHC-C4B-NB	3.44	129.05	124.08
18	4	1304	CLA	C3B-C2B-C1B	-3.44	103.12	107.17
18	B	1220	CLA	CMB-C2B-C1B	3.43	130.65	125.42
18	3	3002	CLA	C4A-NA-C1A	3.43	108.25	106.68
18	1	1008	CLA	C3D-C4D-CHA	-3.43	117.53	125.20
18	L	1125	CLA	CHA-C4D-ND	3.43	129.69	124.84
18	A	1104	CLA	CHC-C1C-NC	3.43	129.38	124.33
18	A	1104	CLA	CHA-C4D-ND	3.43	129.69	124.84
18	A	1137	CLA	CHC-C1C-NC	3.43	129.48	124.31
18	B	1301	CLA	CHA-C4D-ND	3.43	129.69	124.84
18	B	1214	CLA	CHC-C1C-NC	3.43	129.47	124.31
18	4	4013	CLA	C2D-C3D-C4D	-3.43	103.18	107.35
18	L	1502	CLA	CHC-C4B-NB	3.43	129.19	124.05
18	4	4006	CLA	C3D-C4D-CHA	-3.43	117.55	125.20
20	B	6017	BCR	C29-C30-C25	3.43	115.42	110.44
18	3	3010	CLA	C3D-C4D-CHA	-3.43	117.55	125.20
18	3	3003	CLA	CHA-C4D-ND	3.42	129.68	124.84
18	A	1118	CLA	C3D-C4D-CHA	-3.42	117.55	125.20
18	A	1113	CLA	CMD-C2D-C3D	-3.42	119.84	127.69
18	F	1306	CLA	CHA-C4D-ND	3.42	129.68	124.84
18	B	1213	CLA	C3B-C2B-C1B	-3.42	103.00	106.81
18	A	1105	CLA	C1B-NB-C4B	-3.42	103.91	106.31
18	B	1235	CLA	CHC-C1C-C2C	-3.42	117.23	126.95
18	B	1222	CLA	CHC-C1C-NC	3.42	129.46	124.31
18	4	4007	CLA	C2D-C3D-C4D	-3.42	103.20	107.35
18	4	4012	CLA	CHB-C4A-NA	3.42	129.29	124.43
18	A	1109	CLA	C1B-NB-C4B	-3.41	103.92	106.31
18	3	3015	CLA	C1B-NB-C4B	-3.41	103.92	106.31
18	1	1002	CLA	CHA-C4D-ND	3.41	129.66	124.84
18	4	4005	CLA	CHA-C4D-ND	3.41	129.66	124.84
18	B	1222	CLA	C4A-NA-C1A	3.41	108.24	106.68
18	A	1101	CLA	CHA-C4D-ND	3.41	129.66	124.84
18	B	1216	CLA	CED-O2D-CGD	3.41	123.65	115.92
18	A	1123	CLA	O2A-CGA-CBA	3.41	122.23	111.83
18	2	2005	CLA	CHC-C4B-NB	3.41	129.01	124.08
18	J	1307	CLA	C2D-C3D-C4D	-3.41	103.21	107.35
18	2	2013	CLA	C2D-C3D-C4D	-3.41	103.21	107.35

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
18	3	3011	CLA	C3D-C4D-CHA	-3.41	117.59	125.20
18	1	1005	CLA	CHC-C4B-NB	3.41	129.00	124.08
18	B	1222	CLA	C3B-C2B-C1B	-3.41	103.15	107.17
18	2	2005	CLA	C3D-C4D-CHA	-3.41	117.59	125.20
18	B	1218	CLA	C4B-CHC-C1C	-3.41	118.24	126.25
18	B	1203	CLA	C2B-C1B-NB	3.41	113.86	110.33
18	B	1210	CLA	C4C-CHD-C1D	-3.40	116.28	125.98
18	2	2002	CLA	C1C-CHC-C4B	-3.40	117.06	126.04
18	1	1014	CLA	CHC-C4B-NB	3.40	129.00	124.08
18	B	1216	CLA	C4B-CHC-C1C	-3.40	118.25	126.25
18	G	1248	CLA	C3D-C4D-CHA	-3.40	117.60	125.20
18	L	1125	CLA	C2D-C3D-C4D	-3.40	103.22	107.35
18	A	1309	CLA	C2D-C3D-C4D	-3.40	103.22	107.35
18	A	9013	CLA	C4A-NA-C1A	3.40	108.23	106.68
18	F	1240	CLA	CHA-C4D-ND	3.40	129.64	124.84
18	3	3003	CLA	CHC-C4B-NB	3.40	128.99	124.08
20	B	6017	BCR	C34-C9-C10	-3.40	117.31	122.82
18	B	1232	CLA	CED-O2D-CGD	3.40	123.62	115.92
18	A	1152	CLA	CHA-C4D-ND	3.40	129.64	124.84
18	3	3007	CLA	C2D-C3D-C4D	-3.40	103.22	107.35
18	B	1205	CLA	CHC-C4B-NB	3.39	129.14	124.05
18	2	2004	CLA	CHC-C4B-NB	3.39	128.98	124.08
18	B	1217	CLA	C3B-C2B-C1B	-3.39	103.17	107.17
18	1	1002	CLA	C3D-C4D-CHA	-3.39	117.63	125.20
18	2	2002	CLA	CHA-C4D-ND	3.39	129.63	124.84
18	4	4001	CLA	CHC-C4B-NB	3.39	128.98	124.08
18	A	1140	CLA	C2B-C1B-NB	3.39	113.84	110.33
18	B	1201	CLA	C3B-C2B-C1B	-3.39	103.04	106.81
18	3	3008	CLA	CHA-C4D-ND	3.39	129.63	124.84
18	4	4009	CLA	CHC-C4B-NB	3.39	128.97	124.08
18	G	1233	CLA	CHC-C1C-NC	3.38	129.41	124.31
18	3	3009	CLA	C3D-C4D-CHA	-3.38	117.64	125.20
18	A	1146	CLA	C1B-NB-C4B	-3.38	103.94	106.31
18	4	4013	CLA	CHC-C4B-NB	3.38	128.97	124.08
18	A	1126	CLA	CHB-C4A-NA	3.38	129.28	124.40
18	4	4008	CLA	CHC-C4B-NB	3.38	128.97	124.08
18	2	2007	CLA	C3D-C4D-CHA	-3.38	117.65	125.20
18	L	1504	CLA	C2B-C1B-NB	3.38	113.83	110.33
18	1	1008	CLA	C1B-NB-C4B	-3.38	103.94	106.31
18	1	1004	CLA	C2D-C3D-C4D	-3.38	103.24	107.35
18	K	1150	CLA	C3D-C4D-CHA	-3.38	117.66	125.20
18	A	9013	CLA	C2B-C1B-NB	3.38	113.83	110.33

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
18	K	1141	CLA	CHC-C4B-NB	3.38	128.96	124.08
18	A	1146	CLA	CHC-C4B-NB	3.38	128.96	124.08
18	B	1138	CLA	CAA-C2A-C3A	-3.38	103.87	113.00
18	3	3002	CLA	C3B-C2B-C1B	-3.38	103.05	106.81
18	2	2007	CLA	CHC-C4B-NB	3.38	128.96	124.08
18	3	2009	CLA	C3B-C2B-C1B	-3.38	103.05	106.81
18	B	1220	CLA	C4B-C3B-C2B	3.37	111.50	107.30
18	B	1225	CLA	CHC-C4B-NB	3.37	129.11	124.05
18	4	4002	CLA	CHC-C4B-NB	3.37	128.96	124.08
18	B	1227	CLA	C4A-NA-C1A	3.37	108.22	106.68
18	A	1309	CLA	C1B-NB-C4B	-3.37	103.95	106.31
18	4	4005	CLA	C3D-C4D-ND	3.37	114.11	109.50
18	B	1224	CLA	C3B-C2B-C1B	-3.37	103.20	107.17
18	4	4007	CLA	C3D-C4D-CHA	-3.37	117.68	125.20
20	L	6020	BCR	C15-C16-C17	-3.37	116.63	123.52
18	4	4004	CLA	CHC-C4B-NB	3.37	128.95	124.08
18	B	1237	CLA	C3B-C4B-NB	-3.36	107.53	110.53
18	A	1115	CLA	CHC-C1C-C2C	-3.36	117.39	126.95
18	4	4013	CLA	C1B-NB-C4B	-3.36	103.95	106.31
18	H	1505	CLA	CHC-C4B-NB	3.36	128.93	124.08
18	B	1206	CLA	C1C-NC-C4C	-3.36	105.15	106.68
18	2	2004	CLA	C4A-NA-C1A	3.36	108.21	106.68
18	A	1140	CLA	CHB-C1B-NB	-3.36	119.02	124.05
18	3	3012	CLA	C3D-C4D-CHA	-3.36	117.71	125.20
18	B	1227	CLA	CHC-C1C-C2C	-3.36	117.41	126.95
18	4	4012	CLA	C1C-CHC-C4B	-3.35	117.20	126.04
18	B	1231	CLA	CHC-C4B-NB	3.35	129.08	124.05
18	4	4013	CLA	C3B-C2B-C1B	-3.35	103.08	106.81
18	G	1233	CLA	CMD-C2D-C3D	-3.35	120.01	127.69
18	A	1106	CLA	CHC-C1C-NC	3.35	129.35	124.31
18	A	1146	CLA	C4A-NA-C1A	3.34	108.20	106.68
18	B	1234	CLA	O2A-CGA-CBA	3.34	122.03	111.83
18	1	1007	CLA	C2D-C3D-C4D	-3.34	103.29	107.35
18	B	1235	CLA	CMD-C2D-C3D	-3.34	120.02	127.69
18	B	1224	CLA	CMD-C2D-C3D	-3.34	120.03	127.69
18	4	4002	CLA	C1B-NB-C4B	-3.34	103.97	106.31
20	F	6016	BCR	C35-C13-C14	-3.34	117.40	122.82
18	2	2002	CLA	C2D-C3D-C4D	-3.34	103.29	107.35
18	2	2015	CLA	C3D-C4D-CHA	-3.34	117.74	125.20
18	L	1502	CLA	C2B-C1B-NB	3.34	113.79	110.33
18	A	1115	CLA	CAA-C2A-C3A	-3.34	103.98	113.00
18	J	2107	CLA	O2D-CGD-O1D	-3.34	117.36	123.85

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
18	K	1153	CLA	C3D-C4D-CHA	-3.33	117.75	125.20
18	A	1151	CLA	CHA-C4D-ND	3.33	129.55	124.84
18	A	1119	CLA	O2A-CGA-CBA	3.33	122.00	111.83
18	1	1013	CLA	C3D-C4D-CHA	-3.33	117.76	125.20
20	I	6018	BCR	C2-C1-C6	-3.33	105.60	110.44
18	2	2001	CLA	C2D-C3D-C4D	-3.33	103.30	107.35
18	H	1505	CLA	C3D-C4D-CHA	-3.33	117.76	125.20
18	1	1003	CLA	C3D-C4D-CHA	-3.33	117.77	125.20
18	A	1126	CLA	CHD-C4C-C3C	-3.33	119.92	124.77
18	3	3002	CLA	C2D-C3D-C4D	-3.33	103.30	107.35
18	A	1105	CLA	CHA-C4D-ND	3.33	129.54	124.84
18	4	4010	CLA	C3D-C4D-CHA	-3.33	117.77	125.20
18	B	1222	CLA	O2A-CGA-CBA	3.33	121.98	111.83
18	A	1129	CLA	CAA-C2A-C1A	-3.33	101.08	111.97
18	A	1117	CLA	C1B-NB-C4B	-3.33	103.98	106.31
18	A	1131	CLA	CHC-C1C-C2C	-3.32	117.50	126.95
18	A	1120	CLA	CHC-C4B-NB	3.32	128.88	124.08
18	2	2012	CLA	CHC-C4B-NB	3.32	128.88	124.08
18	2	2004	CLA	C1B-NB-C4B	-3.32	103.98	106.31
18	3	3010	CLA	C3B-C2B-C1B	-3.32	103.11	106.81
18	3	3003	CLA	C3D-C4D-CHA	-3.32	117.78	125.20
18	3	3006	CLA	C2D-C3D-C4D	-3.32	103.31	107.35
18	A	1128	CLA	CHC-C4B-NB	3.32	129.03	124.05
18	B	9012	CLA	CMB-C2B-C1B	3.32	130.47	125.42
19	A	5001	PQN	C11-C3-C2	-3.32	119.20	124.89
18	A	1142	CLA	C3D-C4D-CHA	-3.32	117.80	125.20
18	B	1301	CLA	C2D-C3D-C4D	-3.32	103.32	107.35
18	1	1007	CLA	C3B-C2B-C1B	-3.31	103.12	106.81
18	K	1150	CLA	CHA-C4D-ND	3.31	129.52	124.84
18	3	2009	CLA	C3D-C4D-CHA	-3.31	117.80	125.20
18	1	1011	CLA	CHC-C4B-NB	3.31	128.87	124.08
18	B	1217	CLA	CHD-C4C-C3C	-3.31	119.95	124.77
18	B	9023	CLA	CMA-C3A-C4A	-3.31	102.88	111.77
18	A	1123	CLA	CHC-C1C-NC	3.31	129.30	124.31
18	I	1204	CLA	CMD-C2D-C3D	-3.31	120.10	127.69
18	A	1116	CLA	C2D-C3D-C4D	-3.31	103.33	107.35
18	2	2015	CLA	CHA-C4D-ND	3.31	129.51	124.84
20	I	6018	BCR	C28-C27-C26	-3.31	108.16	114.06
18	1	1013	CLA	CHA-C4D-ND	3.31	129.51	124.84
18	B	1226	CLA	C2D-C3D-C4D	-3.30	103.33	107.35
18	B	1230	CLA	C3B-C2B-C1B	-3.30	103.13	106.81
18	B	9012	CLA	CMD-C2D-C3D	-3.30	120.11	127.69

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
18	B	1218	CLA	O2D-CGD-O1D	-3.30	117.42	123.85
20	F	6016	BCR	C12-C13-C14	3.30	124.20	119.01
18	1	1004	CLA	C4A-NA-C1A	3.30	108.18	106.68
20	L	6020	BCR	C21-C20-C19	-3.30	113.64	123.20
18	A	1119	CLA	C3B-C2B-C1B	-3.30	103.28	107.17
18	3	3006	CLA	C3B-C2B-C1B	-3.30	103.14	106.81
18	A	1152	CLA	C3D-C4D-CHA	-3.30	117.84	125.20
18	A	1144	CLA	CHA-C4D-ND	3.29	129.50	124.84
18	3	2009	CLA	CHC-C4B-NB	3.29	128.84	124.08
18	A	1151	CLA	C3D-C4D-CHA	-3.29	117.85	125.20
18	A	1122	CLA	CMD-C2D-C3D	-3.29	120.14	127.69
18	B	1215	CLA	C2A-C1A-CHA	-3.29	118.16	123.87
18	F	1240	CLA	C3D-C4D-ND	3.29	114.00	109.50
18	B	1220	CLA	C1-O2A-CGA	3.29	124.61	116.65
18	A	1119	CLA	C1D-ND-C4D	-3.29	104.00	106.31
18	4	1304	CLA	C4A-NA-C1A	3.29	108.18	106.68
18	2	2012	CLA	C3D-C4D-CHA	-3.29	117.86	125.20
18	4	1009	CLA	C1C-CHC-C4B	-3.29	117.37	126.04
18	B	1228	CLA	CMD-C2D-C3D	-3.29	120.15	127.69
18	1	1007	CLA	C3D-C4D-CHA	-3.29	117.86	125.20
20	I	6018	BCR	C33-C5-C6	-3.28	120.90	124.48
20	F	6016	BCR	C16-C15-C14	-3.28	116.80	123.52
20	F	6016	BCR	C34-C9-C8	3.28	123.10	118.09
18	A	1129	CLA	C2A-C1A-CHA	-3.28	118.17	123.87
18	4	4009	CLA	C3D-C4D-CHA	-3.28	117.88	125.20
18	B	1202	CLA	CHD-C4C-C3C	-3.28	119.99	124.77
18	4	4010	CLA	CHA-C4D-ND	3.28	129.47	124.84
18	A	1126	CLA	C4A-NA-C1A	3.28	108.17	106.68
18	2	2010	CLA	CHA-C4D-ND	3.28	129.47	124.84
18	K	1150	CLA	C2D-C3D-C4D	-3.28	103.37	107.35
18	A	1108	CLA	CHC-C4B-NB	3.28	128.96	124.05
18	2	2001	CLA	CHA-C4D-ND	3.28	129.47	124.84
18	1	1014	CLA	CHA-C4D-ND	3.27	129.47	124.84
18	A	1104	CLA	C2A-C1A-CHA	-3.27	117.05	122.63
18	G	1248	CLA	C3B-C2B-C1B	-3.27	103.17	106.81
18	A	1133	CLA	C2D-C3D-C4D	-3.27	103.38	107.35
18	3	3001	CLA	CHC-C4B-NB	3.27	128.80	124.08
18	A	1111	CLA	CHC-C4B-NB	3.27	128.80	124.08
18	J	1307	CLA	CHC-C1C-NC	3.27	129.13	124.33
18	B	1202	CLA	CAC-C3C-C4C	3.27	129.04	124.79
18	3	3011	CLA	C1B-NB-C4B	-3.27	104.02	106.31
18	K	1141	CLA	C2D-C3D-C4D	-3.27	103.38	107.35

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
18	A	1143	CLA	CHC-C4B-NB	3.26	128.80	124.08
18	2	2003	CLA	CHC-C4B-NB	3.26	128.80	124.08
18	B	9012	CLA	C1-O2A-CGA	3.26	124.55	116.65
20	I	6018	BCR	C8-C7-C6	3.26	135.71	127.00
18	B	1212	CLA	O2D-CGD-O1D	-3.26	117.50	123.85
18	A	1132	CLA	C1C-NC-C4C	-3.26	105.19	106.68
18	A	1102	CLA	CHC-C4B-NB	3.26	128.79	124.08
18	G	1248	CLA	CHA-C4D-ND	3.26	129.45	124.84
18	A	1109	CLA	C1C-CHC-C4B	-3.26	117.44	126.04
18	B	1236	CLA	CHC-C4B-NB	3.26	128.94	124.05
18	2	2007	CLA	CHA-C4D-ND	3.26	129.44	124.84
18	A	1134	CLA	CHC-C4B-NB	3.26	128.79	124.08
18	1	1010	CLA	CHC-C4B-NB	3.26	128.79	124.08
18	B	1225	CLA	O2D-CGD-O1D	-3.26	117.51	123.85
18	3	3010	CLA	C2D-C3D-C4D	-3.25	103.40	107.35
18	4	4003	CLA	C4A-NA-C1A	3.25	108.16	106.68
18	3	3012	CLA	C2D-C3D-C4D	-3.25	103.40	107.35
18	3	3009	CLA	C2D-C3D-C4D	-3.25	103.40	107.35
18	L	1130	CLA	CHC-C4B-NB	3.25	128.93	124.05
18	A	9011	CLA	C4B-C3B-C2B	3.25	111.34	107.30
18	L	1503	CLA	CHC-C4B-NB	3.25	128.92	124.05
18	3	3006	CLA	C1B-NB-C4B	-3.25	104.03	106.31
18	B	1215	CLA	CAA-C2A-C3A	-3.25	104.22	113.00
18	A	1107	CLA	C2B-C1B-NB	3.25	113.69	110.33
18	4	4009	CLA	C2D-C3D-C4D	-3.25	103.41	107.35
18	A	1133	CLA	C1C-CHC-C4B	-3.25	117.48	126.04
18	A	1116	CLA	C3D-C4D-CHA	-3.24	117.95	125.20
18	2	2011	CLA	C1B-NB-C4B	-3.24	104.04	106.31
18	G	1248	CLA	C2D-C3D-C4D	-3.24	103.41	107.35
18	A	1102	CLA	C2D-C3D-C4D	-3.24	103.41	107.35
18	A	1143	CLA	C2D-C3D-C4D	-3.24	103.42	107.35
18	A	1107	CLA	C3B-C4B-NB	-3.24	107.64	110.53
18	B	1222	CLA	O2D-CGD-O1D	-3.24	117.55	123.85
18	A	1146	CLA	C2D-C3D-C4D	-3.23	103.42	107.35
18	F	1305	CLA	C3D-C4D-CHA	-3.23	117.98	125.20
18	H	1501	CLA	O2A-CGA-CBA	3.23	121.69	111.83
18	A	1108	CLA	O2A-CGA-CBA	3.23	121.69	111.83
20	A	6011	BCR	C8-C7-C6	-3.23	118.36	127.00
18	K	1141	CLA	C1B-NB-C4B	-3.23	104.04	106.31
18	3	3004	CLA	CHC-C4B-NB	3.23	128.75	124.08
18	B	1239	CLA	C4A-NA-C1A	3.23	108.15	106.68
18	A	1152	CLA	C2D-C3D-C4D	-3.23	103.42	107.35

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
18	B	1207	CLA	CHC-C1C-NC	3.23	129.18	124.31
18	A	1134	CLA	C3D-C4D-CHA	-3.23	117.99	125.20
18	3	3007	CLA	C1B-NB-C4B	-3.23	104.05	106.31
18	3	3012	CLA	C3B-C2B-C1B	-3.23	103.22	106.81
18	B	1202	CLA	CHC-C1C-C2C	-3.23	117.78	126.95
18	B	1216	CLA	O2A-CGA-CBA	3.23	121.67	111.83
18	3	3001	CLA	CHA-C4D-ND	3.23	129.40	124.84
18	B	1225	CLA	CHB-C4A-NA	3.22	129.05	124.40
18	A	1135	CLA	CHC-C4B-NB	3.22	128.88	124.05
18	B	1229	CLA	CHC-C1C-NC	3.22	129.16	124.31
18	4	4007	CLA	CHA-C4D-ND	3.22	129.39	124.84
20	L	6020	BCR	C34-C9-C8	3.22	123.01	118.09
18	B	1206	CLA	CHC-C1C-NC	3.22	129.06	124.33
18	J	2107	CLA	CHC-C1C-NC	3.22	129.16	124.31
18	A	1148	CLA	CHC-C4B-NB	3.22	128.73	124.08
18	B	1217	CLA	CAA-C2A-C3A	-3.22	104.30	113.00
18	2	2001	CLA	CHC-C4B-NB	3.22	128.73	124.08
18	B	1223	CLA	C3D-C4D-CHA	-3.22	118.02	125.20
18	L	1125	CLA	C1B-NB-C4B	-3.21	104.06	106.31
18	A	1122	CLA	C1-O2A-CGA	3.21	124.43	116.65
18	A	1151	CLA	C3B-C2B-C1B	-3.21	103.23	106.81
18	A	1123	CLA	CHC-C4B-NB	3.21	128.87	124.05
18	B	1232	CLA	O2A-CGA-CBA	3.21	121.63	111.83
20	F	6016	BCR	C30-C25-C26	-3.21	118.25	122.64
18	4	4001	CLA	C4A-NA-C1A	3.21	108.14	106.68
18	B	1213	CLA	C1B-NB-C4B	-3.21	104.06	106.31
18	2	2008	CLA	C3B-C2B-C1B	-3.21	103.24	106.81
18	4	4002	CLA	C3B-C2B-C1B	-3.21	103.24	106.81
18	A	1124	CLA	CHC-C1C-NC	3.21	129.05	124.33
18	B	1234	CLA	CHC-C1C-NC	3.21	129.15	124.31
18	3	3010	CLA	C1B-NB-C4B	-3.21	104.06	106.31
20	A	6011	BCR	C3-C4-C5	-3.21	108.33	114.06
18	F	4015	CLA	C2D-C3D-C4D	-3.21	103.45	107.35
18	B	1216	CLA	CMD-C2D-C3D	-3.21	120.33	127.69
18	A	1126	CLA	CAA-C2A-C1A	-3.21	101.46	111.97
18	B	1229	CLA	CMB-C2B-C1B	3.21	130.30	125.42
18	B	1222	CLA	O2A-CGA-O1A	-3.21	115.61	123.63
18	A	1127	CLA	CHC-C4B-NB	3.21	128.72	124.08
18	B	1241	CLA	C2D-C3D-C4D	-3.21	103.45	107.35
18	B	1208	CLA	CHC-C4B-NB	3.21	128.86	124.05
18	J	1307	CLA	C1B-NB-C4B	-3.21	104.06	106.31
18	1	1010	CLA	CHA-C4D-ND	3.20	129.37	124.84

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
18	B	1138	CLA	CHD-C4C-C3C	-3.20	120.10	124.77
18	A	1120	CLA	CHA-C4D-ND	3.20	129.37	124.84
18	L	1502	CLA	C4-C3-C5	3.20	119.89	116.13
18	A	1102	CLA	C3B-C2B-C1B	-3.20	103.25	106.81
18	F	1303	CLA	C1B-NB-C4B	-3.20	104.07	106.31
18	1	1010	CLA	C3D-C4D-CHA	-3.20	118.06	125.20
18	1	1003	CLA	C4A-NA-C1A	3.20	108.14	106.68
18	B	9022	CLA	CAA-C2A-C1A	3.19	122.44	111.97
18	B	1206	CLA	CHC-C4B-NB	3.19	128.70	124.08
18	B	1208	CLA	C4B-C3B-C2B	3.19	111.27	107.30
18	B	1207	CLA	O2D-CGD-CBD	3.19	116.81	111.23
18	A	1132	CLA	C1C-CHC-C4B	-3.19	117.62	126.04
18	B	9022	CLA	CHC-C1C-C2C	-3.19	117.88	126.95
18	A	1137	CLA	C4-C3-C2	-3.19	115.44	123.63
18	B	1206	CLA	C1C-CHC-C4B	-3.19	117.64	126.04
18	A	1152	CLA	C1B-NB-C4B	-3.19	104.08	106.31
18	1	1011	CLA	C3D-C4D-CHA	-3.19	118.08	125.20
18	A	1124	CLA	CHB-C1B-NB	-3.18	119.48	124.08
18	2	2005	CLA	C4A-NA-C1A	3.18	108.13	106.68
18	3	3015	CLA	C4A-NA-C1A	3.18	108.13	106.68
18	4	4011	CLA	C1B-NB-C4B	-3.18	104.08	106.31
18	A	1137	CLA	CHB-C4A-NA	3.18	128.99	124.40
18	1	1012	CLA	CHB-C4A-NA	3.18	128.96	124.43
18	A	1147	CLA	C3D-C4D-CHA	-3.18	118.10	125.20
18	1	1013	CLA	CHC-C4B-NB	3.18	128.68	124.08
18	A	1103	CLA	O2D-CGD-O1D	-3.18	117.66	123.85
18	3	3009	CLA	CHA-C4D-ND	3.18	129.33	124.84
18	A	1124	CLA	C2D-C3D-C4D	-3.18	103.49	107.35
18	A	1127	CLA	CHA-C4D-ND	3.17	129.33	124.84
18	B	1222	CLA	C4-C3-C5	3.17	120.74	115.23
18	F	1306	CLA	CHC-C4B-NB	3.17	128.66	124.08
18	A	1147	CLA	C3B-C2B-C1B	-3.17	103.28	106.81
18	4	1009	CLA	CHC-C4B-NB	3.17	128.66	124.08
18	B	1242	CLA	CMD-C2D-C3D	-3.17	120.42	127.69
18	B	1218	CLA	C3B-C2B-C1B	-3.17	103.44	107.17
18	B	1239	CLA	CAA-C2A-C3A	-3.17	104.44	113.00
20	B	6017	BCR	C16-C15-C14	3.17	130.00	123.52
18	K	1153	CLA	C3B-C2B-C1B	-3.17	103.29	106.81
18	B	1222	CLA	CHC-C4B-NB	3.17	128.80	124.05
18	4	4006	CLA	CHC-C4B-NB	3.16	128.65	124.08
18	B	1203	CLA	CHB-C4A-NA	3.16	128.97	124.40
18	A	9011	CLA	CHD-C4C-C3C	-3.16	120.16	124.77

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
18	2	2012	CLA	C2D-C3D-C4D	-3.16	103.51	107.35
20	F	6016	BCR	C27-C26-C25	-3.16	118.43	122.70
18	4	4009	CLA	CHA-C4D-ND	3.16	129.31	124.84
18	2	2015	CLA	C2D-C3D-C4D	-3.16	103.51	107.35
18	A	1118	CLA	CHA-C4D-ND	3.16	129.30	124.84
18	J	1307	CLA	C1C-NC-C4C	-3.16	105.24	106.68
18	B	9012	CLA	C4-C3-C2	-3.16	115.52	123.63
18	A	9011	CLA	CHC-C1C-NC	3.16	129.07	124.31
18	B	1215	CLA	C4D-C3D-CAD	3.16	111.53	108.11
20	L	6020	BCR	C20-C21-C22	3.16	131.70	127.28
18	B	1242	CLA	C3B-C2B-C1B	-3.16	103.45	107.17
18	1	1006	CLA	CHA-C4D-ND	3.15	129.30	124.84
18	A	1111	CLA	C3D-C4D-CHA	-3.15	118.16	125.20
18	4	4012	CLA	C3D-C4D-CHA	-3.15	118.16	125.20
18	F	1240	CLA	CHC-C4B-NB	3.15	128.64	124.08
18	K	1153	CLA	C2D-C3D-C4D	-3.15	103.52	107.35
18	1	1004	CLA	CHC-C4B-NB	3.15	128.63	124.08
18	A	1123	CLA	O2D-CGD-O1D	-3.15	117.72	123.85
18	B	1138	CLA	C4-C3-C2	-3.15	115.54	123.63
18	B	1223	CLA	CHC-C4B-NB	3.15	128.63	124.08
18	3	3008	CLA	C3B-C2B-C1B	-3.15	103.31	106.81
18	F	1305	CLA	CHA-C4D-ND	3.15	129.29	124.84
18	A	1115	CLA	O2D-CGD-O1D	-3.15	117.72	123.85
18	A	1126	CLA	C1-O2A-CGA	3.14	124.26	116.65
18	A	1115	CLA	CAC-C3C-C4C	3.14	128.88	124.79
18	1	1013	CLA	C2D-C3D-C4D	-3.14	103.53	107.35
18	B	1219	CLA	C4-C3-C5	3.14	119.83	116.13
18	A	1132	CLA	CHC-C4B-NB	3.14	128.62	124.08
18	L	1504	CLA	C1-O2A-CGA	3.14	124.25	116.65
18	1	1008	CLA	C2D-C3D-C4D	-3.14	103.53	107.35
18	B	1214	CLA	O2A-CGA-CBA	3.14	121.41	111.83
18	B	1209	CLA	C4A-NA-C1A	3.14	108.11	106.68
18	A	1136	CLA	CHC-C1C-NC	3.14	129.04	124.31
18	B	1138	CLA	C4-C3-C5	3.14	120.67	115.23
18	2	2003	CLA	CHA-C4D-ND	3.13	129.27	124.84
18	A	1131	CLA	CHD-C4C-C3C	-3.13	120.21	124.77
18	B	9022	CLA	C2B-C1B-NB	3.13	113.57	110.33
18	4	4004	CLA	C3D-C4D-CHA	-3.13	118.22	125.20
18	L	1504	CLA	CHC-C4B-NB	3.13	128.74	124.05
18	A	1119	CLA	CED-O2D-CGD	3.12	123.00	115.92
18	3	3004	CLA	C3D-C4D-CHA	-3.12	118.23	125.20
18	1	1003	CLA	CHA-C4D-ND	3.12	129.25	124.84

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
18	B	9022	CLA	C4-C3-C5	3.12	120.65	115.23
18	B	9023	CLA	CED-O2D-CGD	3.12	123.00	115.92
18	B	1211	CLA	CHC-C4B-NB	3.12	128.59	124.08
18	4	4003	CLA	C3B-C2B-C1B	-3.12	103.34	106.81
18	I	1204	CLA	CHC-C4B-NB	3.12	128.73	124.05
18	F	1302	CLA	C3B-C2B-C1B	-3.12	103.50	107.17
18	B	1206	CLA	CHB-C4A-NA	3.12	128.86	124.43
18	A	1128	CLA	C2B-C1B-NB	3.11	113.56	110.33
18	4	4005	CLA	C4A-NA-C1A	3.11	108.10	106.68
18	B	1225	CLA	C1D-ND-C4D	-3.11	104.13	106.31
18	4	4003	CLA	C1B-NB-C4B	-3.11	104.13	106.31
18	A	1127	CLA	C3D-C4D-CHA	-3.11	118.26	125.20
18	2	2001	CLA	C3B-C2B-C1B	-3.11	103.35	106.81
18	B	1232	CLA	O2D-CGD-O1D	-3.11	117.80	123.85
18	A	1135	CLA	C2B-C1B-NB	3.11	113.55	110.33
18	B	9023	CLA	CMD-C2D-C3D	-3.10	120.57	127.69
18	B	1138	CLA	C1-O2A-CGA	3.10	124.17	116.65
18	B	1219	CLA	O2D-CGD-O1D	-3.10	117.81	123.85
18	A	1108	CLA	O1D-CGD-CBD	-3.10	118.40	124.52
18	A	1106	CLA	CHC-C1C-C2C	-3.10	118.14	126.95
18	B	1210	CLA	C3D-C4D-CHA	-3.10	118.28	125.20
18	2	2005	CLA	CHA-C4D-ND	3.10	129.22	124.84
18	L	1504	CLA	O2D-CGD-O1D	-3.10	117.81	123.85
18	B	1208	CLA	C4-C3-C2	-3.10	115.67	123.63
18	L	1504	CLA	C3B-C2B-C1B	-3.10	103.52	107.17
18	4	4010	CLA	CHC-C4B-NB	3.10	128.56	124.08
18	3	3002	CLA	C1B-NB-C4B	-3.10	104.14	106.31
18	B	1231	CLA	CHD-C4C-C3C	-3.10	120.26	124.77
18	B	1230	CLA	C1B-NB-C4B	-3.09	104.14	106.31
18	1	1001	CLA	C1B-NB-C4B	-3.09	104.14	106.31
18	F	1139	CLA	C2B-C1B-NB	3.09	113.53	110.33
18	B	1301	CLA	CHC-C4B-NB	3.09	128.55	124.08
18	A	1117	CLA	C2D-C3D-C4D	-3.09	103.59	107.35
18	3	3004	CLA	C2D-C3D-C4D	-3.09	103.59	107.35
18	B	1218	CLA	C6-C5-C3	-3.09	99.04	113.70
18	1	1006	CLA	CHC-C4B-NB	3.09	128.54	124.08
18	B	9023	CLA	O2A-CGA-CBA	3.09	121.25	111.83
18	A	1152	CLA	C4A-NA-C1A	3.09	108.09	106.68
18	B	1220	CLA	CHC-C1C-NC	3.09	128.96	124.31
18	B	1215	CLA	O2A-CGA-CBA	3.09	121.25	111.83
20	B	6017	BCR	C24-C25-C26	-3.09	114.44	121.56
18	F	1305	CLA	C2D-C3D-C4D	-3.09	103.60	107.35

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
18	1	1014	CLA	C3B-C2B-C1B	-3.09	103.38	106.81
18	B	1201	CLA	CHB-C4A-NA	3.09	128.82	124.43
18	A	1133	CLA	CHC-C4B-NB	3.08	128.54	124.08
18	A	1118	CLA	C3B-C2B-C1B	-3.08	103.38	106.81
20	B	6017	BCR	C23-C22-C21	3.08	123.85	119.01
18	A	1135	CLA	O2A-CGA-CBA	3.08	123.73	114.00
18	A	1151	CLA	C2D-C3D-C4D	-3.08	103.61	107.35
18	A	1122	CLA	CHC-C4B-NB	3.08	128.67	124.05
18	B	1218	CLA	O1D-CGD-CBD	-3.08	118.45	124.52
18	H	1501	CLA	C1-O2A-CGA	3.08	124.10	116.65
18	A	1129	CLA	CAC-C3C-C4C	3.08	128.79	124.79
18	B	1229	CLA	CHB-C4A-NA	3.08	128.84	124.40
18	G	1233	CLA	C1-C2-C3	-3.07	121.16	126.20
18	3	3003	CLA	C2D-C3D-C4D	-3.07	103.62	107.35
18	I	1204	CLA	CMB-C2B-C1B	3.07	130.09	125.42
18	3	3011	CLA	C2D-C3D-C4D	-3.07	103.62	107.35
18	B	1231	CLA	C3B-C2B-C1B	-3.07	103.55	107.17
18	1	1012	CLA	CHC-C4B-NB	3.07	128.51	124.08
18	A	1105	CLA	C4A-NA-C1A	3.07	108.08	106.68
18	A	1129	CLA	CHC-C1C-NC	3.07	128.93	124.31
18	B	1219	CLA	C3B-C2B-C1B	-3.06	103.56	107.17
18	4	4006	CLA	C3D-C4D-ND	3.06	113.69	109.50
18	B	1232	CLA	CHC-C4B-NB	3.06	128.64	124.05
18	B	1216	CLA	O2D-CGD-O1D	-3.06	117.89	123.85
18	3	2009	CLA	C2D-C3D-C4D	-3.06	103.63	107.35
18	3	3009	CLA	CHC-C4B-NB	3.06	128.50	124.08
18	K	1150	CLA	CHB-C4A-NA	3.05	128.77	124.43
18	H	1501	CLA	C6-C5-C3	-3.05	106.03	113.47
18	B	1225	CLA	CAA-CBA-CGA	-3.05	104.36	112.49
18	A	1132	CLA	C2D-C3D-C4D	-3.05	103.64	107.35
18	4	1009	CLA	C2D-C3D-C4D	-3.05	103.64	107.35
18	B	1218	CLA	CAA-C2A-C1A	-3.05	101.98	111.97
18	F	1139	CLA	CMB-C2B-C1B	3.05	130.06	125.42
18	B	1214	CLA	O2A-CGA-O1A	-3.05	116.00	123.63
18	A	1122	CLA	CHC-C1C-NC	3.05	128.90	124.31
18	B	1212	CLA	CHC-C4B-NB	3.04	128.62	124.05
18	A	1147	CLA	CHC-C4B-NB	3.04	128.48	124.08
18	A	1132	CLA	C4A-NA-C1A	3.04	108.07	106.68
18	2	2012	CLA	CHA-C4D-ND	3.04	129.14	124.84
18	B	1216	CLA	C3B-C2B-C1B	-3.04	103.58	107.17
18	B	1229	CLA	C4B-CHC-C1C	-3.04	119.10	126.25
18	B	1201	CLA	CHC-C4B-NB	3.04	128.47	124.08

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
18	A	1107	CLA	O2A-C1-C2	3.04	119.79	108.11
18	F	1303	CLA	C2D-C3D-C4D	-3.04	103.66	107.35
18	B	1228	CLA	C1-O2A-CGA	3.03	124.00	116.65
18	A	9011	CLA	CHC-C1C-C2C	-3.03	118.34	126.95
18	B	9010	CLA	O2D-CGD-O1D	-3.03	117.95	123.85
18	F	1302	CLA	O2A-CGA-CBA	3.03	121.07	111.83
18	A	1132	CLA	CHC-C1C-NC	3.03	128.78	124.33
20	B	6017	BCR	C23-C24-C25	-3.03	118.91	127.00
18	A	1111	CLA	CHA-C4D-ND	3.03	129.12	124.84
18	B	1203	CLA	C4D-CHA-C1A	-3.03	117.64	121.24
18	B	1209	CLA	CHC-C1C-C2C	-3.03	118.35	126.95
18	B	1201	CLA	CHA-C4D-ND	3.03	129.12	124.84
18	H	1505	CLA	C2D-C3D-C4D	-3.02	103.67	107.35
18	1	1004	CLA	C3B-C2B-C1B	-3.02	103.44	106.81
18	A	1113	CLA	CHC-C1C-C2C	-3.02	118.36	126.95
20	I	6018	BCR	C40-C30-C25	-3.02	105.50	110.24
18	B	9023	CLA	O2D-CGD-CBD	3.02	116.51	111.23
18	B	1223	CLA	CHA-C4D-ND	3.02	129.11	124.84
18	4	4011	CLA	C3D-C4D-CHA	-3.02	118.46	125.20
18	A	1134	CLA	C4A-NA-C1A	3.02	108.06	106.68
18	F	4015	CLA	C1B-NB-C4B	-3.02	104.20	106.31
18	A	1136	CLA	O2A-CGA-CBA	3.02	121.03	111.83
18	1	1002	CLA	C2D-C3D-C4D	-3.02	103.69	107.35
18	B	1219	CLA	O2A-CGA-CBA	3.01	121.03	111.83
18	A	1126	CLA	C3B-C2B-C1B	-3.01	103.62	107.17
18	A	1116	CLA	CHA-C4D-ND	3.01	129.10	124.84
18	A	1142	CLA	C2D-C3D-C4D	-3.01	103.69	107.35
18	2	2002	CLA	CHC-C4B-NB	3.01	128.44	124.08
18	F	1240	CLA	CHB-C4A-NA	3.01	128.71	124.43
18	A	1137	CLA	CHC-C4B-NB	3.01	128.57	124.05
18	A	1116	CLA	CHC-C4B-NB	3.01	128.43	124.08
18	A	1126	CLA	CHC-C1C-NC	3.00	128.83	124.31
18	B	1239	CLA	O2A-CGA-CBA	3.00	120.99	111.83
18	A	1115	CLA	CMB-C2B-C1B	3.00	129.99	125.42
18	A	1129	CLA	C3B-C2B-C1B	-3.00	103.63	107.17
18	4	4012	CLA	C4D-ND-C1D	-3.00	104.21	106.31
18	A	1151	CLA	CHC-C4B-NB	3.00	128.41	124.08
18	A	9011	CLA	C1-O2A-CGA	3.00	123.91	116.65
18	3	3001	CLA	CHB-C4A-NA	3.00	128.69	124.43
18	B	1224	CLA	CAA-C2A-C3A	-3.00	104.90	113.00
18	B	1223	CLA	C2C-C1C-CHC	-3.00	117.99	125.84
18	A	1142	CLA	C3B-C2B-C1B	-3.00	103.48	106.81

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
18	A	1111	CLA	C2D-C3D-C4D	-3.00	103.71	107.35
18	L	1503	CLA	CED-O2D-CGD	2.99	122.71	115.92
18	4	4012	CLA	CHA-C4D-ND	2.99	129.07	124.84
20	B	6017	BCR	C33-C5-C6	-2.99	121.22	124.48
18	B	9010	CLA	CMD-C2D-C3D	-2.99	120.83	127.69
18	B	1228	CLA	CMA-C3A-C4A	-2.99	103.74	111.77
18	A	1104	CLA	C2D-C3D-C4D	-2.99	103.72	107.35
18	A	1118	CLA	CHC-C4B-NB	2.99	128.40	124.08
18	A	1119	CLA	CHC-C1C-NC	2.98	128.81	124.31
18	A	1103	CLA	CAC-C3C-C4C	2.98	128.67	124.79
18	L	1503	CLA	CAC-C3C-C4C	-2.98	120.91	124.79
19	B	5002	PQN	O1-C1-C10	-2.98	116.80	121.57
20	L	6020	BCR	C28-C27-C26	-2.98	108.74	114.06
18	B	1210	CLA	CHA-C4D-ND	2.98	129.05	124.84
18	A	1107	CLA	CED-O2D-CGD	2.98	122.67	115.92
18	L	1503	CLA	CMB-C2B-C1B	2.98	129.95	125.42
18	A	1113	CLA	O2A-CGA-CBA	2.98	120.91	111.83
18	B	1238	CLA	C2A-C1A-CHA	-2.98	118.70	123.87
18	3	3008	CLA	CHB-C4A-NA	2.97	128.66	124.43
18	I	1204	CLA	C3B-C2B-C1B	-2.97	103.66	107.17
18	A	1129	CLA	C1-C2-C3	-2.97	121.33	126.20
18	A	1101	CLA	C3B-C2B-C1B	-2.97	103.50	106.81
18	B	1203	CLA	CHD-C4C-C3C	-2.97	120.34	125.03
18	B	1228	CLA	O2A-CGA-O1A	-2.97	116.20	123.63
18	A	1115	CLA	O2A-CGA-CBA	2.97	120.89	111.83
18	A	1118	CLA	CHB-C4A-NA	2.97	128.65	124.43
18	A	1129	CLA	CHC-C4B-NB	2.97	128.50	124.05
18	4	4007	CLA	CHC-C4B-NB	2.97	128.37	124.08
18	1	1001	CLA	C3D-C4D-ND	2.97	113.56	109.50
19	B	5002	PQN	C17-C16-C15	-2.97	105.35	113.26
18	4	4004	CLA	CHA-C4D-ND	2.97	129.03	124.84
18	A	1107	CLA	O2A-CGA-CBA	2.97	120.88	111.83
18	B	1201	CLA	C3D-C4D-ND	2.96	113.55	109.50
18	B	1226	CLA	CHC-C4B-NB	2.96	128.36	124.08
18	F	1139	CLA	CHC-C1C-C2C	-2.96	118.53	126.95
18	A	1101	CLA	CHB-C4A-NA	2.96	128.64	124.43
18	1	1006	CLA	C3D-C4D-CHA	-2.96	118.59	125.20
18	B	1138	CLA	CHC-C1C-C2C	-2.96	118.54	126.95
18	1	1007	CLA	CHA-C4D-ND	2.96	129.02	124.84
18	B	1216	CLA	CHB-C4A-NA	2.96	128.67	124.40
18	B	9010	CLA	CHB-C1B-NB	-2.96	119.61	124.05
18	A	1120	CLA	C3D-C4D-ND	2.96	113.54	109.50

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
18	B	1235	CLA	CHC-C4B-NB	2.96	128.49	124.05
18	4	1009	CLA	CHC-C1C-NC	2.96	128.68	124.33
18	B	1238	CLA	C1D-ND-C4D	-2.96	104.24	106.31
18	A	1106	CLA	CHB-C1B-NB	-2.96	119.61	124.05
18	B	1242	CLA	O1D-CGD-CBD	-2.95	118.69	124.52
18	B	1229	CLA	CMD-C2D-C3D	-2.95	120.92	127.69
18	A	1109	CLA	C2A-C3A-C4A	-2.95	100.46	104.64
18	4	1304	CLA	CMB-C2B-C1B	2.95	129.91	125.42
18	2	2003	CLA	C3D-C4D-ND	2.95	113.53	109.50
18	B	9012	CLA	CED-O2D-CGD	2.95	122.60	115.92
18	H	1501	CLA	CED-O2D-CGD	2.95	122.60	115.92
18	B	1215	CLA	CED-O2D-CGD	2.95	122.60	115.92
18	B	1234	CLA	C2A-C1A-CHA	-2.94	118.76	123.87
18	1	1001	CLA	CHA-C4D-ND	2.94	129.00	124.84
20	I	6018	BCR	C19-C18-C17	-2.94	114.38	119.01
18	B	1207	CLA	CMB-C2B-C1B	2.94	129.89	125.42
18	A	1127	CLA	C3B-C2B-C1B	-2.94	103.54	106.81
18	B	1225	CLA	CHC-C1C-C2C	-2.94	118.60	126.95
18	B	1208	CLA	CAC-C3C-C2C	-2.94	122.17	127.56
18	F	1302	CLA	C4A-NA-C1A	2.93	108.02	106.68
18	F	1139	CLA	O2D-CGD-O1D	-2.93	118.14	123.85
18	1	1014	CLA	CHB-C4A-NA	2.93	128.60	124.43
18	K	1150	CLA	CHC-C4B-NB	2.93	128.32	124.08
18	4	4010	CLA	C2D-C3D-C4D	-2.93	103.79	107.35
18	L	1125	CLA	C3B-C2B-C1B	-2.93	103.55	106.81
18	A	1104	CLA	C1B-NB-C4B	-2.93	104.26	106.31
18	A	1107	CLA	CAA-C2A-C1A	-2.93	102.38	111.97
18	B	1236	CLA	C4A-NA-C1A	2.93	108.01	106.68
18	B	9012	CLA	CMA-C3A-C4A	-2.93	103.91	111.77
18	B	1226	CLA	C3B-C2B-C1B	-2.93	103.55	106.81
18	2	2013	CLA	C3B-C2B-C1B	-2.93	103.55	106.81
18	1	1006	CLA	C2D-C3D-C4D	-2.92	103.80	107.35
18	B	1238	CLA	CHC-C1C-C2C	-2.92	118.64	126.95
18	4	1304	CLA	O2D-CGD-O1D	-2.92	118.16	123.85
20	I	6018	BCR	C35-C13-C12	2.92	122.55	118.09
18	A	1104	CLA	C3D-C4D-CHA	-2.92	118.68	125.20
18	B	1215	CLA	CMA-C3A-C2A	-2.92	102.70	113.98
18	F	1302	CLA	CHC-C4B-NB	2.91	128.42	124.05
18	B	1237	CLA	C1-O2A-CGA	2.91	123.70	116.65
18	A	1108	CLA	CHB-C4A-NA	2.91	128.60	124.40
18	A	1128	CLA	C4-C3-C5	2.91	120.28	115.23
18	L	1503	CLA	CGD-CBD-CAD	-2.91	101.42	110.85

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
18	A	1104	CLA	C1C-NC-C4C	-2.91	105.35	106.68
18	B	1222	CLA	C4-C3-C2	-2.91	116.16	123.63
18	B	1220	CLA	C4A-NA-C1A	2.91	108.01	106.68
18	B	1138	CLA	O2A-CGA-CBA	2.91	120.70	111.83
18	L	1130	CLA	CMB-C2B-C1B	2.91	129.85	125.42
18	L	1503	CLA	CHC-C1C-C2C	-2.91	118.68	126.95
18	L	1130	CLA	C3B-C2B-C1B	-2.90	103.75	107.17
18	B	1212	CLA	C1D-ND-C4D	-2.90	104.27	106.31
18	A	1101	CLA	CHC-C4B-NB	2.90	128.28	124.08
18	B	1205	CLA	CHC-C1C-C2C	-2.90	118.70	126.95
18	L	1502	CLA	C3B-C2B-C1B	-2.90	103.75	107.17
18	A	1134	CLA	CHA-C4D-ND	2.90	128.94	124.84
18	2	2003	CLA	CHB-C4A-NA	2.90	128.55	124.43
18	3	3004	CLA	CHA-C4D-ND	2.90	128.93	124.84
18	A	1126	CLA	CMC-C2C-C1C	2.90	129.56	125.03
18	3	3003	CLA	C4A-NA-C1A	2.89	108.00	106.68
18	B	1225	CLA	CMB-C2B-C1B	2.89	129.82	125.42
18	J	2107	CLA	CMD-C2D-C3D	-2.89	121.06	127.69
18	F	1303	CLA	CHB-C4A-NA	2.89	128.54	124.43
18	J	2107	CLA	CHC-C4B-NB	2.88	128.38	124.05
18	B	1225	CLA	CBC-CAC-C3C	-2.88	104.61	112.42
18	1	1011	CLA	C2D-C3D-C4D	-2.88	103.85	107.35
18	B	1203	CLA	CHC-C1C-C2C	-2.88	118.76	126.95
18	A	1109	CLA	CHB-C1B-NB	-2.88	119.92	124.08
18	L	1503	CLA	C3D-C4D-ND	2.88	114.66	109.99
18	B	1239	CLA	C2B-C1B-NB	2.88	113.31	110.33
18	3	3012	CLA	C1B-NB-C4B	-2.88	104.29	106.31
18	L	1130	CLA	C2A-C1A-CHA	-2.87	118.88	123.87
18	L	1504	CLA	O2A-CGA-CBA	2.87	120.59	111.83
20	F	6016	BCR	C32-C1-C6	-2.87	105.74	110.24
18	L	1502	CLA	C4-C3-C2	-2.87	116.26	123.63
18	B	9010	CLA	CAA-CBA-CGA	2.87	121.35	113.21
18	A	9013	CLA	CHB-C4A-NA	2.87	128.54	124.40
18	4	4004	CLA	C2D-C3D-C4D	-2.87	103.87	107.35
18	G	1248	CLA	C3C-C4C-CHD	-2.86	117.79	125.23
18	A	1110	CLA	C1B-NB-C4B	-2.86	104.30	106.31
18	A	1140	CLA	CHC-C1C-C2C	-2.86	118.82	126.95
18	A	1126	CLA	O2A-C1-C2	2.86	119.12	108.11
18	B	1237	CLA	CHC-C1C-C2C	-2.86	118.82	126.95
18	B	1218	CLA	C3D-C4D-ND	2.86	114.64	109.99
18	B	1214	CLA	C1D-ND-C4D	-2.86	104.31	106.31
18	B	9012	CLA	O2D-CGD-O1D	-2.86	118.29	123.85

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
18	A	1111	CLA	CHB-C4A-NA	2.85	128.49	124.43
18	4	4009	CLA	CHB-C4A-NA	2.85	128.49	124.43
18	A	1115	CLA	CHB-C4A-NA	2.85	128.51	124.40
18	G	1248	CLA	CHC-C4B-NB	2.85	128.20	124.08
18	A	1107	CLA	CHC-C1C-C2C	-2.85	118.85	126.95
18	1	1010	CLA	C2D-C3D-C4D	-2.85	103.89	107.35
18	B	1225	CLA	C2A-C1A-CHA	-2.84	118.93	123.87
18	B	1221	CLA	O2A-CGA-O1A	-2.84	116.52	123.63
18	B	1206	CLA	C3D-C4D-ND	2.84	113.38	109.50
18	F	1302	CLA	CHB-C4A-NA	2.84	128.49	124.40
18	B	1208	CLA	O2A-CGA-CBA	2.83	120.48	111.83
18	J	1308	CLA	CHB-C4A-NA	2.83	128.46	124.43
18	B	1206	CLA	C3D-C2D-C1D	2.83	110.79	107.35
18	A	1120	CLA	CHB-C4A-NA	2.83	128.46	124.43
18	B	1220	CLA	C3B-C4B-NB	-2.83	108.00	110.53
18	4	1009	CLA	C1B-NB-C4B	-2.83	104.33	106.31
18	A	1113	CLA	CHB-C4A-NA	2.83	128.48	124.40
18	A	1116	CLA	CHB-C4A-NA	2.83	128.45	124.43
20	I	6018	BCR	C33-C5-C4	2.82	119.61	113.60
18	F	1306	CLA	C3D-C4D-ND	2.82	113.36	109.50
18	B	1221	CLA	C3B-C2B-C1B	-2.82	103.84	107.17
18	B	1217	CLA	C2D-C1D-ND	-2.82	107.33	110.13
18	B	1217	CLA	CHC-C1C-C2C	-2.82	118.93	126.95
18	A	1137	CLA	C6-C5-C3	2.82	120.34	113.47
18	A	1122	CLA	C7-C6-C5	2.82	120.77	113.26
18	A	1124	CLA	CHB-C4A-NA	2.82	128.44	124.43
18	3	3001	CLA	C3D-C4D-ND	2.81	113.35	109.50
18	A	1107	CLA	C1D-ND-C4D	-2.81	104.34	106.31
18	A	1127	CLA	C2C-C1C-CHC	-2.81	118.47	125.84
18	A	9013	CLA	CAA-C2A-C3A	-2.81	105.40	113.00
18	A	1110	CLA	C4A-NA-C1A	2.81	107.96	106.68
18	I	1204	CLA	C4A-NA-C1A	2.81	107.96	106.68
18	2	2004	CLA	C3D-C4D-ND	2.81	113.34	109.50
18	B	1214	CLA	C3D-C4D-ND	2.81	114.55	109.99
18	B	9010	CLA	C4B-C3B-C2B	2.81	110.79	107.30
18	A	1128	CLA	CED-O2D-CGD	2.80	122.28	115.92
18	B	1223	CLA	C2D-C3D-C4D	-2.80	103.94	107.35
18	A	1122	CLA	O1D-CGD-CBD	-2.80	118.99	124.52
20	A	6011	BCR	C4-C5-C6	-2.80	118.92	122.70
18	A	1126	CLA	C4D-CHA-C1A	-2.80	117.91	121.24
18	B	1223	CLA	C3C-C4C-CHD	-2.80	117.97	125.23
18	B	1138	CLA	CMB-C2B-C1B	2.80	129.68	125.42

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
18	A	1105	CLA	C3D-C4D-ND	2.80	113.32	109.50
18	J	1308	CLA	C3D-C4D-ND	2.79	113.32	109.50
18	B	1239	CLA	O2D-CGD-O1D	-2.79	118.41	123.85
20	F	6016	BCR	C39-C30-C25	2.79	114.62	110.24
18	H	1501	CLA	CHC-C1C-C2C	-2.79	119.01	126.95
18	A	1135	CLA	CAC-C3C-C4C	2.79	128.42	124.79
18	B	1236	CLA	C4B-C3B-C2B	2.79	110.77	107.30
18	B	1227	CLA	C3B-C2B-C1B	-2.79	103.88	107.17
18	A	1129	CLA	CED-O2D-CGD	2.79	122.24	115.92
18	B	1220	CLA	O2A-CGA-O1A	-2.79	116.65	123.63
18	B	1236	CLA	CMB-C2B-C1B	2.79	129.67	125.42
18	B	1214	CLA	C3B-C2B-C1B	-2.79	103.88	107.17
18	B	1232	CLA	O1D-CGD-CBD	-2.79	119.02	124.52
18	B	1219	CLA	O2A-C1-C2	2.79	118.83	108.11
18	B	1214	CLA	CBA-CAA-C2A	2.79	122.08	113.79
18	A	1135	CLA	CHC-C1C-C2C	-2.78	119.04	126.95
18	4	4005	CLA	CHB-C1B-NB	-2.78	120.06	124.08
18	B	1222	CLA	CED-O2D-CGD	2.78	122.23	115.92
18	I	1204	CLA	CAA-C2A-C3A	-2.78	105.48	113.00
18	A	1144	CLA	C2C-C1C-CHC	-2.78	118.55	125.84
18	B	1242	CLA	O2A-CGA-CBA	2.78	120.31	111.83
18	A	1115	CLA	CED-O2D-CGD	2.78	122.22	115.92
18	B	1212	CLA	CHB-C4A-NA	2.78	128.41	124.40
18	B	1238	CLA	C4A-NA-C1A	2.78	107.95	106.68
18	2	2008	CLA	C2C-C1C-CHC	-2.78	118.56	125.84
18	K	1153	CLA	C1B-NB-C4B	-2.78	104.36	106.31
18	4	4006	CLA	CHA-C4D-ND	2.78	128.76	124.84
18	B	1230	CLA	C4A-NA-C1A	2.77	107.94	106.68
18	B	1220	CLA	CAA-C2A-C1A	-2.77	102.89	111.97
18	3	3007	CLA	C2C-C1C-CHC	-2.77	118.58	125.84
18	A	1115	CLA	CGD-CBD-CAD	2.77	119.81	110.85
18	F	1305	CLA	C2C-C1C-CHC	-2.77	118.59	125.84
18	B	1231	CLA	CHC-C1C-C2C	-2.77	119.09	126.95
18	4	4005	CLA	CHC-C4B-NB	2.76	128.07	124.08
18	A	9011	CLA	CHB-C1B-NB	-2.76	119.91	124.05
18	A	1117	CLA	C1C-NC-C4C	-2.76	105.42	106.68
18	A	1151	CLA	C3C-C4C-CHD	-2.76	118.06	125.23
18	B	1217	CLA	O2D-CGD-O1D	-2.75	118.49	123.85
18	B	9022	CLA	CAC-C3C-C4C	2.75	128.37	124.79
18	B	1232	CLA	CHC-C1C-C2C	-2.75	119.13	126.95
18	B	1203	CLA	C5-C3-C4	2.75	120.92	114.59
20	A	6011	BCR	C38-C26-C27	2.75	119.46	113.60

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
18	B	1235	CLA	C1-O2A-CGA	2.75	123.30	116.65
19	B	5002	PQN	C16-C17-C18	-2.75	106.84	115.97
18	L	1503	CLA	C4B-C3B-C2B	-2.74	104.45	107.03
18	I	1204	CLA	CHC-C1C-C2C	-2.74	119.16	126.95
18	A	1144	CLA	C3D-C4D-ND	2.74	113.25	109.50
20	A	6011	BCR	C20-C21-C22	-2.74	123.44	127.28
18	B	1220	CLA	O1D-CGD-CBD	-2.74	119.11	124.52
18	A	1113	CLA	CHB-C1B-NB	-2.74	119.94	124.05
18	A	1101	CLA	C3D-C4D-ND	2.74	113.24	109.50
20	F	6016	BCR	C7-C6-C5	-2.74	115.25	121.56
18	B	1209	CLA	CHC-C4B-NB	2.74	128.16	124.05
18	A	1136	CLA	CED-O2D-CGD	2.74	122.12	115.92
18	G	1248	CLA	C2C-C1C-CHC	-2.74	118.67	125.84
18	A	1128	CLA	O2A-CGA-CBA	2.73	120.17	111.83
18	B	1238	CLA	C4-C3-C5	2.73	119.97	115.23
18	B	1203	CLA	CMB-C2B-C1B	2.73	129.58	125.42
18	B	1229	CLA	C4-C3-C2	-2.73	114.46	122.66
18	A	1103	CLA	CHC-C4B-NB	2.73	128.15	124.05
18	2	2007	CLA	C3C-C4C-CHD	-2.73	118.14	125.23
18	A	1103	CLA	C3B-C2B-C1B	-2.73	103.95	107.17
18	1	1005	CLA	CHB-C4A-NA	2.73	128.31	124.43
18	4	4006	CLA	C4D-ND-C1D	-2.73	104.40	106.31
18	G	1233	CLA	CHC-C4B-NB	2.72	128.14	124.05
18	B	1215	CLA	C3D-C4D-ND	2.72	114.41	109.99
18	J	2107	CLA	C4-C3-C5	2.72	119.95	115.23
18	A	1148	CLA	CHB-C4A-NA	2.72	128.30	124.43
18	4	1009	CLA	CHD-C1D-ND	2.72	128.68	124.84
18	A	1147	CLA	C3C-C4C-CHD	-2.72	118.17	125.23
18	B	1210	CLA	C2D-C3D-C4D	-2.72	104.05	107.35
18	3	3004	CLA	CHB-C4A-NA	2.71	128.29	124.43
18	A	1109	CLA	C3A-C4A-CHB	-2.71	120.59	123.91
18	B	1228	CLA	C4D-CHA-C1A	-2.71	118.01	121.24
18	J	2107	CLA	O1D-CGD-CBD	-2.71	119.17	124.52
18	A	1129	CLA	CAA-CBA-CGA	-2.71	105.52	113.21
18	4	4013	CLA	C3C-C4C-CHD	-2.71	118.20	125.23
18	G	1233	CLA	C1D-ND-C4D	-2.71	104.41	106.31
18	A	1142	CLA	C3C-C4C-CHD	-2.70	118.21	125.23
18	B	1207	CLA	C4-C3-C5	2.70	119.92	115.23
18	A	1137	CLA	O1D-CGD-CBD	-2.70	119.19	124.52
18	4	4005	CLA	C3D-C2D-C1D	2.70	110.63	107.35
18	1	1014	CLA	C4D-ND-C1D	-2.70	104.42	106.31
18	2	2010	CLA	C3D-C4D-ND	2.70	113.19	109.50

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
18	G	1233	CLA	CED-O2D-CGD	2.70	122.04	115.92
18	1	1014	CLA	C3D-C4D-ND	2.70	113.19	109.50
18	A	1115	CLA	CHC-C4B-NB	2.70	128.10	124.05
18	B	1214	CLA	CHC-C4B-NB	2.70	128.10	124.05
18	B	1242	CLA	CHB-C4A-NA	2.70	128.29	124.40
18	A	1101	CLA	C2C-C1C-CHC	-2.70	118.78	125.84
18	2	2005	CLA	C3D-C4D-ND	2.70	113.19	109.50
18	B	1209	CLA	CHB-C4A-NA	2.69	128.29	124.40
18	3	3007	CLA	CHB-C4A-NA	2.69	128.26	124.43
18	F	1302	CLA	O2A-CGA-O1A	-2.69	116.90	123.63
18	1	1006	CLA	C3C-C4C-CHD	-2.69	118.25	125.23
18	A	1137	CLA	C4A-NA-C1A	2.69	107.91	106.68
18	A	1140	CLA	CED-O2D-CGD	2.69	122.01	115.92
18	A	1119	CLA	C3D-C4D-ND	2.69	114.36	109.99
18	B	1242	CLA	CHC-C4B-NB	2.69	128.08	124.05
18	I	1204	CLA	O2D-CGD-O1D	-2.68	118.62	123.85
18	1	1002	CLA	C2C-C1C-CHC	-2.68	118.83	125.84
18	F	4015	CLA	C2C-C1C-CHC	-2.68	118.83	125.84
18	4	1304	CLA	O2A-CGA-O1A	-2.68	116.94	123.63
18	4	4004	CLA	CHB-C4A-NA	2.67	128.23	124.43
18	B	9012	CLA	CAA-C2A-C1A	2.67	120.72	111.97
18	B	1215	CLA	O2D-CGD-O1D	-2.67	118.65	123.85
18	3	2009	CLA	C2C-C1C-CHC	-2.67	118.84	125.84
18	3	3002	CLA	C2C-C1C-CHC	-2.67	118.84	125.84
19	B	5002	PQN	C11-C3-C4	-2.67	115.77	118.58
18	4	1304	CLA	CHC-C4B-NB	2.67	128.05	124.05
18	A	1133	CLA	C3D-C4D-ND	2.67	113.15	109.50
18	2	2006	CLA	C3B-C2B-C1B	-2.67	103.84	106.81
18	B	1301	CLA	C3D-C4D-ND	2.67	113.14	109.50
18	A	1118	CLA	C3D-C4D-ND	2.67	113.14	109.50
18	B	1226	CLA	C2C-C1C-CHC	-2.67	118.85	125.84
18	B	1239	CLA	C4-C3-C5	2.67	119.86	115.23
18	A	1123	CLA	CED-O2D-CGD	2.67	121.96	115.92
18	A	1147	CLA	C2C-C1C-CHC	-2.67	118.86	125.84
18	3	3008	CLA	C2C-C1C-CHC	-2.66	118.86	125.84
18	B	1237	CLA	CMB-C2B-C1B	2.66	129.47	125.42
18	F	1305	CLA	CHB-C4A-NA	2.66	128.22	124.43
20	L	6020	BCR	C39-C30-C25	2.66	114.42	110.24
18	A	1143	CLA	CHB-C4A-NA	2.66	128.21	124.43
18	2	2013	CLA	C2C-C1C-CHC	-2.66	118.87	125.84
18	4	4008	CLA	C3D-C4D-ND	2.66	113.13	109.50
18	B	1223	CLA	CHB-C1B-NB	-2.66	120.24	124.08

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
18	B	1228	CLA	CHC-C1C-C2C	-2.66	119.40	126.95
18	A	1126	CLA	CAC-C3C-C4C	2.66	128.25	124.79
18	3	2009	CLA	C3C-C4C-CHD	-2.66	118.33	125.23
18	3	3003	CLA	C3C-C4C-CHD	-2.66	118.33	125.23
18	B	1301	CLA	CHB-C4A-NA	2.65	128.21	124.43
18	K	1153	CLA	C2C-C1C-CHC	-2.65	118.89	125.84
18	B	1202	CLA	CHB-C4A-NA	2.65	128.22	124.40
18	B	1207	CLA	CHC-C1C-C2C	-2.65	119.42	126.95
18	A	1126	CLA	CHC-C4B-NB	2.65	128.02	124.05
18	B	1213	CLA	CHB-C4A-NA	2.65	128.20	124.43
18	L	1130	CLA	C1-O2A-CGA	2.65	123.06	116.65
18	A	1113	CLA	O2A-CGA-O1A	-2.65	117.01	123.63
18	A	1102	CLA	CHB-C4A-NA	2.65	128.19	124.43
18	F	4015	CLA	CHB-C4A-NA	2.65	128.19	124.43
18	1	1007	CLA	C3D-C4D-ND	2.64	113.11	109.50
18	1	1012	CLA	C3D-C4D-ND	2.64	113.11	109.50
18	H	1505	CLA	C3C-C4C-CHD	-2.64	118.36	125.23
18	B	1208	CLA	C2A-C1A-CHA	-2.64	119.28	123.87
18	4	4007	CLA	CHB-C4A-NA	2.64	128.19	124.43
18	B	1215	CLA	C3B-C2B-C1B	-2.64	104.06	107.17
18	2	2010	CLA	C2C-C1C-CHC	-2.64	118.93	125.84
18	B	1206	CLA	C3B-C2B-C1B	-2.64	103.87	106.81
18	A	1134	CLA	C3C-C4C-CHD	-2.64	118.39	125.23
18	4	4012	CLA	C3C-C4C-CHD	-2.63	118.39	125.23
18	3	3005	CLA	C2C-C1C-CHC	-2.63	118.94	125.84
18	B	1208	CLA	CMB-C2B-C1B	2.63	129.43	125.42
18	4	4004	CLA	C3C-C4C-CHD	-2.63	118.39	125.23
18	J	1307	CLA	C4A-NA-C1A	2.63	107.88	106.68
20	F	6016	BCR	C20-C21-C22	2.63	130.97	127.28
18	2	2006	CLA	C3D-C4D-ND	2.63	113.09	109.50
18	H	1501	CLA	CHB-C4A-NA	2.63	128.19	124.40
18	4	1304	CLA	CHC-C1C-C2C	-2.63	119.48	126.95
18	F	1302	CLA	CHC-C1C-C2C	-2.63	119.48	126.95
18	B	1208	CLA	CAA-CBA-CGA	-2.63	105.75	113.21
20	A	6011	BCR	C29-C28-C27	2.62	117.05	111.28
18	3	3013	CLA	C3D-C4D-ND	2.62	113.08	109.50
18	2	2003	CLA	C2C-C1C-CHC	-2.62	118.97	125.84
18	4	4010	CLA	CHB-C4A-NA	2.62	128.16	124.43
18	B	1224	CLA	C4-C3-C5	2.62	119.21	116.13
18	1	1010	CLA	CHB-C4A-NA	2.62	128.16	124.43
18	2	2006	CLA	C2C-C1C-CHC	-2.62	118.97	125.84
18	B	1203	CLA	O2A-CGA-O1A	-2.62	117.08	123.63

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
18	B	1228	CLA	CHC-C4B-NB	2.62	127.98	124.05
18	B	1241	CLA	C1B-NB-C4B	-2.62	104.47	106.31
18	B	1225	CLA	C3D-C4D-ND	2.62	114.24	109.99
18	L	1504	CLA	CHC-C1C-C2C	-2.62	119.51	126.95
18	K	1153	CLA	C1C-NC-C4C	-2.62	105.48	106.68
18	A	1134	CLA	C3D-C4D-ND	2.62	113.08	109.50
18	L	1503	CLA	CHC-C4B-C3B	-2.62	119.83	127.43
18	B	1234	CLA	O1D-CGD-CBD	-2.62	119.36	124.52
18	4	4002	CLA	C3D-C4D-ND	2.61	113.07	109.50
18	4	4011	CLA	C2C-C1C-CHC	-2.61	118.99	125.84
18	2	2015	CLA	CHB-C4A-NA	2.61	128.15	124.43
18	B	1222	CLA	CHB-C4A-NA	2.61	128.17	124.40
18	A	1136	CLA	CHB-C1B-NB	-2.61	120.13	124.05
18	1	1006	CLA	C2C-C1C-CHC	-2.61	119.00	125.84
18	B	1212	CLA	CGD-CBD-CAD	-2.61	102.40	110.85
18	A	1105	CLA	C2C-C1C-CHC	-2.61	119.01	125.84
18	B	1138	CLA	CHB-C4A-NA	2.61	128.16	124.40
19	B	5002	PQN	C14-C13-C15	2.61	119.75	115.23
20	A	6011	BCR	C24-C23-C22	-2.61	122.38	126.23
18	4	4001	CLA	C3D-C4D-ND	2.61	113.06	109.50
18	B	1205	CLA	C4-C3-C5	2.61	119.75	115.23
18	A	1110	CLA	C3D-C2D-C1D	2.61	110.51	107.35
18	4	4007	CLA	C3C-C4C-CHD	-2.61	118.47	125.23
18	4	1304	CLA	CHB-C4A-NA	2.60	128.16	124.40
18	A	1134	CLA	CHB-C4A-NA	2.60	128.13	124.43
18	3	3012	CLA	C2C-C1C-CHC	-2.60	119.02	125.84
18	A	1119	CLA	CHC-C4B-NB	2.60	127.95	124.05
18	A	1147	CLA	C2D-C3D-C4D	-2.60	104.19	107.35
18	B	1237	CLA	O1D-CGD-CBD	-2.60	119.39	124.52
18	H	1501	CLA	O1D-CGD-CBD	-2.60	119.39	124.52
18	A	1127	CLA	C3C-C4C-CHD	-2.60	118.48	125.23
18	4	4012	CLA	CHC-C4B-NB	2.60	127.83	124.08
20	I	6018	BCR	C3-C4-C5	-2.60	109.43	114.06
18	3	2009	CLA	CHB-C4A-NA	2.60	128.12	124.43
18	J	1308	CLA	C2C-C1C-CHC	-2.59	119.04	125.84
18	B	1238	CLA	CED-O2D-CGD	2.59	121.80	115.92
18	3	3012	CLA	C3C-C4C-CHD	-2.59	118.50	125.23
18	3	3005	CLA	CHB-C4A-NA	2.59	128.12	124.43
18	2	2002	CLA	CHB-C4A-NA	2.59	128.12	124.43
18	3	3009	CLA	C3C-C4C-CHD	-2.59	118.50	125.23
18	4	4002	CLA	C3C-C4C-CHD	-2.59	118.50	125.23
20	L	6020	BCR	C11-C12-C13	-2.59	119.26	126.36

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
18	A	1148	CLA	C3C-C4C-CHD	-2.59	118.50	125.23
18	K	1150	CLA	C3C-C4C-CHD	-2.59	118.50	125.23
18	3	3010	CLA	C2C-C1C-CHC	-2.59	119.06	125.84
18	B	1208	CLA	C3D-C4D-ND	2.59	114.19	109.99
18	A	1124	CLA	C3C-C4C-CHD	-2.59	118.51	125.23
18	B	1211	CLA	C3D-C4D-ND	2.59	113.03	109.50
18	1	1012	CLA	C3C-C4C-CHD	-2.58	118.52	125.23
18	2	2004	CLA	C2C-C1C-CHC	-2.58	119.07	125.84
19	B	5002	PQN	C19-C18-C17	-2.58	102.07	111.27
18	1	1011	CLA	C3C-C4C-CHD	-2.58	118.52	125.23
18	B	9010	CLA	CED-O2D-CGD	2.58	121.77	115.92
18	B	1216	CLA	CAC-C3C-C4C	2.58	128.15	124.79
18	A	1128	CLA	C3D-C4D-ND	2.58	114.18	109.99
18	A	1115	CLA	C4A-NA-C1A	2.58	107.86	106.68
20	B	6017	BCR	C19-C18-C17	2.58	123.07	119.01
18	3	3009	CLA	C3D-C4D-ND	2.58	113.03	109.50
18	4	4009	CLA	C2C-C1C-CHC	-2.58	119.08	125.84
18	B	9022	CLA	CAA-C2A-C3A	-2.58	106.03	113.00
18	2	2001	CLA	C3D-C4D-ND	2.58	113.02	109.50
18	A	1137	CLA	O2A-CGA-CBA	2.58	119.69	111.83
18	B	1237	CLA	C4A-NA-C1A	2.58	107.85	106.68
18	B	1212	CLA	CED-O2D-CGD	2.57	121.76	115.92
18	A	1110	CLA	C3D-C4D-ND	2.57	113.02	109.50
18	A	1129	CLA	O2A-C1-C2	2.57	118.01	108.11
20	F	6016	BCR	C29-C30-C25	-2.57	106.70	110.44
18	A	1108	CLA	CMB-C2B-C1B	2.57	129.34	125.42
18	3	3005	CLA	C3D-C4D-ND	2.57	113.02	109.50
18	1	1005	CLA	C3D-C4D-ND	2.57	113.01	109.50
18	A	1151	CLA	CHB-C4A-NA	2.57	128.09	124.43
18	2	2005	CLA	CHB-C4A-NA	2.57	128.09	124.43
18	B	1229	CLA	CHC-C4B-NB	2.57	127.90	124.05
18	L	1130	CLA	CHC-C1C-C2C	-2.57	119.64	126.95
18	B	1201	CLA	C2C-C1C-CHC	-2.57	119.11	125.84
18	A	1127	CLA	C2D-C3D-C4D	-2.57	104.23	107.35
18	B	1222	CLA	CHB-C1B-NB	-2.57	120.19	124.05
18	H	1505	CLA	CHB-C4A-NA	2.57	128.08	124.43
18	B	9012	CLA	C5-C3-C2	2.57	126.93	121.17
18	2	2001	CLA	C2C-C1C-CHC	-2.57	119.12	125.84
20	F	6016	BCR	C4-C5-C6	-2.57	119.24	122.70
18	4	4006	CLA	CHB-C4A-NA	2.57	128.08	124.43
18	A	1122	CLA	C5-C3-C2	-2.56	115.41	121.17
18	B	1207	CLA	C4D-CHA-C1A	-2.56	118.19	121.24

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
18	1	1001	CLA	C4A-NA-C1A	2.56	107.85	106.68
18	1	1002	CLA	C3C-C4C-CHD	-2.56	118.57	125.23
18	3	3006	CLA	C2C-C1C-CHC	-2.56	119.12	125.84
18	2	2012	CLA	C3D-C4D-ND	2.56	113.00	109.50
18	B	1210	CLA	C4D-ND-C1D	-2.56	104.51	106.31
18	A	1110	CLA	C3C-C4C-CHD	-2.56	118.58	125.23
18	4	1009	CLA	C3B-C2B-C1B	-2.56	103.96	106.81
18	B	1239	CLA	CMB-C2B-C1B	2.56	129.32	125.42
18	4	4005	CLA	C2C-C1C-CHC	-2.56	119.14	125.84
18	B	9023	CLA	CHC-C1C-C2C	-2.56	119.68	126.95
18	A	1134	CLA	C2C-C1C-CHC	-2.56	119.14	125.84
18	A	1148	CLA	C3D-C4D-ND	2.56	112.99	109.50
18	B	1226	CLA	CHB-C4A-NA	2.55	128.06	124.43
18	1	1004	CLA	C3C-C4C-CHD	-2.55	118.61	125.23
18	A	1152	CLA	C3C-C4C-CHD	-2.55	118.61	125.23
18	1	1003	CLA	C3D-C4D-ND	2.55	112.98	109.50
18	2	2007	CLA	CHB-C4A-NA	2.55	128.05	124.43
18	B	1206	CLA	C2C-C1C-CHC	-2.55	119.17	125.84
18	2	2008	CLA	C3D-C4D-ND	2.55	112.98	109.50
18	4	4006	CLA	C3C-C4C-CHD	-2.54	118.63	125.23
18	A	1144	CLA	CHB-C4A-NA	2.54	128.04	124.43
18	4	1009	CLA	C2C-C1C-CHC	-2.54	119.19	125.84
18	A	1151	CLA	C2C-C1C-CHC	-2.53	119.20	125.84
18	L	1130	CLA	C4A-NA-C1A	2.53	107.83	106.68
18	J	2107	CLA	C5-C3-C2	-2.53	115.48	121.17
18	A	1107	CLA	CHB-C1B-NB	-2.53	120.25	124.05
18	B	1219	CLA	O2A-CGA-O1A	-2.53	117.29	123.63
18	1	1007	CLA	C2C-C1C-CHC	-2.53	119.20	125.84
20	I	6018	BCR	C34-C9-C8	-2.53	114.22	118.09
18	1	1011	CLA	CHB-C4A-NA	2.53	128.03	124.43
18	A	1122	CLA	O2A-CGA-CBA	2.53	119.55	111.83
18	A	1115	CLA	C1-O2A-CGA	2.53	123.86	116.67
18	B	1210	CLA	C2C-C1C-CHC	-2.53	119.21	125.84
18	1	1010	CLA	C2C-C1C-CHC	-2.53	119.21	125.84
18	A	1122	CLA	C6-C5-C3	2.53	119.63	113.47
18	I	1204	CLA	CAA-C2A-C1A	-2.53	103.69	111.97
18	B	1211	CLA	CHB-C1B-NB	-2.53	120.43	124.08
18	A	1120	CLA	C2C-C1C-CHC	-2.53	119.22	125.84
18	B	1230	CLA	C2C-C1C-CHC	-2.53	119.22	125.84
18	A	1147	CLA	CHB-C4A-NA	2.53	128.02	124.43
18	K	1141	CLA	CHB-C4A-NA	2.53	128.02	124.43
18	4	4002	CLA	C2C-C1C-CHC	-2.53	119.22	125.84

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
18	2	2003	CLA	C3C-C4C-CHD	-2.53	118.67	125.23
18	B	1202	CLA	CAC-C3C-C2C	-2.53	122.92	127.56
18	L	1125	CLA	CHB-C4A-NA	2.52	128.02	124.43
18	1	1002	CLA	CHB-C4A-NA	2.52	128.02	124.43
18	G	1248	CLA	C3D-C4D-ND	2.52	112.95	109.50
18	1	1012	CLA	C2C-C1C-CHC	-2.52	119.23	125.84
18	1	1008	CLA	CHB-C4A-NA	2.52	128.02	124.43
18	A	1116	CLA	C2C-C1C-CHC	-2.52	119.23	125.84
18	4	4012	CLA	CHB-C1B-NB	-2.52	120.43	124.08
18	A	1116	CLA	C3D-C4D-ND	2.52	112.94	109.50
18	1	1008	CLA	C2C-C1C-CHC	-2.52	119.24	125.84
18	B	1221	CLA	CHC-C4B-C3B	-2.52	116.44	127.37
18	2	2015	CLA	C2C-C1C-CHC	-2.52	119.24	125.84
18	J	2107	CLA	C6-C7-C8	-2.51	107.61	115.97
18	A	1131	CLA	CHC-C4B-C3B	-2.51	120.13	127.43
18	A	1152	CLA	C2C-C1C-CHC	-2.51	119.25	125.84
18	A	1132	CLA	CHB-C4A-NA	2.51	128.00	124.43
18	2	2006	CLA	CHB-C4A-NA	2.51	128.00	124.43
18	A	1137	CLA	CHC-C1C-C2C	-2.51	119.81	126.95
18	3	3013	CLA	C2C-C1C-CHC	-2.51	119.26	125.84
18	A	1309	CLA	CHB-C4A-NA	2.51	128.00	124.43
18	4	4007	CLA	C3D-C4D-ND	2.51	112.93	109.50
18	A	1309	CLA	C2C-C1C-CHC	-2.51	119.26	125.84
18	B	1218	CLA	CHC-C4B-NB	2.51	127.81	124.05
18	4	4010	CLA	C3C-C4C-CHD	-2.51	118.72	125.23
18	B	1226	CLA	C3D-C4D-ND	2.51	112.93	109.50
18	B	1237	CLA	CHB-C4A-NA	2.51	128.02	124.40
18	B	1211	CLA	C2C-C1C-CHC	-2.51	119.28	125.84
18	B	1214	CLA	C4A-NA-C1A	2.51	107.82	106.68
18	1	1004	CLA	C1C-NC-C4C	-2.51	105.54	106.68
18	3	3002	CLA	C3C-C4C-CHD	-2.50	118.72	125.23
18	B	1219	CLA	C4D-CHA-C1A	-2.50	118.26	121.24
20	F	6016	BCR	C34-C9-C10	-2.50	118.76	122.82
18	3	3004	CLA	C2C-C1C-CHC	-2.50	119.28	125.84
18	A	1106	CLA	C3B-C4B-NB	-2.50	108.30	110.53
18	2	2001	CLA	C3C-C4C-CHD	-2.50	118.73	125.23
18	A	1137	CLA	C3D-C4D-ND	2.50	114.05	109.99
18	A	1109	CLA	CHB-C4A-NA	2.50	127.99	124.43
18	1	1006	CLA	CHB-C4A-NA	2.50	127.98	124.43
18	2	2013	CLA	C3D-C4D-ND	2.50	112.92	109.50
18	A	1134	CLA	C4D-ND-C1D	-2.50	104.56	106.31
18	2	2012	CLA	C2C-C1C-CHC	-2.50	119.29	125.84

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
18	B	1138	CLA	C1-C2-C3	2.50	130.29	126.20
18	A	1127	CLA	CHB-C4A-NA	2.50	127.98	124.43
18	B	1227	CLA	C2A-C1A-CHA	-2.50	119.54	123.87
18	A	9013	CLA	O2A-CGA-CBA	2.50	121.57	112.14
18	B	1220	CLA	CHB-C1B-NB	-2.50	120.31	124.05
18	A	1142	CLA	C2C-C1C-CHC	-2.49	119.31	125.84
18	1	1013	CLA	C2C-C1C-CHC	-2.49	119.31	125.84
18	2	2007	CLA	C3D-C4D-ND	2.49	112.91	109.50
18	G	1248	CLA	CHB-C1B-NB	-2.49	120.48	124.08
18	B	1222	CLA	CHC-C1C-C2C	-2.49	119.87	126.95
18	B	1224	CLA	C1-C2-C3	-2.49	122.12	126.20
18	F	1303	CLA	C3C-C4C-CHD	-2.49	118.77	125.23
18	A	1108	CLA	CHC-C1C-C2C	-2.49	119.87	126.95
18	A	9011	CLA	C2C-C1C-NC	2.49	112.60	109.98
18	L	1125	CLA	C3D-C4D-ND	2.49	112.90	109.50
18	A	1136	CLA	CHB-C4A-NA	2.49	127.99	124.40
18	B	1208	CLA	C1D-ND-C4D	-2.49	104.57	106.31
18	H	1501	CLA	CMB-C2B-C1B	2.49	129.20	125.42
18	2	2010	CLA	C3C-C4C-CHD	-2.48	118.78	125.23
18	B	1238	CLA	CHB-C4A-NA	2.48	127.98	124.40
18	1	1014	CLA	C2C-C1C-CHC	-2.48	119.34	125.84
18	4	4002	CLA	CHB-C4A-NA	2.48	127.96	124.43
18	1	1003	CLA	C2C-C1C-CHC	-2.48	119.34	125.84
18	4	4011	CLA	C1C-NC-C4C	-2.48	105.55	106.68
18	2	2007	CLA	C2C-C1C-CHC	-2.48	119.34	125.84
18	1	1004	CLA	C2C-C1C-CHC	-2.48	119.34	125.84
18	F	1302	CLA	C1-C2-C3	2.48	130.26	126.20
18	H	1501	CLA	CHB-C1B-NB	-2.48	120.33	124.05
18	K	1141	CLA	C3D-C4D-ND	2.48	112.89	109.50
18	A	1117	CLA	CHB-C4A-NA	2.48	127.95	124.43
18	4	4006	CLA	CHB-C1B-NB	-2.48	120.50	124.08
18	B	1222	CLA	C1-O2A-CGA	2.48	122.65	116.65
18	2	2011	CLA	C3C-C4C-CHD	-2.48	118.80	125.23
18	G	1248	CLA	CHB-C4A-NA	2.48	127.95	124.43
18	4	4013	CLA	CHB-C4A-NA	2.48	127.95	124.43
18	A	1118	CLA	C2C-C1C-CHC	-2.48	119.35	125.84
18	B	1242	CLA	CED-O2D-CGD	2.48	121.53	115.92
18	3	3008	CLA	C3D-C4D-ND	2.48	112.88	109.50
18	3	3004	CLA	C3C-C4C-CHD	-2.47	118.80	125.23
18	B	1241	CLA	C4A-NA-C1A	2.47	107.81	106.68
18	A	1128	CLA	C2A-C1A-CHA	-2.47	119.57	123.87
18	B	1202	CLA	CHB-C1B-NB	-2.47	120.34	124.05

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
18	1	1012	CLA	C4D-ND-C1D	-2.47	104.58	106.31
18	3	3011	CLA	C2C-C1C-CHC	-2.47	119.37	125.84
18	B	1209	CLA	C4-C3-C5	2.47	119.52	115.23
18	L	1502	CLA	O2A-CGA-CBA	2.47	119.37	111.83
19	B	5002	PQN	C2M-C2-C1	2.47	121.22	116.68
18	B	1219	CLA	CHC-C1C-C2C	-2.47	119.93	126.95
18	A	1108	CLA	CGD-CBD-CAD	-2.47	102.85	110.85
18	B	1234	CLA	CHC-C1C-C2C	-2.47	119.93	126.95
18	B	1223	CLA	C3D-C4D-ND	2.47	112.87	109.50
18	3	3011	CLA	C3C-C4C-CHD	-2.47	118.82	125.23
18	B	1234	CLA	C3D-C4D-ND	2.47	114.00	109.99
18	B	1226	CLA	C3C-C4C-CHD	-2.47	118.82	125.23
18	A	1133	CLA	C3C-C4C-CHD	-2.47	118.83	125.23
18	4	4010	CLA	C2C-C1C-CHC	-2.47	119.38	125.84
18	A	1143	CLA	C3C-C4C-CHD	-2.47	118.83	125.23
18	B	1224	CLA	O2A-CGA-CBA	2.46	119.35	111.83
18	B	1236	CLA	CHB-C4A-NA	2.46	127.95	124.40
18	B	1215	CLA	O1D-CGD-CBD	-2.46	119.66	124.52
18	J	1307	CLA	CHD-C1D-ND	2.46	128.32	124.84
18	B	1218	CLA	CMD-C2D-C3D	-2.46	122.04	127.69
18	L	1502	CLA	C3D-C4D-ND	2.46	113.99	109.99
18	2	2002	CLA	C3D-C4D-ND	2.46	112.86	109.50
18	4	4003	CLA	C3D-C4D-ND	2.46	112.86	109.50
18	A	1113	CLA	C4B-C3B-C2B	2.46	110.36	107.30
18	B	1215	CLA	O2A-CGA-O1A	-2.46	117.48	123.63
18	4	4013	CLA	C3D-C4D-ND	2.46	112.86	109.50
18	A	1131	CLA	C1B-C2B-C3B	-2.46	104.72	107.03
18	L	1503	CLA	CBC-CAC-C3C	-2.46	105.76	112.42
18	A	1137	CLA	C1D-ND-C4D	-2.46	104.59	106.31
18	B	1202	CLA	O2A-CGA-O1A	-2.46	117.49	123.63
18	A	1111	CLA	C3C-C4C-CHD	-2.45	118.86	125.23
18	B	1241	CLA	C3C-C4C-CHD	-2.45	118.86	125.23
18	2	2012	CLA	C3C-C4C-CHD	-2.45	118.86	125.23
18	A	1103	CLA	CAA-C2A-C3A	-2.45	106.37	113.00
18	A	9013	CLA	CMB-C2B-C1B	2.45	129.16	125.42
18	2	2002	CLA	C2C-C1C-CHC	-2.45	119.42	125.84
18	3	3009	CLA	C2C-C1C-CHC	-2.45	119.42	125.84
18	3	3003	CLA	C2C-C1C-CHC	-2.45	119.42	125.84
18	2	2010	CLA	CHB-C4A-NA	2.45	127.92	124.43
18	4	4011	CLA	C3C-C4C-CHD	-2.45	118.87	125.23
18	B	1216	CLA	CHC-C1C-C2C	-2.45	119.98	126.95
18	F	1240	CLA	C3D-C2D-C1D	2.45	110.32	107.35

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
18	B	1216	CLA	CHB-C1B-NB	-2.45	120.38	124.05
18	2	2011	CLA	C3D-C4D-ND	2.45	112.84	109.50
18	4	1009	CLA	C3C-C4C-CHD	-2.45	118.88	125.23
18	B	1224	CLA	CHC-C4B-NB	2.45	127.72	124.05
18	B	1213	CLA	C3D-C4D-ND	2.45	112.84	109.50
18	A	1148	CLA	C2C-C1C-CHC	-2.45	119.43	125.84
18	A	1101	CLA	CHB-C1B-NB	-2.44	120.55	124.08
18	B	1202	CLA	C2D-C1D-ND	-2.44	107.71	110.13
18	3	3005	CLA	C3C-C4C-CHD	-2.44	118.89	125.23
18	3	3004	CLA	C3D-C4D-ND	2.44	112.84	109.50
18	4	4005	CLA	C3C-C4C-CHD	-2.44	118.89	125.23
18	B	1229	CLA	CHB-C1B-NB	-2.44	120.39	124.05
18	B	1221	CLA	C2D-C1D-ND	-2.44	107.71	110.13
18	4	4004	CLA	C2C-C1C-CHC	-2.44	119.45	125.84
18	2	2005	CLA	C2C-C1C-CHC	-2.44	119.45	125.84
18	3	3010	CLA	CHB-C4A-NA	2.44	127.90	124.43
18	L	1125	CLA	C2C-C1C-CHC	-2.44	119.45	125.84
18	B	1227	CLA	C2B-C1B-NB	2.44	112.85	110.33
18	A	1109	CLA	C3C-C4C-CHD	-2.44	118.90	125.23
18	L	1130	CLA	CMA-C3A-C2A	-2.43	104.57	113.98
18	B	1207	CLA	CHB-C1B-NB	-2.43	120.40	124.05
18	1	1013	CLA	CHB-C4A-NA	2.43	127.89	124.43
18	A	1132	CLA	CHD-C1D-ND	2.43	128.28	124.84
18	H	1505	CLA	C2C-C1C-CHC	-2.43	119.47	125.84
18	K	1150	CLA	C3D-C4D-ND	2.43	112.82	109.50
18	A	1105	CLA	C3C-C4C-CHD	-2.43	118.92	125.23
18	L	1125	CLA	C3C-C4C-CHD	-2.43	118.92	125.23
18	B	1215	CLA	CHB-C4A-NA	2.43	127.91	124.40
18	B	1238	CLA	CAC-C3C-C4C	2.43	127.95	124.79
18	A	9011	CLA	O2A-CGA-O1A	-2.43	117.55	123.63
18	4	4005	CLA	CHB-C4A-NA	2.43	127.88	124.43
18	1	1008	CLA	C3C-C4C-CHD	-2.43	118.92	125.23
18	A	1110	CLA	C2C-C1C-CHC	-2.43	119.48	125.84
18	B	1215	CLA	CHC-C4B-C3B	-2.43	116.83	127.37
18	B	1231	CLA	CMB-C2B-C1B	2.43	129.12	125.42
18	A	1136	CLA	CMC-C2C-C1C	2.43	128.83	125.03
18	A	1117	CLA	C3C-C4C-CHD	-2.43	118.93	125.23
18	B	1230	CLA	C3C-C4C-CHD	-2.43	118.93	125.23
18	2	2005	CLA	C3C-C4C-CHD	-2.43	118.93	125.23
18	4	4001	CLA	C2C-C1C-CHC	-2.43	119.49	125.84
18	4	4009	CLA	C3D-C4D-ND	2.42	112.81	109.50
18	B	1222	CLA	C1D-ND-C4D	-2.42	104.61	106.31

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
18	F	1302	CLA	CHB-C1B-NB	-2.42	120.41	124.05
20	L	6020	BCR	C31-C1-C6	-2.42	106.44	110.24
18	A	1119	CLA	O1D-CGD-CBD	-2.42	119.74	124.52
18	A	1146	CLA	CHB-C4A-NA	2.42	127.87	124.43
18	3	3009	CLA	CHB-C4A-NA	2.42	127.87	124.43
18	3	3007	CLA	C3C-C4C-CHD	-2.42	118.94	125.23
18	A	1122	CLA	CBC-CAC-C3C	2.42	118.98	112.42
18	B	1235	CLA	CHD-C4C-NC	2.42	127.98	124.23
18	2	2008	CLA	CHB-C4A-NA	2.42	127.87	124.43
18	4	4003	CLA	C2C-C1C-CHC	-2.42	119.50	125.84
18	B	1202	CLA	C1-O2A-CGA	2.42	122.51	116.65
18	B	1221	CLA	C2B-C1B-NB	2.42	112.83	110.33
18	2	2002	CLA	C3C-C4C-CHD	-2.42	118.95	125.23
18	3	3006	CLA	C3D-C4D-ND	2.42	112.81	109.50
18	2	2011	CLA	C2C-C1C-CHC	-2.42	119.50	125.84
18	B	9012	CLA	O1D-CGD-CBD	-2.42	119.75	124.52
18	1	1013	CLA	C3C-C4C-CHD	-2.42	118.95	125.23
18	3	3008	CLA	C3C-C4C-CHD	-2.42	118.95	125.23
18	A	1128	CLA	O2A-CGA-O1A	-2.42	117.58	123.63
18	B	1212	CLA	CHB-C1B-NB	-2.42	120.42	124.05
18	L	1503	CLA	O2A-CGA-O1A	-2.42	117.58	123.63
20	B	6017	BCR	C34-C9-C8	2.42	121.78	118.09
18	B	1215	CLA	C2C-C1C-NC	2.42	112.52	109.98
18	A	1117	CLA	C2C-C1C-CHC	-2.42	119.51	125.84
18	A	1122	CLA	CMB-C2B-C1B	2.41	129.10	125.42
18	L	1504	CLA	C4-C3-C5	2.41	119.42	115.23
18	L	1504	CLA	CMB-C2B-C1B	2.41	129.09	125.42
18	A	1106	CLA	C2C-C1C-NC	2.41	112.51	109.98
18	4	4001	CLA	CHB-C1B-NB	-2.41	120.60	124.08
18	B	1241	CLA	C1C-NC-C4C	-2.41	105.58	106.68
18	B	1230	CLA	C3D-C4D-ND	2.41	112.79	109.50
18	1	1004	CLA	C3D-C4D-ND	2.41	112.79	109.50
18	F	1139	CLA	CAA-C2A-C1A	2.41	119.86	111.97
18	4	4013	CLA	C2C-C1C-CHC	-2.41	119.53	125.84
18	A	1113	CLA	CBA-CAA-C2A	2.41	120.95	113.79
18	A	1102	CLA	C2C-C1C-CHC	-2.41	119.54	125.84
18	B	1208	CLA	C3A-C2A-C1A	2.40	104.94	101.34
18	A	1118	CLA	C3C-C4C-CHD	-2.40	118.99	125.23
18	2	2004	CLA	CHB-C4A-NA	2.40	127.85	124.43
18	B	1209	CLA	O2A-CGA-O1A	-2.40	117.61	123.63
18	B	1221	CLA	CHB-C1B-NB	-2.40	120.44	124.05
18	F	1306	CLA	CHB-C1B-NB	-2.40	120.61	124.08

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
18	3	3010	CLA	C3C-C4C-CHD	-2.40	118.99	125.23
18	3	3004	CLA	CHB-C1B-NB	-2.40	120.61	124.08
18	1	1011	CLA	C2C-C1C-CHC	-2.40	119.55	125.84
20	F	6016	BCR	C29-C28-C27	2.40	116.56	111.28
18	B	1210	CLA	CHB-C1B-NB	-2.40	120.61	124.08
18	A	1123	CLA	C3D-C4D-ND	2.40	113.89	109.99
18	B	1301	CLA	CHB-C1B-NB	-2.40	120.61	124.08
18	F	1240	CLA	C2C-C1C-CHC	-2.40	119.55	125.84
18	B	1229	CLA	C5-C3-C4	2.40	120.11	114.59
18	B	1231	CLA	CMA-C3A-C4A	-2.40	105.32	111.77
18	L	1504	CLA	C2A-C1A-CHA	-2.40	119.70	123.87
18	A	1113	CLA	CMB-C2B-C1B	2.40	129.07	125.42
18	B	1211	CLA	C3C-C4C-CHD	-2.40	119.00	125.23
18	1	1014	CLA	C3C-C4C-CHD	-2.40	119.00	125.23
20	I	6018	BCR	C4-C5-C6	-2.40	119.46	122.70
18	B	1206	CLA	CHD-C1D-ND	2.40	128.23	124.84
18	A	1144	CLA	C3C-C4C-CHD	-2.40	119.00	125.23
18	B	1242	CLA	CHC-C1C-C2C	-2.40	120.13	126.95
18	F	1303	CLA	C3D-C4D-ND	2.40	112.78	109.50
18	A	1128	CLA	CHC-C1C-C2C	-2.40	120.14	126.95
18	3	3006	CLA	C3C-C4C-CHD	-2.40	119.01	125.23
18	B	1231	CLA	CAC-C3C-C4C	2.39	127.91	124.79
20	B	6017	BCR	C1-C6-C7	2.39	122.14	115.65
18	L	1503	CLA	C4D-CHA-C1A	-2.39	118.39	121.24
18	4	4012	CLA	C3D-C4D-ND	2.39	112.77	109.50
18	4	4008	CLA	CHB-C4A-NA	2.39	127.83	124.43
18	A	1113	CLA	C1D-ND-C4D	-2.39	104.63	106.31
18	A	1136	CLA	C4-C3-C5	2.39	119.38	115.23
18	F	1306	CLA	C2C-C1C-CHC	-2.39	119.58	125.84
18	L	1130	CLA	CHB-C4A-NA	2.39	127.85	124.40
18	B	1138	CLA	CAA-C2A-C1A	-2.39	104.14	111.97
18	3	3015	CLA	C3D-C4D-ND	2.39	112.76	109.50
18	3	3015	CLA	C2C-C1C-CHC	-2.39	119.59	125.84
18	4	4007	CLA	C2C-C1C-CHC	-2.39	119.59	125.84
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	F	4015	CLA	C3C-C4C-CHD	-2.39	119.03	125.23
20	I	6018	BCR	C1-C6-C5	-2.39	119.38	122.64
18	A	1110	CLA	CHD-C1D-ND	2.39	128.21	124.84
18	4	4005	CLA	CHD-C1D-ND	2.39	128.21	124.84
18	B	1216	CLA	C1D-ND-C4D	-2.38	104.64	106.31

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
18	2	2012	CLA	CHB-C1B-NB	-2.38	120.64	124.08
18	A	1146	CLA	C3C-C4C-CHD	-2.38	119.04	125.23
18	4	4009	CLA	C3C-C4C-CHD	-2.38	119.04	125.23
18	4	4010	CLA	C3D-C4D-ND	2.38	112.75	109.50
18	B	9010	CLA	O2A-CGA-CBA	2.38	119.09	111.83
18	B	1231	CLA	CHB-C4A-NA	2.38	127.84	124.40
18	4	1304	CLA	C4-C3-C5	2.38	119.36	115.23
18	4	4011	CLA	C2D-C3D-C4D	-2.38	104.46	107.35
18	A	1101	CLA	C4D-ND-C1D	-2.38	104.64	106.31
18	B	1205	CLA	CHB-C4A-NA	2.38	127.83	124.40
18	B	1238	CLA	O2A-CGA-CBA	2.38	119.08	111.83
18	B	1215	CLA	C2B-C1B-NB	2.38	112.79	110.33
18	4	4008	CLA	C2C-C1C-CHC	-2.38	119.61	125.84
18	3	3006	CLA	CHB-C4A-NA	2.38	127.81	124.43
18	4	4004	CLA	C3D-C4D-ND	2.38	112.75	109.50
18	A	1102	CLA	C3C-C4C-CHD	-2.38	119.06	125.23
18	A	1135	CLA	C4A-NA-C1A	2.37	107.76	106.68
18	A	1140	CLA	O1D-CGD-CBD	-2.37	119.84	124.52
18	2	2015	CLA	C3D-C4D-ND	2.37	112.74	109.50
18	B	1209	CLA	C1-C2-C3	2.37	130.09	126.20
18	B	1205	CLA	CED-O2D-CGD	2.37	121.30	115.92
18	1	1007	CLA	CHB-C4A-NA	2.37	127.80	124.43
18	2	2005	CLA	C4D-ND-C1D	-2.37	104.65	106.31
18	A	1102	CLA	C3D-C4D-ND	2.37	112.74	109.50
18	A	1124	CLA	C3D-C4D-ND	2.37	112.74	109.50
18	B	9012	CLA	CHC-C1C-C2C	-2.37	120.21	126.95
18	1	1008	CLA	CHD-C1D-ND	2.37	128.19	124.84
18	A	1126	CLA	CMA-C3A-C4A	-2.37	105.40	111.77
18	B	9012	CLA	C1D-ND-C4D	-2.37	104.65	106.31
18	A	1132	CLA	C2C-C1C-CHC	-2.37	119.63	125.84
18	A	1309	CLA	C3D-C4D-ND	2.37	112.74	109.50
18	B	1238	CLA	C3D-C4D-ND	2.37	113.84	109.99
18	F	1305	CLA	C3C-C4C-CHD	-2.37	119.08	125.23
18	F	1305	CLA	C3D-C4D-ND	2.37	112.74	109.50
18	1	1013	CLA	C3D-C4D-ND	2.37	112.73	109.50
18	A	1128	CLA	C4A-NA-C1A	2.37	107.76	106.68
18	B	1239	CLA	CHB-C4A-NA	2.37	127.81	124.40
18	F	1139	CLA	CGD-CBD-CAD	-2.36	103.19	110.85
18	B	9010	CLA	CAA-C2A-C3A	-2.36	106.61	113.00
18	A	1104	CLA	C2C-C1C-CHC	-2.36	119.65	125.84
18	A	1140	CLA	O2A-CGA-O1A	-2.36	117.72	123.63
18	1	1008	CLA	C3D-C4D-ND	2.36	112.73	109.50

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
18	3	3004	CLA	C4D-ND-C1D	-2.36	104.66	106.31
18	G	1233	CLA	O1D-CGD-CBD	-2.36	119.86	124.52
18	A	1122	CLA	CHC-C1C-C2C	-2.36	120.24	126.95
18	1	1003	CLA	C3C-C4C-CHD	-2.36	119.10	125.23
18	A	1111	CLA	C3D-C4D-ND	2.36	112.72	109.50
18	A	1146	CLA	C3D-C4D-ND	2.36	112.72	109.50
18	B	1218	CLA	C1D-ND-C4D	-2.36	104.66	106.31
18	1	1010	CLA	C3C-C4C-CHD	-2.36	119.11	125.23
18	B	1238	CLA	CMB-C2B-C3B	2.36	132.09	126.55
18	A	1123	CLA	CHC-C1C-C2C	-2.35	120.26	126.95
18	3	3007	CLA	C3D-C4D-ND	2.35	112.72	109.50
18	4	4001	CLA	C3C-C4C-CHD	-2.35	119.12	125.23
18	A	1143	CLA	C3D-C4D-ND	2.35	112.72	109.50
20	F	6016	BCR	C1-C6-C5	-2.35	119.42	122.64
18	B	1202	CLA	CED-O2D-CGD	2.35	121.25	115.92
18	B	1221	CLA	C2C-C1C-NC	2.35	112.45	109.98
18	B	1235	CLA	C2C-C1C-NC	2.35	112.45	109.98
18	B	1236	CLA	CMA-C3A-C2A	-2.35	104.89	113.98
18	K	1150	CLA	C2C-C1C-CHC	-2.35	119.68	125.84
18	A	1140	CLA	CAC-C3C-C4C	2.35	127.85	124.79
18	B	1241	CLA	C2C-C1C-CHC	-2.35	119.68	125.84
18	B	1217	CLA	C3D-C4D-ND	2.35	113.81	109.99
18	B	1219	CLA	CHB-C4A-NA	2.35	127.79	124.40
18	1	1005	CLA	CHB-C1B-NB	-2.35	120.69	124.08
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	1	1002	CLA	C3D-C4D-ND	2.35	112.71	109.50
18	A	1103	CLA	CED-O2D-CGD	2.35	121.24	115.92
18	F	1306	CLA	C3C-C4C-CHD	-2.35	119.14	125.23
18	3	3011	CLA	CHB-C4A-NA	2.34	127.76	124.43
18	J	2107	CLA	CHC-C1C-C2C	-2.34	120.29	126.95
18	A	1126	CLA	O2A-CGA-O1A	-2.34	117.77	123.63
18	A	1119	CLA	C1-O2A-CGA	2.34	122.32	116.65
18	3	3015	CLA	C3C-C4C-CHD	-2.34	119.15	125.23
18	3	3002	CLA	CHB-C4A-NA	2.34	127.76	124.43
18	A	1136	CLA	O2D-CGD-O1D	-2.34	119.29	123.85
18	A	1111	CLA	C2C-C1C-CHC	-2.34	119.71	125.84
18	4	4006	CLA	C2C-C1C-CHC	-2.34	119.71	125.84
18	B	1205	CLA	CBC-CAC-C3C	-2.34	106.08	112.42
20	I	6018	BCR	C21-C20-C19	2.34	129.97	123.20
18	J	1307	CLA	C3D-C4D-ND	2.34	112.69	109.50
18	2	2008	CLA	C3C-C4C-CHD	-2.34	119.16	125.23

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
18	B	1218	CLA	CGD-CBD-CAD	2.33	118.40	110.85
18	B	1241	CLA	CHD-C1D-ND	2.33	128.14	124.84
18	B	9010	CLA	C3B-C4B-NB	-2.33	108.45	110.53
18	B	1232	CLA	C4-C3-C5	2.33	119.27	115.23
18	B	1210	CLA	CHB-C4A-NA	2.33	127.74	124.43
18	1	1004	CLA	CHD-C1D-ND	2.33	128.13	124.84
18	B	1208	CLA	CED-O2D-CGD	2.33	121.20	115.92
18	A	1119	CLA	O2D-CGD-O1D	-2.33	119.32	123.85
18	1	1001	CLA	C2C-C1C-CHC	-2.33	119.74	125.84
18	3	3001	CLA	C2C-C1C-CHC	-2.33	119.75	125.84
18	A	9013	CLA	C4B-C3B-C2B	2.33	110.19	107.30
18	3	3015	CLA	C1C-NC-C4C	-2.33	105.62	106.68
18	K	1141	CLA	C3C-C4C-CHD	-2.33	119.19	125.23
18	B	9022	CLA	C2D-C1D-ND	-2.32	107.83	110.13
18	A	1136	CLA	CHC-C1C-C2C	-2.32	120.34	126.95
18	B	1214	CLA	CHB-C4A-NA	2.32	127.75	124.40
18	F	1303	CLA	C2C-C1C-CHC	-2.32	119.75	125.84
18	B	1210	CLA	C3D-C4D-ND	2.32	112.67	109.50
18	A	1146	CLA	CHD-C1D-ND	2.32	128.12	124.84
18	B	1213	CLA	C2C-C1C-CHC	-2.32	119.76	125.84
18	A	1101	CLA	C3C-C4C-CHD	-2.32	119.20	125.23
18	1	1001	CLA	C3C-C4C-CHD	-2.32	119.20	125.23
18	A	1127	CLA	CHB-C1B-NB	-2.32	120.72	124.08
18	A	1119	CLA	C2A-C1A-CHA	-2.32	119.84	123.87
18	B	1212	CLA	CHC-C1C-C2C	-2.32	120.35	126.95
18	B	9012	CLA	C6-C5-C3	-2.32	107.82	113.47
18	B	9022	CLA	C3B-C4B-NB	-2.32	108.46	110.53
18	B	1218	CLA	O2A-CGA-CBA	2.32	118.90	111.83
18	A	1140	CLA	C2A-C1A-CHA	-2.31	119.85	123.87
18	B	9023	CLA	CHB-C1B-NB	-2.31	120.58	124.05
18	L	1503	CLA	C2B-C1B-NB	2.31	112.72	110.33
18	B	1225	CLA	C4B-C3B-C2B	2.31	110.18	107.30
18	3	3001	CLA	C3C-C4C-CHD	-2.31	119.23	125.23
18	A	1124	CLA	C1C-CHC-C4B	-2.31	119.95	126.04
18	F	1302	CLA	O1D-CGD-CBD	-2.31	119.96	124.52
18	2	2007	CLA	CHB-C1B-NB	-2.31	120.74	124.08
18	A	1309	CLA	C3C-C4C-CHD	-2.31	119.23	125.23
18	B	1220	CLA	CHC-C1C-C2C	-2.31	120.39	126.95
18	B	9010	CLA	O1D-CGD-CBD	-2.31	119.97	124.52
18	4	1304	CLA	CHB-C1B-NB	-2.31	120.59	124.05
18	1	1011	CLA	CHB-C1B-NB	-2.30	120.75	124.08
18	A	1131	CLA	CED-O2D-CGD	2.30	121.14	115.92

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
18	4	4003	CLA	CHB-C4A-NA	2.30	127.70	124.43
18	J	1307	CLA	CHB-C4A-NA	2.30	127.70	124.43
18	L	1130	CLA	C3D-C4D-ND	2.30	113.72	109.99
18	4	1304	CLA	C4-C3-C2	-2.30	117.73	123.63
18	B	1301	CLA	C3C-C4C-CHD	-2.29	119.27	125.23
18	A	1117	CLA	CHD-C1D-ND	2.29	128.08	124.84
18	F	1302	CLA	CED-O2D-CGD	2.29	121.12	115.92
19	A	5001	PQN	C14-C13-C15	2.29	119.21	115.23
18	2	2003	CLA	C4D-ND-C1D	-2.29	104.70	106.31
18	A	1110	CLA	CHB-C4A-NA	2.29	127.69	124.43
20	L	6020	BCR	C16-C15-C14	2.29	128.21	123.52
18	A	1123	CLA	C1D-ND-C4D	-2.29	104.70	106.31
18	A	1116	CLA	CHB-C1B-NB	-2.29	120.77	124.08
18	B	1202	CLA	O2A-CGA-CBA	2.29	118.82	111.83
18	B	1235	CLA	CBC-CAC-C3C	2.29	118.62	112.42
18	B	1216	CLA	CMB-C2B-C1B	2.29	128.90	125.42
18	B	9010	CLA	O2A-CGA-O1A	-2.29	117.91	123.63
18	B	1223	CLA	C3B-C2B-C1B	-2.29	104.26	106.81
18	B	1213	CLA	CHD-C1D-ND	2.29	128.07	124.84
20	L	6020	BCR	C1-C6-C7	2.29	121.85	115.65
18	A	1129	CLA	CBA-CAA-C2A	2.29	120.60	113.79
18	A	1104	CLA	C3C-C4C-CHD	-2.29	119.29	125.23
18	B	1208	CLA	C5-C3-C2	2.29	126.30	121.17
18	B	1205	CLA	C1-O2A-CGA	2.29	122.18	116.65
18	2	2013	CLA	C3C-C4C-CHD	-2.28	119.30	125.23
18	B	1138	CLA	C3A-C2A-C1A	2.28	104.76	101.34
18	3	3002	CLA	C3D-C4D-ND	2.28	112.62	109.50
18	2	2012	CLA	CHB-C4A-NA	2.28	127.68	124.43
18	3	3015	CLA	CHB-C4A-NA	2.28	127.67	124.43
18	4	4008	CLA	C3C-C4C-CHD	-2.28	119.31	125.23
18	B	1235	CLA	C2D-C1D-ND	-2.28	107.87	110.13
18	A	1116	CLA	C3C-C4C-CHD	-2.28	119.31	125.23
18	A	1136	CLA	C4-C3-C2	-2.28	117.77	123.63
18	2	2004	CLA	C3C-C4C-CHD	-2.28	119.31	125.23
18	B	1216	CLA	C2A-C1A-CHA	-2.28	119.91	123.87
18	B	1237	CLA	C2D-C1D-ND	-2.28	107.87	110.13
18	B	1217	CLA	O2A-CGA-O1A	-2.28	117.93	123.63
18	A	1123	CLA	O2A-CGA-O1A	-2.28	117.94	123.63
20	A	6011	BCR	C19-C18-C17	2.27	122.59	119.01
18	A	1123	CLA	C4-C3-C5	2.27	119.17	115.23
19	A	5001	PQN	O4-C4-C3	2.27	124.32	120.67
18	B	1217	CLA	C1-O2A-CGA	2.27	122.15	116.65

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
20	F	6016	BCR	C30-C25-C24	2.27	121.81	115.65
18	B	9012	CLA	C3D-C4D-ND	2.27	113.68	109.99
18	A	1108	CLA	C1D-ND-C4D	-2.27	104.72	106.31
18	B	1221	CLA	CMB-C2B-C1B	2.27	128.88	125.42
18	A	1132	CLA	C3C-C4C-CHD	-2.27	119.34	125.23
18	1	1007	CLA	C4D-ND-C1D	-2.27	104.72	106.31
18	B	1138	CLA	CAC-C3C-C4C	2.27	127.74	124.79
18	B	1138	CLA	O2D-CGD-O1D	-2.27	119.44	123.85
18	A	1151	CLA	C3D-C4D-ND	2.27	112.60	109.50
18	A	1103	CLA	CHD-C4C-C3C	-2.27	121.47	124.77
18	A	1106	CLA	CGD-CBD-CAD	2.27	118.18	110.85
18	B	1239	CLA	CAC-C3C-C4C	2.26	127.74	124.79
18	B	1217	CLA	O2A-CGA-CBA	2.26	118.74	111.83
20	B	6017	BCR	C31-C1-C6	-2.26	106.69	110.24
18	1	1005	CLA	C2C-C1C-CHC	-2.26	119.91	125.84
18	F	1240	CLA	C3C-C4C-CHD	-2.26	119.36	125.23
18	A	9013	CLA	CHB-C1B-NB	-2.26	120.66	124.05
18	A	1133	CLA	CHB-C4A-NA	2.26	127.64	124.43
18	B	1207	CLA	CAA-C2A-C1A	-2.26	104.57	111.97
18	B	1213	CLA	C3C-C4C-CHD	-2.26	119.36	125.23
18	A	1136	CLA	O2A-CGA-O1A	-2.26	117.97	123.63
18	B	1301	CLA	C2C-C1C-CHC	-2.26	119.92	125.84
18	3	3013	CLA	CHB-C4A-NA	2.26	127.64	124.43
18	A	1152	CLA	CHB-C4A-NA	2.26	127.64	124.43
18	B	1218	CLA	CHC-C1C-C2C	-2.26	120.53	126.95
18	K	1153	CLA	C3C-C4C-CHD	-2.26	119.37	125.23
20	L	6020	BCR	C35-C13-C12	-2.26	114.64	118.09
18	F	1306	CLA	CHB-C4A-NA	2.26	127.64	124.43
18	J	2107	CLA	O2A-CGA-CBA	2.26	118.71	111.83
18	G	1248	CLA	C4D-ND-C1D	-2.25	104.73	106.31
18	B	1208	CLA	CBC-CAC-C3C	2.25	118.53	112.42
18	L	1504	CLA	C3D-C4D-ND	2.25	113.65	109.99
18	A	1118	CLA	CHB-C1B-NB	-2.25	120.83	124.08
18	A	1147	CLA	CHB-C1B-NB	-2.25	120.83	124.08
20	L	6020	BCR	C29-C28-C27	2.25	116.22	111.28
18	3	3011	CLA	C3D-C4D-ND	2.25	112.58	109.50
18	A	1146	CLA	C2C-C1C-CHC	-2.25	119.95	125.84
18	A	1123	CLA	CHB-C4A-NA	2.25	127.64	124.40
18	B	1214	CLA	CHC-C1C-C2C	-2.25	120.56	126.95
18	B	1224	CLA	O1D-CGD-CBD	-2.25	120.09	124.52
18	K	1141	CLA	C2C-C1C-CHC	-2.25	119.95	125.84
18	A	1123	CLA	C4A-NA-C1A	2.25	107.70	106.68

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
18	4	4012	CLA	C2D-C3D-C4D	-2.25	104.62	107.35
18	1	1010	CLA	C3D-C4D-ND	2.24	112.57	109.50
18	L	1130	CLA	O2A-C1-C2	2.24	116.75	108.11
18	B	1224	CLA	CED-O2D-CGD	2.24	121.01	115.92
18	F	1302	CLA	CMA-C3A-C2A	-2.24	105.31	113.98
18	B	1227	CLA	CHC-C4B-C3B	-2.24	117.64	127.37
18	A	1143	CLA	C2C-C1C-CHC	-2.24	119.97	125.84
18	3	3002	CLA	CHD-C1D-ND	2.24	128.01	124.84
20	A	6011	BCR	C29-C30-C25	2.24	113.69	110.44
18	2	2015	CLA	C3C-C4C-CHD	-2.24	119.41	125.23
18	B	1208	CLA	CHB-C4A-NA	2.24	127.63	124.40
18	A	1140	CLA	C4B-C3B-C2B	2.24	110.09	107.30
18	F	1240	CLA	CHB-C1B-NB	-2.24	120.85	124.08
18	3	3012	CLA	CHB-C4A-NA	2.24	127.61	124.43
18	B	1201	CLA	C3C-C4C-CHD	-2.24	119.42	125.23
18	J	1307	CLA	C3C-C4C-CHD	-2.23	119.43	125.23
18	B	1205	CLA	CAA-C2A-C3A	-2.23	106.96	113.00
18	4	1304	CLA	C1-O2A-CGA	2.23	122.06	116.65
18	2	2013	CLA	CHB-C4A-NA	2.23	127.61	124.43
18	B	1234	CLA	C2B-C1B-NB	2.23	112.64	110.33
20	B	6017	BCR	C35-C13-C12	2.23	121.50	118.09
18	B	1218	CLA	C1-O2A-CGA	2.23	122.06	116.65
18	B	1211	CLA	CHB-C4A-NA	2.23	127.60	124.43
18	3	3013	CLA	C3C-C4C-CHD	-2.23	119.44	125.23
18	A	1103	CLA	O2A-CGA-CBA	2.23	118.64	111.83
18	B	1215	CLA	CMC-C2C-C3C	2.23	132.18	126.15
18	A	1131	CLA	CHC-C4B-NB	2.23	127.39	124.05
18	4	4003	CLA	CHD-C1D-ND	2.23	127.99	124.84
18	3	3010	CLA	C3D-C4D-ND	2.23	112.54	109.50
20	B	6017	BCR	C12-C13-C14	-2.23	115.51	119.01
18	4	4013	CLA	CHD-C1D-ND	2.22	127.99	124.84
18	L	1502	CLA	C4A-NA-C1A	2.22	107.69	106.68
18	A	1129	CLA	C3D-C4D-ND	2.22	113.60	109.99
18	4	4001	CLA	CHB-C4A-NA	2.22	127.59	124.43
18	J	2107	CLA	CAA-CBA-CGA	-2.22	106.89	113.21
18	2	2011	CLA	CHB-C4A-NA	2.22	127.59	124.43
18	A	1134	CLA	C1C-NC-C4C	-2.22	105.67	106.68
18	1	1001	CLA	CHB-C4A-NA	2.22	127.59	124.43
18	B	1241	CLA	C3D-C4D-ND	2.22	112.54	109.50
18	3	3012	CLA	C3D-C4D-ND	2.22	112.53	109.50
18	3	3003	CLA	C3D-C4D-ND	2.22	112.53	109.50
20	L	6020	BCR	C34-C9-C10	-2.22	119.22	122.82

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
18	3	3006	CLA	CHB-C1B-NB	-2.22	120.87	124.08
18	4	4003	CLA	C3C-C4C-CHD	-2.22	119.47	125.23
18	A	1126	CLA	CHC-C1C-C2C	-2.22	120.64	126.95
18	1	1004	CLA	CHB-C4A-NA	2.22	127.58	124.43
18	A	1126	CLA	C3A-C2A-C1A	2.22	104.66	101.34
18	B	1227	CLA	C5-C3-C4	2.22	119.69	114.59
18	B	1210	CLA	C3C-C4C-CHD	-2.22	119.47	125.23
18	B	1208	CLA	CHC-C1C-C2C	-2.22	120.65	126.95
18	B	1234	CLA	C4D-CHA-C1A	2.22	123.89	121.24
18	A	1133	CLA	CHB-C1B-NB	-2.22	120.88	124.08
18	4	4007	CLA	CHB-C1B-NB	-2.21	120.88	124.08
18	B	1228	CLA	CBC-CAC-C3C	-2.21	106.42	112.42
18	B	1217	CLA	CHB-C4A-NA	2.21	127.59	124.40
18	I	1204	CLA	C3D-C4D-ND	2.21	113.58	109.99
18	2	2012	CLA	C4D-ND-C1D	-2.21	104.76	106.31
18	B	1224	CLA	CMB-C2B-C1B	2.21	128.79	125.42
18	A	1152	CLA	C3D-C4D-ND	2.21	112.52	109.50
18	B	1226	CLA	CHB-C1B-NB	-2.21	120.89	124.08
18	B	1234	CLA	C5-C3-C4	2.21	119.67	114.59
18	B	1229	CLA	O1D-CGD-CBD	-2.21	120.16	124.52
18	1	1012	CLA	CHB-C1B-NB	-2.21	120.89	124.08
18	A	9011	CLA	O2D-CGD-O1D	-2.21	119.55	123.85
18	F	4015	CLA	C3D-C4D-ND	2.21	112.52	109.50
18	A	1129	CLA	C4-C3-C5	2.21	119.06	115.23
18	A	1128	CLA	C4D-CHA-C1A	-2.20	118.61	121.24
18	B	1201	CLA	CHB-C1B-NB	-2.20	120.89	124.08
18	A	1143	CLA	CHB-C1B-NB	-2.20	120.89	124.08
18	B	1222	CLA	O1D-CGD-CBD	-2.20	120.17	124.52
18	H	1505	CLA	C3D-C4D-ND	2.20	112.51	109.50
18	L	1502	CLA	CHC-C1C-C2C	-2.20	120.69	126.95
18	A	1120	CLA	C3C-C4C-CHD	-2.20	119.51	125.23
18	A	1131	CLA	CHB-C1B-NB	-2.20	120.75	124.05
18	1	1014	CLA	CHB-C1B-NB	-2.20	120.90	124.08
18	B	1212	CLA	CMB-C2B-C1B	2.20	128.77	125.42
18	A	1135	CLA	CHB-C4A-NA	2.20	127.58	124.40
18	B	1209	CLA	C1-O2A-CGA	2.20	121.97	116.65
18	A	1131	CLA	CAA-C2A-C3A	-2.20	107.06	113.00
18	L	1502	CLA	C1D-ND-C4D	-2.20	104.77	106.31
18	A	1107	CLA	CHB-C4A-NA	2.20	127.57	124.40
20	I	6018	BCR	C15-C14-C13	2.20	130.36	127.28
18	H	1501	CLA	CAA-C2A-C3A	2.20	118.93	113.00
18	A	1131	CLA	C2A-C1A-CHA	-2.19	120.06	123.87

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
18	B	1208	CLA	C4A-NA-C1A	2.19	107.68	106.68
18	3	3005	CLA	C2B-C3B-C4B	2.19	109.25	106.81
18	B	1232	CLA	C1-O2A-CGA	2.19	121.95	116.65
18	1	1005	CLA	C3C-C4C-CHD	-2.19	119.55	125.23
18	3	3006	CLA	CHD-C1D-ND	2.19	127.93	124.84
18	A	1128	CLA	CMA-C3A-C2A	-2.19	105.52	113.98
18	2	2004	CLA	CHD-C1D-ND	2.19	127.93	124.84
18	3	3012	CLA	CHD-C1D-ND	2.19	127.93	124.84
18	A	1128	CLA	C1-C2-C3	-2.19	122.62	126.20
18	A	1107	CLA	C3D-C4D-ND	2.18	113.54	109.99
18	3	3013	CLA	CHD-C1D-ND	2.18	127.93	124.84
18	A	1135	CLA	CHB-C1B-NB	-2.18	120.78	124.05
18	4	1304	CLA	C3D-C4D-ND	2.18	113.53	109.99
18	B	1221	CLA	CAA-C2A-C3A	2.18	118.89	113.00
18	B	1222	CLA	CMB-C2B-C1B	2.18	128.74	125.42
18	A	1119	CLA	CHB-C4A-NA	2.18	127.55	124.40
18	3	2009	CLA	C3D-C4D-ND	2.18	112.48	109.50
18	1	1006	CLA	CHB-C1B-NB	-2.18	120.93	124.08
18	A	1120	CLA	CHB-C1B-NB	-2.18	120.93	124.08
18	B	1232	CLA	CHB-C4A-NA	2.18	127.54	124.40
18	A	1103	CLA	CHB-C1B-NB	-2.18	120.78	124.05
18	B	1234	CLA	C1D-ND-C4D	-2.18	104.78	106.31
18	B	1203	CLA	CAC-C3C-C2C	-2.18	122.23	126.75
18	1	1003	CLA	CHB-C4A-NA	2.18	127.52	124.43
18	1	1010	CLA	CHB-C1B-NB	-2.18	120.94	124.08
18	2	2003	CLA	CHB-C1B-NB	-2.17	120.94	124.08
18	A	1118	CLA	C4D-ND-C1D	-2.17	104.79	106.31
18	B	1230	CLA	CHB-C4A-NA	2.17	127.52	124.43
18	B	1207	CLA	CAC-C3C-C2C	2.17	131.54	127.56
18	A	1119	CLA	CMA-C3A-C2A	-2.17	105.59	113.98
18	B	1138	CLA	CBA-CAA-C2A	2.17	120.25	113.79
18	A	1142	CLA	CHB-C4A-NA	2.17	127.51	124.43
18	4	4002	CLA	CHD-C1D-ND	2.17	127.91	124.84
18	B	1234	CLA	C4A-NA-C1A	2.17	107.67	106.68
18	A	1102	CLA	CHB-C1B-NB	-2.17	120.95	124.08
18	2	2002	CLA	CHB-C1B-NB	-2.17	120.95	124.08
18	3	3009	CLA	CHB-C1B-NB	-2.17	120.95	124.08
18	A	1142	CLA	C3D-C4D-ND	2.16	112.46	109.50
18	B	1229	CLA	O2A-CGA-CBA	2.16	118.44	111.83
18	B	9023	CLA	O2A-CGA-O1A	-2.16	118.21	123.63
18	G	1233	CLA	O2D-CGD-O1D	-2.16	119.64	123.85
18	1	1013	CLA	CHB-C1B-NB	-2.16	120.96	124.08

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
18	J	1307	CLA	C2C-C1C-CHC	-2.16	120.18	125.84
18	1	1007	CLA	C3C-C4C-CHD	-2.16	119.62	125.23
18	B	1224	CLA	CHC-C1C-C2C	-2.16	120.81	126.95
18	B	1231	CLA	C1-O2A-CGA	2.16	122.98	116.07
18	4	4010	CLA	CHB-C1B-NB	-2.16	120.96	124.08
18	B	1227	CLA	O2A-CGA-CBA	2.16	118.41	111.83
18	A	1148	CLA	CHD-C1D-ND	2.15	127.89	124.84
18	B	1222	CLA	C3D-C4D-ND	2.15	113.49	109.99
18	B	9012	CLA	CAA-CBA-CGA	2.15	119.32	113.21
18	A	1129	CLA	O2A-CGA-O1A	-2.15	118.24	123.63
18	A	1131	CLA	O2D-CGD-CBD	2.15	114.99	111.23
18	A	9011	CLA	C1-C2-C3	-2.15	122.68	126.20
18	B	9012	CLA	CHB-C1B-NB	-2.15	120.83	124.05
18	B	1236	CLA	CHC-C1C-C2C	-2.15	120.85	126.95
20	I	6018	BCR	C36-C18-C19	2.15	121.37	118.09
18	B	1207	CLA	CBC-CAC-C3C	2.14	118.23	112.42
18	A	1128	CLA	C1D-ND-C4D	-2.14	104.81	106.31
18	B	1227	CLA	O2D-CGD-O1D	-2.14	119.68	123.85
18	B	1237	CLA	O2A-CGA-O1A	-2.14	118.27	123.63
20	B	6017	BCR	C20-C19-C18	2.14	132.24	126.36
18	2	2006	CLA	C3C-C4C-CHD	-2.14	119.67	125.23
20	I	6018	BCR	C23-C22-C21	2.14	122.37	119.01
18	4	4008	CLA	CHD-C1D-ND	2.14	127.86	124.84
18	A	1123	CLA	C1-O2A-CGA	2.14	121.82	116.65
18	A	1129	CLA	CHC-C1C-C2C	-2.13	120.88	126.95
18	B	1214	CLA	O2A-C1-C2	2.13	114.07	108.99
18	A	1108	CLA	CHB-C1B-NB	-2.13	120.85	124.05
18	F	4015	CLA	C2B-C3B-C4B	2.13	109.18	106.81
18	B	9022	CLA	CHA-C4D-ND	2.13	136.95	132.55
20	F	6016	BCR	C37-C22-C23	2.13	121.34	118.09
18	A	1127	CLA	C3D-C4D-ND	2.13	112.41	109.50
18	J	1308	CLA	C3C-C4C-CHD	-2.13	119.70	125.23
18	B	1227	CLA	C2D-C1D-ND	-2.13	108.02	110.13
18	B	1138	CLA	C4A-NA-C1A	2.13	107.65	106.68
18	A	1105	CLA	CHB-C4A-NA	2.13	127.45	124.43
18	B	1301	CLA	C4D-ND-C1D	-2.13	104.82	106.31
18	2	2004	CLA	CHB-C1B-NB	-2.12	121.01	124.08
18	L	1502	CLA	C2A-C1A-CHA	-2.12	120.18	123.87
18	B	1203	CLA	CHA-C4D-ND	2.12	136.93	132.55
18	B	1237	CLA	CHB-C1B-NB	-2.12	120.87	124.05
18	B	1217	CLA	C5-C3-C4	2.12	119.47	114.59
18	B	1239	CLA	C3B-C2B-C1B	-2.12	104.67	107.17

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
18	B	1216	CLA	C3D-C4D-ND	2.12	113.43	109.99
18	4	4011	CLA	CHB-C4A-NA	2.12	127.44	124.43
20	B	6017	BCR	C27-C26-C25	-2.12	119.84	122.70
18	B	1207	CLA	O1D-CGD-CBD	2.12	128.70	124.52
20	L	6020	BCR	C36-C18-C19	2.12	121.32	118.09
18	B	1212	CLA	C3D-C4D-ND	2.12	113.43	109.99
18	B	1229	CLA	C4B-C3B-C2B	2.12	109.03	107.03
18	A	1131	CLA	C3D-C4D-ND	2.12	113.43	109.99
18	H	1501	CLA	CAA-CBA-CGA	-2.11	107.20	113.21
18	B	1235	CLA	C6-C7-C8	-2.11	106.50	115.94
18	A	1113	CLA	C1C-C2C-C3C	-2.11	104.76	106.98
18	B	9012	CLA	C4B-C3B-C2B	2.11	109.93	107.30
18	A	1136	CLA	C1D-ND-C4D	-2.11	104.83	106.31
18	1	1001	CLA	C4D-ND-C1D	-2.11	104.83	106.31
18	A	1142	CLA	CHD-C1D-ND	2.11	127.83	124.84
18	B	1227	CLA	CHB-C1B-NB	-2.11	120.88	124.05
18	A	1134	CLA	C2B-C3B-C4B	2.11	109.15	106.81
18	B	1203	CLA	C4B-C3B-C2B	2.11	109.92	107.30
18	B	1231	CLA	C3D-C4D-ND	2.11	113.42	109.99
18	3	3015	CLA	CHD-C1D-ND	2.11	127.82	124.84
18	A	1133	CLA	CHD-C1D-ND	2.11	127.82	124.84
18	A	1129	CLA	CMB-C2B-C1B	2.11	128.63	125.42
18	H	1501	CLA	C4-C3-C5	2.11	118.88	115.23
18	B	1236	CLA	CED-O2D-CGD	2.11	120.69	115.92
18	4	4012	CLA	C2C-C1C-CHC	-2.10	120.33	125.84
18	A	1104	CLA	CHD-C1D-ND	2.10	127.81	124.84
18	K	1153	CLA	C3B-C4B-CHC	-2.10	119.32	126.76
18	3	3009	CLA	C4D-ND-C1D	-2.10	104.84	106.31
18	B	9023	CLA	C1-O2A-CGA	2.10	122.63	116.67
18	3	3003	CLA	CHB-C4A-NA	2.10	127.41	124.43
18	A	9013	CLA	CHC-C4B-C3B	-2.10	118.27	127.37
18	A	1108	CLA	CED-O2D-CGD	2.10	120.67	115.92
18	B	1225	CLA	O2A-CGA-CBA	2.09	120.62	114.00
18	B	1234	CLA	C3B-C2B-C1B	-2.09	104.70	107.17
18	B	1227	CLA	C3D-C4D-ND	2.09	113.39	109.99
18	L	1130	CLA	O2A-CGA-O1A	-2.09	118.39	123.63
18	J	2107	CLA	CBC-CAC-C3C	2.09	118.09	112.42
18	B	1238	CLA	CMC-C2C-C1C	2.09	128.30	125.03
18	B	1205	CLA	C5-C3-C2	-2.08	116.49	121.17
18	B	1201	CLA	C4D-ND-C1D	-2.08	104.85	106.31
18	B	1234	CLA	CGD-CBD-CAD	-2.08	104.10	110.85
18	B	1224	CLA	CMC-C2C-C1C	2.08	128.29	125.03

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
18	A	1137	CLA	O2D-CGD-O1D	-2.08	119.79	123.85
18	I	1204	CLA	C3A-C2A-C1A	2.08	104.46	101.34
18	1	1010	CLA	C4D-ND-C1D	-2.08	104.85	106.31
18	L	1502	CLA	C3A-C2A-C1A	2.08	104.45	101.34
18	B	9010	CLA	CGD-CBD-CAD	-2.08	104.11	110.85
18	B	1215	CLA	CMA-C3A-C4A	2.08	117.36	111.77
18	B	1238	CLA	C1-O2A-CGA	2.08	121.68	116.65
18	L	1130	CLA	C1D-ND-C4D	-2.08	104.85	106.31
18	2	2011	CLA	CHB-C1B-NB	-2.08	121.08	124.08
18	B	9010	CLA	C2C-C1C-NC	2.08	112.16	109.98
18	G	1233	CLA	C3D-C4D-ND	2.08	113.36	109.99
18	A	1147	CLA	CHD-C1D-ND	2.07	127.77	124.84
18	B	9022	CLA	C4B-C3B-C2B	2.07	109.88	107.30
18	A	1105	CLA	CHD-C1D-ND	2.07	127.77	124.84
18	4	1304	CLA	C1D-ND-C4D	-2.07	104.86	106.31
18	2	2013	CLA	CHB-C1B-NB	-2.07	121.09	124.08
18	A	1127	CLA	C4D-ND-C1D	-2.07	104.86	106.31
18	I	1204	CLA	C1-O2A-CGA	2.07	121.66	116.65
18	K	1153	CLA	CHD-C1D-ND	2.07	127.77	124.84
20	A	6011	BCR	C24-C25-C26	-2.07	116.79	121.56
18	A	1131	CLA	C3B-C4B-NB	2.07	112.47	110.33
18	2	2008	CLA	CHD-C1D-ND	2.07	127.76	124.84
18	4	4002	CLA	C3D-C2D-C1D	2.07	109.86	107.35
18	2	2004	CLA	C3D-C2D-C1D	2.07	109.86	107.35
18	B	1214	CLA	C2A-C1A-CHA	-2.07	120.28	123.87
18	A	1126	CLA	C3D-C4D-ND	2.06	113.34	109.99
18	A	1136	CLA	CAA-C2A-C3A	-2.06	107.43	113.00
18	A	1111	CLA	C4D-ND-C1D	-2.06	104.86	106.31
18	2	2007	CLA	C4D-ND-C1D	-2.06	104.86	106.31
18	F	1240	CLA	CHD-C1D-ND	2.06	127.75	124.84
18	4	4003	CLA	C1C-NC-C4C	-2.06	105.74	106.68
18	A	1126	CLA	C2D-C1D-ND	-2.06	108.09	110.13
18	2	2011	CLA	CHD-C1D-ND	2.06	127.75	124.84
18	B	1208	CLA	CAA-C2A-C1A	-2.06	105.23	111.97
18	B	1225	CLA	CHB-C1B-NB	-2.06	120.96	124.05
18	F	1306	CLA	C4D-ND-C1D	-2.06	104.87	106.31
18	2	2001	CLA	CHB-C1B-NB	-2.06	121.11	124.08
18	B	1215	CLA	CHD-C1D-ND	-2.06	121.91	124.80
18	B	1239	CLA	CHB-C1B-NB	-2.05	120.97	124.05
18	3	3005	CLA	CHD-C1D-ND	2.05	127.75	124.84
18	B	1227	CLA	CAA-CBA-CGA	-2.05	107.38	113.21
18	F	1139	CLA	C3D-C4D-ND	2.05	113.32	109.99

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
18	B	1220	CLA	CHB-C4A-NA	2.05	127.36	124.40
18	B	1242	CLA	O2D-CGD-O1D	-2.05	119.86	123.85
18	3	3013	CLA	CHB-C1B-NB	-2.05	121.12	124.08
18	1	1007	CLA	CHB-C1B-NB	-2.05	121.12	124.08
18	H	1501	CLA	C3D-C4D-ND	2.05	113.31	109.99
18	I	1204	CLA	CHB-C4A-NA	2.04	127.35	124.40
18	B	1225	CLA	O1D-CGD-CBD	-2.04	120.49	124.52
18	B	1209	CLA	C7-C6-C5	-2.04	107.82	113.26
18	B	1219	CLA	C4-C3-C2	-2.04	118.38	123.63
20	A	6011	BCR	C37-C22-C23	2.04	121.21	118.09
18	B	1238	CLA	C3A-C2A-C1A	2.04	104.39	101.34
20	I	6018	BCR	C7-C6-C5	2.04	126.25	121.56
18	K	1150	CLA	CHB-C1B-NB	-2.04	121.13	124.08
18	B	1203	CLA	CHB-C1B-NB	-2.04	120.99	124.05
18	H	1501	CLA	CBC-CAC-C3C	-2.04	106.89	112.42
18	I	1204	CLA	C1D-ND-C4D	-2.04	104.88	106.31
18	B	1211	CLA	CHD-C1D-ND	2.03	127.72	124.84
18	A	1132	CLA	C3D-C4D-ND	2.03	112.28	109.50
18	1	1011	CLA	CHD-C1D-ND	2.03	127.72	124.84
18	2	2008	CLA	CHB-C1B-NB	-2.03	121.14	124.08
18	A	1140	CLA	O1A-CGA-CBA	-2.03	115.83	123.78
18	B	1226	CLA	C1C-NC-C4C	-2.03	105.75	106.68
18	B	9023	CLA	CAA-C2A-C3A	-2.03	107.51	113.00
18	K	1150	CLA	C4D-ND-C1D	-2.03	104.89	106.31
18	3	3001	CLA	CHB-C1B-NB	-2.03	121.15	124.08
18	A	9011	CLA	CAC-C3C-C4C	2.03	127.43	124.79
18	A	1131	CLA	CMB-C2B-C1B	2.03	128.50	125.42
18	A	1122	CLA	CMB-C2B-C3B	2.03	131.32	126.55
18	L	1502	CLA	CAA-C2A-C1A	-2.03	105.33	111.97
18	B	1209	CLA	O2D-CGD-O1D	-2.02	119.91	123.85
18	A	1151	CLA	CHD-C1D-ND	2.02	127.70	124.84
18	A	1143	CLA	CHD-C1D-ND	2.02	127.70	124.84
18	B	9010	CLA	CMB-C2B-C1B	2.02	128.50	125.42
18	A	1109	CLA	C2C-C1C-CHC	-2.02	120.54	125.84
18	A	1119	CLA	CHC-C1C-C2C	-2.02	121.20	126.95
18	B	1206	CLA	C3C-C4C-CHD	-2.02	119.98	125.23
18	B	1239	CLA	O1D-CGD-CBD	-2.02	120.53	124.52
18	B	1221	CLA	CMC-C2C-C3C	2.02	131.61	126.15
18	B	1225	CLA	CED-O2D-CGD	2.02	120.50	115.92
18	2	2006	CLA	C3D-C2D-C1D	2.02	109.80	107.35
20	A	6011	BCR	C33-C5-C4	2.02	117.90	113.60
18	K	1153	CLA	CHB-C4A-NA	2.02	127.30	124.43

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
18	A	1124	CLA	CHC-C4B-NB	2.02	127.00	124.08
20	B	6017	BCR	C33-C5-C4	2.02	117.89	113.60
18	F	4015	CLA	CHD-C1D-ND	2.02	127.69	124.84
18	F	1305	CLA	C4D-ND-C1D	-2.02	104.90	106.31
18	H	1505	CLA	CHB-C1B-NB	-2.01	121.17	124.08
18	B	1224	CLA	C3D-C4D-ND	2.01	113.26	109.99
18	3	2009	CLA	CHD-C1D-ND	2.01	127.69	124.84
18	B	1209	CLA	CMB-C2B-C3B	2.01	131.28	126.55
18	H	1501	CLA	C1D-ND-C4D	-2.01	104.90	106.31
18	2	2010	CLA	CHB-C1B-NB	-2.01	121.17	124.08
18	A	1106	CLA	CED-O2D-CGD	2.01	120.47	115.92
18	F	1139	CLA	CHB-C1B-NB	-2.01	121.04	124.05
18	J	2107	CLA	CED-O2D-CGD	2.01	120.47	115.92
18	4	1009	CLA	C3D-C4D-ND	2.01	112.24	109.50
18	B	1228	CLA	C1-C2-C3	2.01	129.48	126.20
18	A	1144	CLA	C4D-ND-C1D	-2.00	104.91	106.31
18	L	1504	CLA	O1D-CGD-CBD	-2.00	120.57	124.52
18	B	1232	CLA	O2A-CGA-O1A	-2.00	118.62	123.63

All (33) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
18	A	1107	CLA	C8
18	A	1119	CLA	C8
18	A	1122	CLA	C8
18	A	1123	CLA	C8
18	A	1126	CLA	C8
18	A	1128	CLA	C8
18	A	1129	CLA	C8
18	A	1136	CLA	C8
18	A	1137	CLA	C8
18	A	1140	CLA	C8
18	A	9011	CLA	C8
18	B	1138	CLA	C8
18	B	9012	CLA	C8
18	B	1205	CLA	C8
18	B	1207	CLA	C8
18	B	1208	CLA	C8
18	B	1209	CLA	C8
18	B	1212	CLA	C8
18	B	1216	CLA	C8
18	B	1220	CLA	C8

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Mol	Chain	Res	Type	Atom
18	B	1222	CLA	C8
18	B	1228	CLA	C8
18	B	1232	CLA	C8
18	B	1235	CLA	C8
18	B	1239	CLA	C8
18	F	1302	CLA	C8
18	H	1501	CLA	C8
18	I	1204	CLA	C8
18	J	2107	CLA	C8
18	L	1504	CLA	C8
18	4	1304	CLA	C8
19	A	5001	PQN	C23
19	B	5002	PQN	C23

All (770) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
18	A	1103	CLA	C1A-C2A-CAA-CBA
18	A	1106	CLA	CHA-CBD-CGD-O1D
18	A	1106	CLA	CHA-CBD-CGD-O2D
18	A	1107	CLA	C2-C1-O2A-CGA
18	A	1107	CLA	C2B-C3B-CAB-CBB
18	A	1107	CLA	CBD-CGD-O2D-CED
18	A	1108	CLA	C1A-C2A-CAA-CBA
18	A	1113	CLA	C4B-C3B-CAB-CBB
18	A	1113	CLA	CBD-CGD-O2D-CED
18	A	1115	CLA	C2B-C3B-CAB-CBB
18	A	1119	CLA	C4B-C3B-CAB-CBB
18	A	1119	CLA	CBD-CGD-O2D-CED
18	A	1122	CLA	C1A-C2A-CAA-CBA
18	A	1122	CLA	C3A-C2A-CAA-CBA
18	A	1122	CLA	C2B-C3B-CAB-CBB
18	A	1122	CLA	C4B-C3B-CAB-CBB
18	A	1122	CLA	CBD-CGD-O2D-CED
18	A	1123	CLA	C1A-C2A-CAA-CBA
18	A	1123	CLA	C2B-C3B-CAB-CBB
18	A	1126	CLA	C4B-C3B-CAB-CBB
18	A	1126	CLA	CBD-CGD-O2D-CED
18	A	1128	CLA	C4B-C3B-CAB-CBB
18	A	1131	CLA	C1A-C2A-CAA-CBA
18	A	1131	CLA	CBD-CGD-O2D-CED
18	A	1131	CLA	O1D-CGD-O2D-CED

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Mol	Chain	Res	Type	Atoms
18	A	1135	CLA	C1A-C2A-CAA-CBA
18	A	1135	CLA	C3A-C2A-CAA-CBA
18	A	1135	CLA	C2B-C3B-CAB-CBB
18	A	1135	CLA	CBD-CGD-O2D-CED
18	A	1136	CLA	C2B-C3B-CAB-CBB
18	A	1136	CLA	CAD-CBD-CGD-O2D
18	A	1137	CLA	C1A-C2A-CAA-CBA
18	A	1137	CLA	C2B-C3B-CAB-CBB
18	A	1140	CLA	C1A-C2A-CAA-CBA
18	A	1140	CLA	C3A-C2A-CAA-CBA
18	A	1140	CLA	C4B-C3B-CAB-CBB
18	A	9011	CLA	C1A-C2A-CAA-CBA
18	A	9011	CLA	C4B-C3B-CAB-CBB
18	A	9011	CLA	CBD-CGD-O2D-CED
18	B	1138	CLA	C4B-C3B-CAB-CBB
18	B	1138	CLA	CBD-CGD-O2D-CED
18	B	1138	CLA	O1D-CGD-O2D-CED
18	B	9010	CLA	C1A-C2A-CAA-CBA
18	B	9010	CLA	C3A-C2A-CAA-CBA
18	B	9010	CLA	CBD-CGD-O2D-CED
18	B	9012	CLA	CBA-CGA-O2A-C1
18	B	9012	CLA	O1A-CGA-O2A-C1
18	B	9012	CLA	C2B-C3B-CAB-CBB
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	9022	CLA	CHA-CBD-CGD-O1D
18	B	9022	CLA	CHA-CBD-CGD-O2D
18	B	9022	CLA	CBD-CGD-O2D-CED
18	B	9023	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	C4B-C3B-CAB-CBB
18	B	1203	CLA	C1A-C2A-CAA-CBA
18	B	1203	CLA	CBD-CGD-O2D-CED
18	B	1205	CLA	CHA-CBD-CGD-O1D
18	B	1205	CLA	CHA-CBD-CGD-O2D
18	B	1207	CLA	C3A-C2A-CAA-CBA
18	B	1208	CLA	C1A-C2A-CAA-CBA
18	B	1208	CLA	CBA-CGA-O2A-C1
18	B	1208	CLA	O1A-CGA-O2A-C1

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Mol	Chain	Res	Type	Atoms
18	B	1209	CLA	C1A-C2A-CAA-CBA
18	B	1209	CLA	C4B-C3B-CAB-CBB
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	1212	CLA	C2-C1-O2A-CGA
18	B	1212	CLA	C2B-C3B-CAB-CBB
18	B	1212	CLA	CHA-CBD-CGD-O1D
18	B	1212	CLA	CHA-CBD-CGD-O2D
18	B	1214	CLA	C1A-C2A-CAA-CBA
18	B	1215	CLA	C4B-C3B-CAB-CBB
18	B	1215	CLA	CBD-CGD-O2D-CED
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	1216	CLA	CHA-CBD-CGD-O2D
18	B	1217	CLA	C1A-C2A-CAA-CBA
18	B	1217	CLA	C2B-C3B-CAB-CBB
18	B	1218	CLA	CAD-CBD-CGD-O1D
18	B	1218	CLA	CAD-CBD-CGD-O2D
18	B	1218	CLA	CBD-CGD-O2D-CED
18	B	1219	CLA	C1A-C2A-CAA-CBA
18	B	1219	CLA	C3A-C2A-CAA-CBA
18	B	1219	CLA	CHA-CBD-CGD-O1D
18	B	1219	CLA	CHA-CBD-CGD-O2D
18	B	1219	CLA	C2-C3-C5-C6
18	B	1220	CLA	C2B-C3B-CAB-CBB
18	B	1220	CLA	C4B-C3B-CAB-CBB
18	B	1220	CLA	C6-C7-C8-C10
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	B	1222	CLA	C2-C1-O2A-CGA
18	B	1222	CLA	C4B-C3B-CAB-CBB
18	B	1222	CLA	CBD-CGD-O2D-CED
18	B	1224	CLA	C2B-C3B-CAB-CBB
18	B	1225	CLA	CBD-CGD-O2D-CED
18	B	1227	CLA	C1A-C2A-CAA-CBA
18	B	1227	CLA	C3A-C2A-CAA-CBA
18	B	1227	CLA	CBD-CGD-O2D-CED
18	B	1228	CLA	CBA-CGA-O2A-C1
18	B	1228	CLA	O1A-CGA-O2A-C1

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Mol	Chain	Res	Type	Atoms
18	B	1228	CLA	CHA-CBD-CGD-O1D
18	B	1228	CLA	CHA-CBD-CGD-O2D
18	B	1228	CLA	O2A-C1-C2-C3
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	1231	CLA	C3A-C2A-CAA-CBA
18	B	1231	CLA	CBA-CGA-O2A-C1
18	B	1231	CLA	C2B-C3B-CAB-CBB
18	B	1231	CLA	CBD-CGD-O2D-CED
18	B	1232	CLA	CBD-CGD-O2D-CED
18	B	1234	CLA	C1A-C2A-CAA-CBA
18	B	1235	CLA	C4B-C3B-CAB-CBB
18	B	1235	CLA	C2C-C3C-CAC-CBC
18	B	1235	CLA	C4C-C3C-CAC-CBC
18	B	1235	CLA	CAD-CBD-CGD-O1D
18	B	1235	CLA	CAD-CBD-CGD-O2D
18	B	1236	CLA	C2B-C3B-CAB-CBB
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	1238	CLA	C3A-C2A-CAA-CBA
18	B	1238	CLA	O1A-CGA-O2A-C1
18	B	1238	CLA	CBD-CGD-O2D-CED
18	B	1242	CLA	C1A-C2A-CAA-CBA
18	B	1242	CLA	C2B-C3B-CAB-CBB
18	F	1139	CLA	CAD-CBD-CGD-O2D
18	F	1139	CLA	CBD-CGD-O2D-CED
18	F	1139	CLA	O1D-CGD-O2D-CED
18	F	1302	CLA	C4B-C3B-CAB-CBB
18	F	1302	CLA	CBD-CGD-O2D-CED
18	G	1233	CLA	C3A-C2A-CAA-CBA
18	G	1233	CLA	CBD-CGD-O2D-CED
18	G	1233	CLA	C2-C3-C5-C6
18	H	1501	CLA	C3A-C2A-CAA-CBA
18	H	1501	CLA	C4B-C3B-CAB-CBB
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	J	2107	CLA	C1A-C2A-CAA-CBA
18	J	2107	CLA	C3A-C2A-CAA-CBA

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Mol	Chain	Res	Type	Atoms
18	J	2107	CLA	C2B-C3B-CAB-CBB
18	L	1130	CLA	CBA-CGA-O2A-C1
18	L	1130	CLA	O1A-CGA-O2A-C1
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	L	1503	CLA	C1A-C2A-CAA-CBA
18	4	1304	CLA	C1A-C2A-CAA-CBA
18	4	1304	CLA	CAD-CBD-CGD-O1D
18	4	1304	CLA	CAD-CBD-CGD-O2D
18	4	1304	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
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
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
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
20	L	6020	BCR	C7-C8-C9-C10
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	C23-C24-C25-C26
20	L	6020	BCR	C23-C24-C25-C30

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Mol	Chain	Res	Type	Atoms
18	B	1207	CLA	C4C-C3C-CAC-CBC
18	B	1221	CLA	C4C-C3C-CAC-CBC
18	A	1129	CLA	O1D-CGD-O2D-CED
18	B	1207	CLA	O1D-CGD-O2D-CED
18	B	1212	CLA	O1D-CGD-O2D-CED
18	B	1238	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	C2C-C3C-CAC-CBC
18	A	1103	CLA	O1D-CGD-O2D-CED
18	A	1119	CLA	O1D-CGD-O2D-CED
18	A	9011	CLA	O1D-CGD-O2D-CED
18	B	9010	CLA	O1D-CGD-O2D-CED
18	B	1221	CLA	O1D-CGD-O2D-CED
18	B	1222	CLA	O1D-CGD-O2D-CED
18	B	1225	CLA	O1D-CGD-O2D-CED
18	4	1304	CLA	O1D-CGD-O2D-CED
18	A	1103	CLA	CBD-CGD-O2D-CED
18	A	1108	CLA	CBD-CGD-O2D-CED
18	A	1128	CLA	CBD-CGD-O2D-CED
18	A	1129	CLA	CBD-CGD-O2D-CED
18	A	9013	CLA	CBD-CGD-O2D-CED
18	B	1207	CLA	CBD-CGD-O2D-CED
18	B	1208	CLA	CBD-CGD-O2D-CED
18	B	1212	CLA	CBD-CGD-O2D-CED
18	B	1220	CLA	CBD-CGD-O2D-CED
18	B	1221	CLA	CBD-CGD-O2D-CED
18	B	1236	CLA	CBD-CGD-O2D-CED
18	B	1237	CLA	CBD-CGD-O2D-CED
18	B	1239	CLA	CBD-CGD-O2D-CED
18	L	1504	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	I	1204	CLA	C4C-C3C-CAC-CBC
18	B	1221	CLA	C2C-C3C-CAC-CBC
18	A	1113	CLA	O1D-CGD-O2D-CED
18	B	1231	CLA	O1D-CGD-O2D-CED
18	B	1138	CLA	C5-C6-C7-C8
18	L	1503	CLA	C2C-C3C-CAC-CBC
18	A	1107	CLA	O1D-CGD-O2D-CED

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Mol	Chain	Res	Type	Atoms
18	A	1108	CLA	O1D-CGD-O2D-CED
18	A	1128	CLA	O1D-CGD-O2D-CED
18	B	1218	CLA	O1D-CGD-O2D-CED
18	B	1232	CLA	O1D-CGD-O2D-CED
18	B	1236	CLA	O1D-CGD-O2D-CED
18	B	1218	CLA	CBA-CGA-O2A-C1
18	B	1227	CLA	CBA-CGA-O2A-C1
18	B	1214	CLA	CBD-CGD-O2D-CED
18	A	1103	CLA	O1A-CGA-O2A-C1
18	B	1209	CLA	O1A-CGA-O2A-C1
18	B	1214	CLA	O1A-CGA-O2A-C1
18	B	1220	CLA	O1A-CGA-O2A-C1
18	B	1224	CLA	O1A-CGA-O2A-C1
18	B	1237	CLA	O1A-CGA-O2A-C1
18	F	1302	CLA	O1A-CGA-O2A-C1
18	L	1502	CLA	O1A-CGA-O2A-C1
18	L	1504	CLA	O1A-CGA-O2A-C1
18	4	1304	CLA	O1A-CGA-O2A-C1
18	A	1137	CLA	C2C-C3C-CAC-CBC
18	B	1220	CLA	C2C-C3C-CAC-CBC
18	I	1204	CLA	C2C-C3C-CAC-CBC
18	B	9012	CLA	O1D-CGD-O2D-CED
18	B	9022	CLA	O1D-CGD-O2D-CED
18	B	1203	CLA	O1D-CGD-O2D-CED
18	B	1215	CLA	O1D-CGD-O2D-CED
18	B	1227	CLA	O1D-CGD-O2D-CED
18	I	1204	CLA	O1D-CGD-O2D-CED
18	A	1137	CLA	C4C-C3C-CAC-CBC
18	A	1122	CLA	O1D-CGD-O2D-CED
18	A	1126	CLA	O1D-CGD-O2D-CED
19	B	5002	PQN	C20-C21-C22-C23
18	A	9011	CLA	O1A-CGA-O2A-C1
18	B	1215	CLA	C4C-C3C-CAC-CBC
18	L	1503	CLA	C4C-C3C-CAC-CBC
18	B	1236	CLA	CBA-CGA-O2A-C1
18	A	1119	CLA	C3-C5-C6-C7
18	A	1126	CLA	C3-C5-C6-C7
18	A	1128	CLA	C3-C5-C6-C7
18	A	1136	CLA	C3-C5-C6-C7
18	A	1140	CLA	C3-C5-C6-C7
18	B	1205	CLA	C3-C5-C6-C7
19	A	5001	PQN	C13-C15-C16-C17

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Mol	Chain	Res	Type	Atoms
18	B	1215	CLA	C2C-C3C-CAC-CBC
18	A	1135	CLA	O1D-CGD-O2D-CED
18	A	1103	CLA	CBA-CGA-O2A-C1
18	A	1113	CLA	CBA-CGA-O2A-C1
18	A	1140	CLA	CBA-CGA-O2A-C1
18	B	1209	CLA	CBA-CGA-O2A-C1
18	B	1212	CLA	CBA-CGA-O2A-C1
18	B	1214	CLA	CBA-CGA-O2A-C1
18	B	1220	CLA	CBA-CGA-O2A-C1
18	B	1229	CLA	CBA-CGA-O2A-C1
18	B	1238	CLA	CBA-CGA-O2A-C1
18	L	1502	CLA	CBA-CGA-O2A-C1
18	L	1504	CLA	CBA-CGA-O2A-C1
18	4	1304	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	C4C-C3C-CAC-CBC
18	B	9023	CLA	O1D-CGD-O2D-CED
18	L	1504	CLA	O1D-CGD-O2D-CED
18	A	9013	CLA	O1A-CGA-O2A-C1
18	A	1131	CLA	C2C-C3C-CAC-CBC
18	A	1126	CLA	C4-C3-C5-C6
18	A	1137	CLA	C4-C3-C5-C6
18	B	1138	CLA	C4-C3-C5-C6
18	B	9022	CLA	C4-C3-C5-C6
18	B	1235	CLA	C4-C3-C5-C6
18	B	1239	CLA	C4-C3-C5-C6
18	A	1126	CLA	C2-C3-C5-C6
18	A	1137	CLA	C2-C3-C5-C6
18	B	1138	CLA	C2-C3-C5-C6
18	B	9022	CLA	C2-C3-C5-C6
18	B	1235	CLA	C2-C3-C5-C6
18	B	1239	CLA	C2-C3-C5-C6
18	B	1207	CLA	C2A-CAA-CBA-CGA
18	B	1209	CLA	C2A-CAA-CBA-CGA
18	A	1140	CLA	O1A-CGA-O2A-C1
18	A	1107	CLA	C3-C5-C6-C7
18	B	9022	CLA	CBA-CGA-O2A-C1
18	B	1224	CLA	CBA-CGA-O2A-C1
18	B	1237	CLA	CBA-CGA-O2A-C1
18	F	1302	CLA	CBA-CGA-O2A-C1
18	B	1236	CLA	O1A-CGA-O2A-C1

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Mol	Chain	Res	Type	Atoms
18	A	1103	CLA	C2-C1-O2A-CGA
20	A	6011	BCR	C9-C10-C11-C12
20	A	6011	BCR	C13-C14-C15-C16
20	B	6017	BCR	C9-C10-C11-C12
20	B	6017	BCR	C13-C14-C15-C16
20	B	6017	BCR	C19-C20-C21-C22
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	L	6020	BCR	C13-C14-C15-C16
20	L	6020	BCR	C15-C16-C17-C18
18	A	1107	CLA	O1A-CGA-O2A-C1
18	B	1203	CLA	O1A-CGA-O2A-C1
18	B	1229	CLA	O1A-CGA-O2A-C1
18	A	9013	CLA	CBA-CGA-O2A-C1
18	A	1131	CLA	C4C-C3C-CAC-CBC
18	A	9011	CLA	C2C-C3C-CAC-CBC
18	A	1137	CLA	C3-C5-C6-C7
18	B	1232	CLA	C3-C5-C6-C7
18	J	2107	CLA	C3-C5-C6-C7
18	A	1115	CLA	CBD-CGD-O2D-CED
18	A	1140	CLA	C2C-C3C-CAC-CBC
18	B	1208	CLA	O1D-CGD-O2D-CED
18	B	1220	CLA	O1D-CGD-O2D-CED
18	B	1237	CLA	O1D-CGD-O2D-CED
18	A	1129	CLA	CBA-CGA-O2A-C1
18	B	1203	CLA	CBA-CGA-O2A-C1
18	A	1113	CLA	O1A-CGA-O2A-C1
18	B	9022	CLA	O1A-CGA-O2A-C1
18	B	1239	CLA	O1D-CGD-O2D-CED
18	B	1219	CLA	CBD-CGD-O2D-CED
18	B	1219	CLA	C2C-C3C-CAC-CBC
18	B	1237	CLA	C2C-C3C-CAC-CBC
18	F	1139	CLA	C2C-C3C-CAC-CBC
18	A	9013	CLA	O1D-CGD-O2D-CED
18	A	1123	CLA	C3-C5-C6-C7
18	A	1107	CLA	CBA-CGA-O2A-C1
18	A	9011	CLA	CBA-CGA-O2A-C1
18	A	9011	CLA	C4-C3-C5-C6
19	B	5002	PQN	C14-C13-C15-C16
18	A	9011	CLA	C2-C3-C5-C6
19	B	5002	PQN	C12-C13-C15-C16

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Mol	Chain	Res	Type	Atoms
18	B	1234	CLA	C2A-CAA-CBA-CGA
18	B	9010	CLA	CBA-CGA-O2A-C1
18	B	1224	CLA	CBD-CGD-O2D-CED
18	H	1501	CLA	CBD-CGD-O2D-CED
18	B	1232	CLA	O1A-CGA-O2A-C1
18	A	1122	CLA	O1A-CGA-O2A-C1
18	A	1129	CLA	O1A-CGA-O2A-C1
18	B	9010	CLA	O1A-CGA-O2A-C1
18	A	1115	CLA	CBA-CGA-O2A-C1
18	A	1122	CLA	CBA-CGA-O2A-C1
18	A	1123	CLA	CBA-CGA-O2A-C1
18	A	1126	CLA	CBA-CGA-O2A-C1
18	A	1136	CLA	CBA-CGA-O2A-C1
18	A	1137	CLA	CBA-CGA-O2A-C1
18	B	1232	CLA	CBA-CGA-O2A-C1
18	B	1235	CLA	CBA-CGA-O2A-C1
18	B	1242	CLA	CBA-CGA-O2A-C1
18	G	1233	CLA	CBA-CGA-O2A-C1
18	B	1214	CLA	O1D-CGD-O2D-CED
18	B	1234	CLA	O1D-CGD-O2D-CED
18	B	9022	CLA	C3-C5-C6-C7
18	B	1222	CLA	C11-C10-C8-C9
19	A	5001	PQN	C19-C18-C20-C21
18	A	1136	CLA	O1D-CGD-O2D-CED
18	A	1115	CLA	O1A-CGA-O2A-C1
18	A	1126	CLA	O1A-CGA-O2A-C1
20	A	6011	BCR	C36-C18-C19-C20
20	L	6020	BCR	C37-C22-C23-C24
18	B	1215	CLA	C3-C5-C6-C7
18	4	1304	CLA	C2A-CAA-CBA-CGA
18	A	1136	CLA	O1A-CGA-O2A-C1
18	B	1235	CLA	O1A-CGA-O2A-C1
18	B	1138	CLA	C3-C5-C6-C7
18	J	2107	CLA	CBA-CGA-O2A-C1
18	B	1209	CLA	C2-C1-O2A-CGA
18	B	1217	CLA	C2-C1-O2A-CGA
18	A	1107	CLA	C2C-C3C-CAC-CBC
18	A	9011	CLA	C4C-C3C-CAC-CBC
18	A	1123	CLA	CBD-CGD-O2D-CED
19	A	5001	PQN	C22-C23-C25-C26
20	A	6011	BCR	C19-C20-C21-C22
20	I	6018	BCR	C19-C20-C21-C22

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Mol	Chain	Res	Type	Atoms
18	A	1123	CLA	C2C-C3C-CAC-CBC
18	B	1238	CLA	C3-C5-C6-C7
18	A	1140	CLA	C5-C6-C7-C8
18	B	1219	CLA	C4C-C3C-CAC-CBC
18	B	1242	CLA	O1A-CGA-O2A-C1
18	G	1233	CLA	O1A-CGA-O2A-C1
18	J	2107	CLA	O1A-CGA-O2A-C1
18	B	1216	CLA	C2A-CAA-CBA-CGA
18	B	1225	CLA	C2A-CAA-CBA-CGA
18	B	1231	CLA	C2A-CAA-CBA-CGA
18	A	1140	CLA	C4C-C3C-CAC-CBC
20	B	6017	BCR	C10-C11-C12-C13
18	A	1123	CLA	C5-C6-C7-C8
18	A	1129	CLA	C5-C6-C7-C8
18	A	1137	CLA	O1A-CGA-O2A-C1
18	B	1216	CLA	CBD-CGD-O2D-CED
19	A	5001	PQN	C18-C20-C21-C22
18	A	1123	CLA	O1A-CGA-O2A-C1
18	A	1107	CLA	C8-C10-C11-C12
18	B	1232	CLA	C5-C6-C7-C8
18	B	9012	CLA	C5-C6-C7-C8
18	A	1137	CLA	C5-C6-C7-C8
18	A	1119	CLA	C2A-CAA-CBA-CGA
18	A	1129	CLA	C2A-CAA-CBA-CGA
18	B	9010	CLA	C2A-CAA-CBA-CGA
18	B	1222	CLA	C2A-CAA-CBA-CGA
18	B	1234	CLA	CBA-CGA-O2A-C1
18	F	1139	CLA	C4C-C3C-CAC-CBC
18	B	1205	CLA	C5-C6-C7-C8
18	B	1208	CLA	C5-C6-C7-C8
19	A	5001	PQN	C23-C25-C26-C27
18	B	1216	CLA	C5-C6-C7-C8
18	H	1501	CLA	C4-C3-C5-C6
18	J	2107	CLA	C8-C10-C11-C12
18	B	1235	CLA	C5-C6-C7-C8
18	A	1137	CLA	C6-C7-C8-C10
20	B	6017	BCR	C11-C12-C13-C35
20	A	6011	BCR	C17-C18-C19-C20
20	B	6017	BCR	C21-C22-C23-C24
20	L	6020	BCR	C21-C22-C23-C24
18	A	1126	CLA	C2A-CAA-CBA-CGA
18	A	1135	CLA	C2A-CAA-CBA-CGA

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Mol	Chain	Res	Type	Atoms
18	B	9022	CLA	C2A-CAA-CBA-CGA
18	F	1302	CLA	C2A-CAA-CBA-CGA
18	B	1220	CLA	C5-C6-C7-C8
18	B	1219	CLA	O1D-CGD-O2D-CED
18	L	1130	CLA	O2A-C1-C2-C3
18	A	1123	CLA	C6-C7-C8-C9
18	B	9012	CLA	C6-C7-C8-C9
18	B	1208	CLA	C6-C7-C8-C10
18	B	1209	CLA	C6-C7-C8-C10
18	B	1228	CLA	C6-C7-C8-C10
20	A	6011	BCR	C11-C10-C9-C8
18	B	1221	CLA	O2A-C1-C2-C3
18	A	1128	CLA	C6-C7-C8-C9
18	A	1136	CLA	C6-C7-C8-C9
18	A	1115	CLA	O1D-CGD-O2D-CED
18	F	1139	CLA	C2A-CAA-CBA-CGA
18	B	1237	CLA	C4C-C3C-CAC-CBC
18	A	1106	CLA	C4B-C3B-CAB-CBB
18	B	9023	CLA	C4B-C3B-CAB-CBB
18	B	1238	CLA	C4B-C3B-CAB-CBB
18	A	1119	CLA	C6-C7-C8-C9
18	A	1119	CLA	C6-C7-C8-C10
18	A	1137	CLA	C6-C7-C8-C9
18	B	1208	CLA	C6-C7-C8-C9
18	B	1209	CLA	C6-C7-C8-C9
18	B	9012	CLA	C2A-CAA-CBA-CGA
18	A	1128	CLA	C5-C6-C7-C8
18	H	1501	CLA	O1D-CGD-O2D-CED
18	B	1234	CLA	O1A-CGA-O2A-C1
18	A	1108	CLA	C3A-C2A-CAA-CBA
18	A	1123	CLA	C3A-C2A-CAA-CBA
18	A	1131	CLA	C3A-C2A-CAA-CBA
18	A	1137	CLA	C3A-C2A-CAA-CBA
18	A	9011	CLA	C3A-C2A-CAA-CBA
18	B	1214	CLA	C3A-C2A-CAA-CBA
18	B	1232	CLA	C3A-C2A-CAA-CBA
18	B	1234	CLA	C3A-C2A-CAA-CBA
18	B	1242	CLA	C3A-C2A-CAA-CBA
18	I	1204	CLA	C3A-C2A-CAA-CBA
18	L	1503	CLA	C3A-C2A-CAA-CBA
18	4	1304	CLA	C3A-C2A-CAA-CBA
18	A	1123	CLA	C6-C7-C8-C10

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Mol	Chain	Res	Type	Atoms
18	B	1228	CLA	C6-C7-C8-C9
18	H	1501	CLA	C6-C7-C8-C9
18	B	1224	CLA	O1D-CGD-O2D-CED
18	B	1242	CLA	C2C-C3C-CAC-CBC
18	A	1136	CLA	C6-C7-C8-C10
18	A	9011	CLA	C2B-C3B-CAB-CBB
18	B	1227	CLA	C2B-C3B-CAB-CBB
18	B	1234	CLA	C2B-C3B-CAB-CBB
18	B	1238	CLA	C2B-C3B-CAB-CBB
18	L	1130	CLA	C2B-C3B-CAB-CBB
20	B	6017	BCR	C23-C24-C25-C30
18	A	1140	CLA	C2A-CAA-CBA-CGA
18	B	1212	CLA	C4-C3-C5-C6
20	I	6018	BCR	C10-C11-C12-C13
18	B	9012	CLA	C6-C7-C8-C10
18	B	1205	CLA	CBA-CGA-O2A-C1
18	A	1129	CLA	C3-C5-C6-C7
20	I	6018	BCR	C13-C14-C15-C16
20	B	6017	BCR	C37-C22-C23-C24
20	B	6017	BCR	C11-C12-C13-C14
18	A	1128	CLA	C6-C7-C8-C10
18	A	1119	CLA	C4-C3-C5-C6
18	B	1212	CLA	C2-C3-C5-C6
18	B	1207	CLA	C5-C6-C7-C8
18	B	1205	CLA	O1A-CGA-O2A-C1
18	B	1238	CLA	C5-C6-C7-C8
18	J	2107	CLA	C2-C1-O2A-CGA
18	A	1123	CLA	C4C-C3C-CAC-CBC
18	A	1107	CLA	C4C-C3C-CAC-CBC
18	H	1501	CLA	C6-C7-C8-C10
18	A	1119	CLA	C1A-C2A-CAA-CBA
18	A	1128	CLA	C1A-C2A-CAA-CBA
18	B	1207	CLA	C1A-C2A-CAA-CBA
18	B	1218	CLA	C1A-C2A-CAA-CBA
18	B	1221	CLA	C1A-C2A-CAA-CBA
18	B	1231	CLA	C1A-C2A-CAA-CBA
18	B	1232	CLA	C1A-C2A-CAA-CBA
18	B	1238	CLA	C1A-C2A-CAA-CBA
18	G	1233	CLA	C1A-C2A-CAA-CBA
18	H	1501	CLA	C1A-C2A-CAA-CBA
18	B	1222	CLA	C15-C16-C17-C18
18	B	1220	CLA	C11-C10-C8-C7

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Mol	Chain	Res	Type	Atoms
19	A	5001	PQN	C17-C18-C20-C21
18	A	1126	CLA	C6-C7-C8-C10
18	B	1215	CLA	C4-C3-C5-C6
18	A	1119	CLA	C2-C3-C5-C6
18	B	1222	CLA	C13-C15-C16-C17
18	B	1216	CLA	O1D-CGD-O2D-CED
18	B	1203	CLA	C2A-CAA-CBA-CGA
18	J	2107	CLA	C2A-CAA-CBA-CGA
18	B	1212	CLA	C11-C10-C8-C9
20	L	6020	BCR	C11-C12-C13-C35
20	B	6017	BCR	C17-C18-C19-C20
18	B	1222	CLA	C8-C10-C11-C12
18	A	1137	CLA	C2A-CAA-CBA-CGA
20	F	6016	BCR	C15-C16-C17-C18
18	B	1215	CLA	C2-C3-C5-C6
18	B	1217	CLA	CBD-CGD-O2D-CED
18	B	1216	CLA	C3-C5-C6-C7
18	A	1119	CLA	C2C-C3C-CAC-CBC
18	A	1119	CLA	CBA-CGA-O2A-C1
19	B	5002	PQN	C15-C16-C17-C18
18	I	1204	CLA	C6-C7-C8-C10
18	B	9012	CLA	C4-C3-C5-C6
19	B	5002	PQN	C18-C20-C21-C22
18	B	9022	CLA	C6-C7-C8-C9
18	A	1107	CLA	C11-C10-C8-C9
18	B	1220	CLA	C11-C10-C8-C9
18	B	1222	CLA	C14-C13-C15-C16
18	A	1107	CLA	C4B-C3B-CAB-CBB
18	B	1227	CLA	C4B-C3B-CAB-CBB
18	4	1304	CLA	C4B-C3B-CAB-CBB
18	B	1212	CLA	C2C-C3C-CAC-CBC
18	B	1212	CLA	C11-C10-C8-C7
18	J	2107	CLA	C11-C12-C13-C15
18	A	1126	CLA	C5-C6-C7-C8
18	A	1103	CLA	C3A-C2A-CAA-CBA
18	B	9012	CLA	C3A-C2A-CAA-CBA
18	B	1208	CLA	C3A-C2A-CAA-CBA
18	B	1209	CLA	C3A-C2A-CAA-CBA
18	B	1212	CLA	C3A-C2A-CAA-CBA
18	B	1216	CLA	C3A-C2A-CAA-CBA
18	B	1218	CLA	C3A-C2A-CAA-CBA
18	A	1123	CLA	O1D-CGD-O2D-CED

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Mol	Chain	Res	Type	Atoms
18	H	1501	CLA	C2-C3-C5-C6
20	L	6020	BCR	C9-C10-C11-C12
18	B	1219	CLA	C4-C3-C5-C6
18	G	1233	CLA	C4-C3-C5-C6
20	L	6020	BCR	C11-C12-C13-C14
18	A	1103	CLA	C2A-CAA-CBA-CGA
18	B	1208	CLA	C2A-CAA-CBA-CGA
18	B	1208	CLA	C3-C5-C6-C7
18	B	1205	CLA	C4-C3-C5-C6
18	A	1108	CLA	C2B-C3B-CAB-CBB
18	B	1212	CLA	CAA-CBA-CGA-O2A
18	B	1239	CLA	C6-C7-C8-C10
18	I	1204	CLA	C3-C5-C6-C7
18	J	2107	CLA	C11-C12-C13-C14
18	B	1222	CLA	C3-C5-C6-C7
18	I	1204	CLA	C2A-CAA-CBA-CGA
20	F	6016	BCR	C11-C10-C9-C34
18	B	1239	CLA	C6-C7-C8-C9
19	B	5002	PQN	C23-C25-C26-C27
19	B	5002	PQN	C25-C26-C27-C28
20	B	6017	BCR	C36-C18-C19-C20
18	A	1107	CLA	C6-C7-C8-C10
18	B	1138	CLA	C6-C7-C8-C10
18	A	1126	CLA	C6-C7-C8-C9
18	J	2107	CLA	C10-C11-C12-C13
18	A	1119	CLA	O1A-CGA-O2A-C1
18	B	1227	CLA	C2C-C3C-CAC-CBC
18	B	1220	CLA	C2A-CAA-CBA-CGA
18	B	1235	CLA	C3-C5-C6-C7
18	A	1107	CLA	C6-C7-C8-C9
18	B	1202	CLA	O1D-CGD-O2D-CED
18	B	9022	CLA	C2-C1-O2A-CGA
18	G	1233	CLA	C2C-C3C-CAC-CBC
19	B	5002	PQN	C26-C27-C28-C29
18	B	9012	CLA	C3-C5-C6-C7
18	L	1504	CLA	C3-C5-C6-C7
18	I	1204	CLA	C6-C7-C8-C9
18	A	1129	CLA	C4B-C3B-CAB-CBB
18	B	1218	CLA	C4B-C3B-CAB-CBB
18	B	1219	CLA	C4B-C3B-CAB-CBB
18	B	1228	CLA	C4B-C3B-CAB-CBB
18	L	1502	CLA	C1A-C2A-CAA-CBA

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Mol	Chain	Res	Type	Atoms
18	B	1222	CLA	C11-C10-C8-C7
18	B	1238	CLA	C2C-C3C-CAC-CBC
18	B	1215	CLA	C2A-CAA-CBA-CGA
20	B	6017	BCR	C15-C16-C17-C18
18	B	1214	CLA	O2A-C1-C2-C3
18	A	1107	CLA	CAD-CBD-CGD-O2D
18	B	1138	CLA	CAD-CBD-CGD-O2D
18	B	1203	CLA	CAD-CBD-CGD-O2D
18	B	1221	CLA	CAD-CBD-CGD-O2D
18	B	1215	CLA	CBA-CGA-O2A-C1
18	B	1207	CLA	C6-C7-C8-C10
18	B	1209	CLA	C3-C5-C6-C7
18	A	1103	CLA	CHA-CBD-CGD-O1D
18	A	1103	CLA	CHA-CBD-CGD-O2D
18	A	1107	CLA	CAD-CBD-CGD-O1D
18	A	1123	CLA	CHA-CBD-CGD-O1D
18	A	1123	CLA	CHA-CBD-CGD-O2D
18	A	1136	CLA	CAD-CBD-CGD-O1D
18	B	1138	CLA	CAD-CBD-CGD-O1D
18	B	1203	CLA	CAD-CBD-CGD-O1D
18	B	1216	CLA	CHA-CBD-CGD-O1D
18	B	1221	CLA	CAD-CBD-CGD-O1D
18	F	1139	CLA	CAD-CBD-CGD-O1D
18	F	1302	CLA	CAD-CBD-CGD-O1D
18	I	1204	CLA	CHA-CBD-CGD-O1D
20	I	6018	BCR	C15-C16-C17-C18
18	A	1103	CLA	C2B-C3B-CAB-CBB
18	B	1205	CLA	C2B-C3B-CAB-CBB
18	B	1225	CLA	C2B-C3B-CAB-CBB
18	B	1232	CLA	C2B-C3B-CAB-CBB
18	L	1502	CLA	C2B-C3B-CAB-CBB
18	L	1504	CLA	C2B-C3B-CAB-CBB
20	B	6017	BCR	C5-C6-C7-C8
18	B	1205	CLA	C2-C3-C5-C6
18	L	1504	CLA	C6-C7-C8-C10
19	A	5001	PQN	C26-C27-C28-C29
18	B	1220	CLA	C10-C11-C12-C13
18	B	1222	CLA	C11-C12-C13-C14
18	B	1222	CLA	C12-C13-C15-C16
18	B	1228	CLA	C3-C5-C6-C7
18	B	1242	CLA	C4C-C3C-CAC-CBC
18	A	1108	CLA	CAA-CBA-CGA-O2A

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Mol	Chain	Res	Type	Atoms
18	B	1207	CLA	CAA-CBA-CGA-O2A
18	I	1204	CLA	C4-C3-C5-C6
18	B	1231	CLA	C2C-C3C-CAC-CBC
18	B	1203	CLA	C4B-C3B-CAB-CBB
18	I	1204	CLA	C4B-C3B-CAB-CBB
18	B	1212	CLA	C5-C6-C7-C8
18	B	1215	CLA	O1A-CGA-O2A-C1
18	A	1115	CLA	C3A-C2A-CAA-CBA
18	B	1203	CLA	C3A-C2A-CAA-CBA
18	B	1220	CLA	C3A-C2A-CAA-CBA
18	B	1229	CLA	C3A-C2A-CAA-CBA
20	A	6011	BCR	C16-C17-C18-C36
20	F	6016	BCR	C35-C13-C14-C15
20	L	6020	BCR	C20-C21-C22-C37
18	A	1126	CLA	C2-C1-O2A-CGA
18	B	1208	CLA	C2-C1-O2A-CGA
19	A	5001	PQN	C24-C23-C25-C26
18	B	1203	CLA	CAA-CBA-CGA-O2A
19	A	5001	PQN	C25-C26-C27-C28
18	B	1202	CLA	CBD-CGD-O2D-CED
18	I	1204	CLA	C2-C3-C5-C6
18	B	1212	CLA	C1A-C2A-CAA-CBA
18	B	1229	CLA	C1A-C2A-CAA-CBA
18	F	1139	CLA	C1A-C2A-CAA-CBA
20	A	6011	BCR	C16-C17-C18-C19
20	F	6016	BCR	C12-C13-C14-C15
20	L	6020	BCR	C20-C21-C22-C23
18	B	9022	CLA	C2B-C3B-CAB-CBB
18	B	9023	CLA	C2B-C3B-CAB-CBB
18	B	1221	CLA	C2B-C3B-CAB-CBB
18	I	1204	CLA	C2B-C3B-CAB-CBB
20	B	6017	BCR	C1-C6-C7-C8
18	B	1208	CLA	C2C-C3C-CAC-CBC
19	A	5001	PQN	C21-C22-C23-C25
18	L	1504	CLA	C6-C7-C8-C9
18	A	1135	CLA	CAA-CBA-CGA-O1A
18	B	1225	CLA	CAA-CBA-CGA-O1A
18	L	1503	CLA	C2-C1-O2A-CGA
18	B	9023	CLA	C2-C1-O2A-CGA
18	A	1136	CLA	C2A-CAA-CBA-CGA
18	B	1220	CLA	C6-C7-C8-C9
18	B	1227	CLA	C4C-C3C-CAC-CBC

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Mol	Chain	Res	Type	Atoms
18	B	1225	CLA	CAA-CBA-CGA-O2A
18	B	9012	CLA	C2-C3-C5-C6
18	B	1222	CLA	O1A-CGA-O2A-C1
18	B	1205	CLA	C2A-CAA-CBA-CGA
18	B	1242	CLA	C2-C1-O2A-CGA
18	A	1107	CLA	C5-C6-C7-C8
18	J	2107	CLA	C5-C6-C7-C8
18	B	1217	CLA	O1D-CGD-O2D-CED
18	A	1135	CLA	CAA-CBA-CGA-O2A
18	J	2107	CLA	C2C-C3C-CAC-CBC
18	B	1229	CLA	CAA-CBA-CGA-O2A
18	G	1233	CLA	CAA-CBA-CGA-O2A
18	B	1205	CLA	C2-C1-O2A-CGA
18	B	1219	CLA	C2-C1-O2A-CGA
18	B	1232	CLA	C2-C1-O2A-CGA
18	B	1234	CLA	C2-C1-O2A-CGA
18	B	1222	CLA	CBA-CGA-O2A-C1
18	B	1217	CLA	C3A-C2A-CAA-CBA
18	A	1119	CLA	C4C-C3C-CAC-CBC
18	B	1138	CLA	O1A-CGA-O2A-C1
18	B	1222	CLA	C2C-C3C-CAC-CBC
19	A	5001	PQN	C26-C27-C28-C30
18	A	1128	CLA	O1A-CGA-O2A-C1
18	B	1212	CLA	C4C-C3C-CAC-CBC
18	B	1205	CLA	CAA-CBA-CGA-O2A
18	L	1502	CLA	C2C-C3C-CAC-CBC
18	B	1242	CLA	O1D-CGD-O2D-CED
18	B	1221	CLA	C2A-CAA-CBA-CGA
18	A	1129	CLA	C2B-C3B-CAB-CBB
18	B	1219	CLA	C2B-C3B-CAB-CBB
18	A	1136	CLA	C2-C1-O2A-CGA
18	B	1222	CLA	C10-C11-C12-C13
18	B	1207	CLA	C6-C7-C8-C9
18	B	1242	CLA	CBD-CGD-O2D-CED
18	A	1107	CLA	CAA-CBA-CGA-O2A
18	B	1218	CLA	C2A-CAA-CBA-CGA
18	B	1220	CLA	CAA-CBA-CGA-O2A
18	A	1115	CLA	CAA-CBA-CGA-O2A
18	B	1212	CLA	CAA-CBA-CGA-O1A
20	A	6011	BCR	C37-C22-C23-C24
18	B	1215	CLA	CAA-CBA-CGA-O2A
18	A	1113	CLA	C1A-C2A-CAA-CBA

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Mol	Chain	Res	Type	Atoms
18	B	1232	CLA	C4B-C3B-CAB-CBB
18	L	1504	CLA	C1A-C2A-CAA-CBA
18	B	1242	CLA	CAA-CBA-CGA-O2A
18	L	1503	CLA	CAA-CBA-CGA-O2A
20	A	6011	BCR	C21-C22-C23-C24
18	A	1128	CLA	CBA-CGA-O2A-C1
18	B	1228	CLA	C5-C6-C7-C8
18	B	1212	CLA	C11-C12-C13-C15
18	B	1138	CLA	C2-C1-O2A-CGA
18	B	1218	CLA	C2-C1-O2A-CGA
18	A	1140	CLA	C6-C7-C8-C9
18	B	1202	CLA	C3A-C2A-CAA-CBA
18	L	1504	CLA	C3A-C2A-CAA-CBA
18	B	1205	CLA	CAA-CBA-CGA-O1A
18	A	1107	CLA	CAA-CBA-CGA-O1A
18	B	1138	CLA	CBA-CGA-O2A-C1
18	B	1220	CLA	CAA-CBA-CGA-O1A
18	A	1115	CLA	CAA-CBA-CGA-O1A
18	B	1222	CLA	CAA-CBA-CGA-O2A
19	B	5002	PQN	C26-C27-C28-C30
18	B	1207	CLA	C4-C3-C5-C6
18	B	1217	CLA	CAD-CBD-CGD-O2D
18	B	9023	CLA	CAA-CBA-CGA-O2A
18	A	1129	CLA	C2C-C3C-CAC-CBC
18	B	1215	CLA	CAA-CBA-CGA-O1A
18	B	1242	CLA	CAA-CBA-CGA-O1A
18	B	9012	CLA	C2-C1-O2A-CGA
18	H	1501	CLA	C2-C1-O2A-CGA
18	A	1140	CLA	CAA-CBA-CGA-O2A
18	B	1237	CLA	CAA-CBA-CGA-O2A
18	A	1140	CLA	CAA-CBA-CGA-O1A

There are no ring outliers.

131 monomers are involved in 1317 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
18	2	2003	CLA	1	0
18	A	1101	CLA	4	0
18	A	1113	CLA	6	0
18	2	2002	CLA	2	0
18	4	4001	CLA	3	0
18	B	1238	CLA	21	0

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
18	A	1123	CLA	25	0
18	B	1223	CLA	5	0
18	A	1103	CLA	21	0
18	B	1222	CLA	12	0
18	4	4011	CLA	1	0
18	B	1226	CLA	5	0
18	I	1204	CLA	9	0
20	L	6020	BCR	17	0
18	A	1122	CLA	4	0
18	A	9013	CLA	19	0
18	A	1105	CLA	3	0
18	A	1106	CLA	13	0
18	A	1140	CLA	23	0
18	3	3006	CLA	1	0
18	1	1013	CLA	3	0
18	F	1139	CLA	18	0
18	1	1006	CLA	2	0
18	4	4013	CLA	1	0
18	B	1205	CLA	15	0
18	B	1230	CLA	6	0
18	A	1115	CLA	8	0
18	4	1304	CLA	9	0
18	B	1235	CLA	18	0
18	B	1212	CLA	13	0
18	B	1242	CLA	20	0
18	3	3004	CLA	2	0
18	F	4015	CLA	2	0
18	A	1135	CLA	6	0
18	A	9011	CLA	22	0
18	K	1141	CLA	5	0
18	B	9022	CLA	19	0
18	2	2006	CLA	2	0
18	A	1127	CLA	6	0
18	A	1108	CLA	11	0
18	B	1221	CLA	19	0
20	I	6018	BCR	13	0
18	A	1128	CLA	13	0
21	C	3103	SF4	7	0
18	B	1203	CLA	15	0
18	F	1303	CLA	2	0
18	A	1137	CLA	18	0
20	B	6017	BCR	17	0

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
18	B	1217	CLA	14	0
18	B	1301	CLA	3	0
18	A	1124	CLA	14	0
18	J	2107	CLA	8	0
18	1	1012	CLA	3	0
18	4	4012	CLA	1	0
18	B	1210	CLA	15	0
18	A	1111	CLA	2	0
18	A	1134	CLA	7	0
18	B	1241	CLA	6	0
18	G	1248	CLA	4	0
20	F	6016	BCR	13	0
18	A	1119	CLA	8	0
18	A	1118	CLA	7	0
19	A	5001	PQN	30	0
18	A	1133	CLA	2	0
18	B	1225	CLA	41	0
18	A	1126	CLA	23	0
18	B	1227	CLA	20	0
18	B	1228	CLA	22	0
18	A	1147	CLA	6	0
18	F	1302	CLA	17	0
18	B	9012	CLA	18	0
18	A	1129	CLA	17	0
18	B	1239	CLA	29	0
18	A	1131	CLA	10	0
18	B	1236	CLA	11	0
18	2	2004	CLA	3	0
18	L	1130	CLA	20	0
18	B	1206	CLA	5	0
18	B	1224	CLA	14	0
18	B	1209	CLA	39	0
18	A	1132	CLA	11	0
18	H	1505	CLA	2	0
18	A	1107	CLA	18	0
18	1	1008	CLA	1	0
18	L	1504	CLA	11	0
18	B	1232	CLA	7	0
18	3	3010	CLA	2	0
18	L	1502	CLA	19	0
18	4	4010	CLA	1	0
21	C	3102	SF4	8	0

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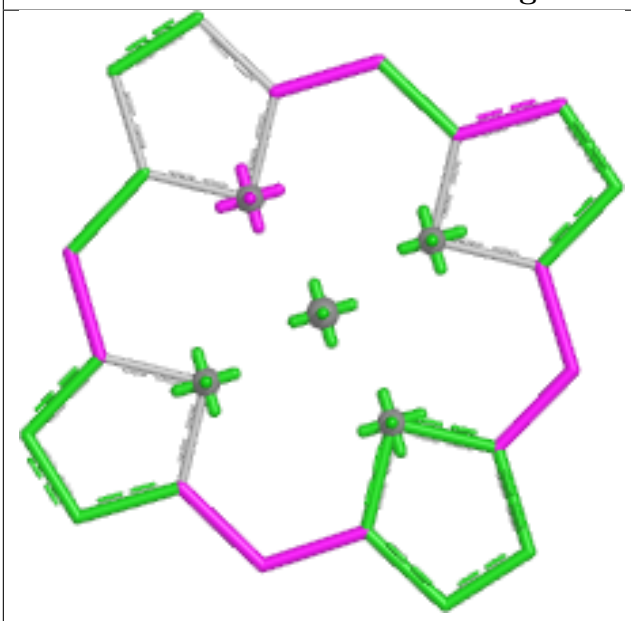
Mol	Chain	Res	Type	Clashes	Symm-Clashes
21	B	3101	SF4	4	0
18	B	9023	CLA	14	0
20	A	6011	BCR	17	0
18	B	1219	CLA	11	0
18	B	1213	CLA	1	0
18	L	1503	CLA	56	0
18	2	2011	CLA	1	0
18	1	1003	CLA	3	0
18	2	2005	CLA	1	0
18	A	1110	CLA	3	0
18	A	1136	CLA	22	0
18	G	1233	CLA	8	0
18	3	3005	CLA	5	0
18	F	1240	CLA	2	0
18	B	1215	CLA	21	0
18	3	3002	CLA	2	0
18	A	1146	CLA	1	0
18	B	9010	CLA	26	0
18	A	1148	CLA	4	0
18	B	1216	CLA	23	0
18	B	1218	CLA	46	0
18	B	1220	CLA	26	0
18	2	2012	CLA	5	0
18	2	2007	CLA	2	0
18	A	1116	CLA	5	0
18	B	1138	CLA	24	0
18	H	1501	CLA	12	0
18	3	3007	CLA	1	0
18	B	1211	CLA	8	0
18	A	1120	CLA	1	0
18	B	1202	CLA	42	0
18	B	1208	CLA	11	0
18	B	1214	CLA	31	0
18	B	1231	CLA	2	0
18	B	1234	CLA	26	0
18	B	1229	CLA	14	0
18	4	4005	CLA	1	0
19	B	5002	PQN	20	0
18	B	1237	CLA	11	0
18	A	1109	CLA	12	0
18	B	1207	CLA	16	0

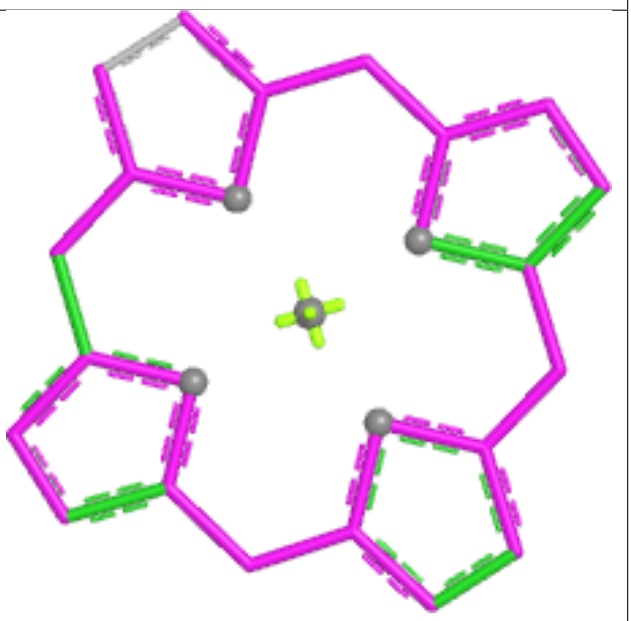
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths,

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

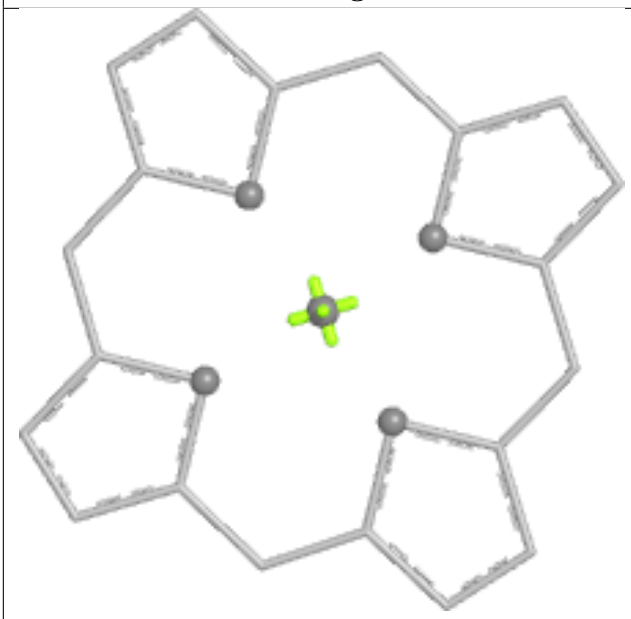
Ligand CLA 2 2015



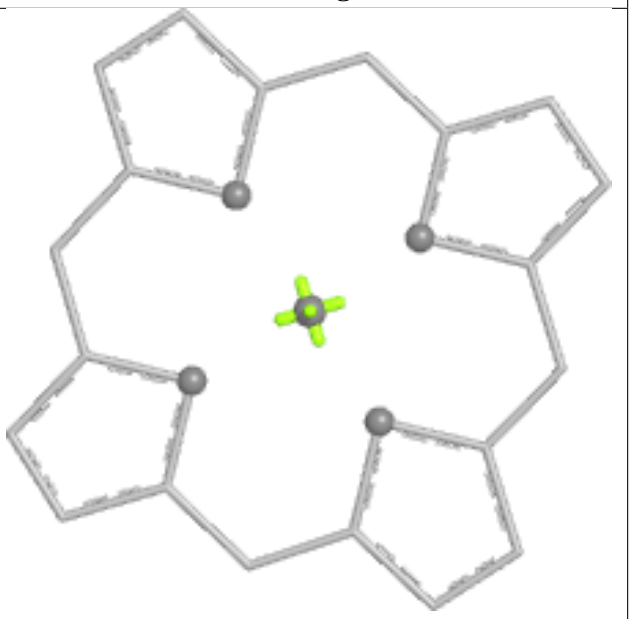
Bond lengths



Bond angles

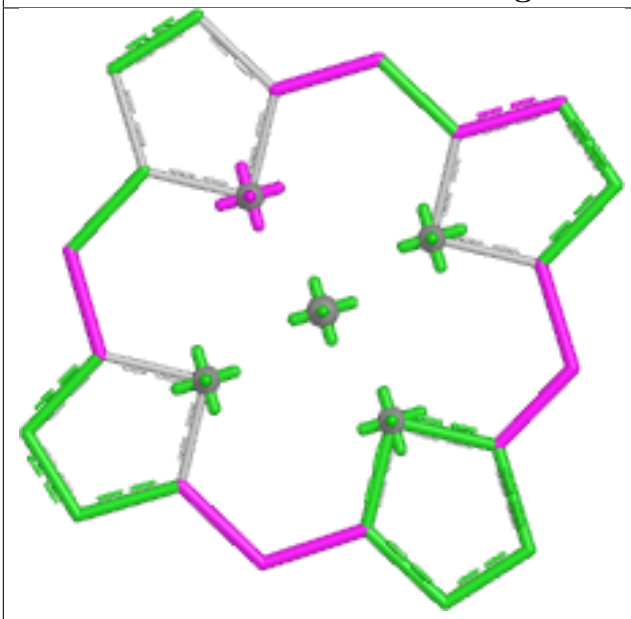


Torsions

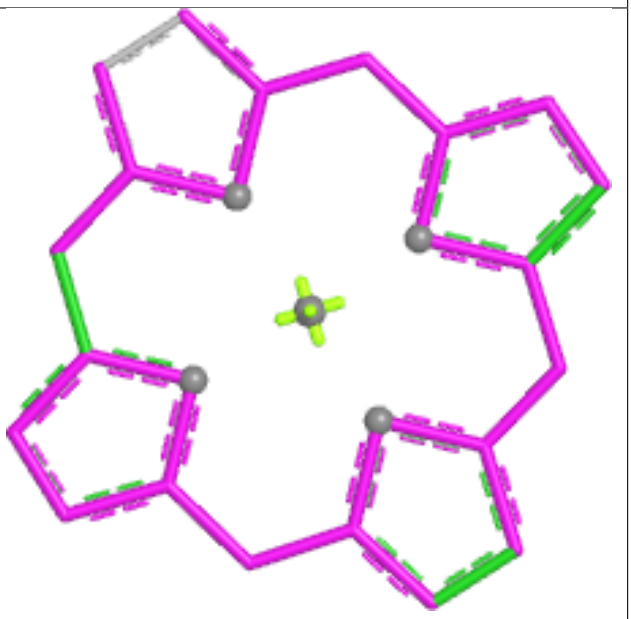


Rings

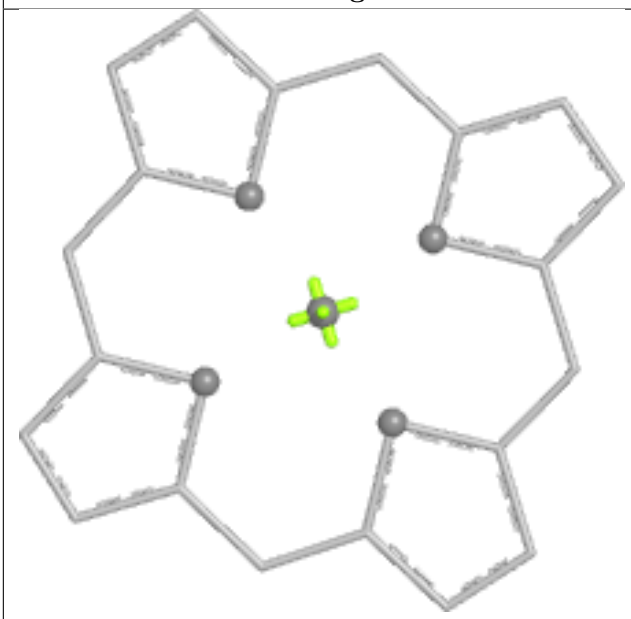
Ligand CLA K 1153



Bond lengths



Bond angles



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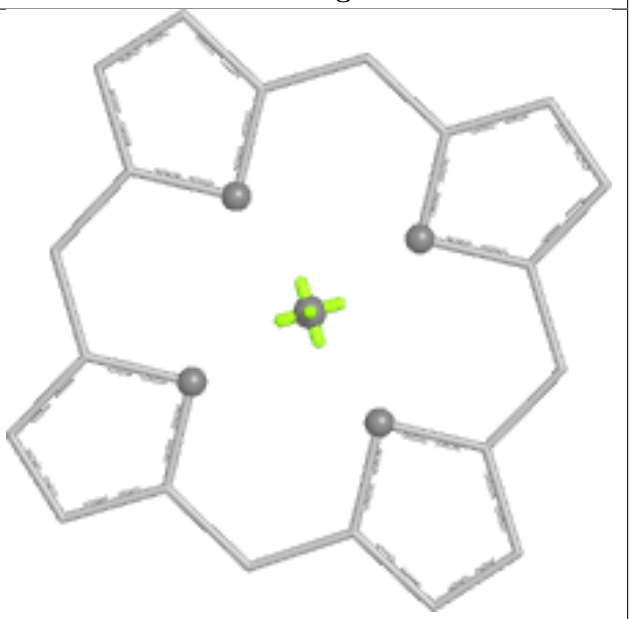
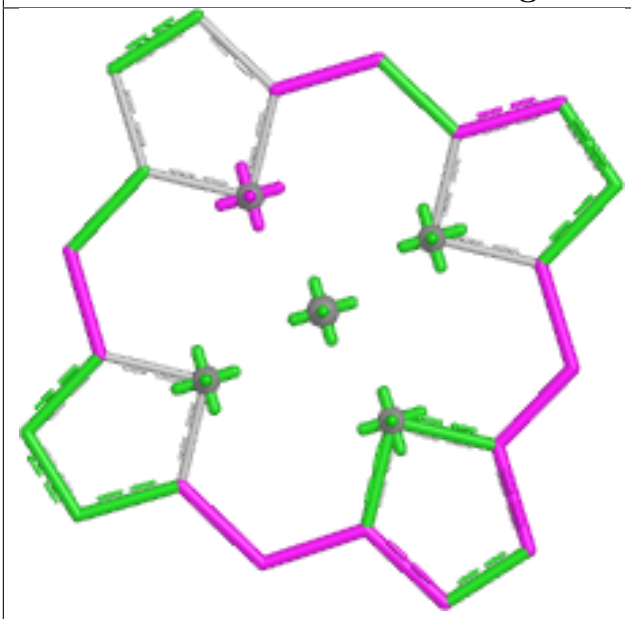
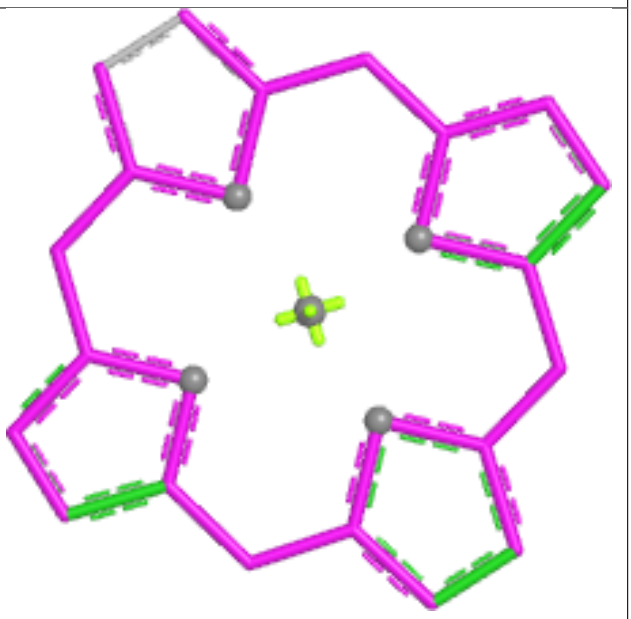


Rings

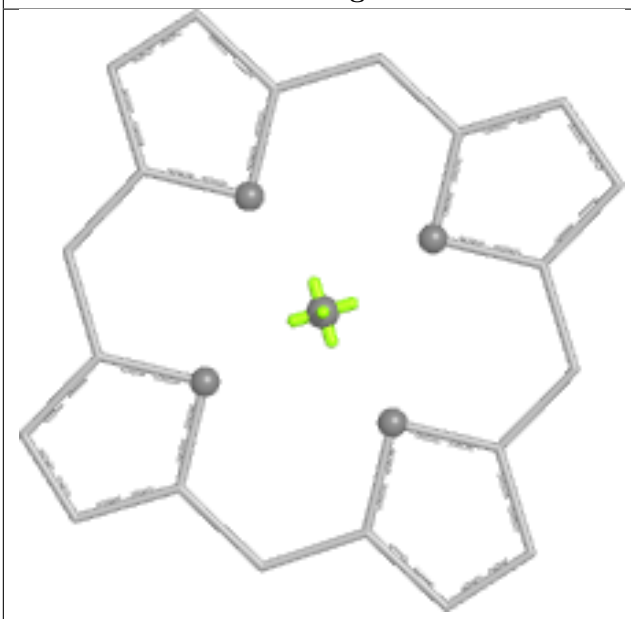
Ligand CLA 2 2003



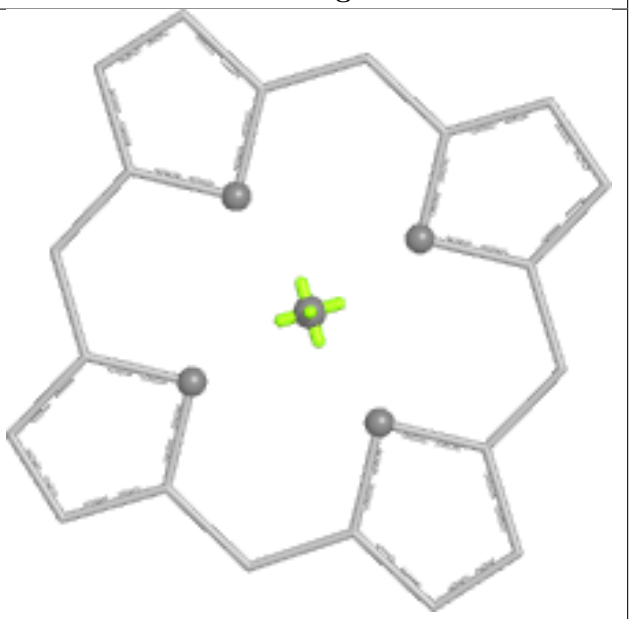
Bond lengths



Bond angles

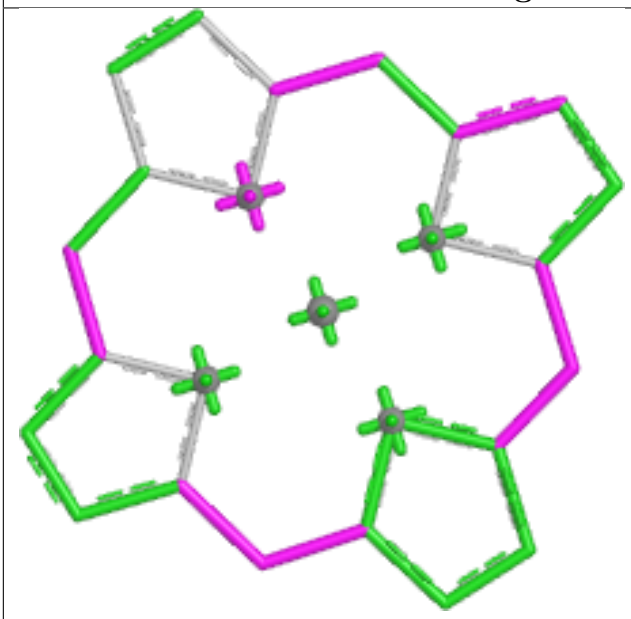


Torsions



Rings

Ligand CLA A 1101



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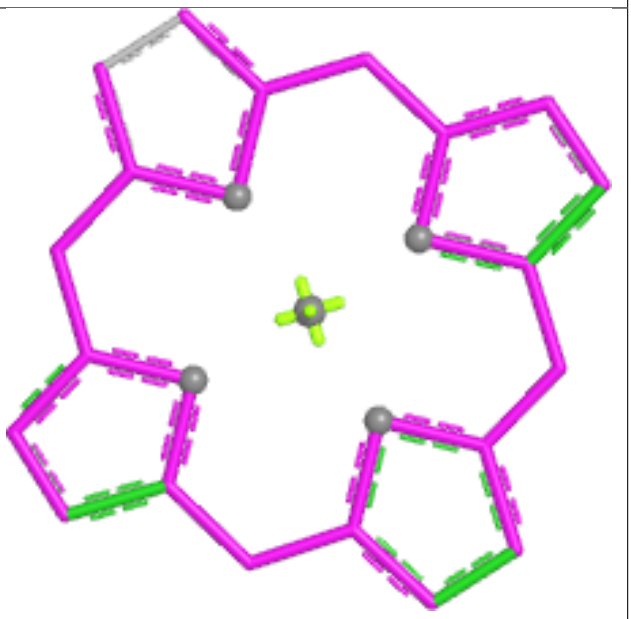
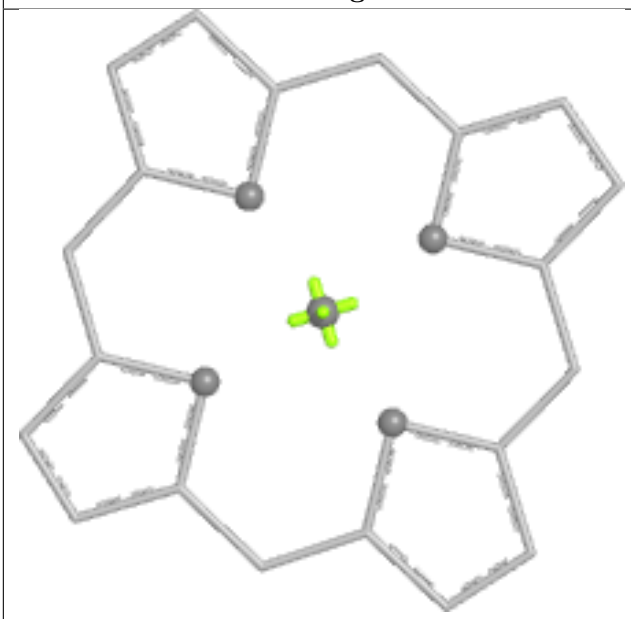


Bond angles



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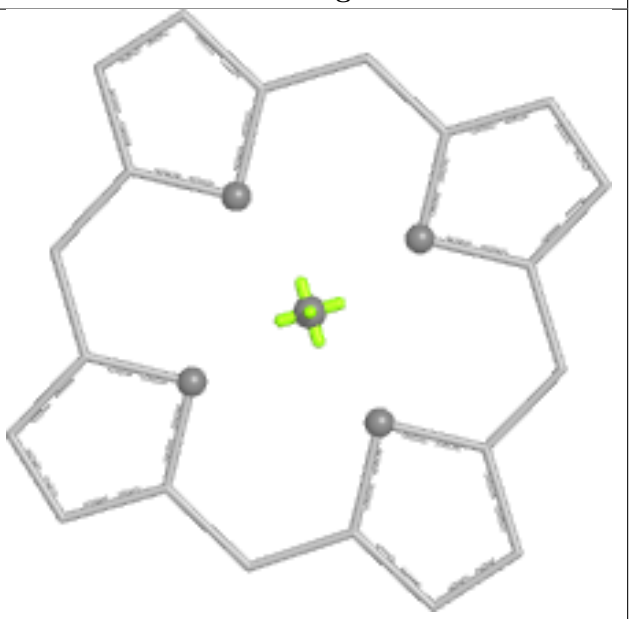
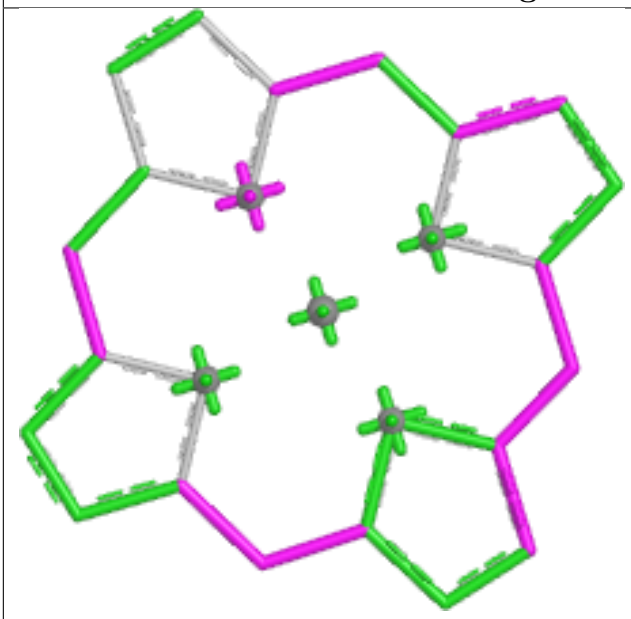


Rings

Ligand CLA 3 3009



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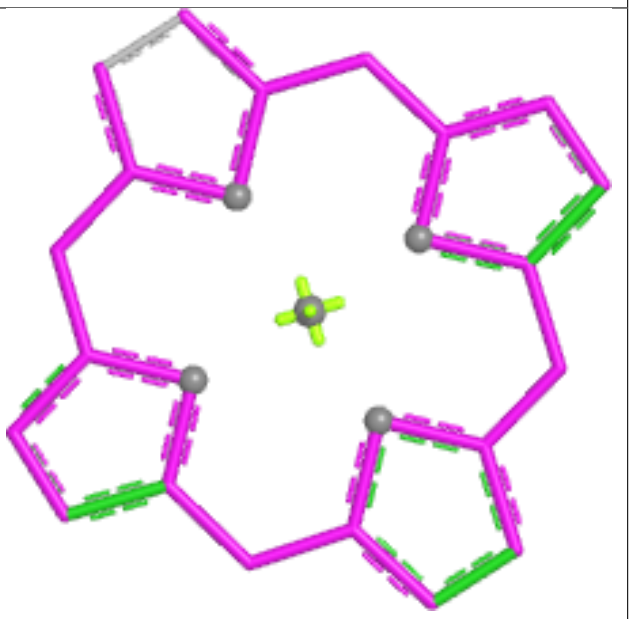

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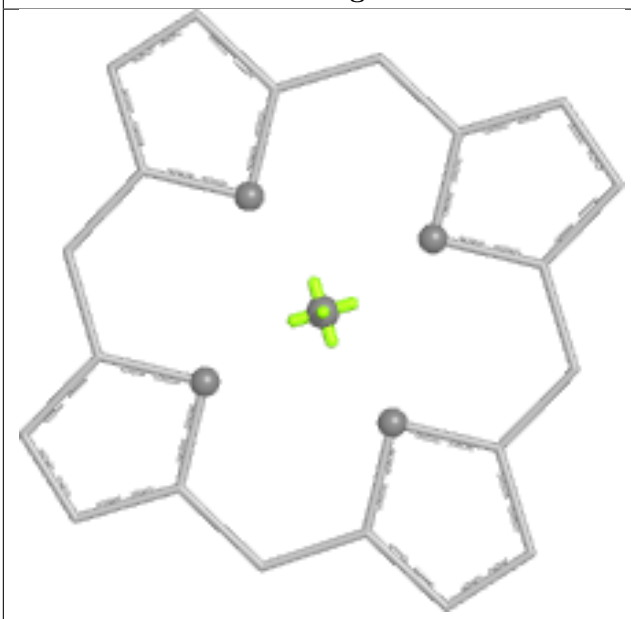

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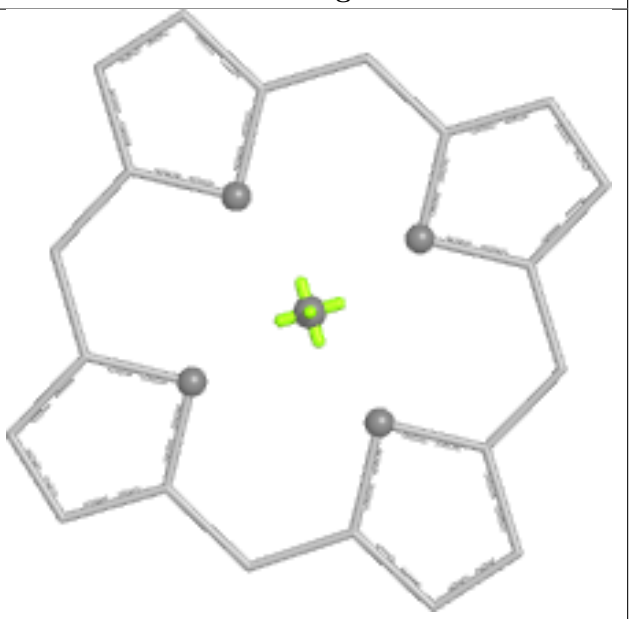
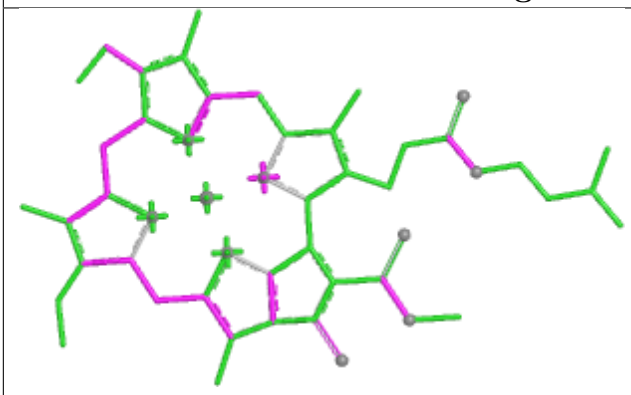


Rings

Ligand CLA A 1113



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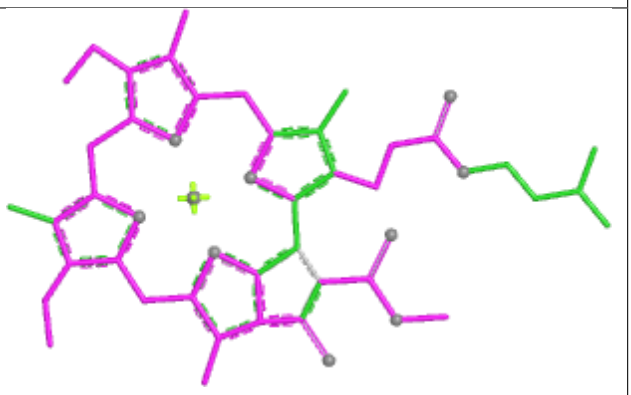

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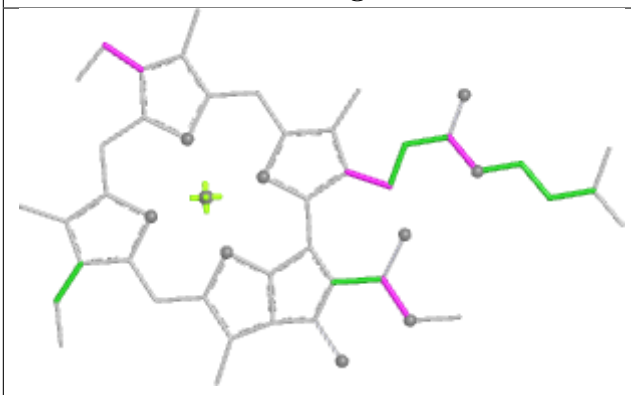

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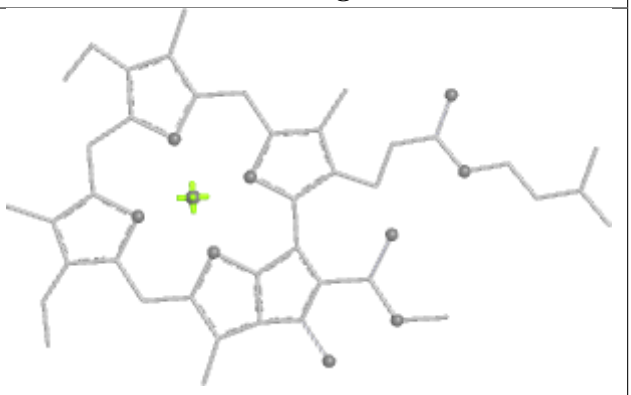
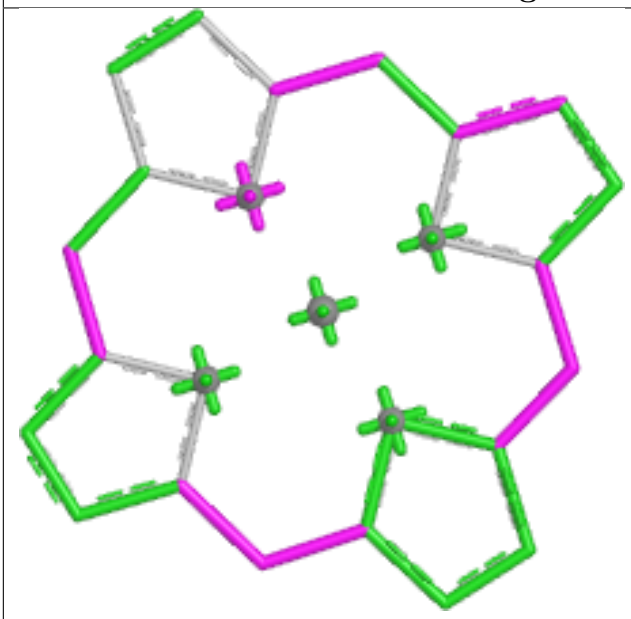


Rings

Ligand CLA 2 2002



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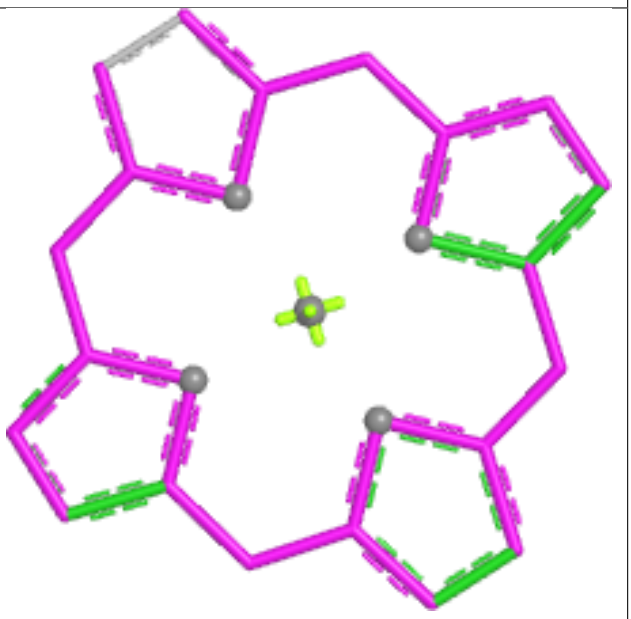

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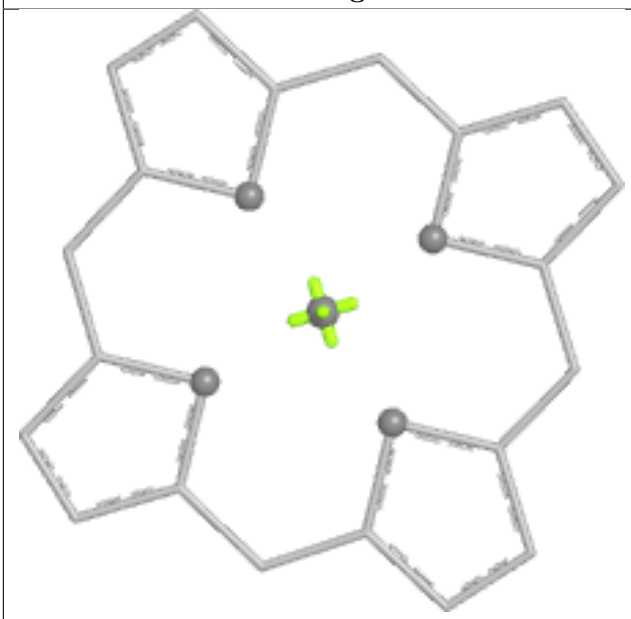

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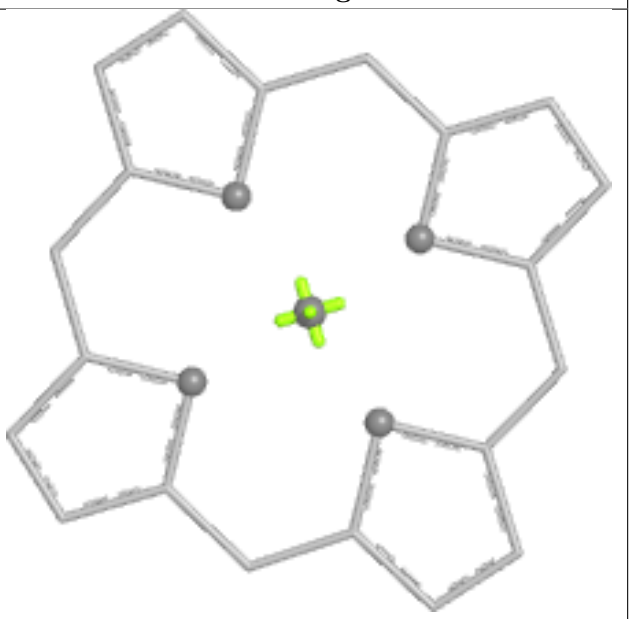
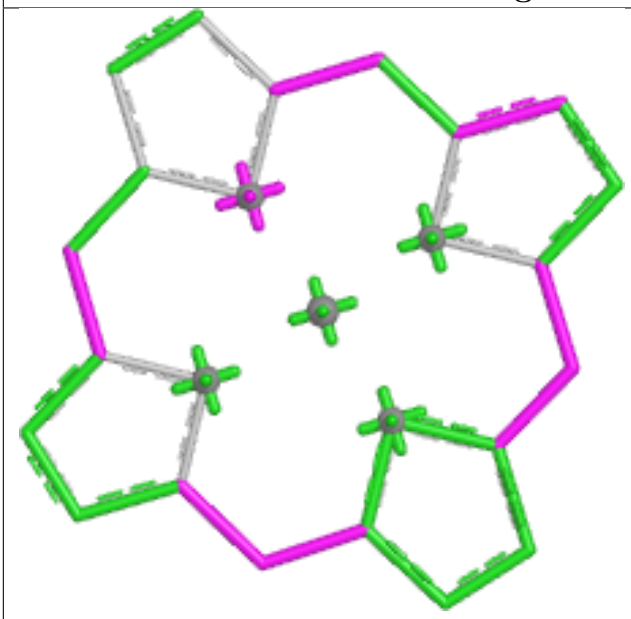


Rings

Ligand CLA A 1309



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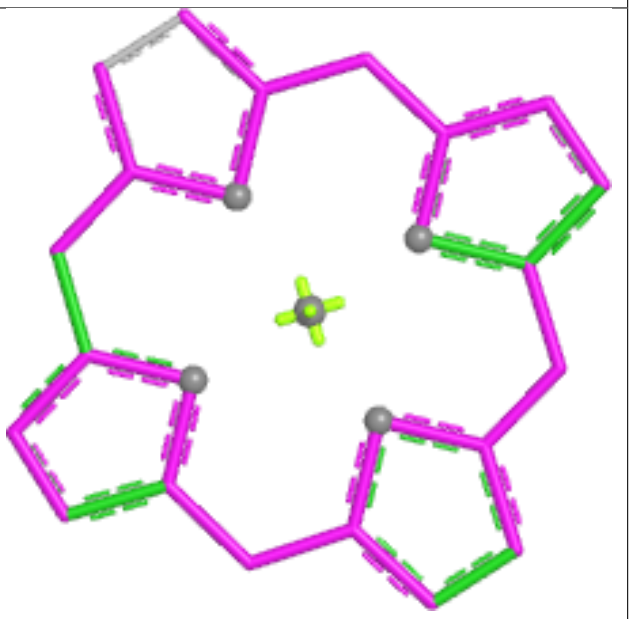

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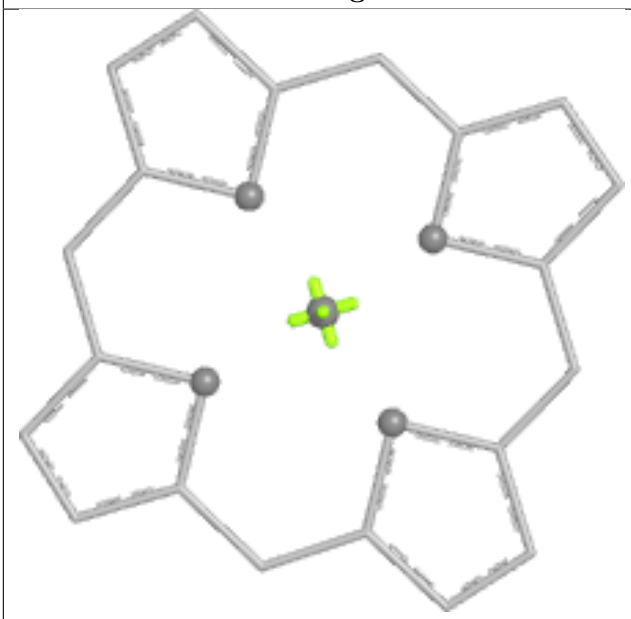

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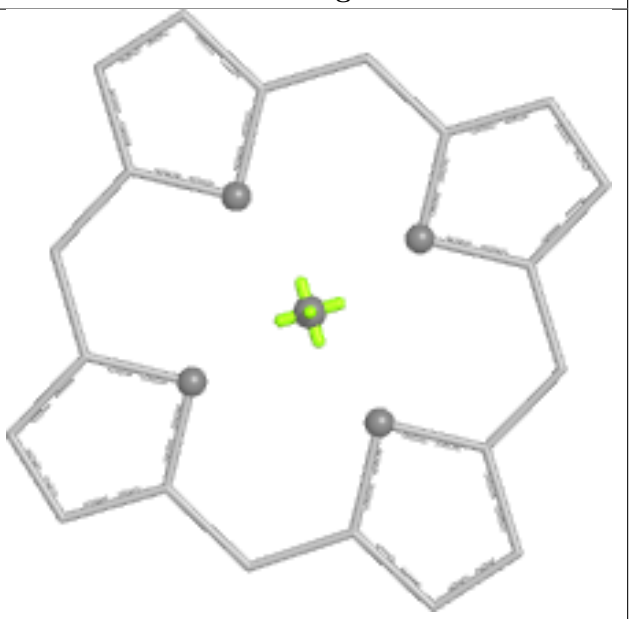
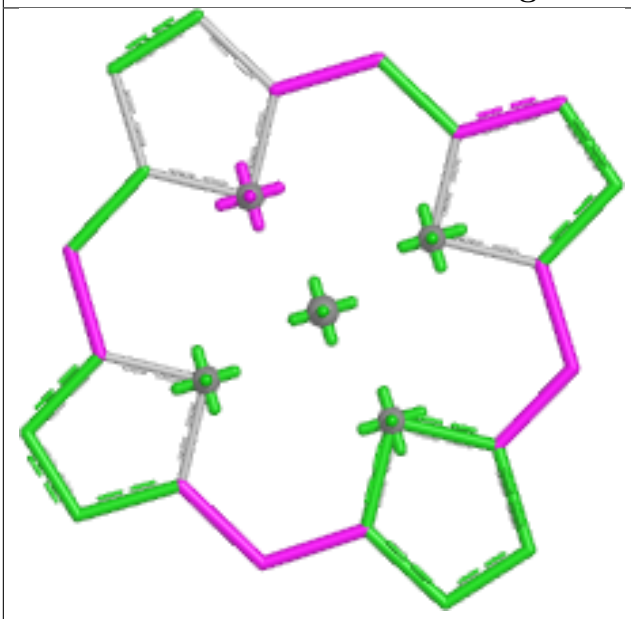


Rings

Ligand CLA 4 4001



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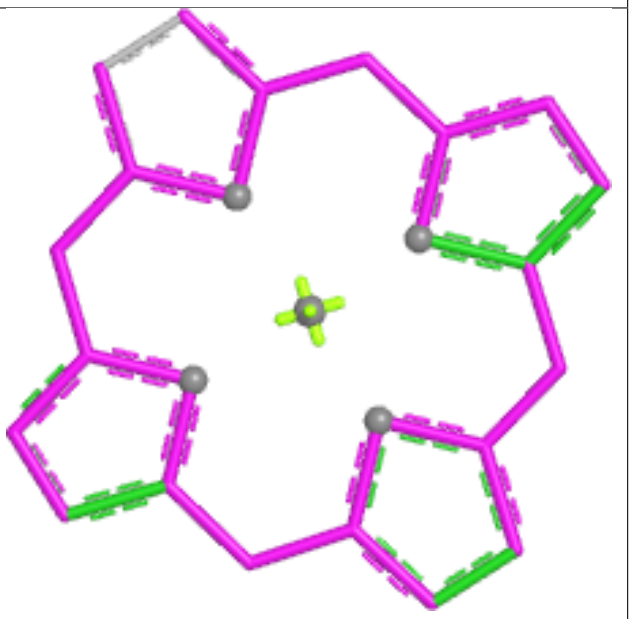
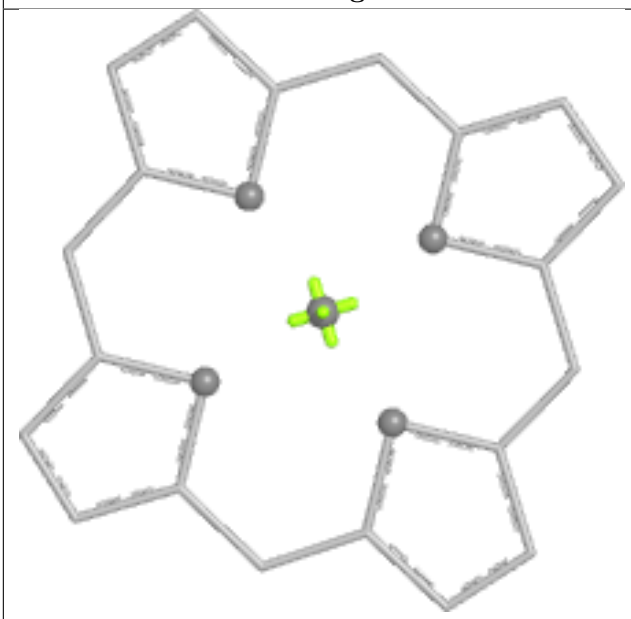


Bond angles



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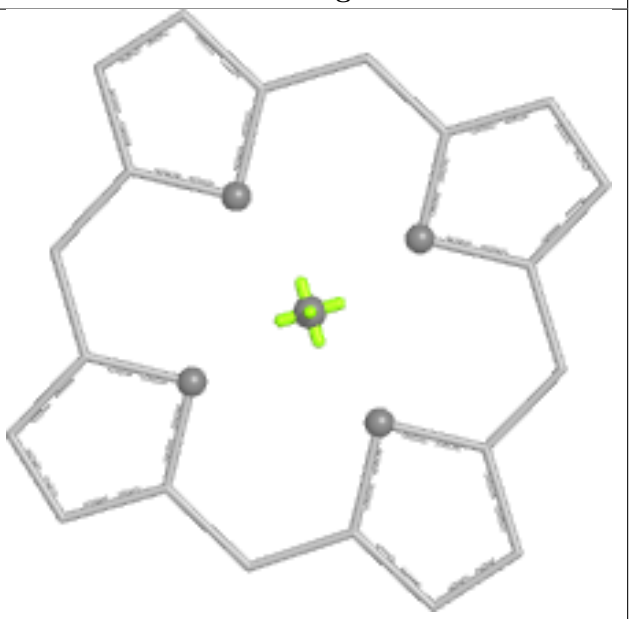
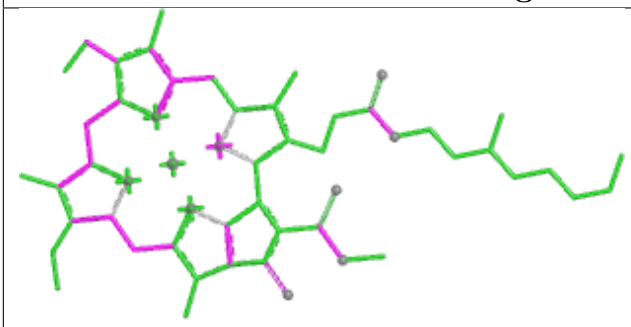
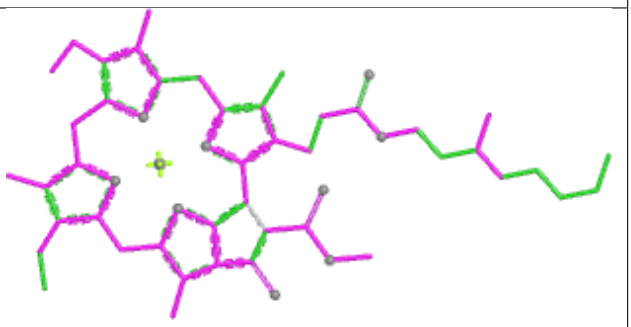
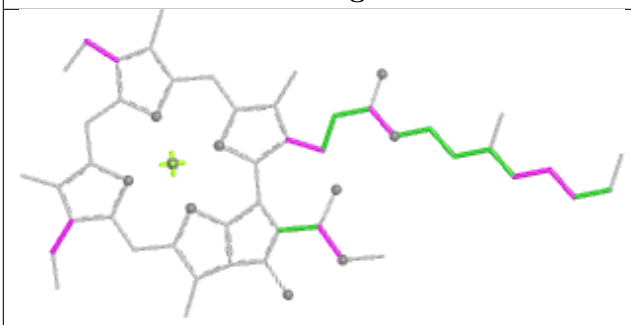
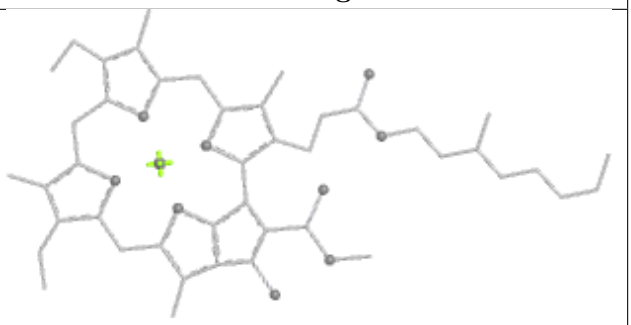
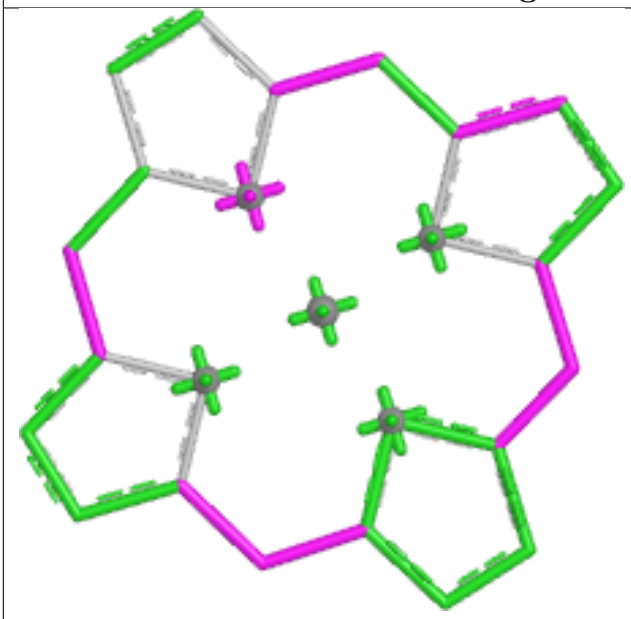


Rings

Ligand CLA B 1238	
 Bond lengths	 Bond angles
 Torsions	 Rings

Ligand CLA 4 4007



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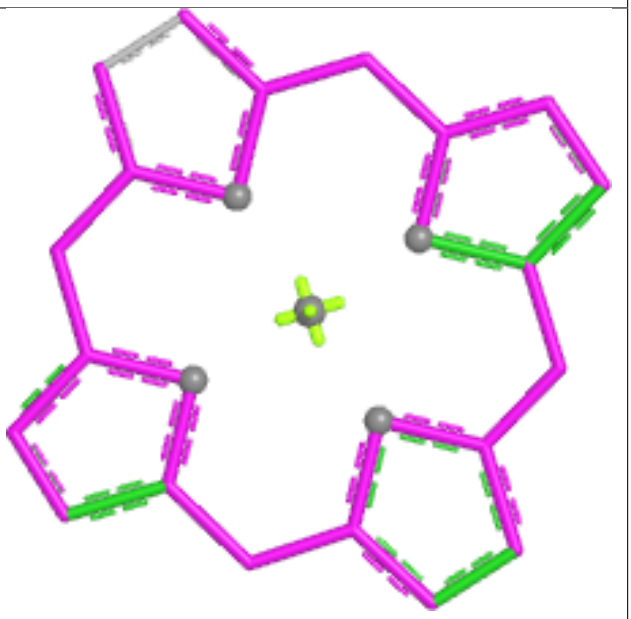

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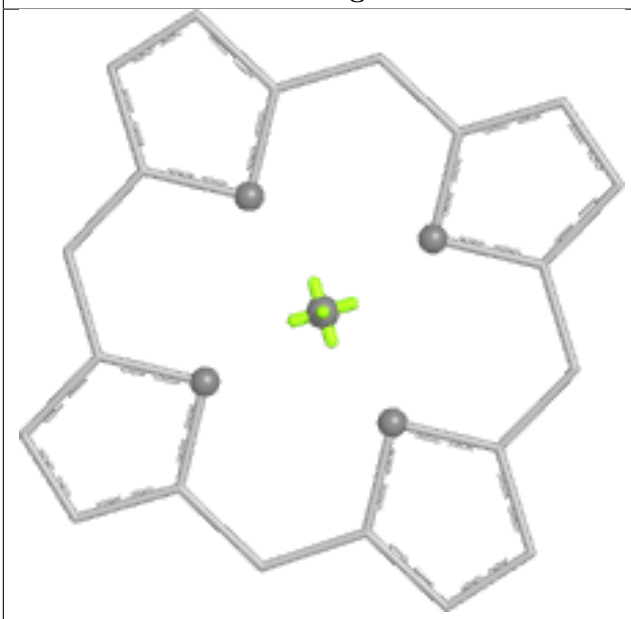

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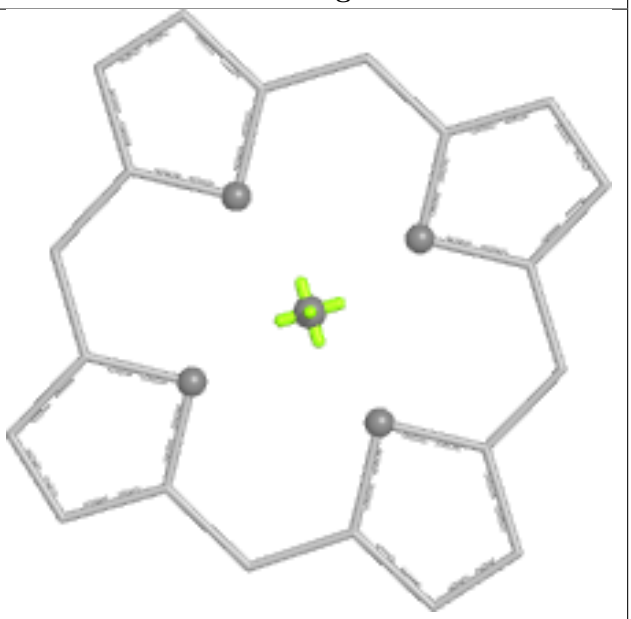
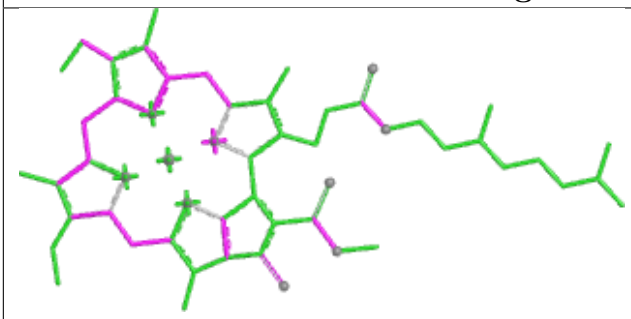
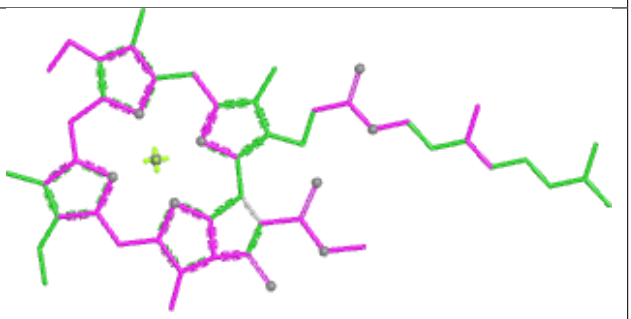
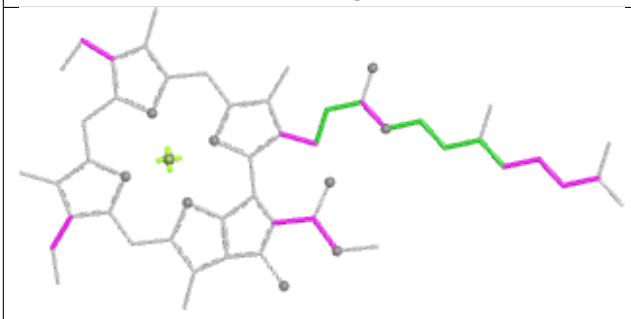
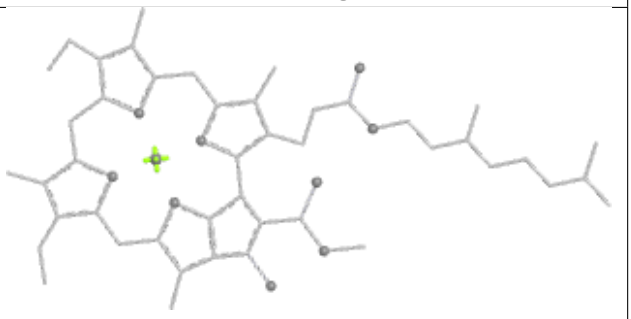
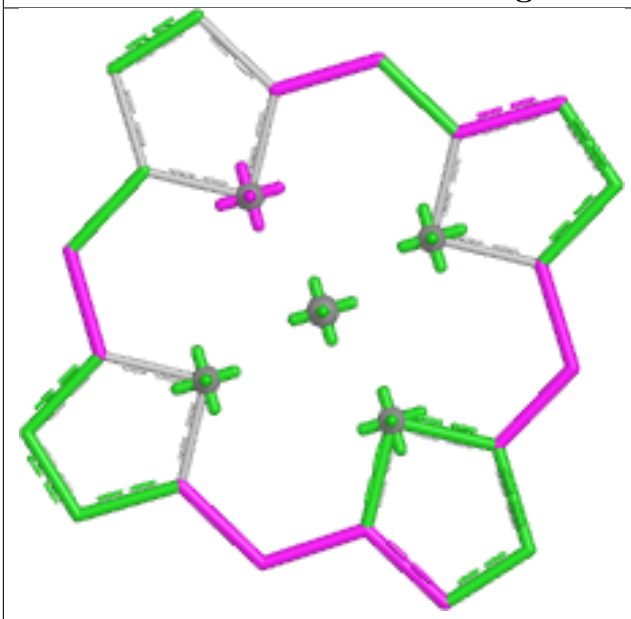


Rings

Ligand CLA A 1123	
 Bond lengths	 Bond angles
 Torsions	 Rings

Ligand CLA B 1223



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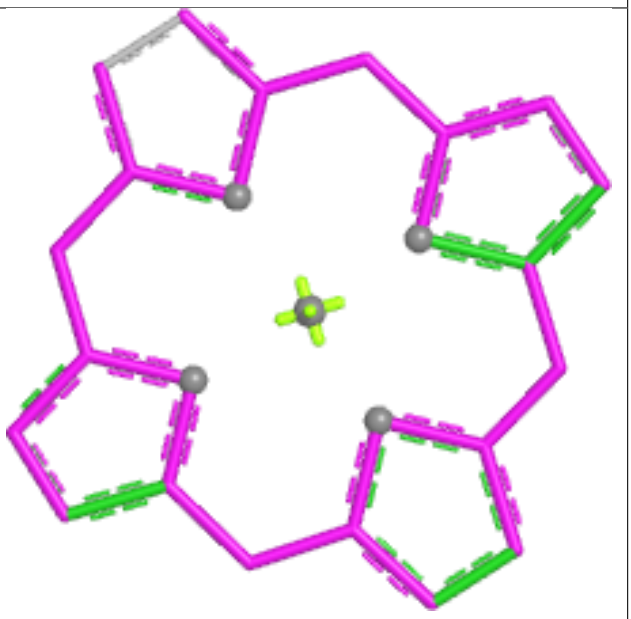
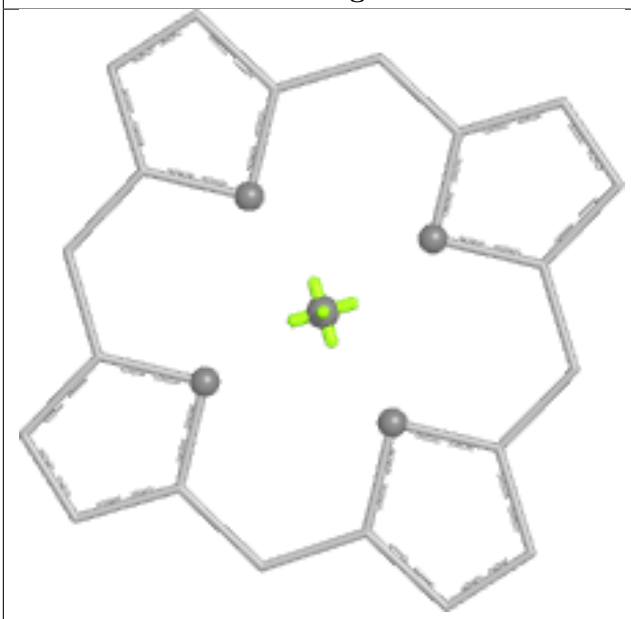


Bond angles



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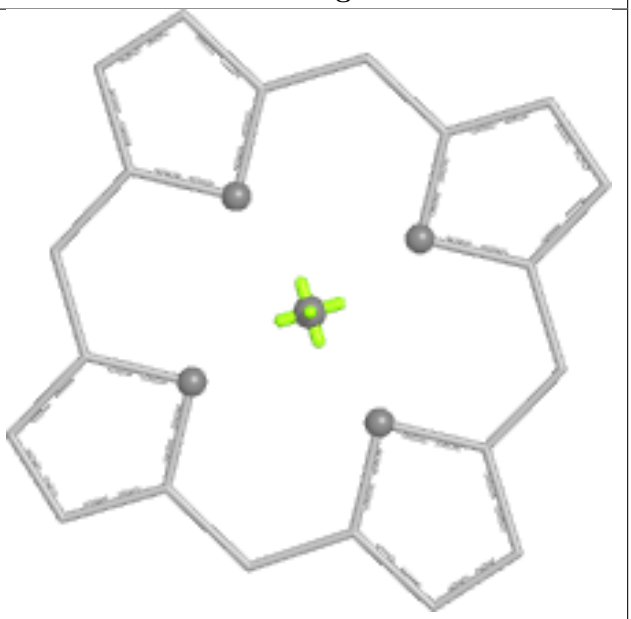
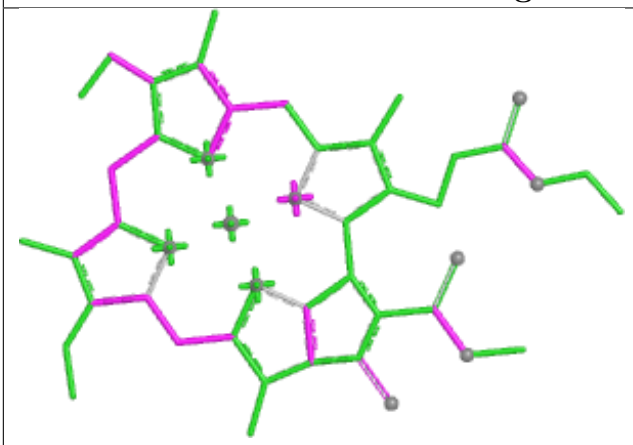


Rings

Ligand CLA A 1103



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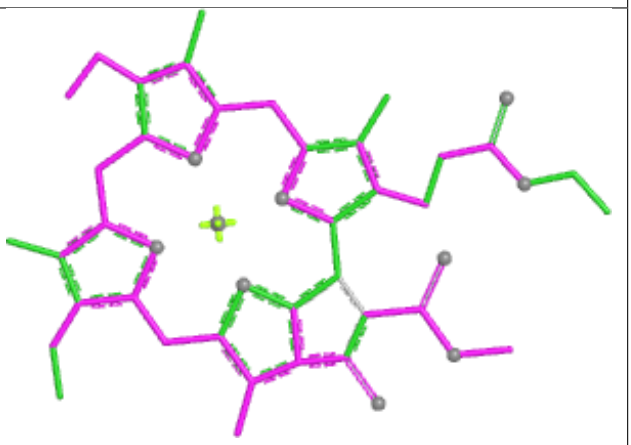
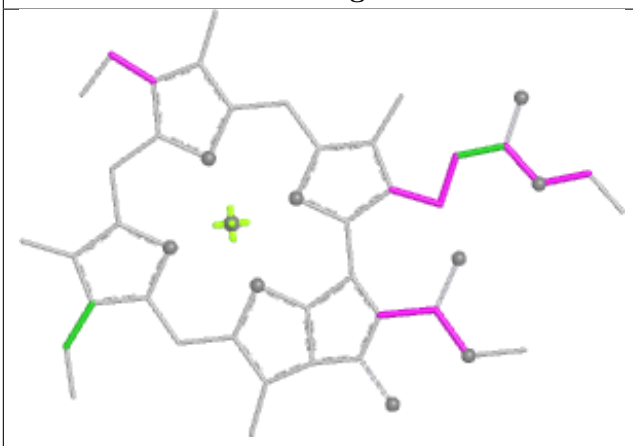


Bond angles



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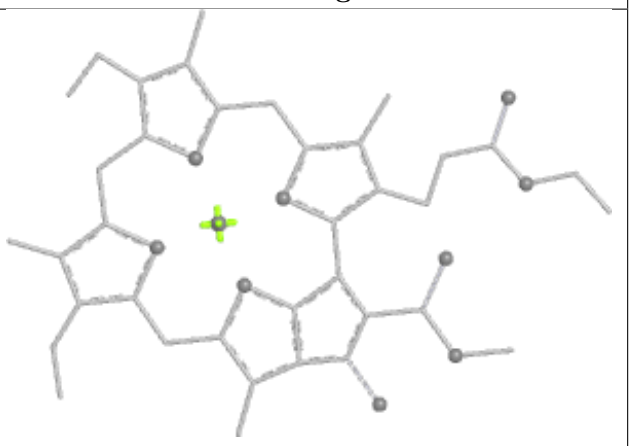
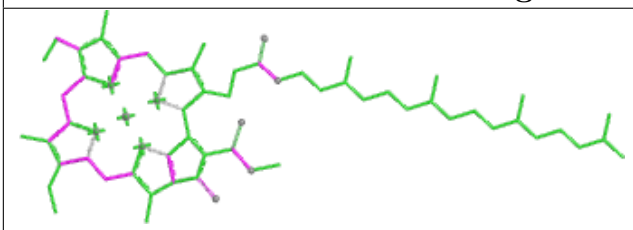


Rings

Ligand CLA B 1222



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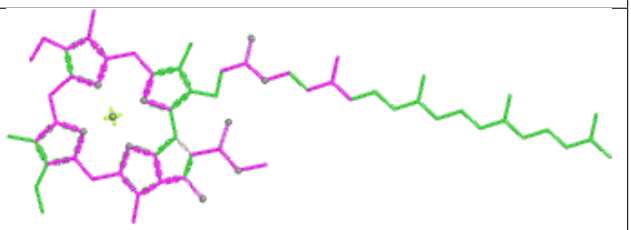
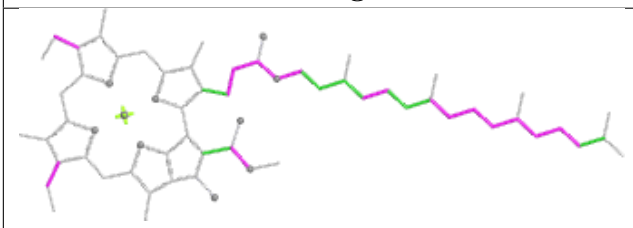


Bond angles



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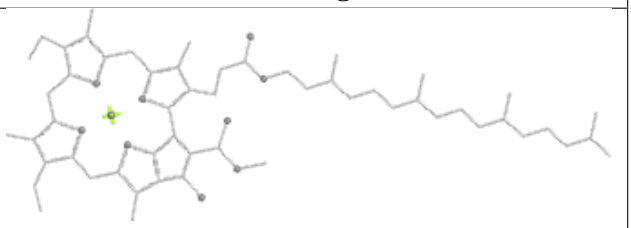
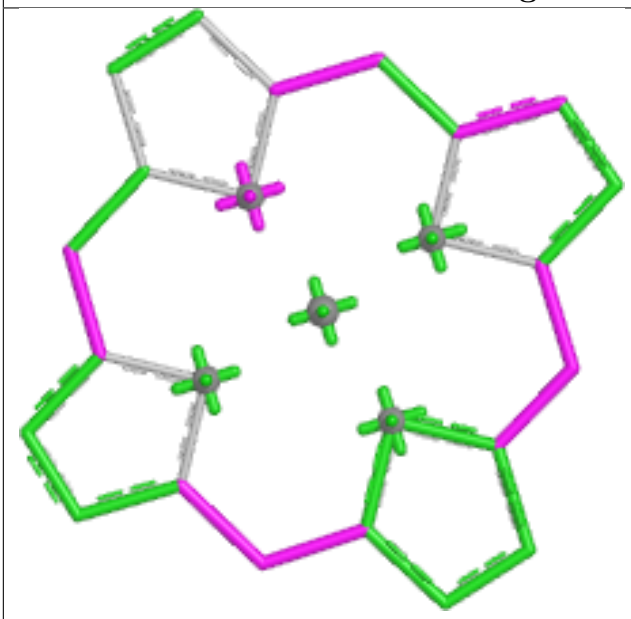


Rings

Ligand CLA 1 1001



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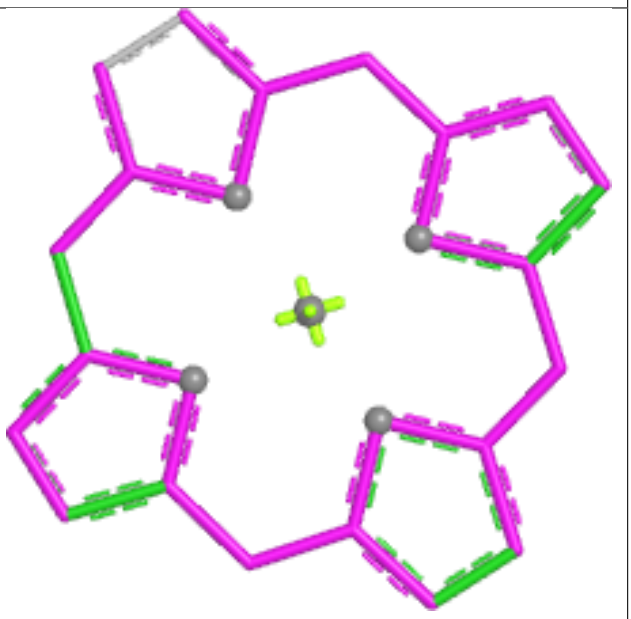
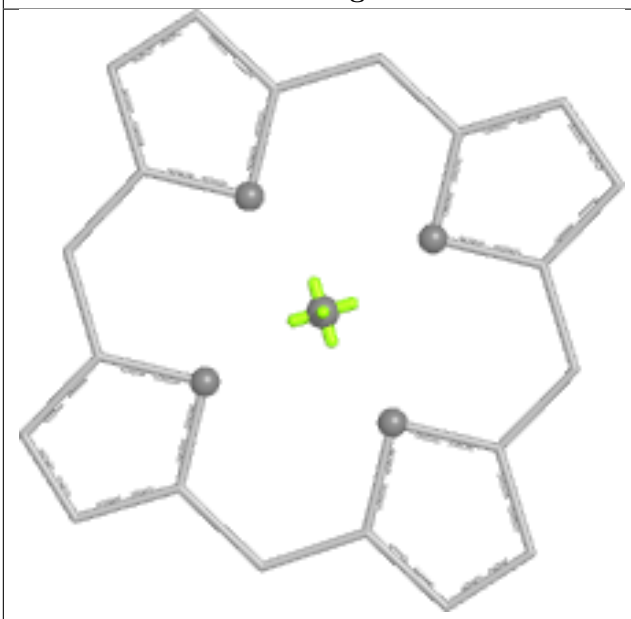


Bond angles



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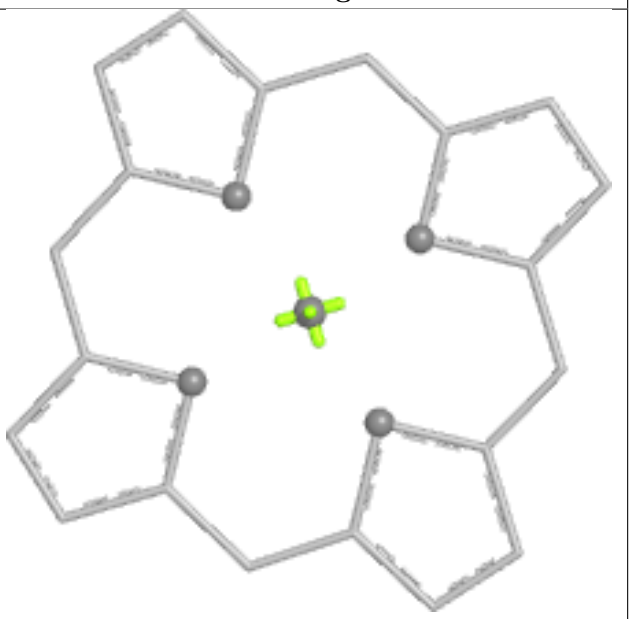
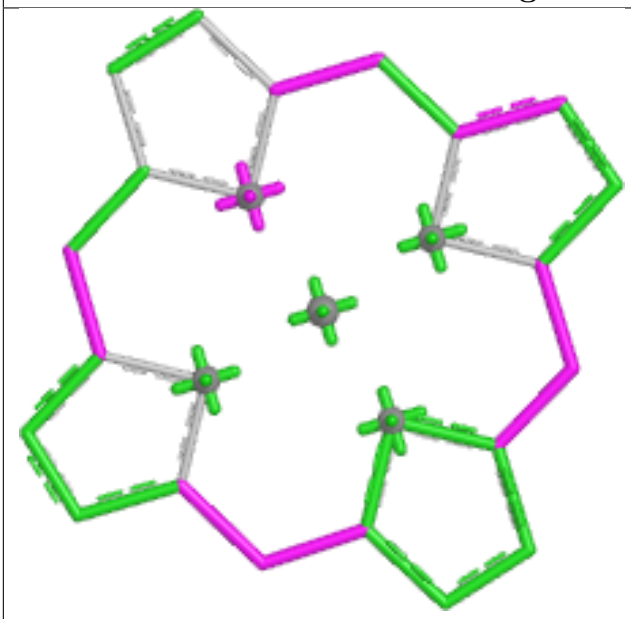


Rings

Ligand CLA 4 4011



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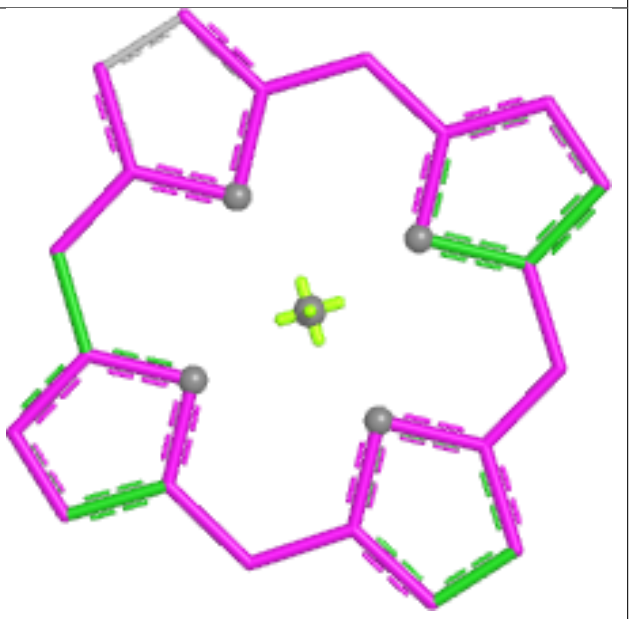
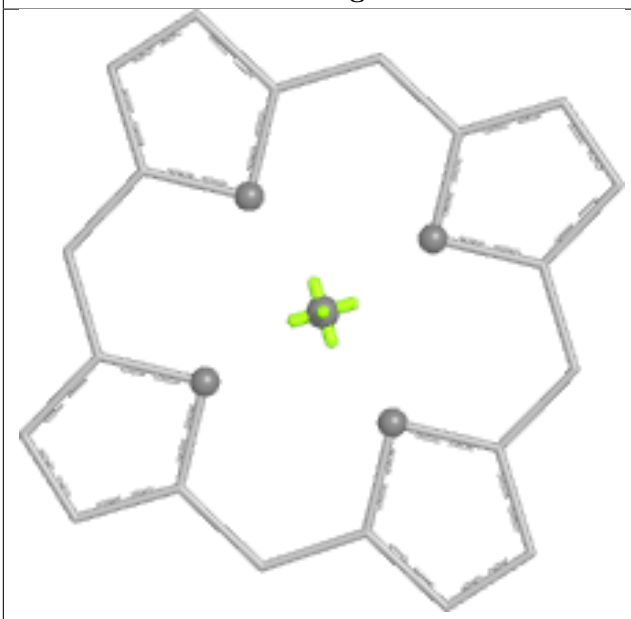


Bond angles



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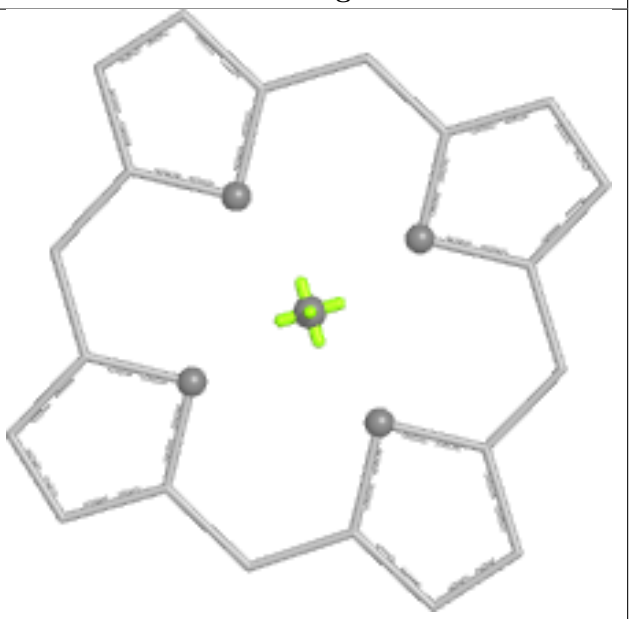
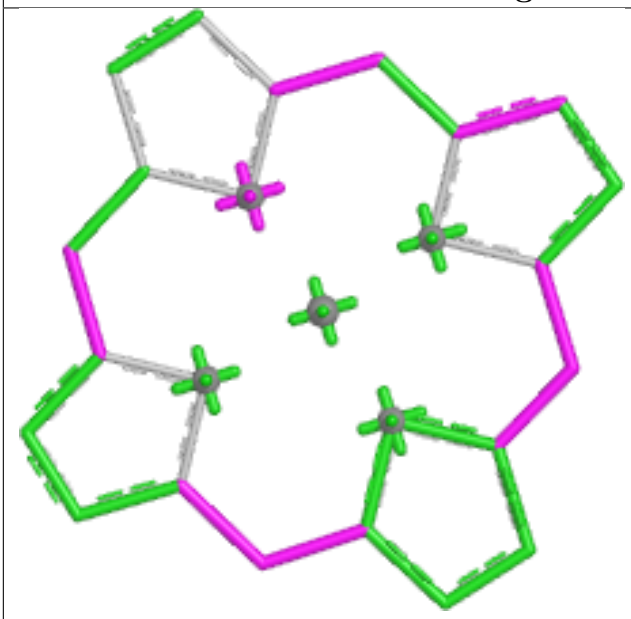
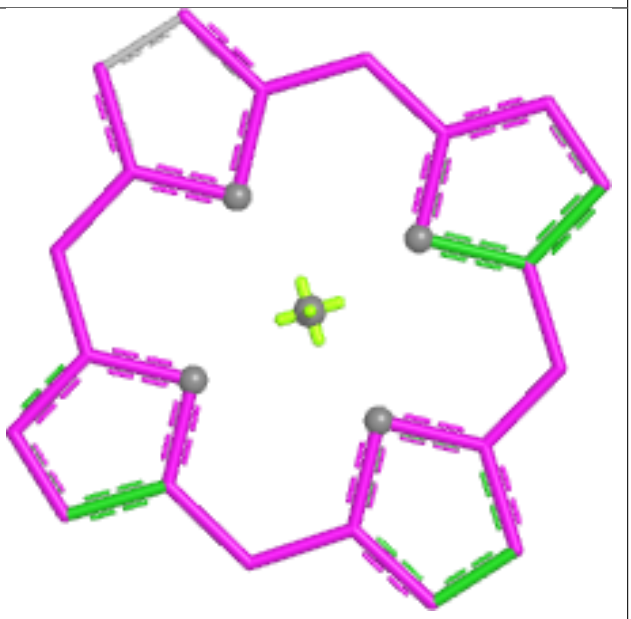


Rings

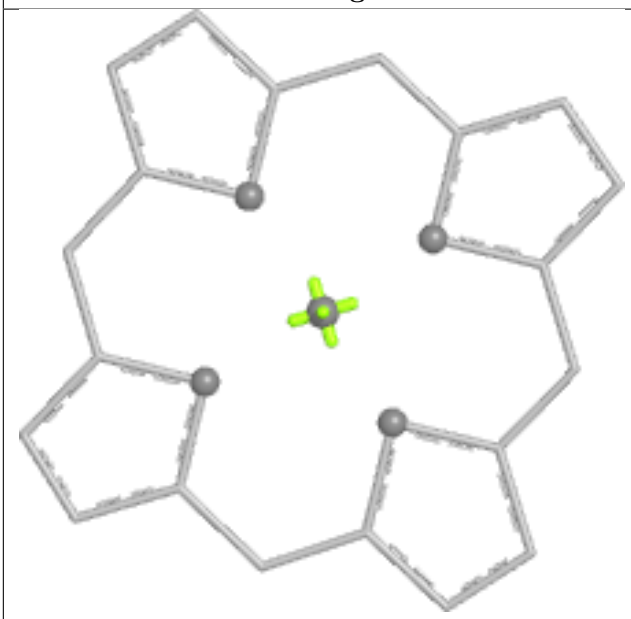
Ligand CLA B 1226



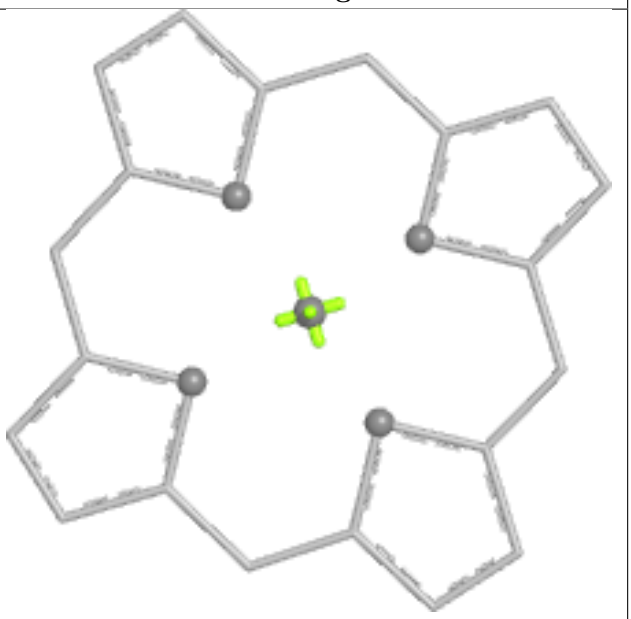
Bond lengths



Bond angles

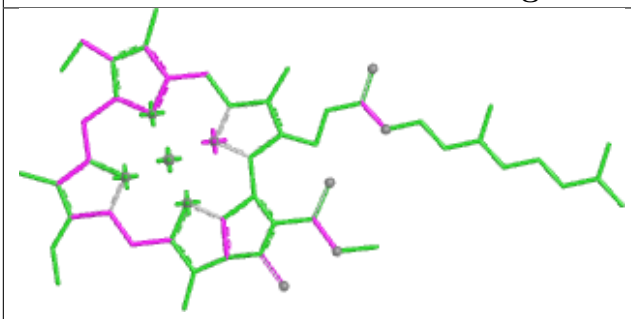


Torsions



Rings

Ligand CLA I 1204



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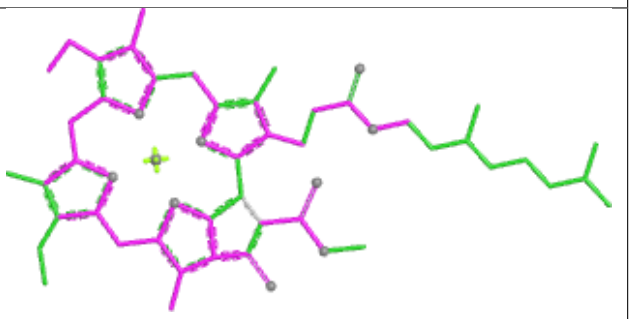

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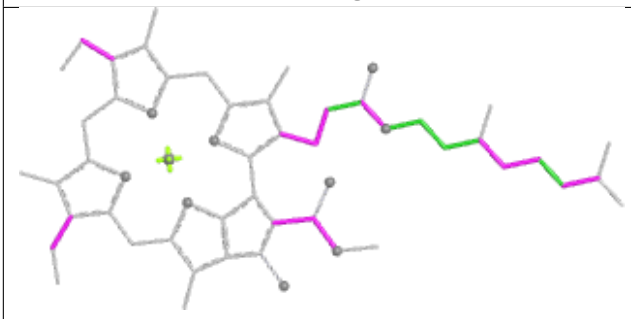

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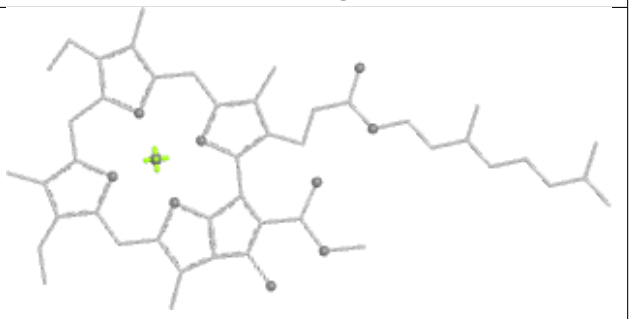
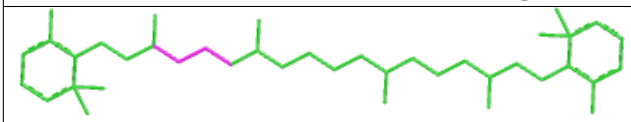


Rings

Ligand BCR L 6020



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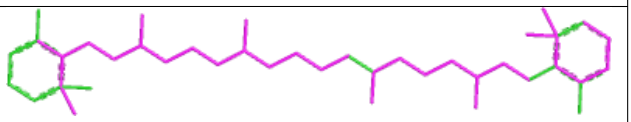

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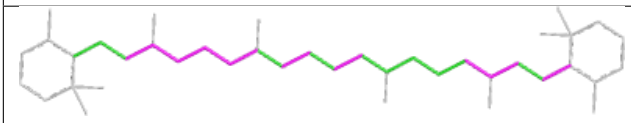

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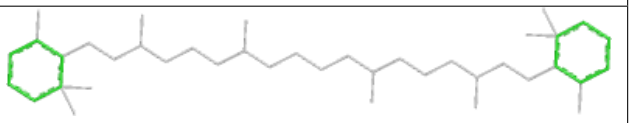
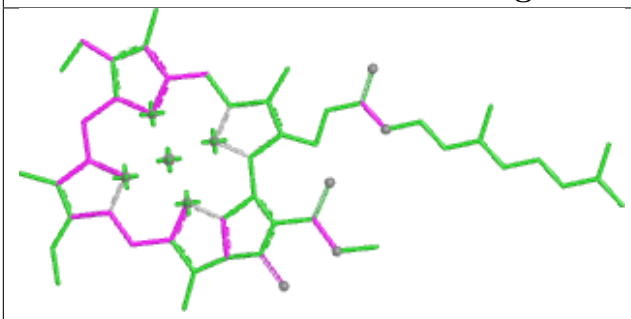


Rings

Ligand CLA A 1122



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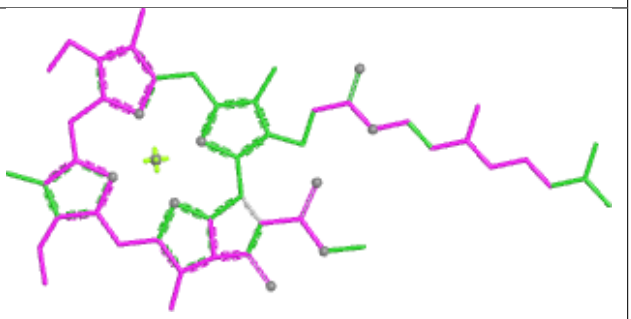

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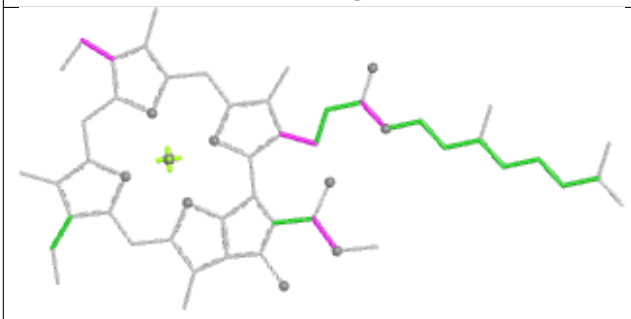

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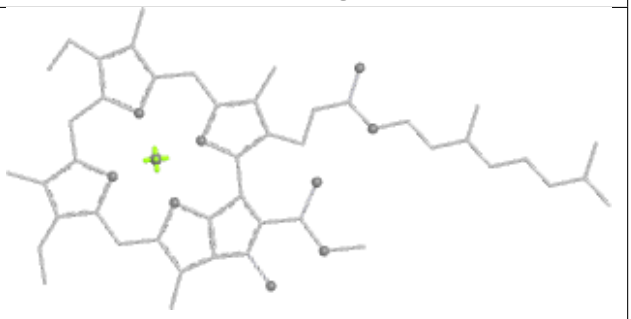
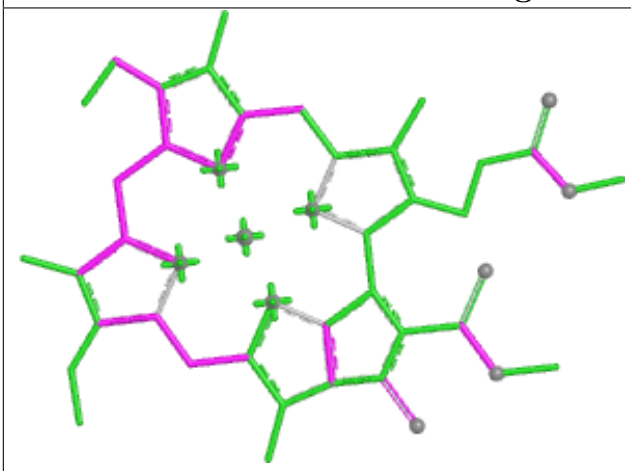


Rings

Ligand CLA A 9013



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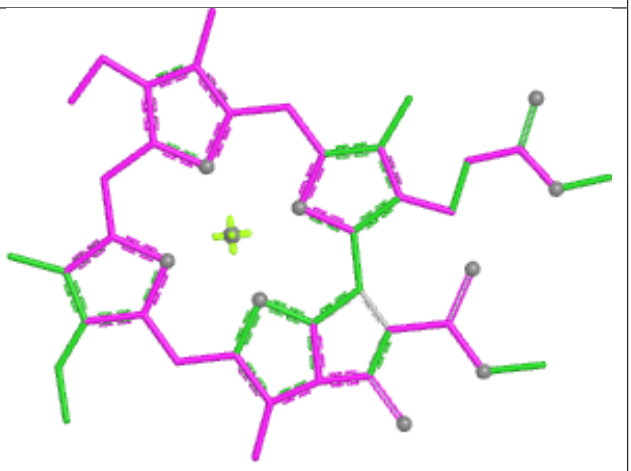

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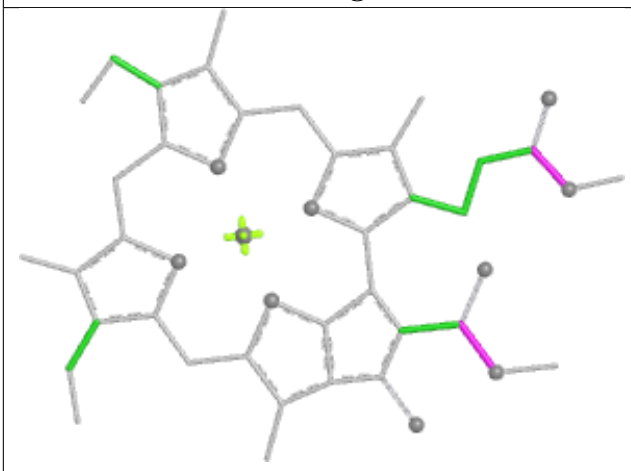

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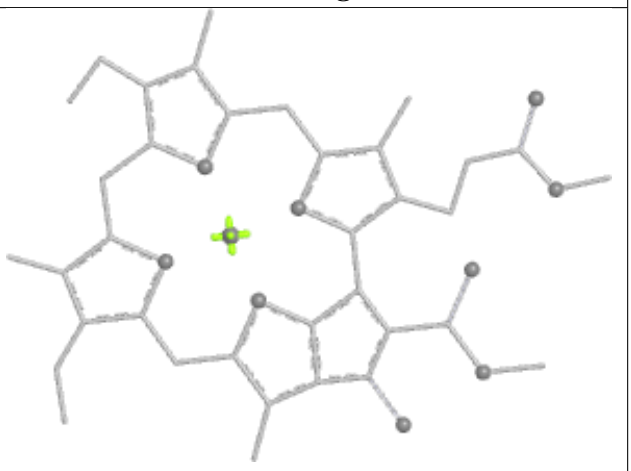
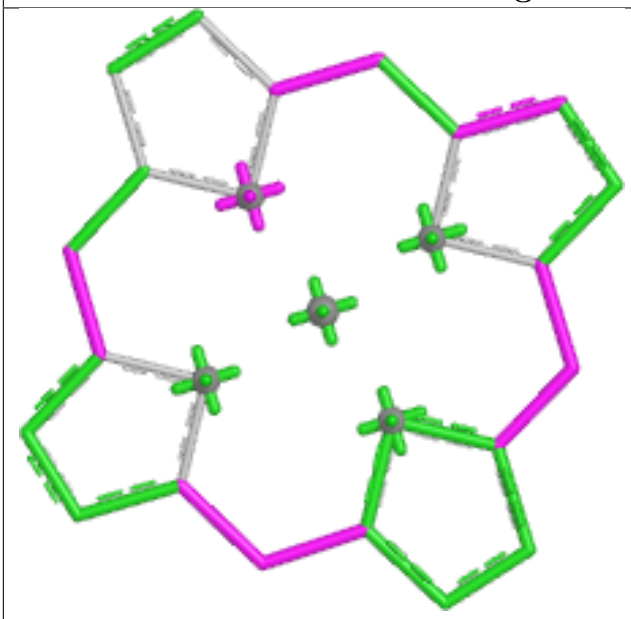


Rings

Ligand CLA A 1105



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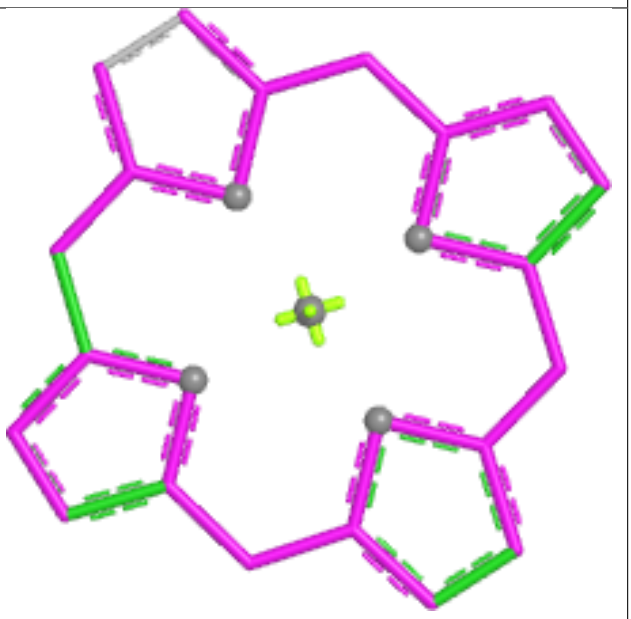
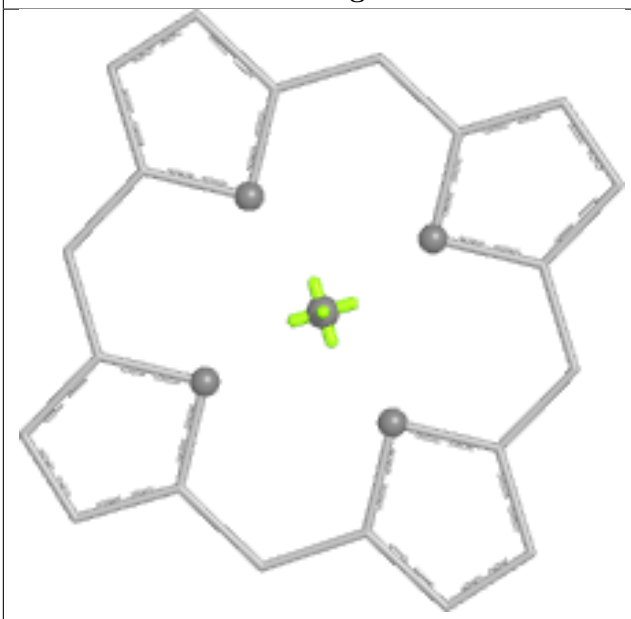


Bond angles



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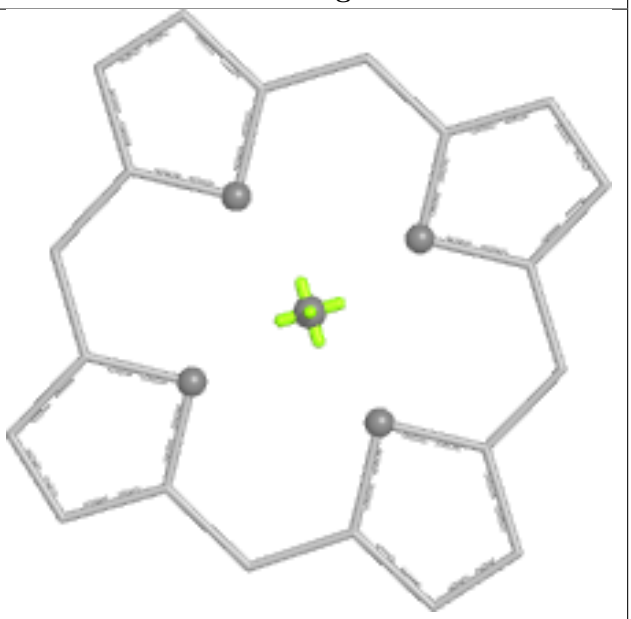
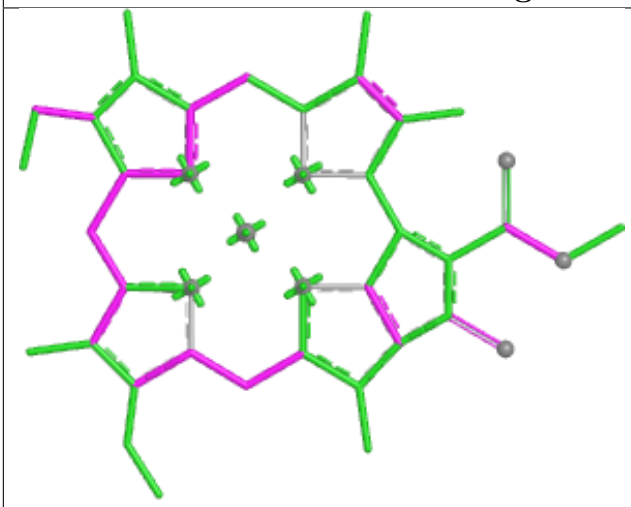


Rings

Ligand CLA A 1106



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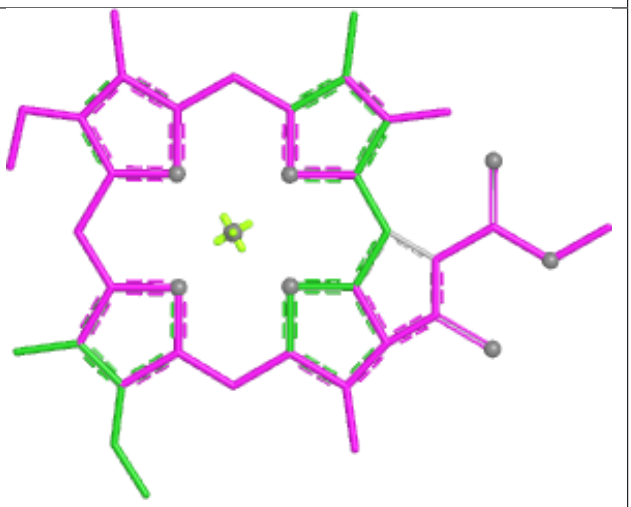

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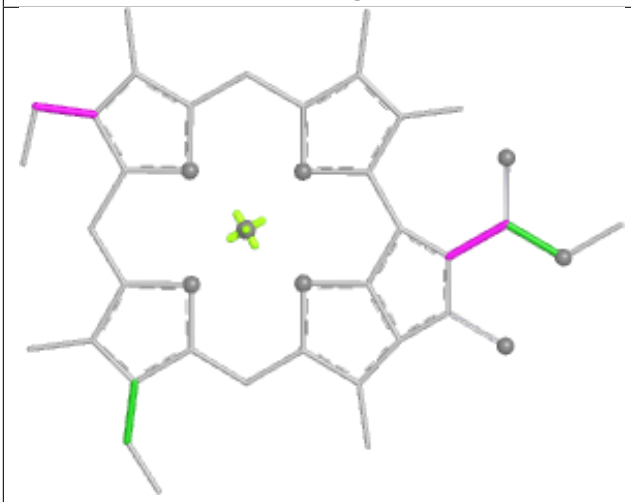

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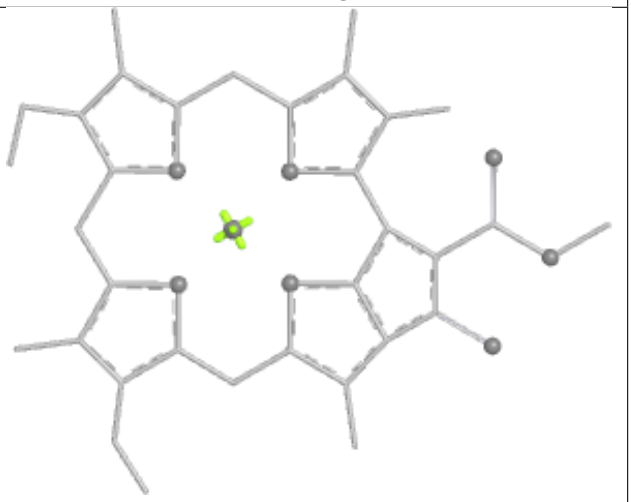
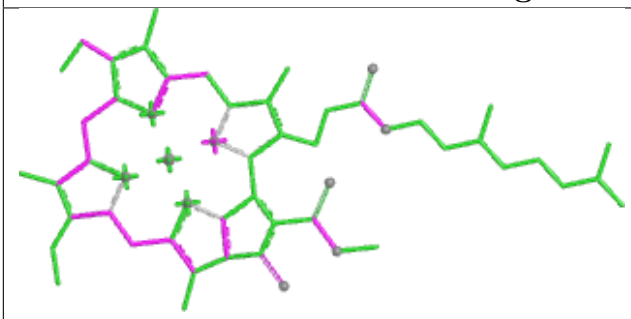
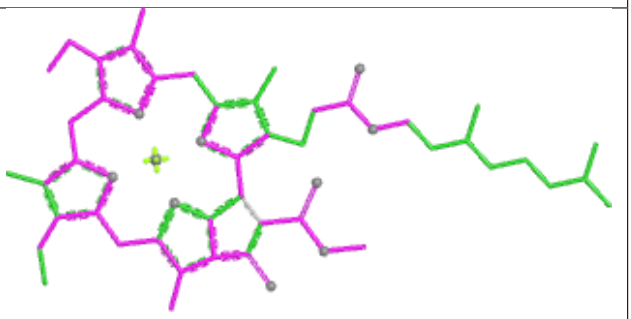
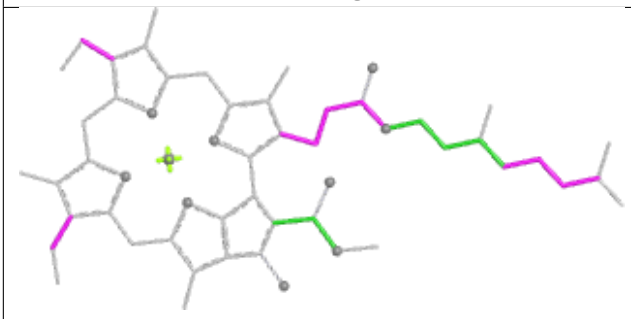
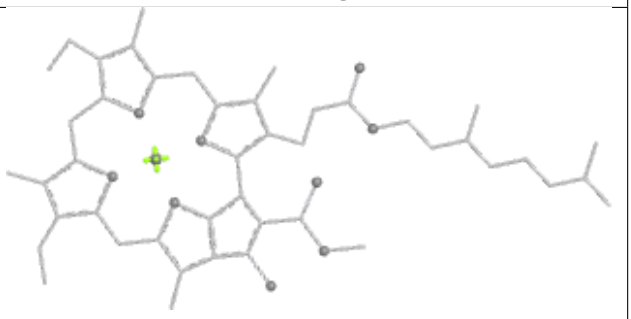
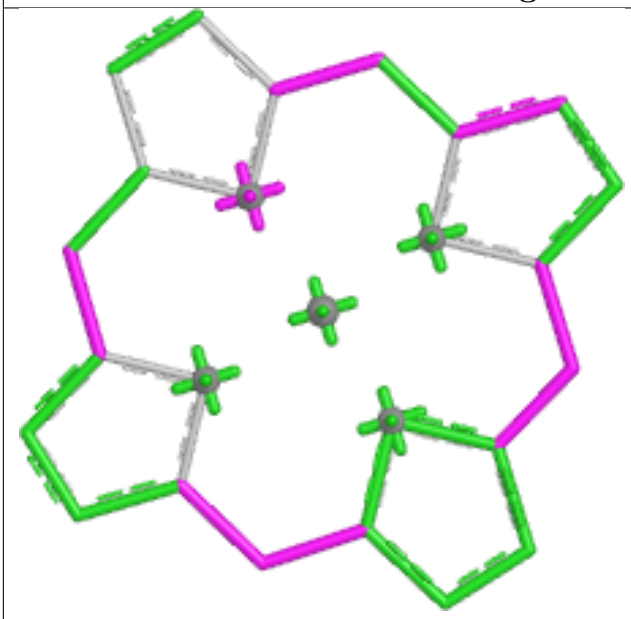


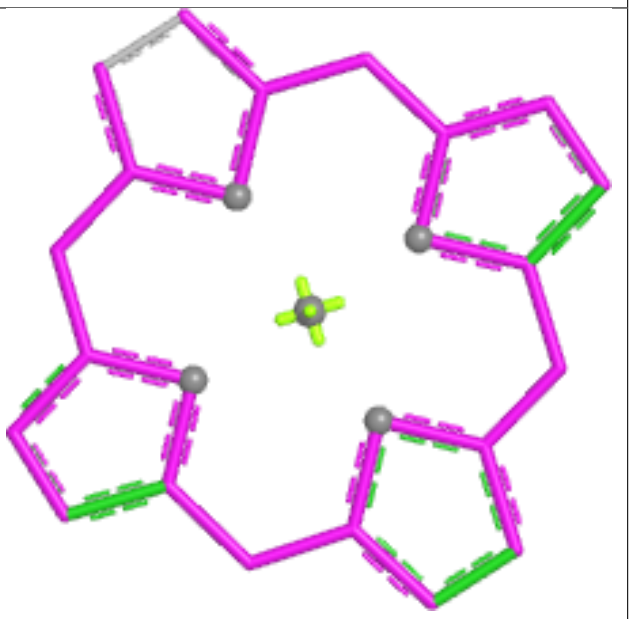
Rings

Ligand CLA A 1140	
 Bond lengths	 Bond angles
 Torsions	 Rings

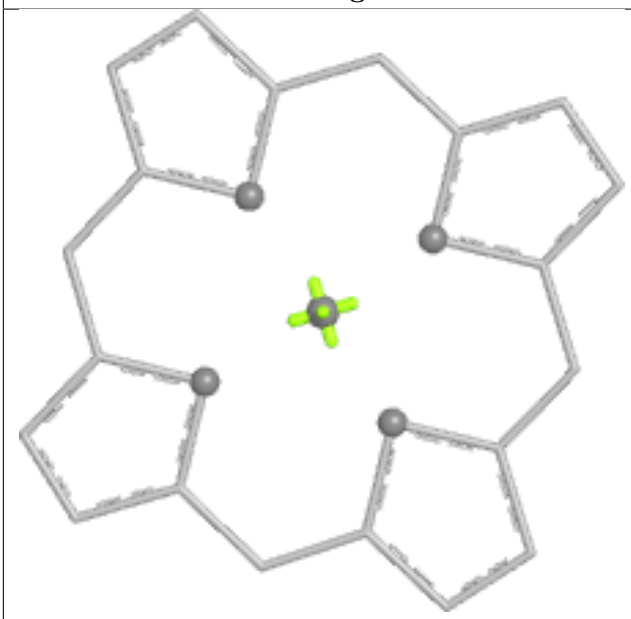
Ligand CLA 3 3006



Bond lengths



Bond angles



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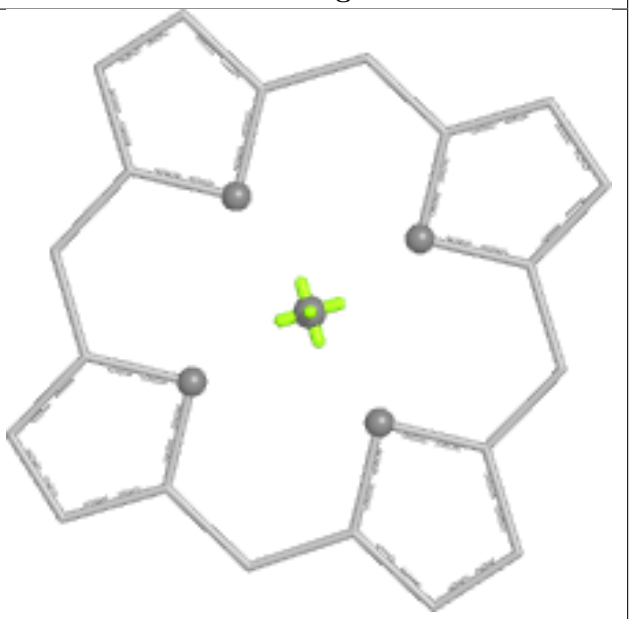
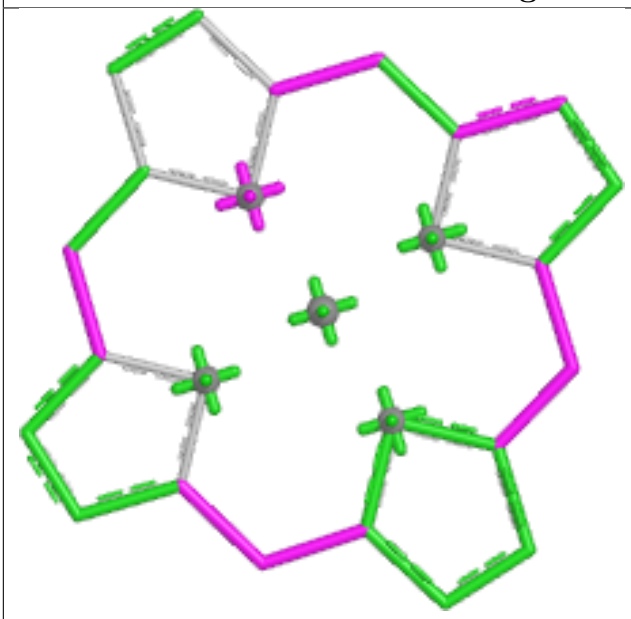


Rings

Ligand CLA 1 1013



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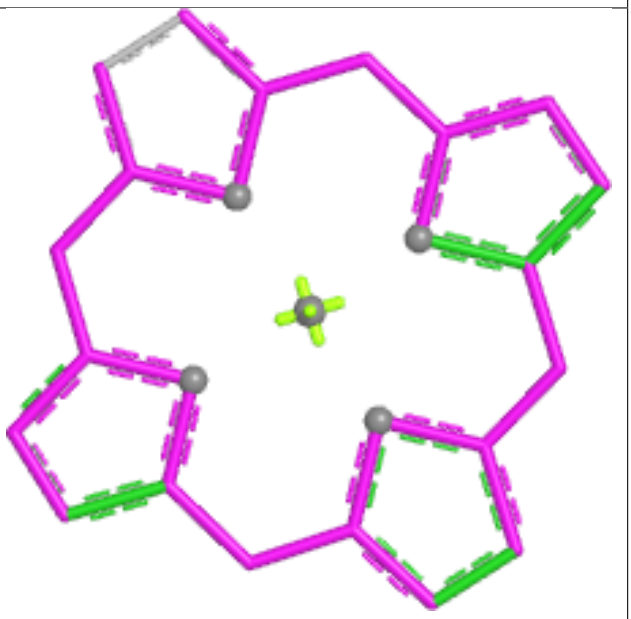

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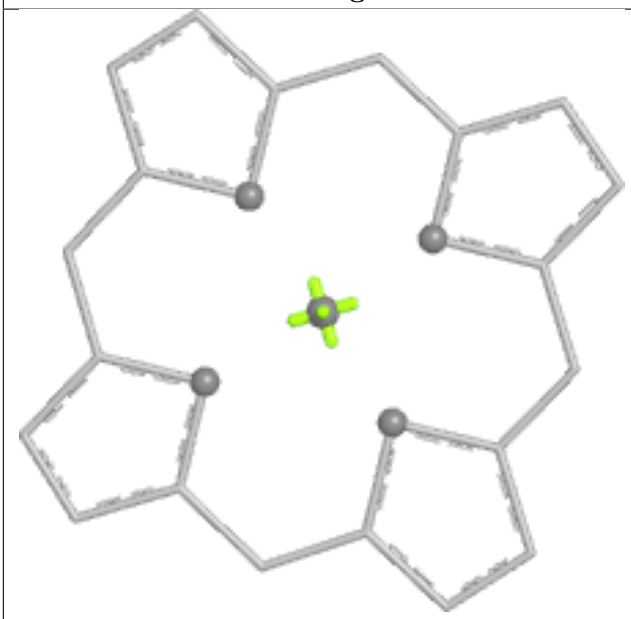

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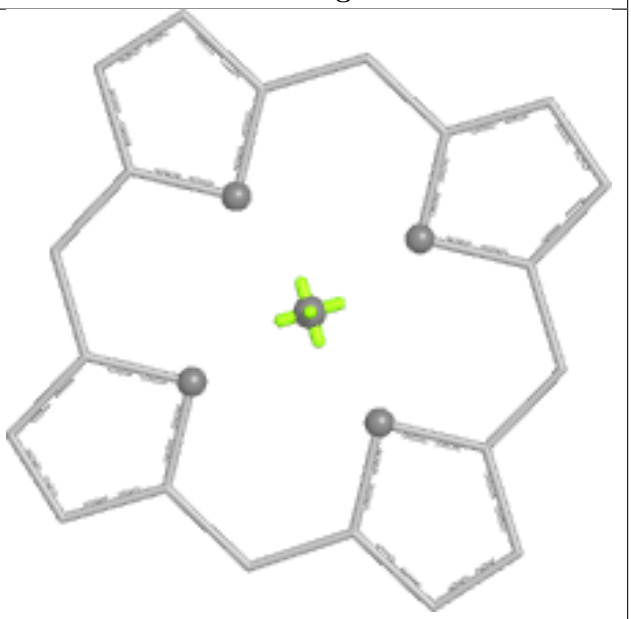
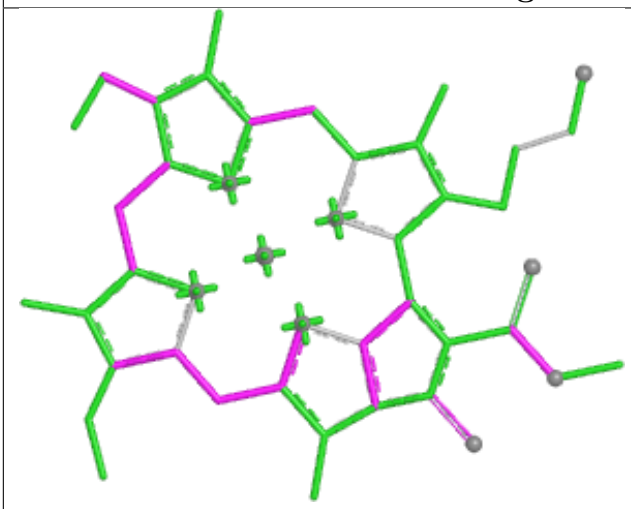


Rings

Ligand CLA F 1139



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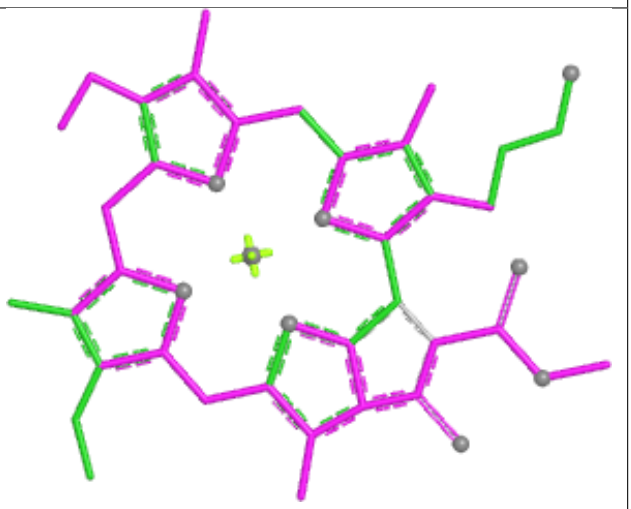

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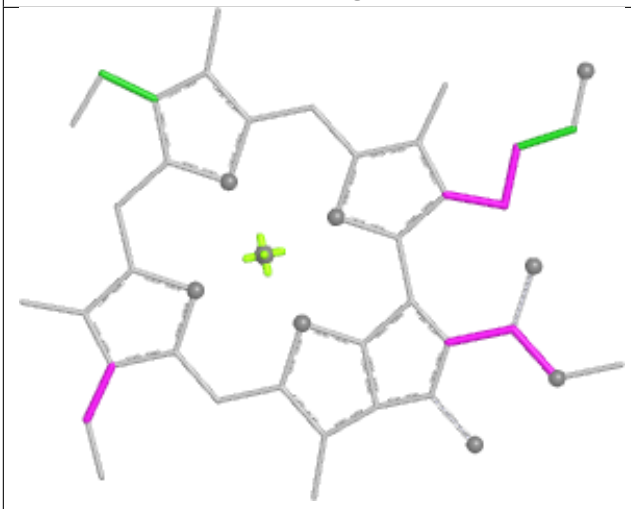
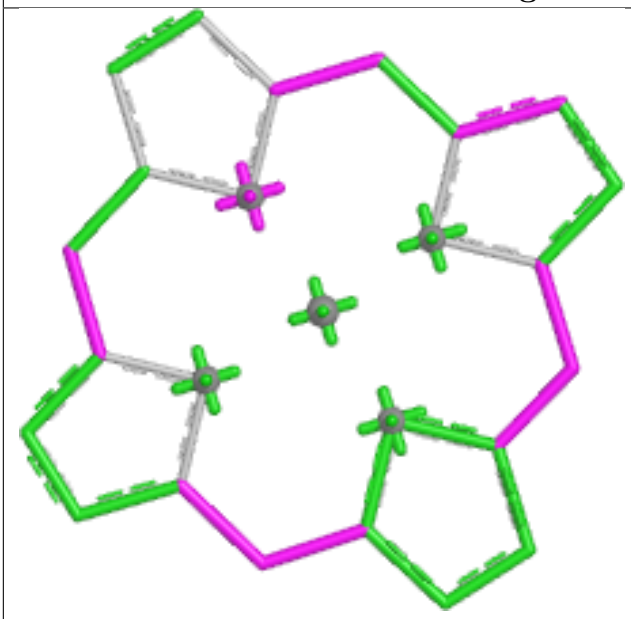


Torsions

Rings

Ligand CLA 1 1006



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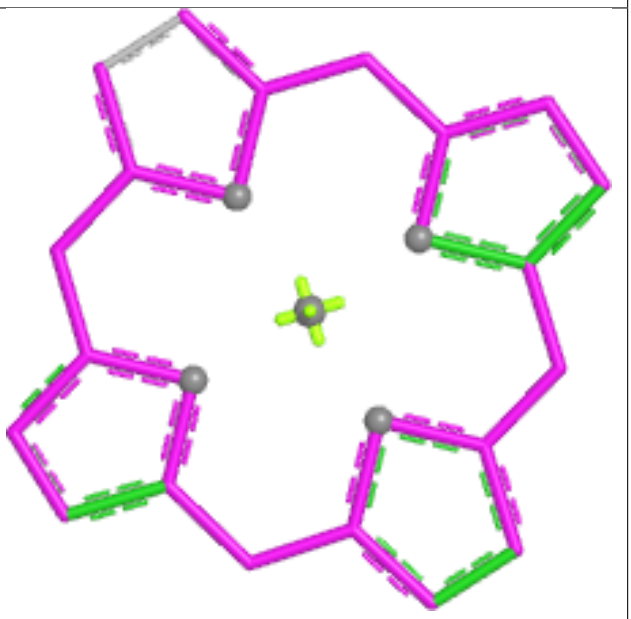

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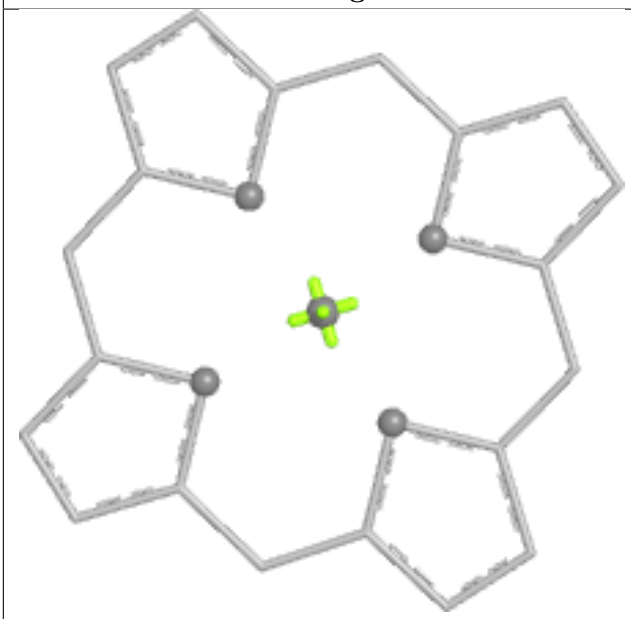

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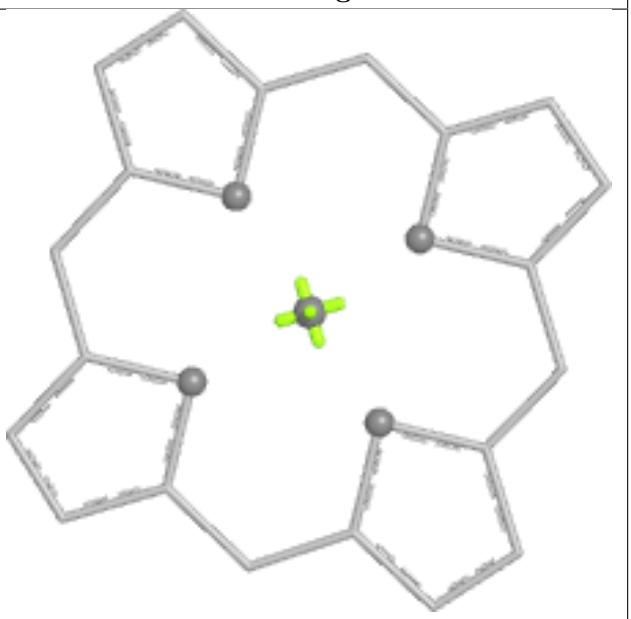
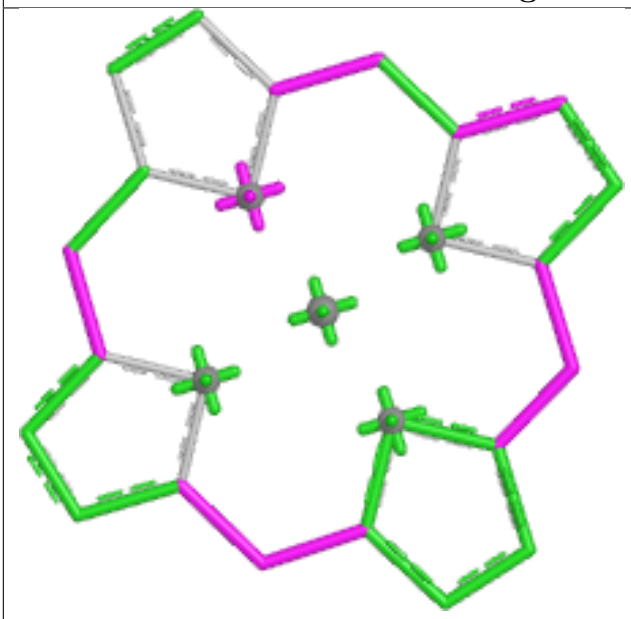
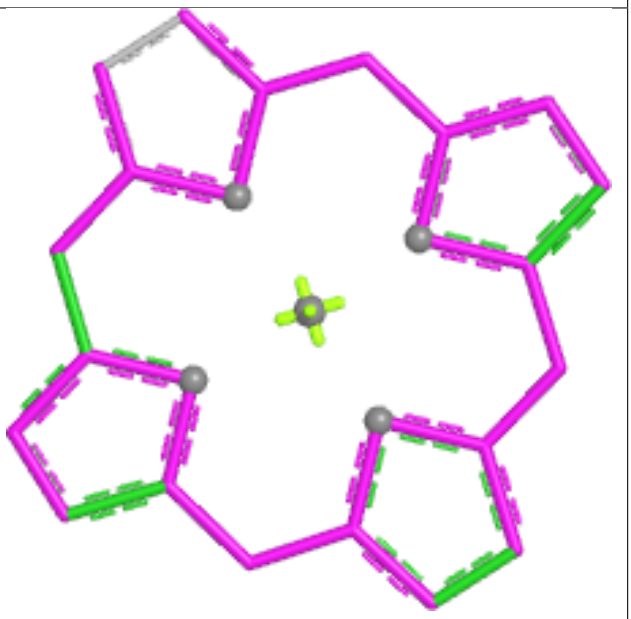


Rings

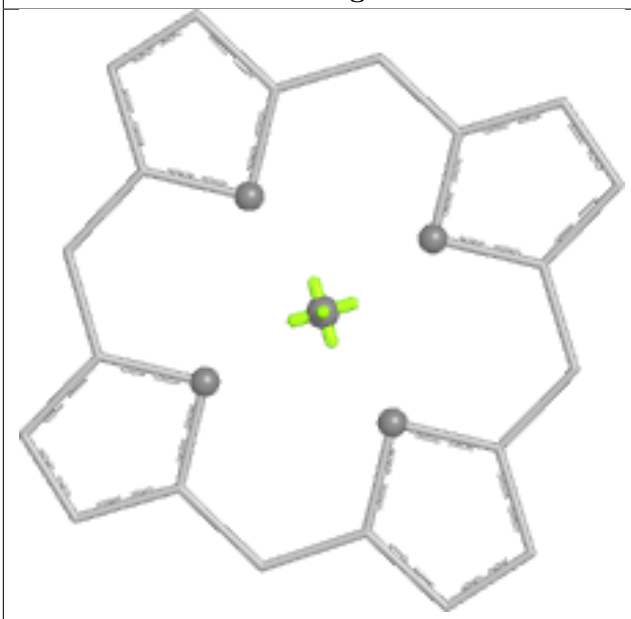
Ligand CLA 4 4013



Bond lengths



Bond angles



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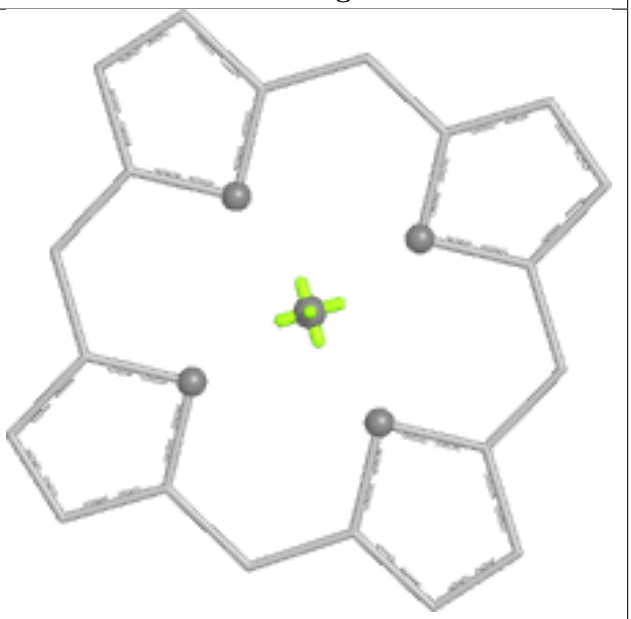
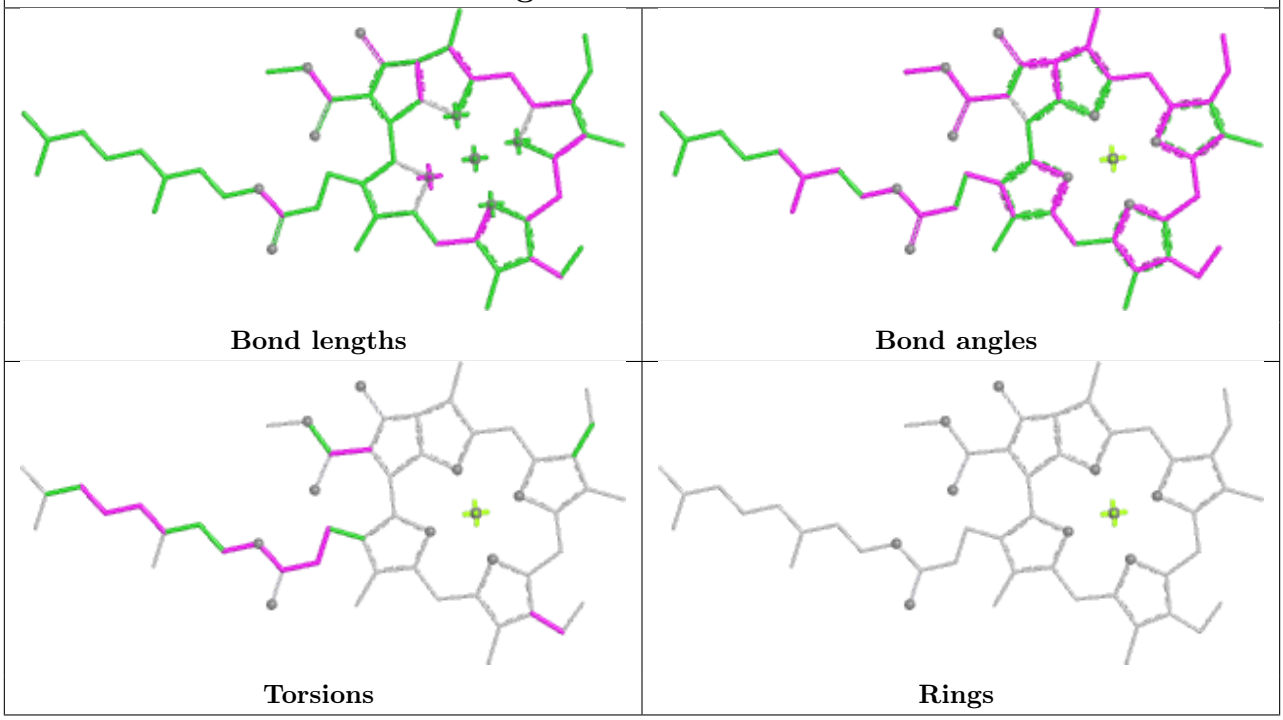
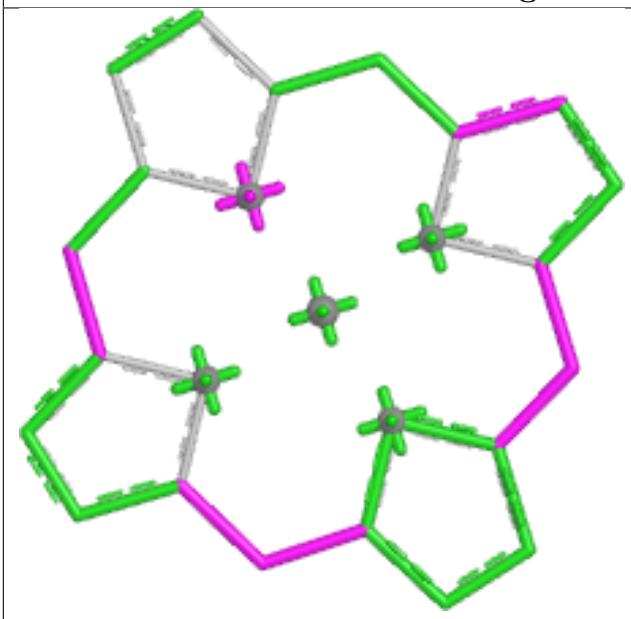


Rings

Ligand CLA B 1205



Ligand CLA 4 1009



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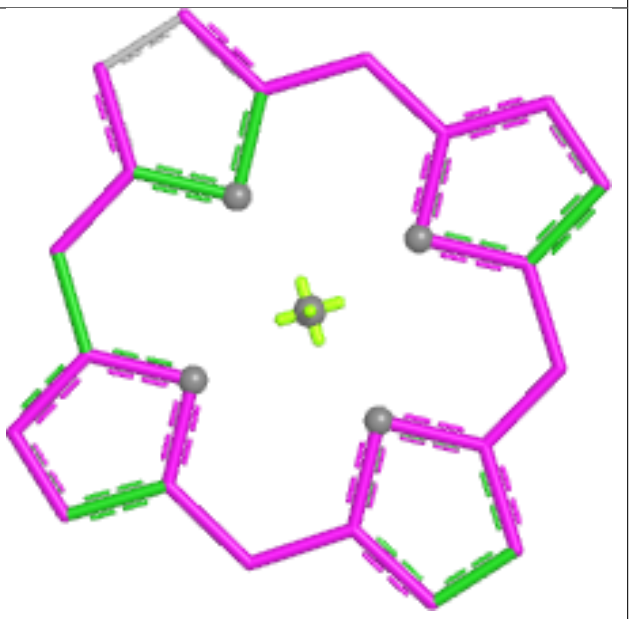
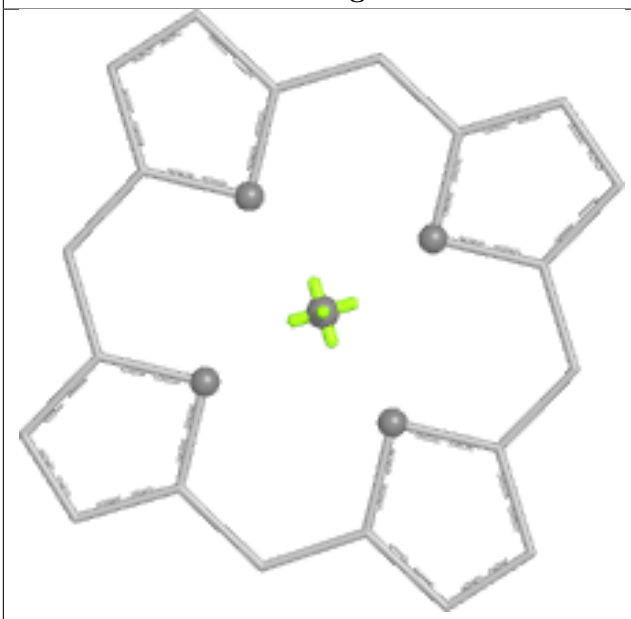


Bond angles



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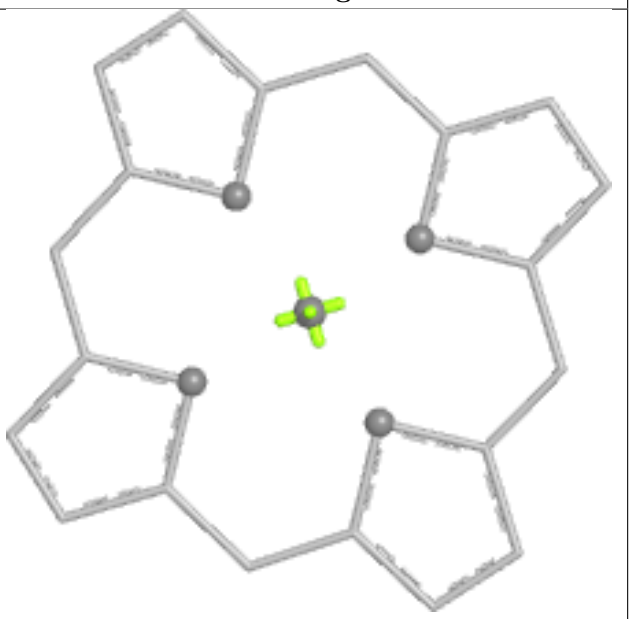
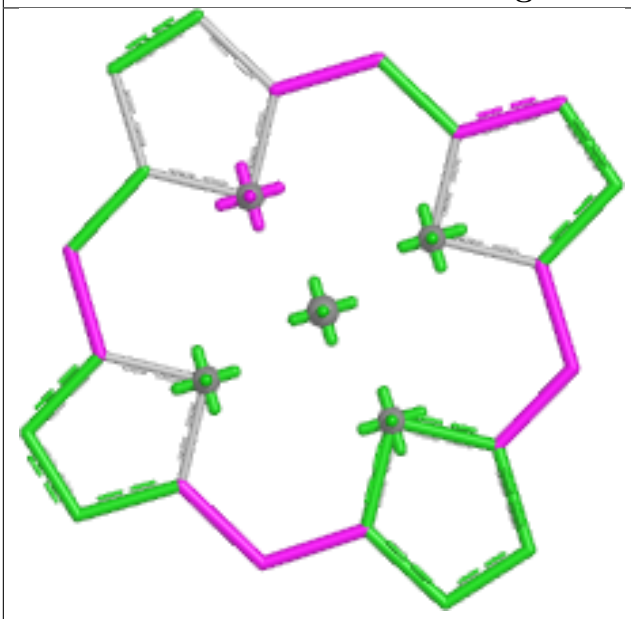
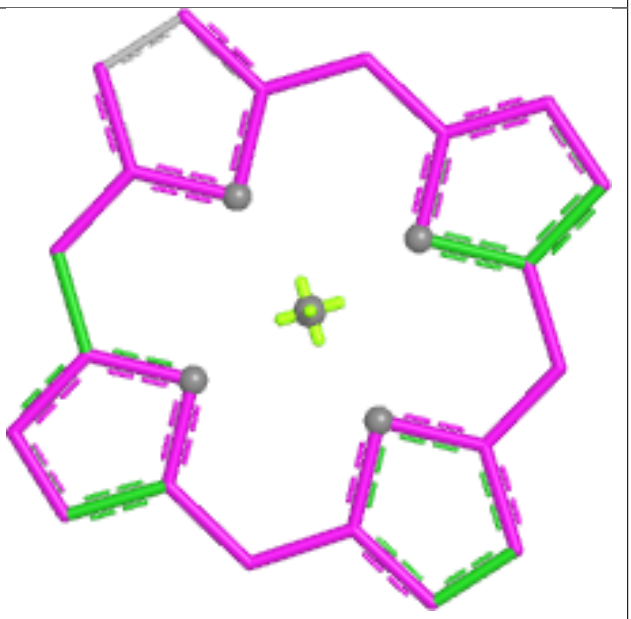


Rings

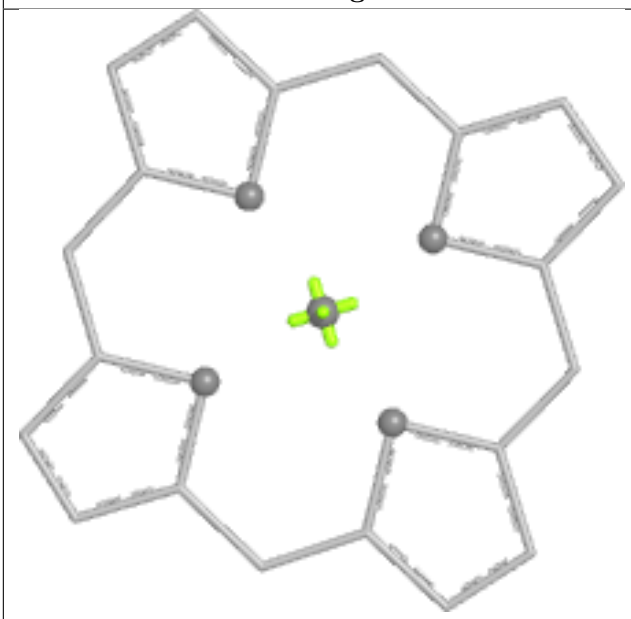
Ligand CLA B 1230



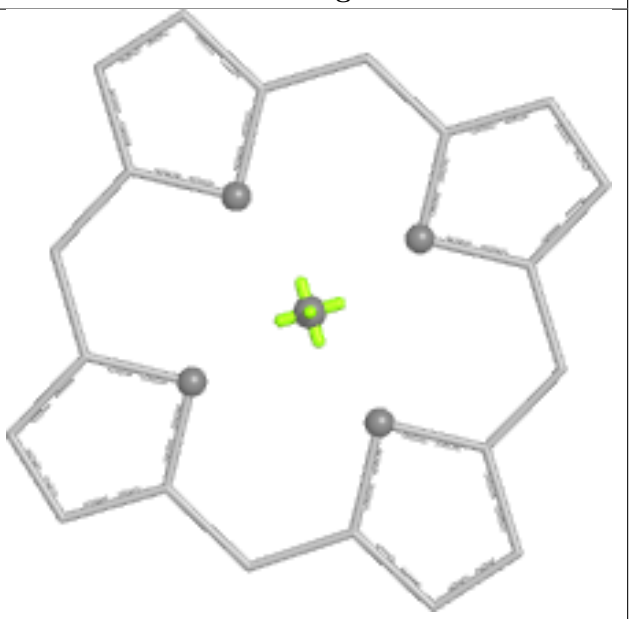
Bond lengths



Bond angles

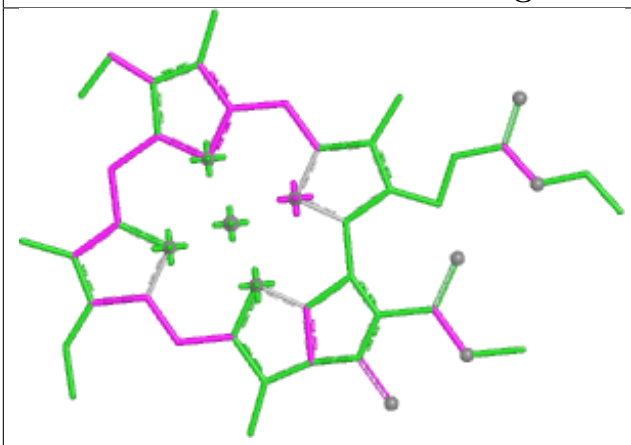


Torsions



Rings

Ligand CLA A 1115



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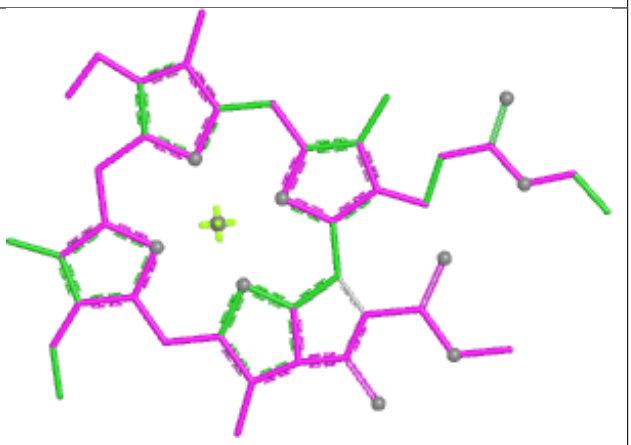

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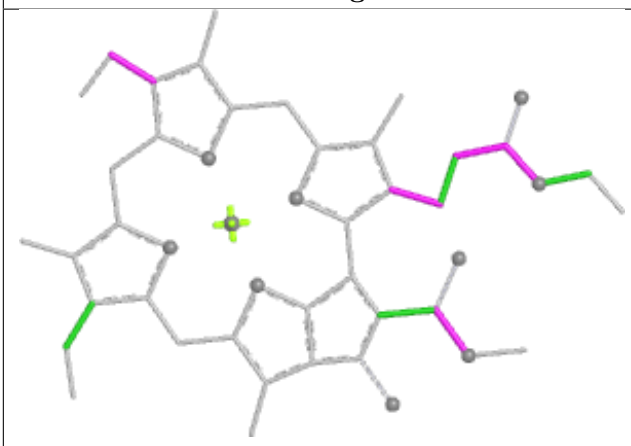

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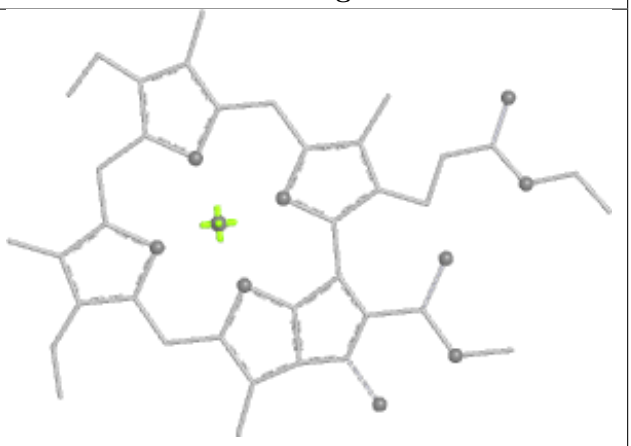
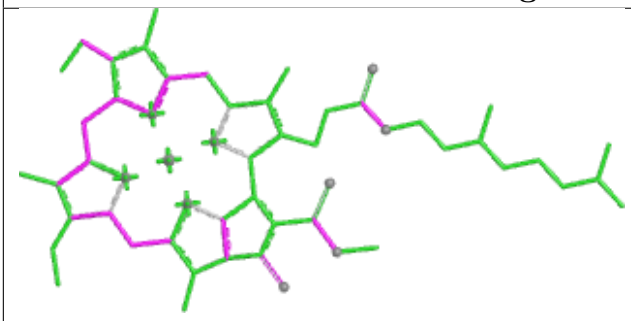


Rings

Ligand CLA 4 1304



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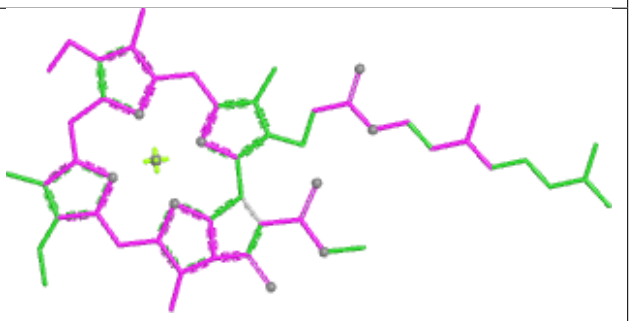
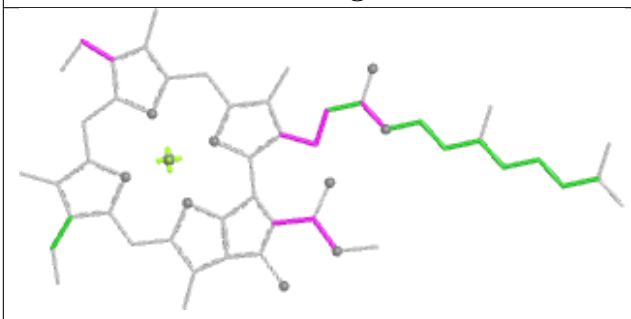


Bond angles



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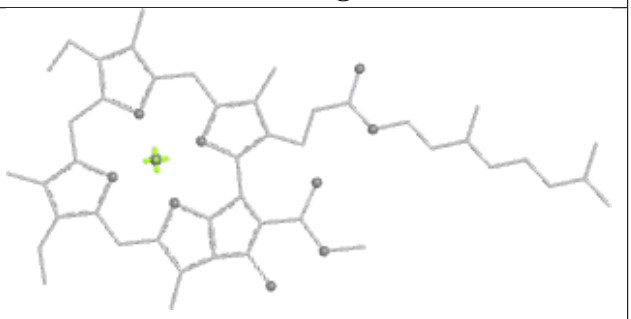
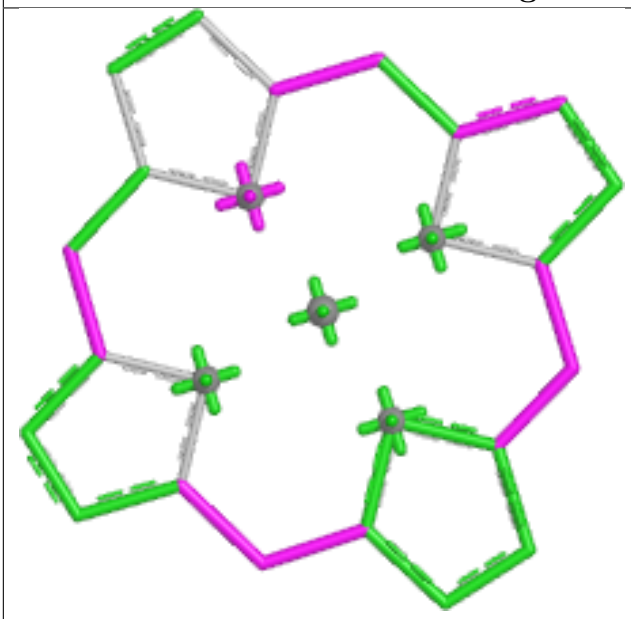


Rings

Ligand CLA 2 2001



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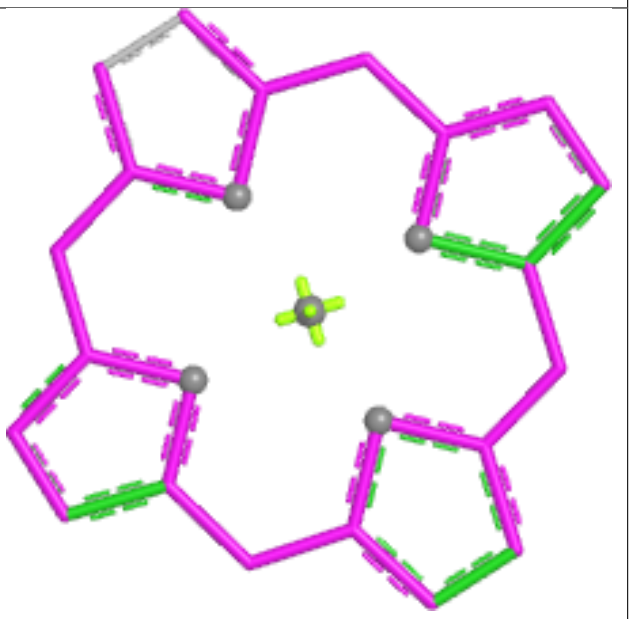
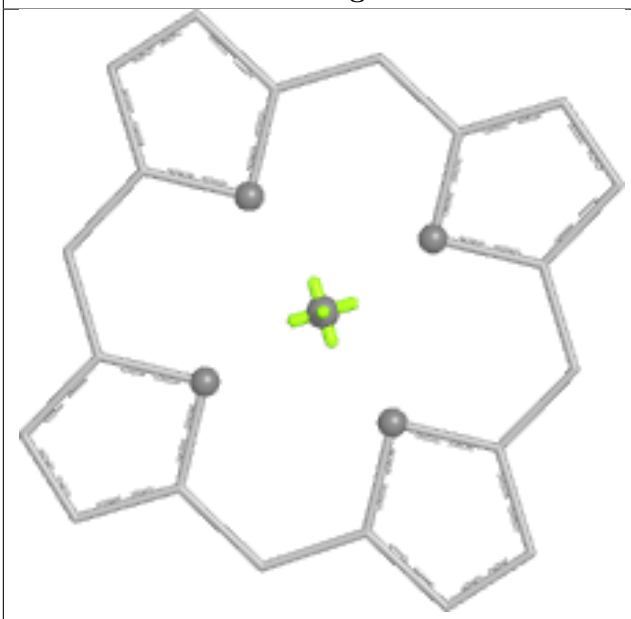


Bond angles



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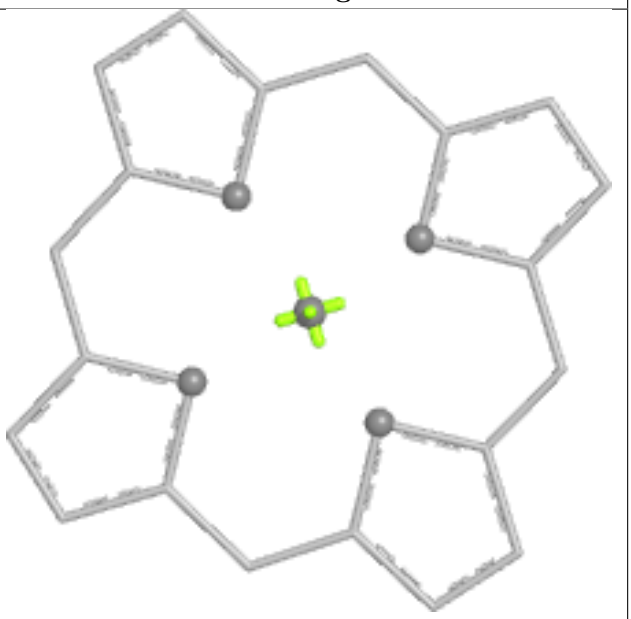
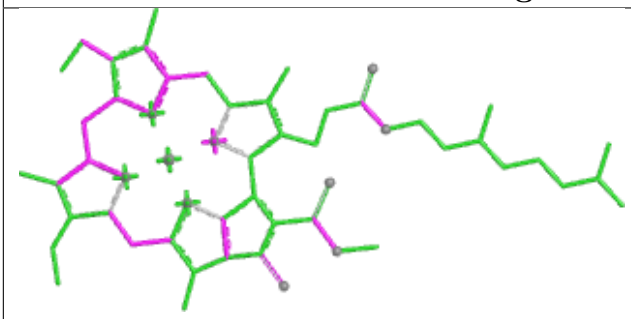
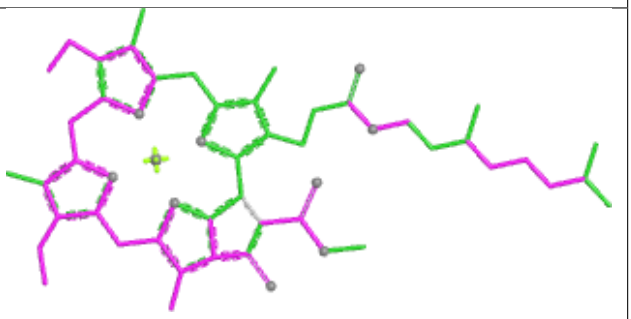
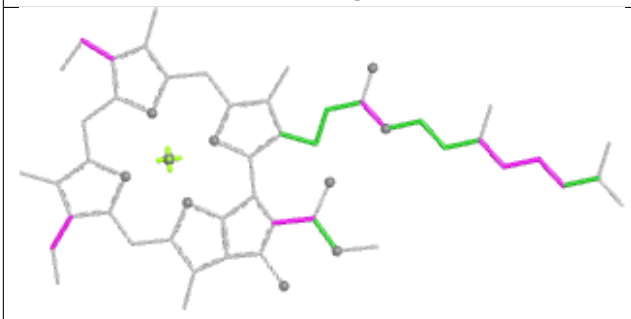
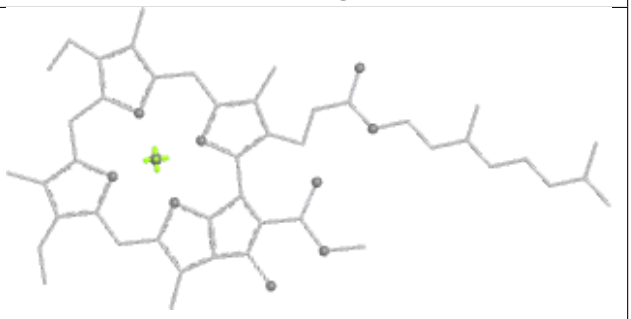


Rings

Ligand CLA B 1235	
 Bond lengths	 Bond angles
 Torsions	 Rings

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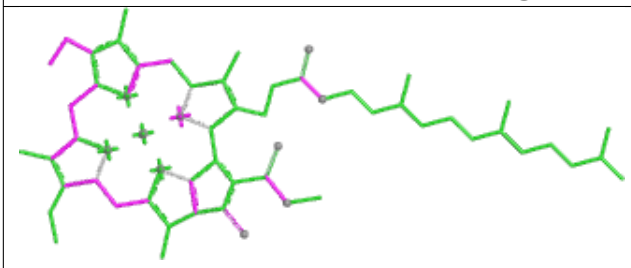
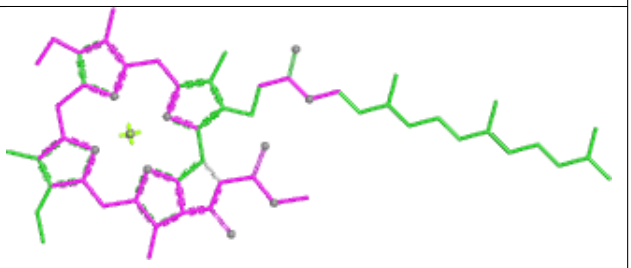
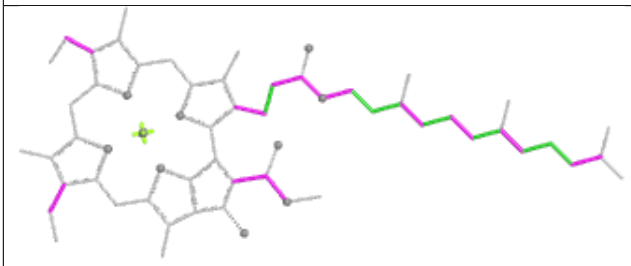
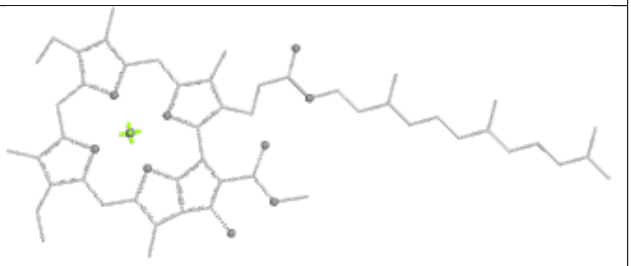
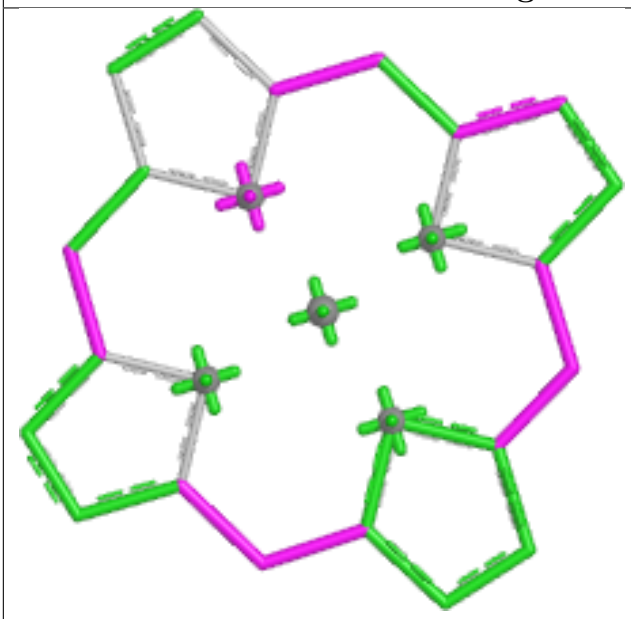
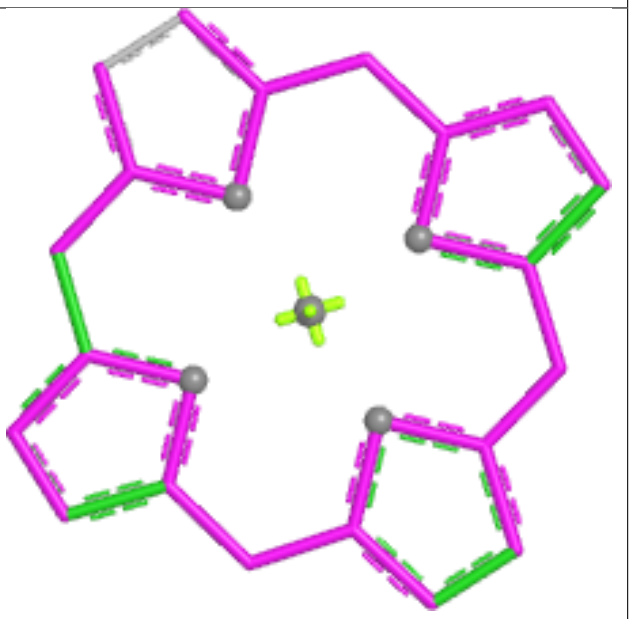
 Bond lengths	 Bond angles
 Torsions	 Rings

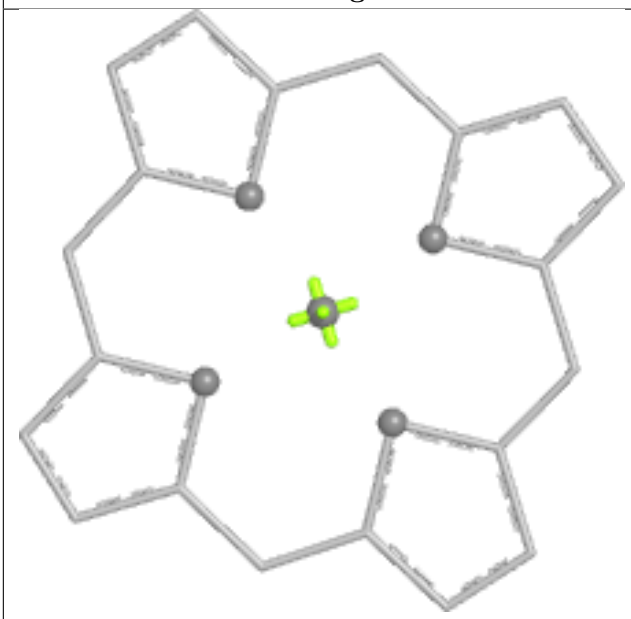
Ligand CLA F 1305



Bond lengths



Bond angles



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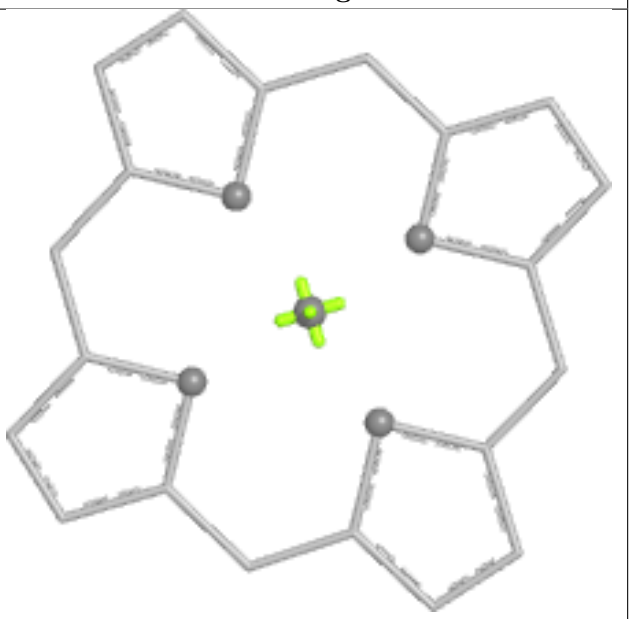
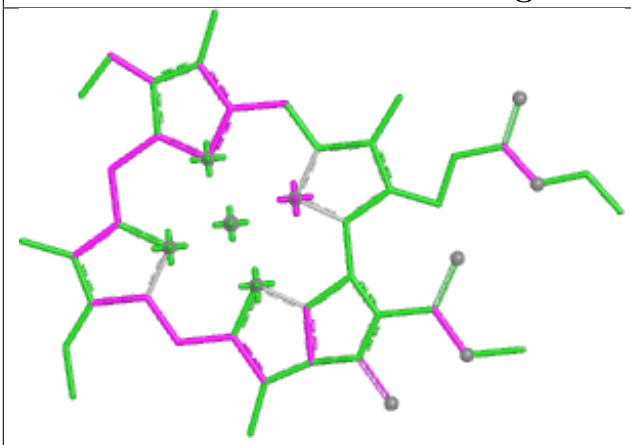


Rings

Ligand CLA B 1242



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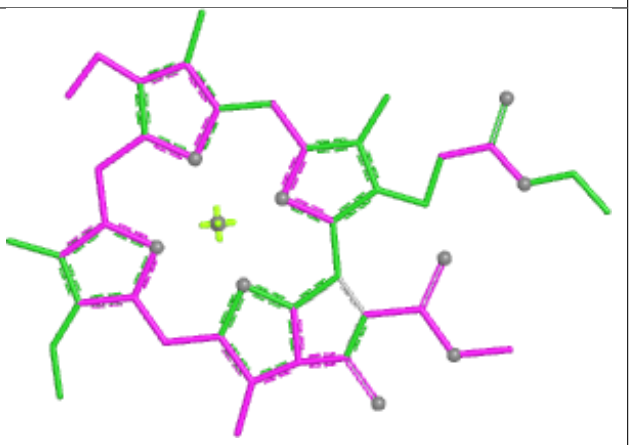

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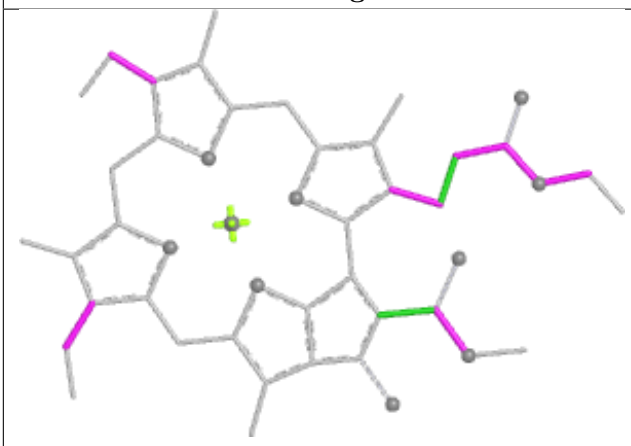

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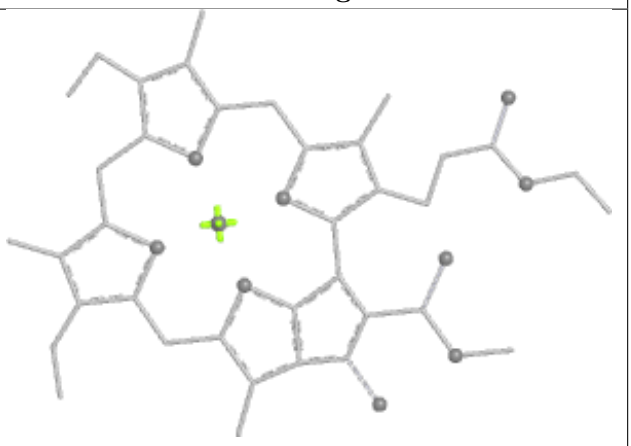
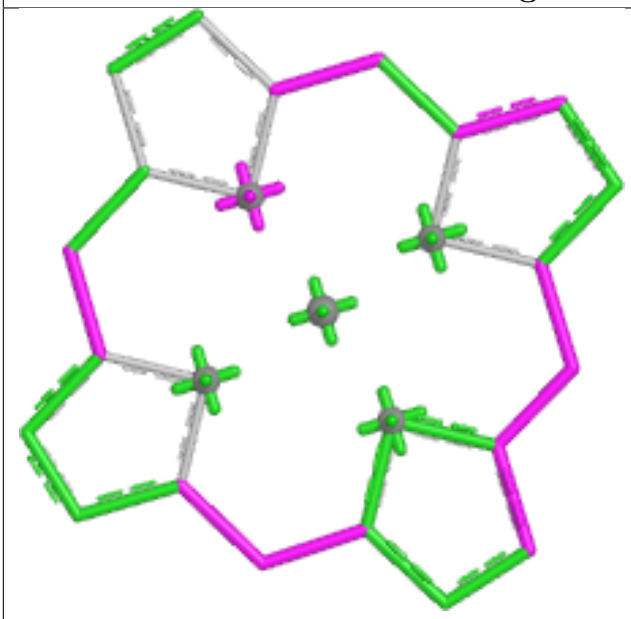


Rings

Ligand CLA 3 3004



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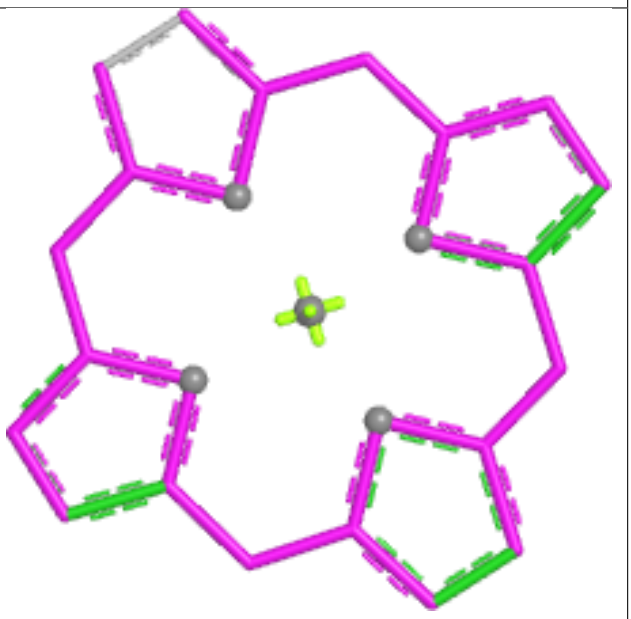
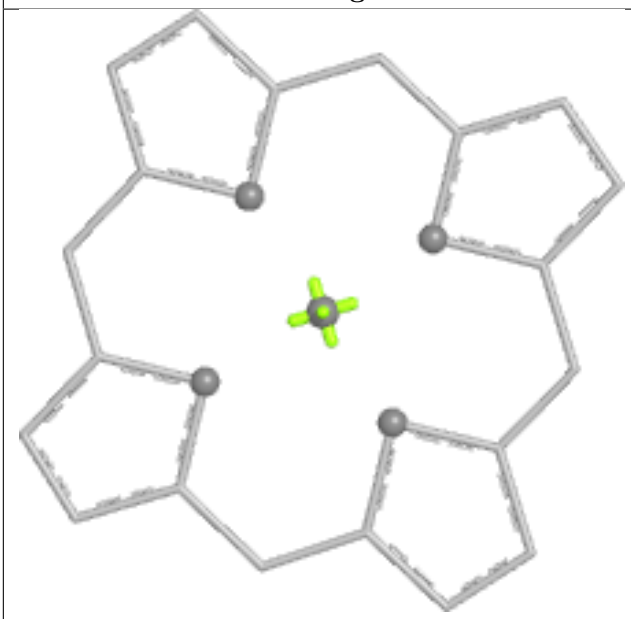


Bond angles



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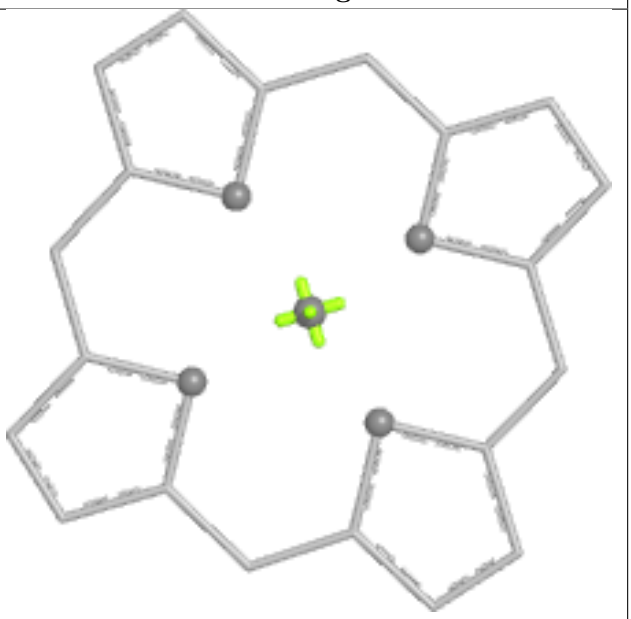
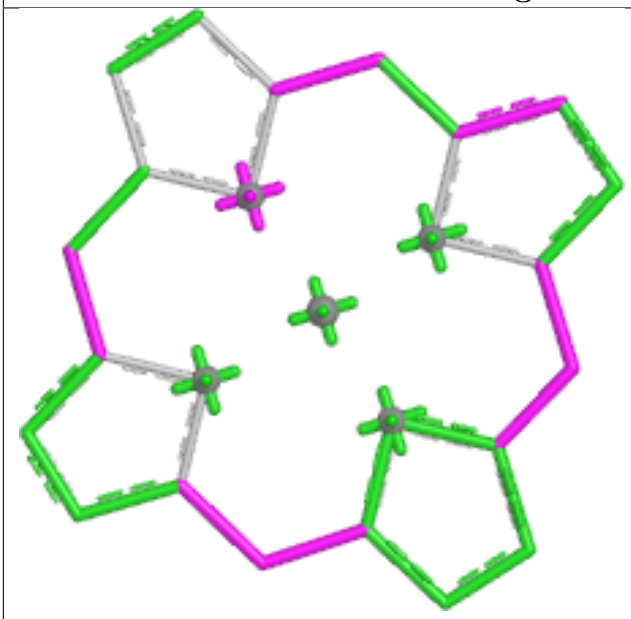


Rings

Ligand CLA A 1144



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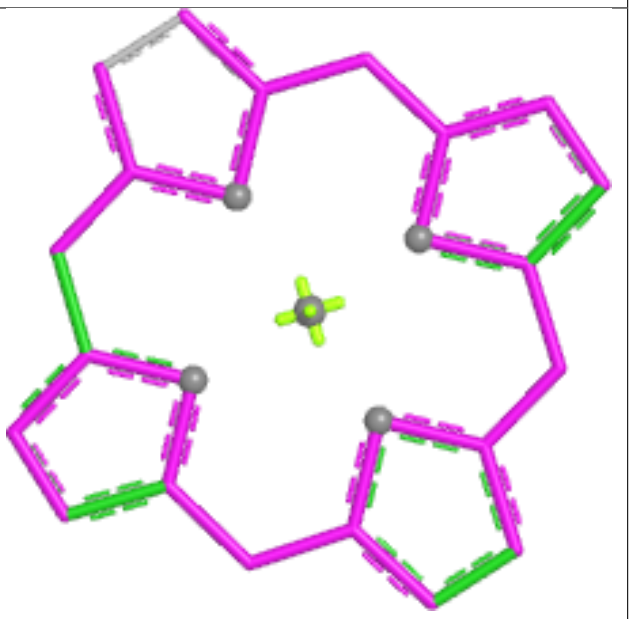
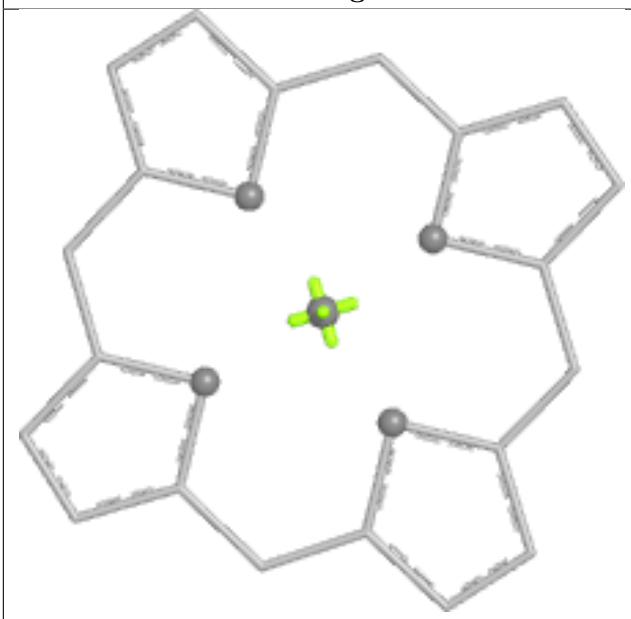


Bond angles



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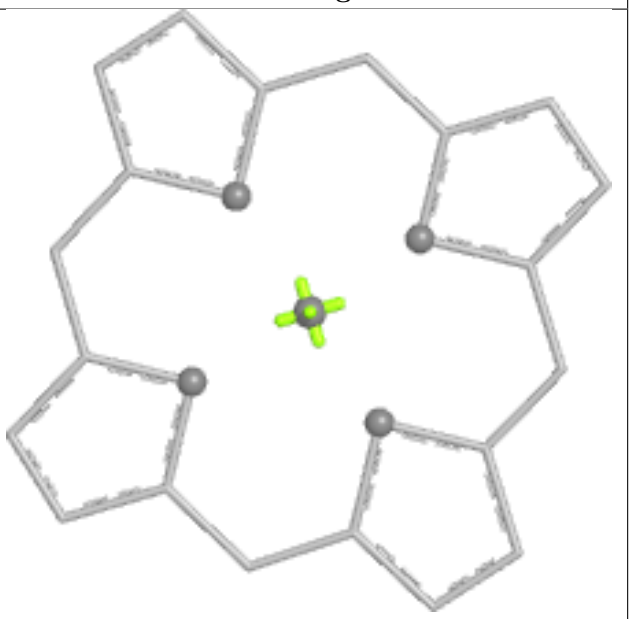
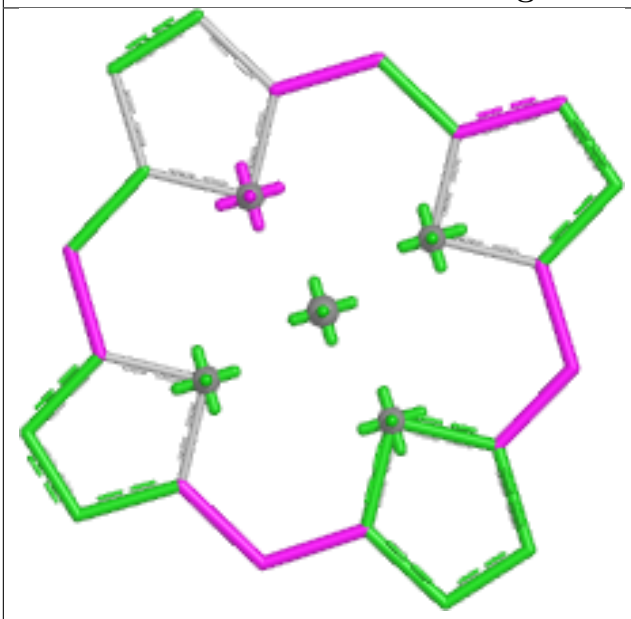


Rings

Ligand CLA F 4015



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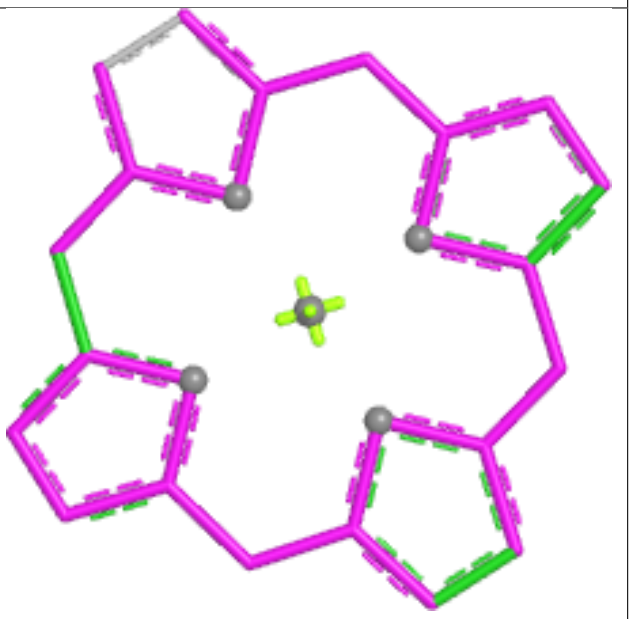

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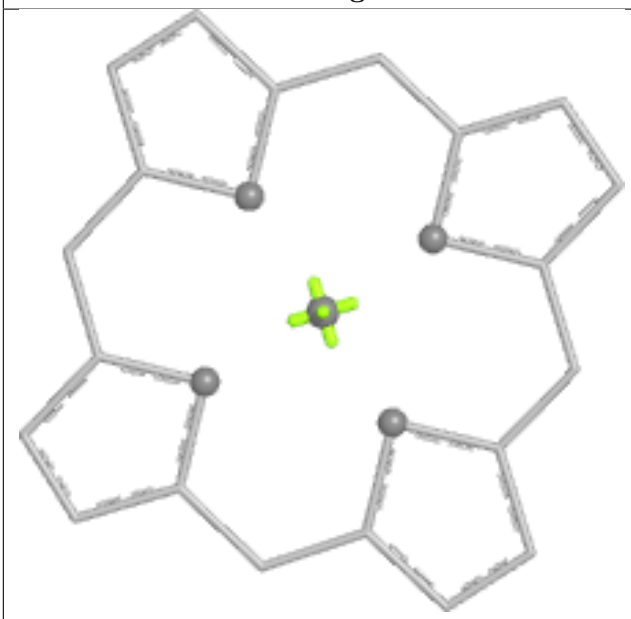

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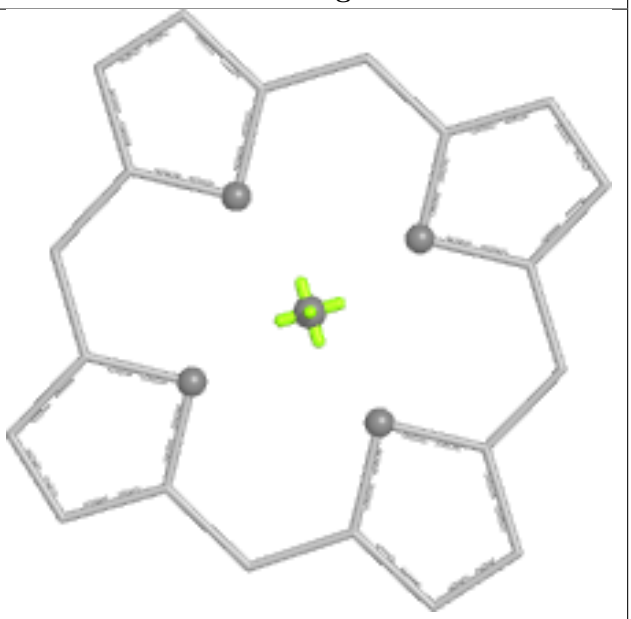
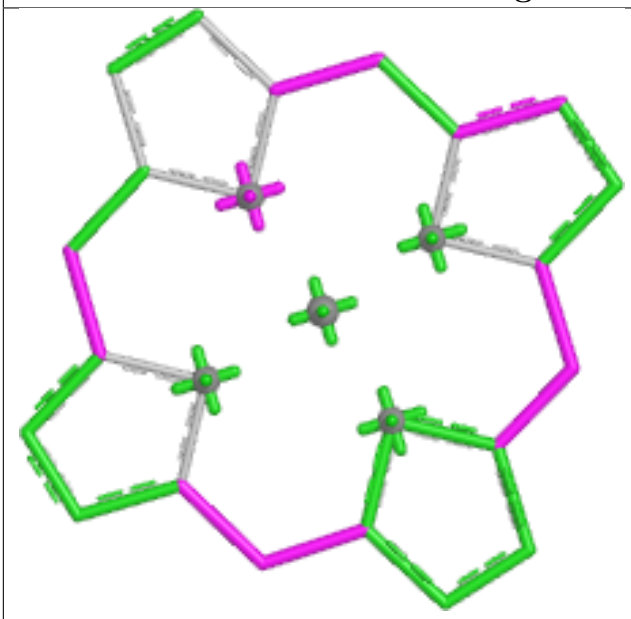


Rings

Ligand CLA A 1152



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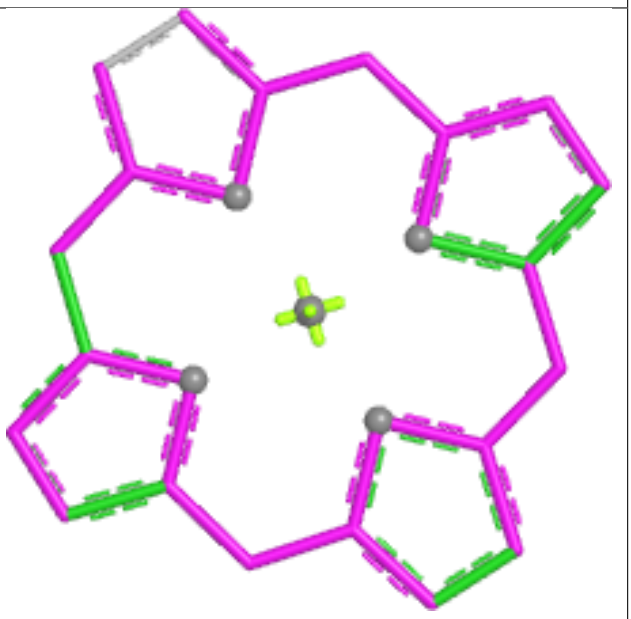
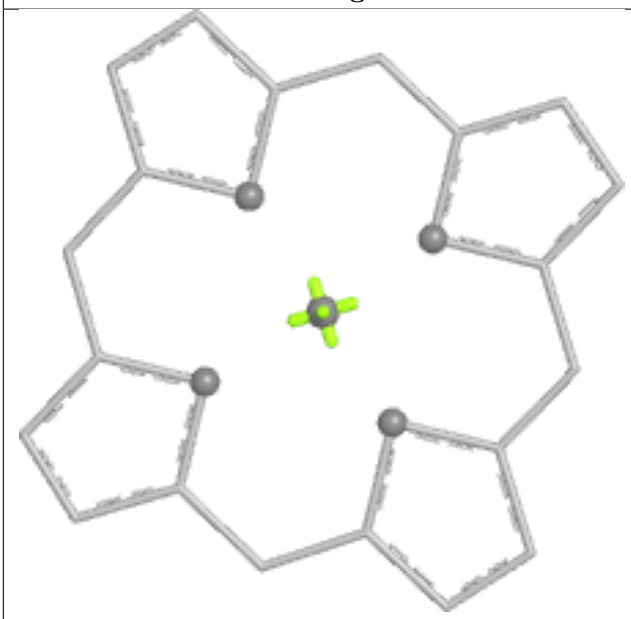


Bond angles



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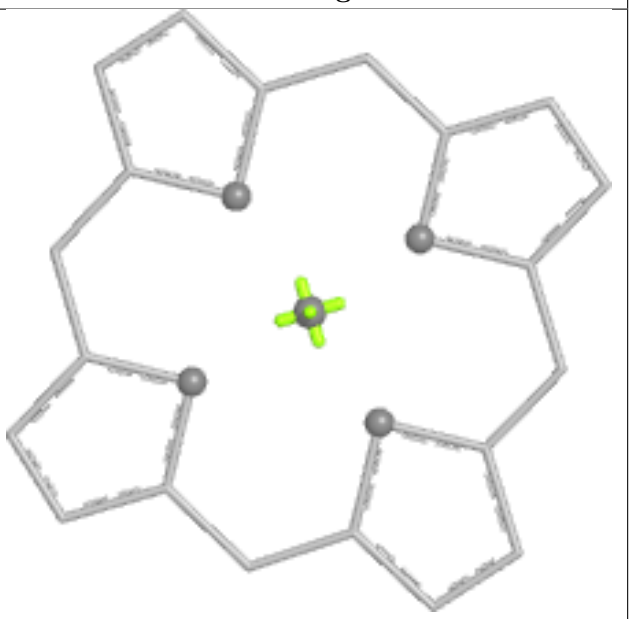
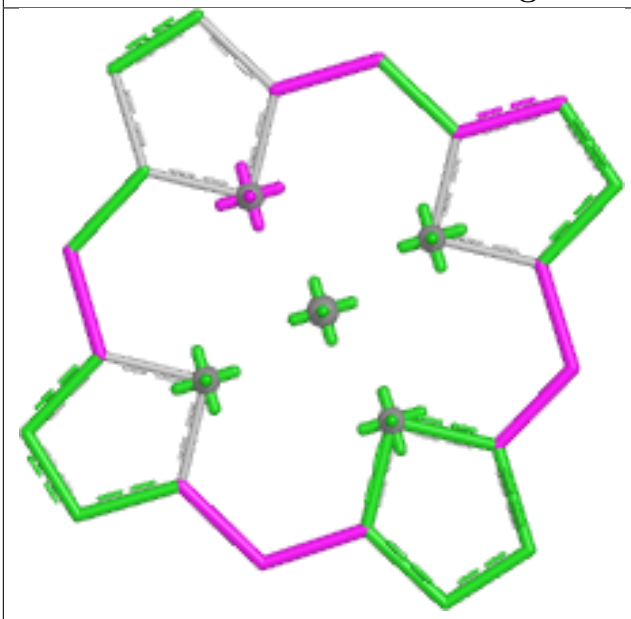


Rings

Ligand CLA 1 1010



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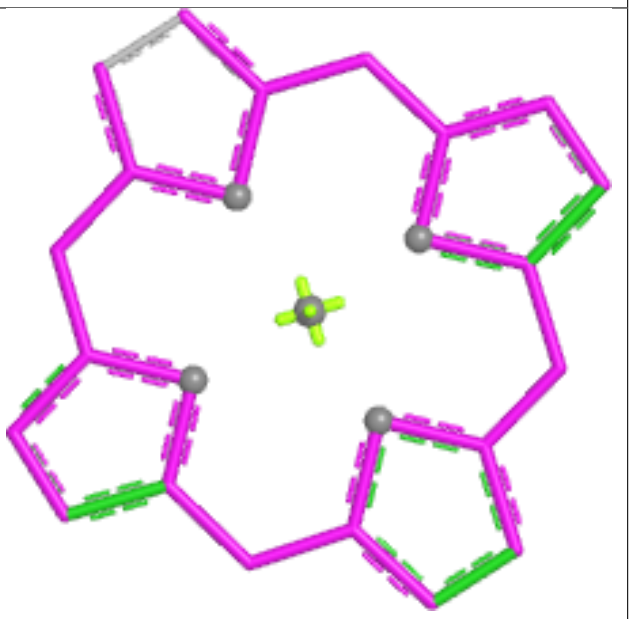
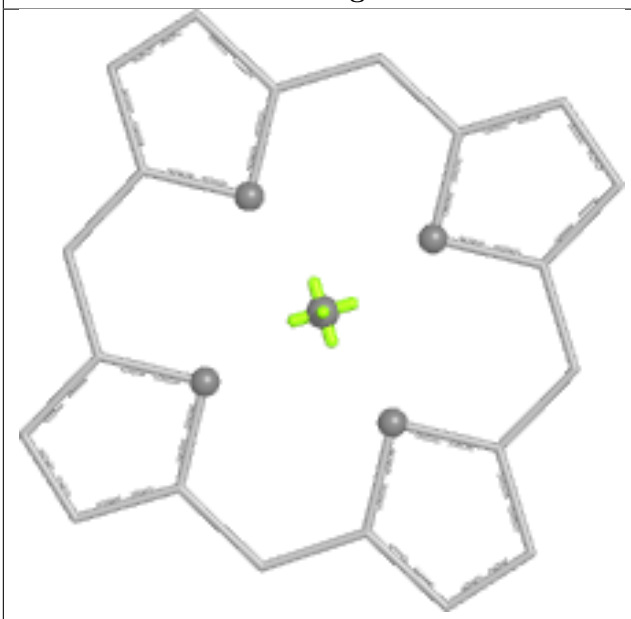


Bond angles



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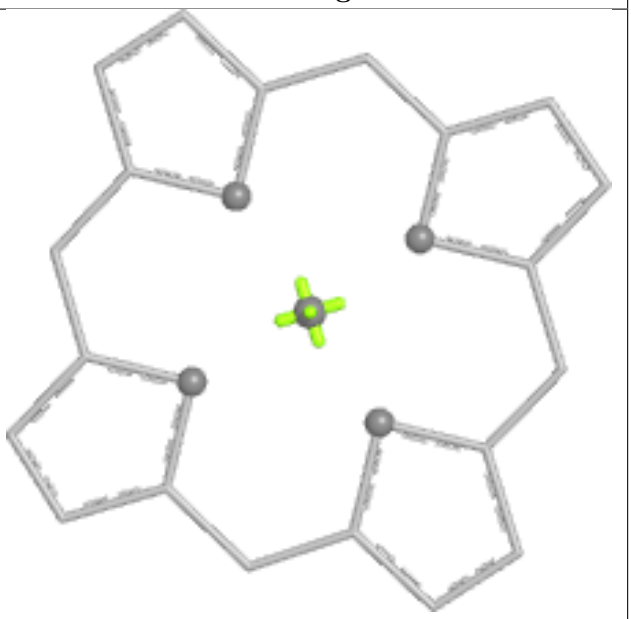
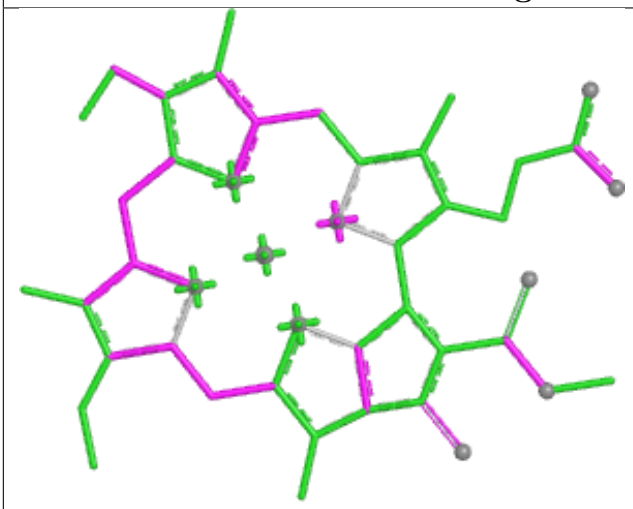


Rings

Ligand CLA A 1135



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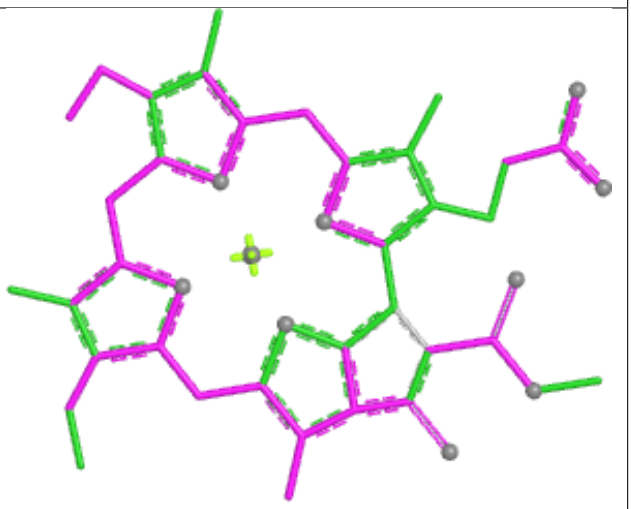
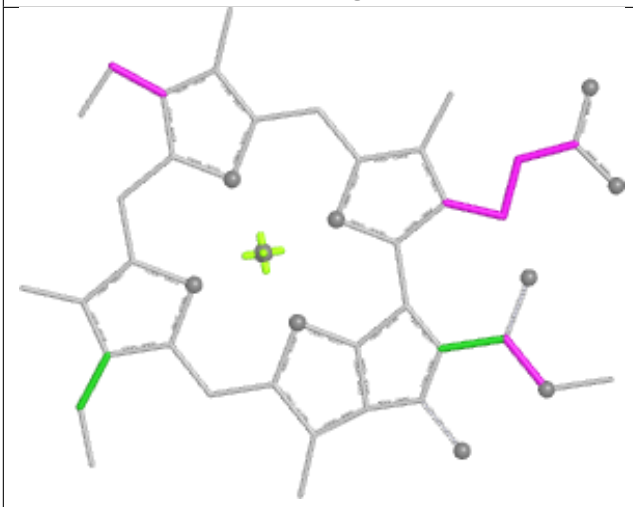
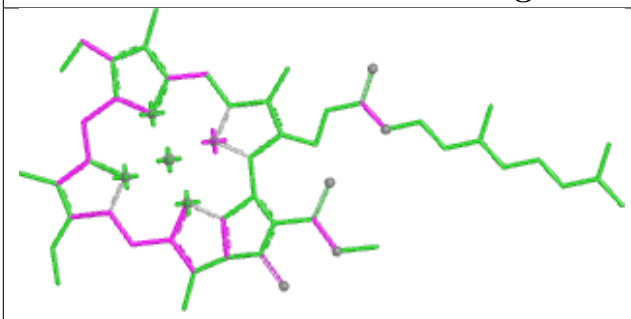
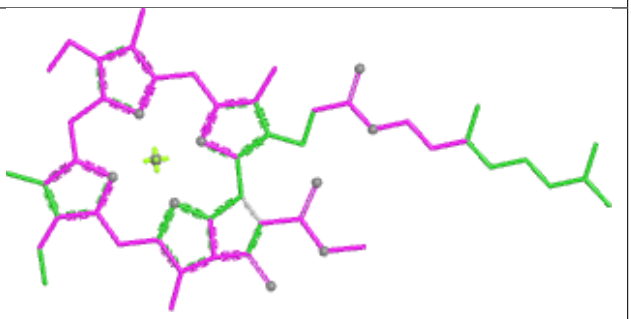
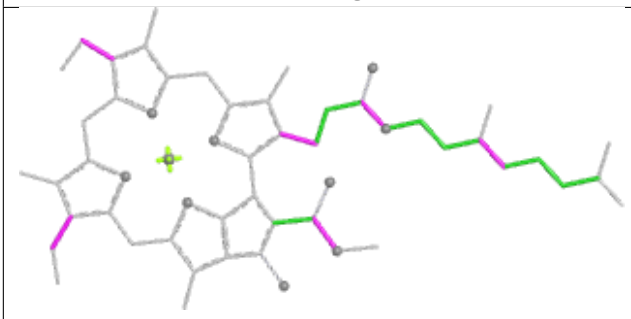
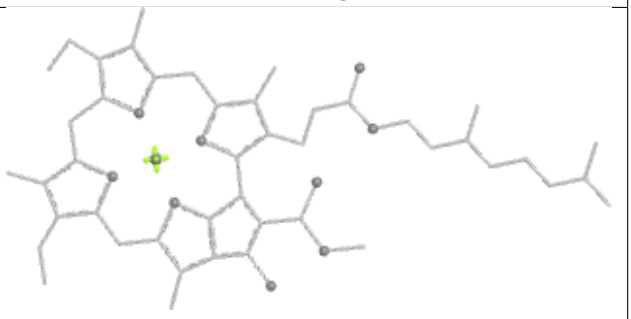


Bond angles

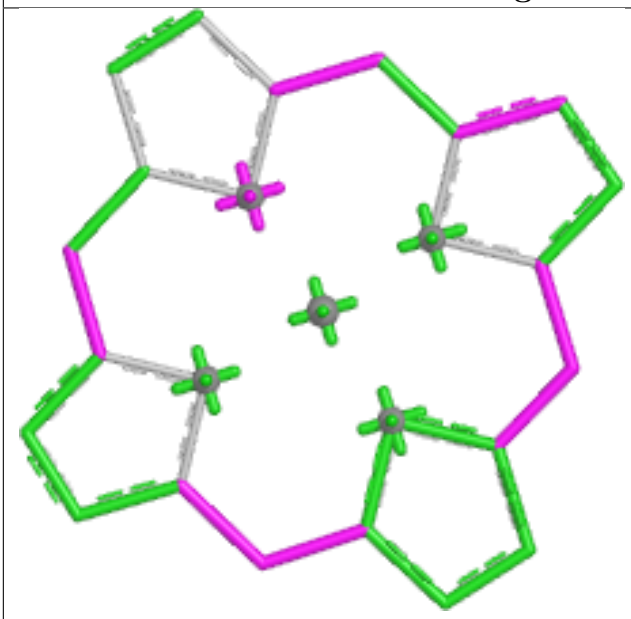


Torsions

Rings

Ligand CLA A 9011	
 Bond lengths	 Bond angles
 Torsions	 Rings

Ligand CLA K 1141



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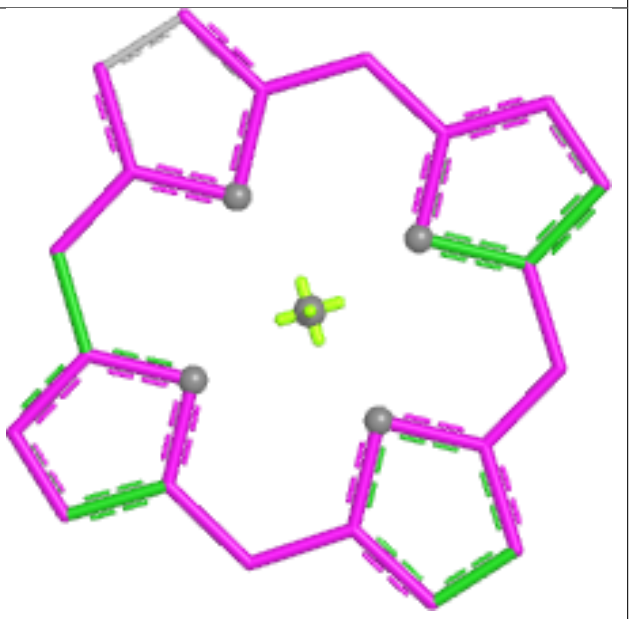
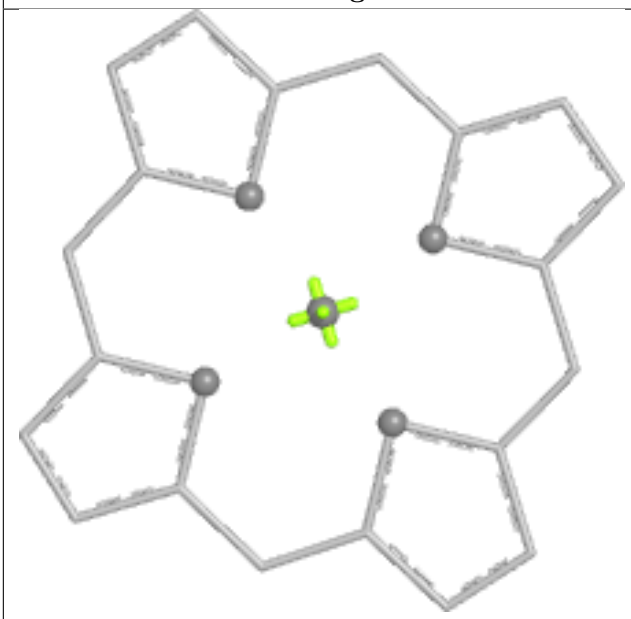


Bond angles



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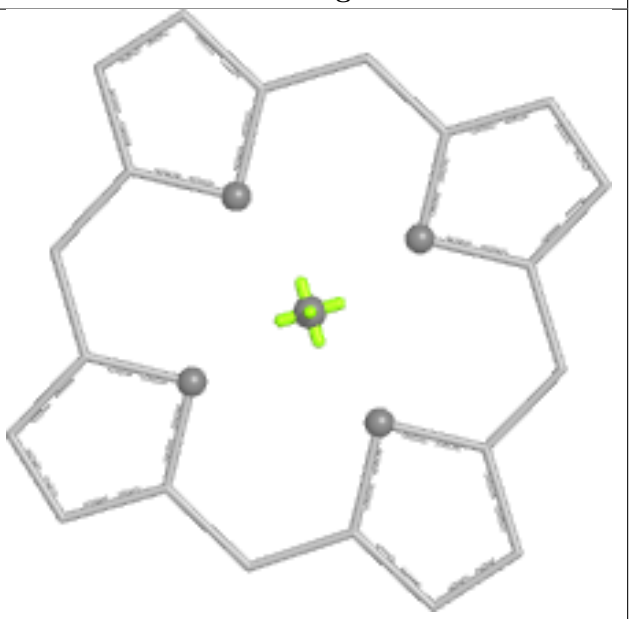
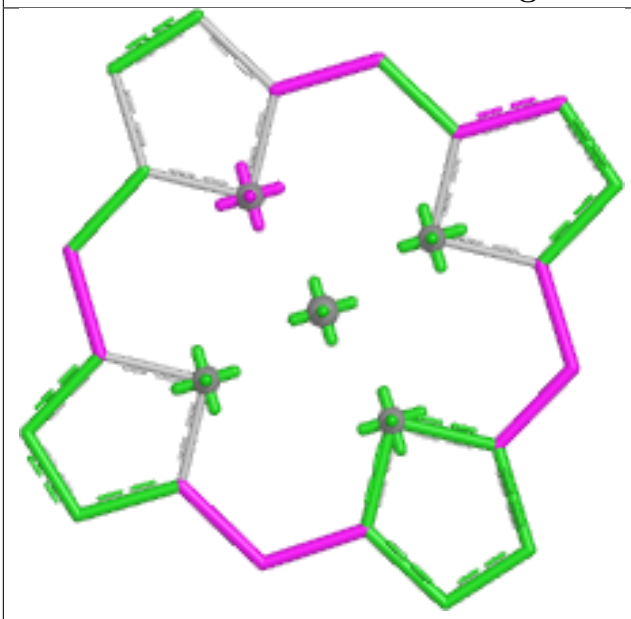


Rings

Ligand CLA 4 4002



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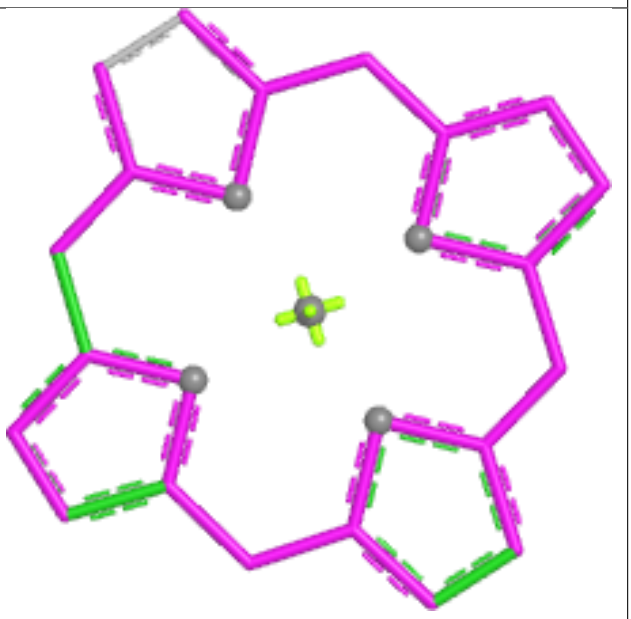

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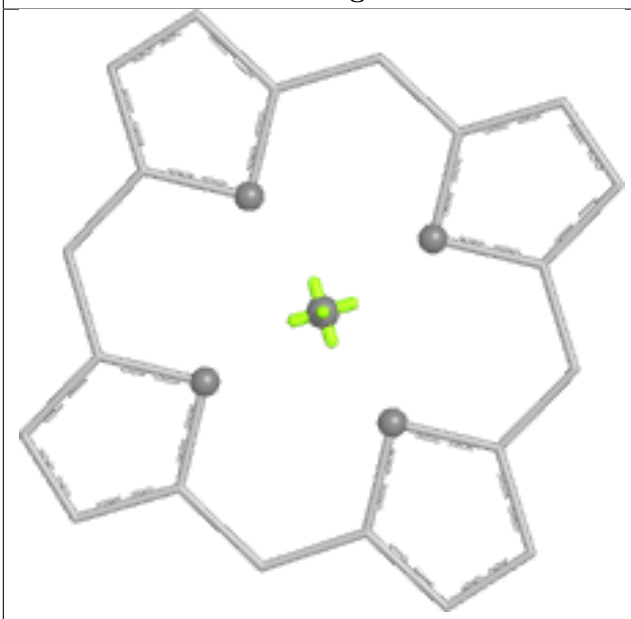

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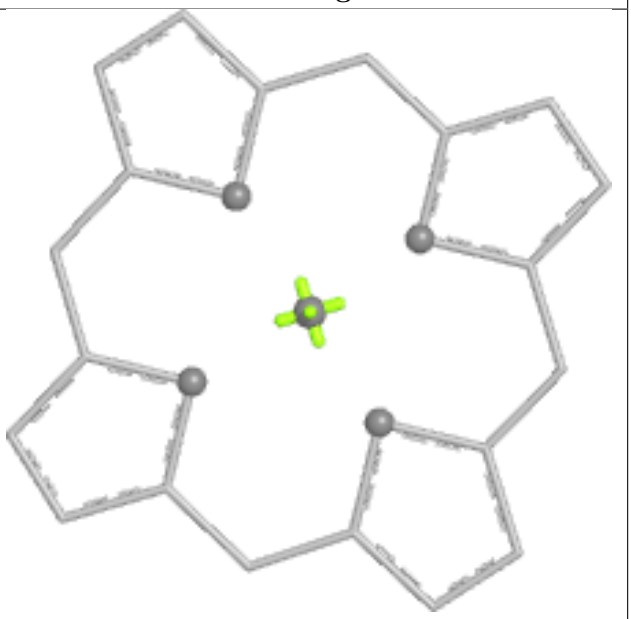

Rings

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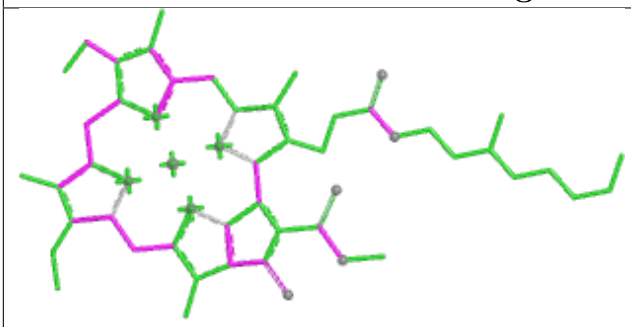
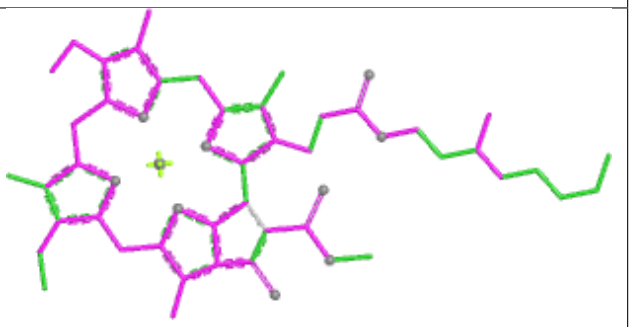
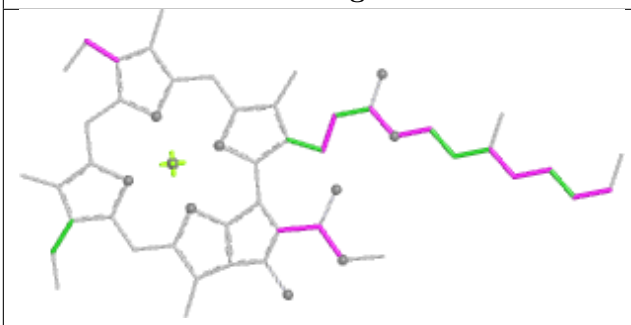
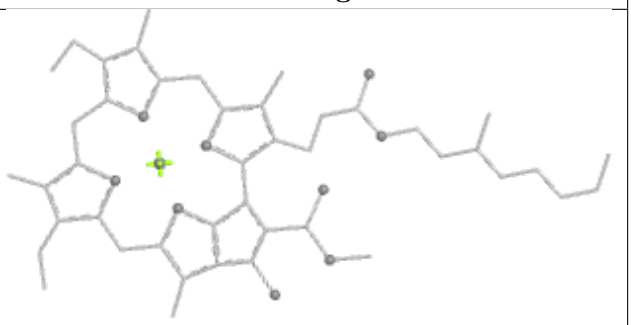
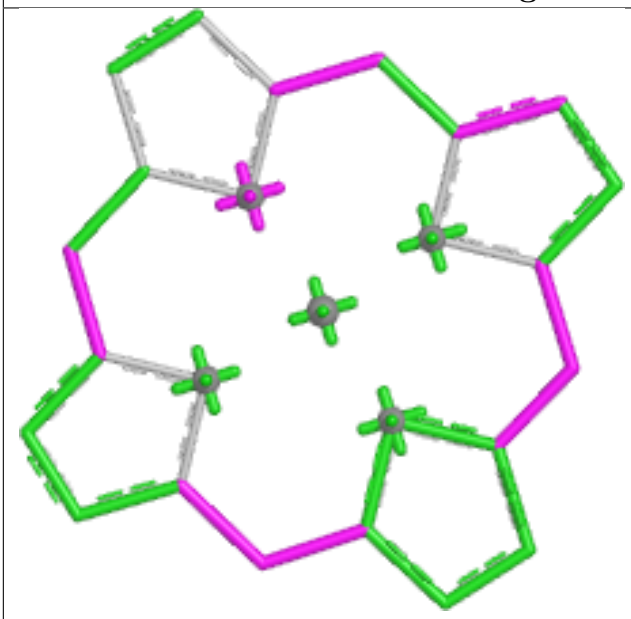
 Bond lengths	 Bond angles
 Torsions	 Rings

Ligand CLA 2 2006



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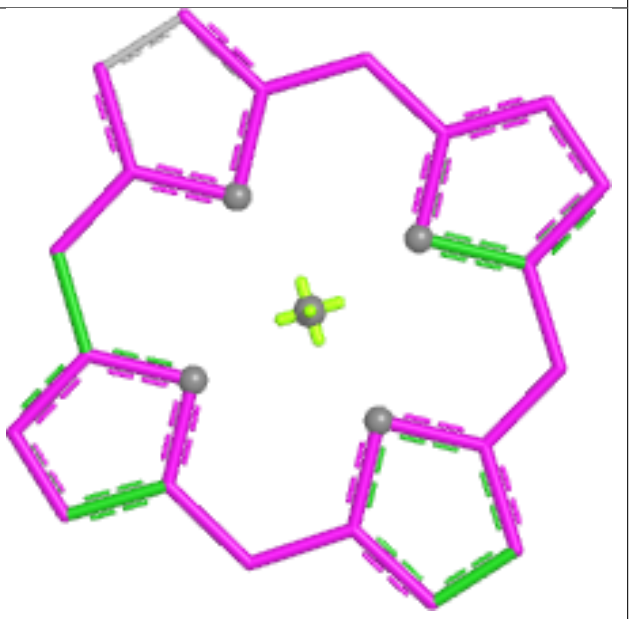

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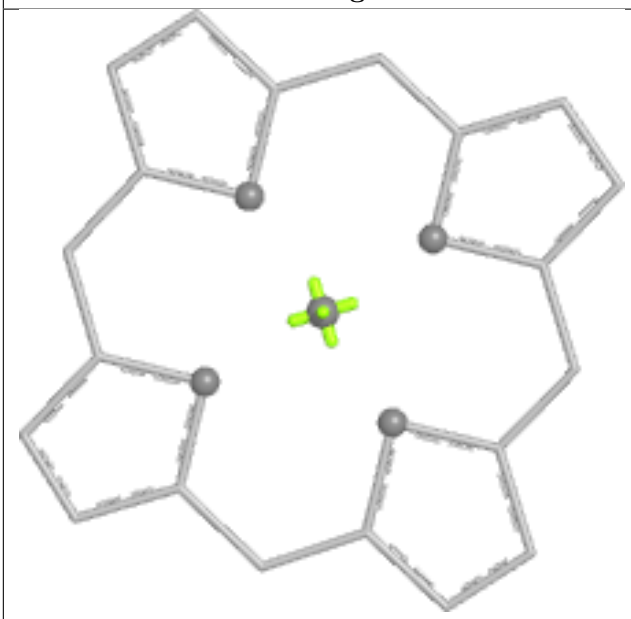

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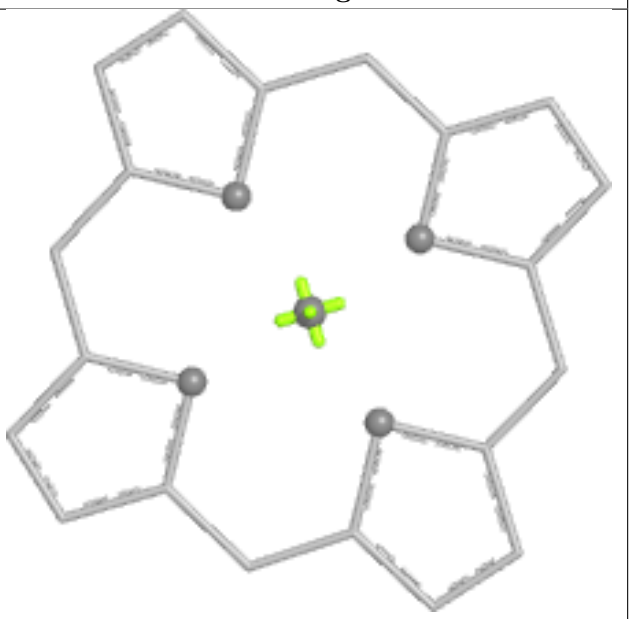
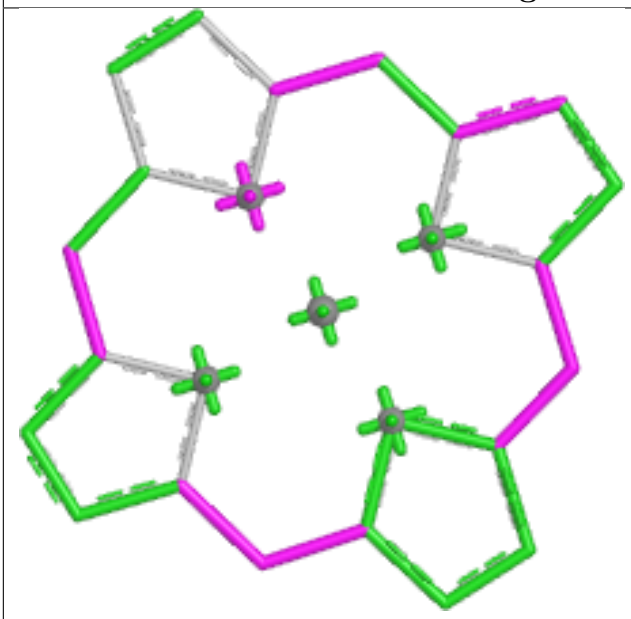


Rings

Ligand CLA 3 3001



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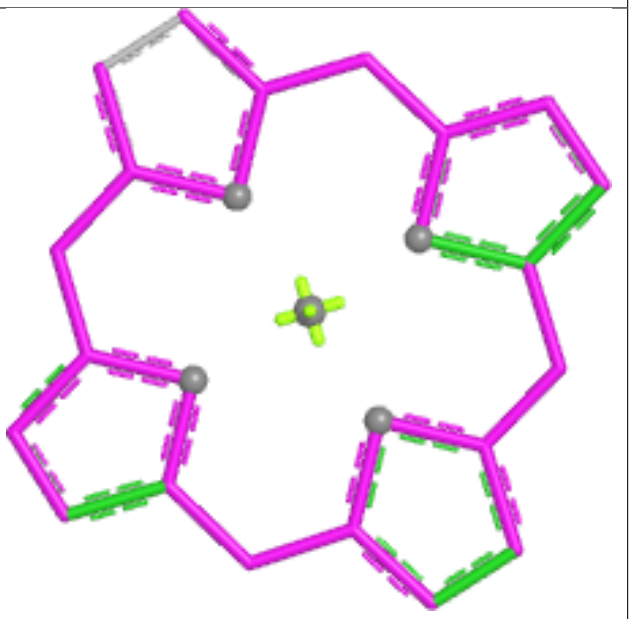

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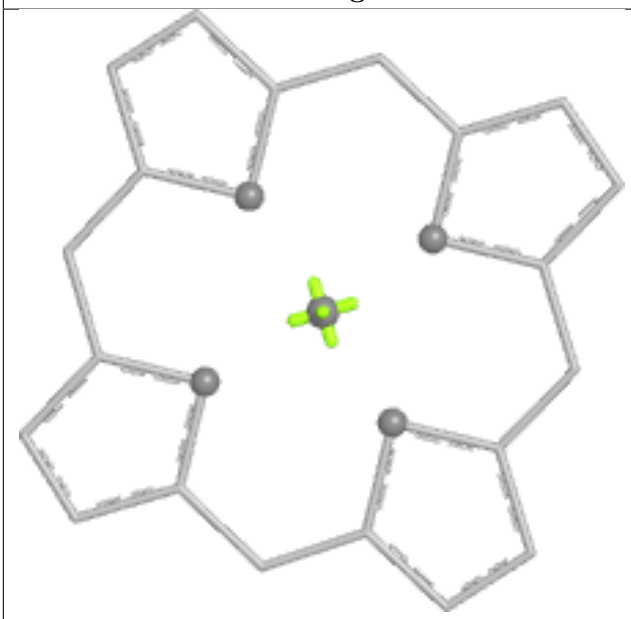

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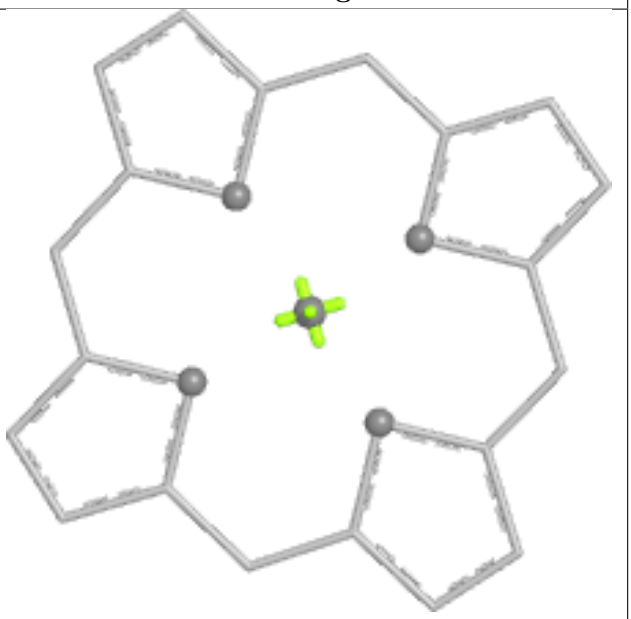
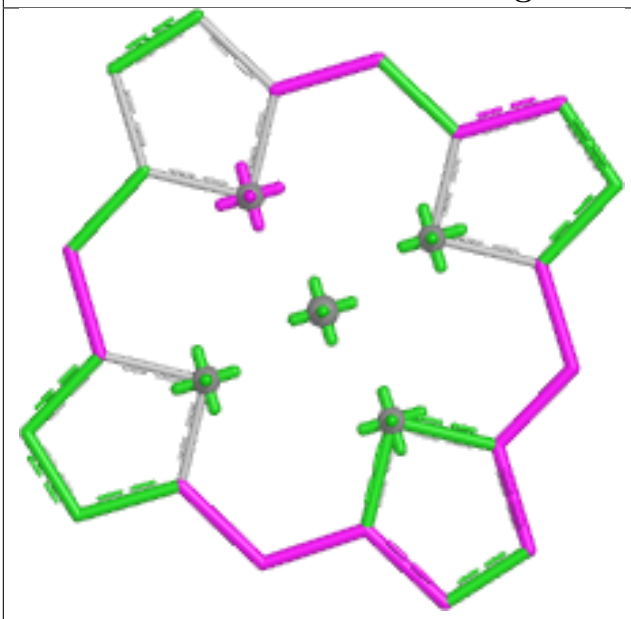


Rings

Ligand CLA A 1127



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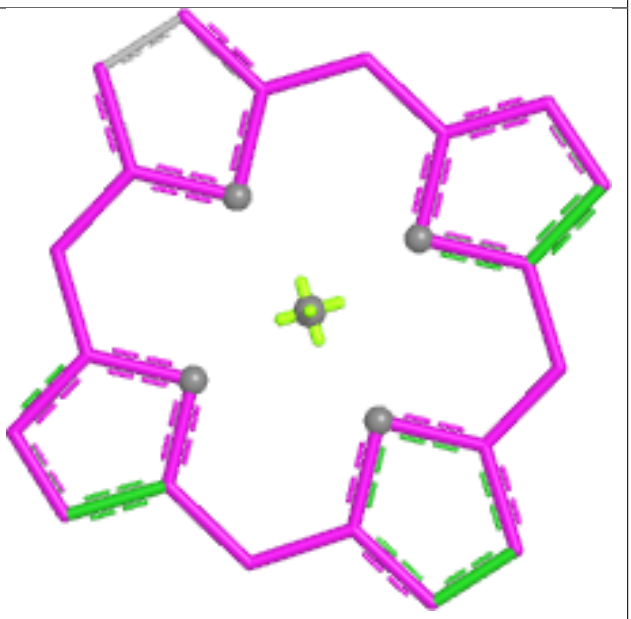

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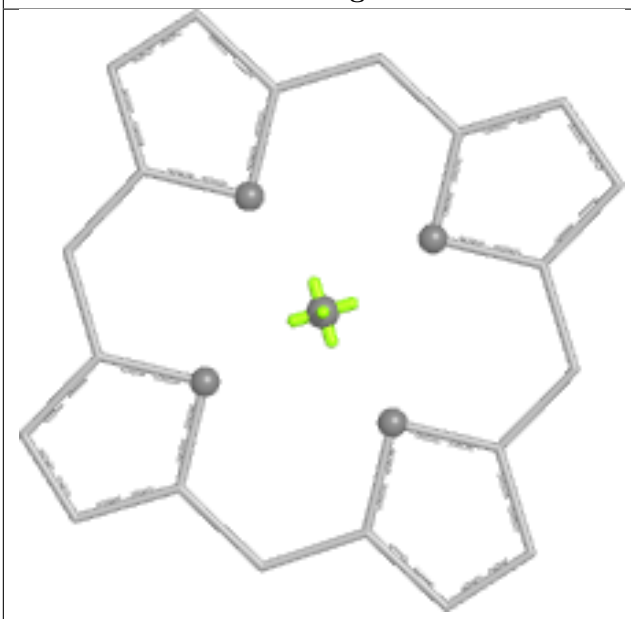

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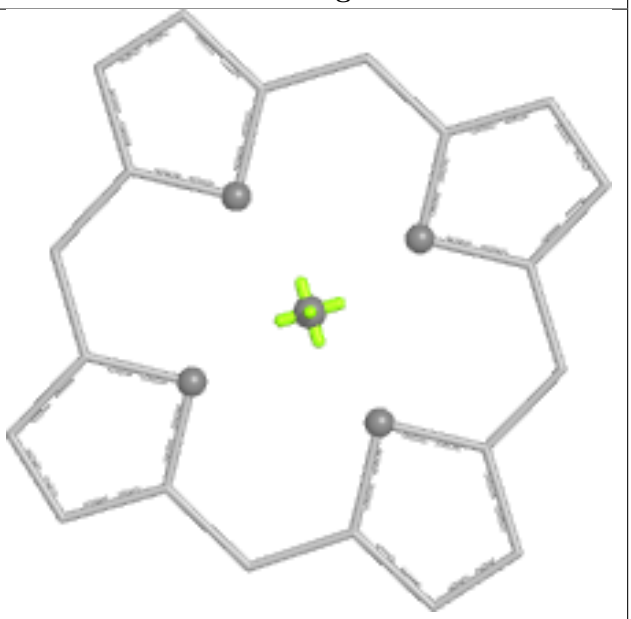
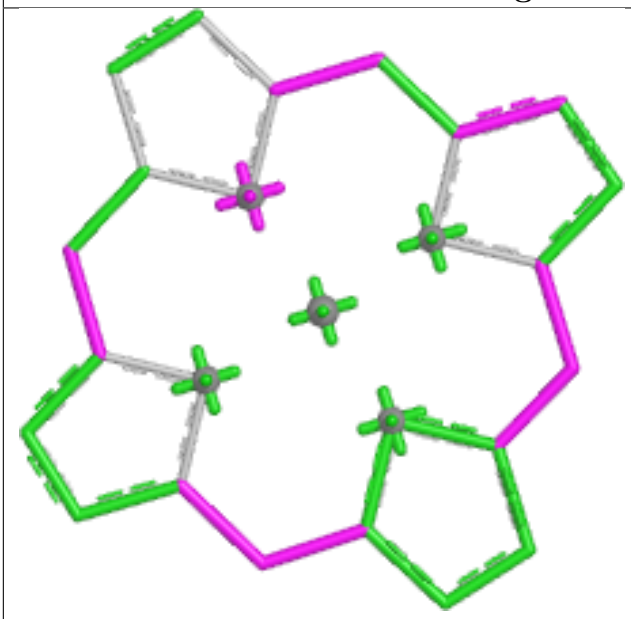


Rings

Ligand CLA A 1102



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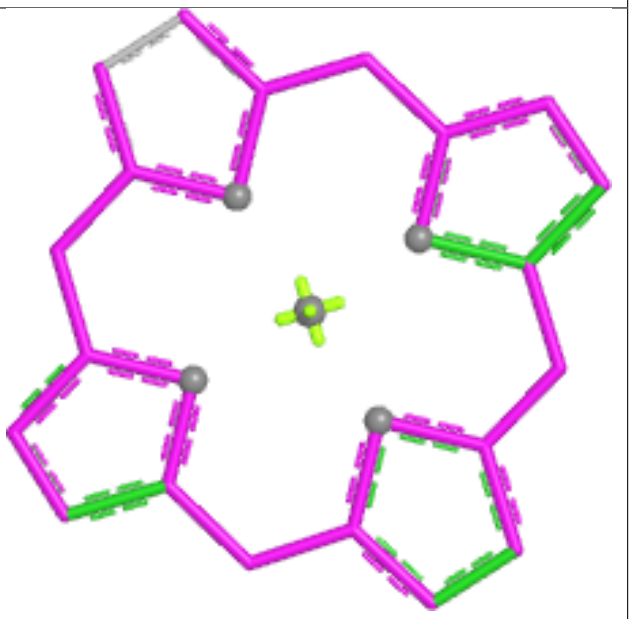

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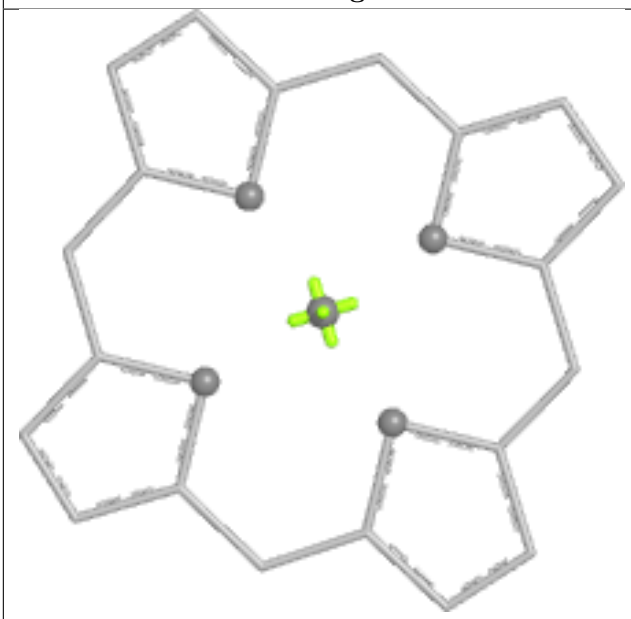

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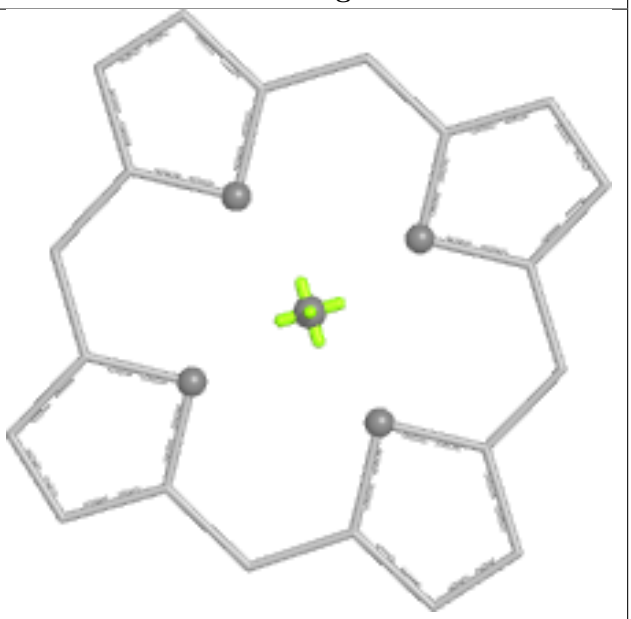
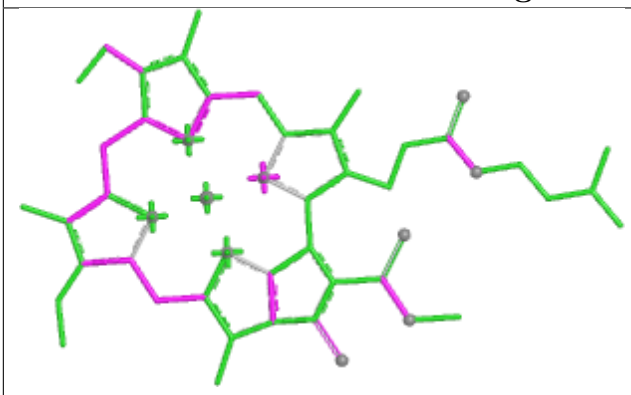


Rings

Ligand CLA A 1108



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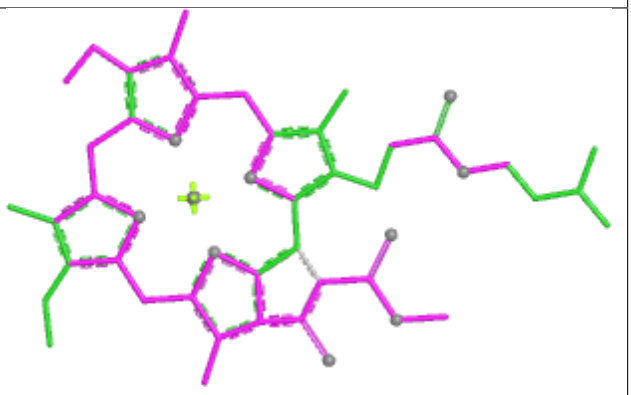

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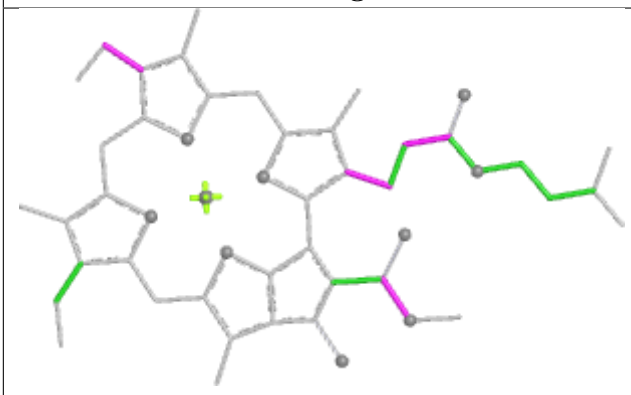

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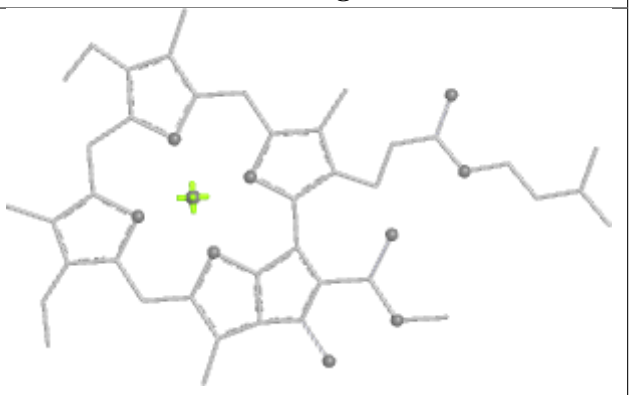
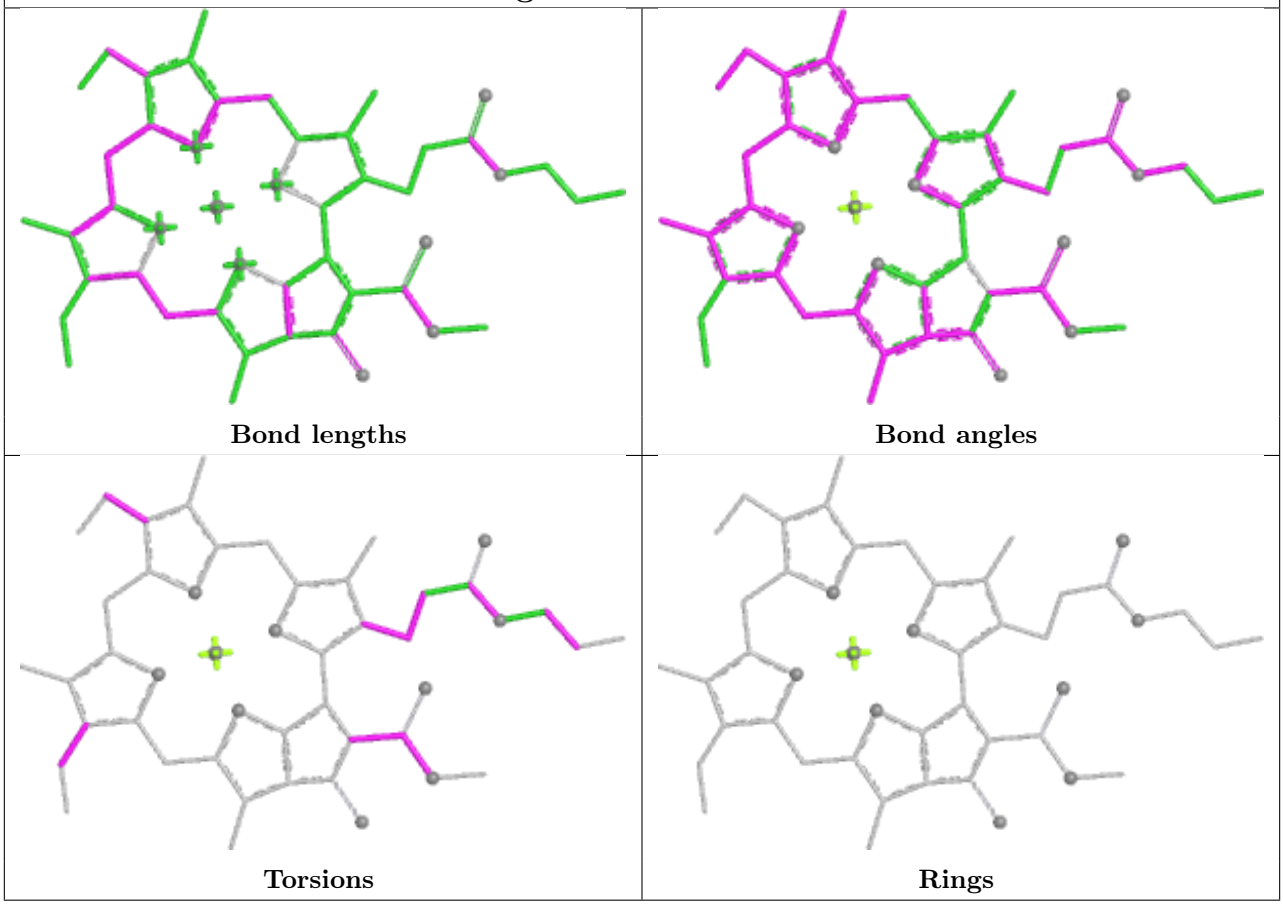


Rings

Ligand CLA B 1221



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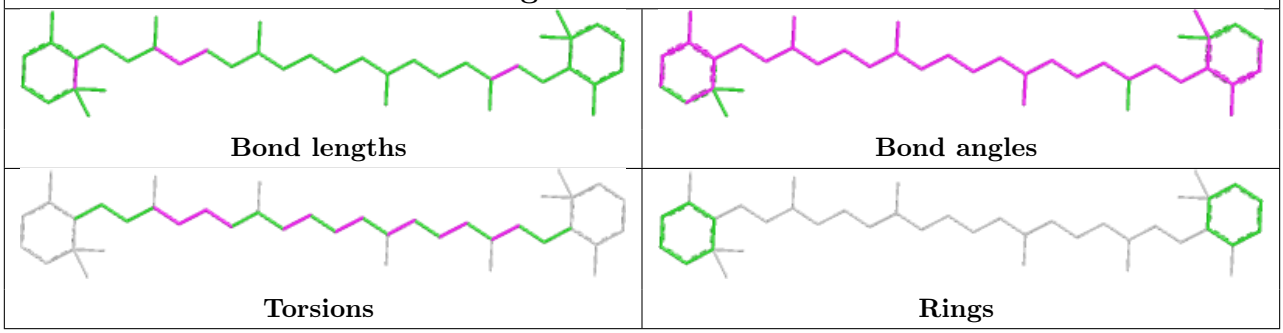

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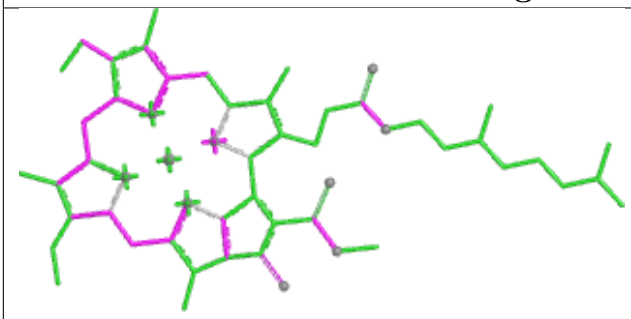

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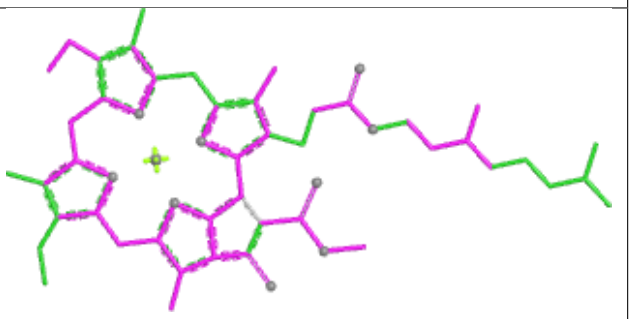

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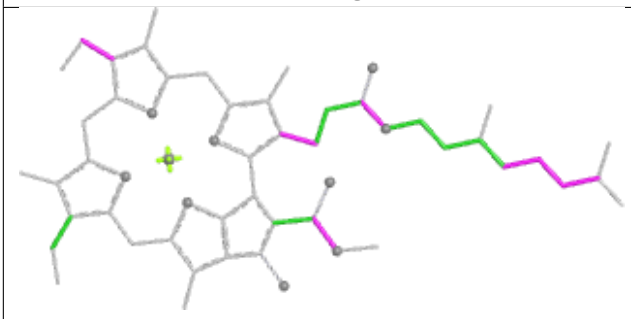

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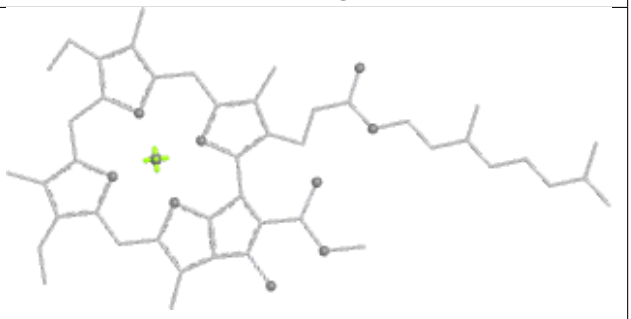

Rings

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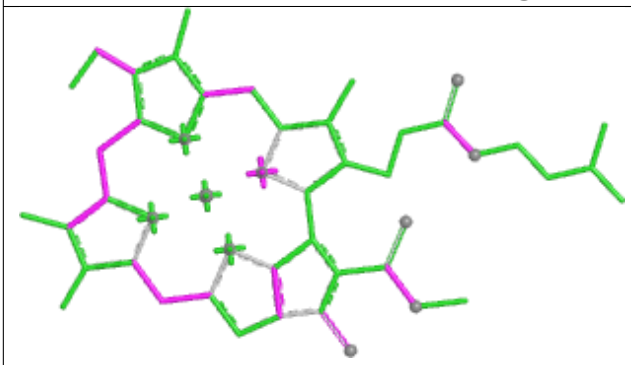

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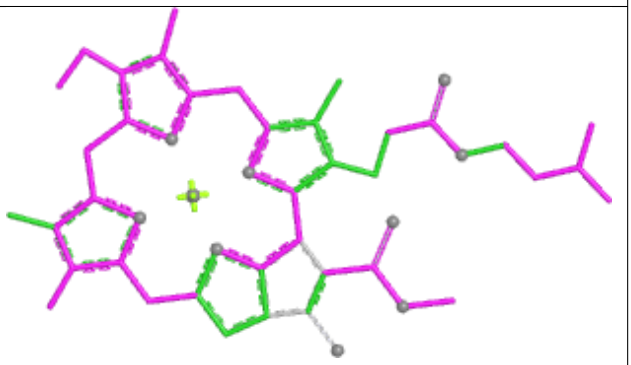

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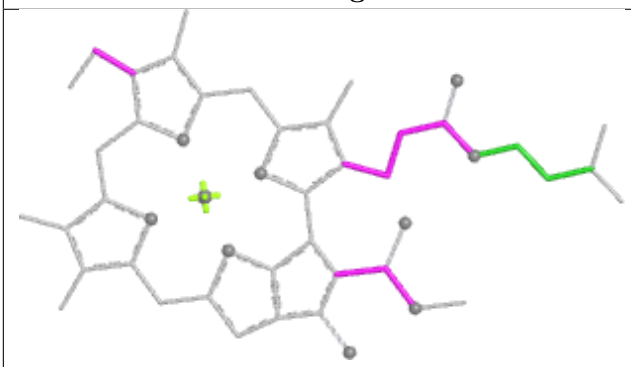

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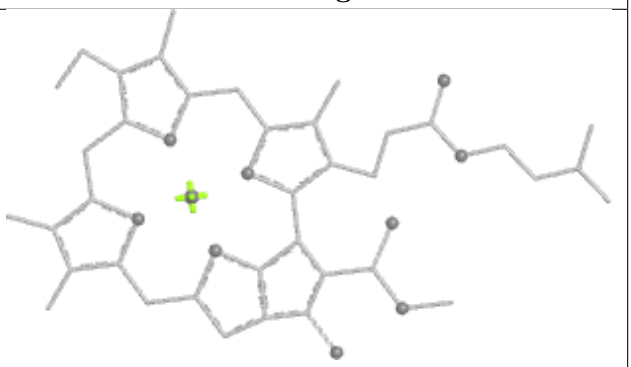

Rings

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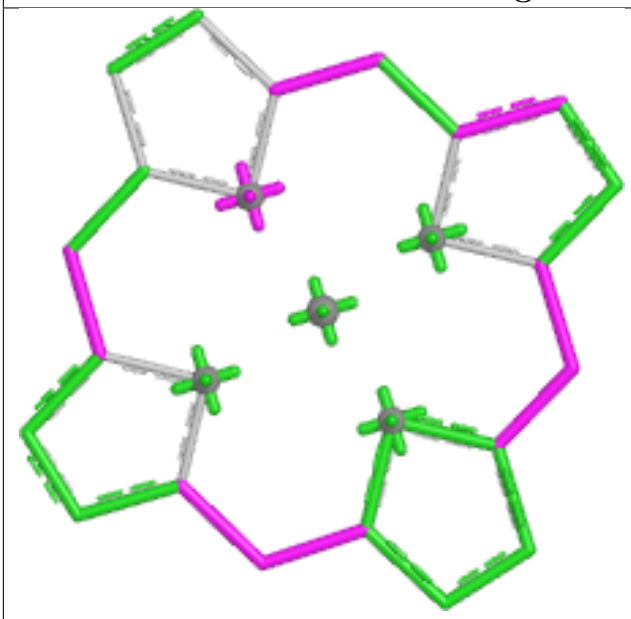

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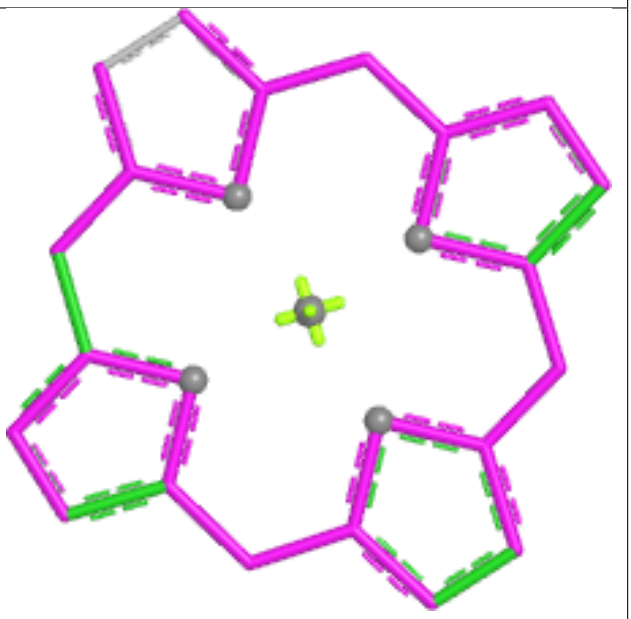
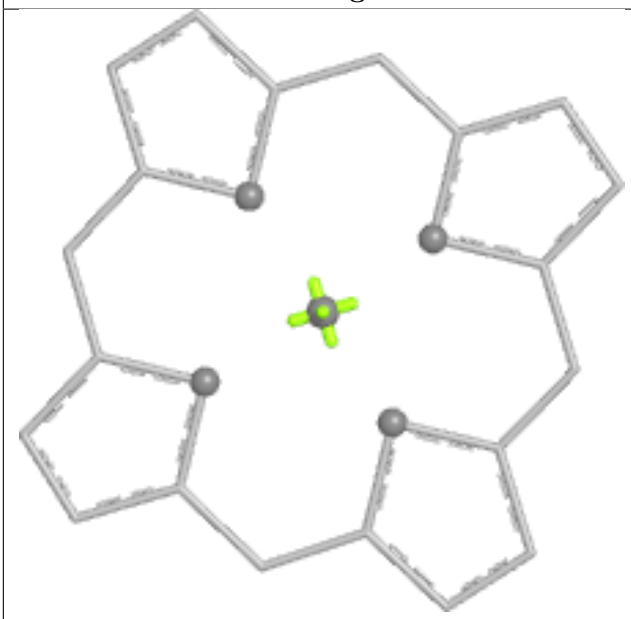


Bond angles



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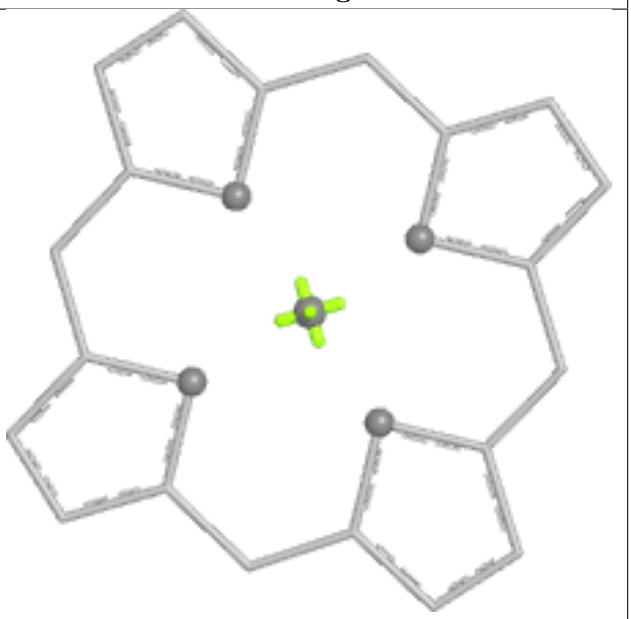
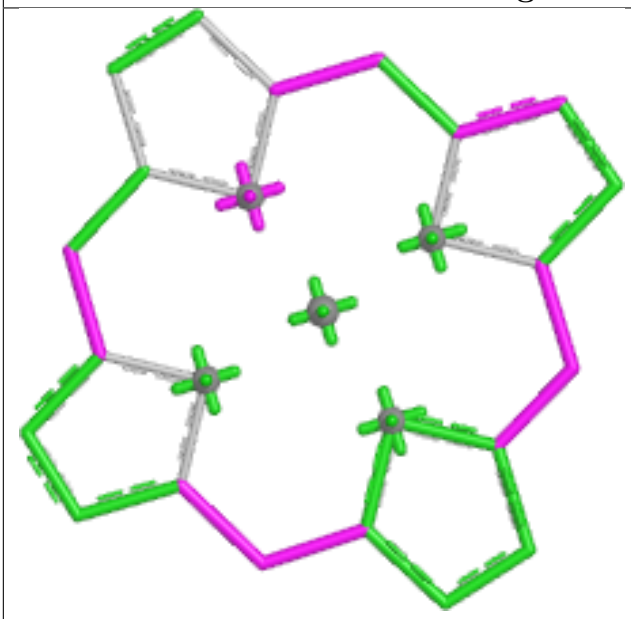


Rings

Ligand CLA F 1303



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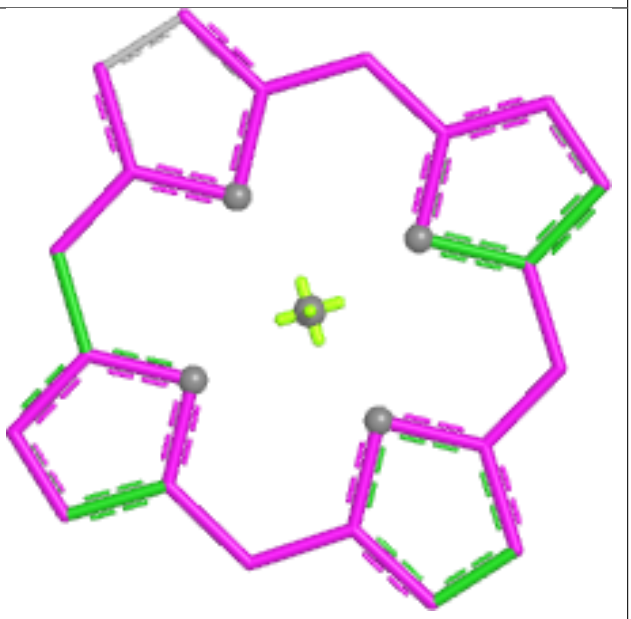
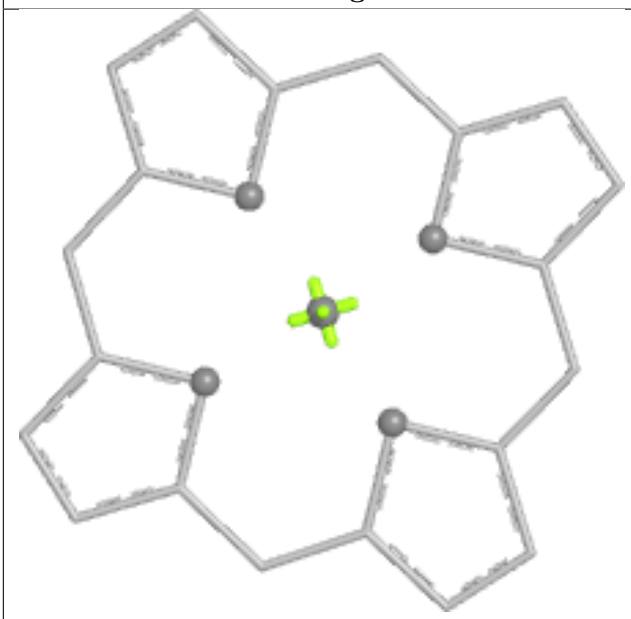


Bond angles



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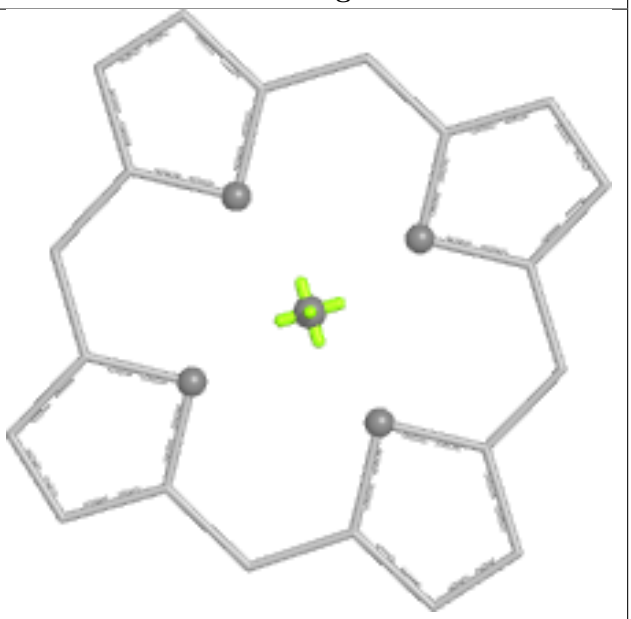
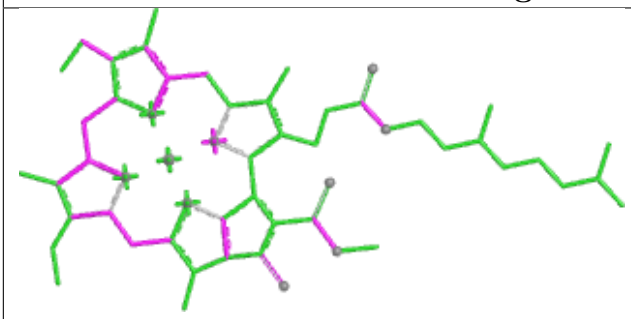
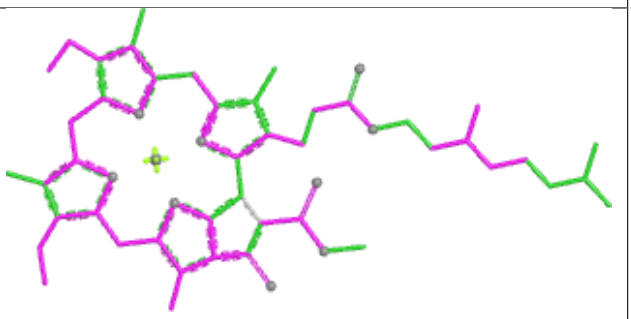
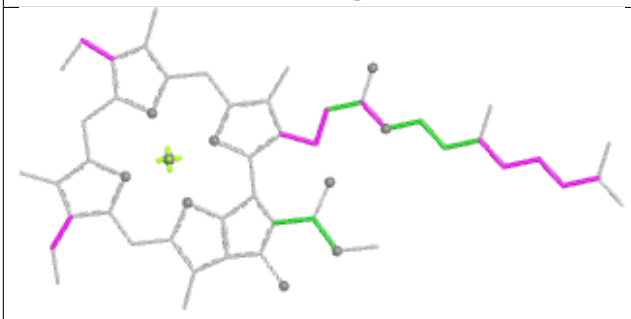
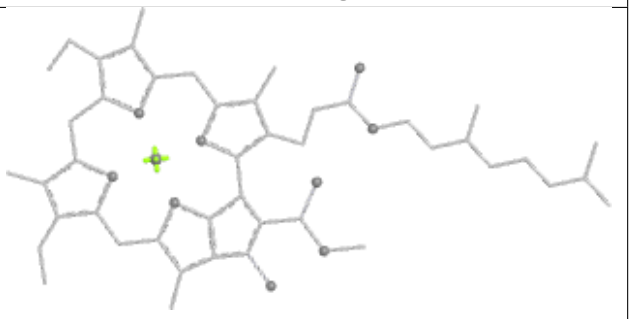
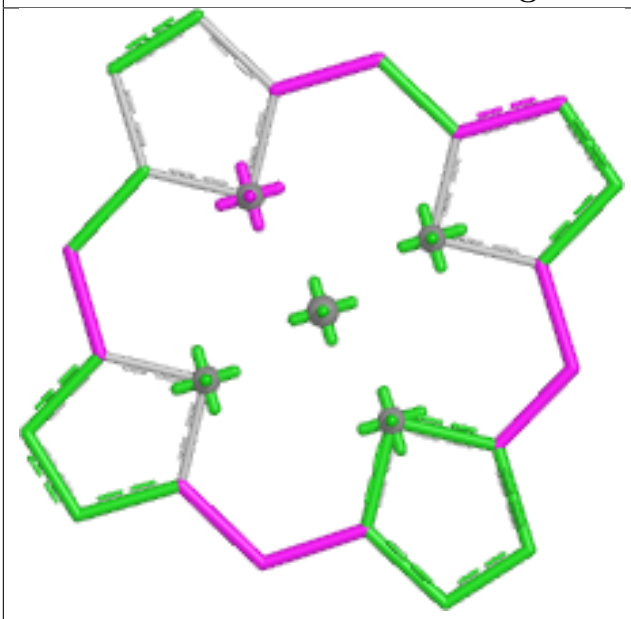


Rings

Ligand CLA A 1137	
 Bond lengths	 Bond angles
 Torsions	 Rings

Ligand CLA 1 1011



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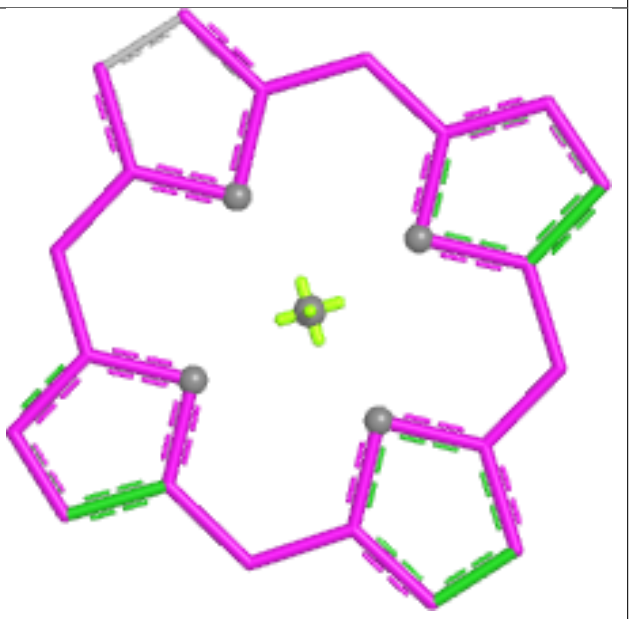
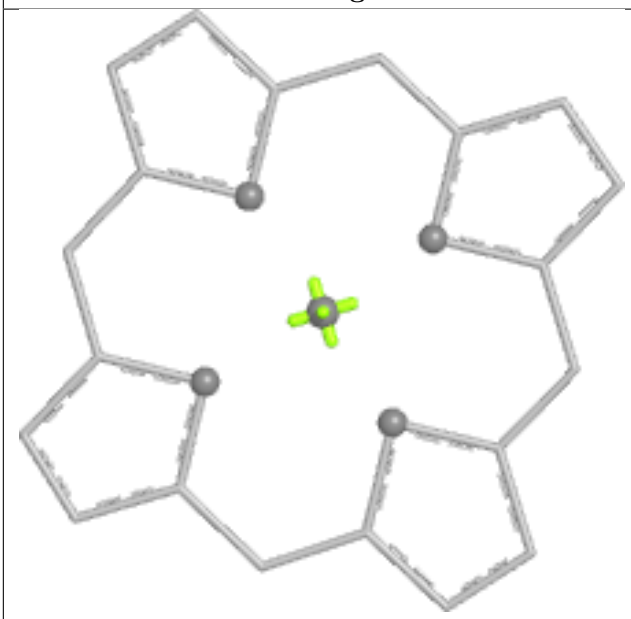
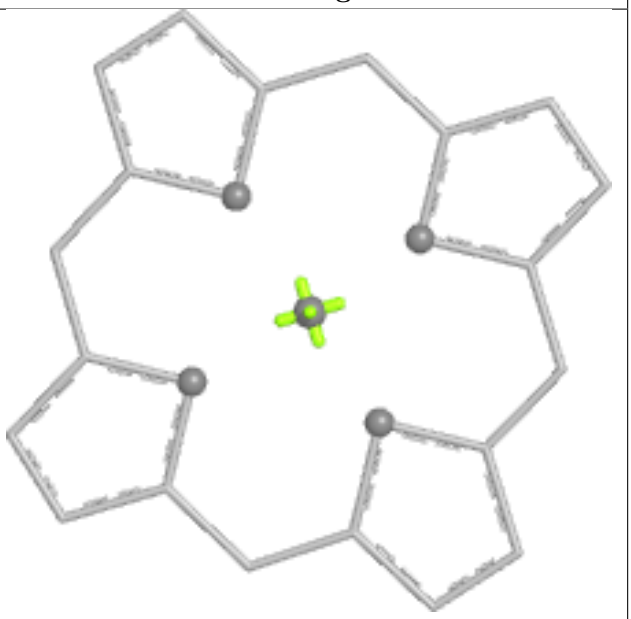


Bond angles

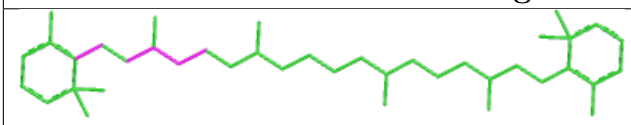


Torsions



Rings

Ligand BCR B 6017



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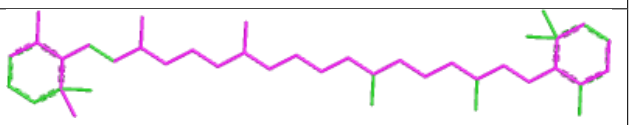

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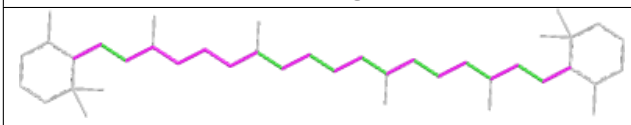

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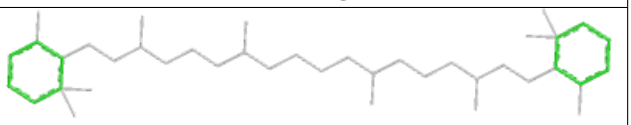
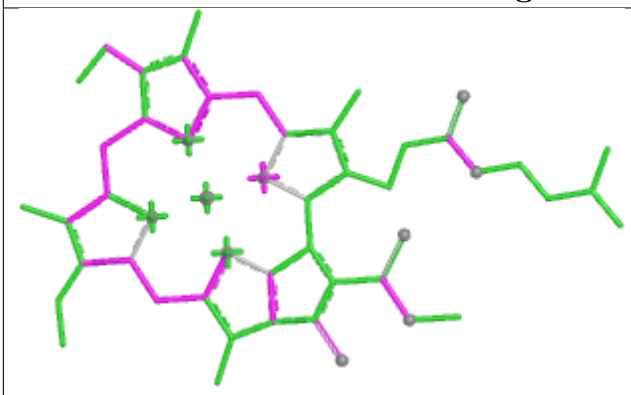


Rings

Ligand CLA B 1217



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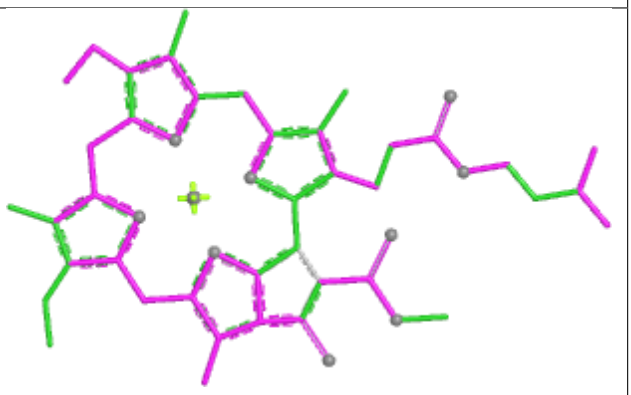

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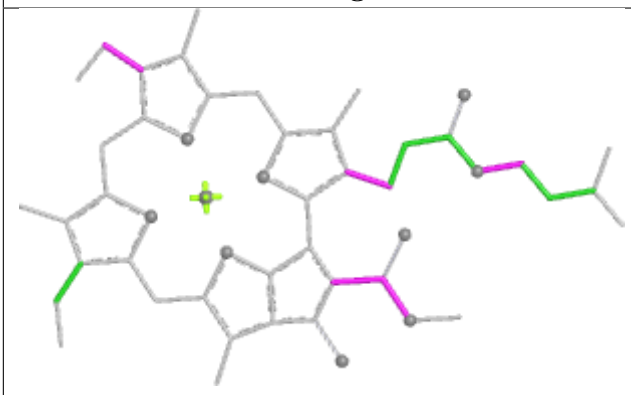

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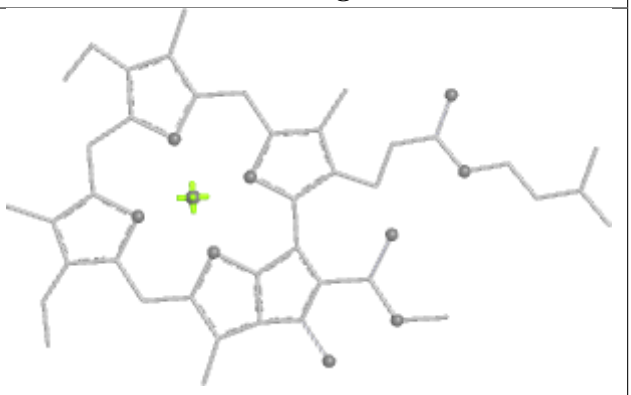
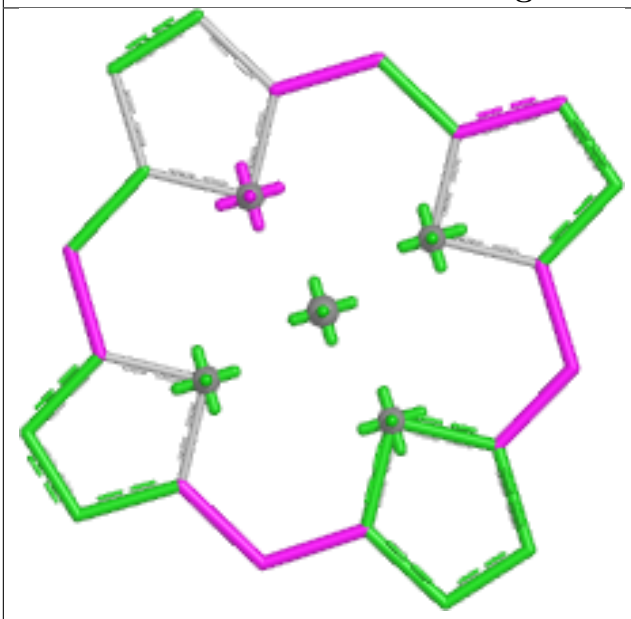


Rings

Ligand CLA B 1301



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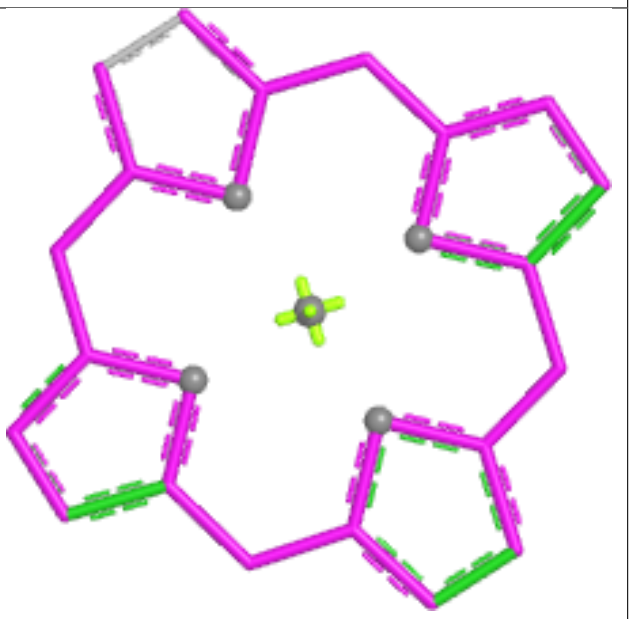

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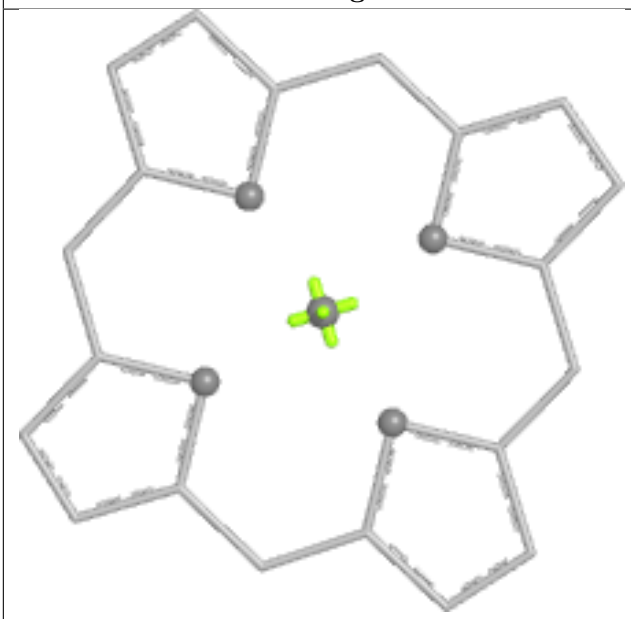

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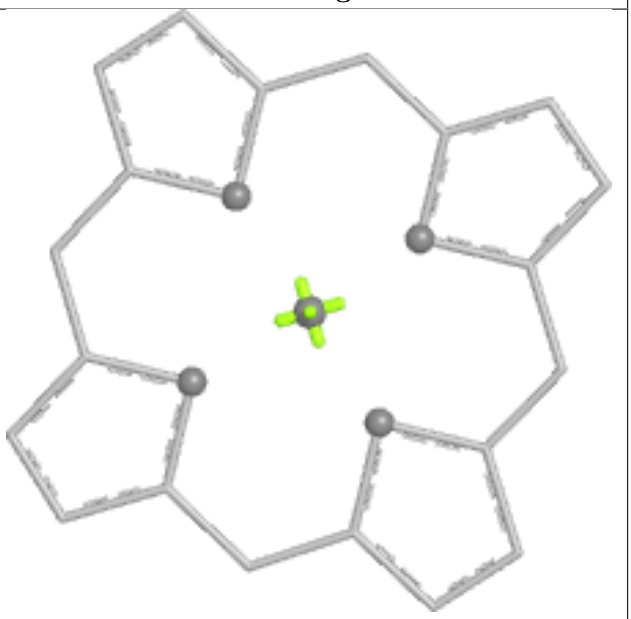
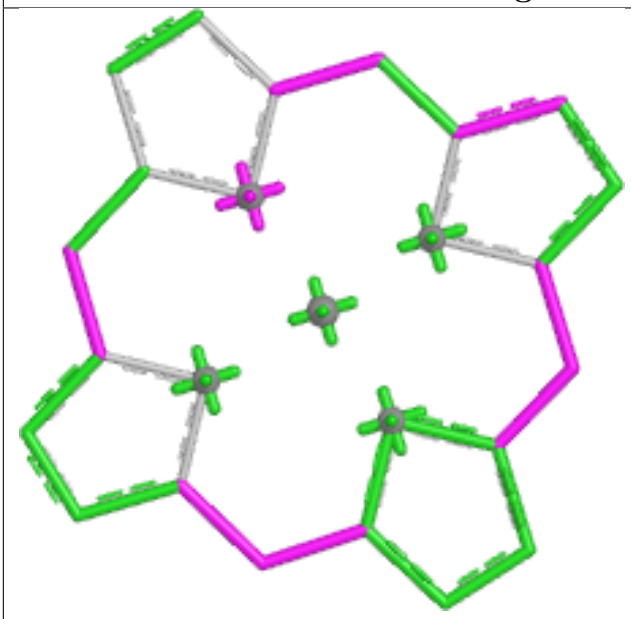


Rings

Ligand CLA A 1117



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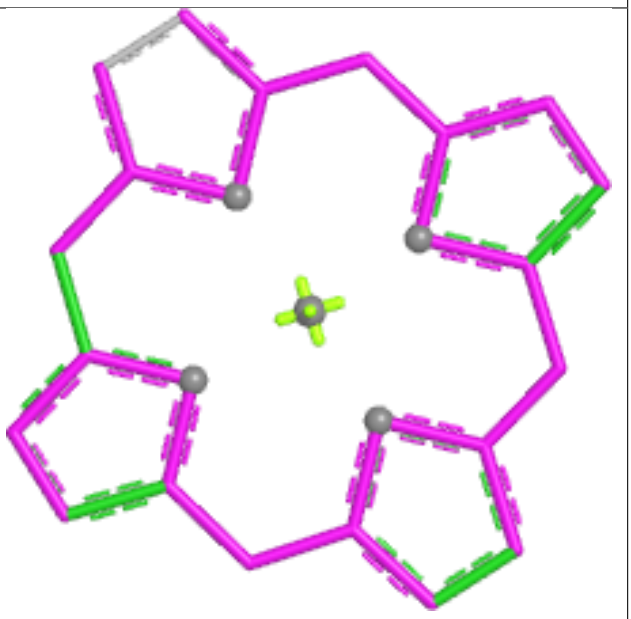

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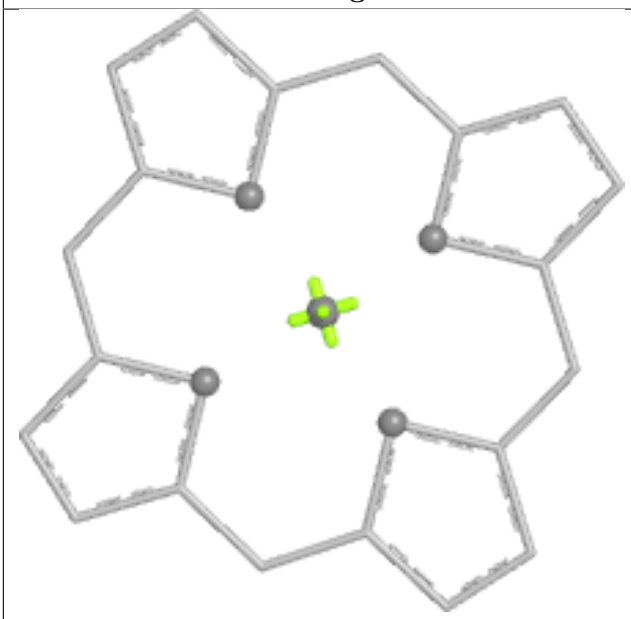

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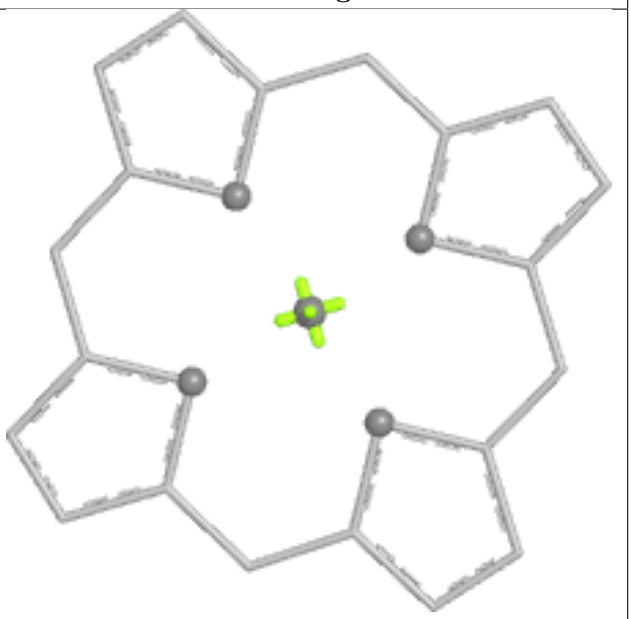
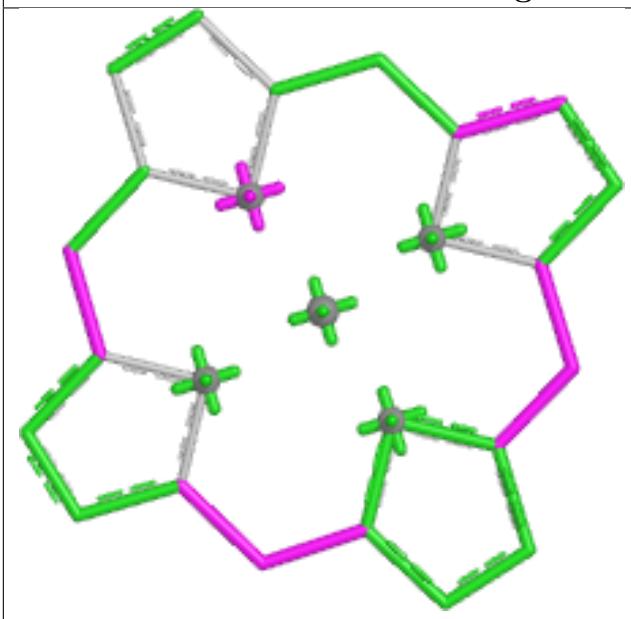


Rings

Ligand CLA A 1124



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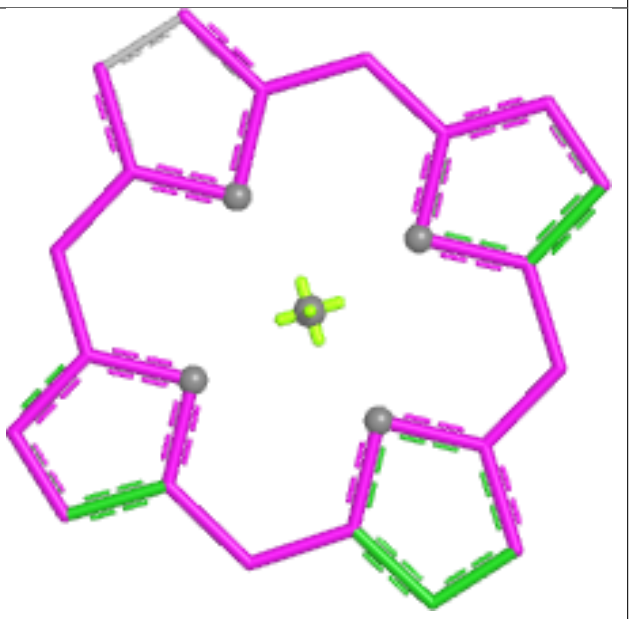

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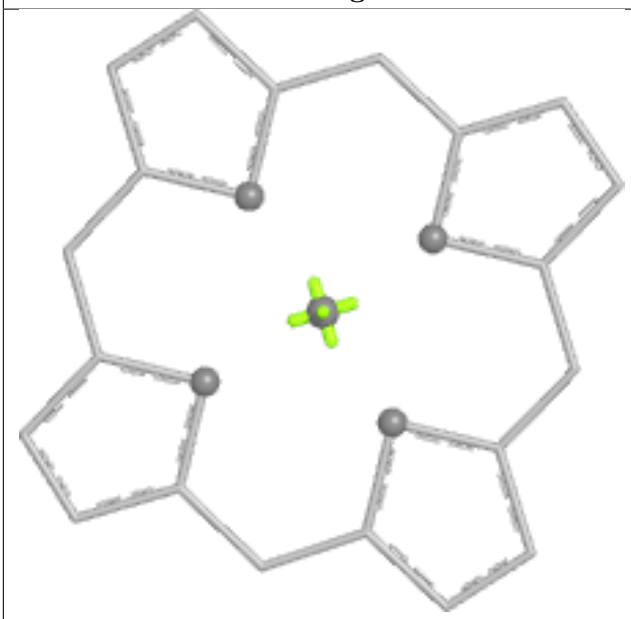

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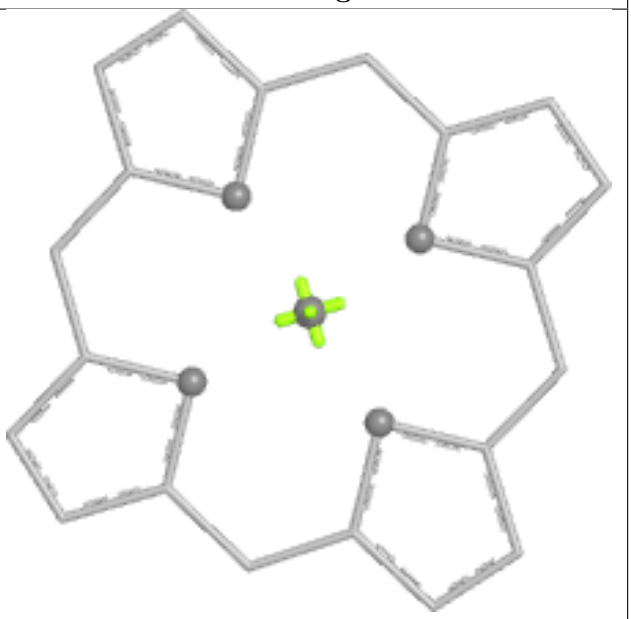
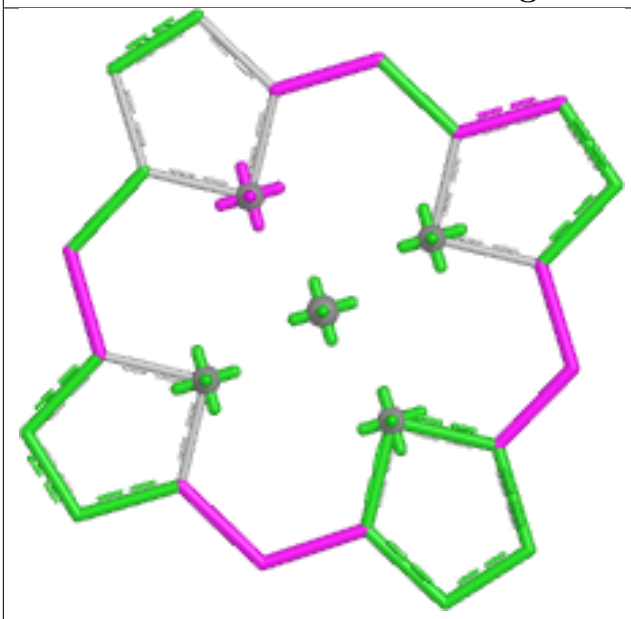


Rings

Ligand CLA 4 4003



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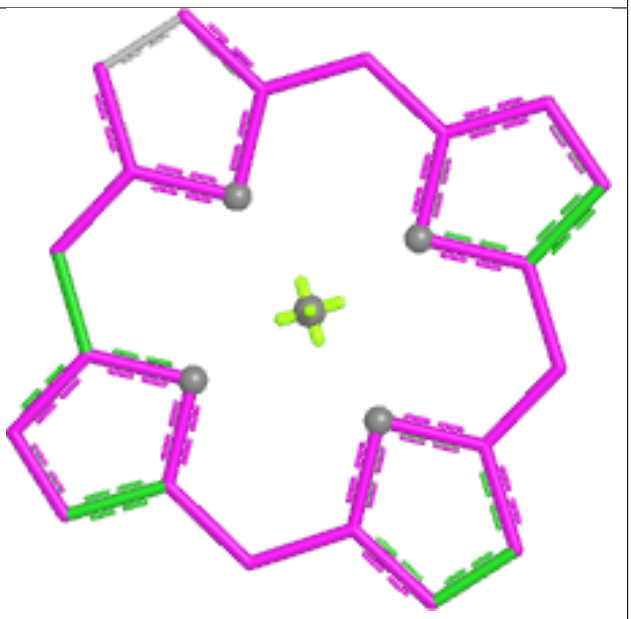

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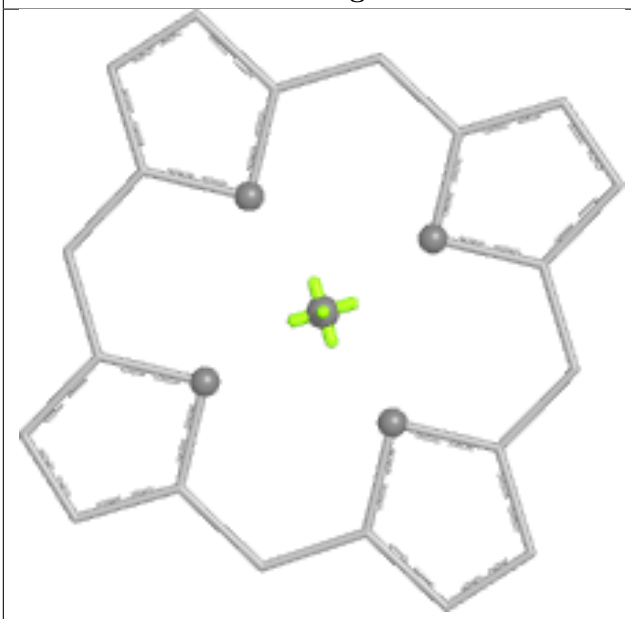

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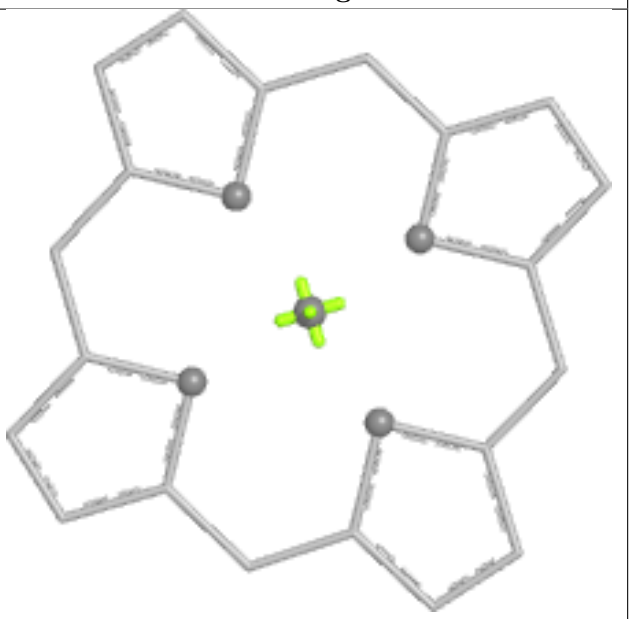
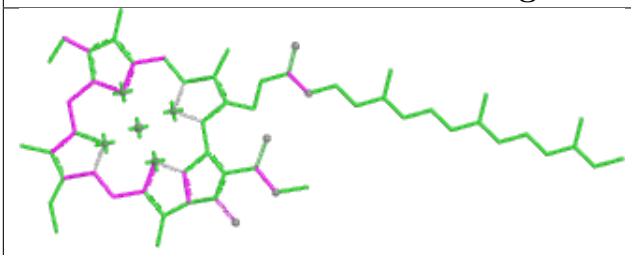
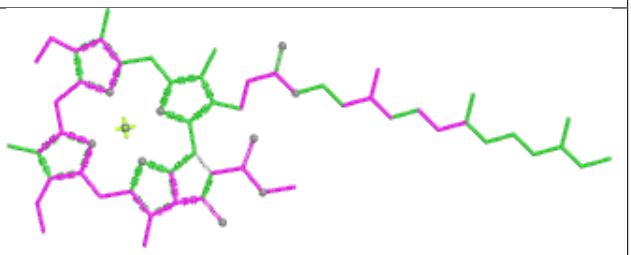
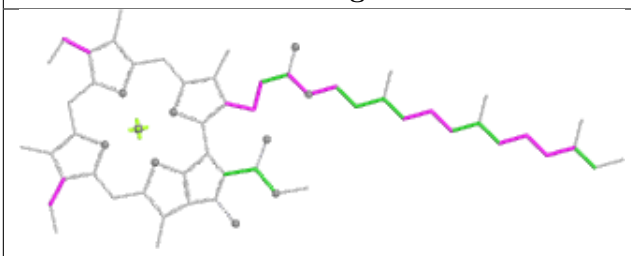
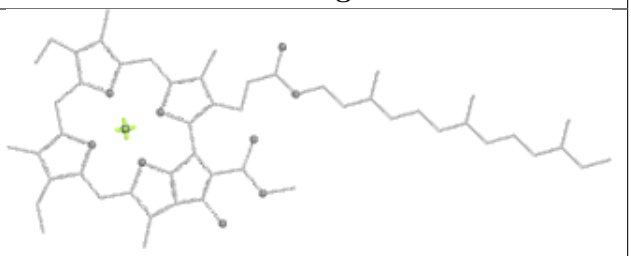
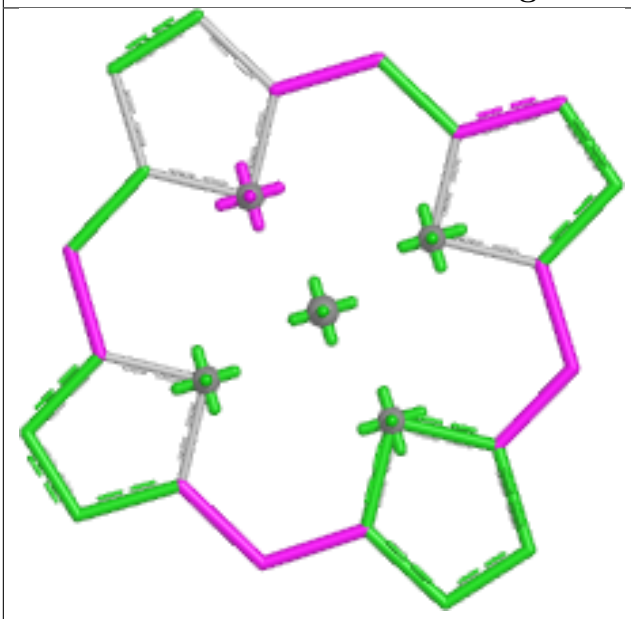


Rings

Ligand CLA J 2107	
 Bond lengths	 Bond angles
 Torsions	 Rings

Ligand CLA 1 1012



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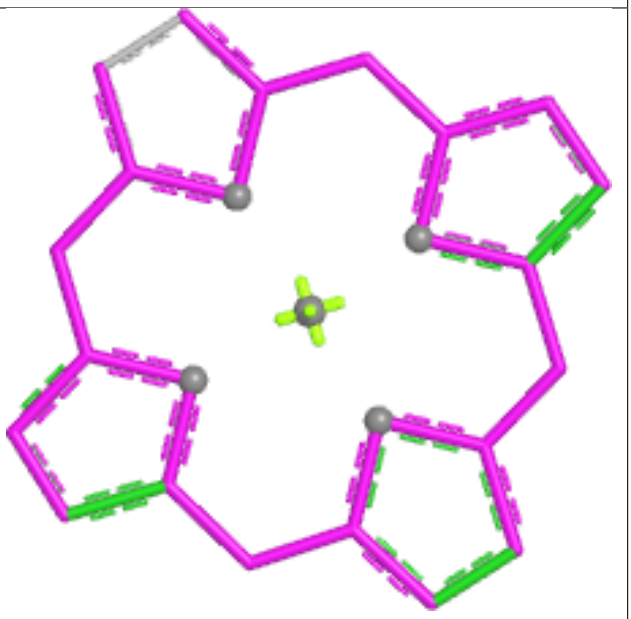
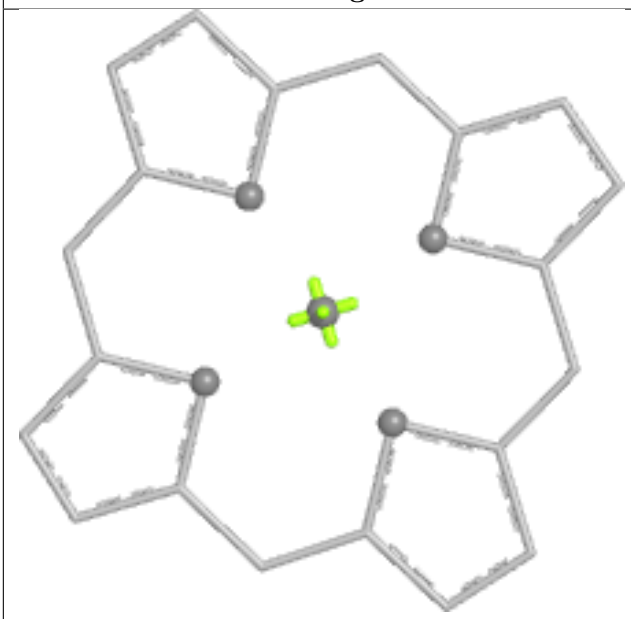


Bond angles



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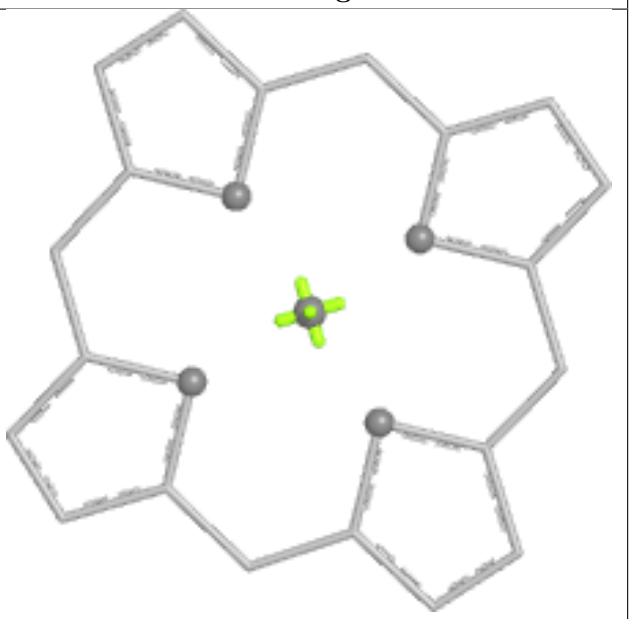
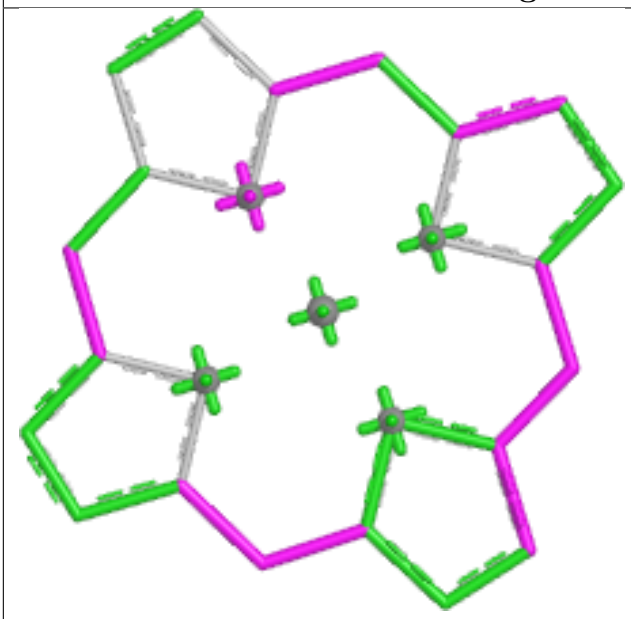


Rings

Ligand CLA 4 4012



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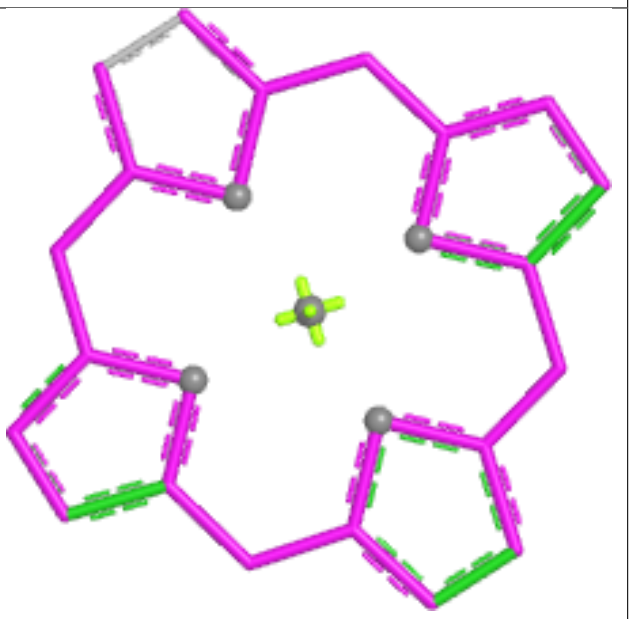

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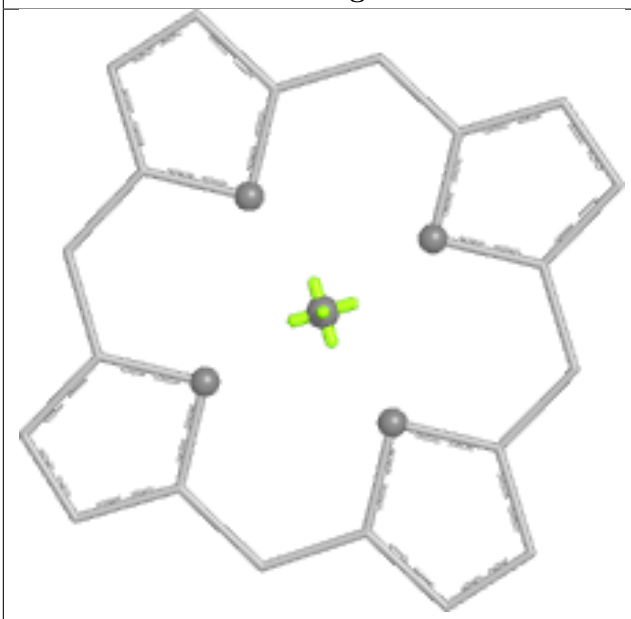

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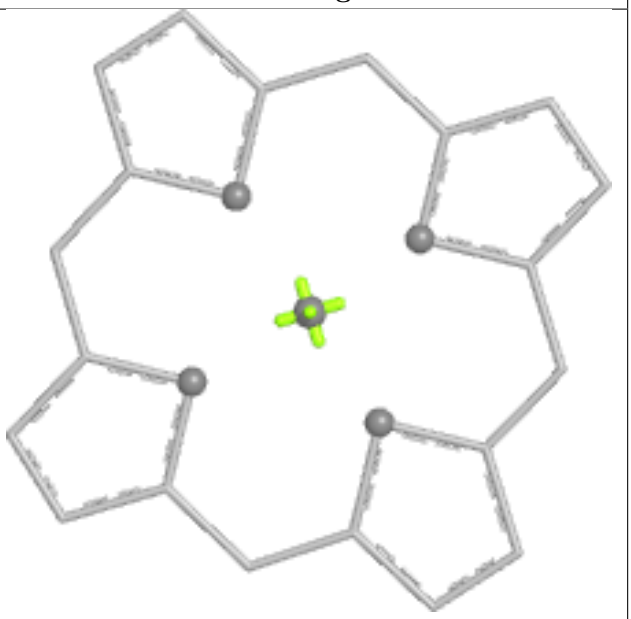
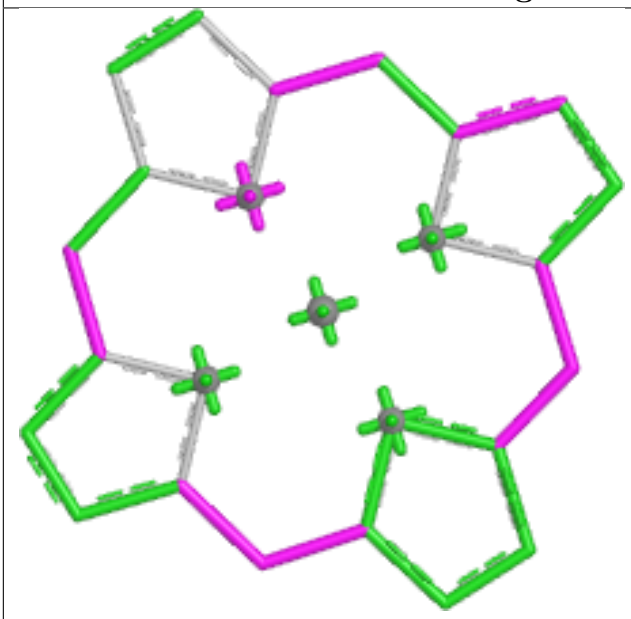


Rings

Ligand CLA B 1210



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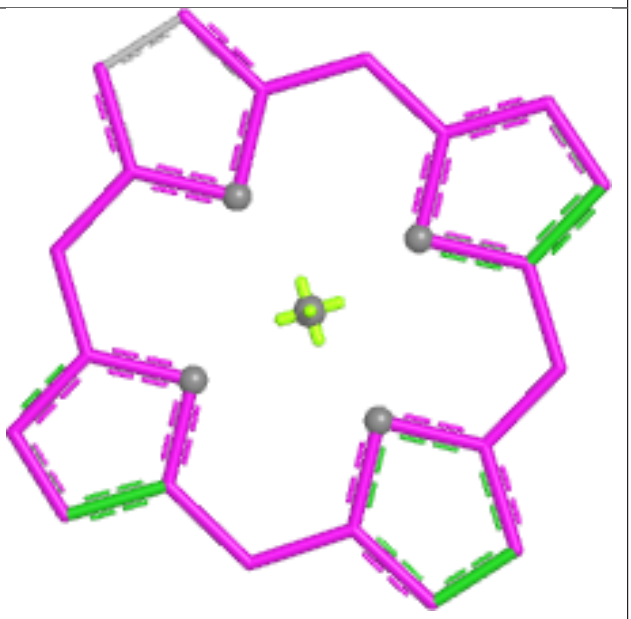

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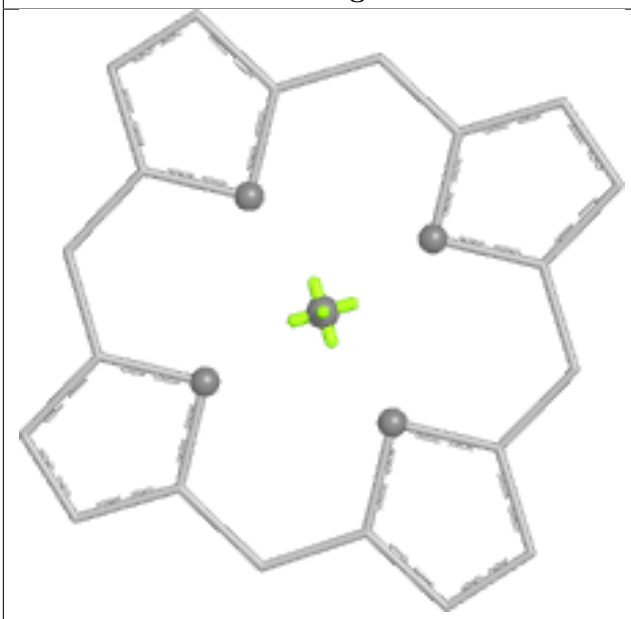

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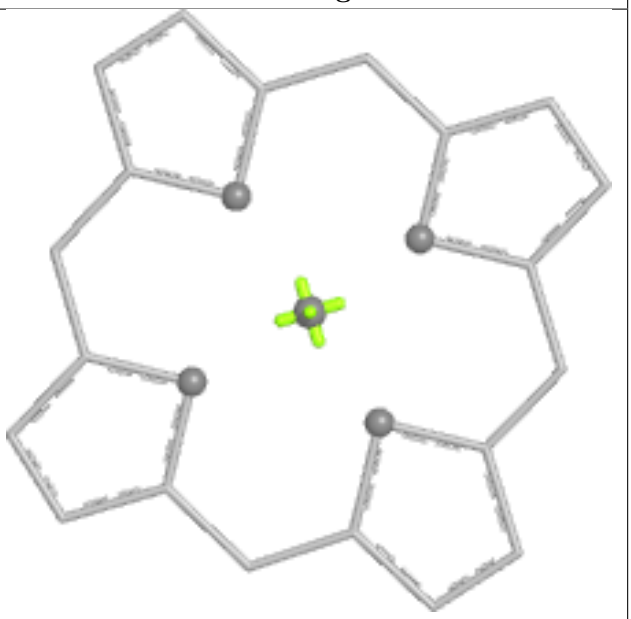
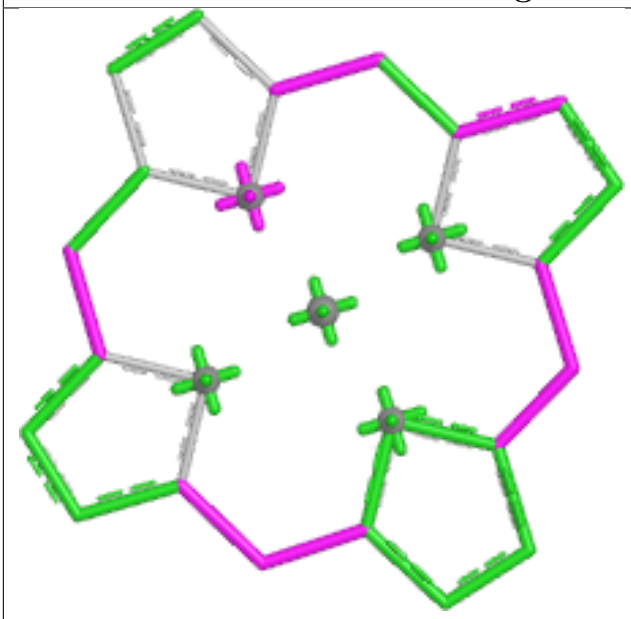


Rings

Ligand CLA A 1111



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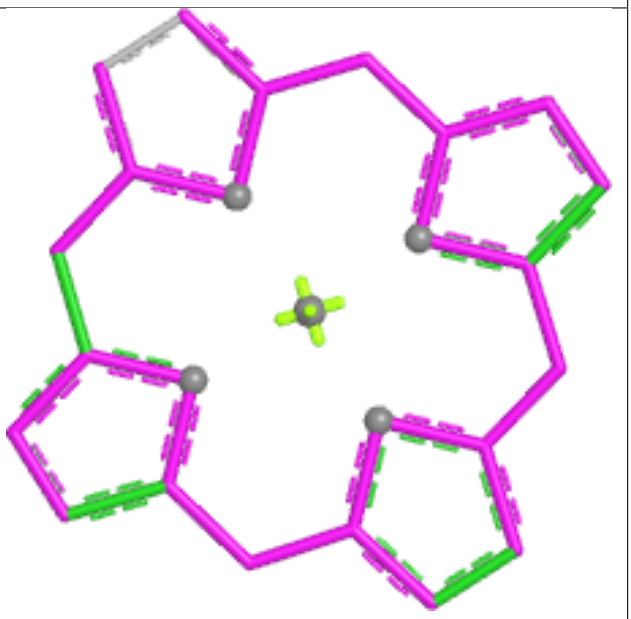

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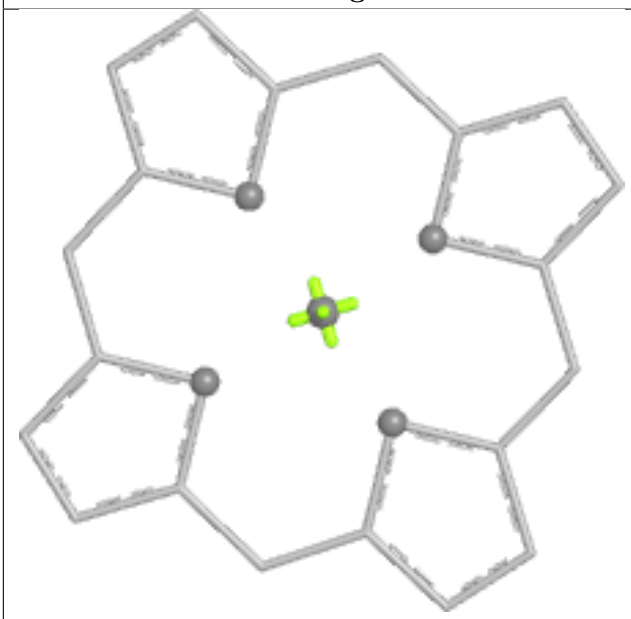

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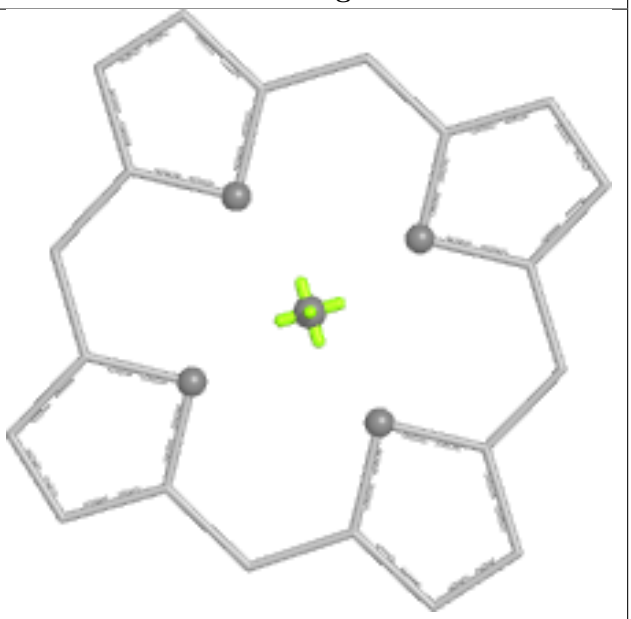
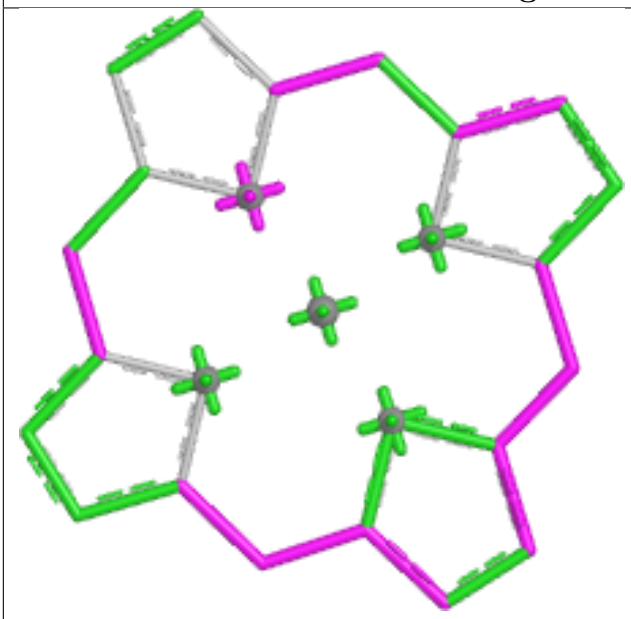


Rings

Ligand CLA 4 4004



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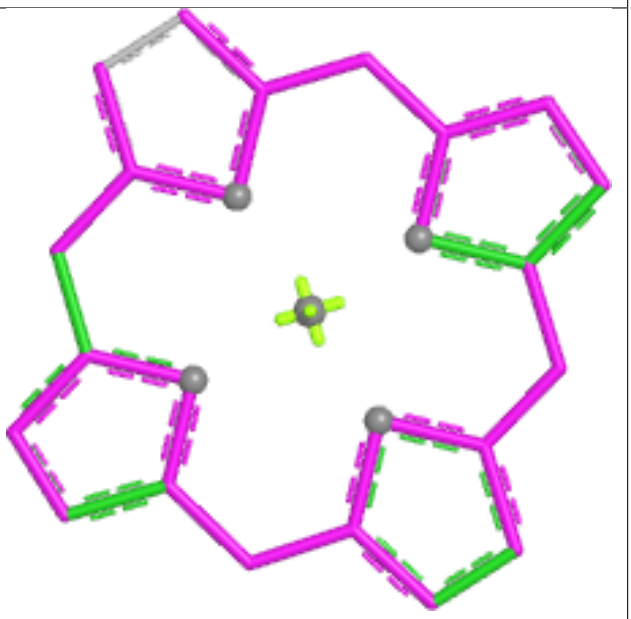

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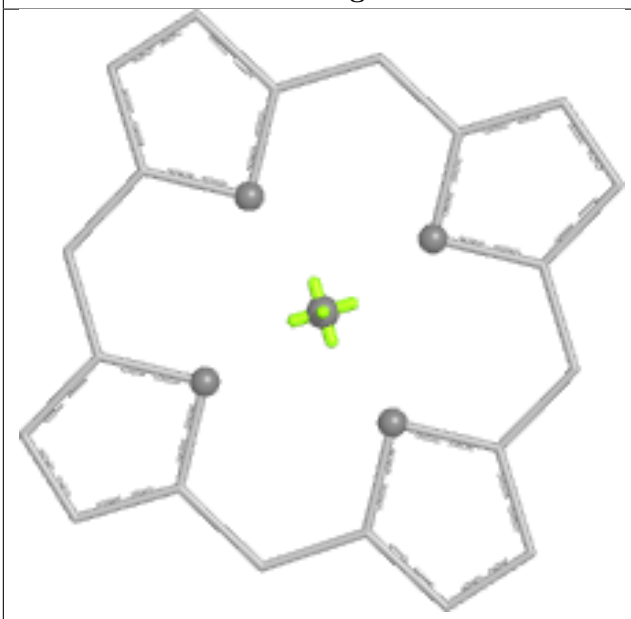

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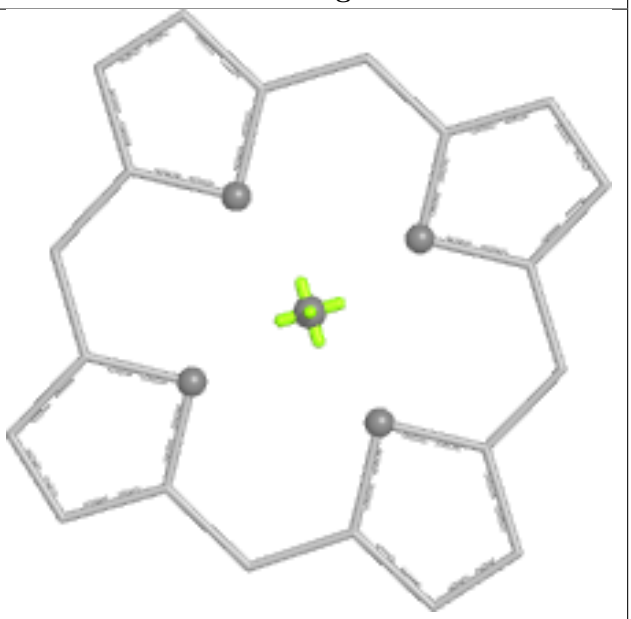
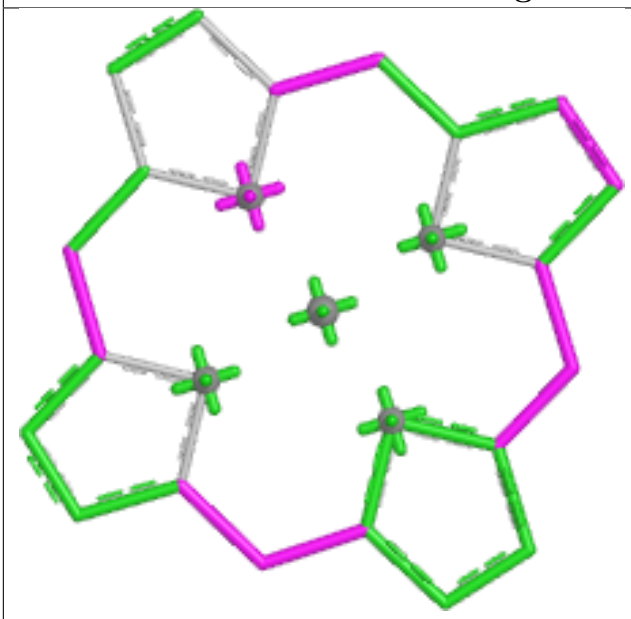


Rings

Ligand CLA A 1134



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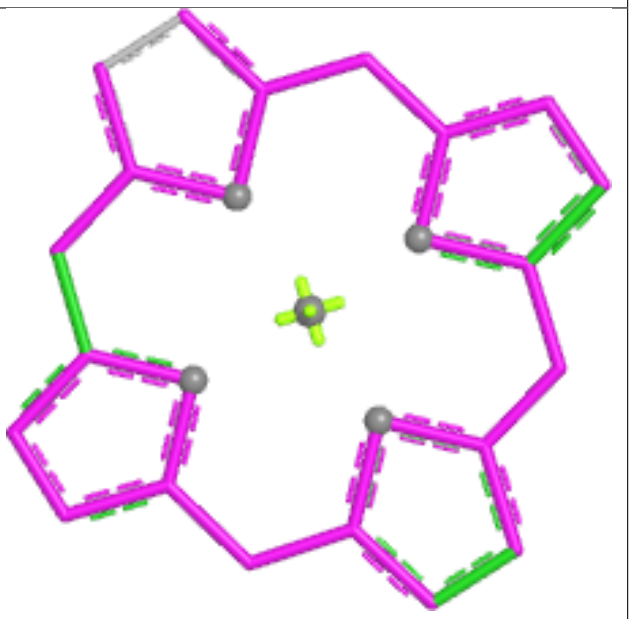
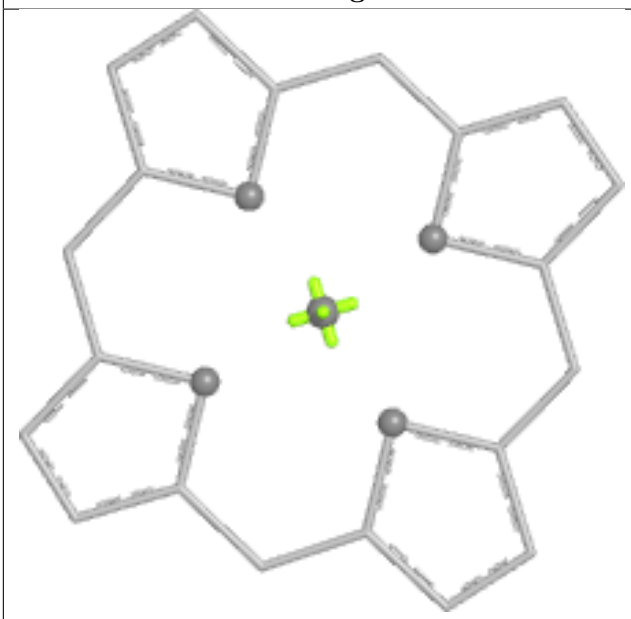


Bond angles



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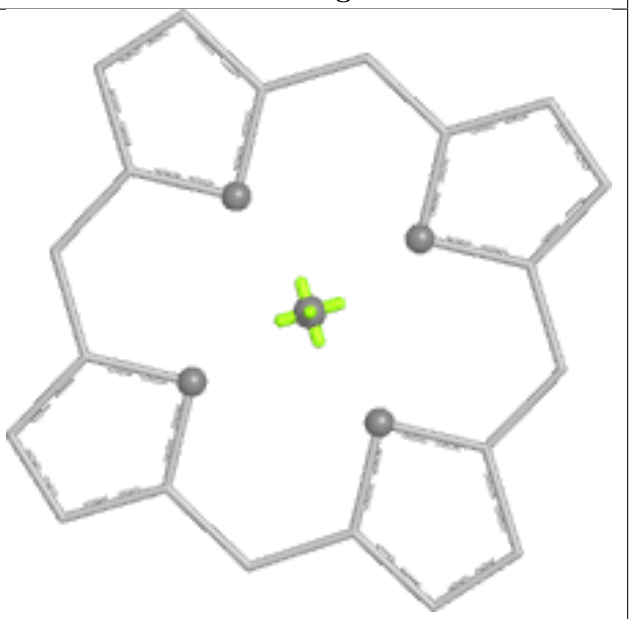
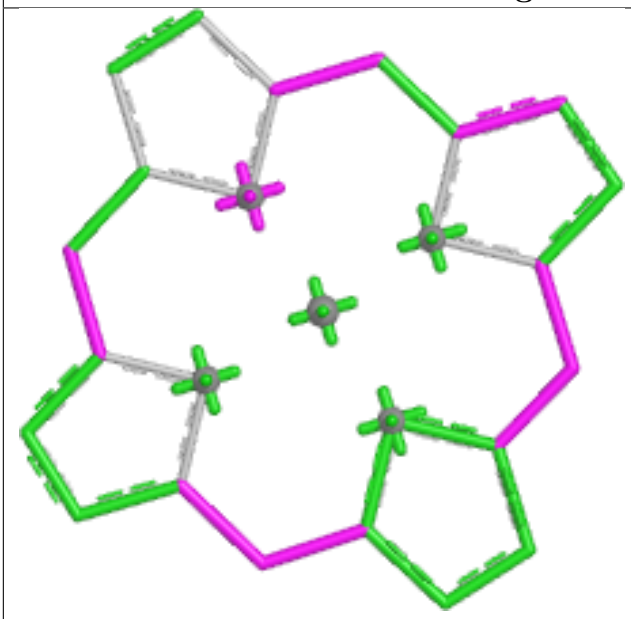


Rings

Ligand CLA B 1241



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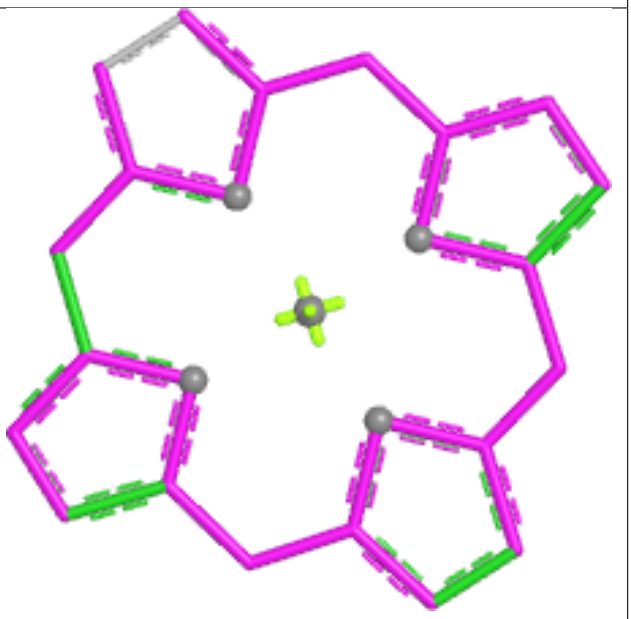
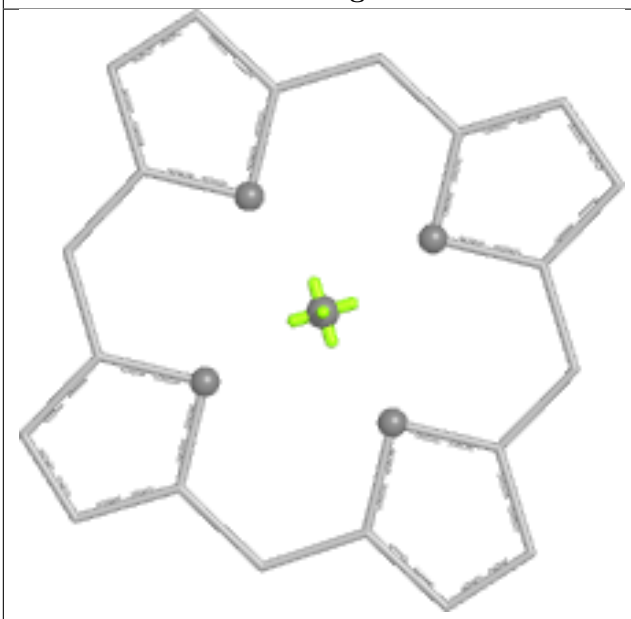
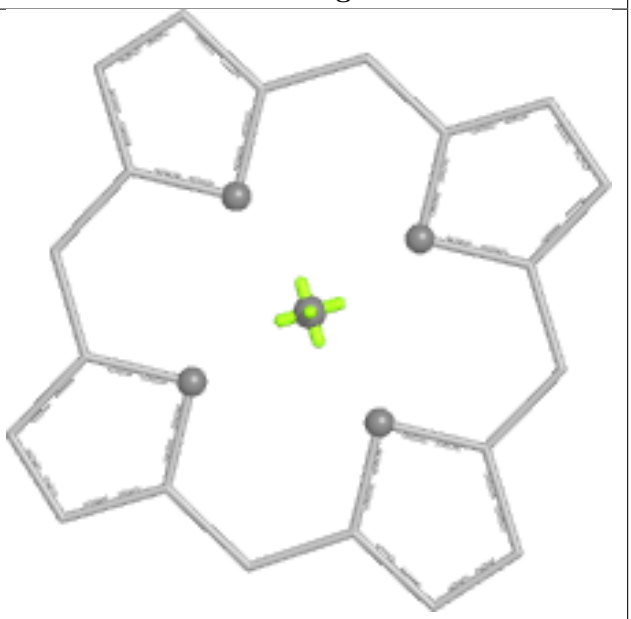


Bond angles

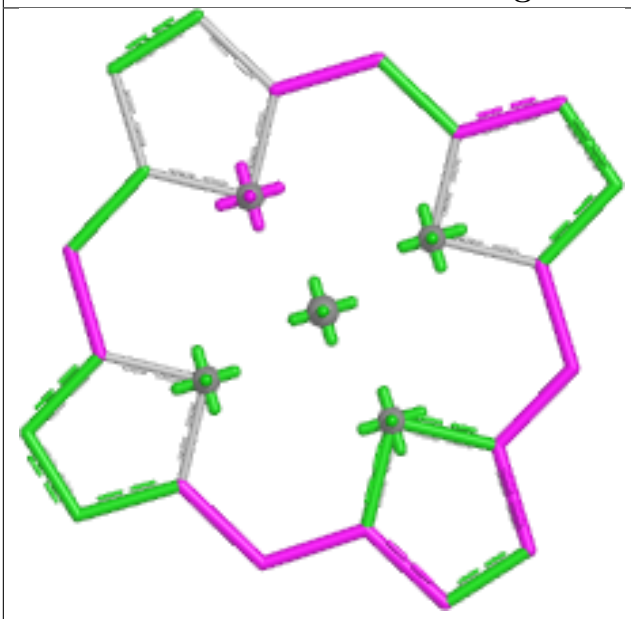


Torsions



Rings

Ligand CLA G 1248



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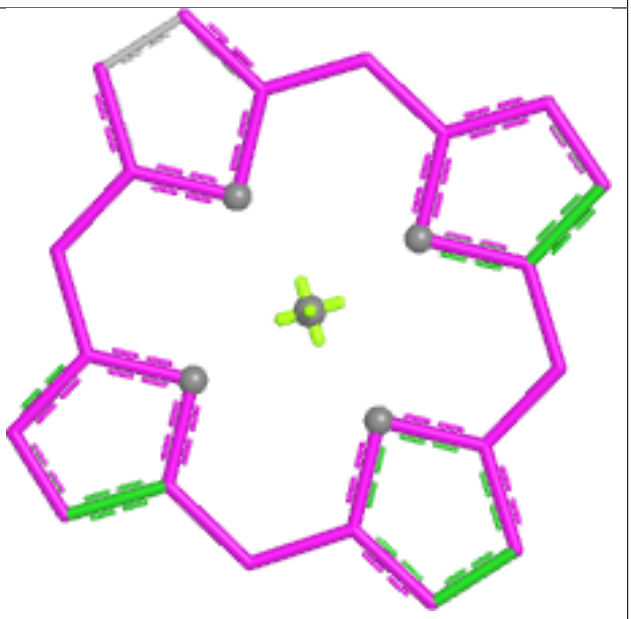
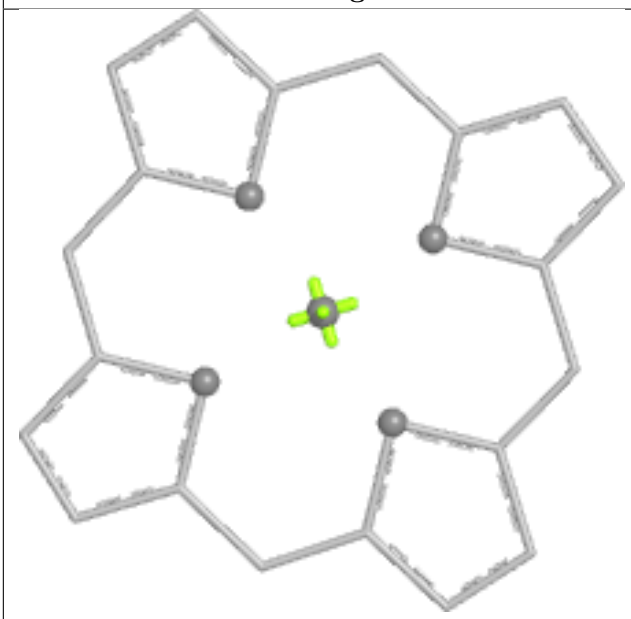


Bond angles



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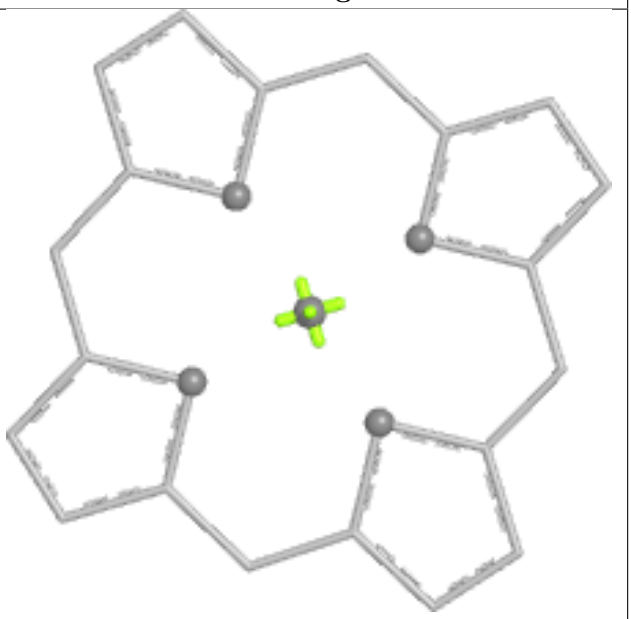
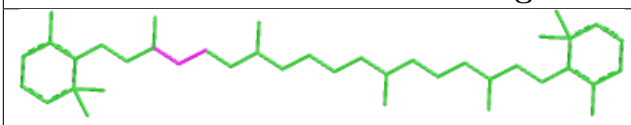


Rings

Ligand BCR F 6016



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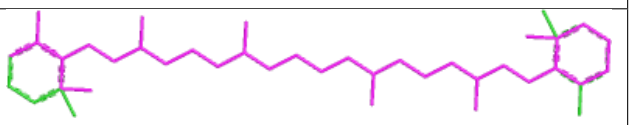

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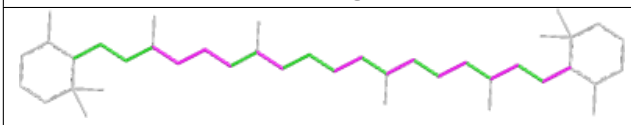

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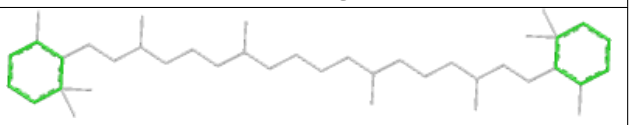
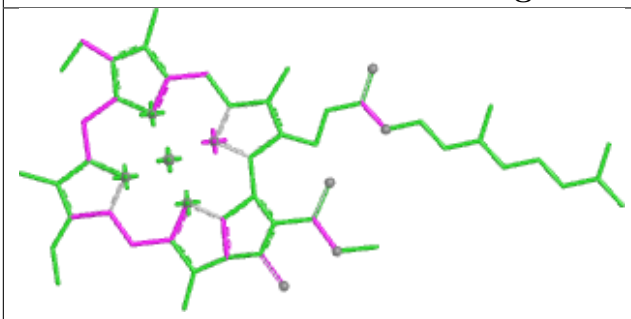
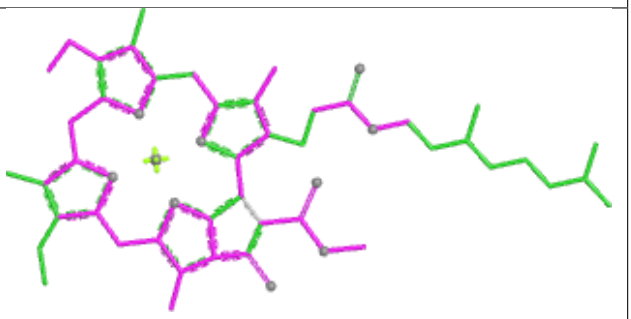
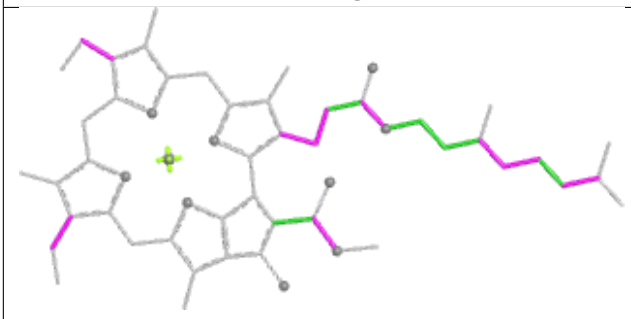
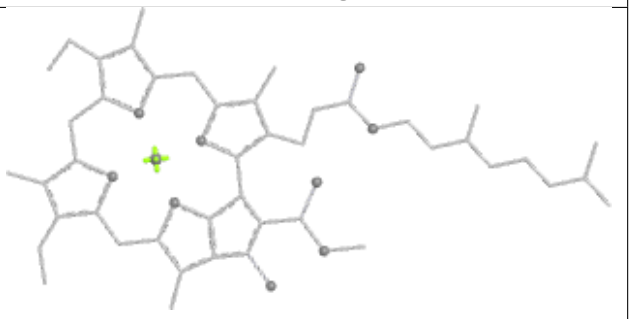
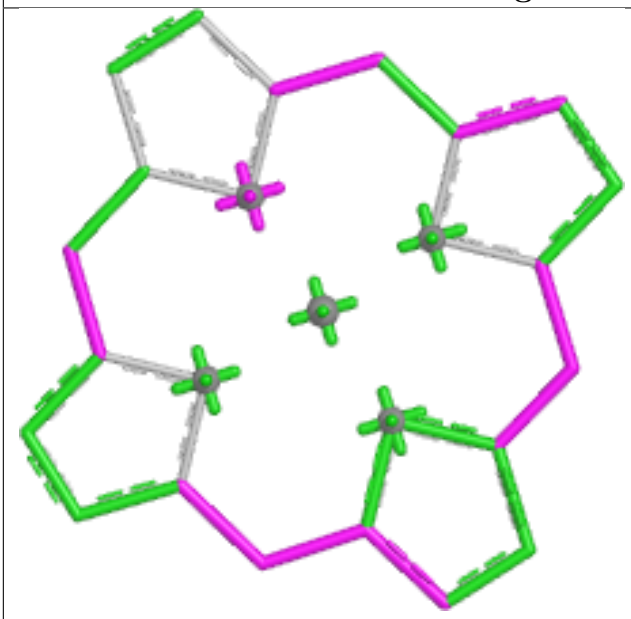


Rings

Ligand CLA A 1119	
 Bond lengths	 Bond angles
 Torsions	 Rings

Ligand CLA A 1118



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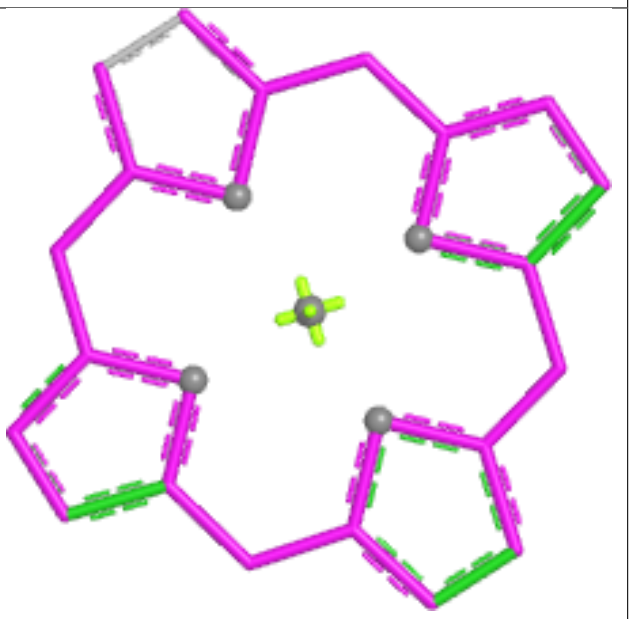

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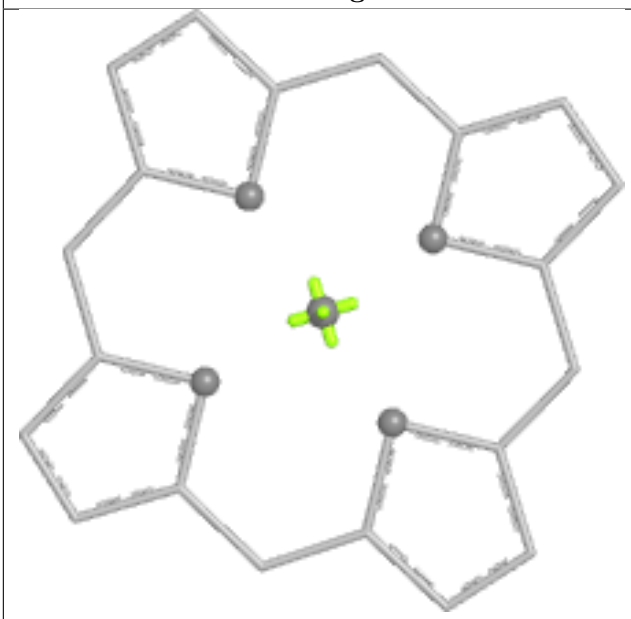

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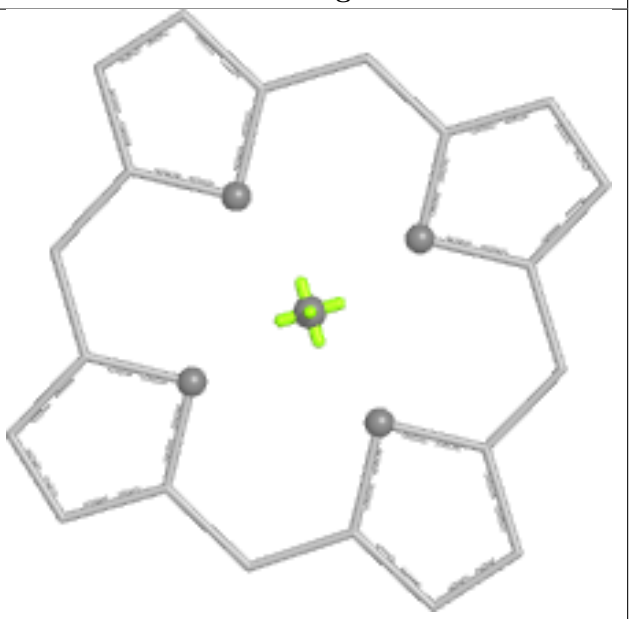
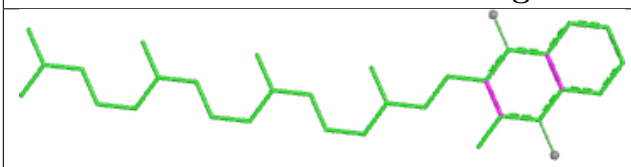


Rings

Ligand PQN A 5001



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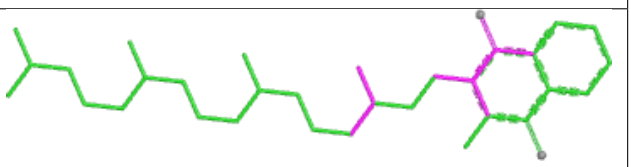

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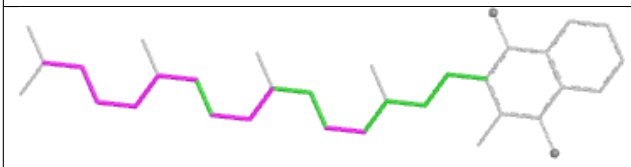

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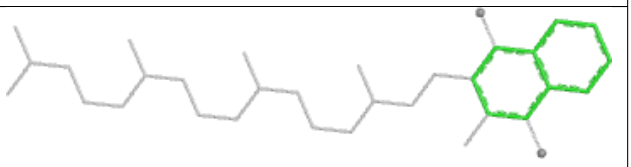
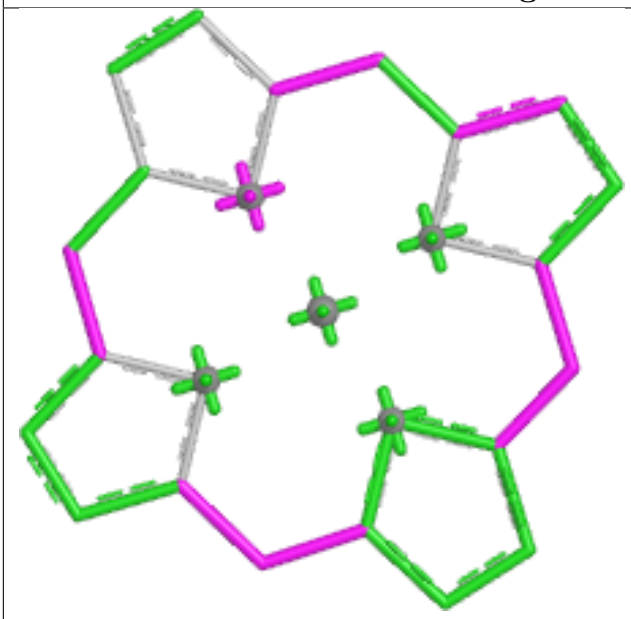


Rings

Ligand CLA 2 2010



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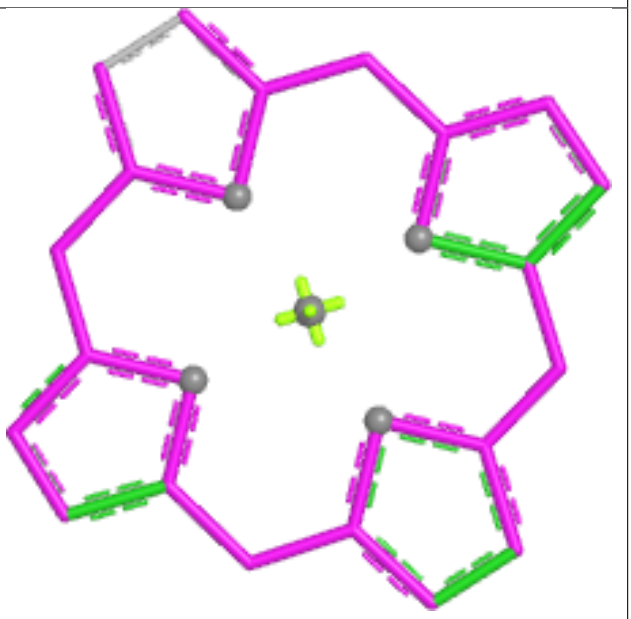

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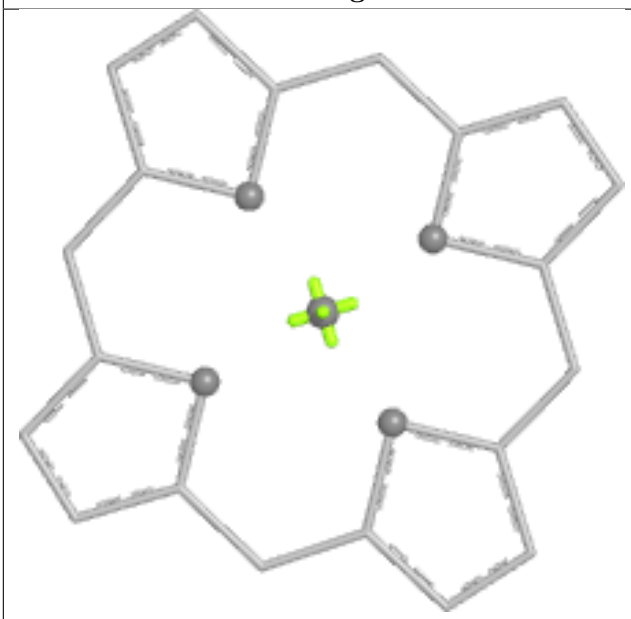

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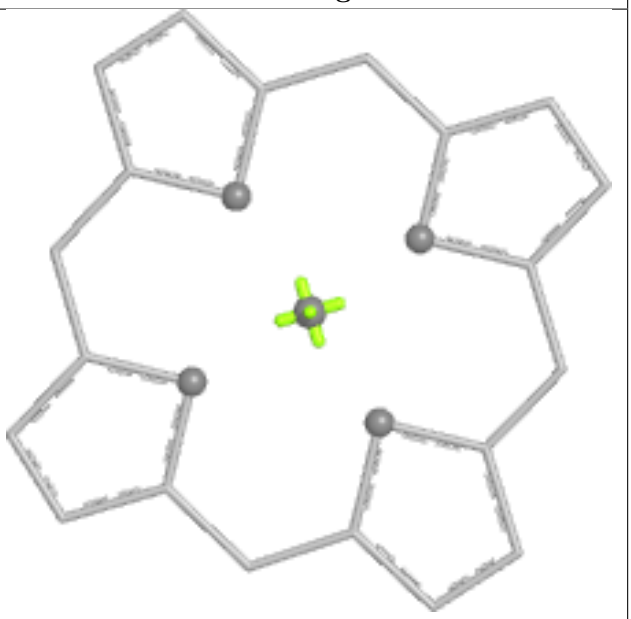
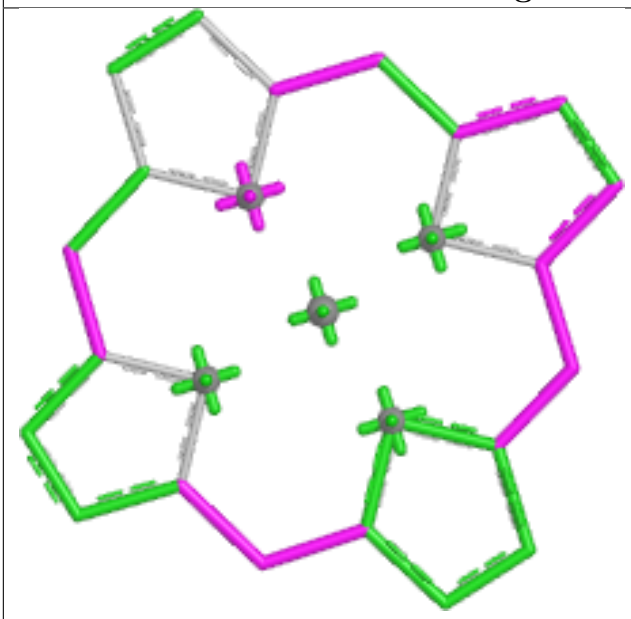


Rings

Ligand CLA A 1133



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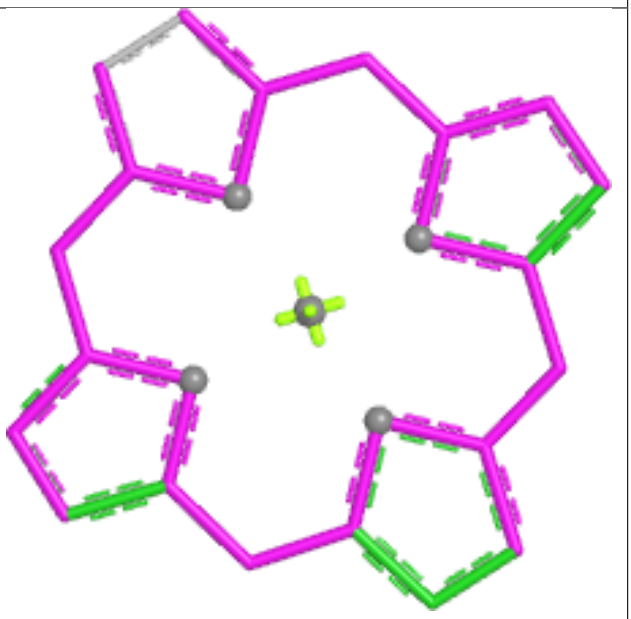

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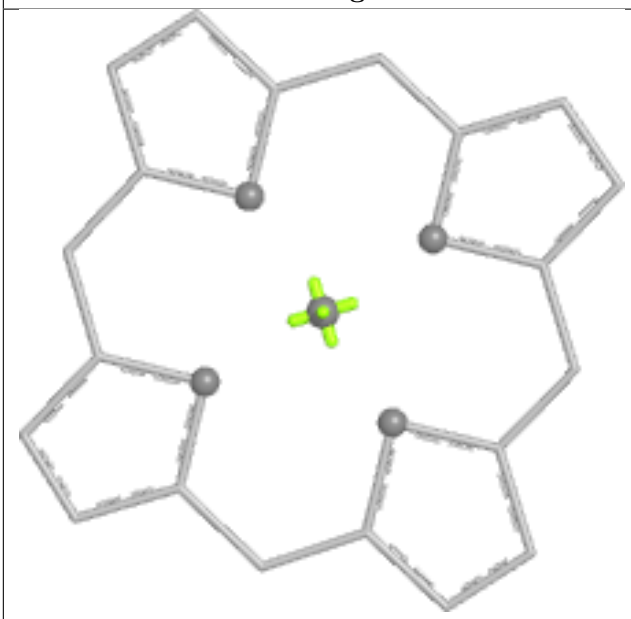

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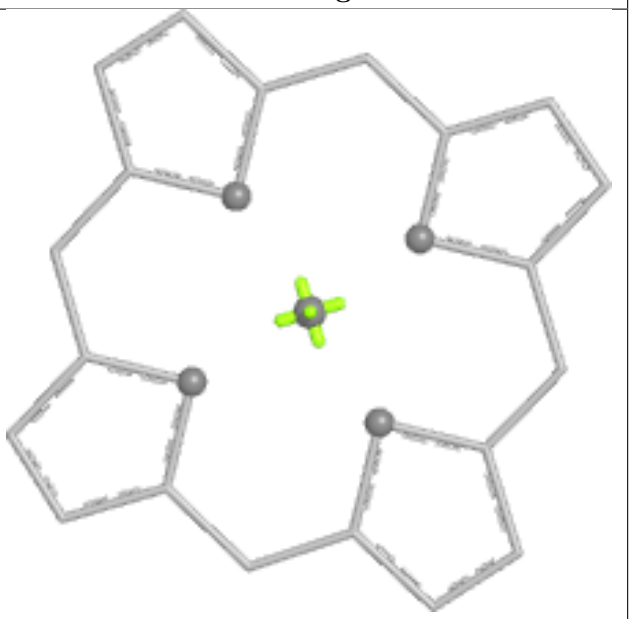
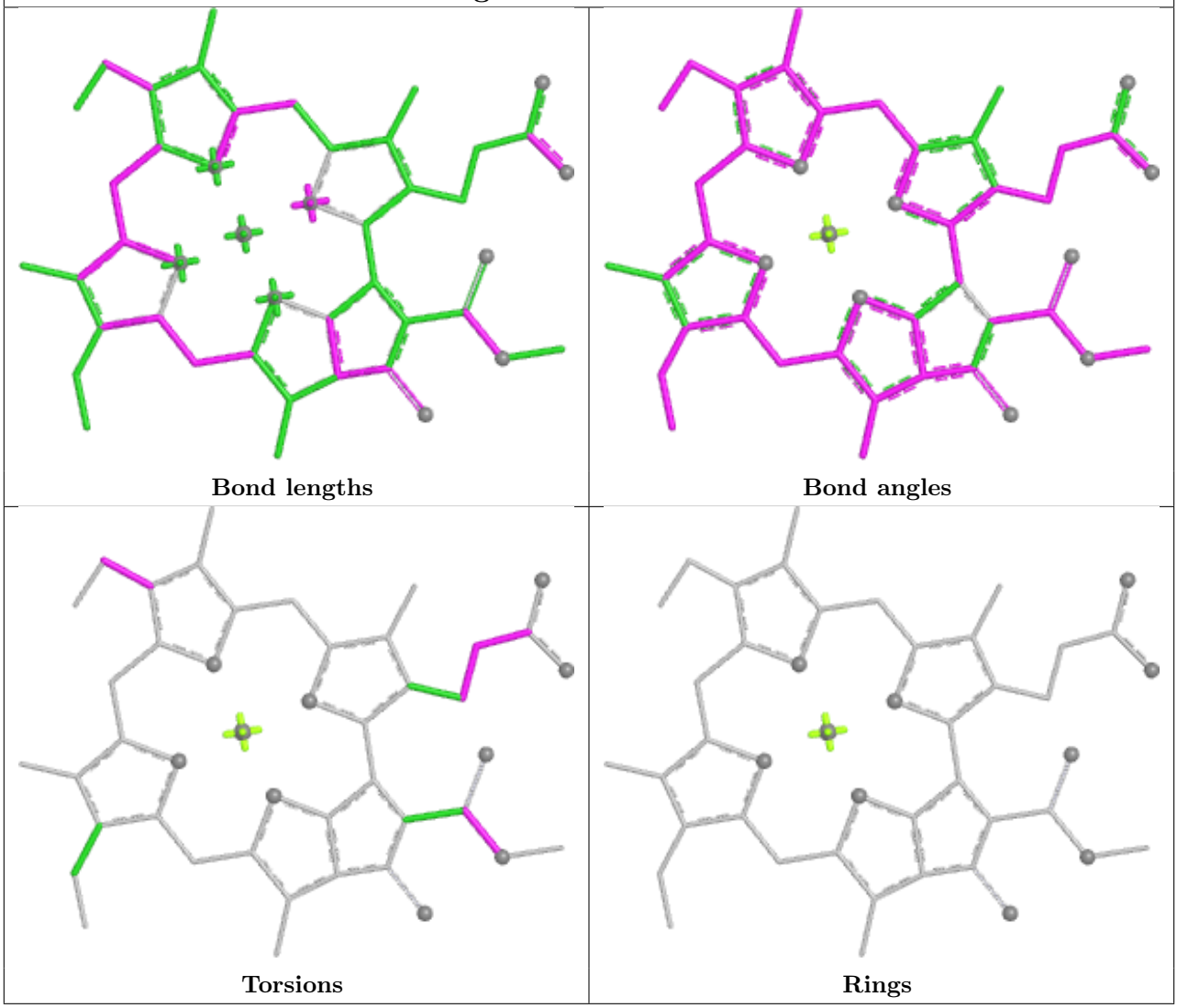


Rings

Ligand CLA B 1225



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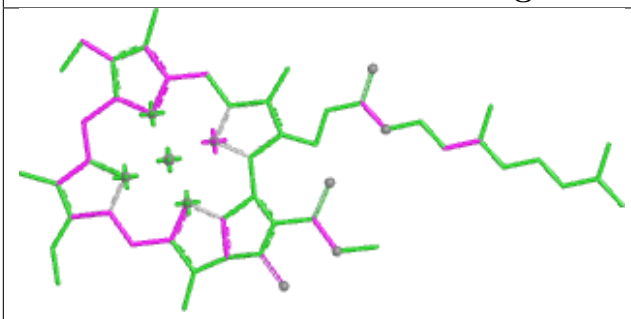

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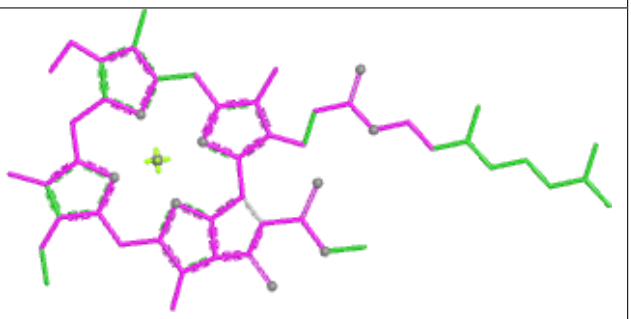
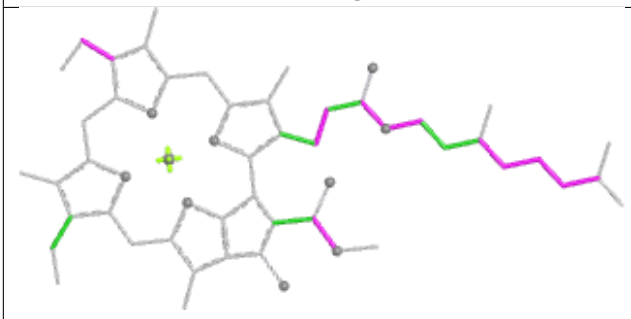


Bond angles



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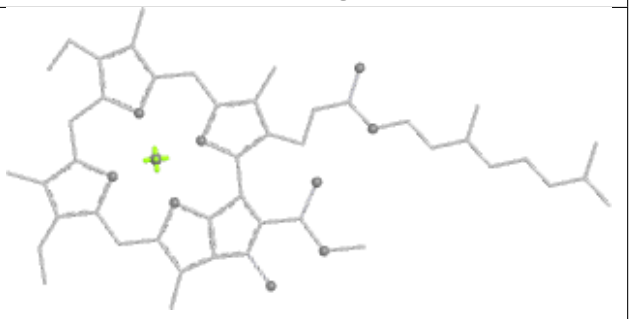
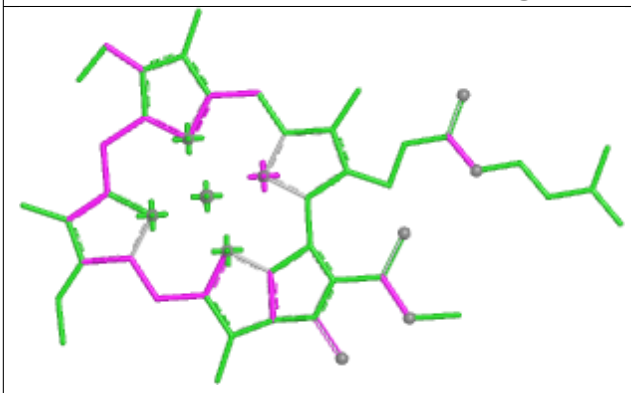


Rings

Ligand CLA B 1227



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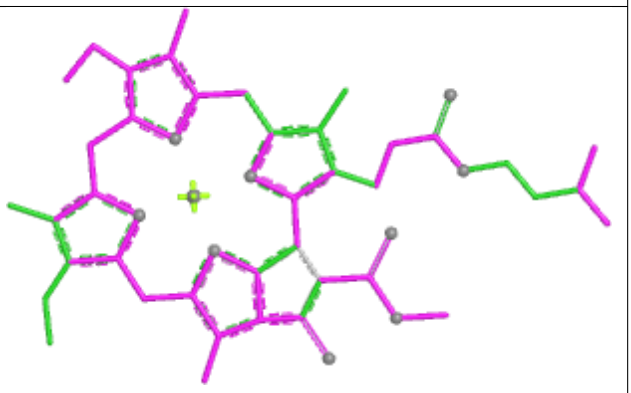
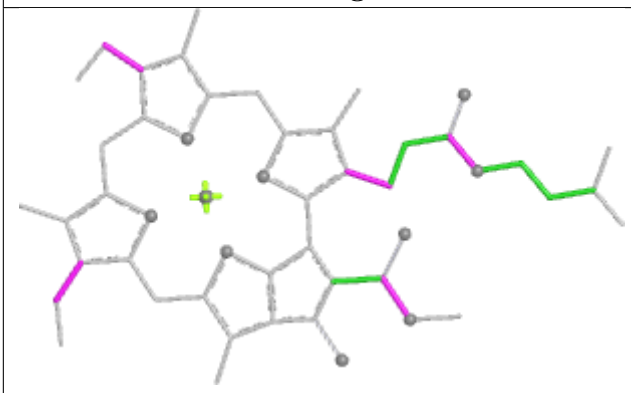


Bond angles



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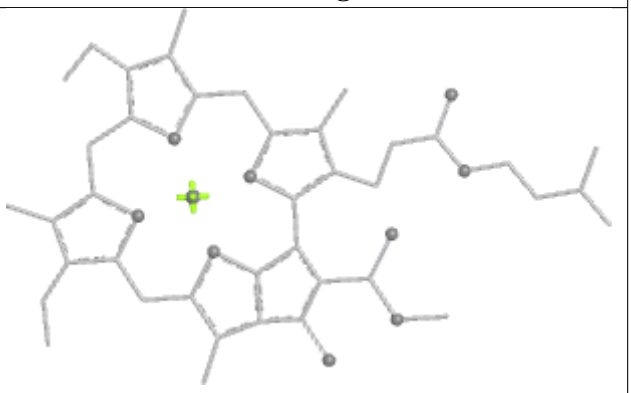

Rings

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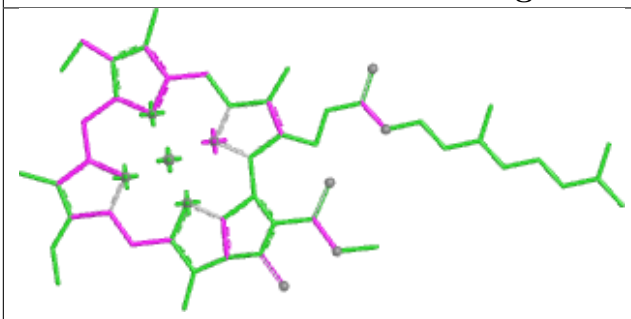
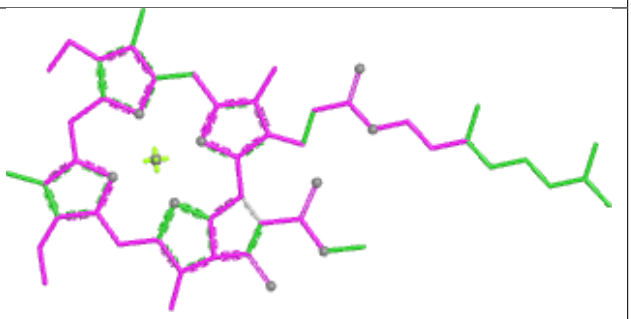
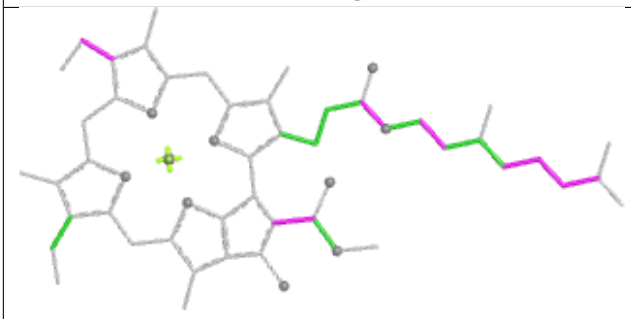
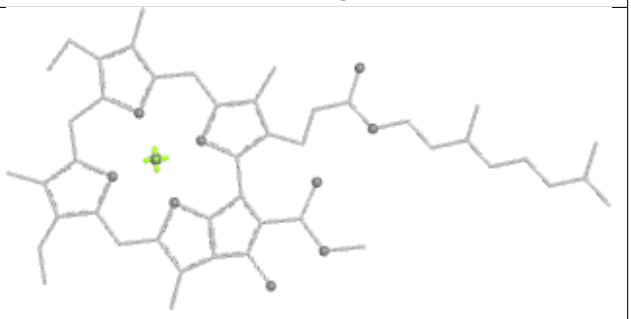
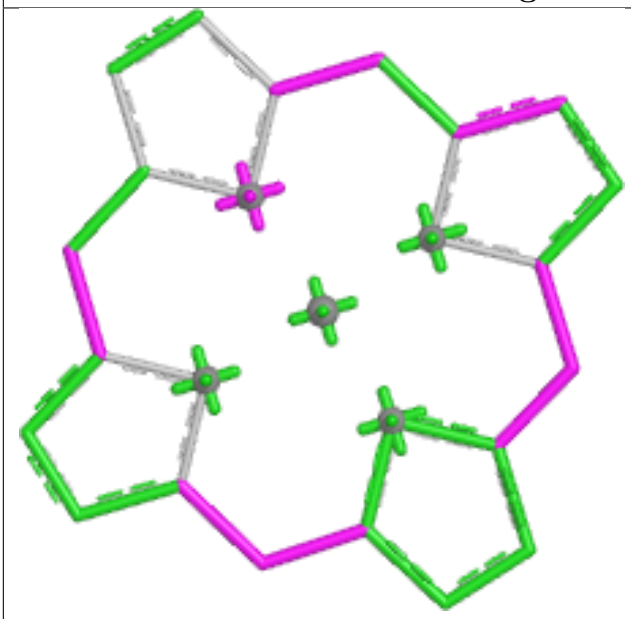
 Bond lengths	 Bond angles
 Torsions	 Rings

Ligand CLA 1 1007



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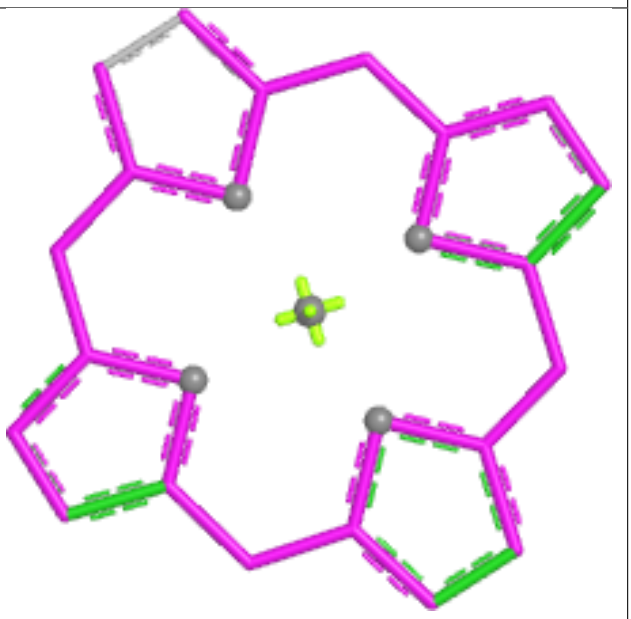
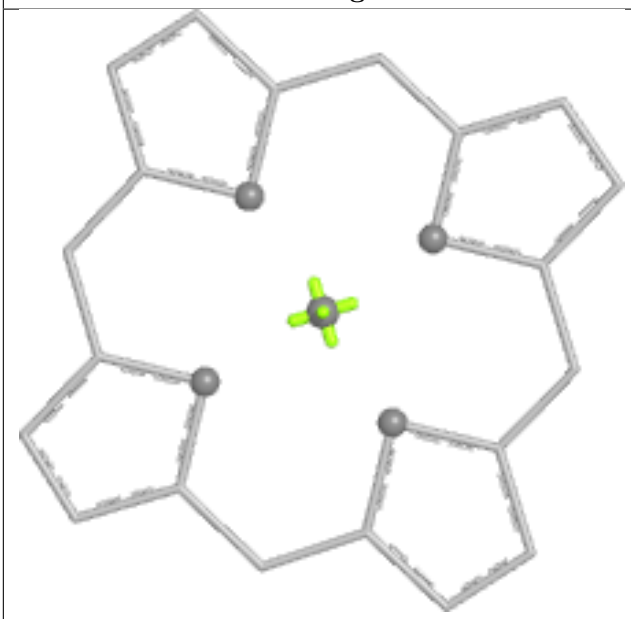


Bond angles



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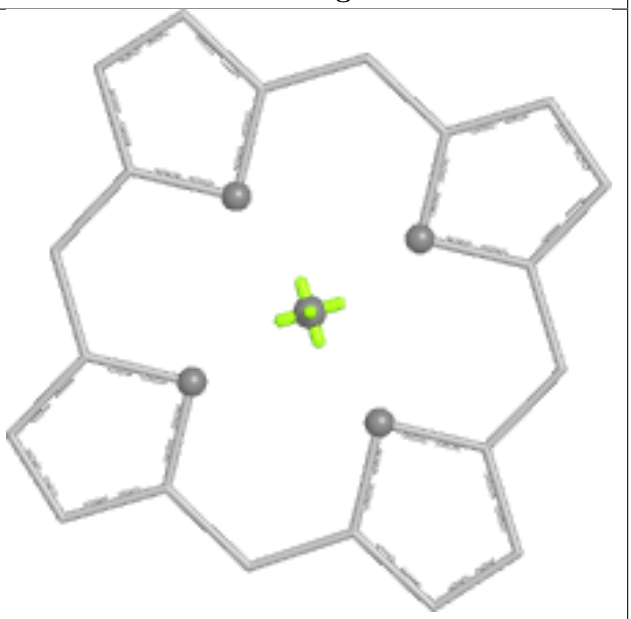
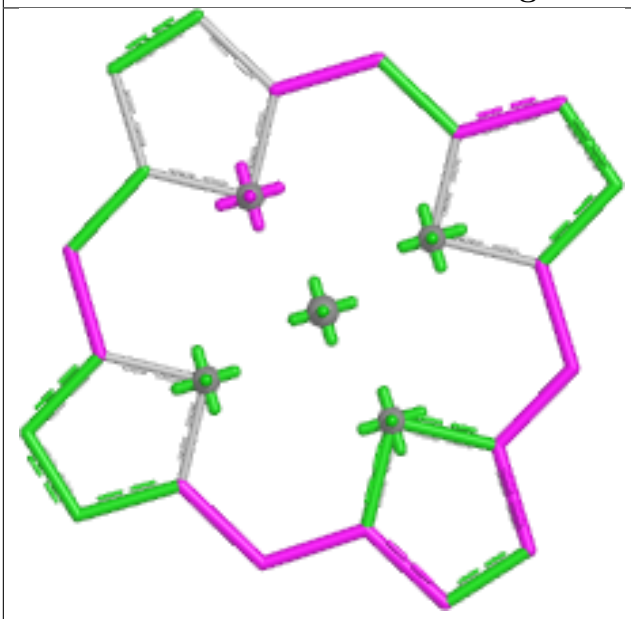


Rings

Ligand CLA 3 3012



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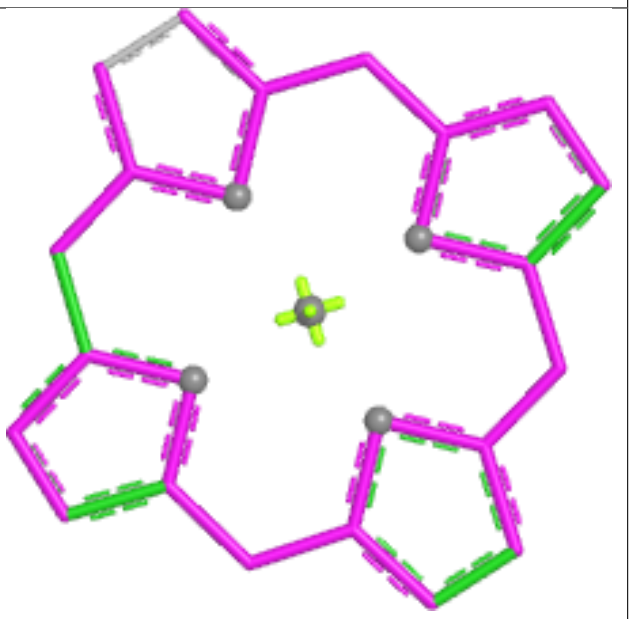

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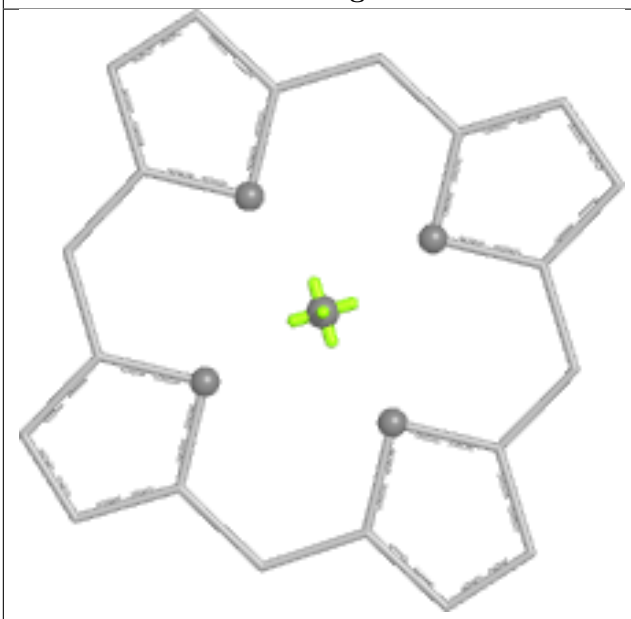

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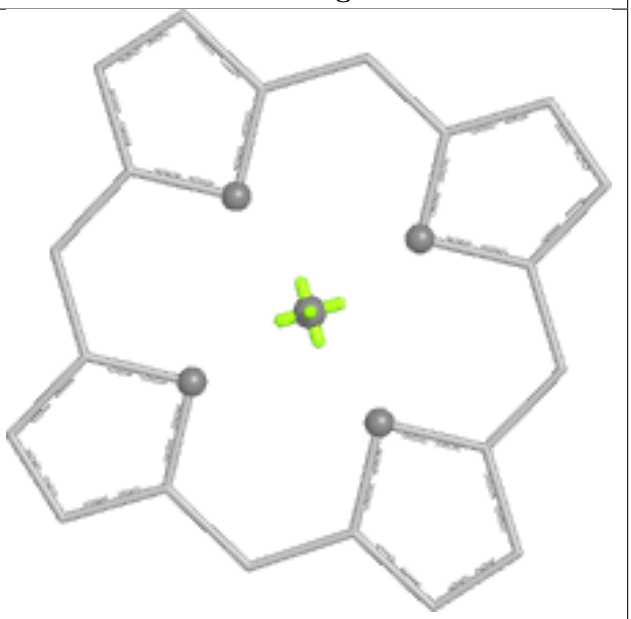
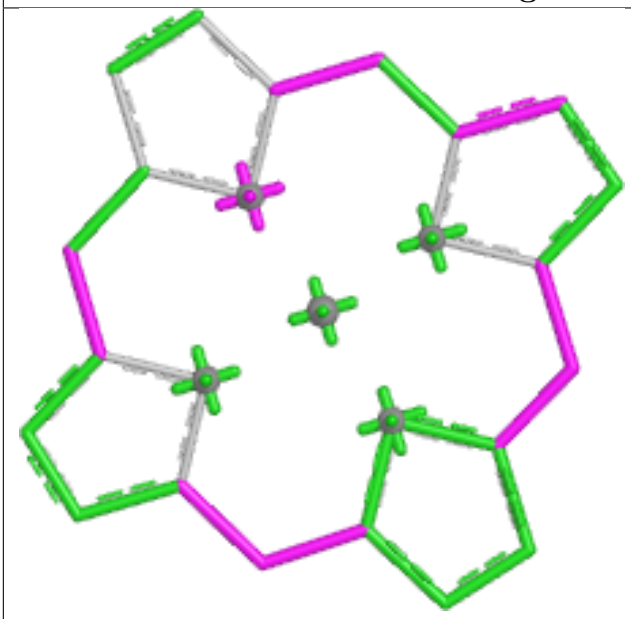


Rings

Ligand CLA 4 4009



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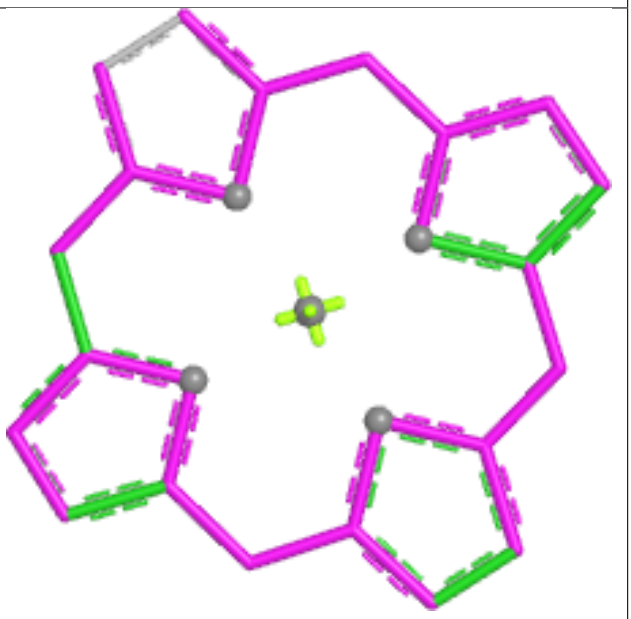
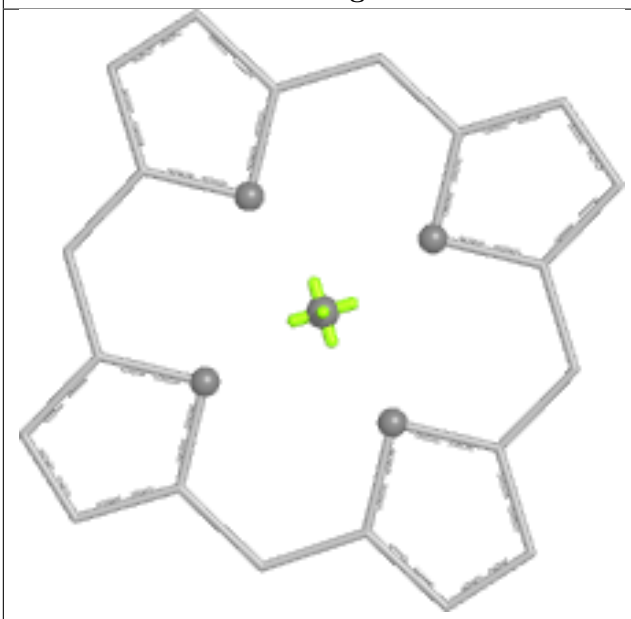


Bond angles



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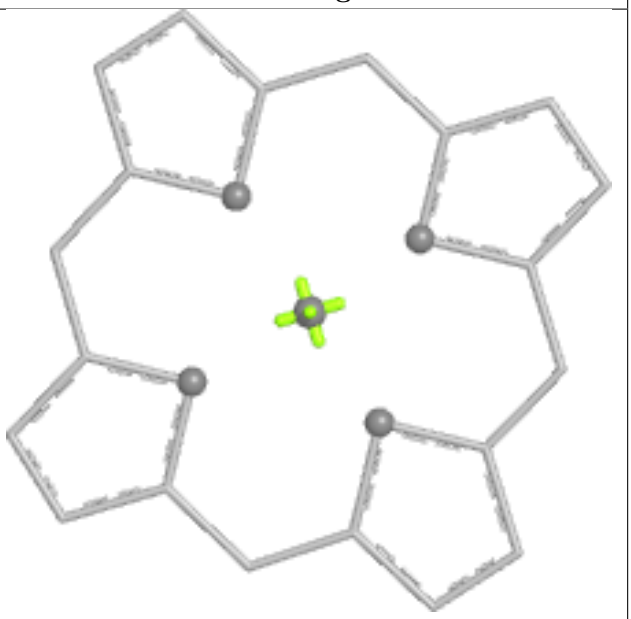
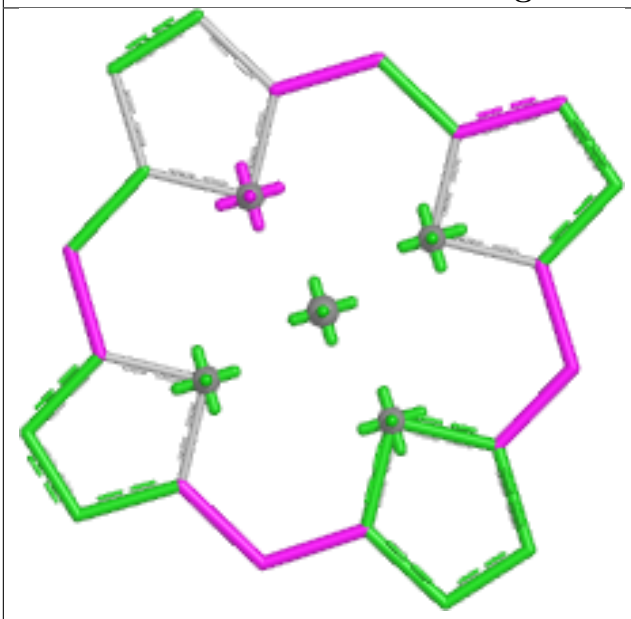


Rings

Ligand CLA A 1147



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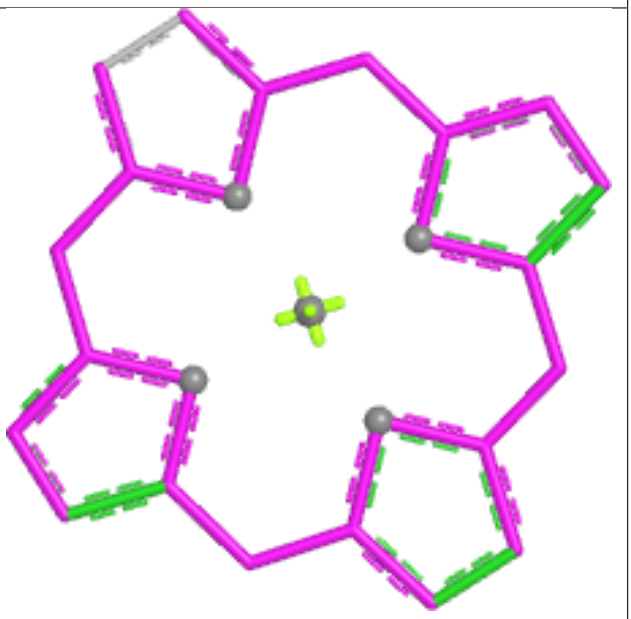
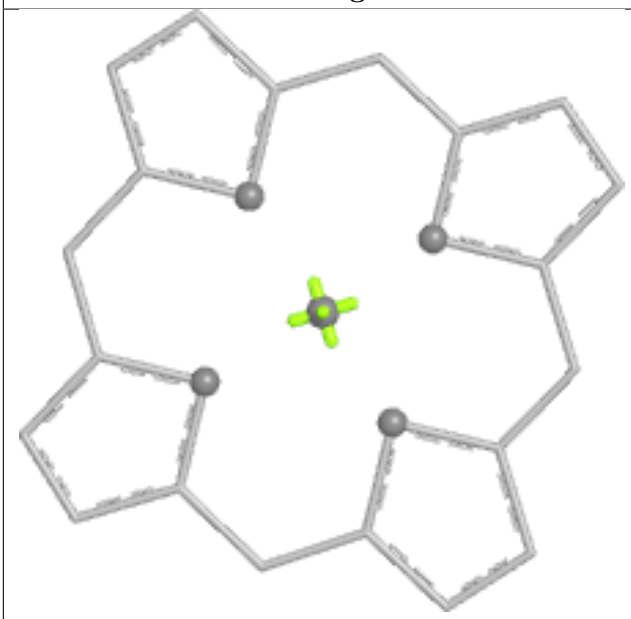
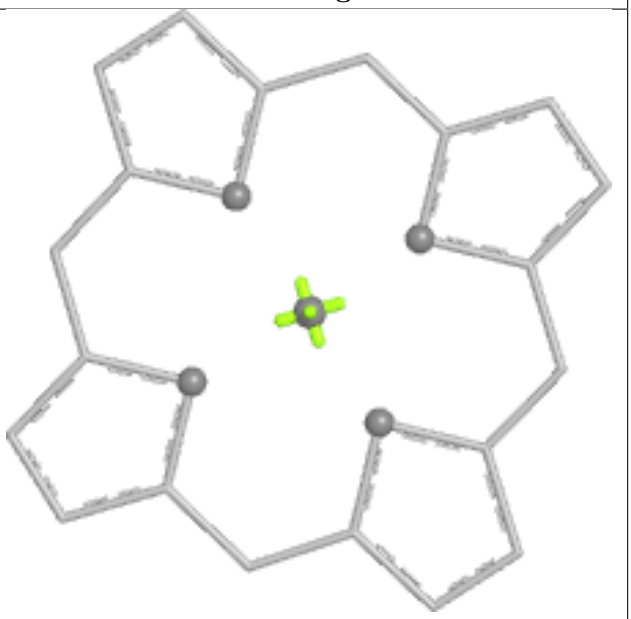


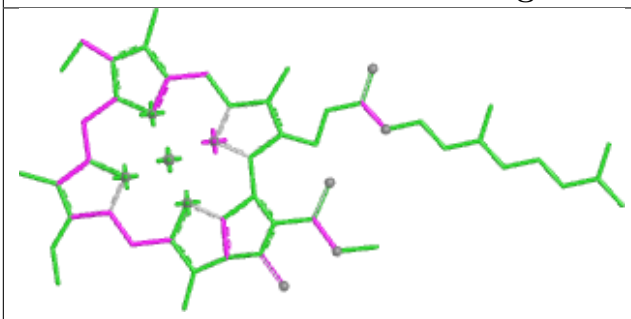
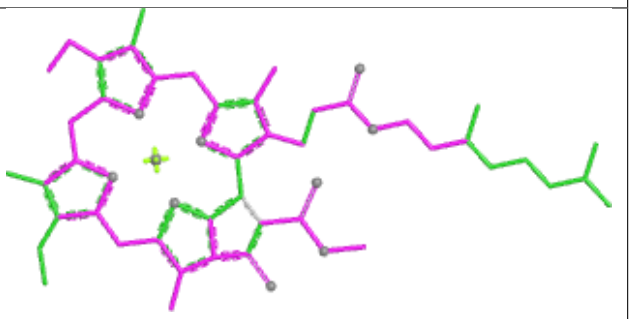
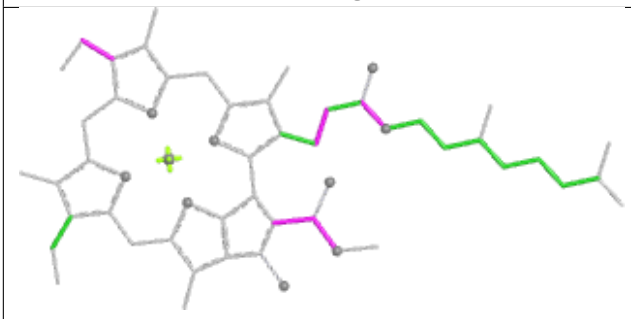
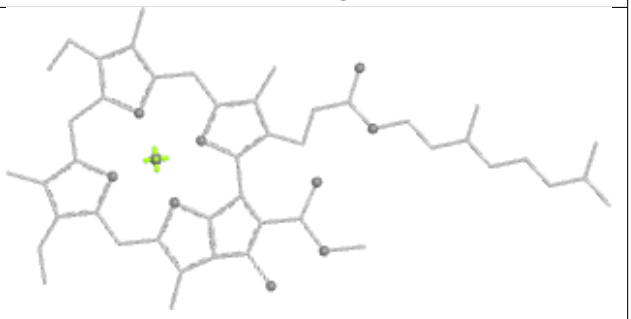
Bond angles



Torsions



Rings

Ligand CLA F 1302	
 Bond lengths	 Bond angles
 Torsions	 Rings

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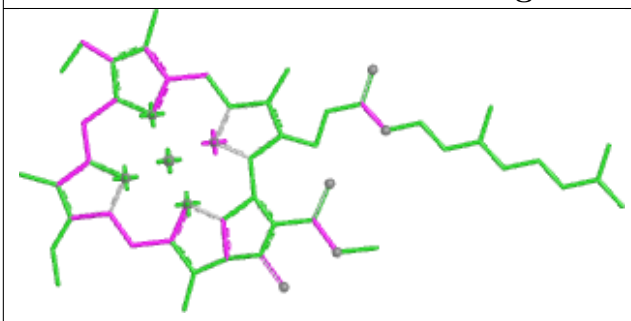
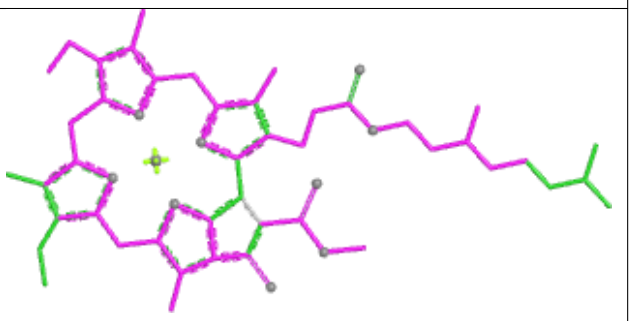
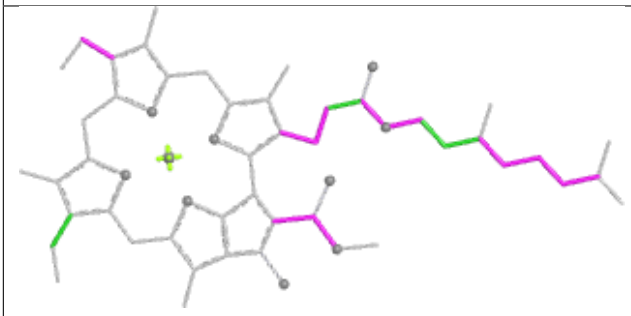
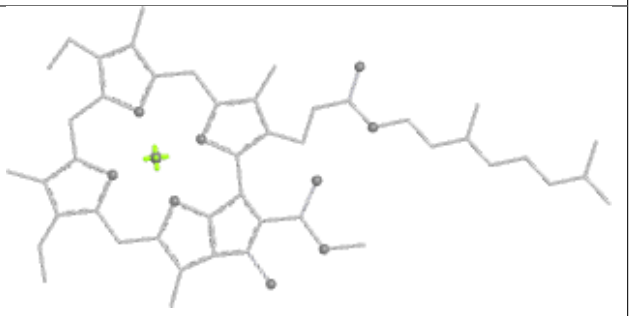
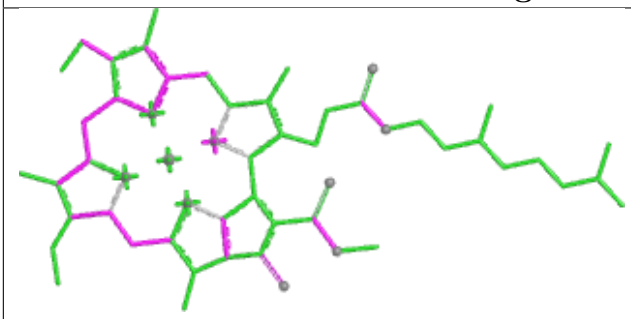
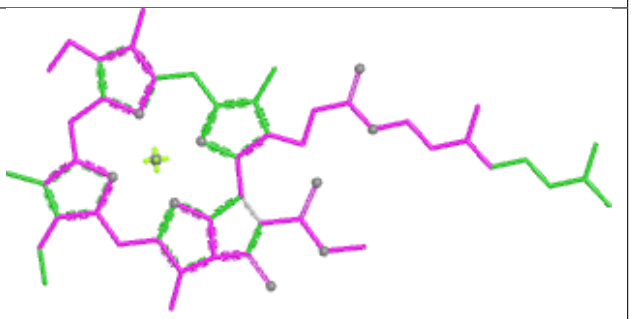
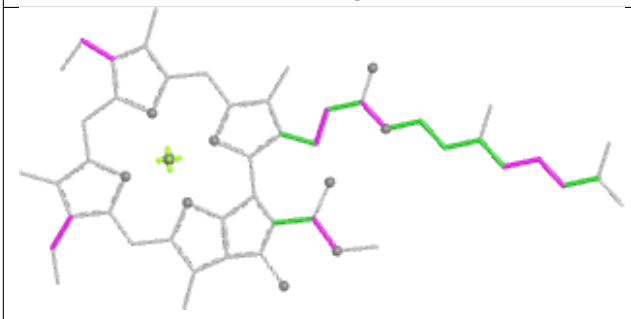
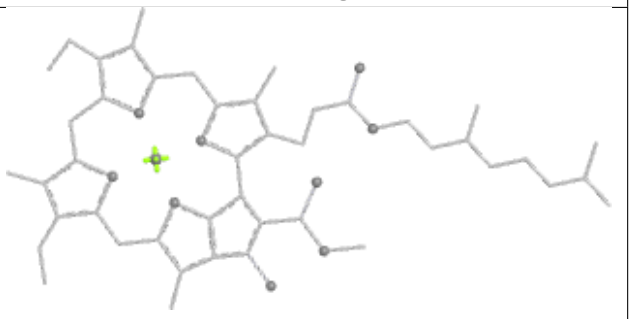
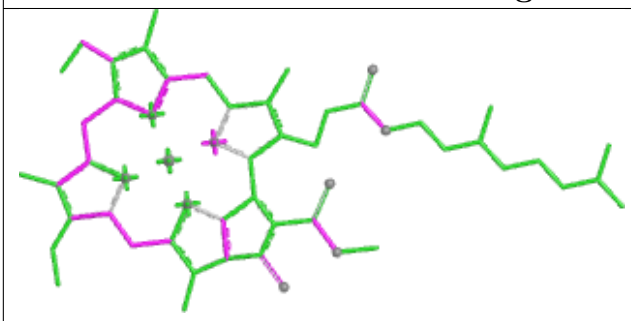
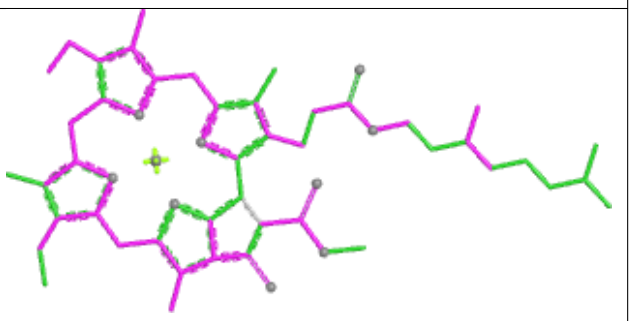
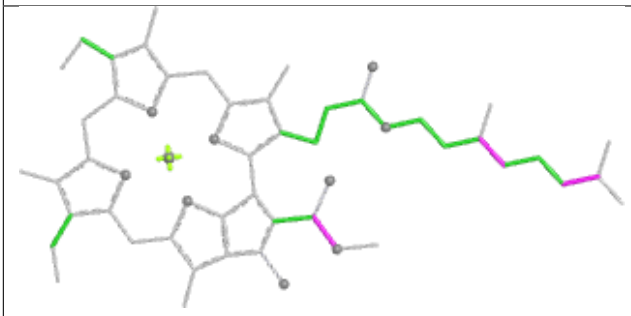
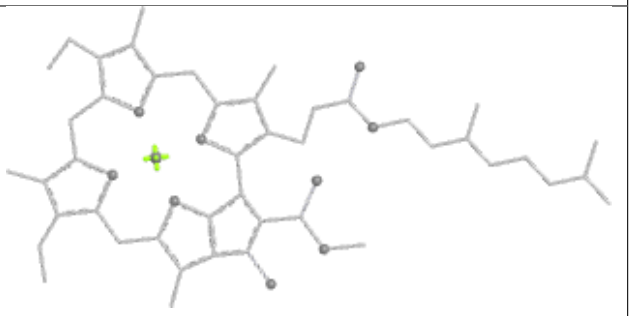
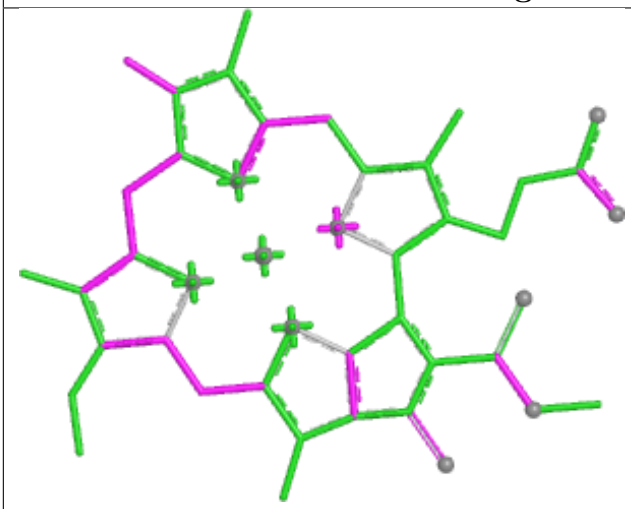
 Bond lengths	 Bond angles
 Torsions	 Rings

Ligand CLA A 1129	
 Bond lengths	 Bond angles
 Torsions	 Rings

Ligand CLA B 1239	
 Bond lengths	 Bond angles
 Torsions	 Rings

Ligand CLA A 1131



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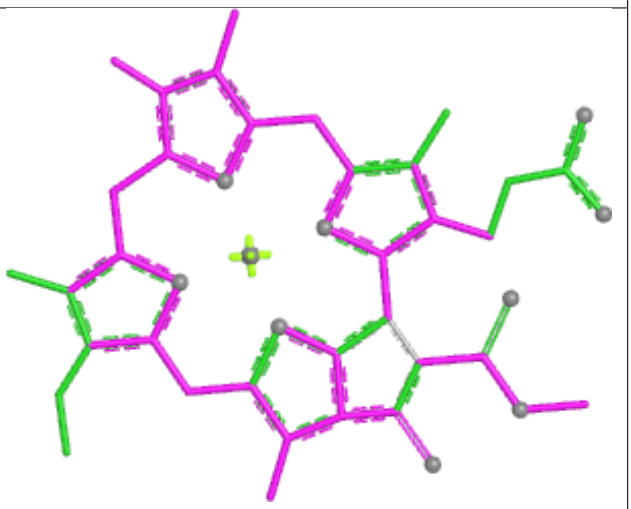

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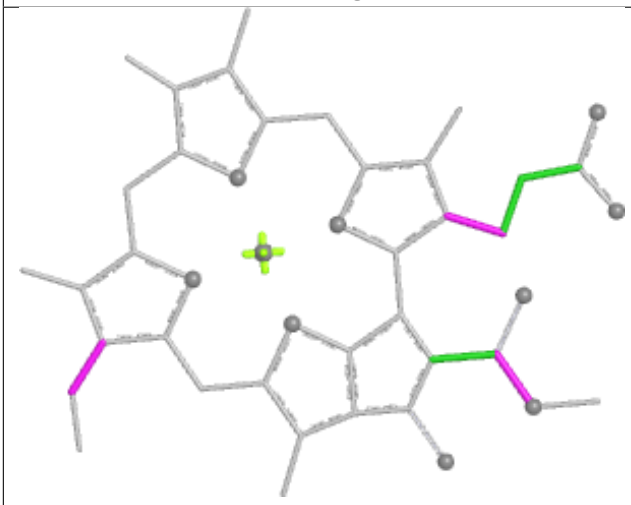

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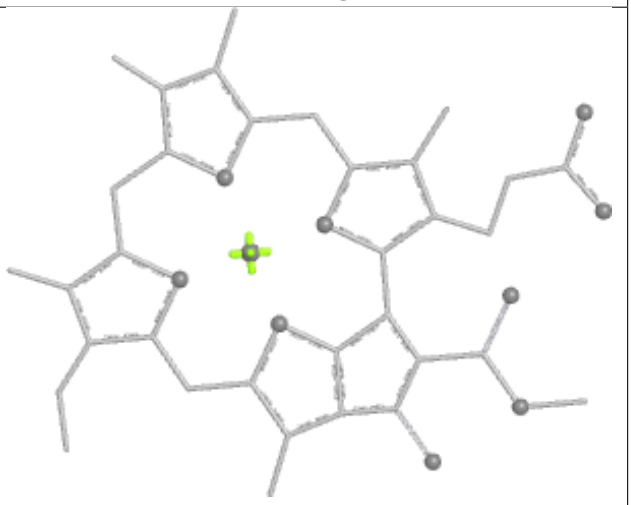
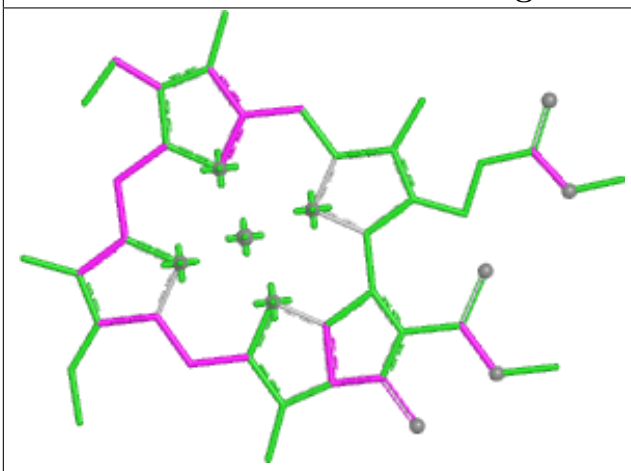


Rings

Ligand CLA B 1236



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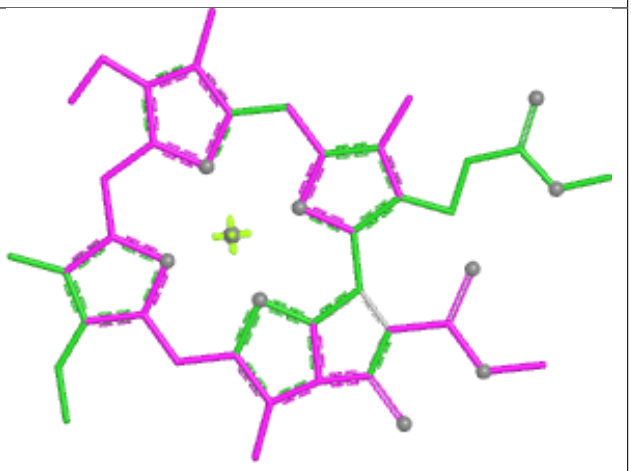

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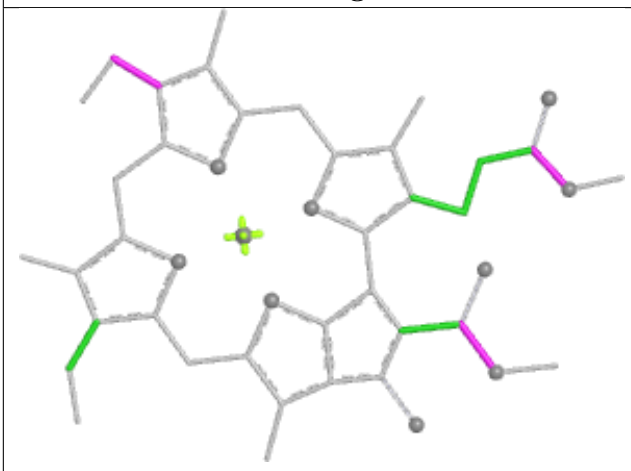

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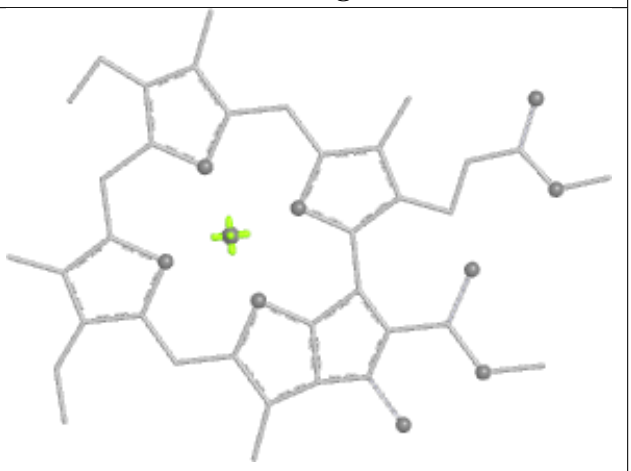
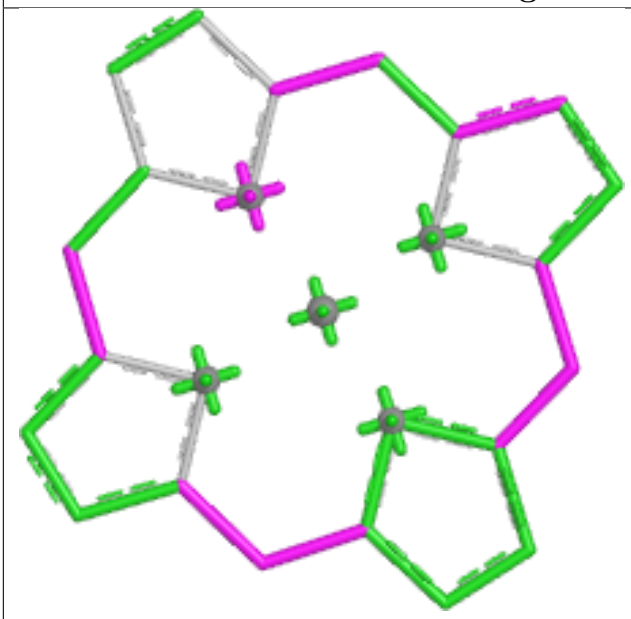


Rings

Ligand CLA 2 2004



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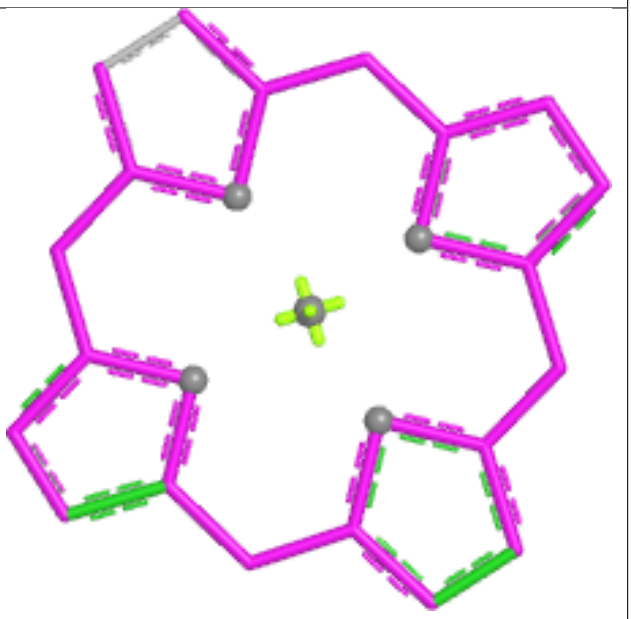
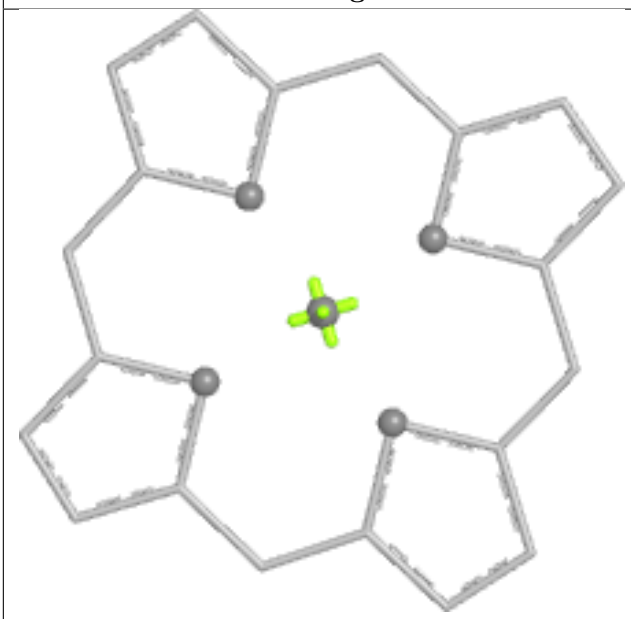


Bond angles



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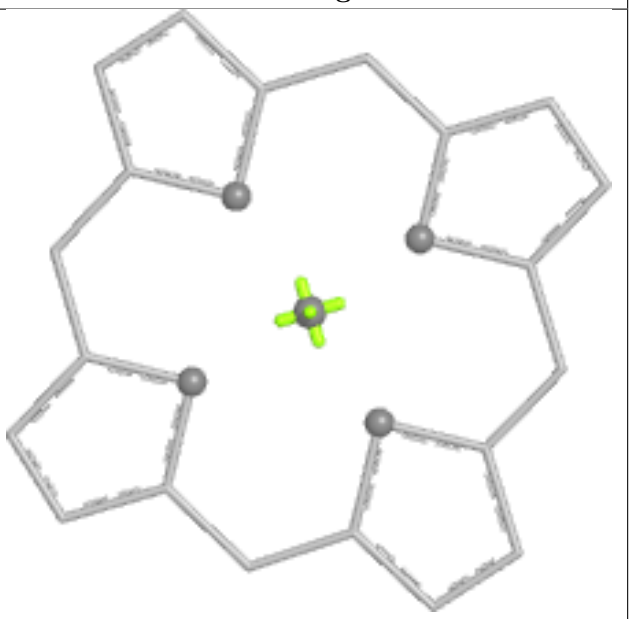
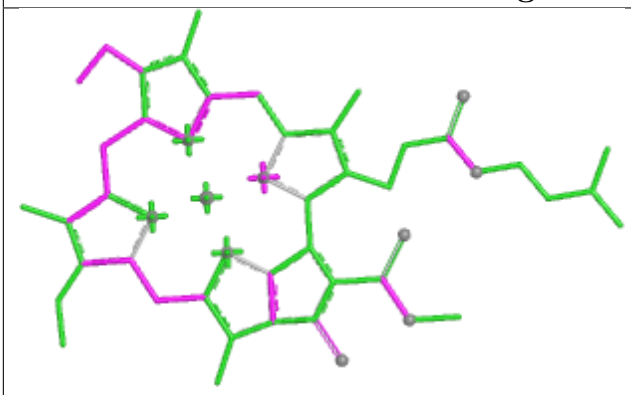


Rings

Ligand CLA L 1130



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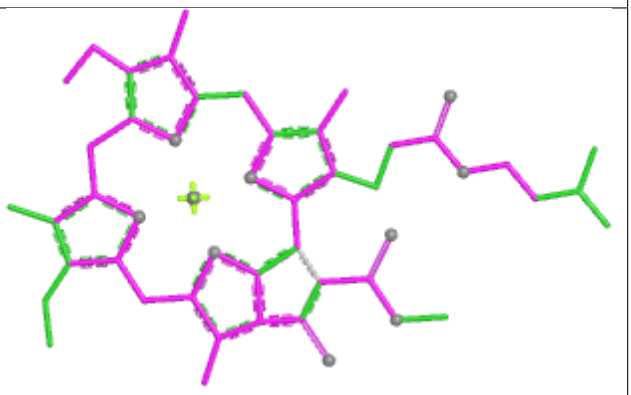
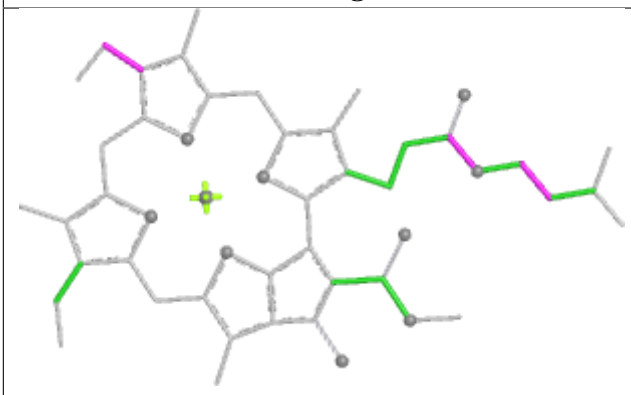


Bond angles



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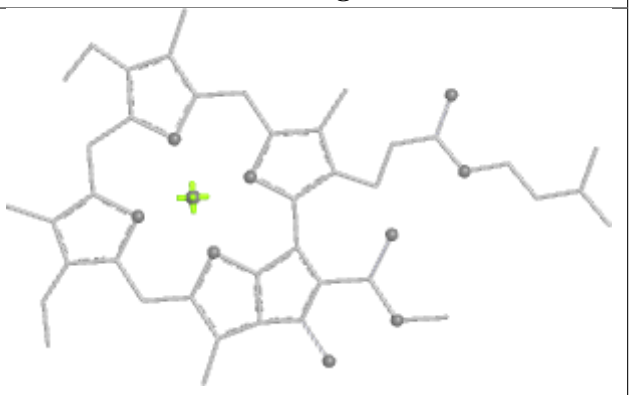
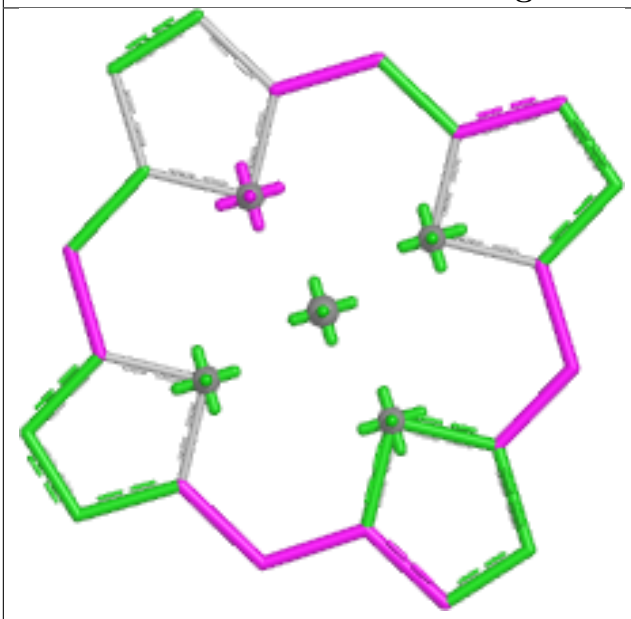


Rings

Ligand CLA B 1206



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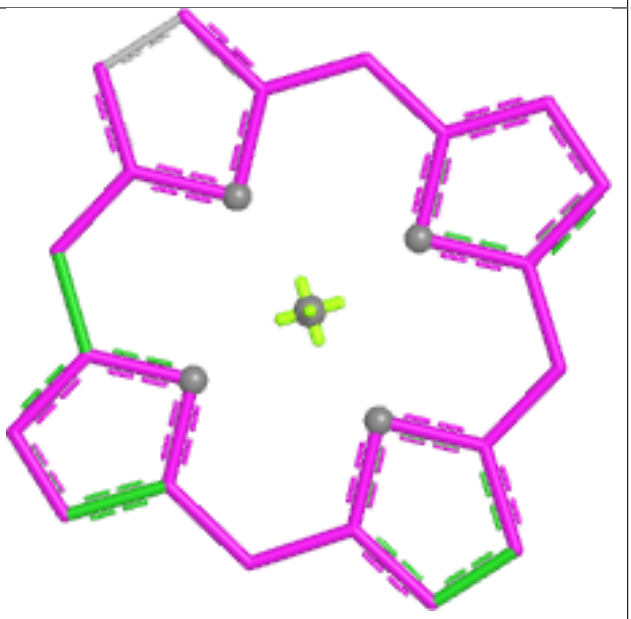
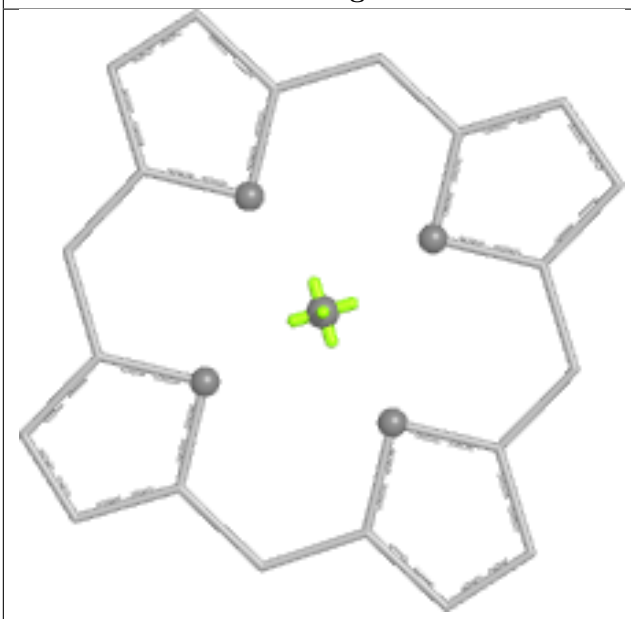


Bond angles



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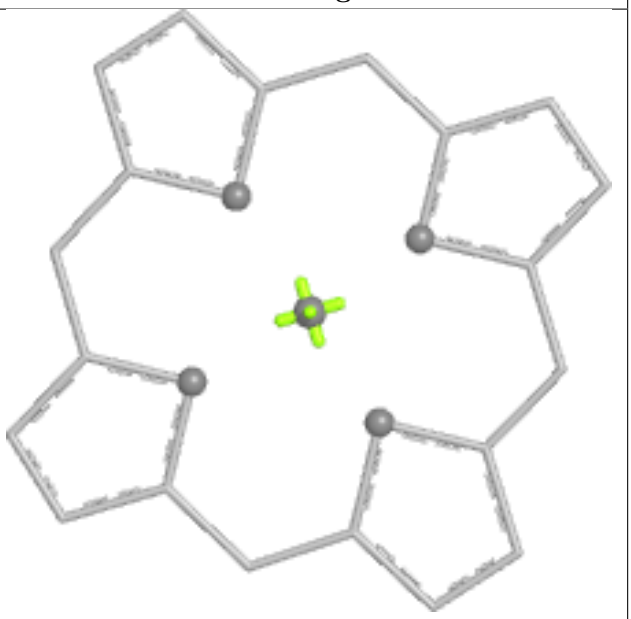
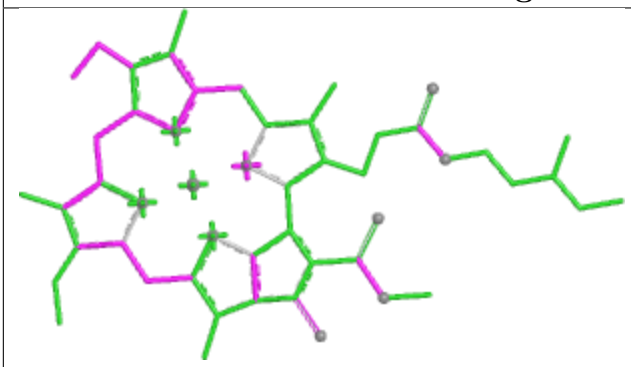
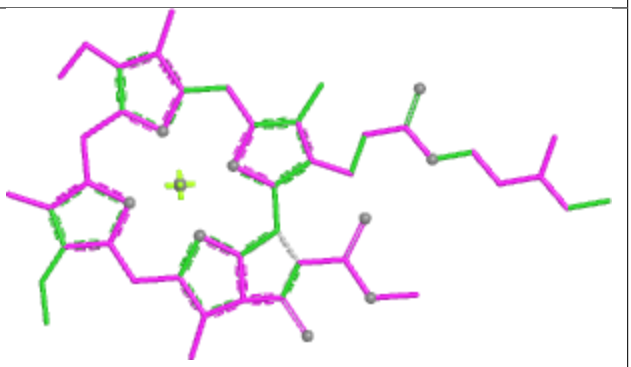
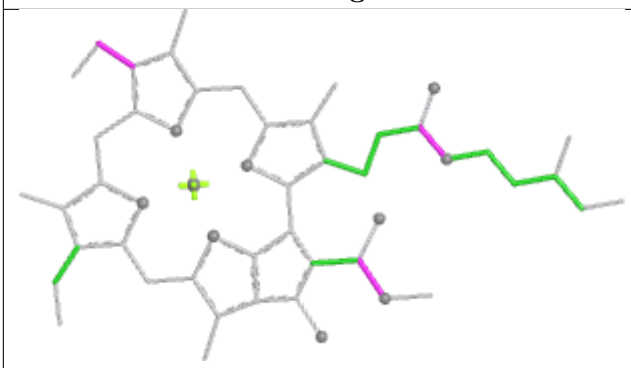
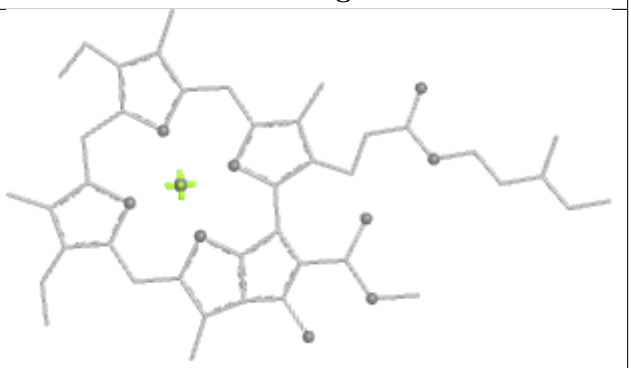
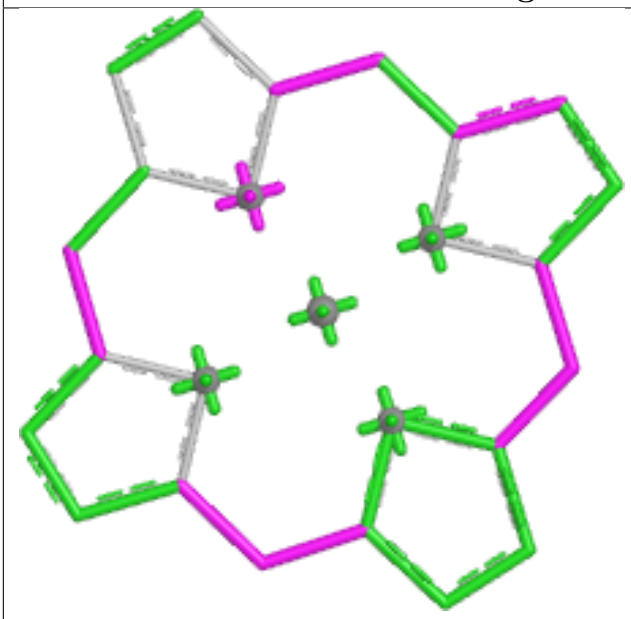


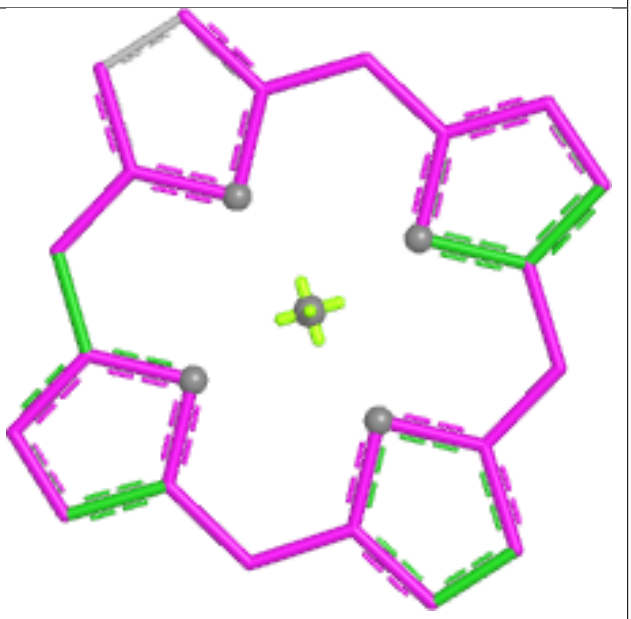
Rings

Ligand CLA B 1224	
 Bond lengths	 Bond angles
 Torsions	 Rings

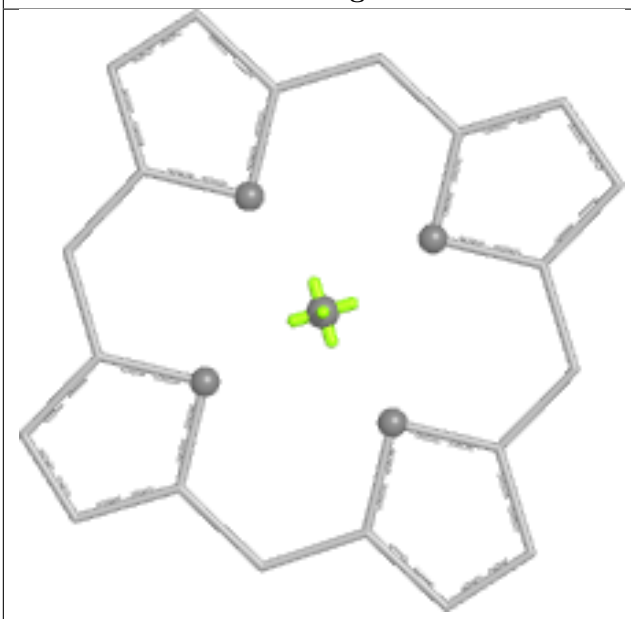
Ligand CLA L 1125



Bond lengths



Bond angles



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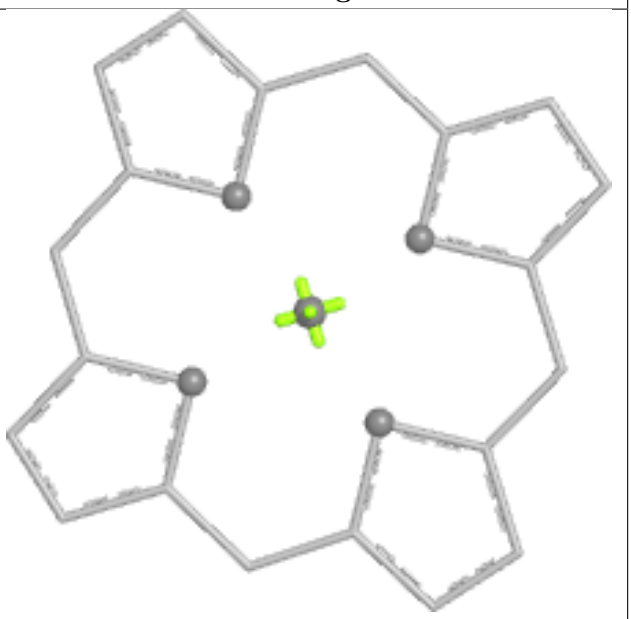
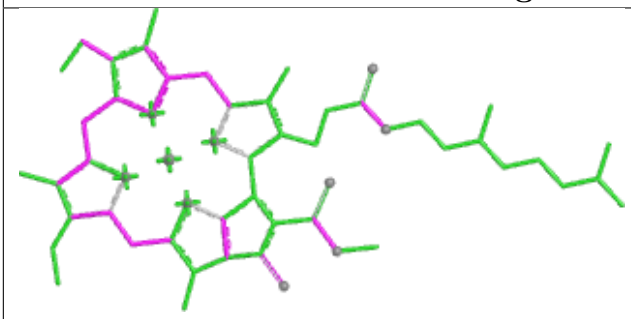
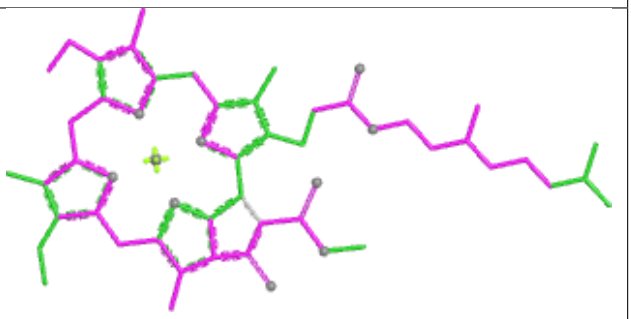
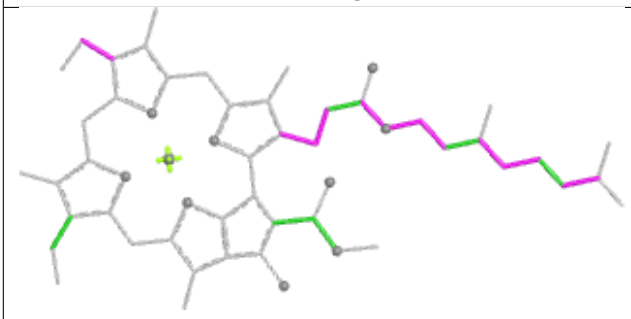
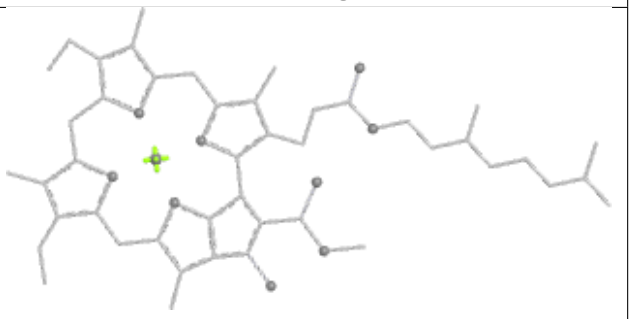
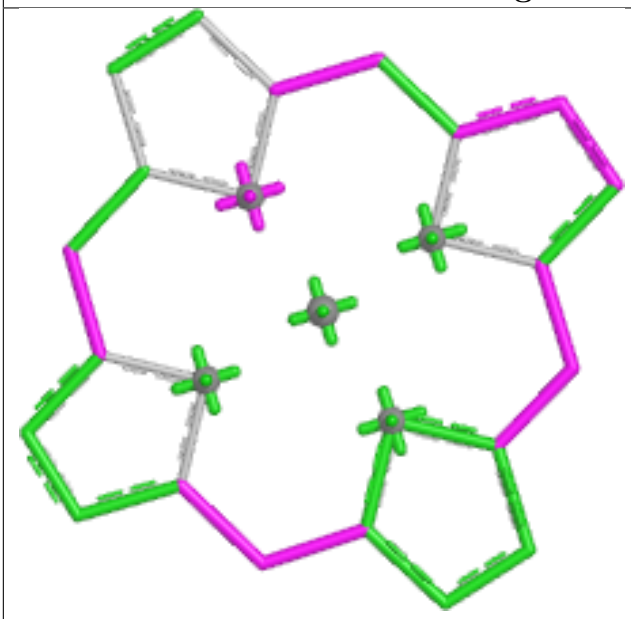


Rings

Ligand CLA B 1209	
 Bond lengths	 Bond angles
 Torsions	 Rings

Ligand CLA A 1132



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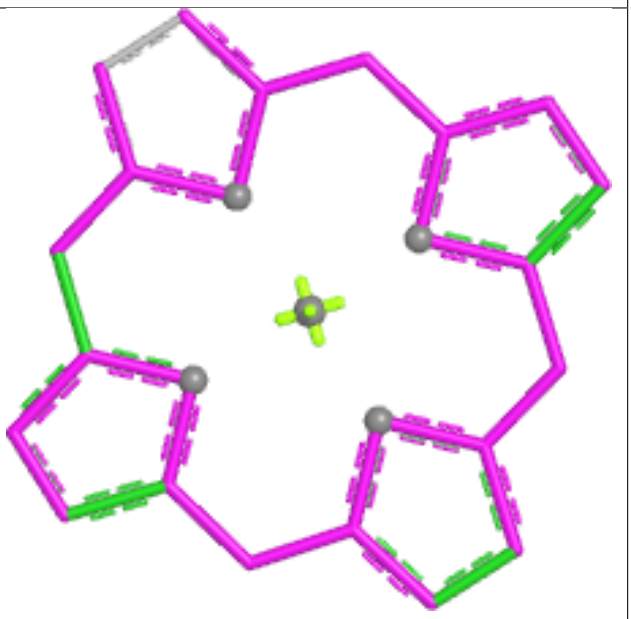
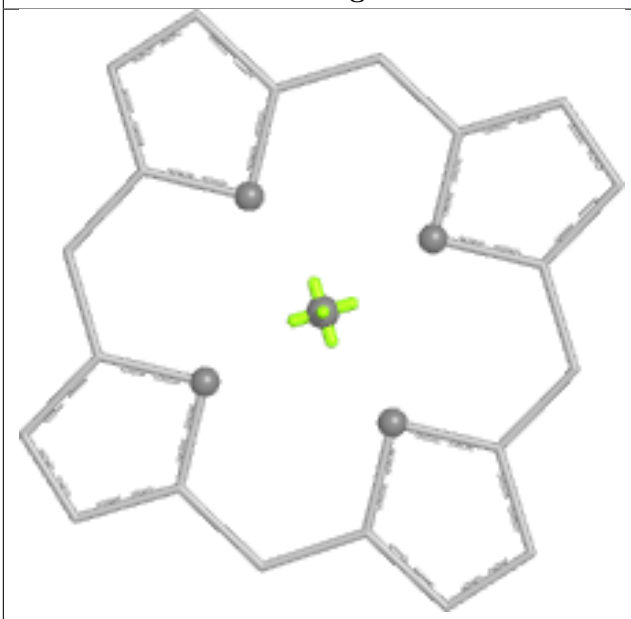


Bond angles



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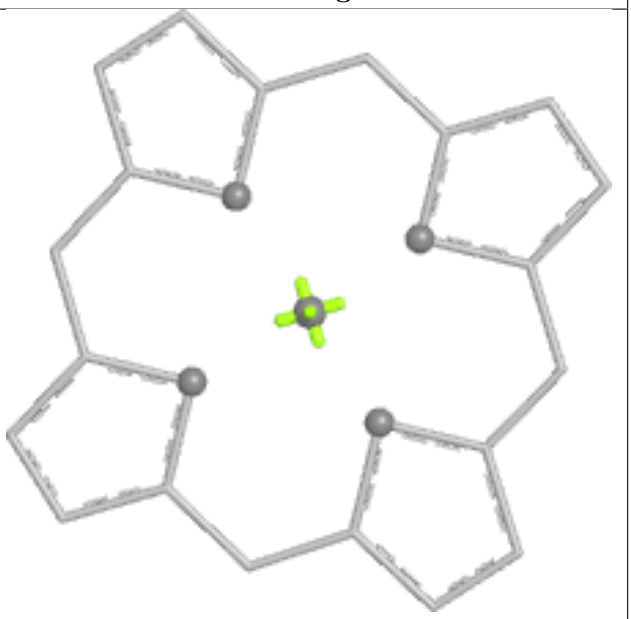
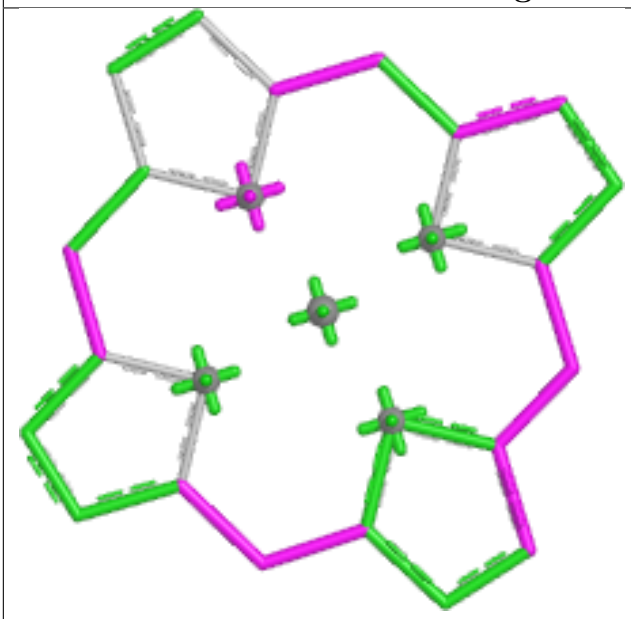


Rings

Ligand CLA H 1505



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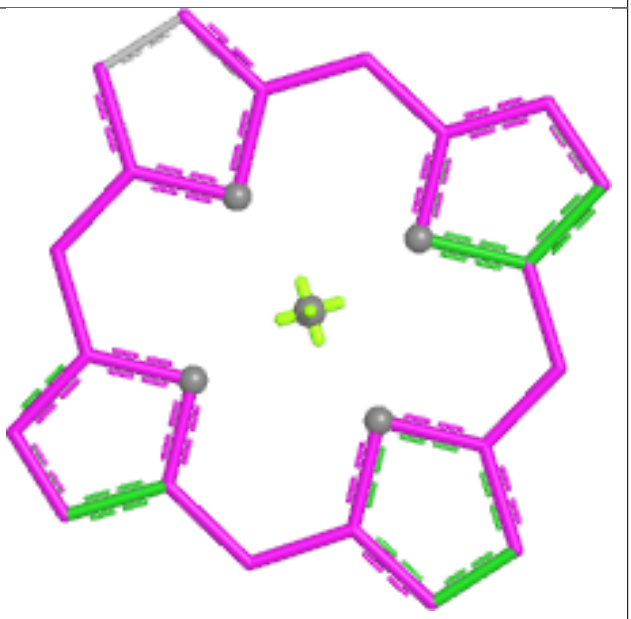
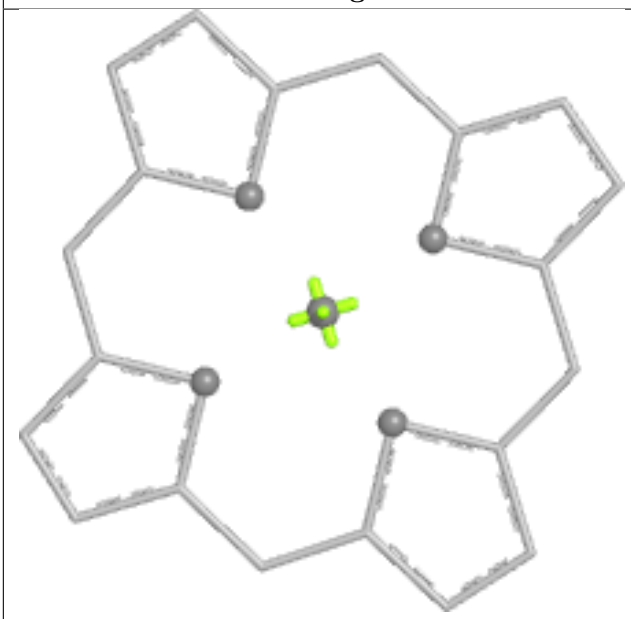


Bond angles



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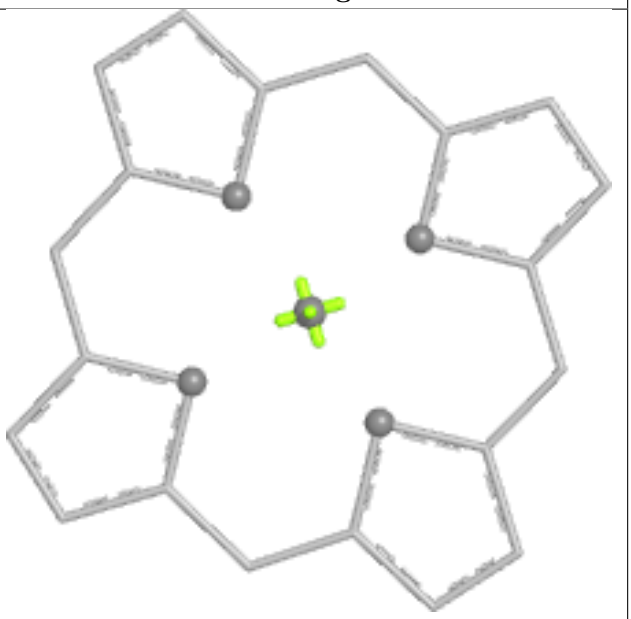
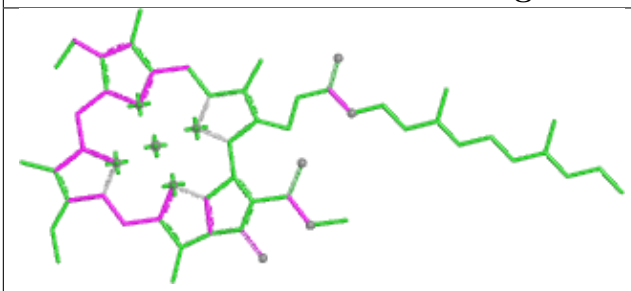
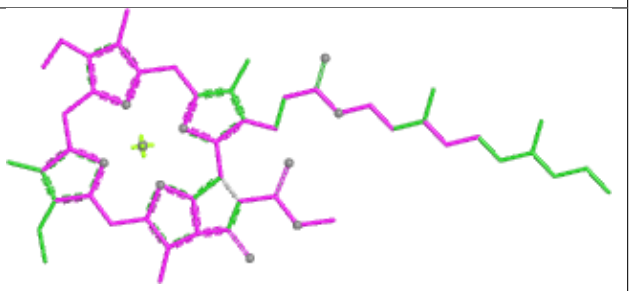
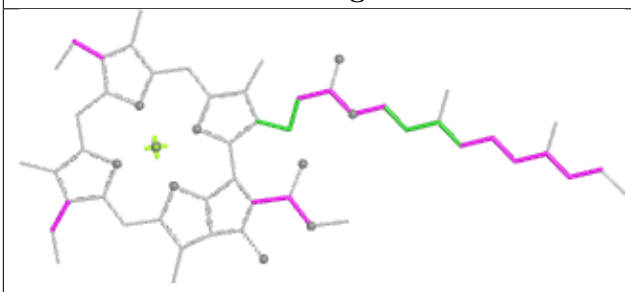
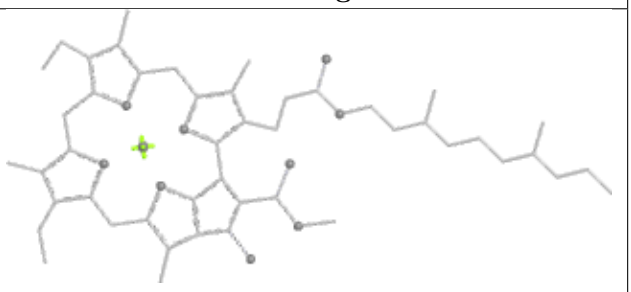
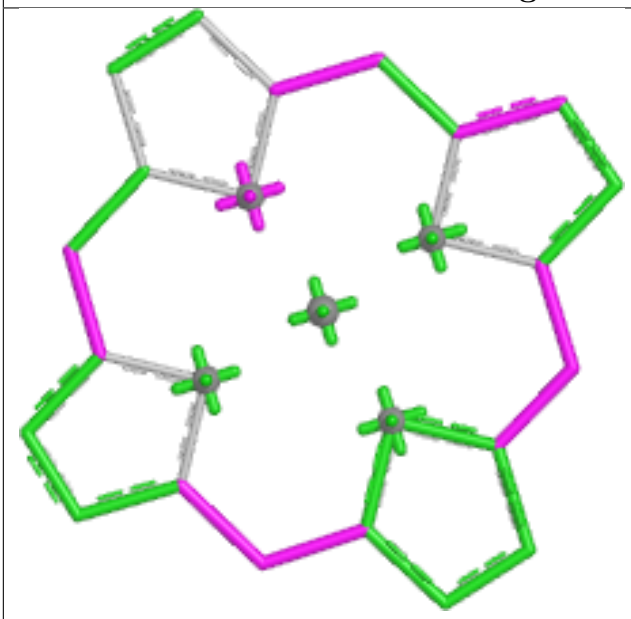


Rings

Ligand CLA A 1107	
 Bond lengths	 Bond angles
 Torsions	 Rings

Ligand CLA 1 1008



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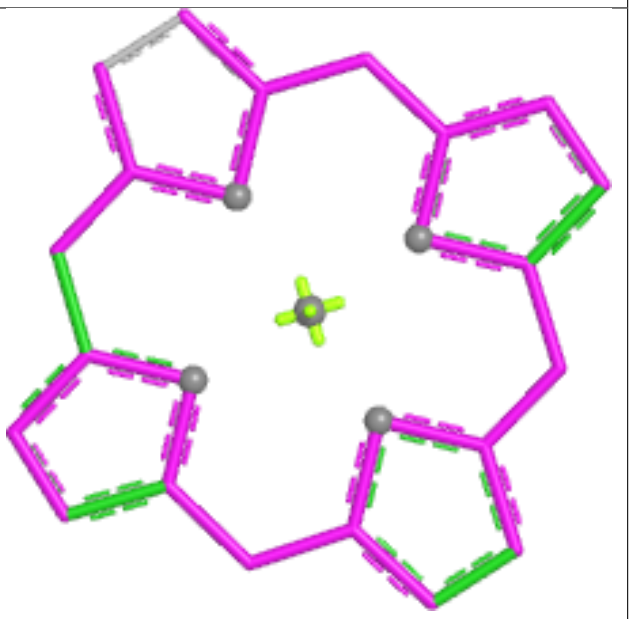

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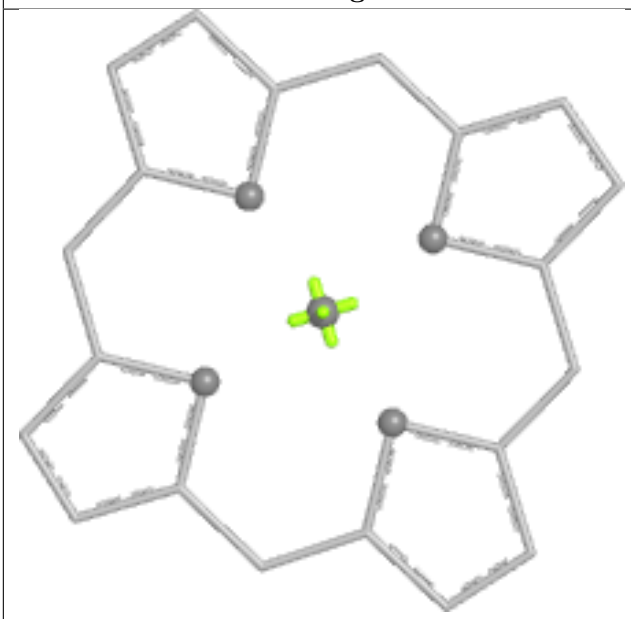

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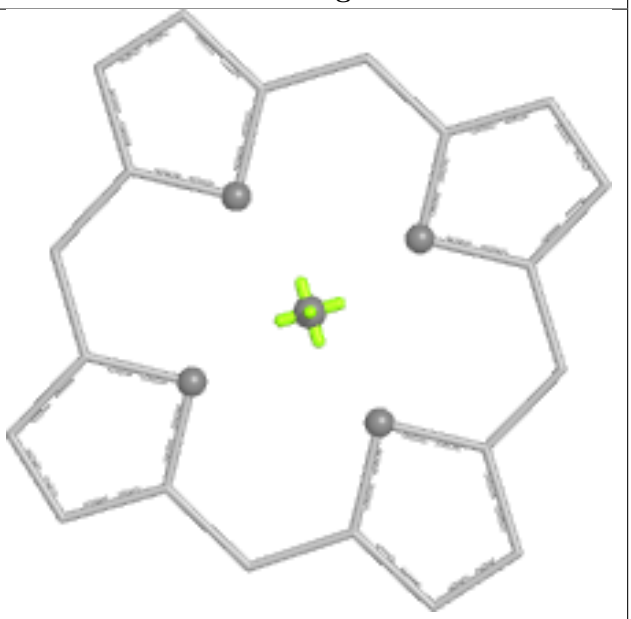
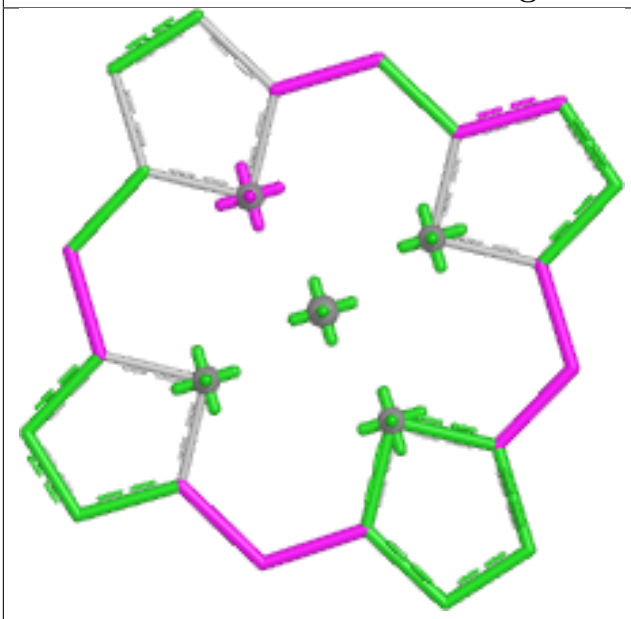


Rings

Ligand CLA 3 2009



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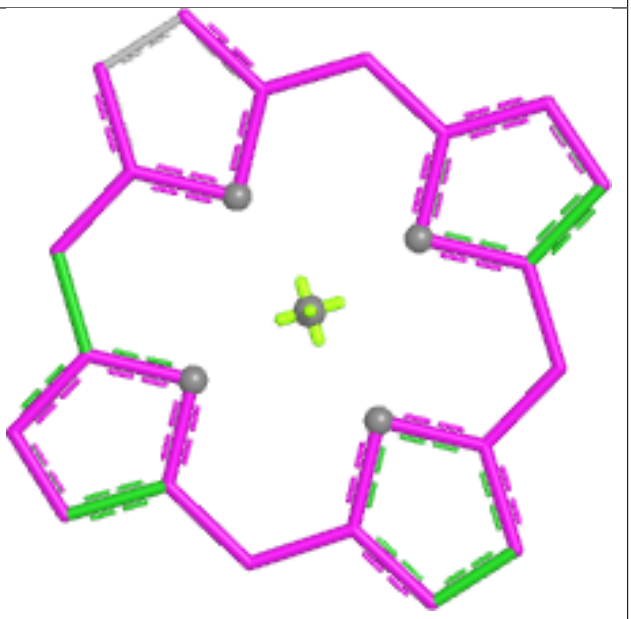

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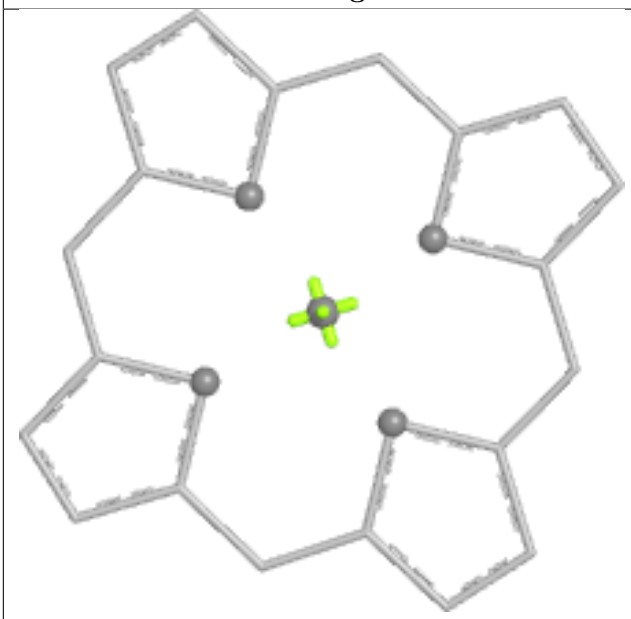

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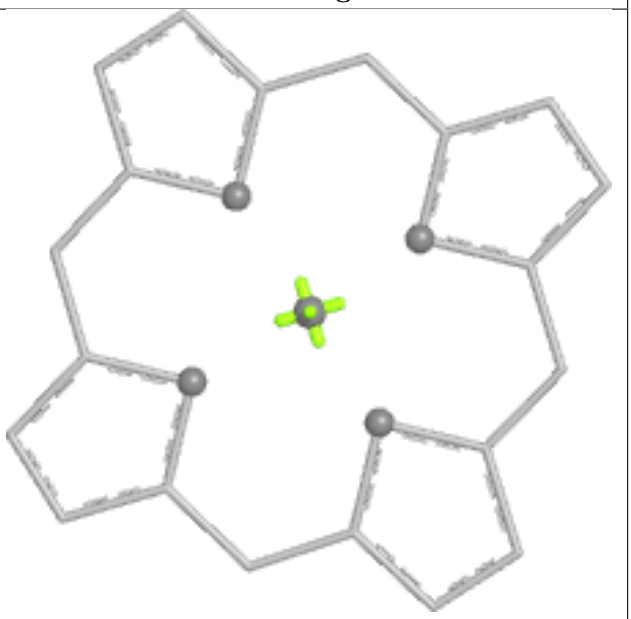
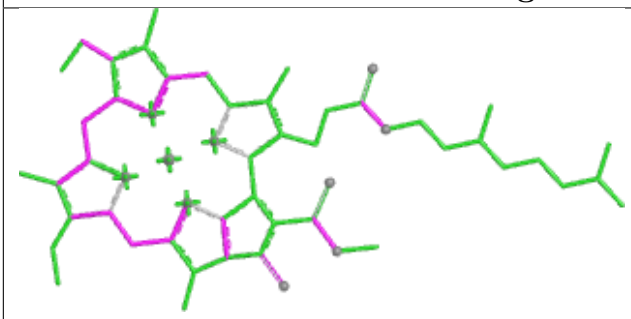


Rings

Ligand CLA L 1504



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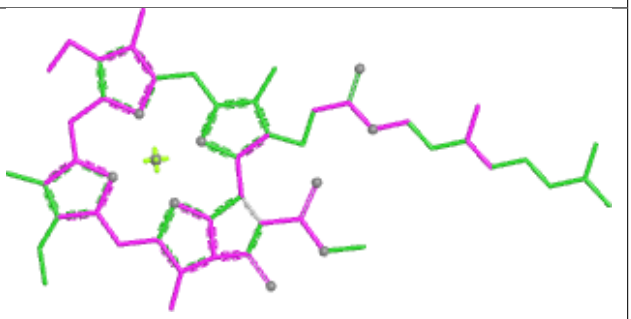

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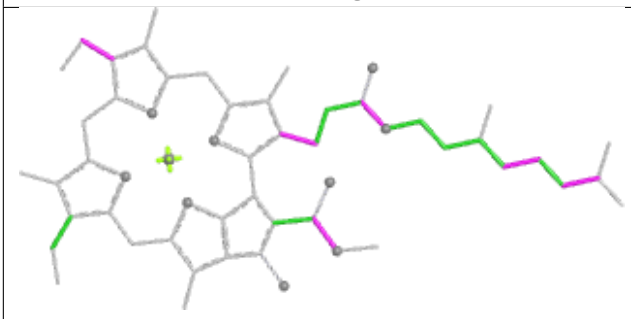

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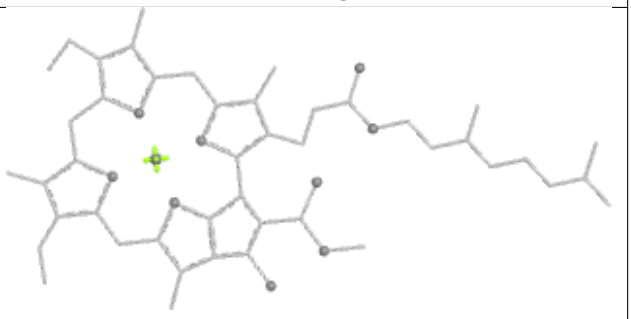
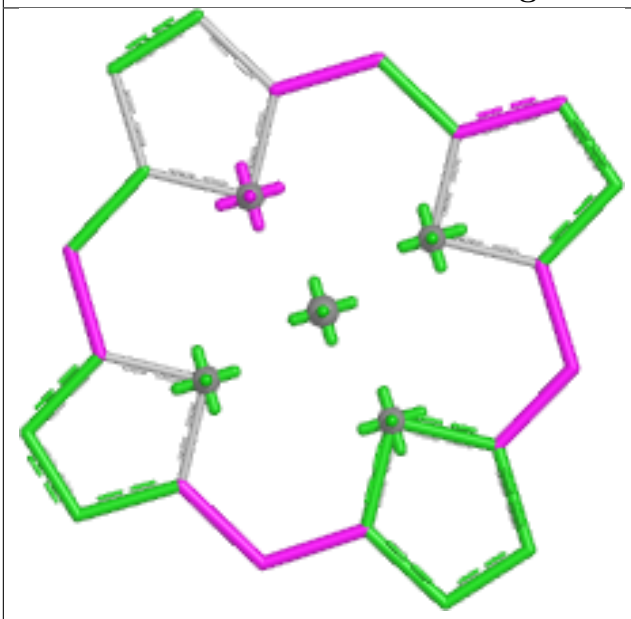


Rings

Ligand CLA 3 3003



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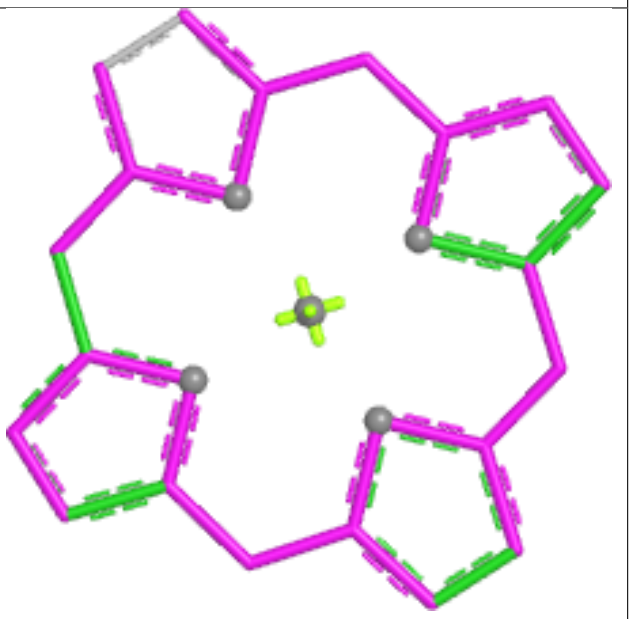
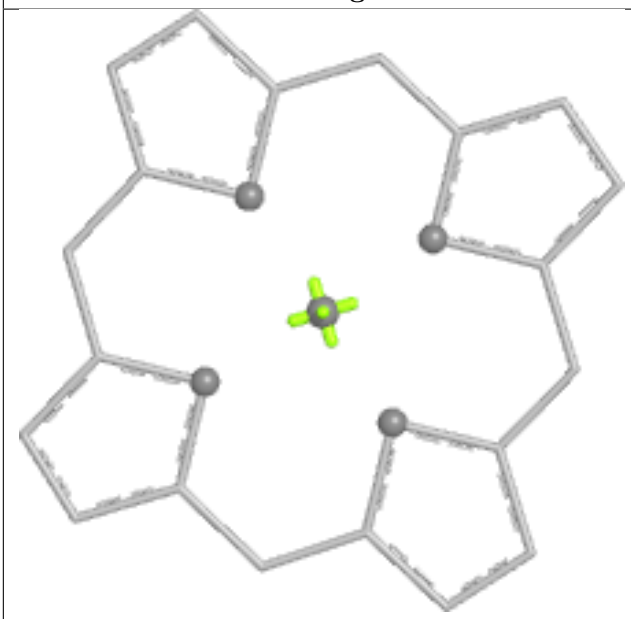


Bond angles



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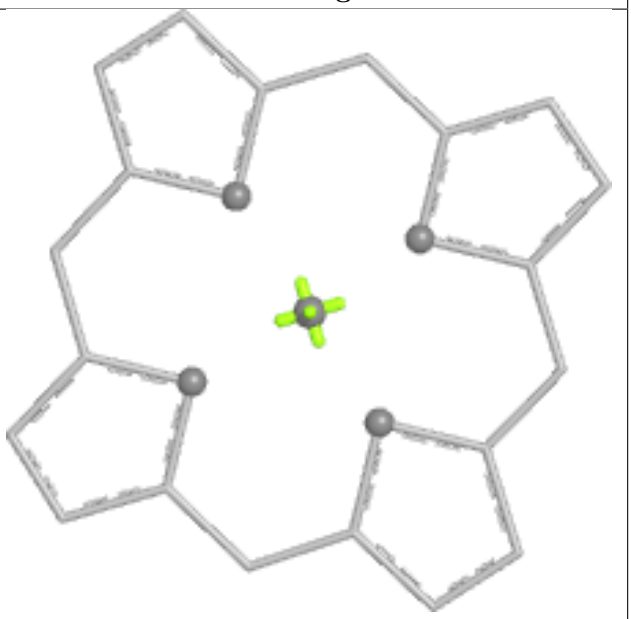
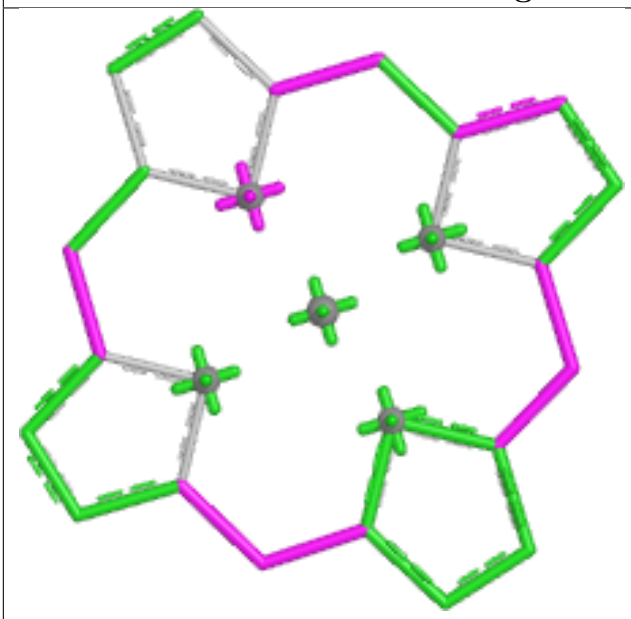


Rings

Ligand CLA A 1104



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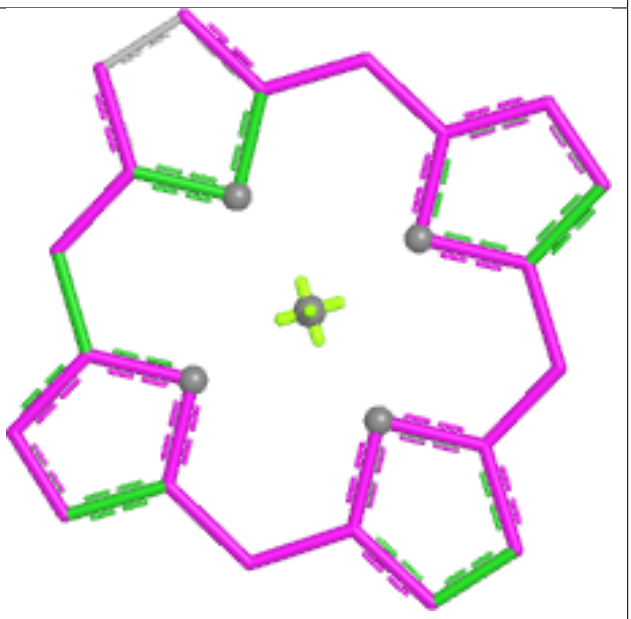

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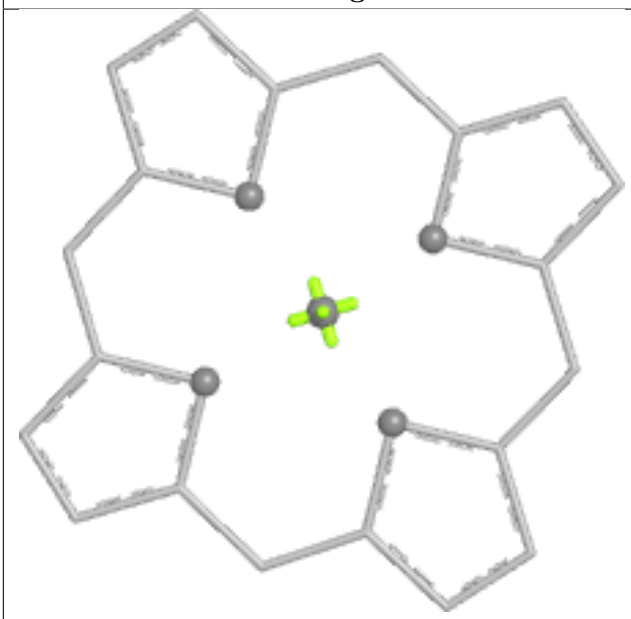

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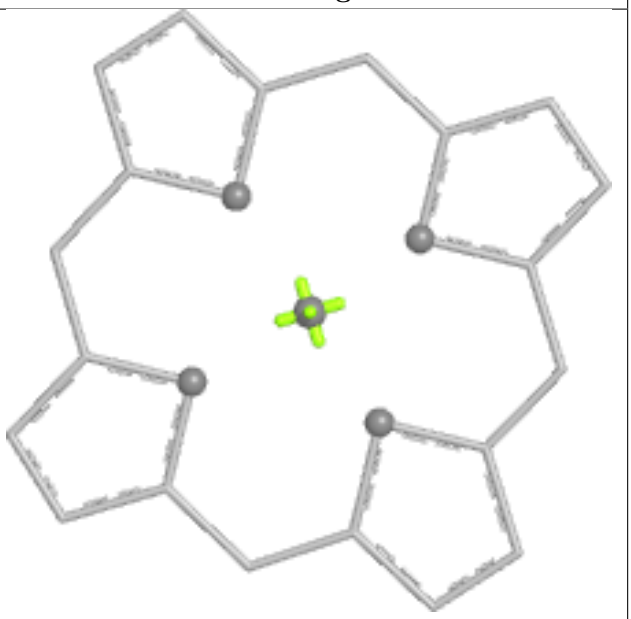
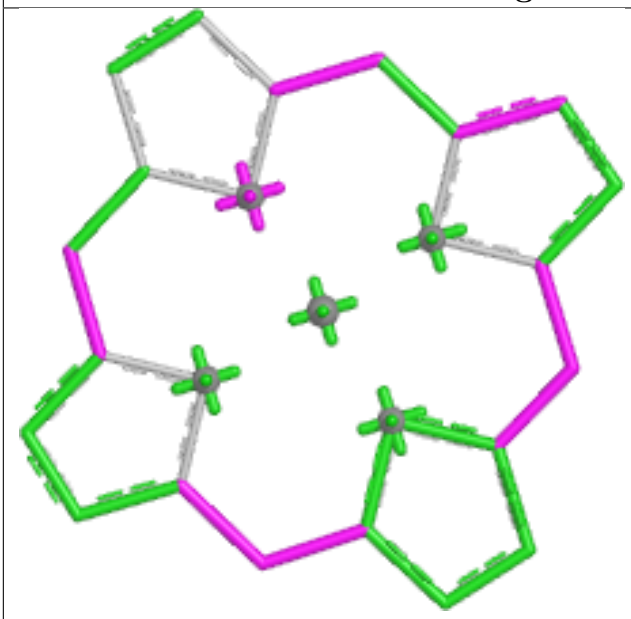


Rings

Ligand CLA B 1201



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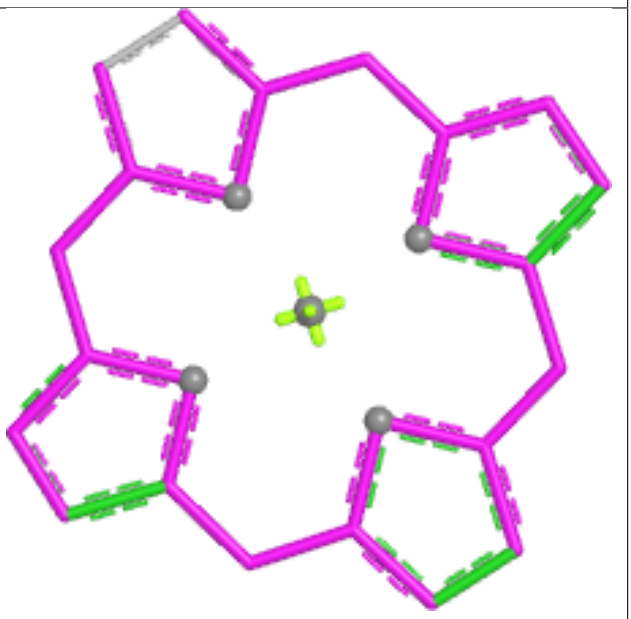

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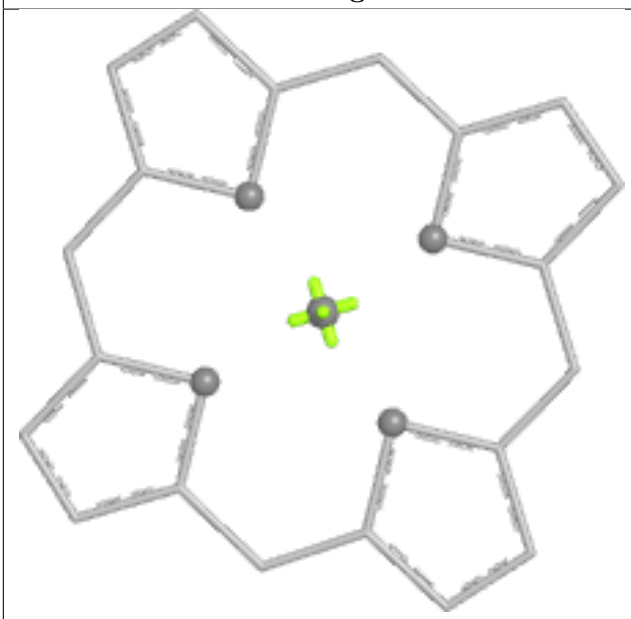

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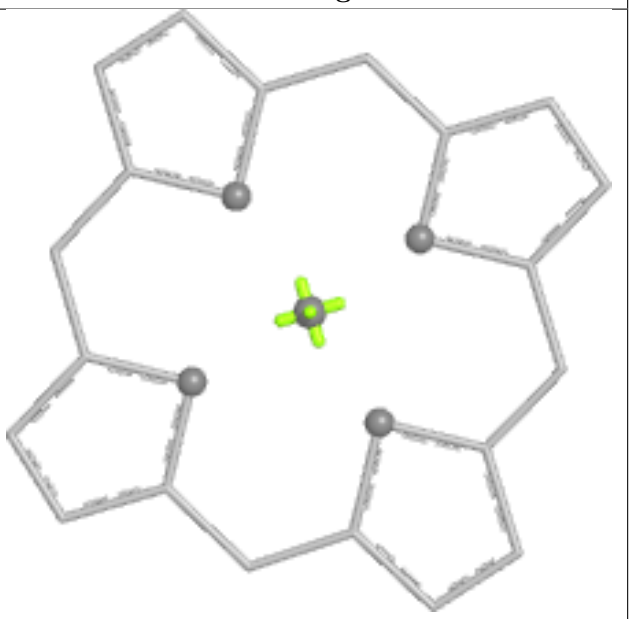
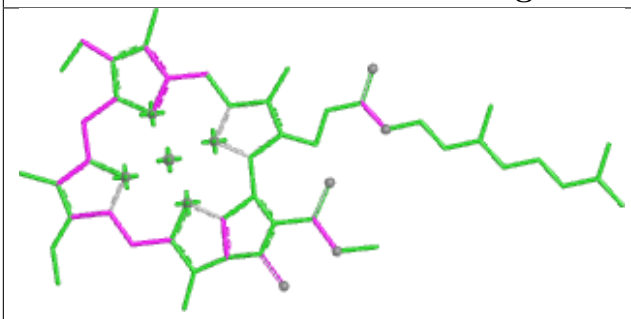
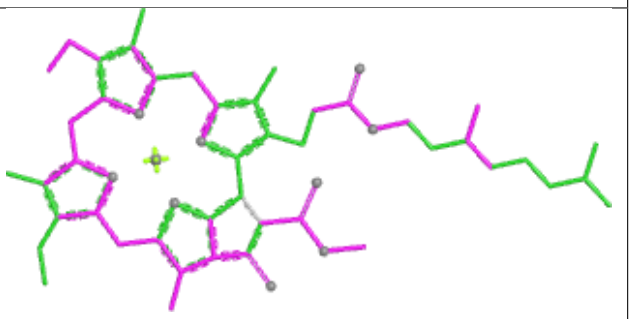
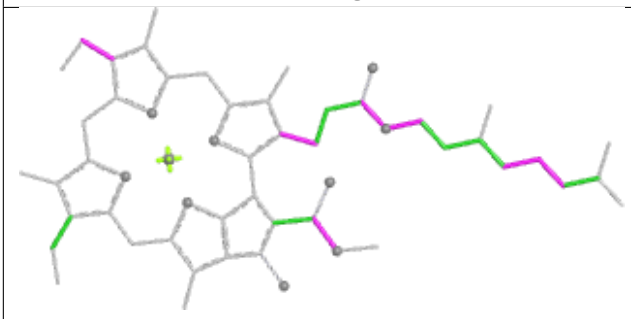
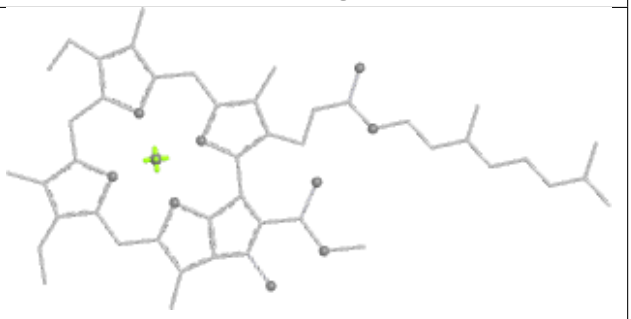
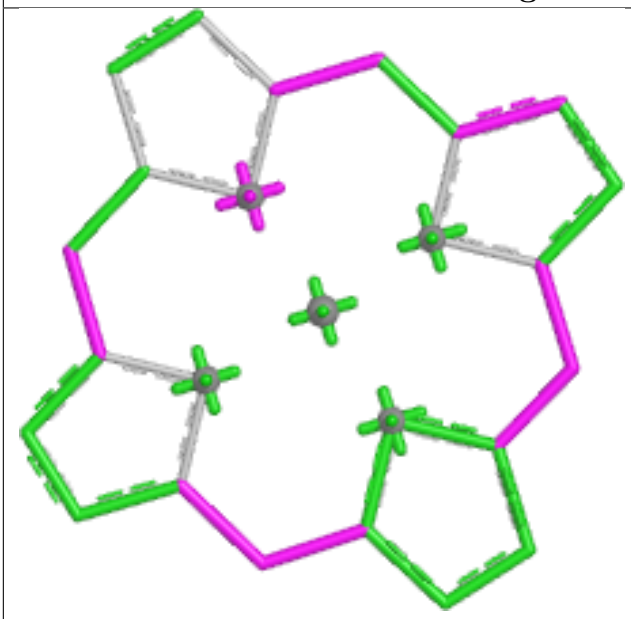


Rings

Ligand CLA B 1232	
 Bond lengths	 Bond angles
 Torsions	 Rings

Ligand CLA 3 3010



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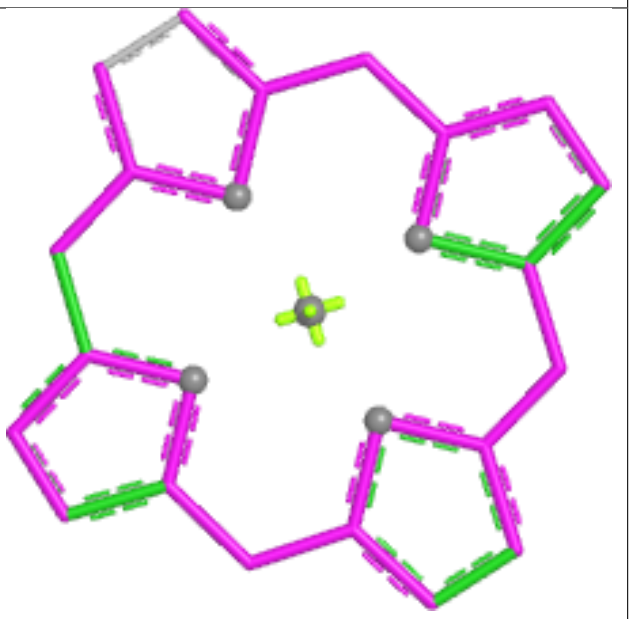

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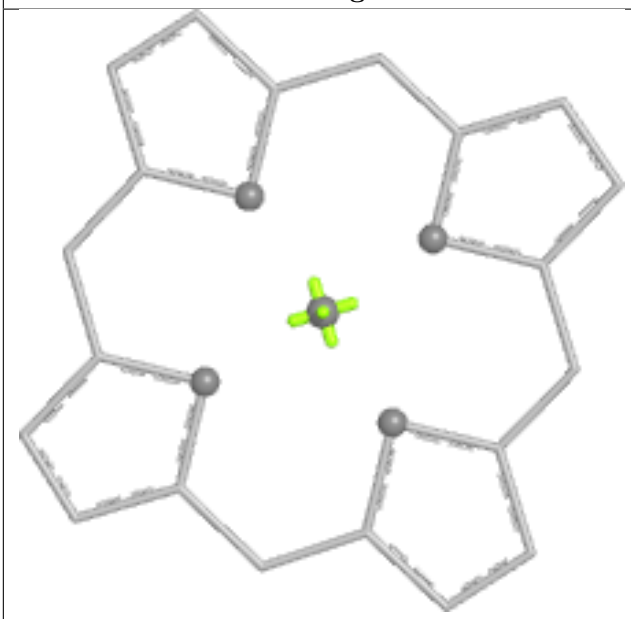

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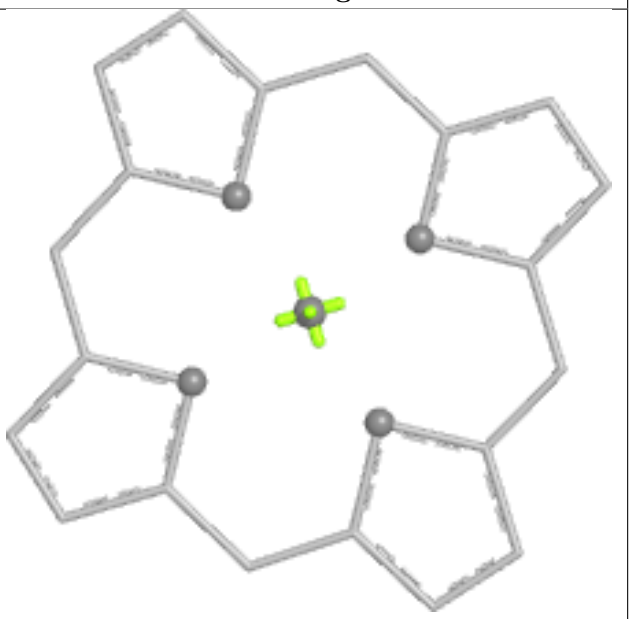
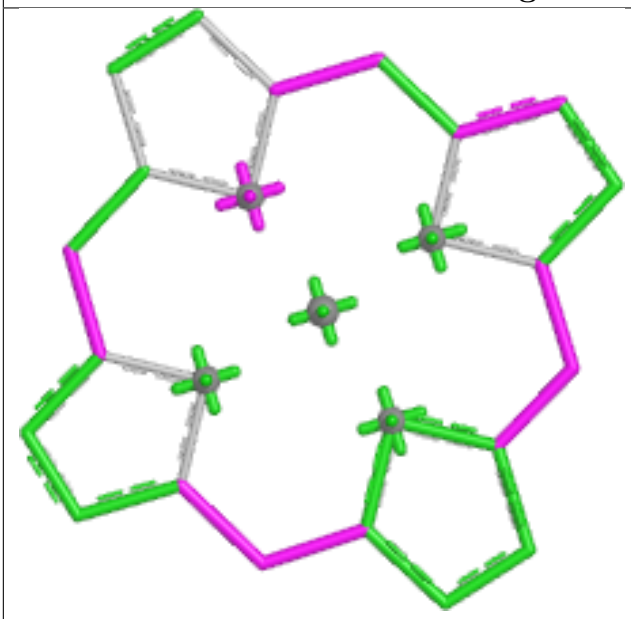


Rings

Ligand CLA J 1307



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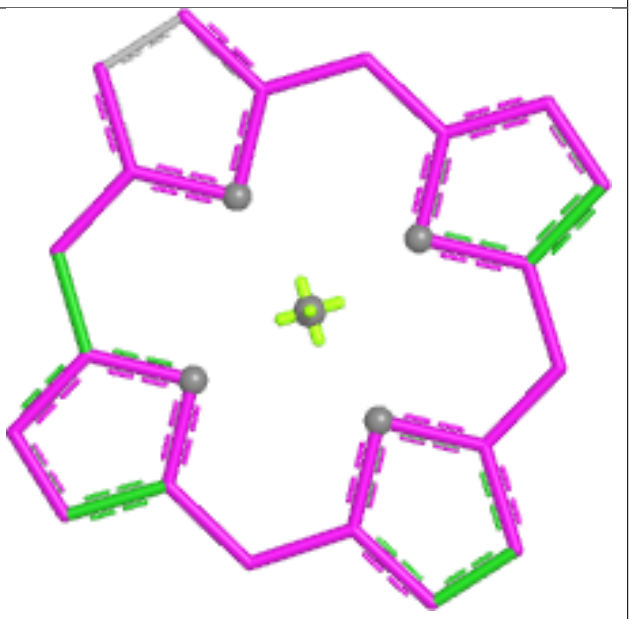

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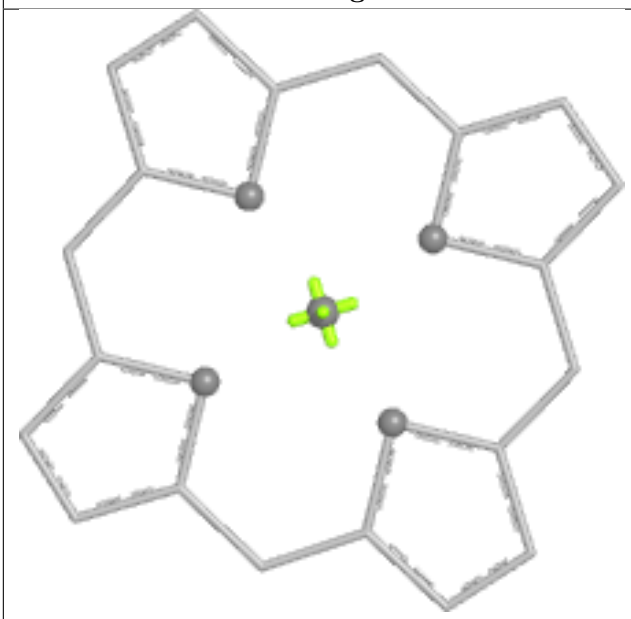

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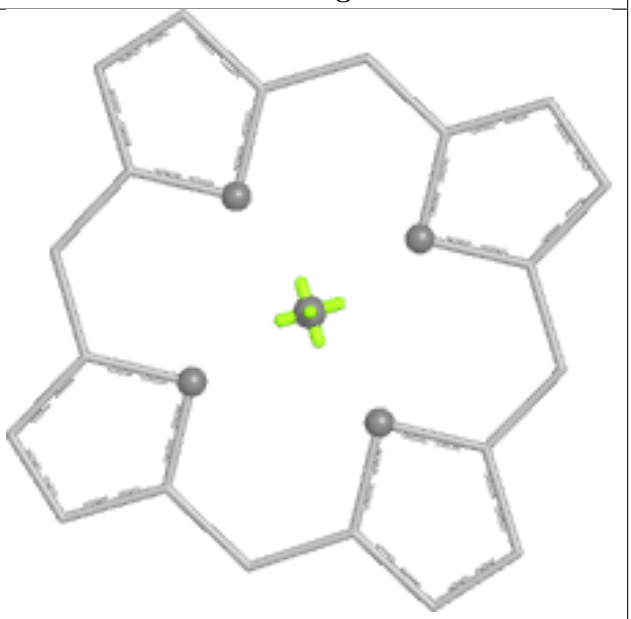
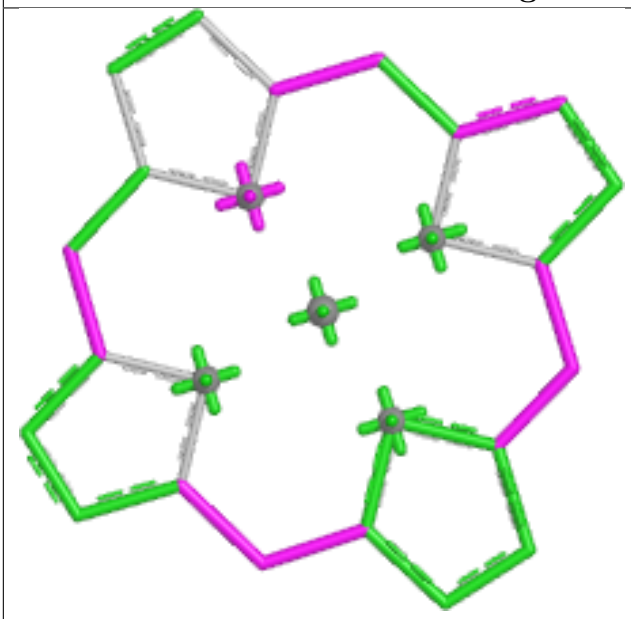


Rings

Ligand CLA 3 3015



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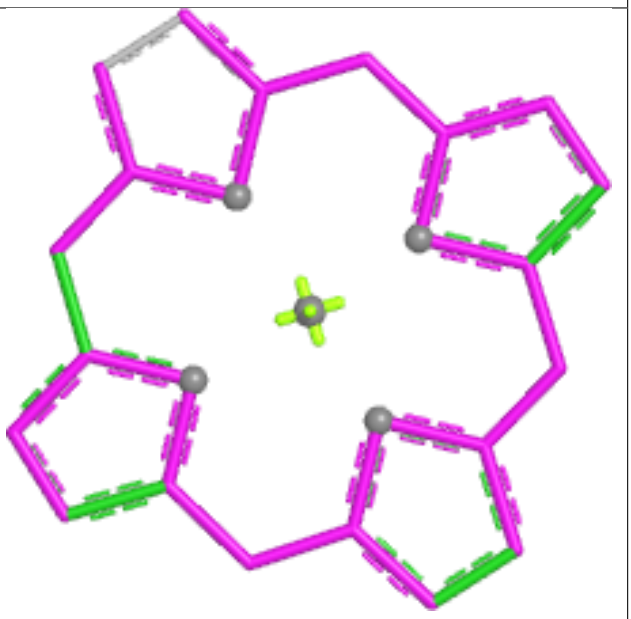

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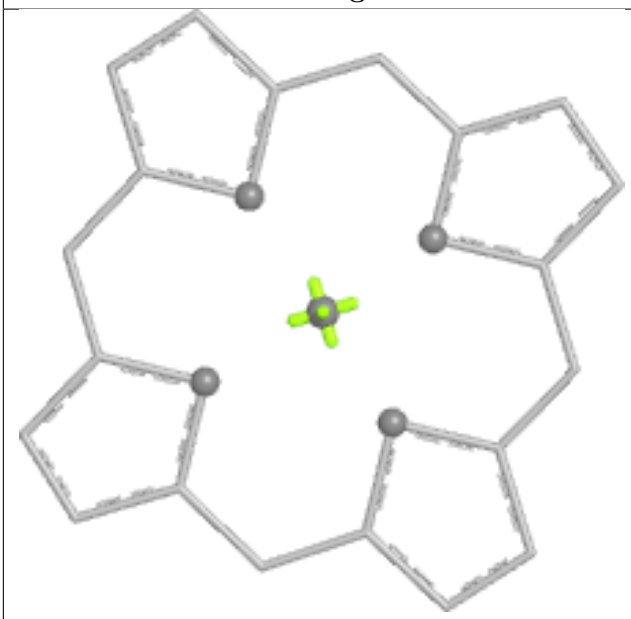

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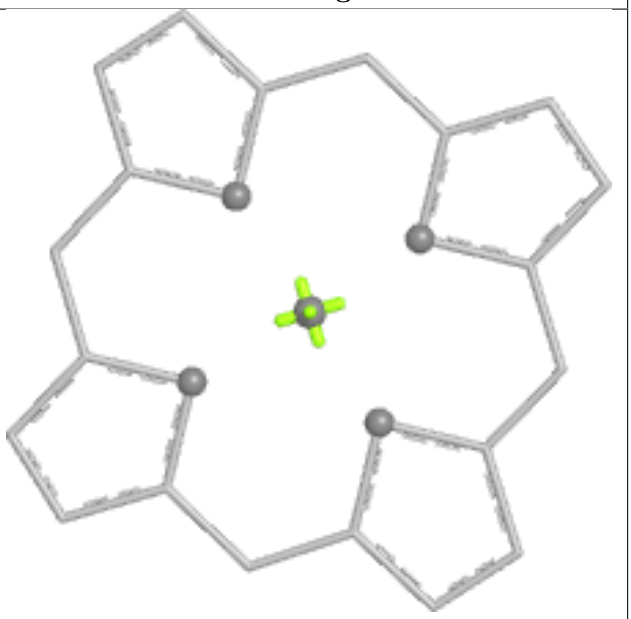
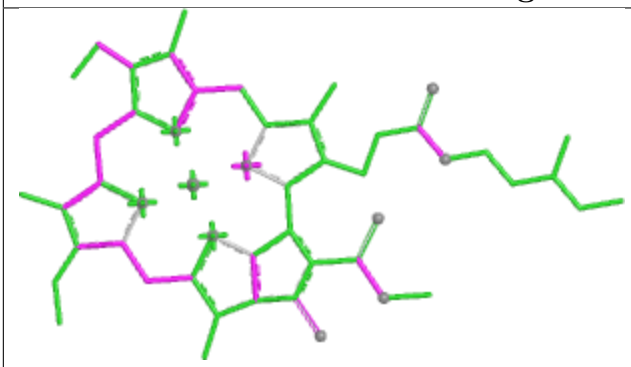


Rings

Ligand CLA L 1502



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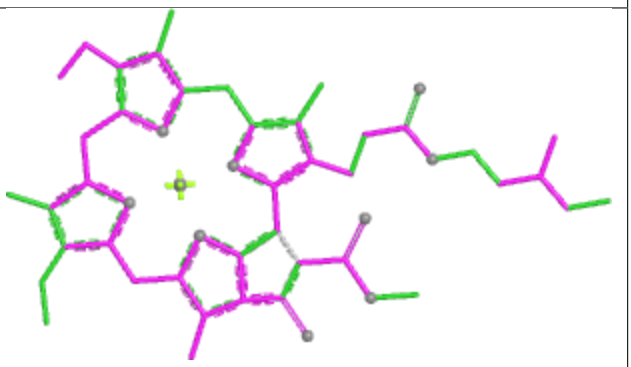

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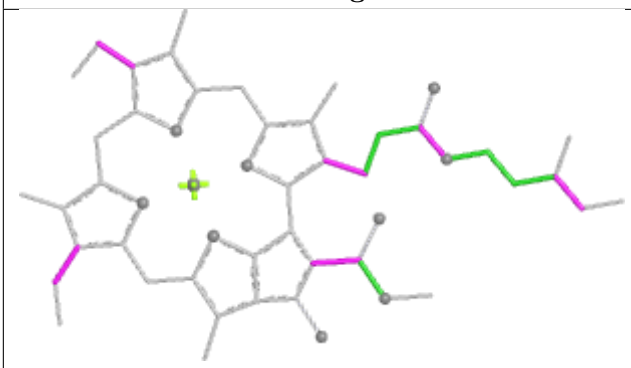

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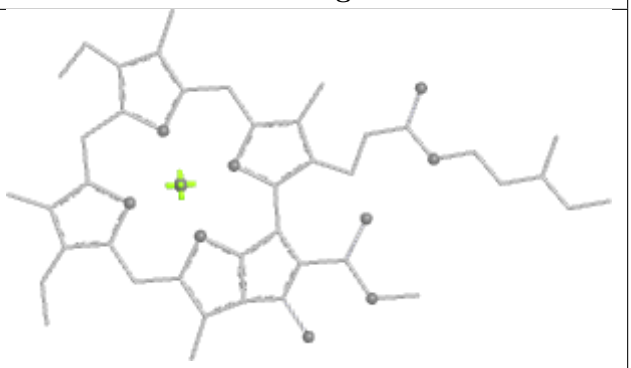
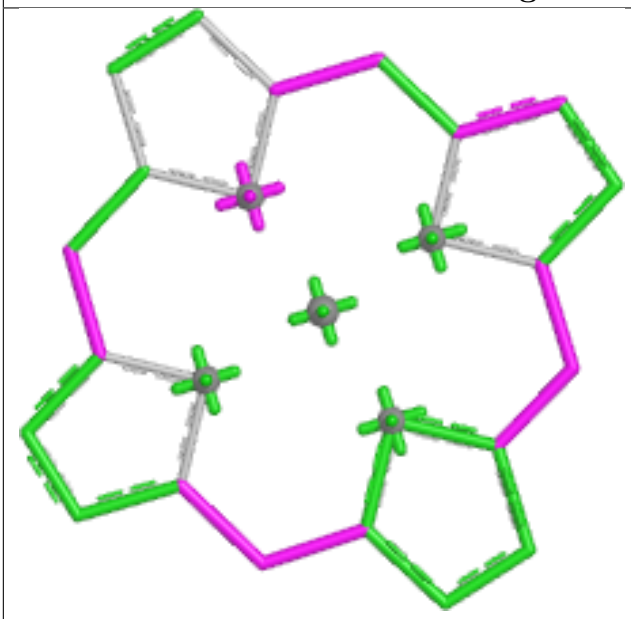


Rings

Ligand CLA 4 4010



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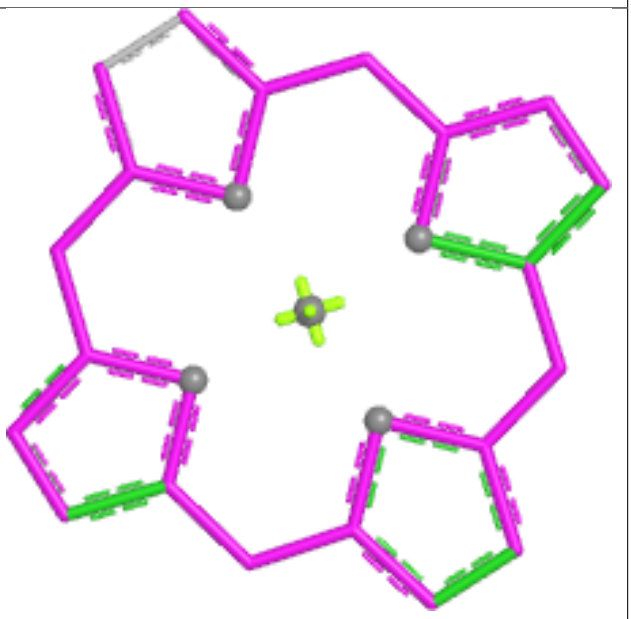

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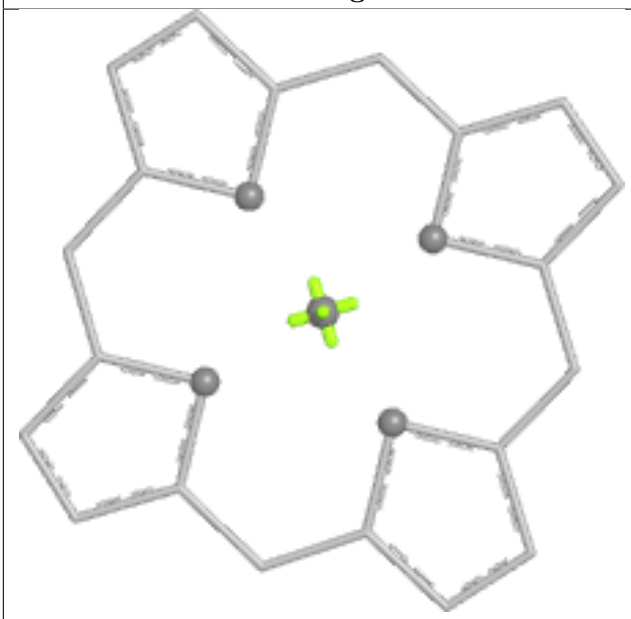

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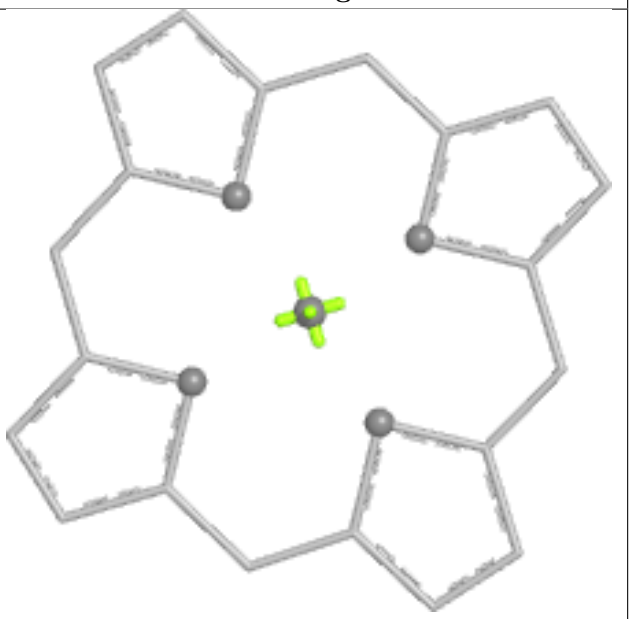
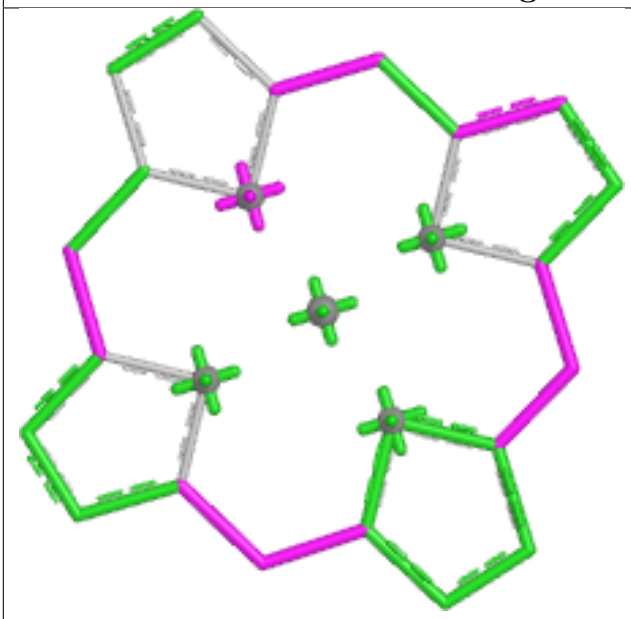


Rings

Ligand CLA 2 2008



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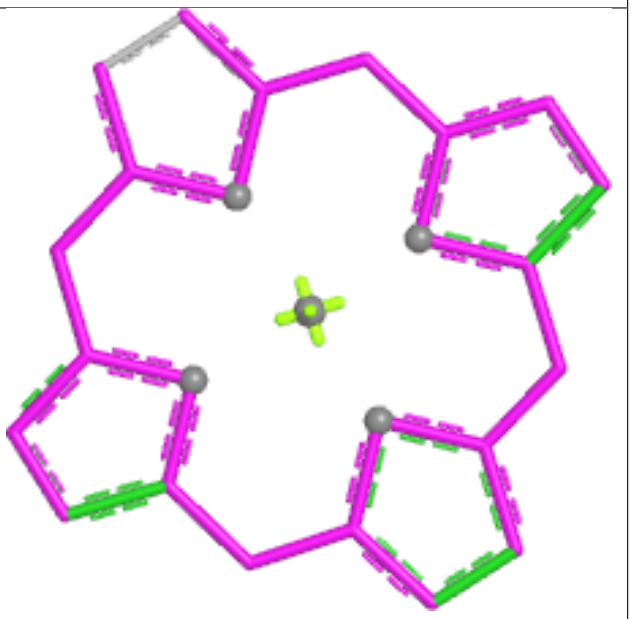
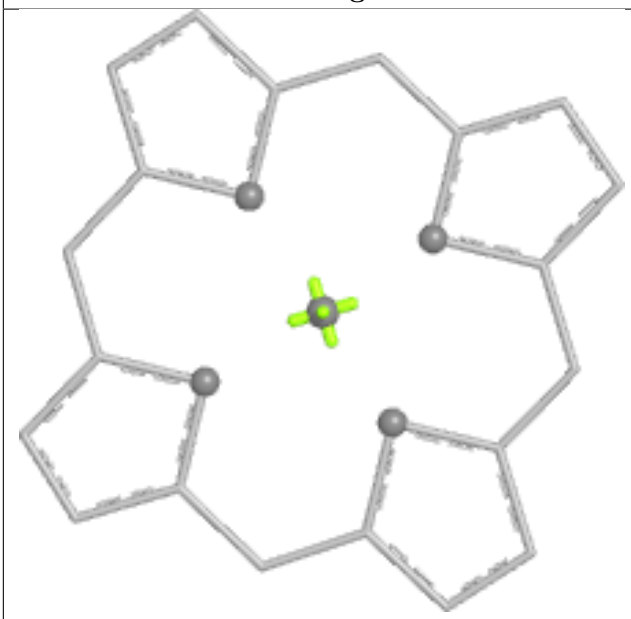


Bond angles



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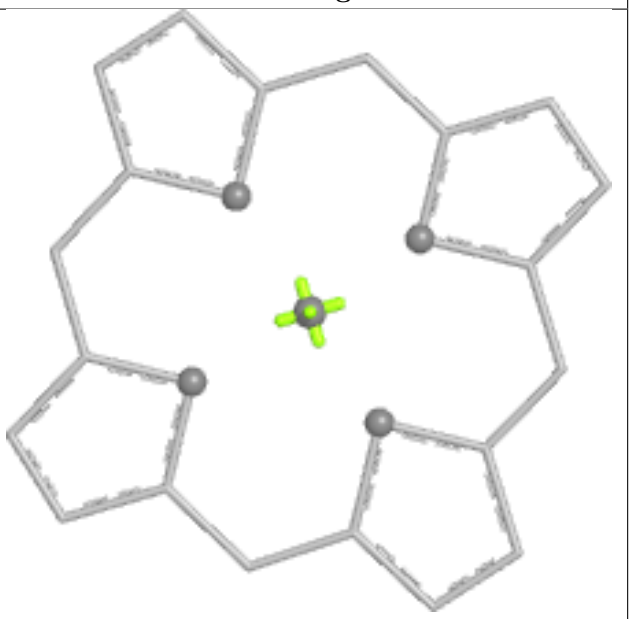
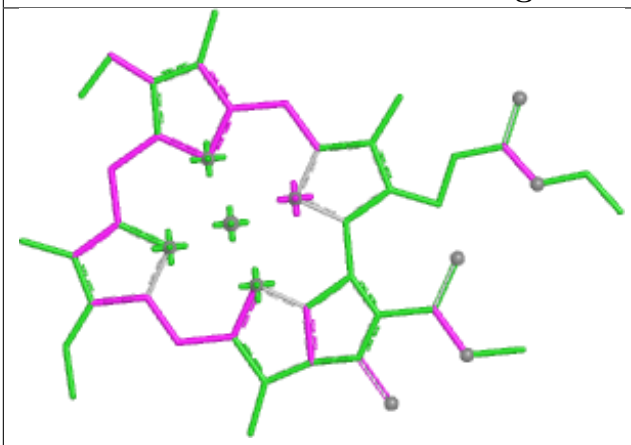


Rings

Ligand CLA B 9023



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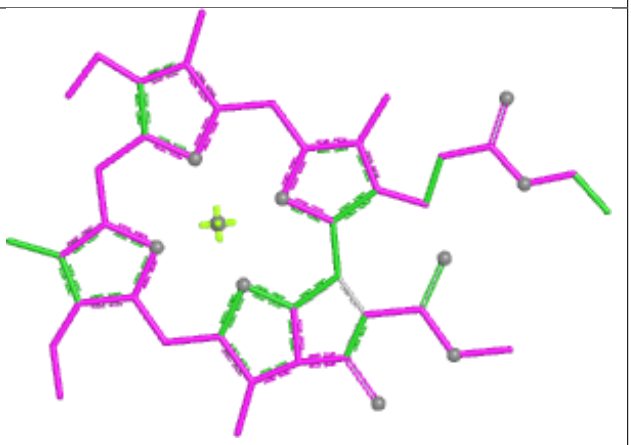
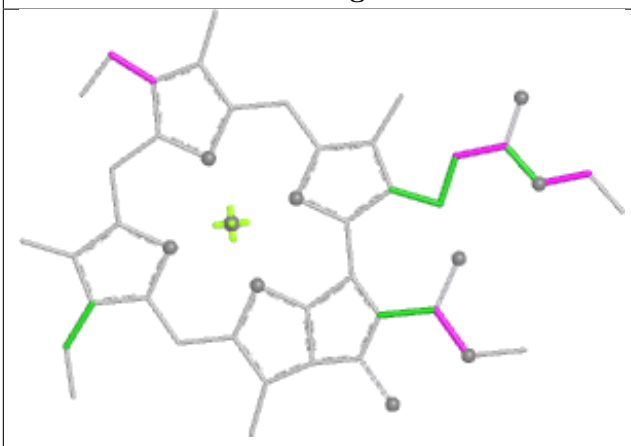


Bond angles



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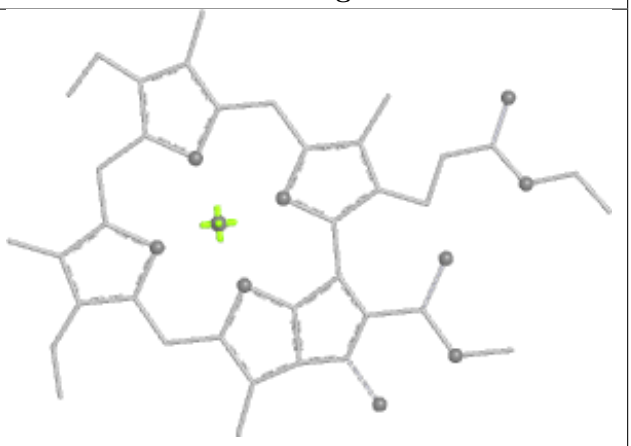

Rings

Ligand BCR A 6011

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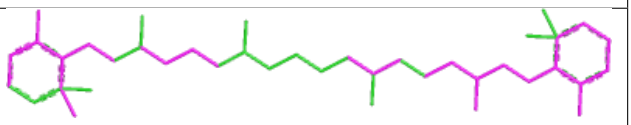

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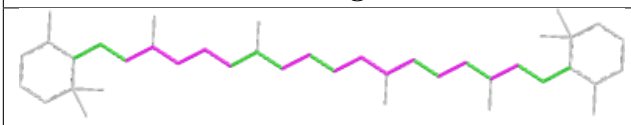

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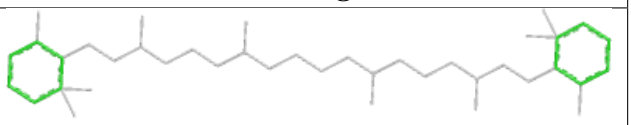
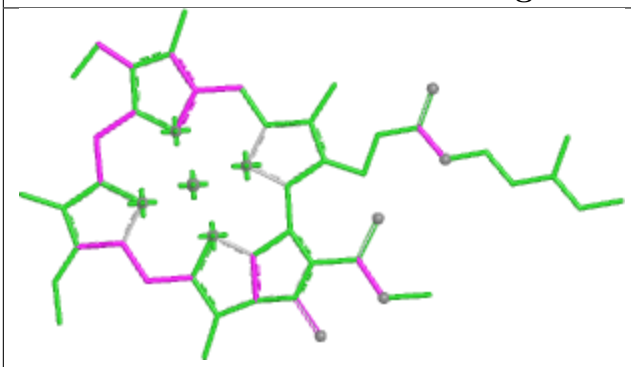


Rings

Ligand CLA B 1219



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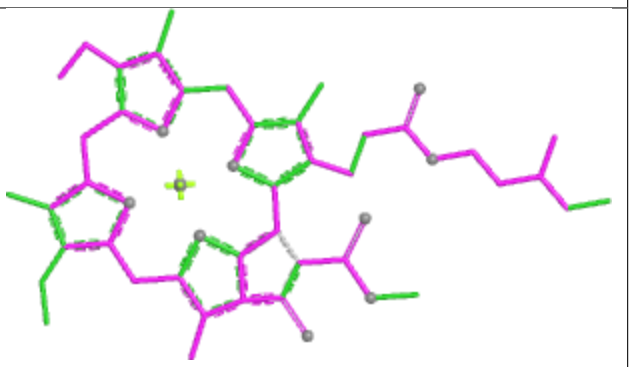

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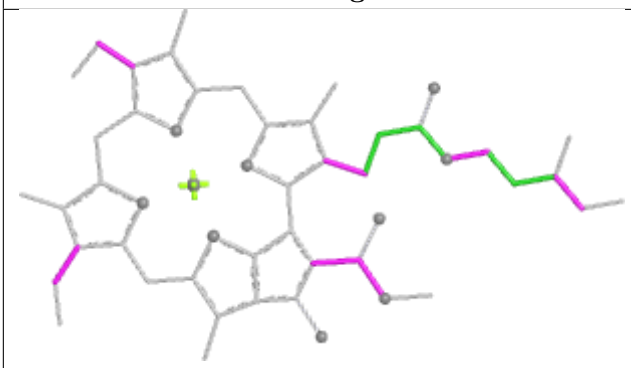

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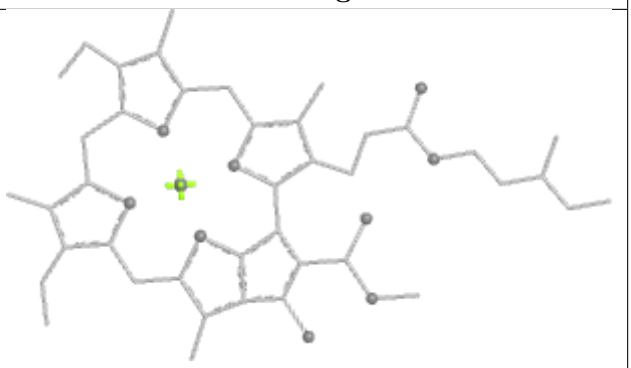
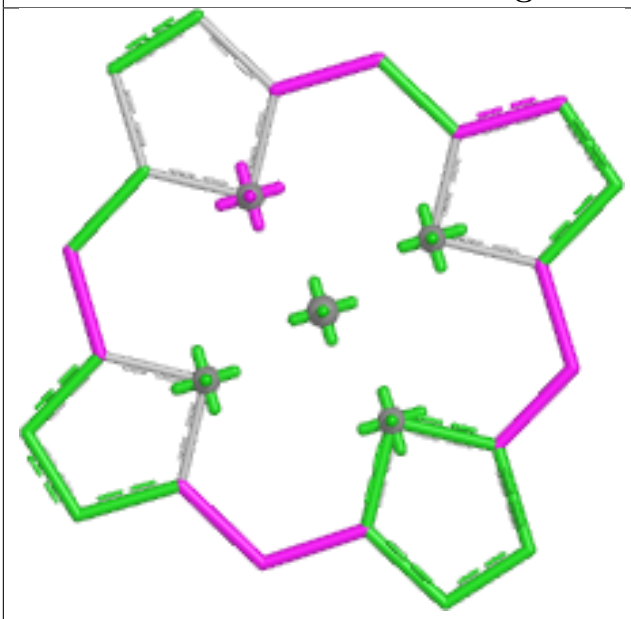


Rings

Ligand CLA B 1213



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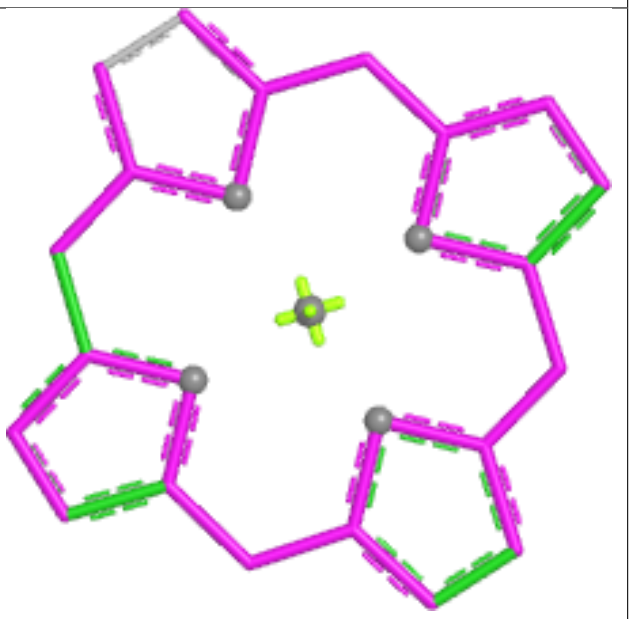

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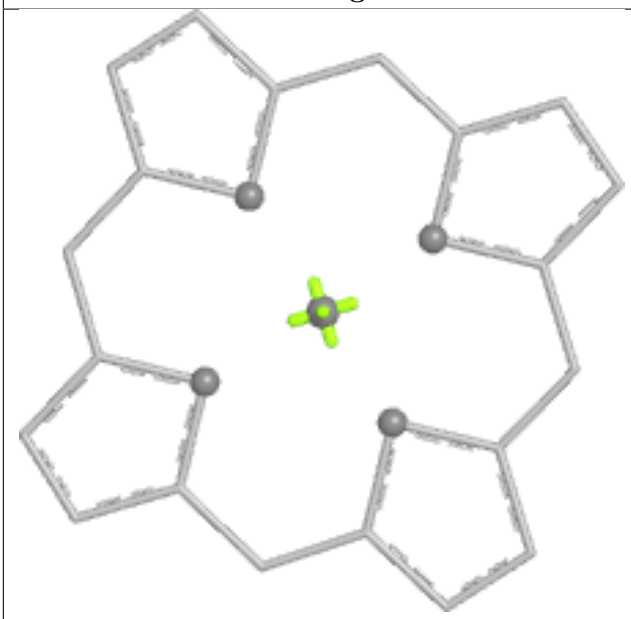

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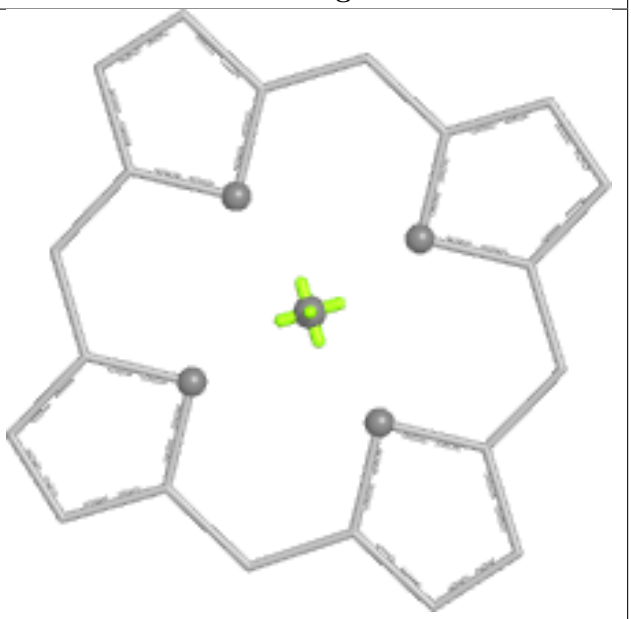
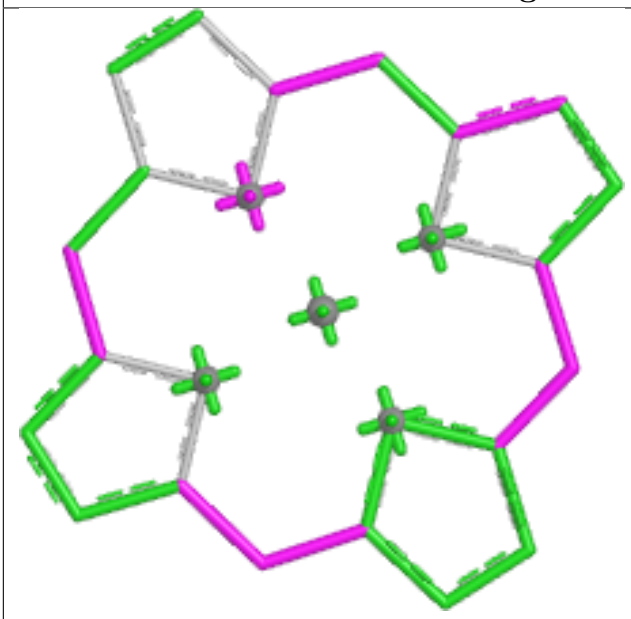


Rings

Ligand CLA 4 4008



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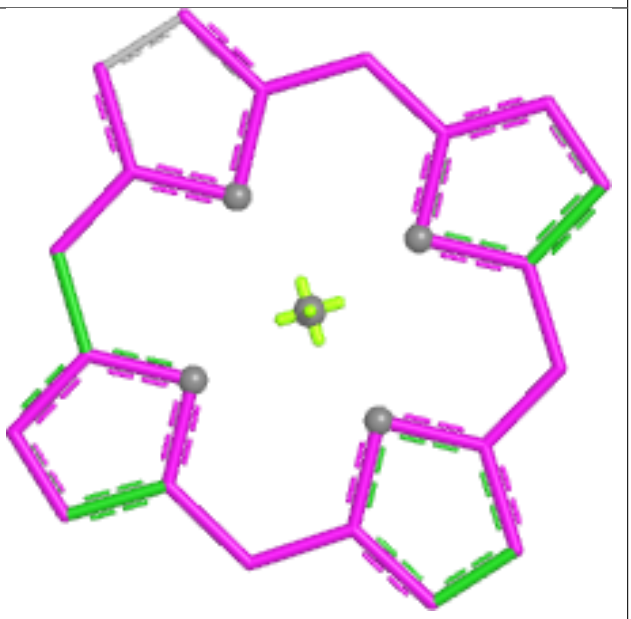

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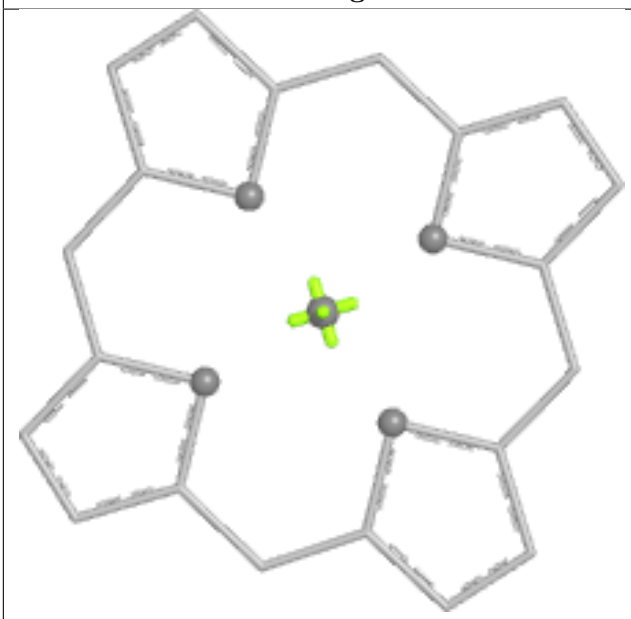

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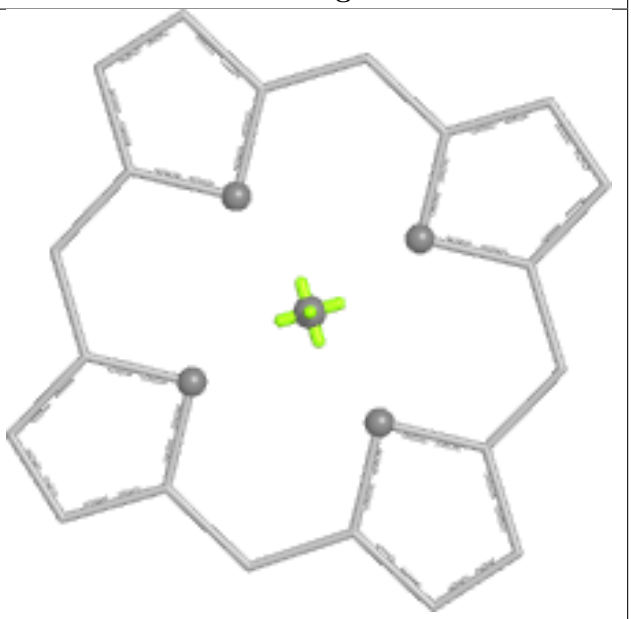
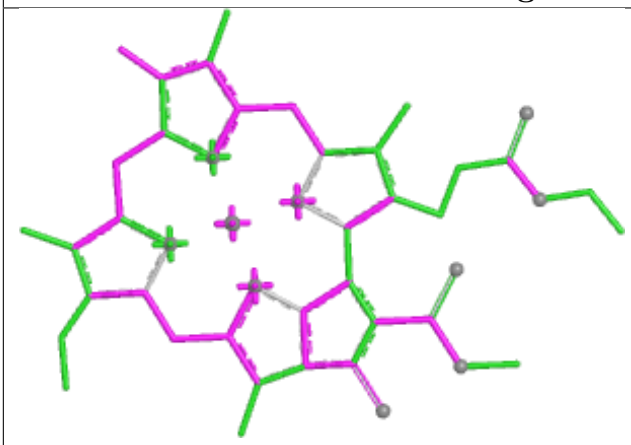


Rings

Ligand CLA L 1503



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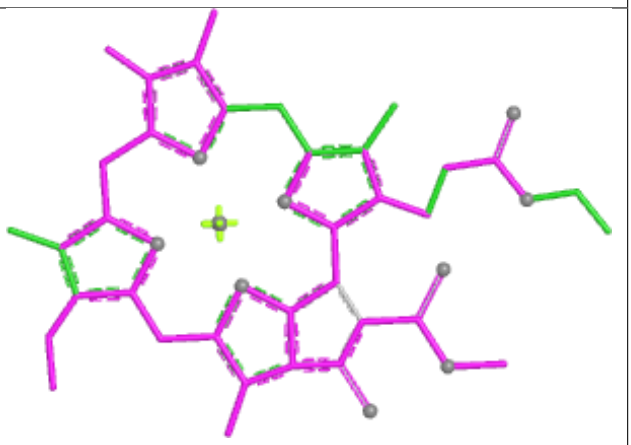

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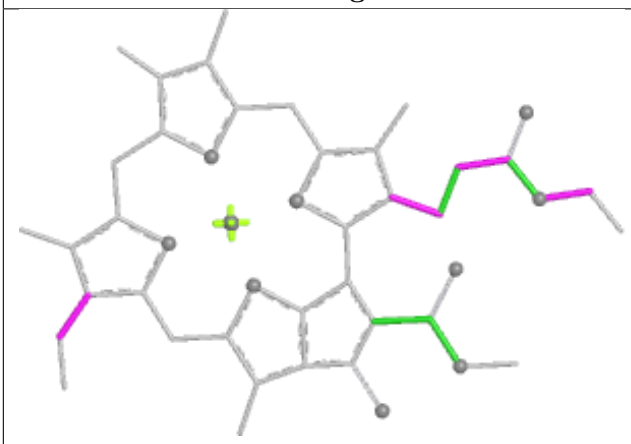

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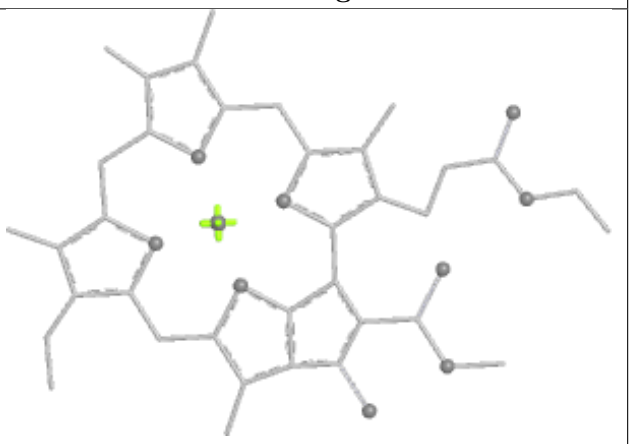
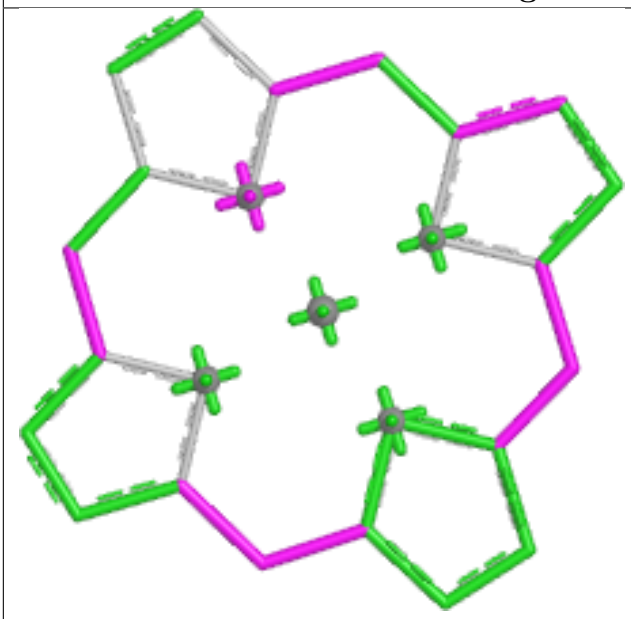


Rings

Ligand CLA 2 2011



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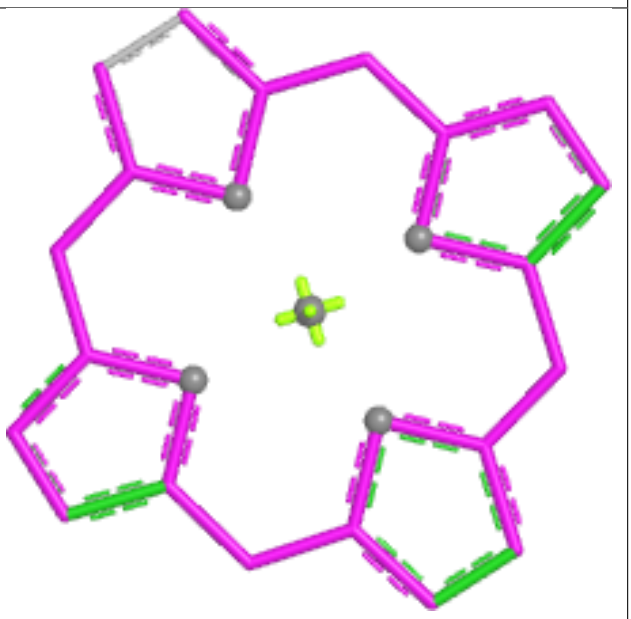
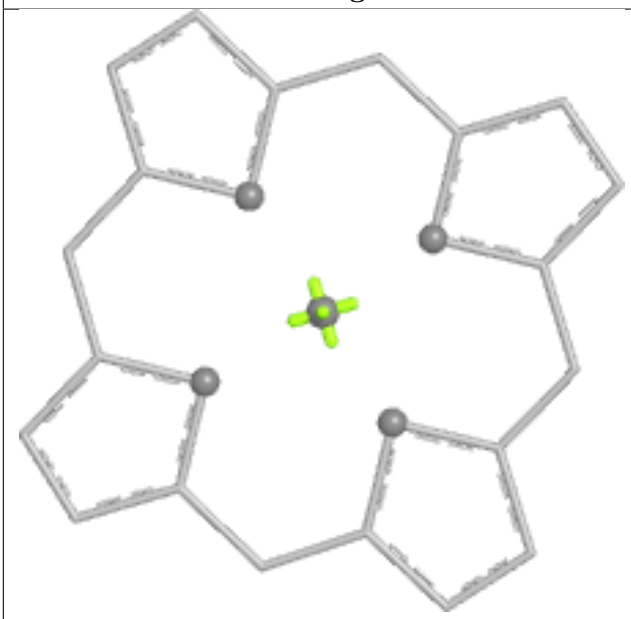


Bond angles



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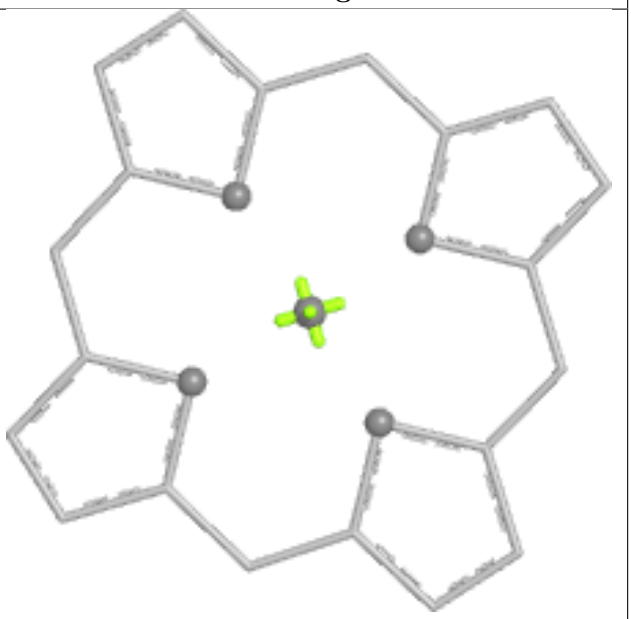
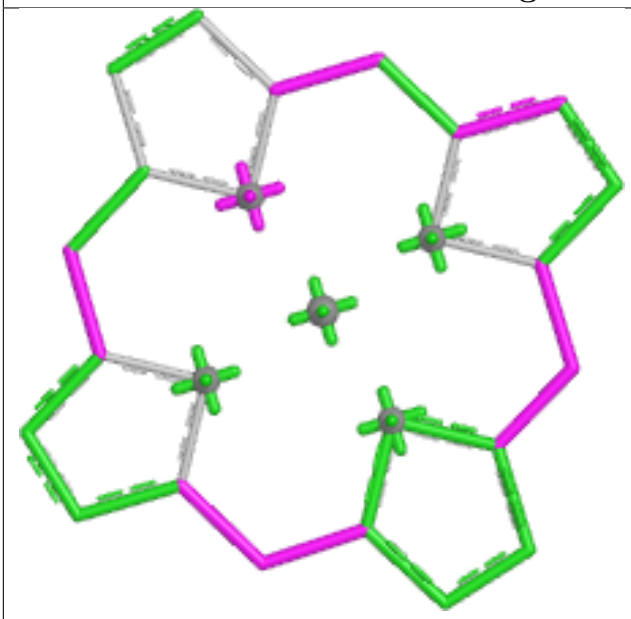


Rings

Ligand CLA 3 3013



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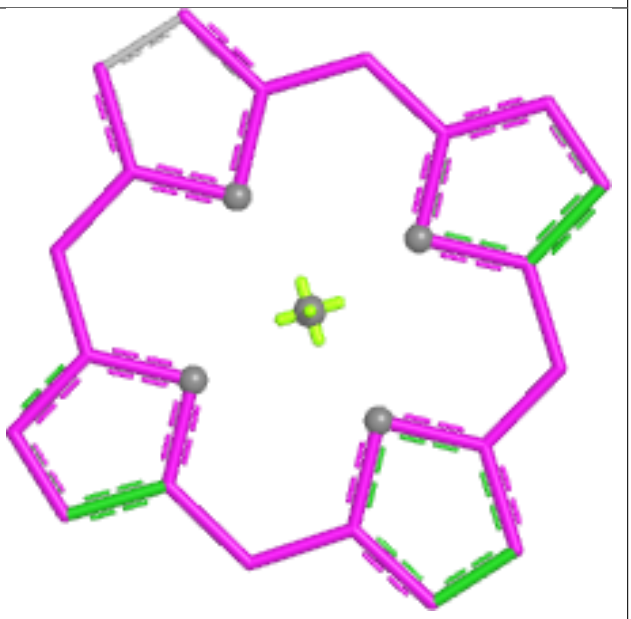

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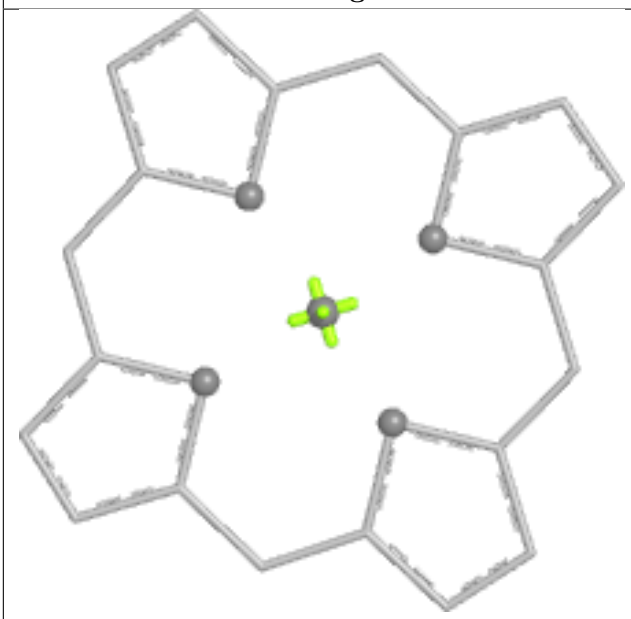

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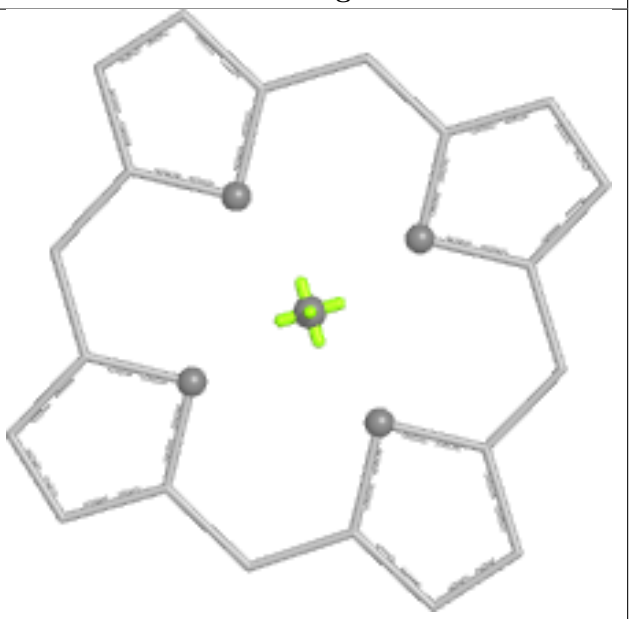
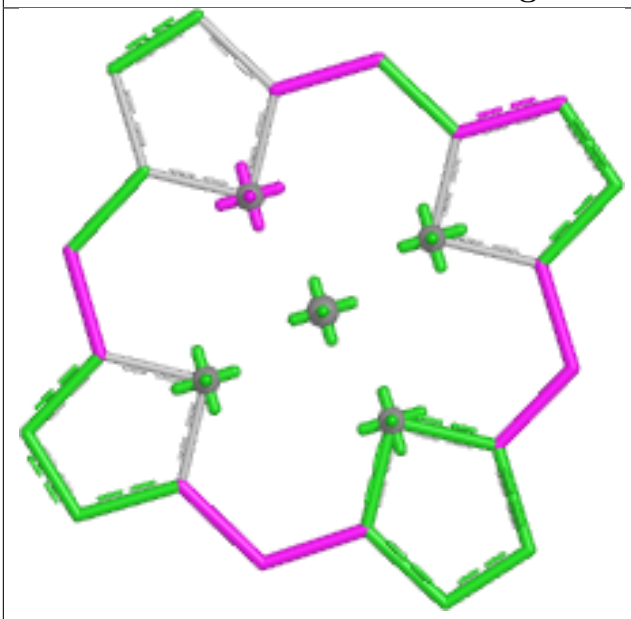


Rings

Ligand CLA 1 1003



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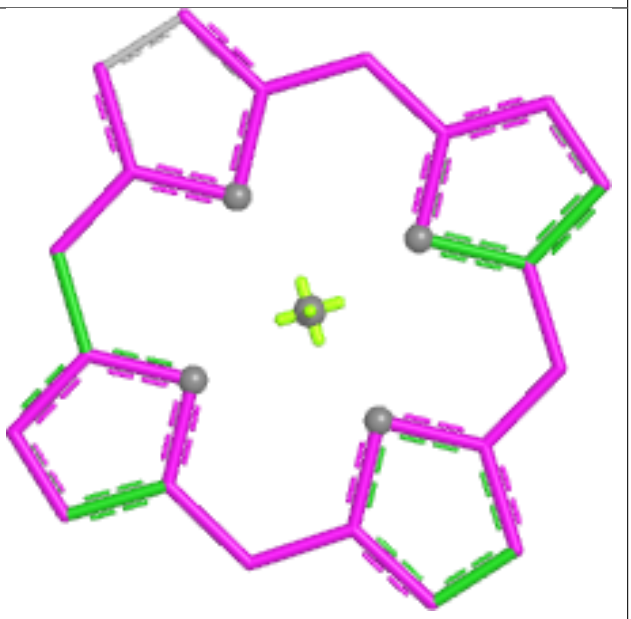

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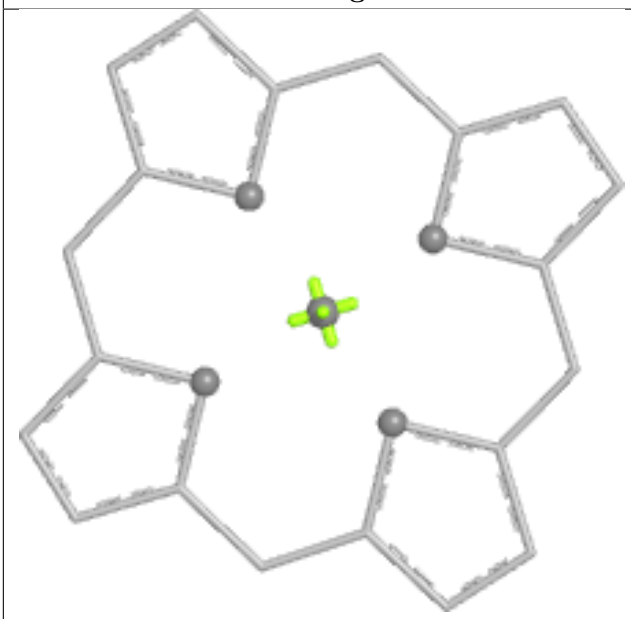

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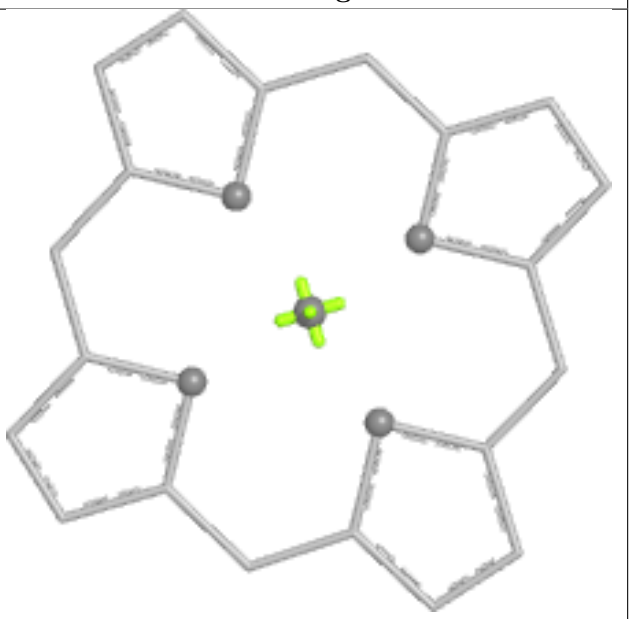
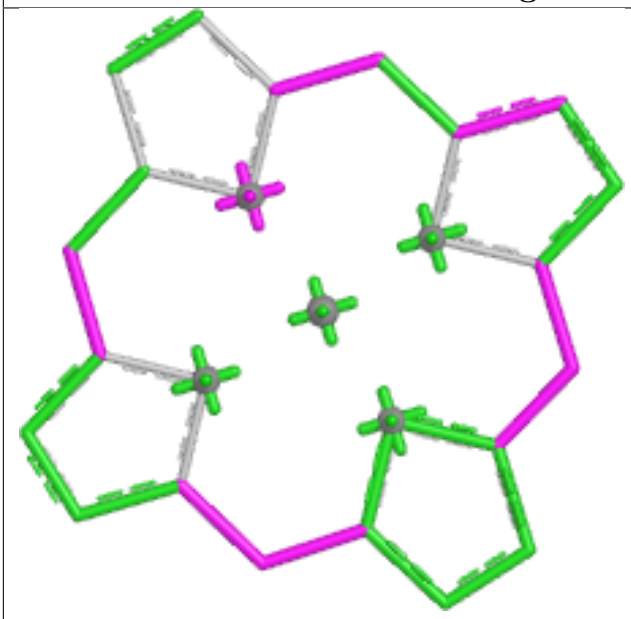


Rings

Ligand CLA 2 2005



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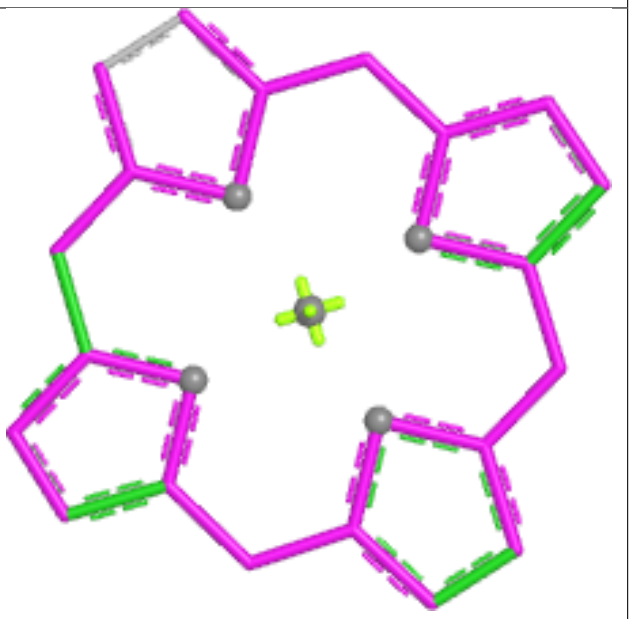

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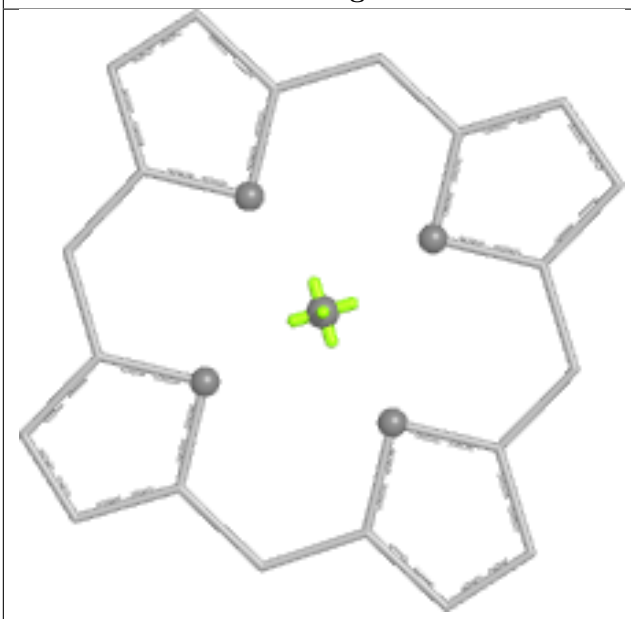

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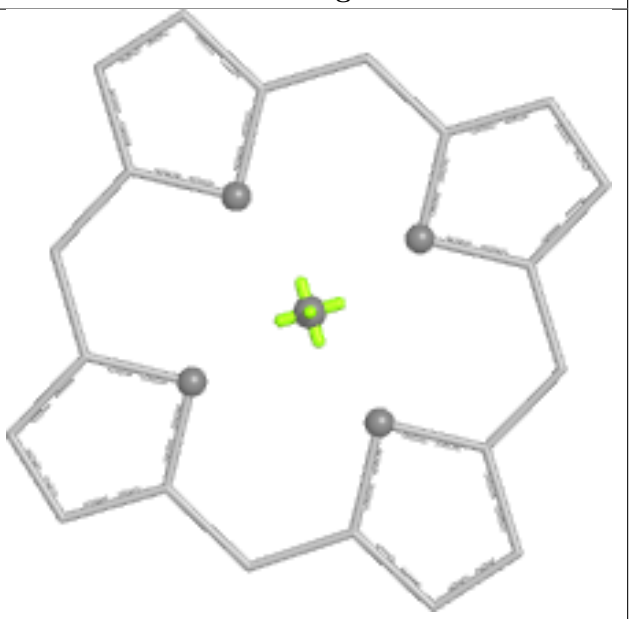
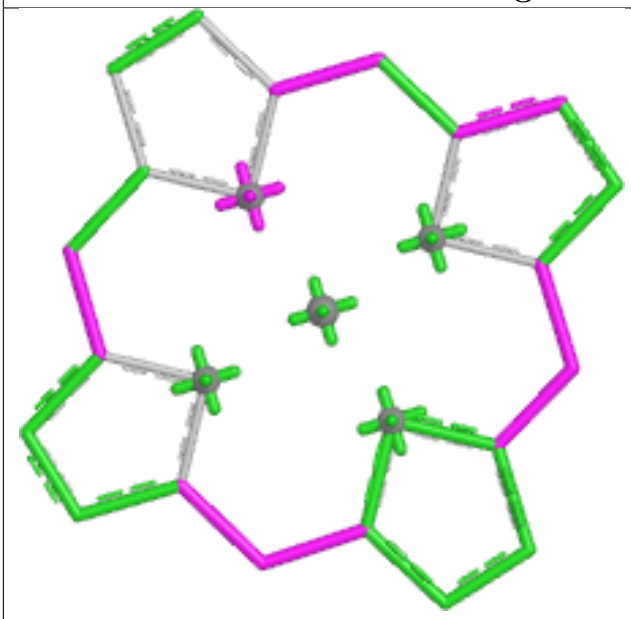


Rings

Ligand CLA A 1110



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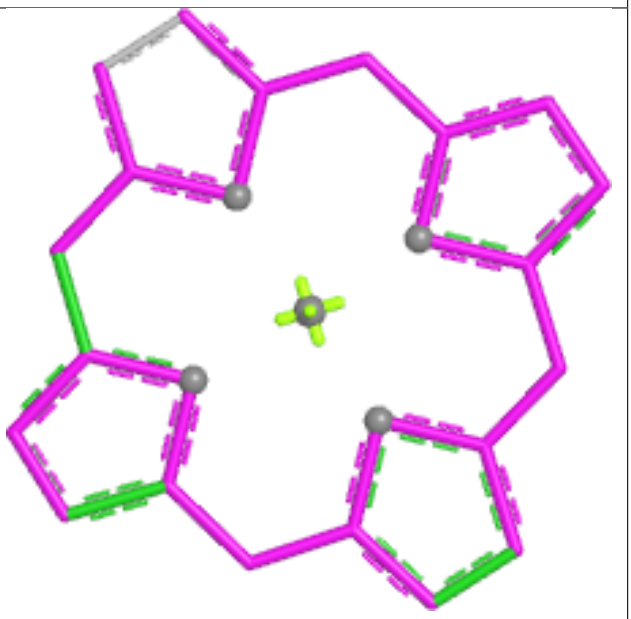

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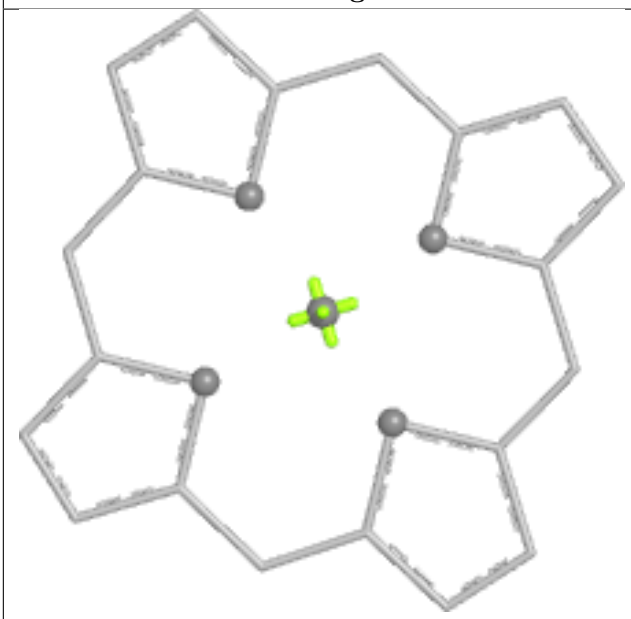

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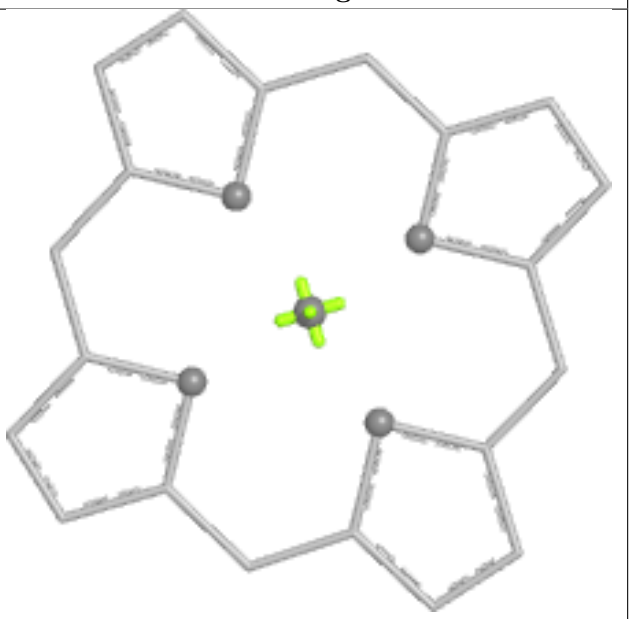
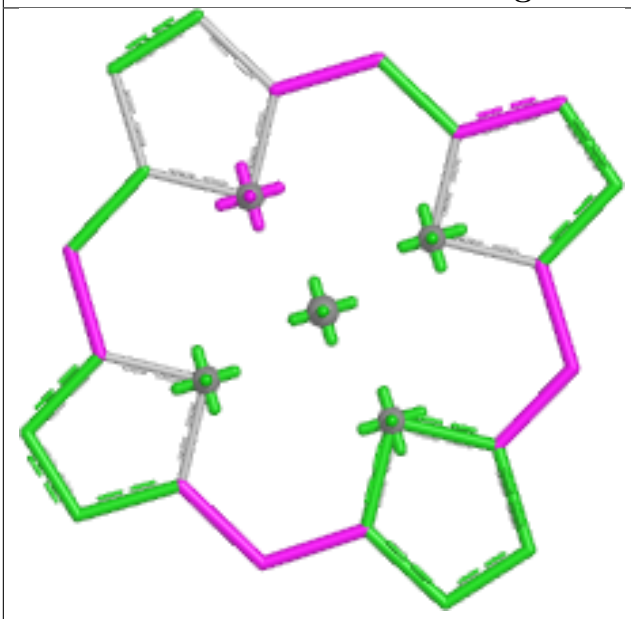


Rings

Ligand CLA K 1150



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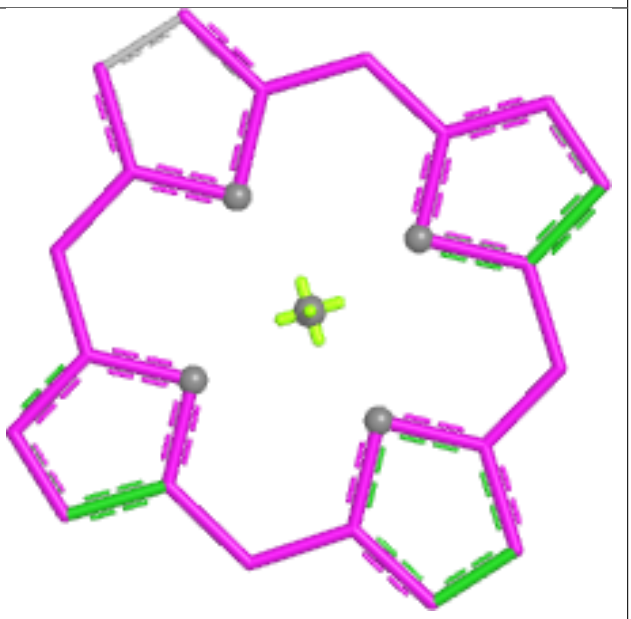

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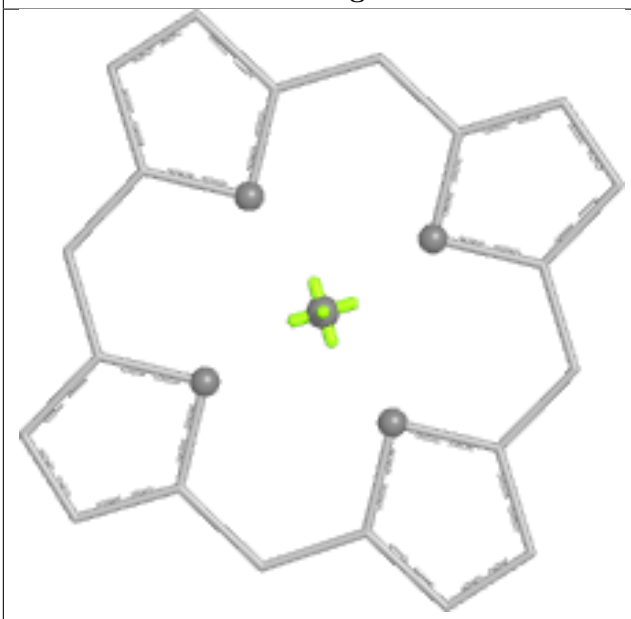

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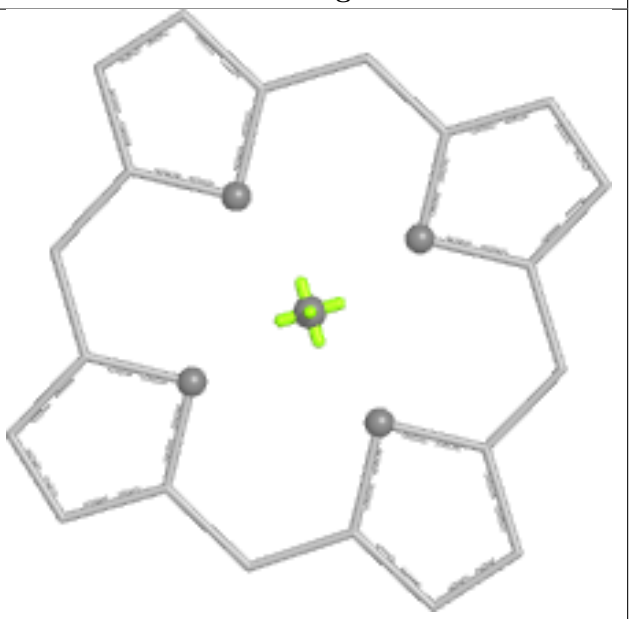
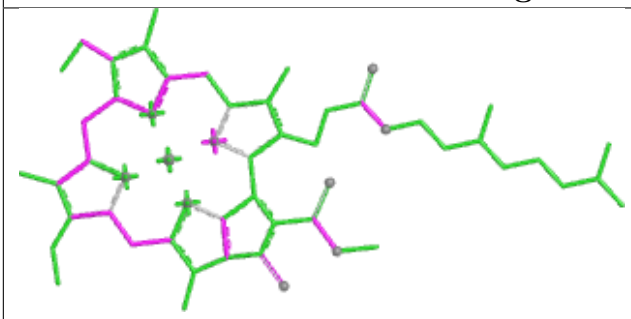


Rings

Ligand CLA A 1136



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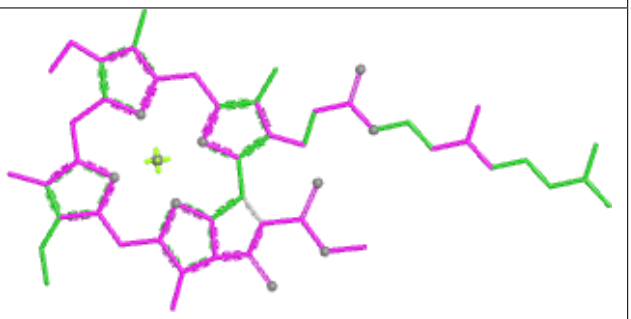

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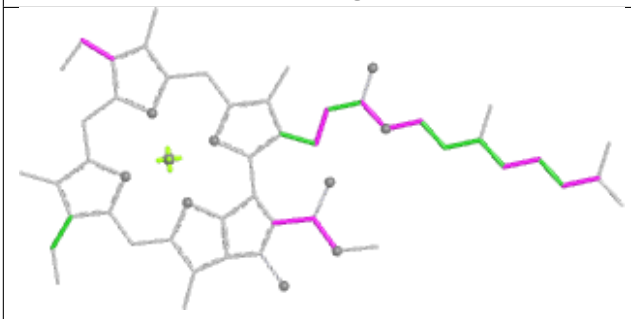

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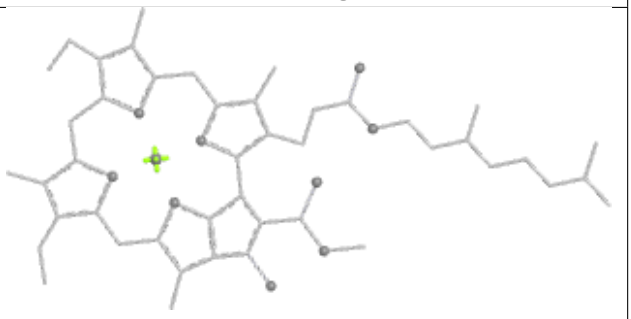
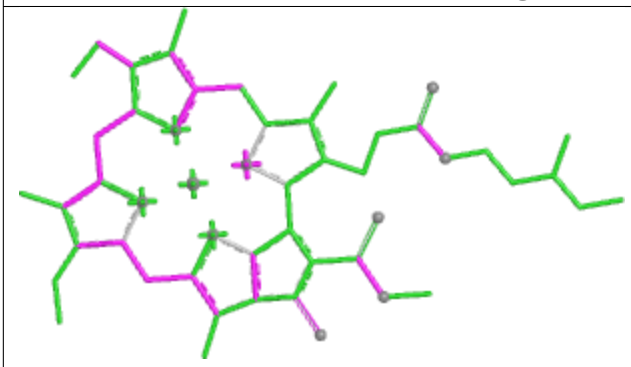


Rings

Ligand CLA G 1233



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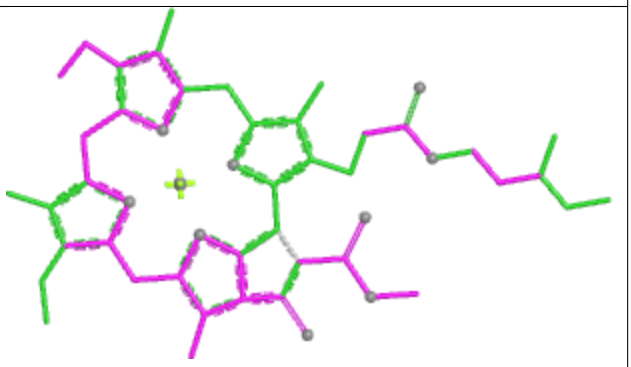
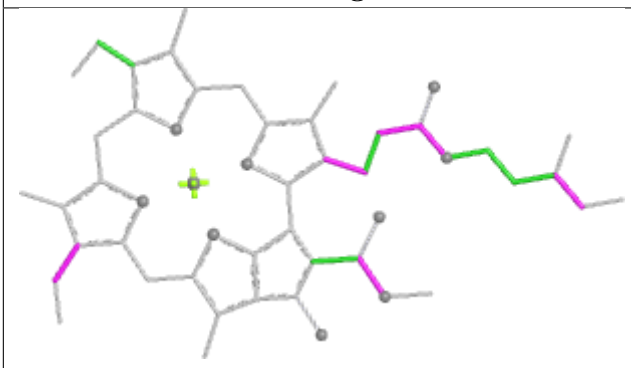


Bond angles



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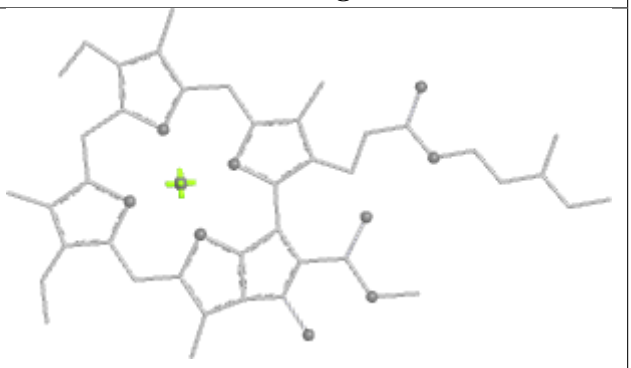
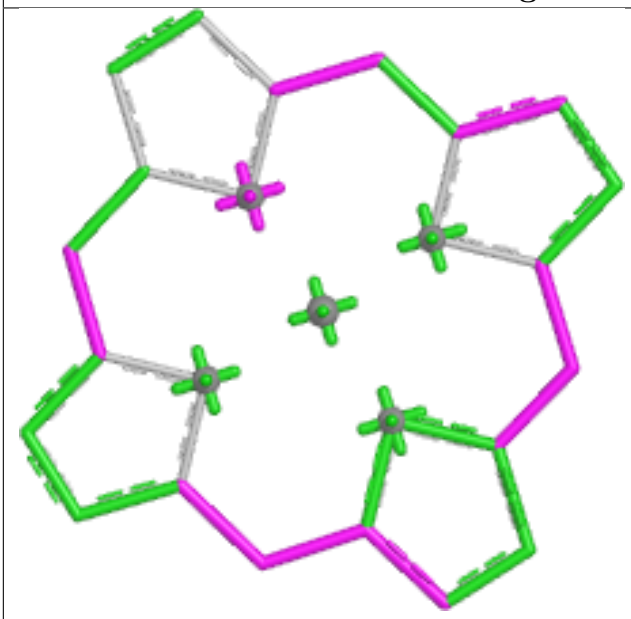


Rings

Ligand CLA 3 3005



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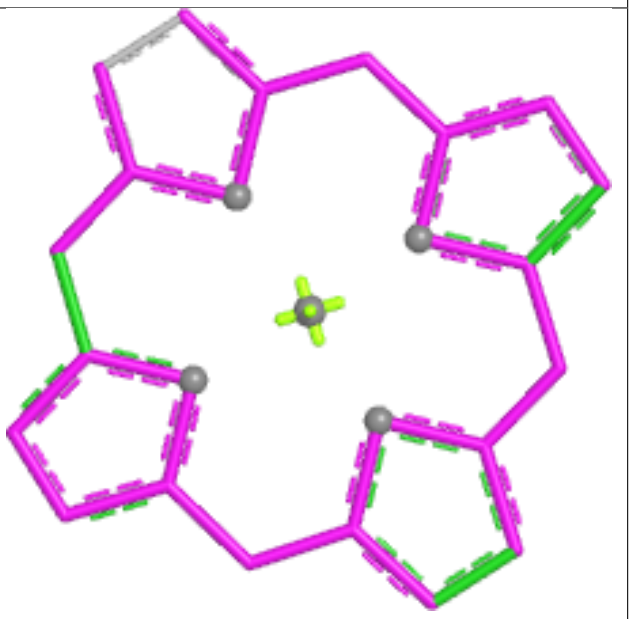
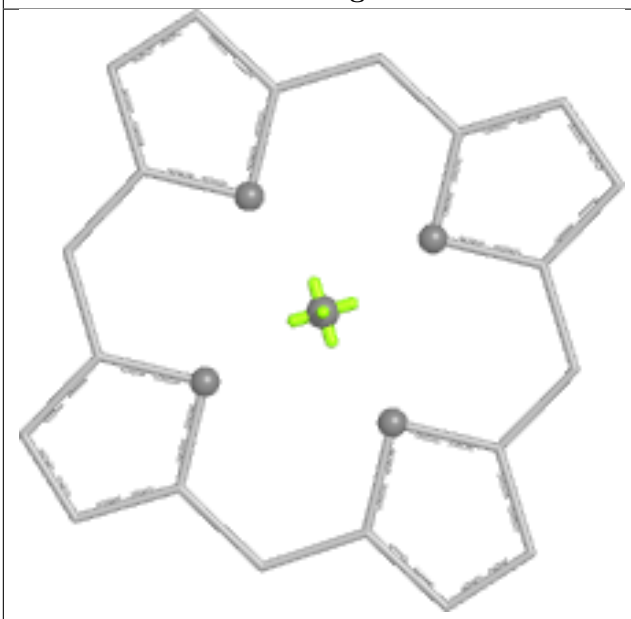


Bond angles



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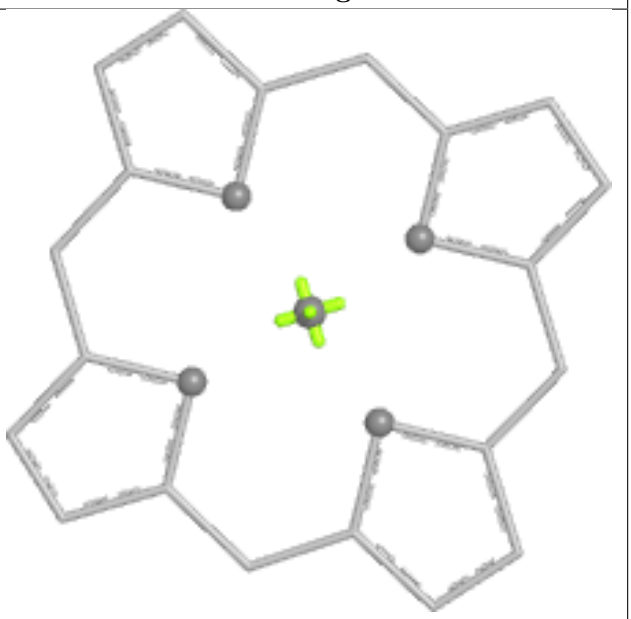
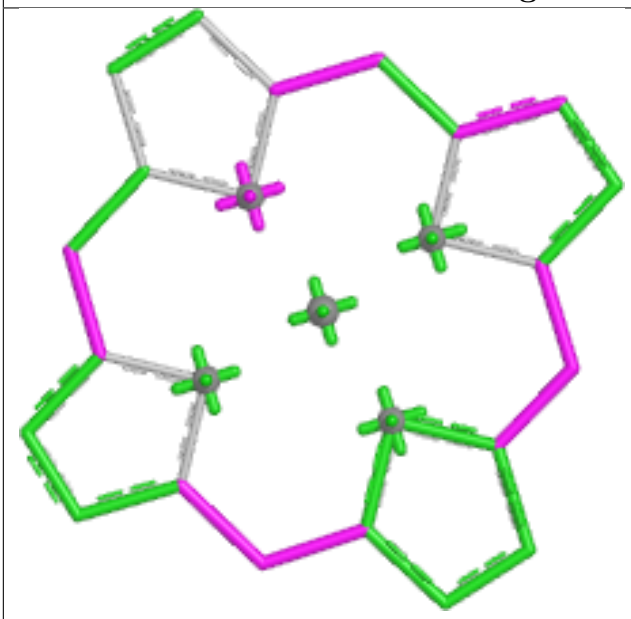


Rings

Ligand CLA 3 3008



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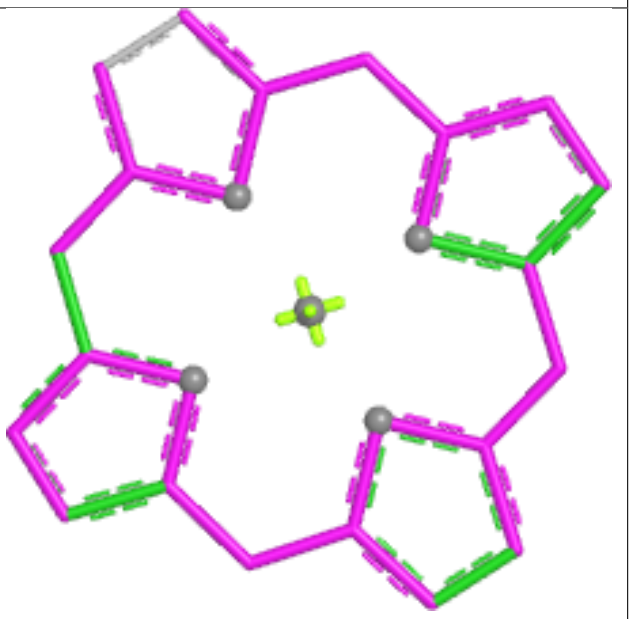

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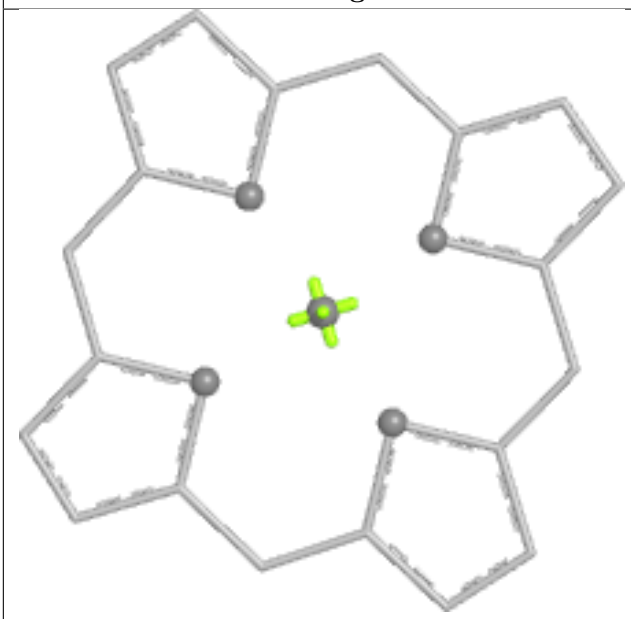
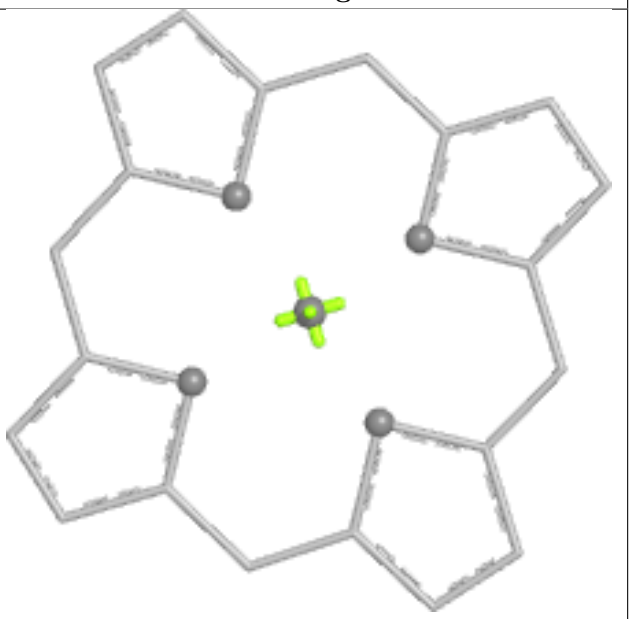
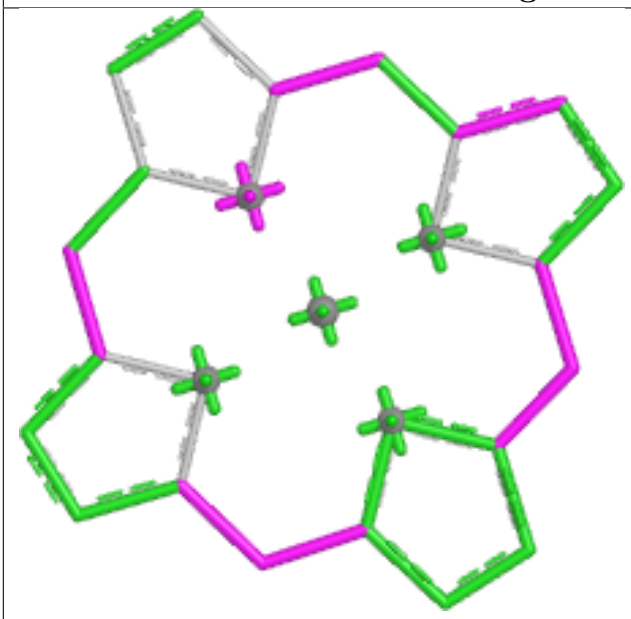


Torsions



Rings

Ligand CLA 1 1004



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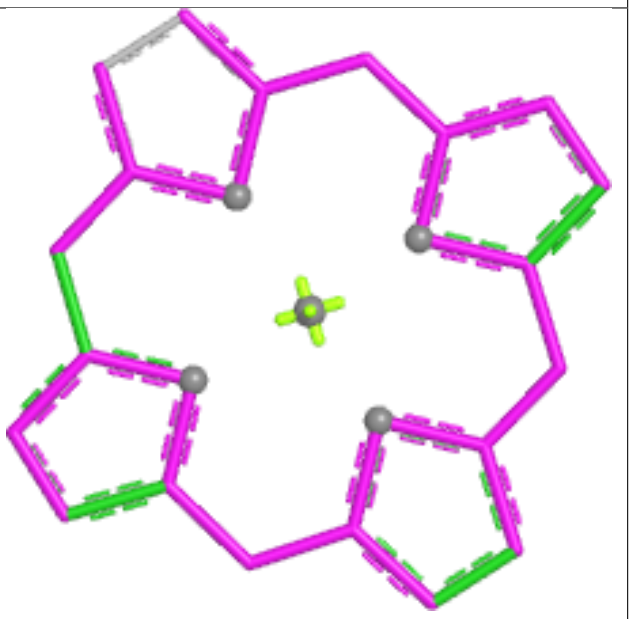

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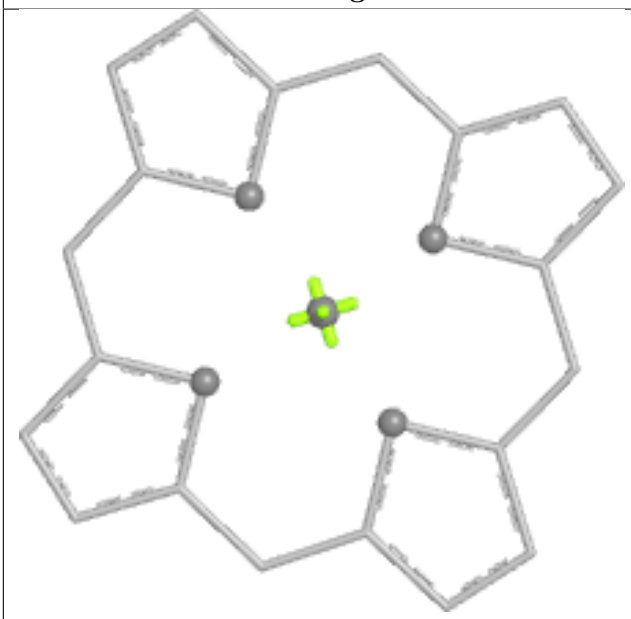

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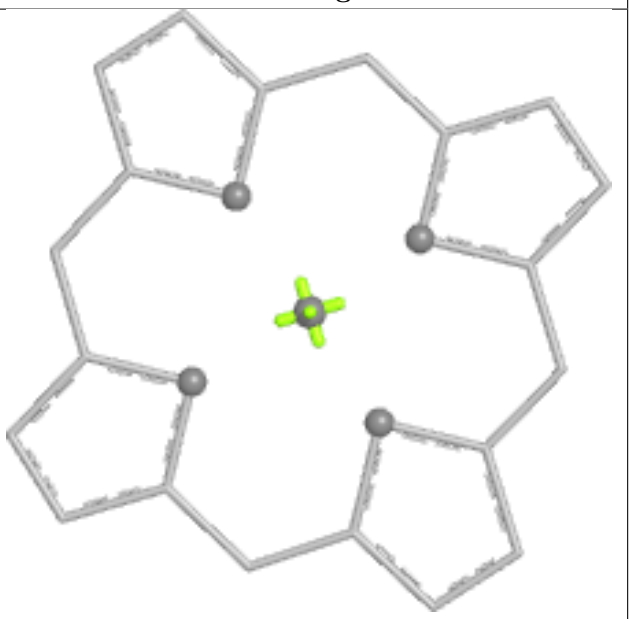
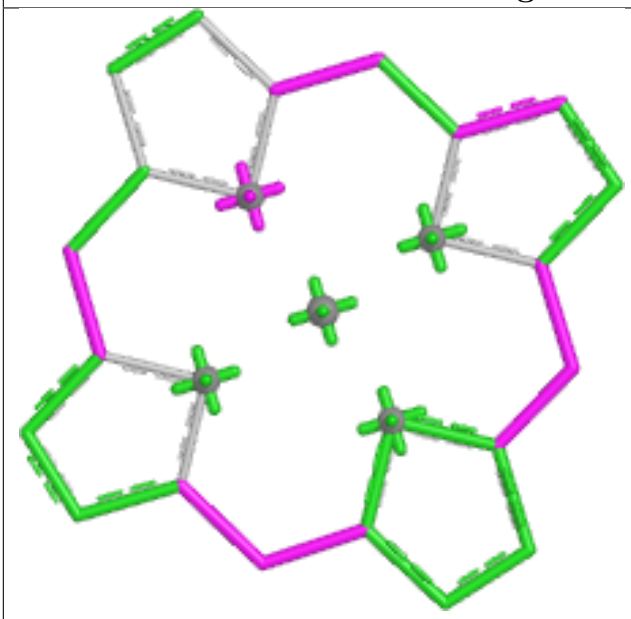


Rings

Ligand CLA F 1240



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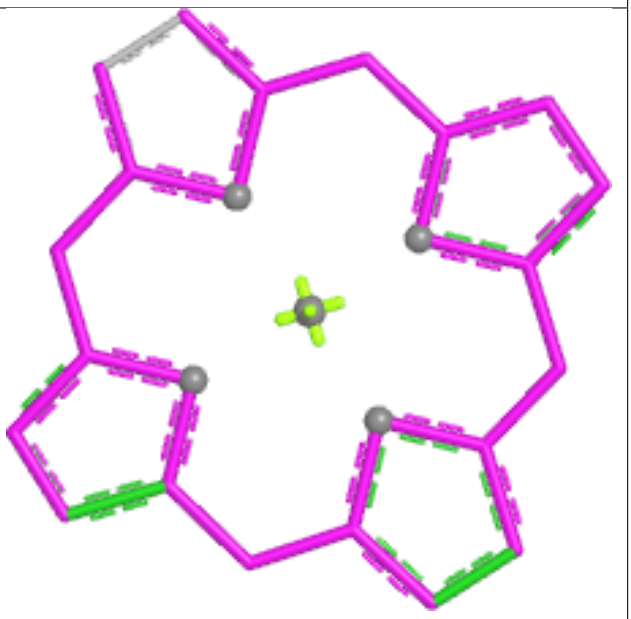

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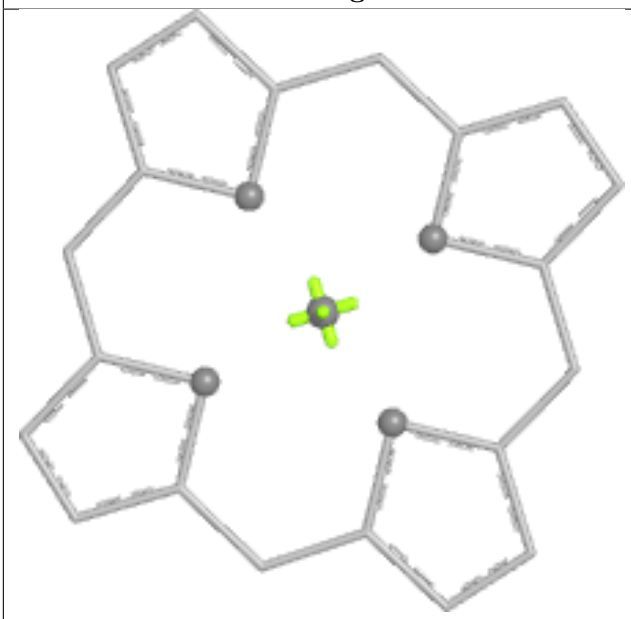

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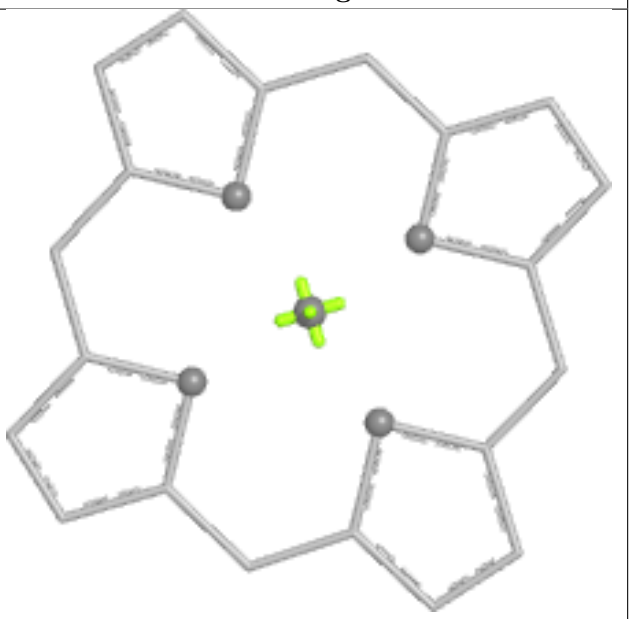

Rings

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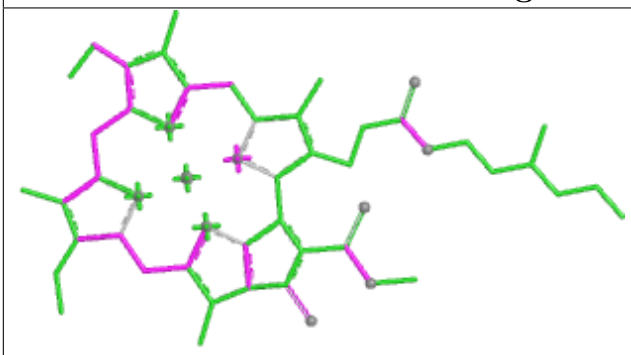
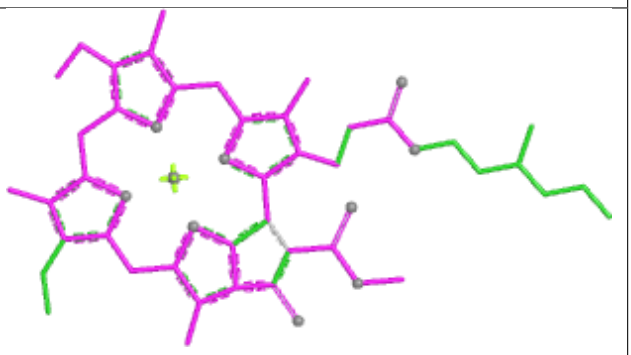
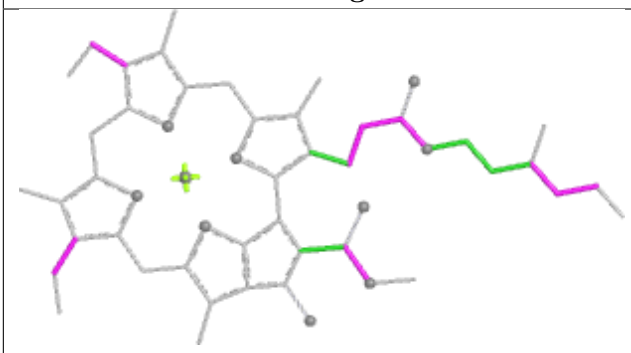
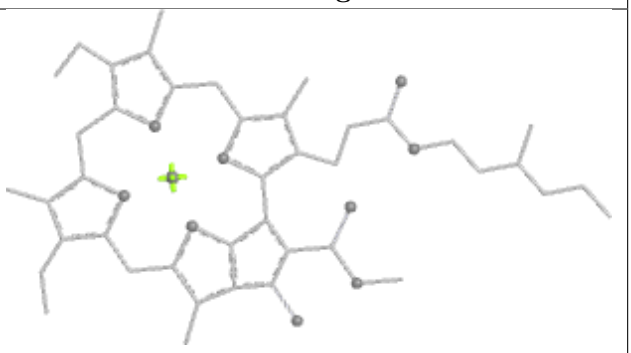
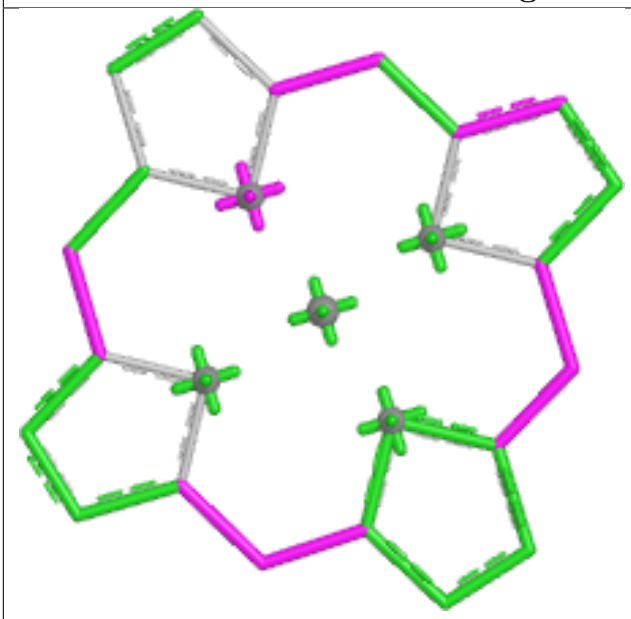
 Bond lengths	 Bond angles
 Torsions	 Rings

Ligand CLA 3 3002



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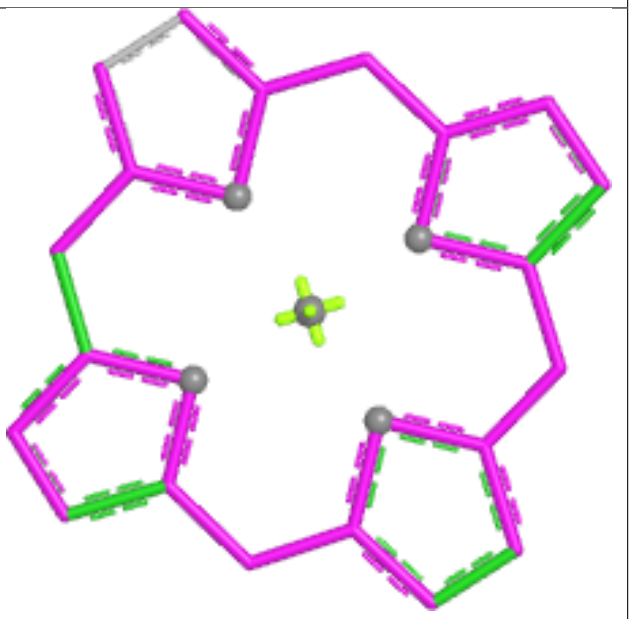

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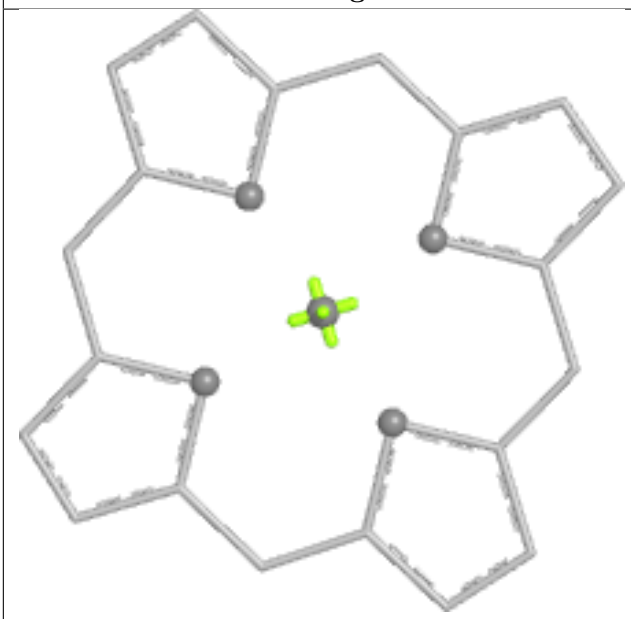

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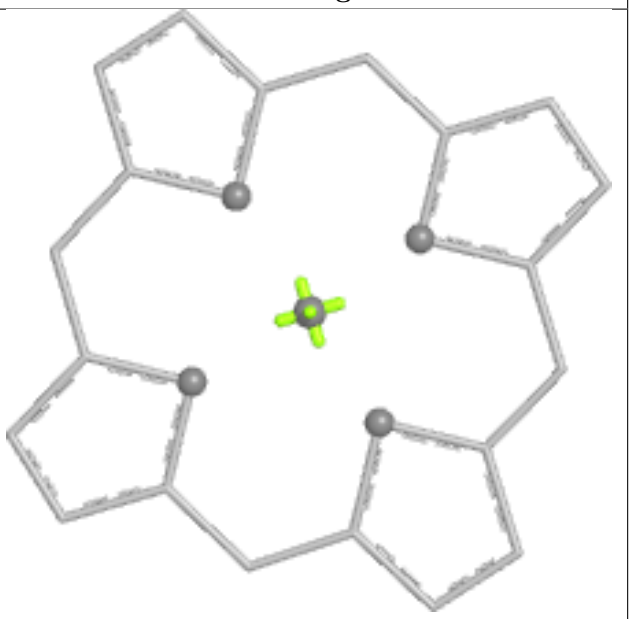
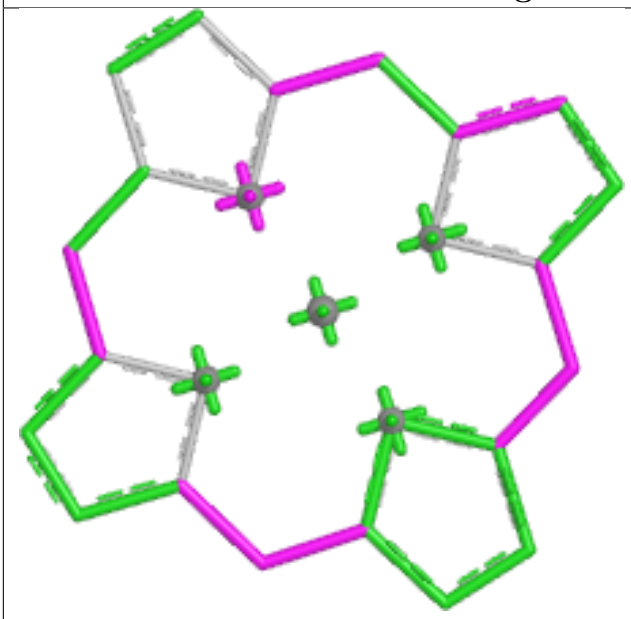


Rings

Ligand CLA A 1146



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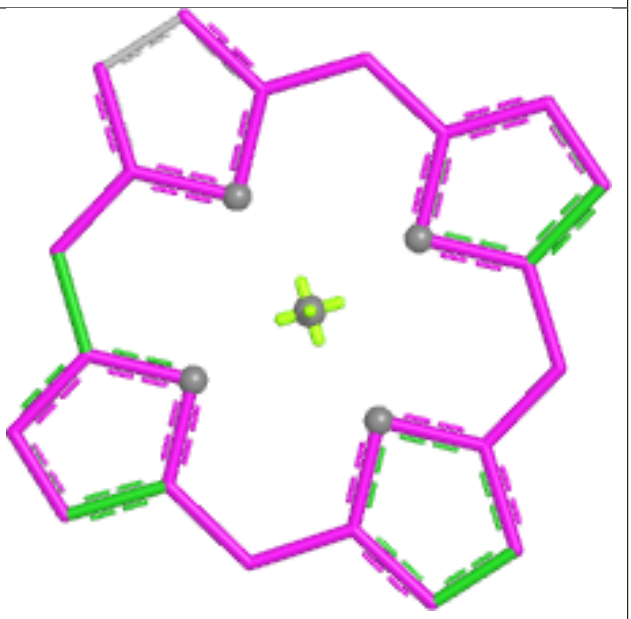

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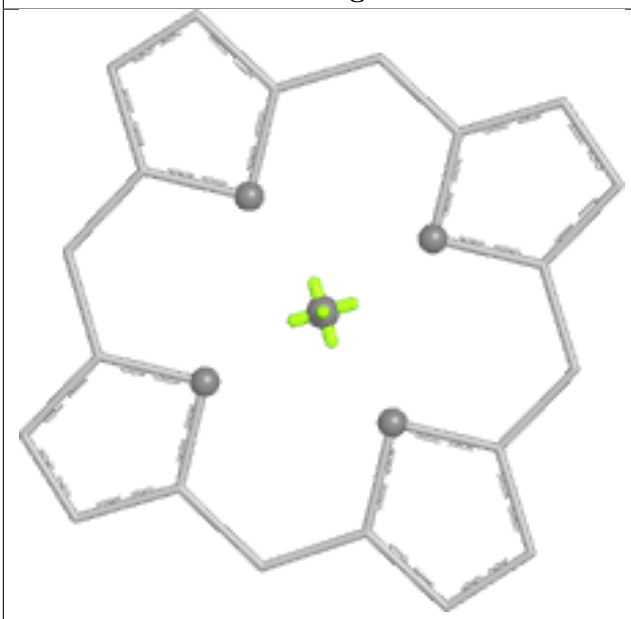

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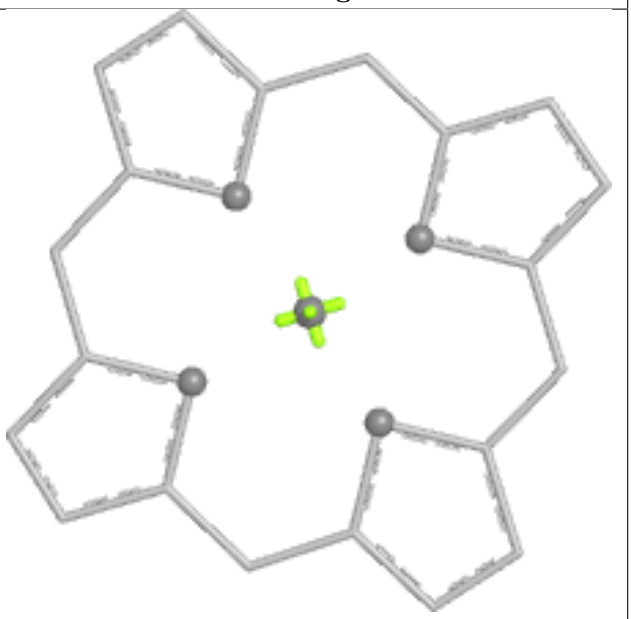
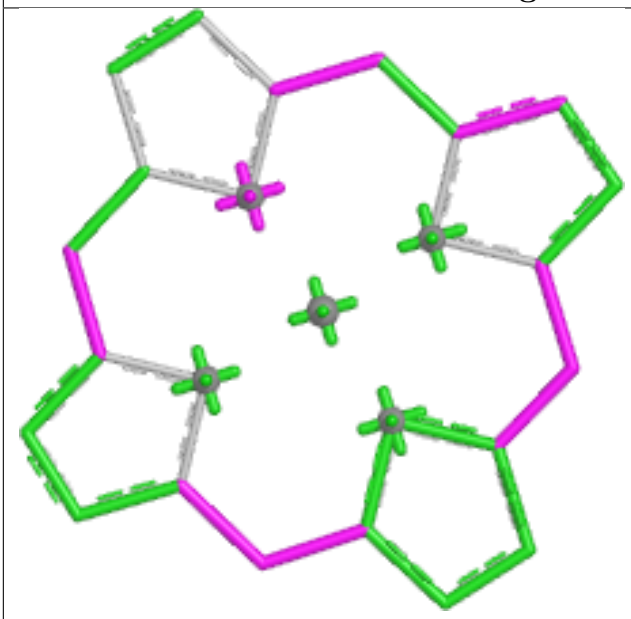


Rings

Ligand CLA 1 1002



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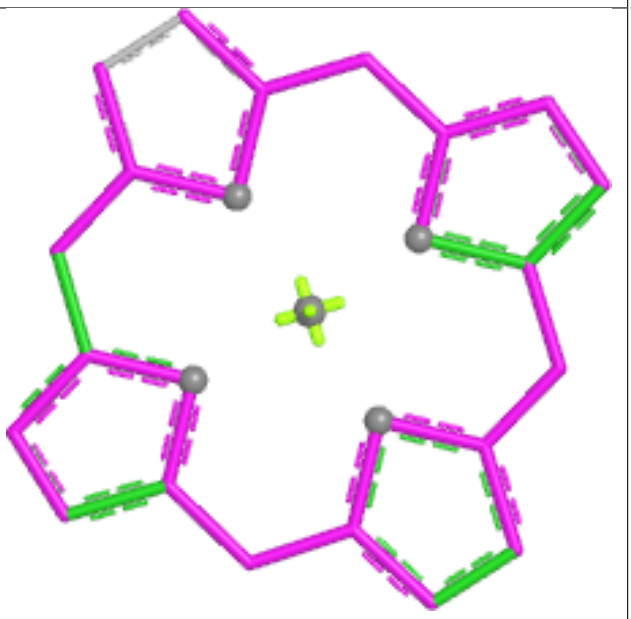

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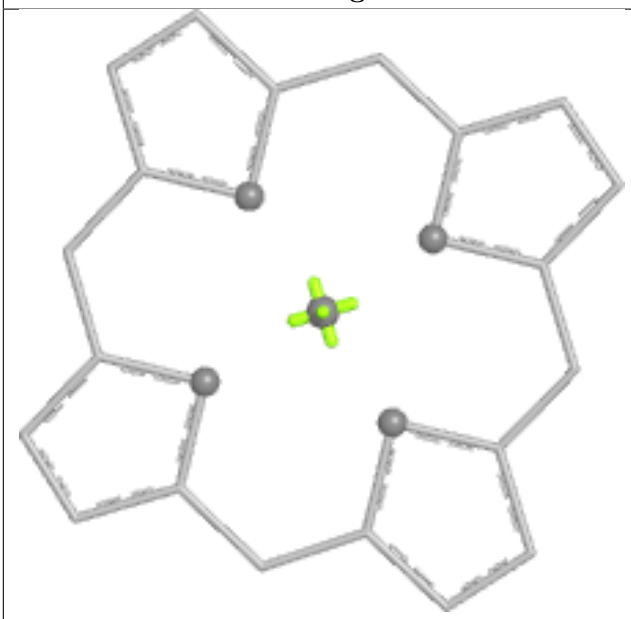

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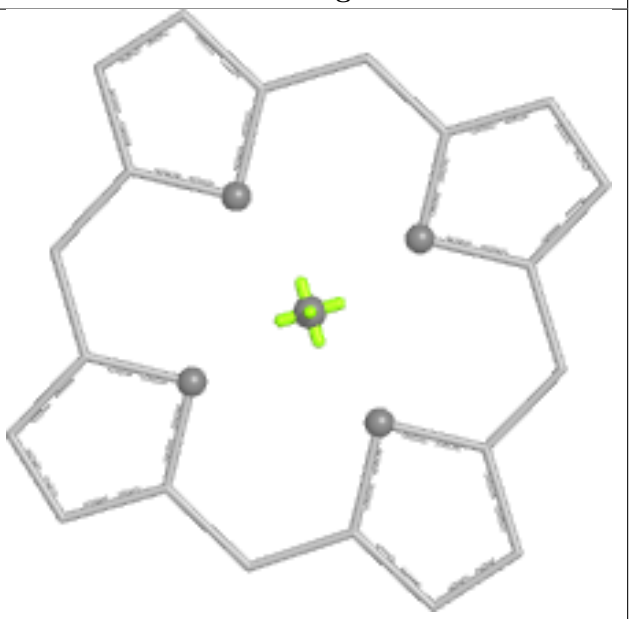
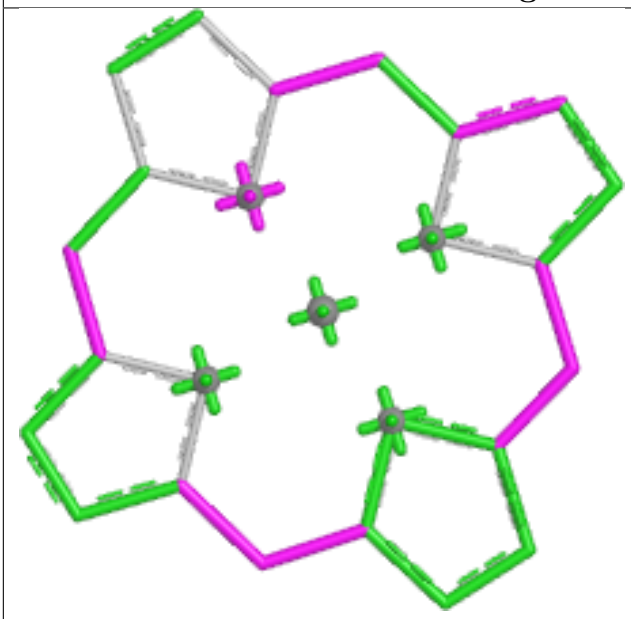


Rings

Ligand CLA 4 4006



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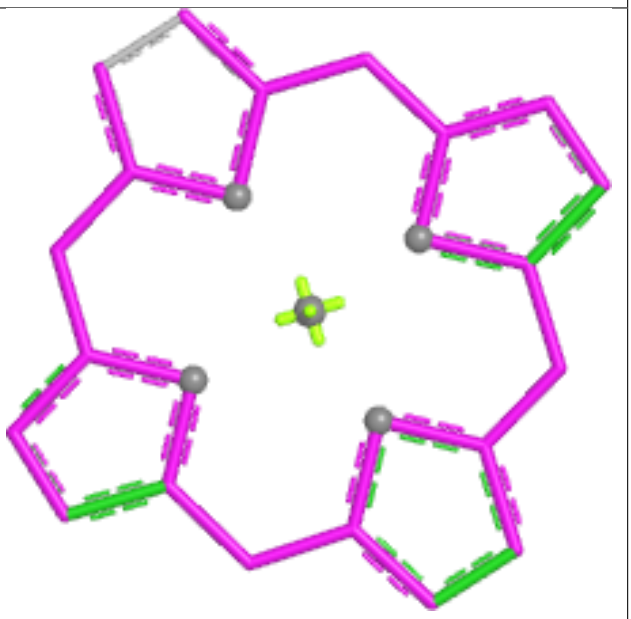

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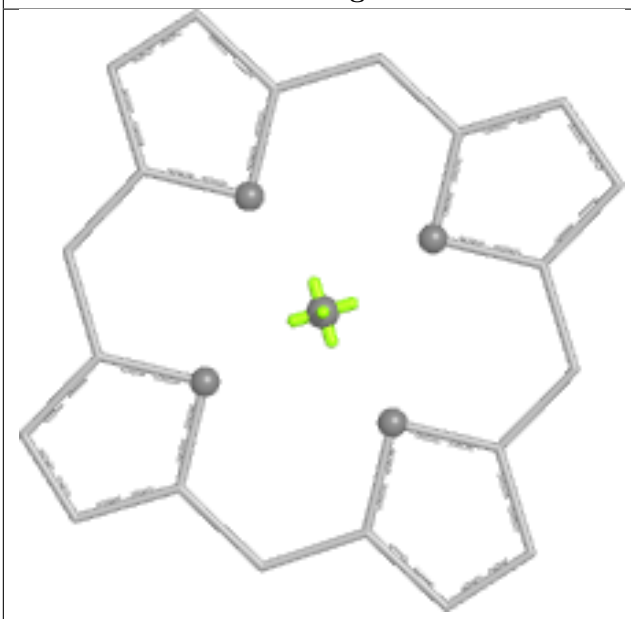

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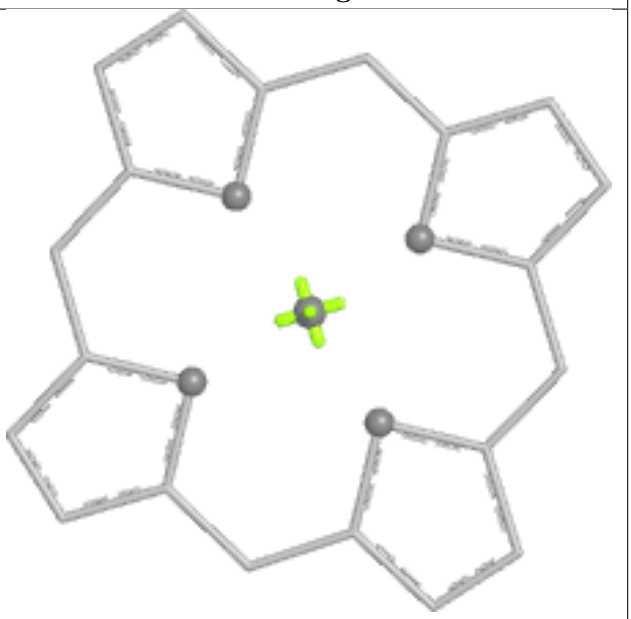
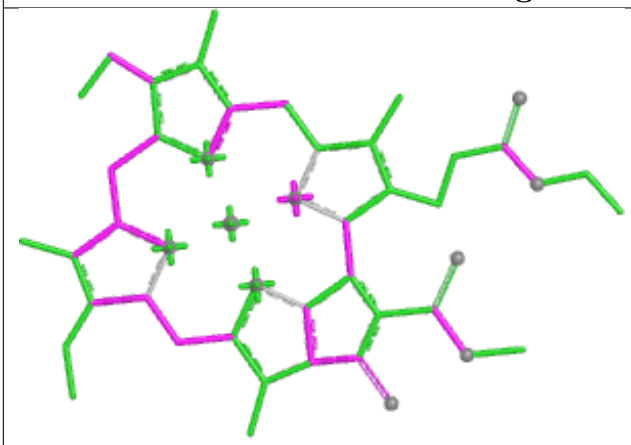


Rings

Ligand CLA B 9010



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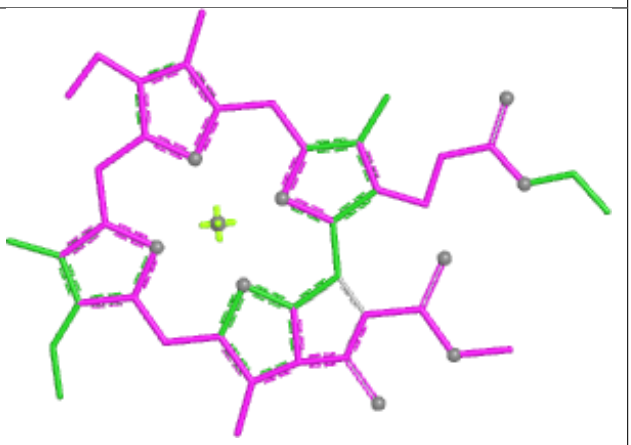

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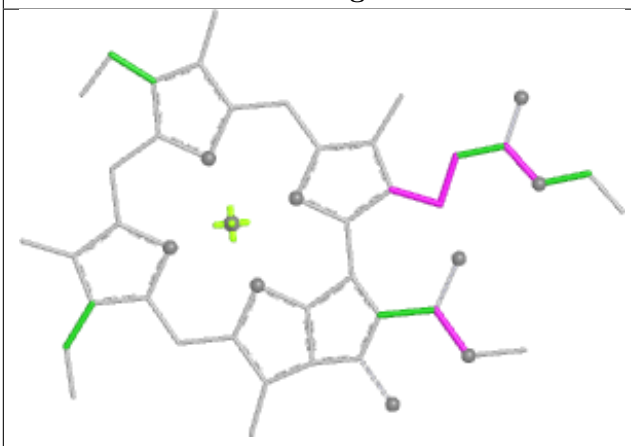

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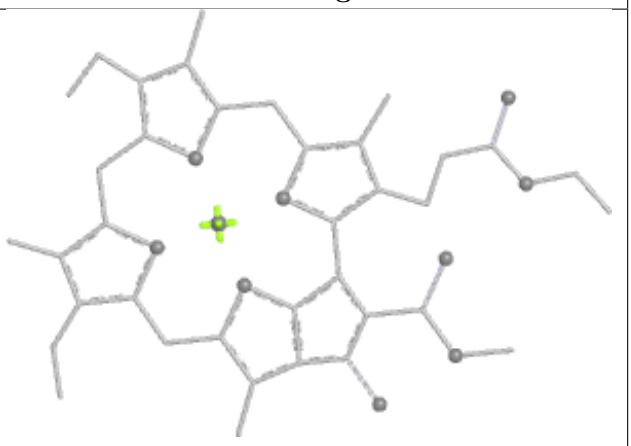
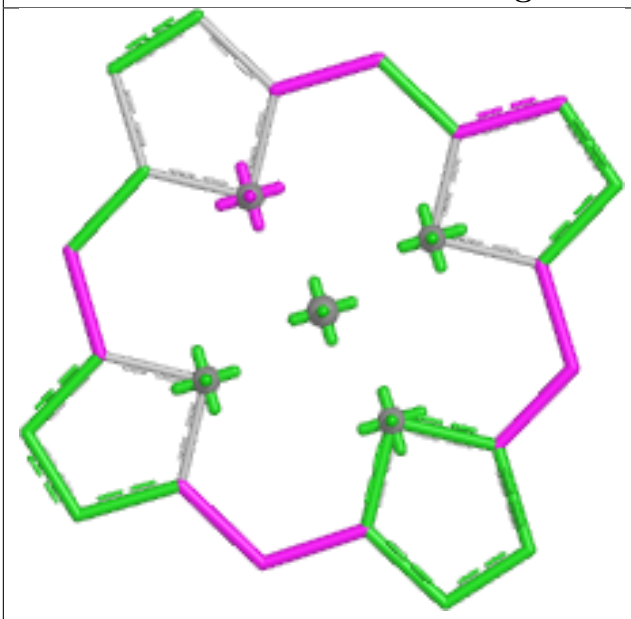


Rings

Ligand CLA A 1148



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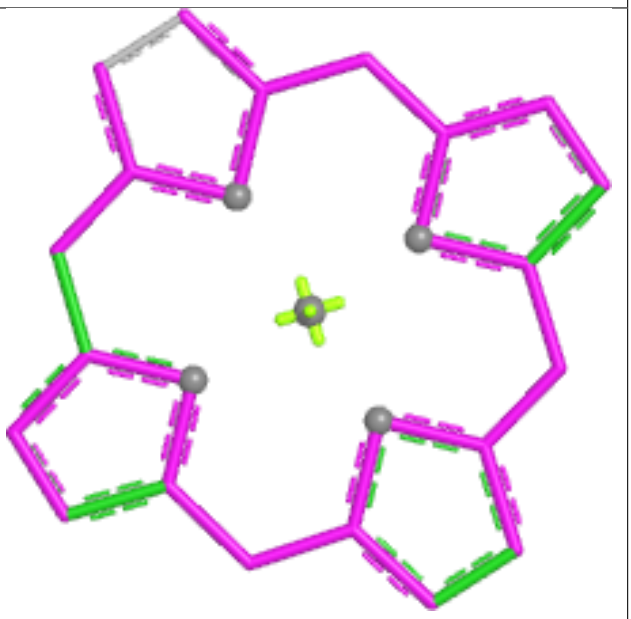

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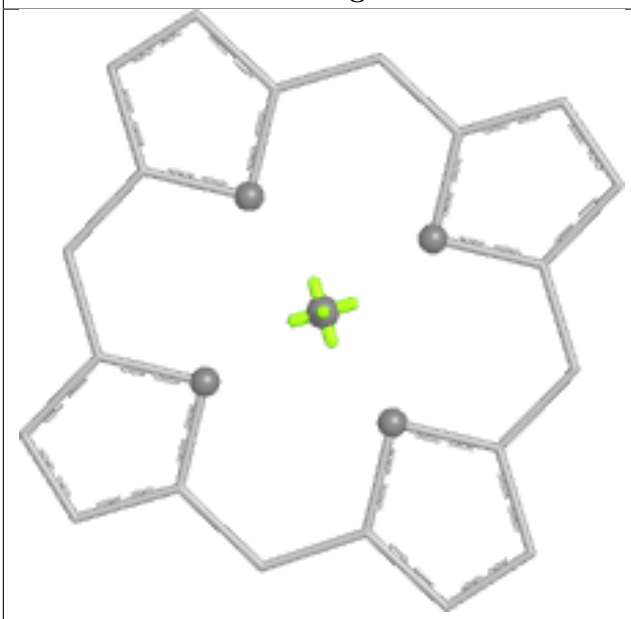

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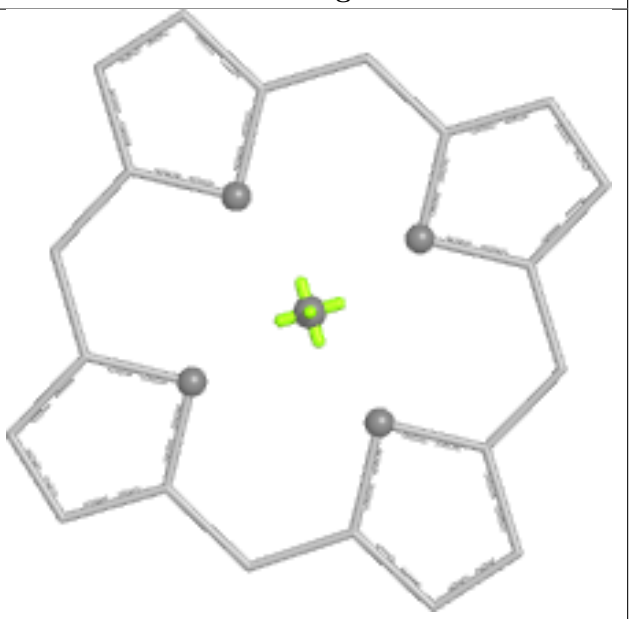
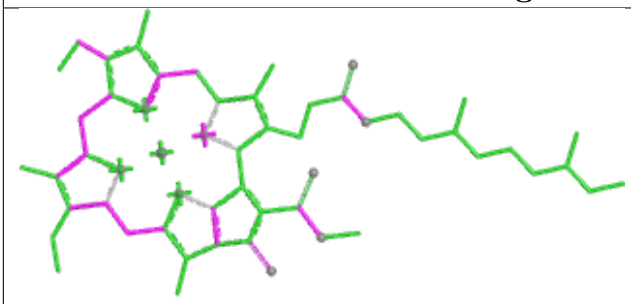


Rings

Ligand CLA B 1216



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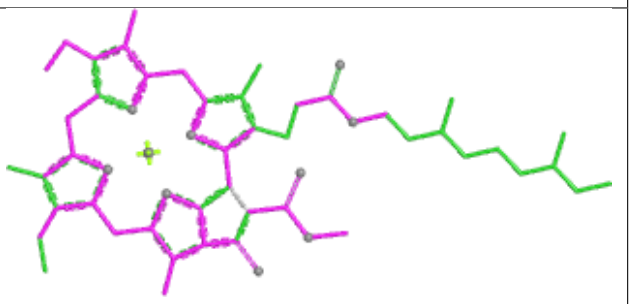

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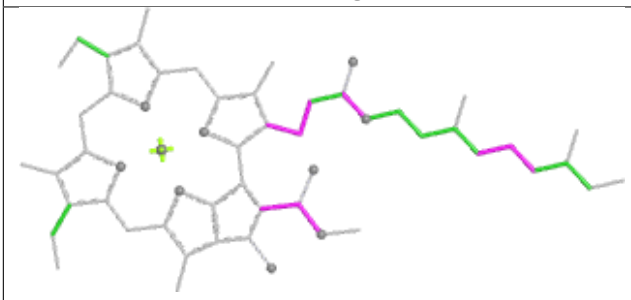

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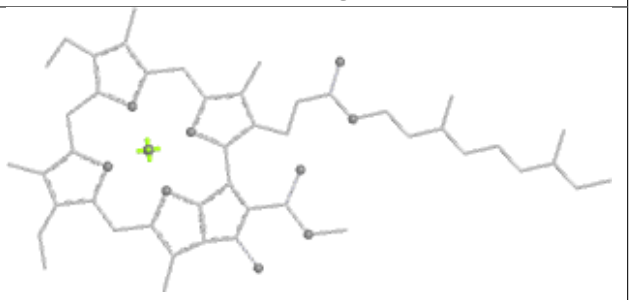
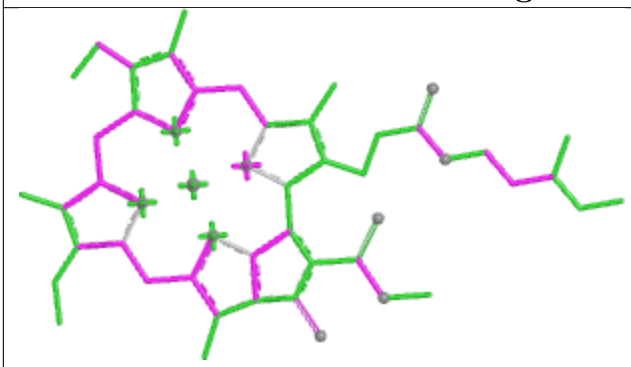


Rings

Ligand CLA B 1218



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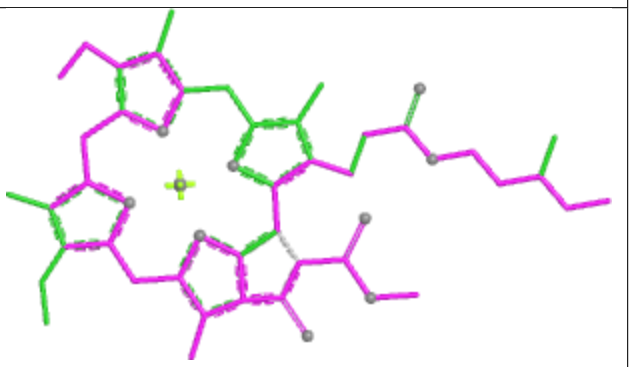

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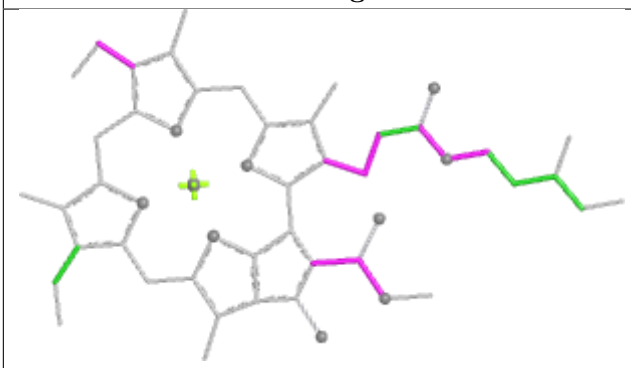

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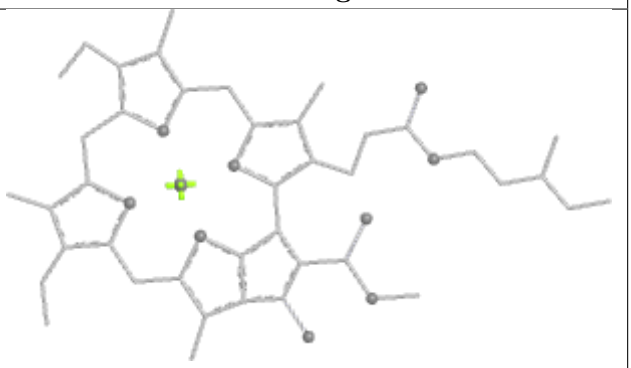
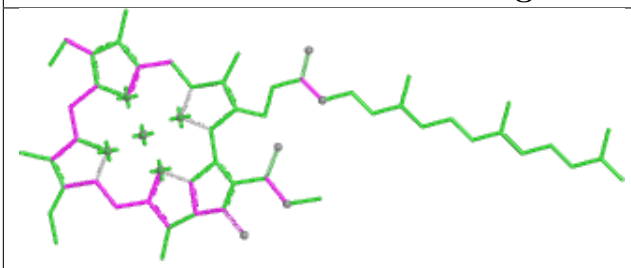
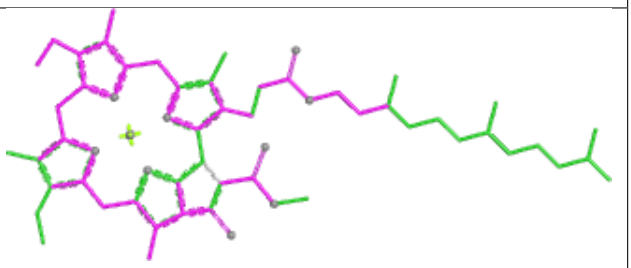
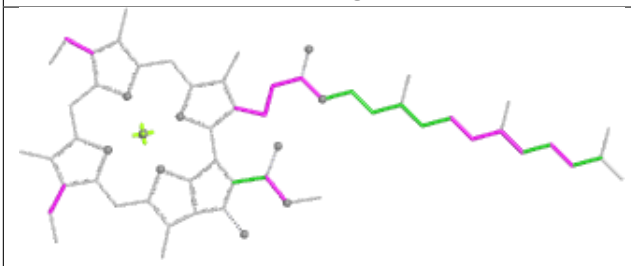
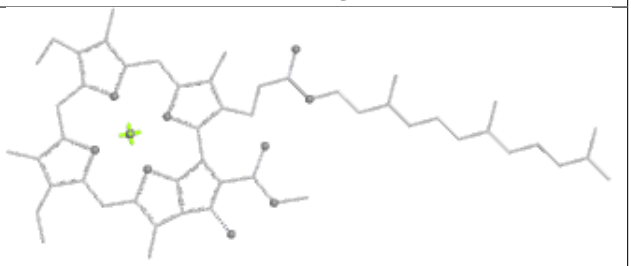
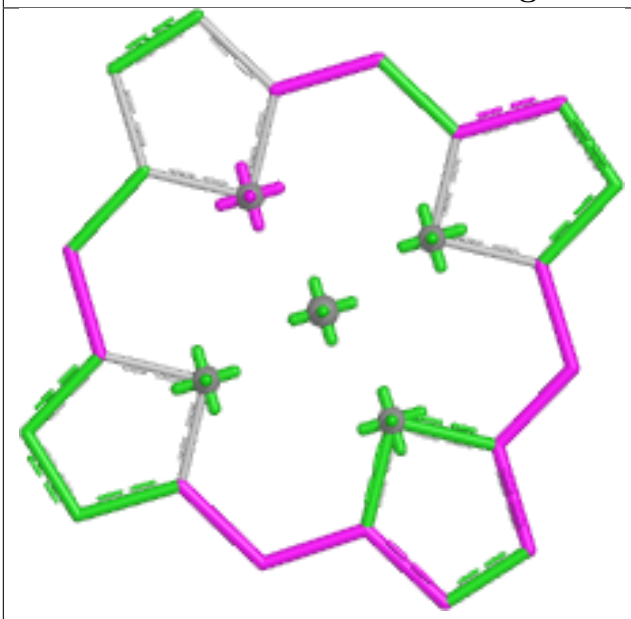


Rings

Ligand CLA B 1220	
 Bond lengths	 Bond angles
 Torsions	 Rings

Ligand CLA 2 2012



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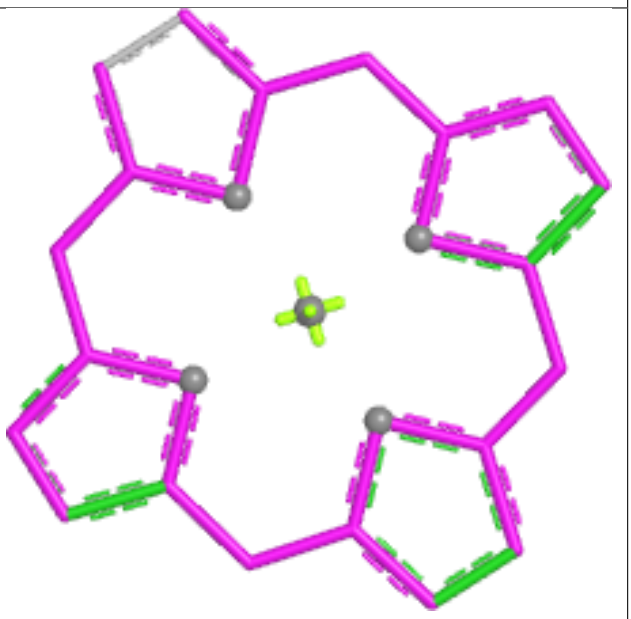
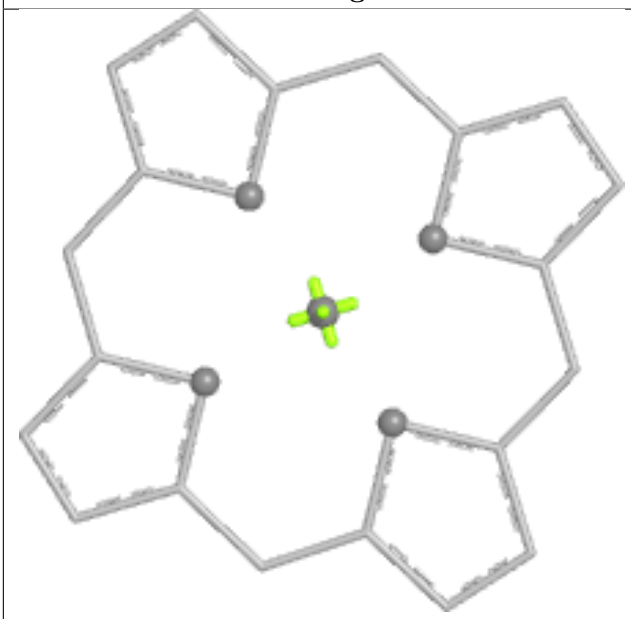


Bond angles



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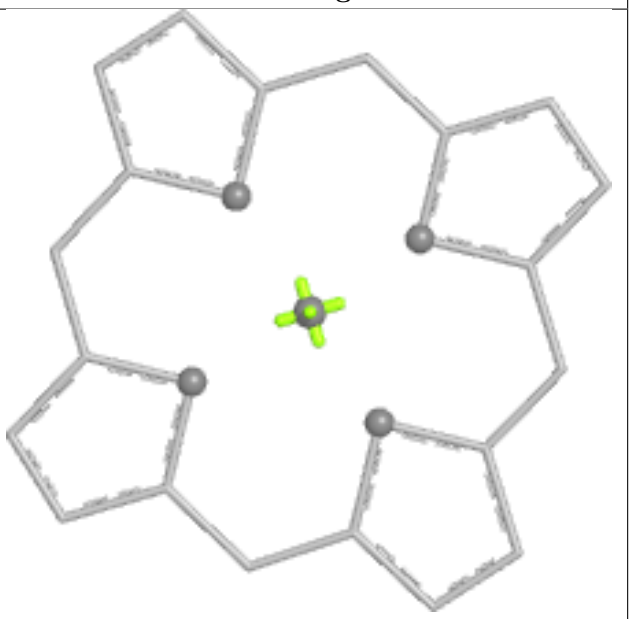
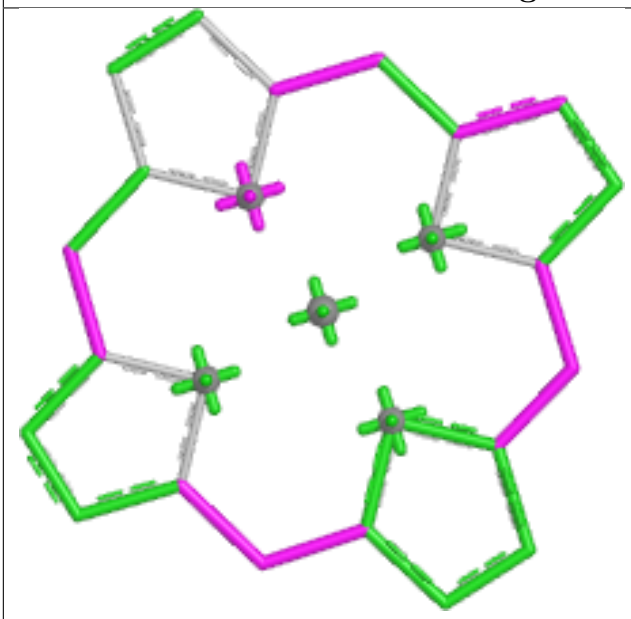


Rings

Ligand CLA 2 2007



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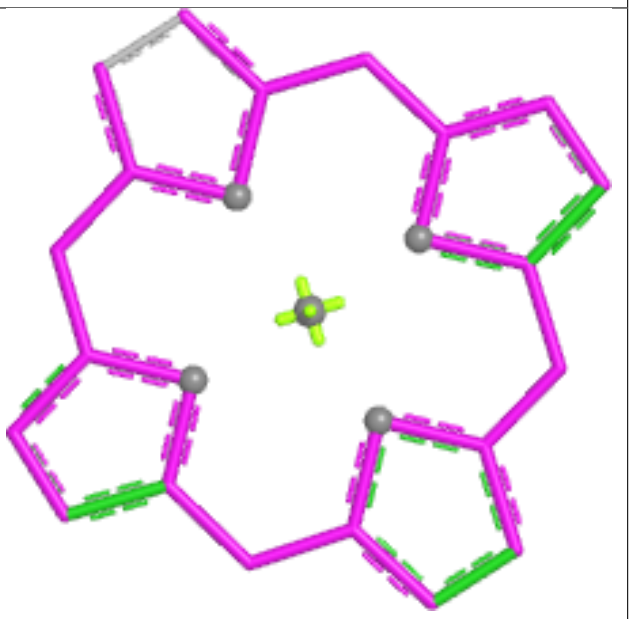
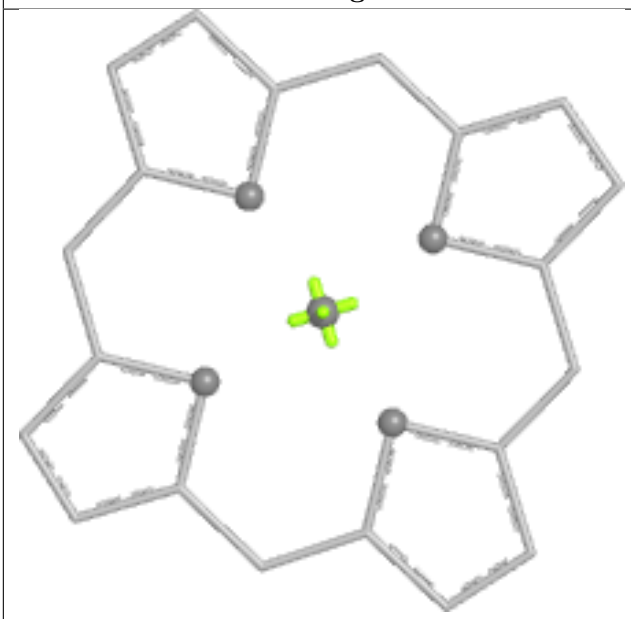
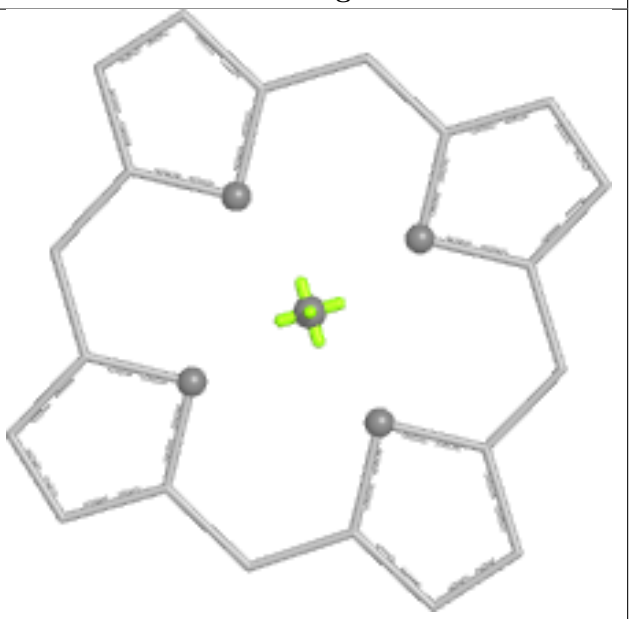


Bond angles

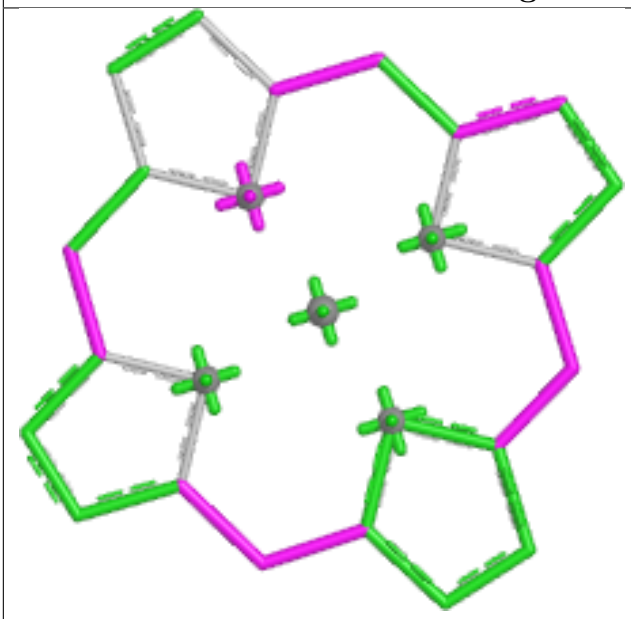


Torsions



Rings

Ligand CLA 1 1005



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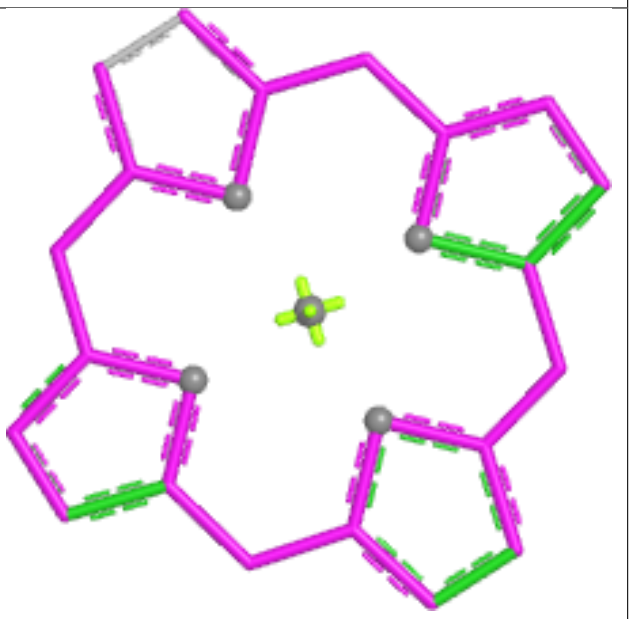

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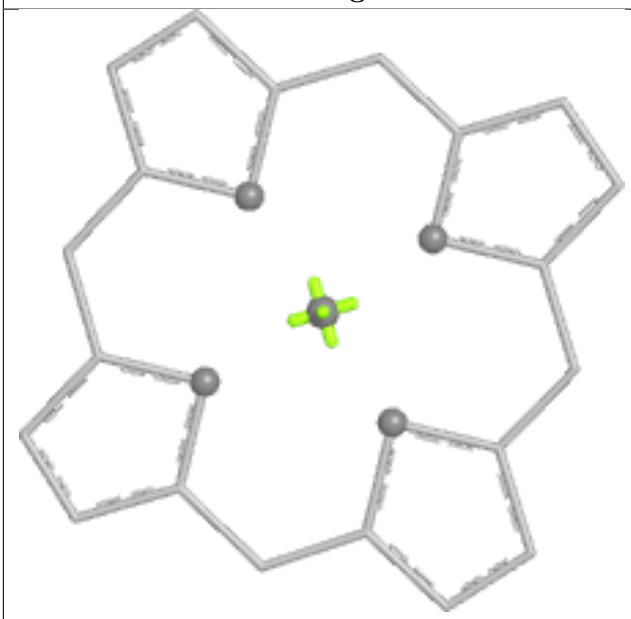

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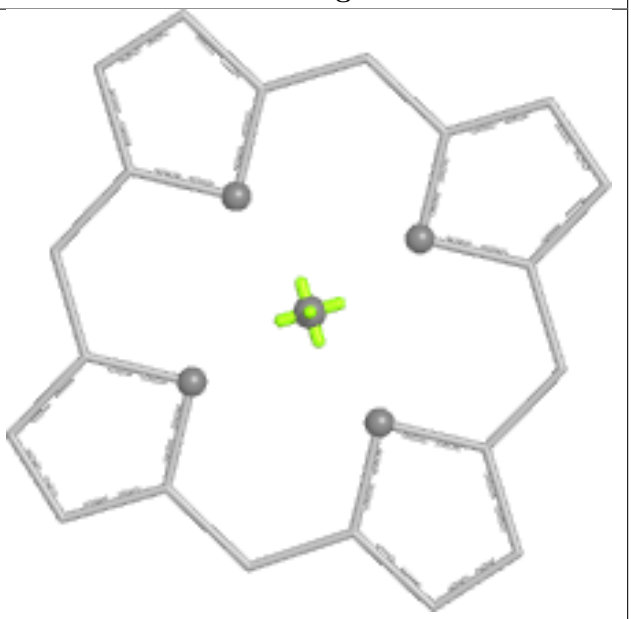
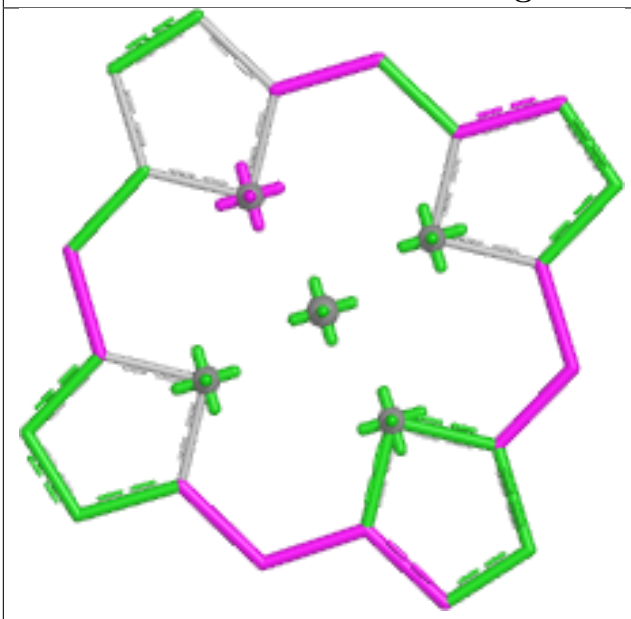


Rings

Ligand CLA A 1116



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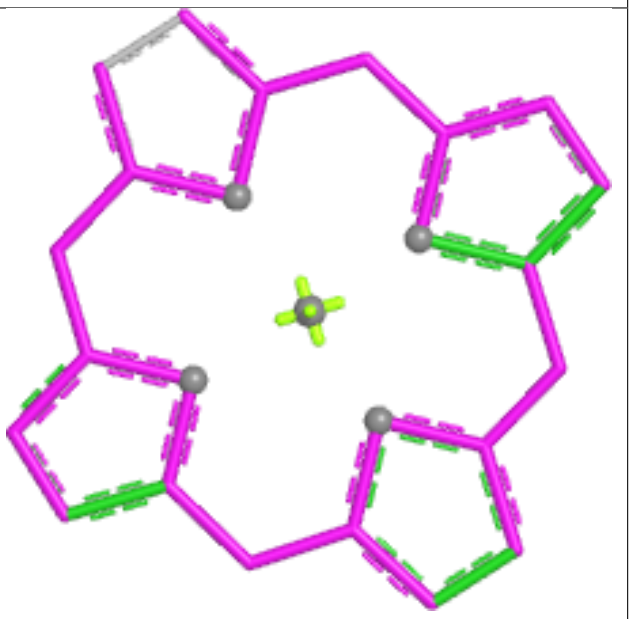

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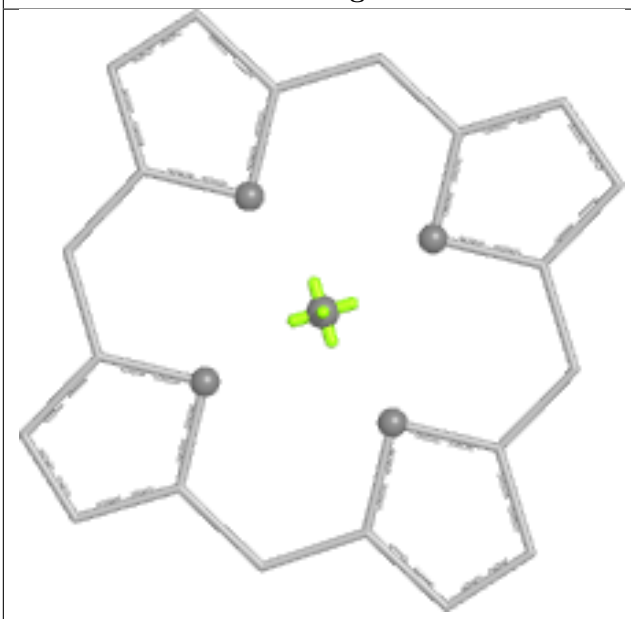

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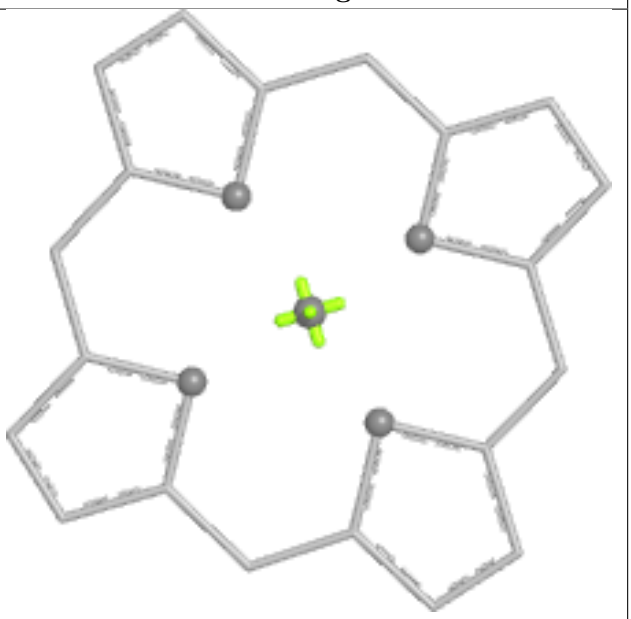
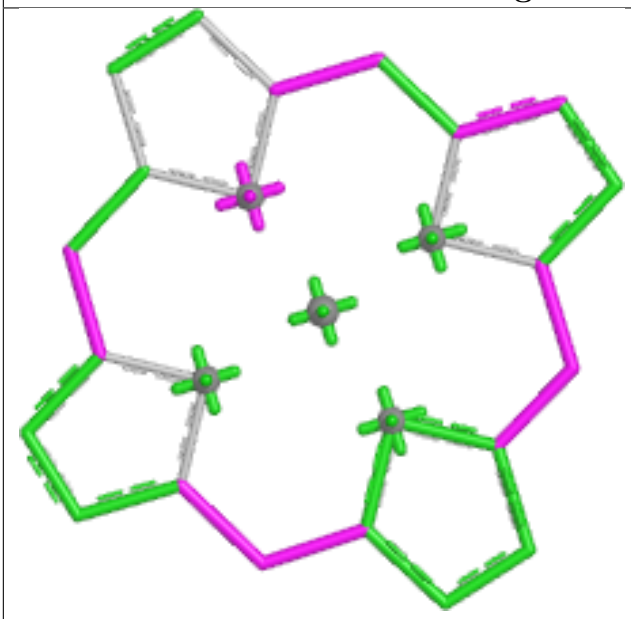


Rings

Ligand CLA A 1151



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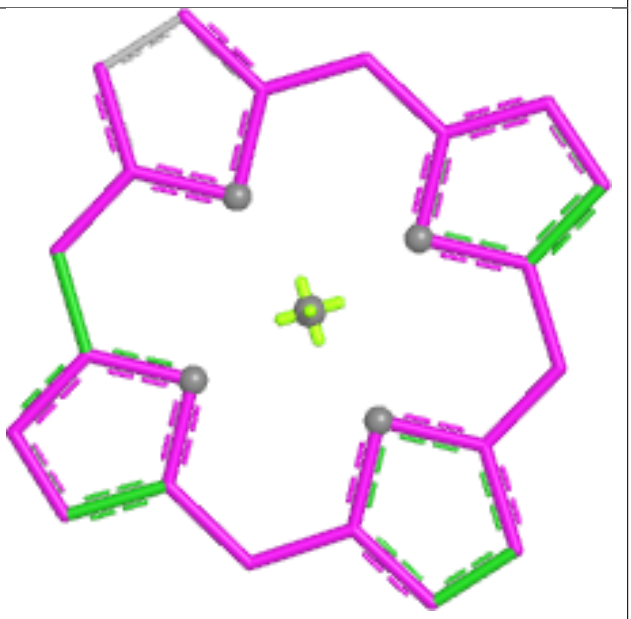

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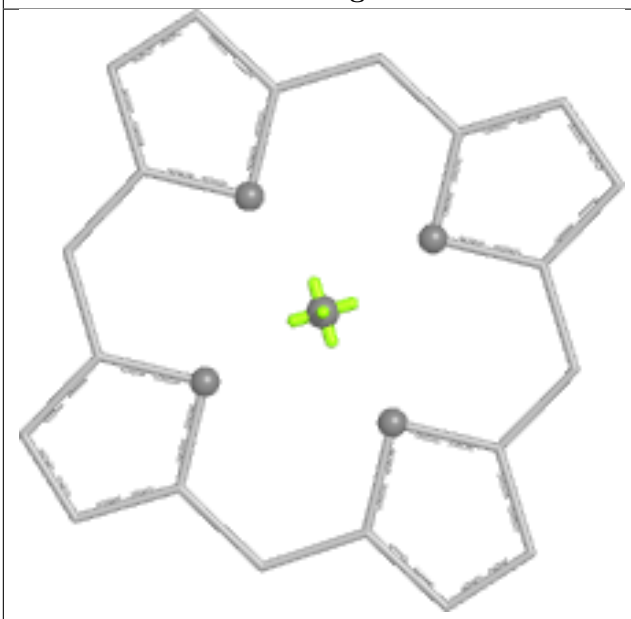

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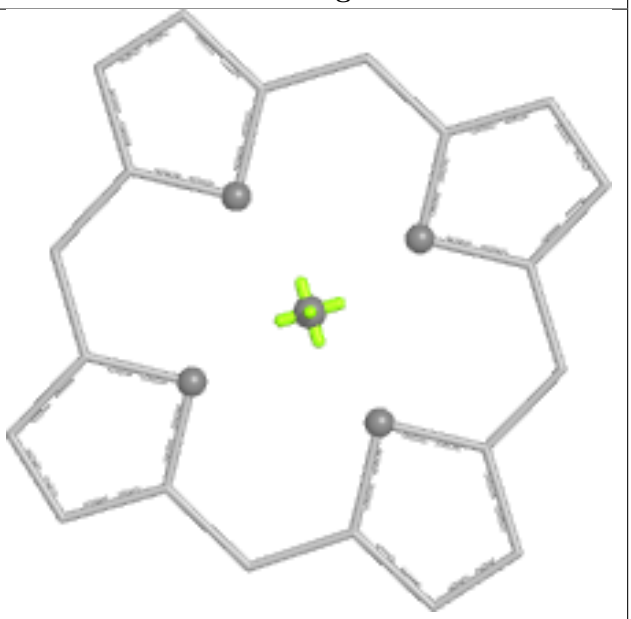
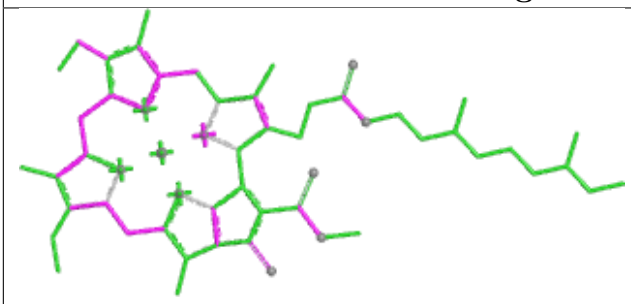


Rings

Ligand CLA B 1138



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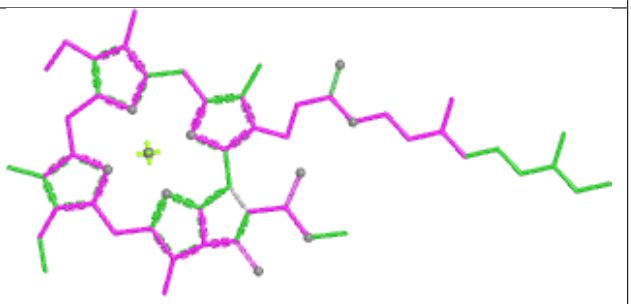

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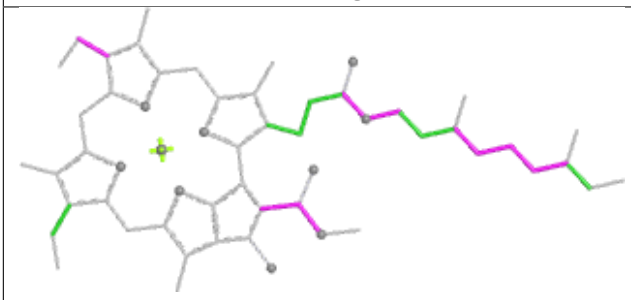

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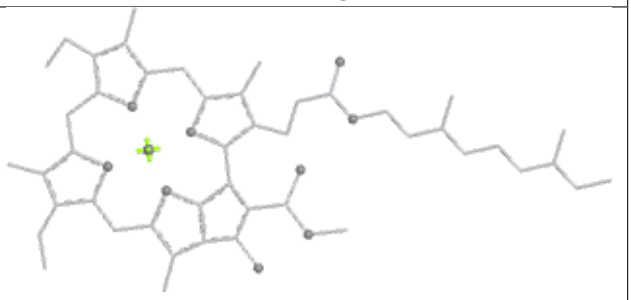
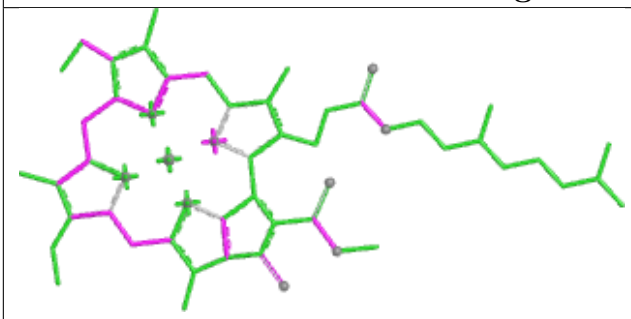


Rings

Ligand CLA H 1501



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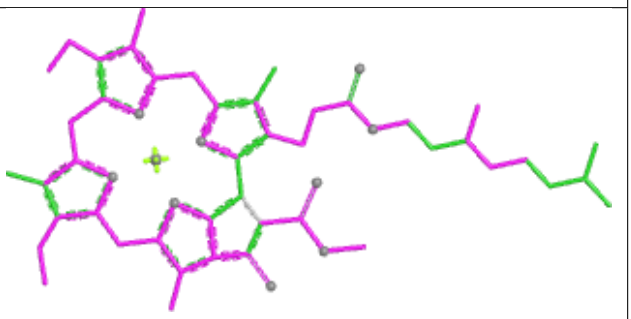
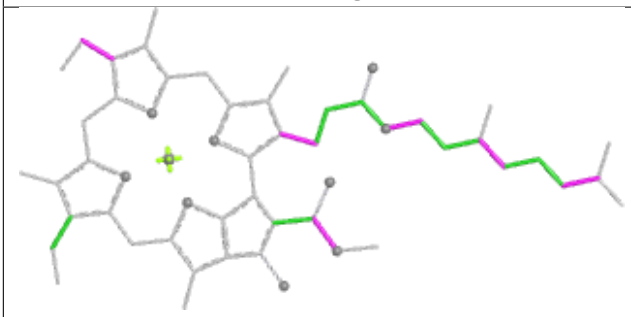


Bond angles



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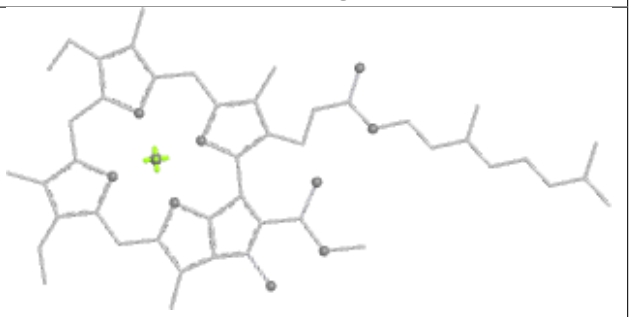
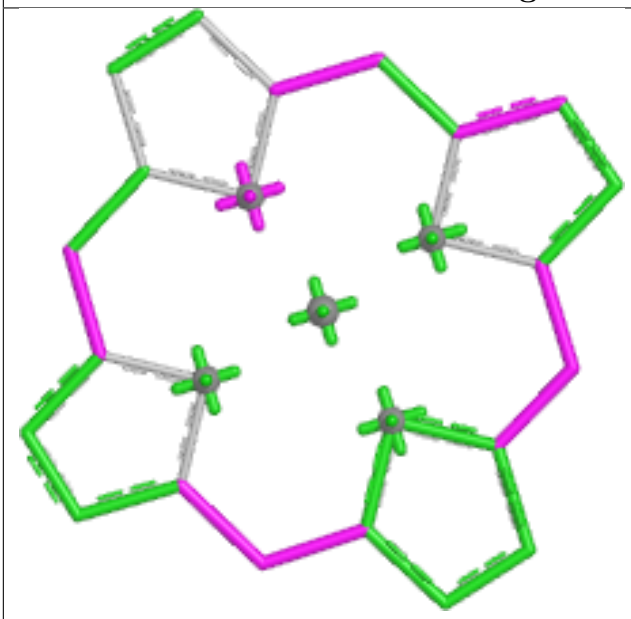


Rings

Ligand CLA 3 3007



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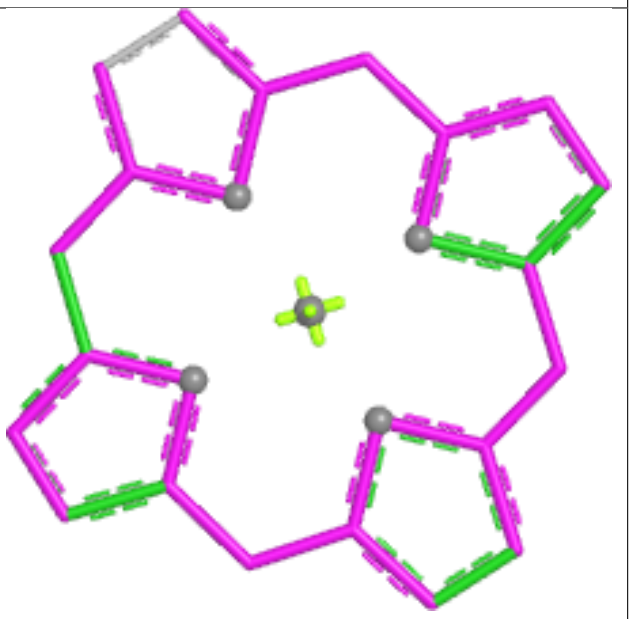
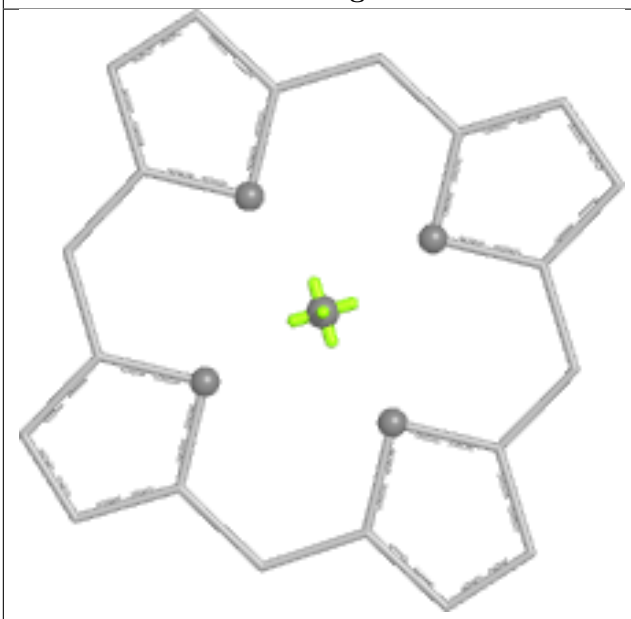


Bond angles



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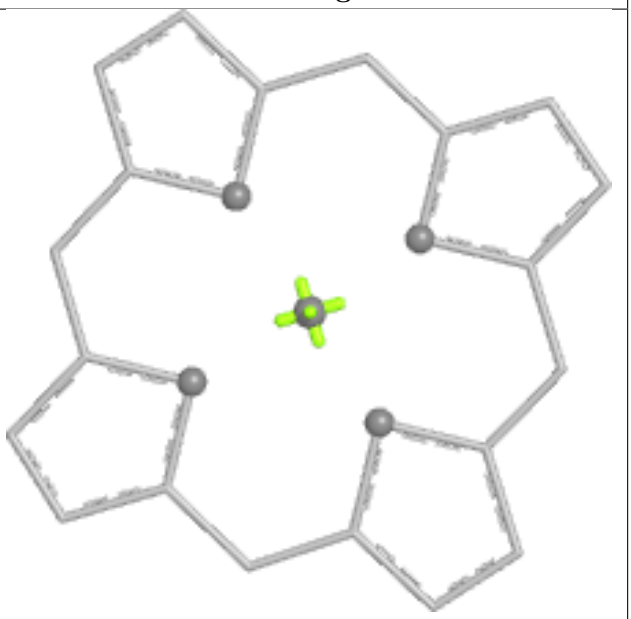
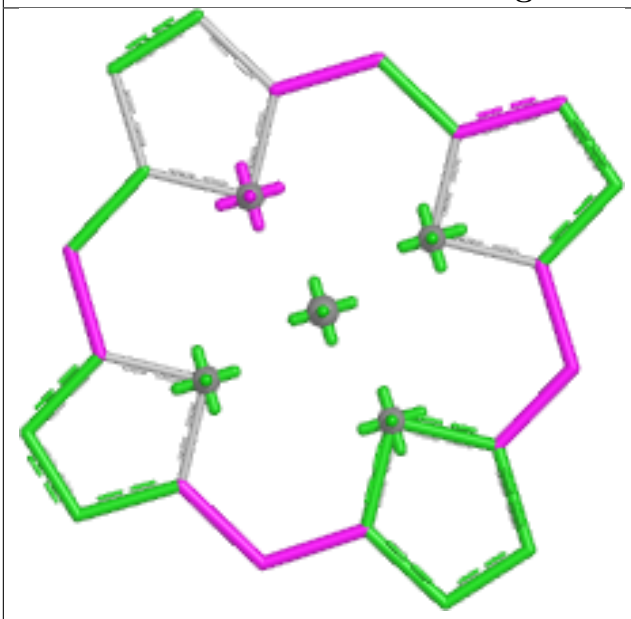


Rings

Ligand CLA B 1211



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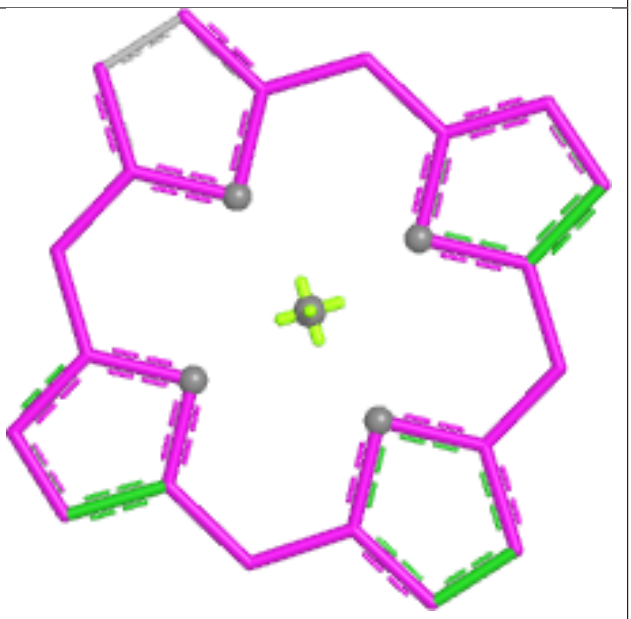

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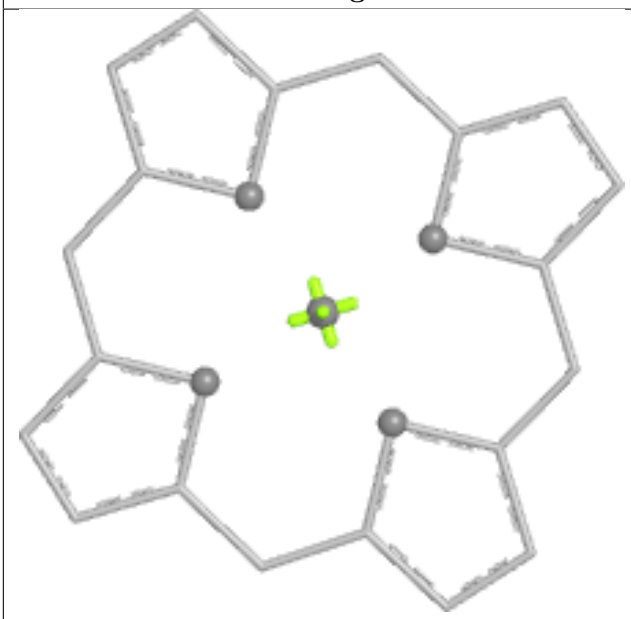

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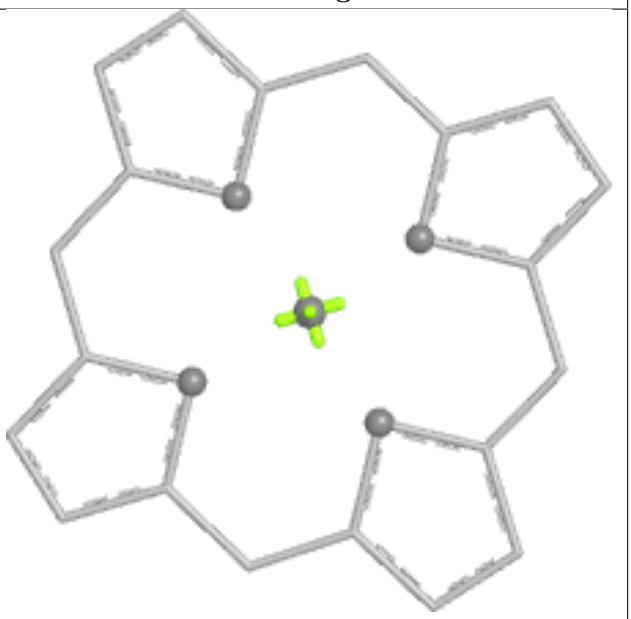
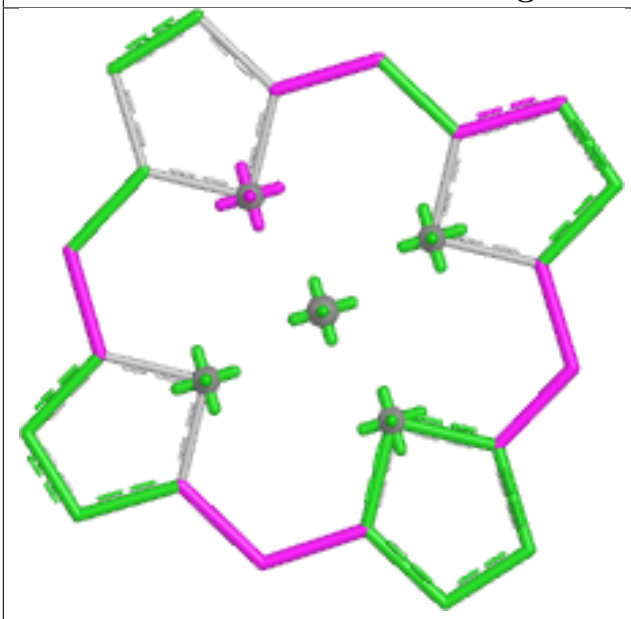


Rings

Ligand CLA F 1306



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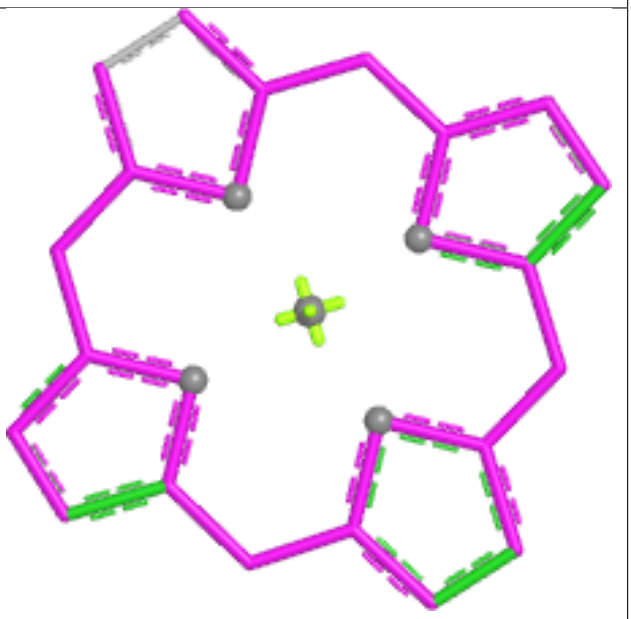
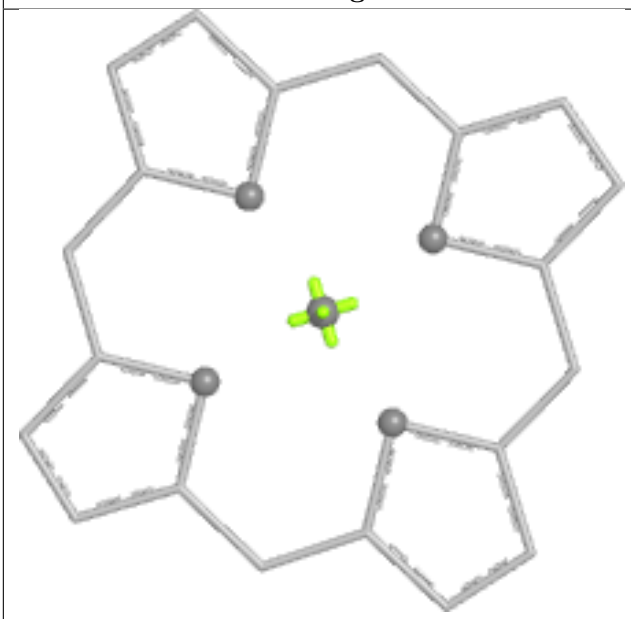


Bond angles



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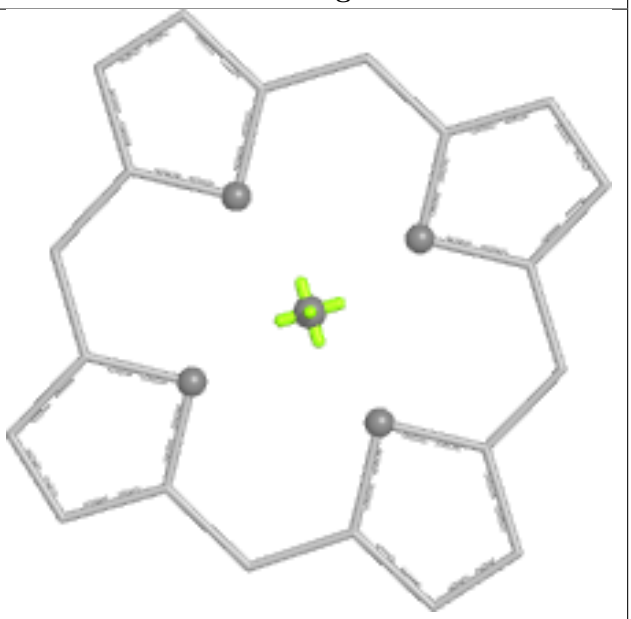
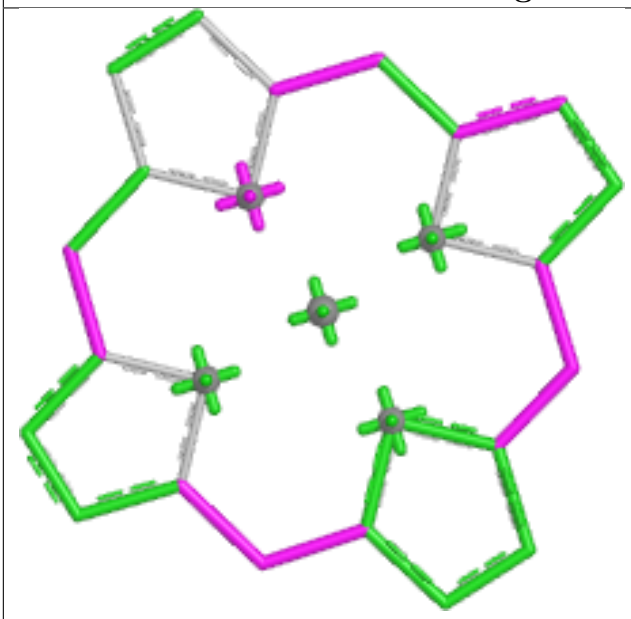


Rings

Ligand CLA A 1120



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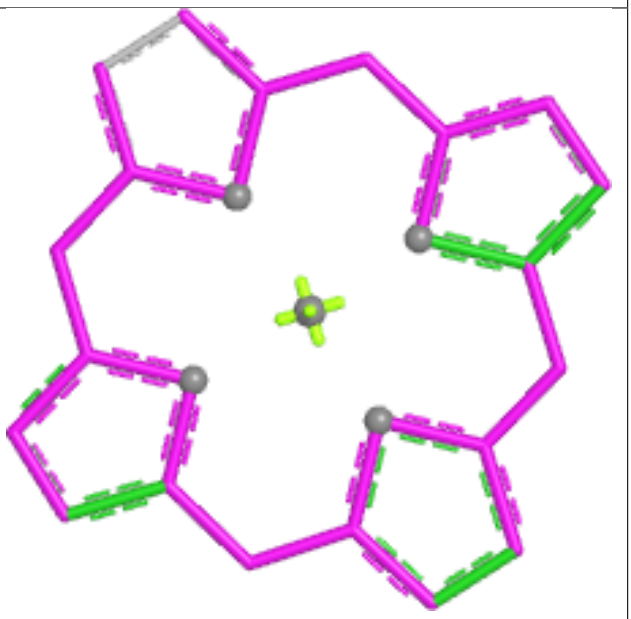
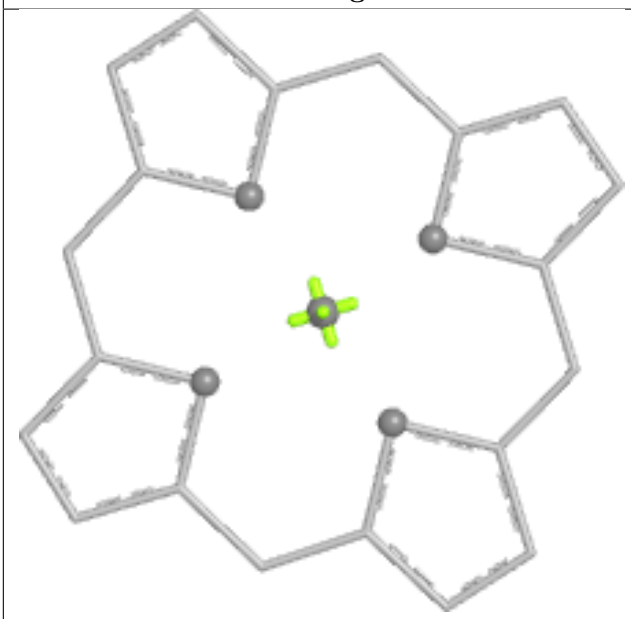


Bond angles



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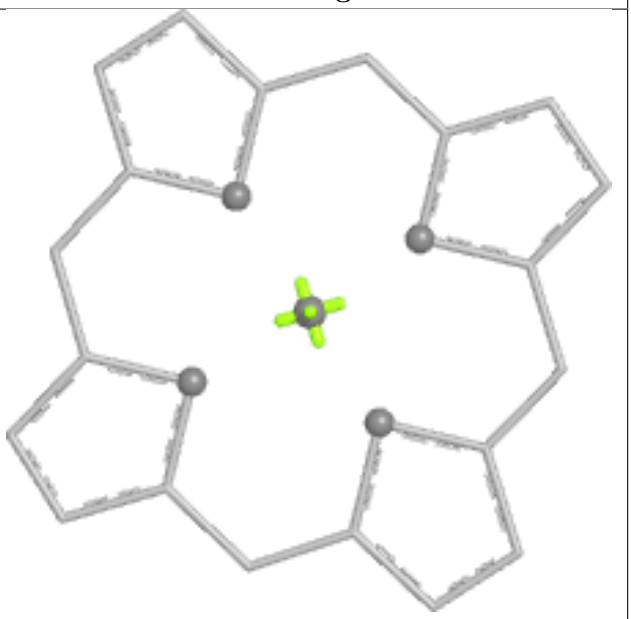
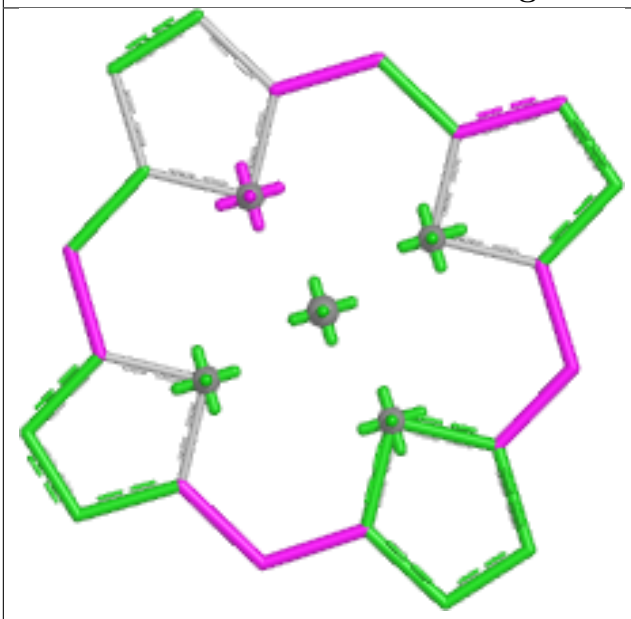


Rings

Ligand CLA J 1308



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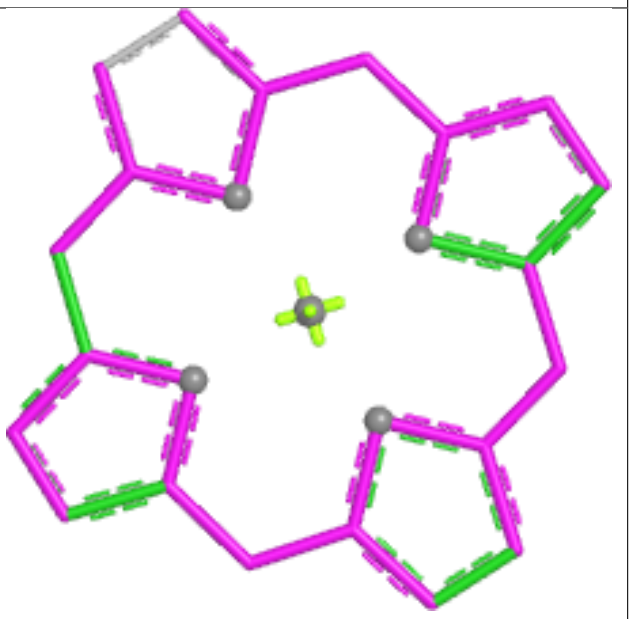

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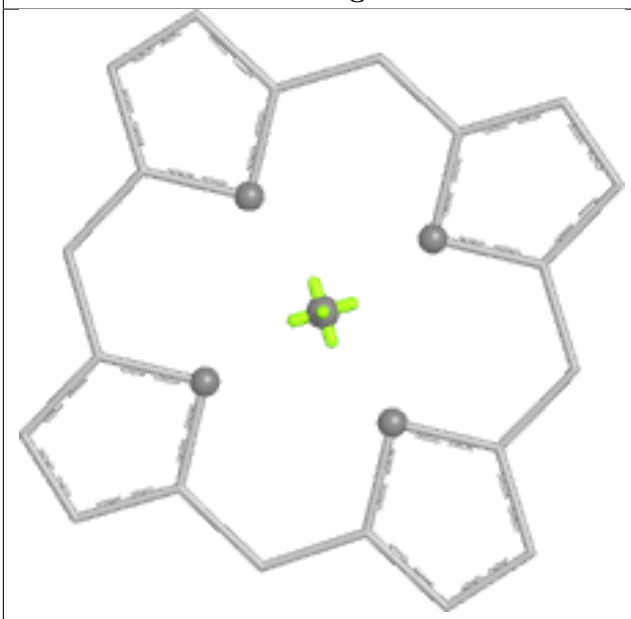

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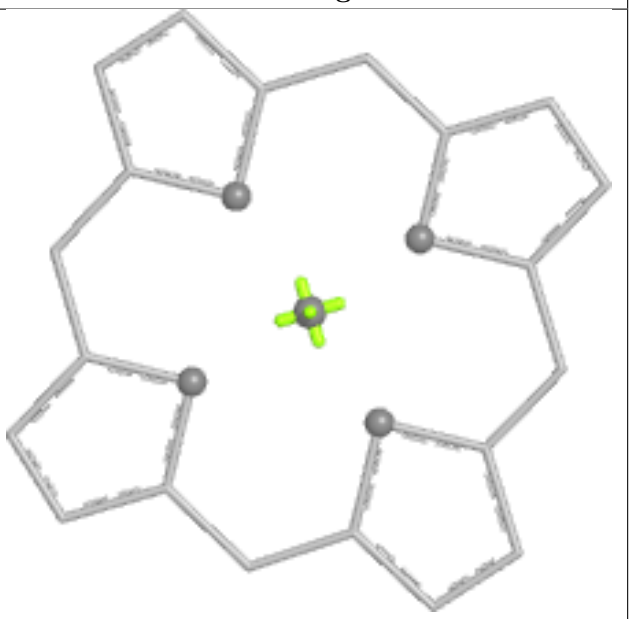
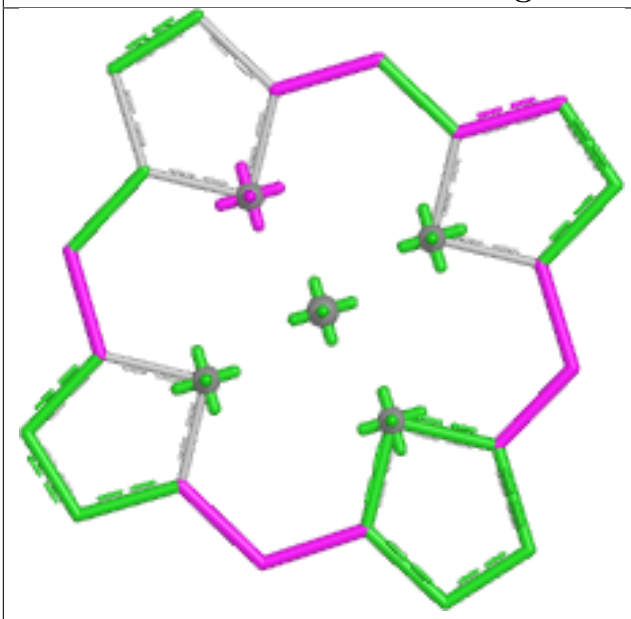


Rings

Ligand CLA A 1143



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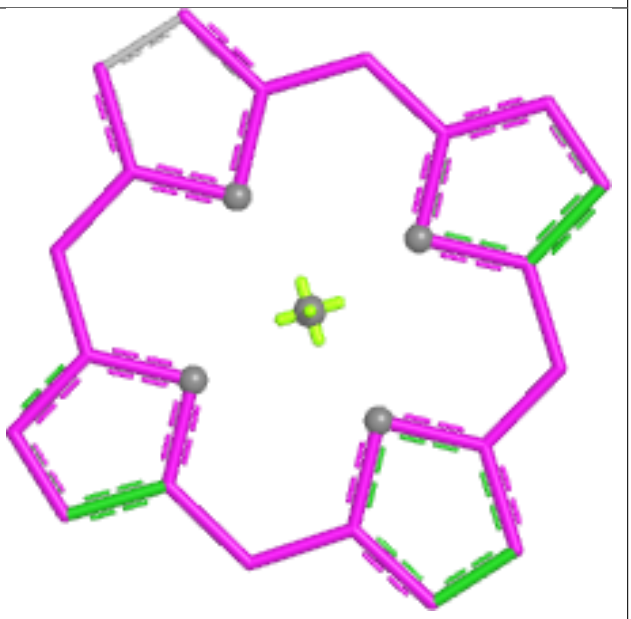
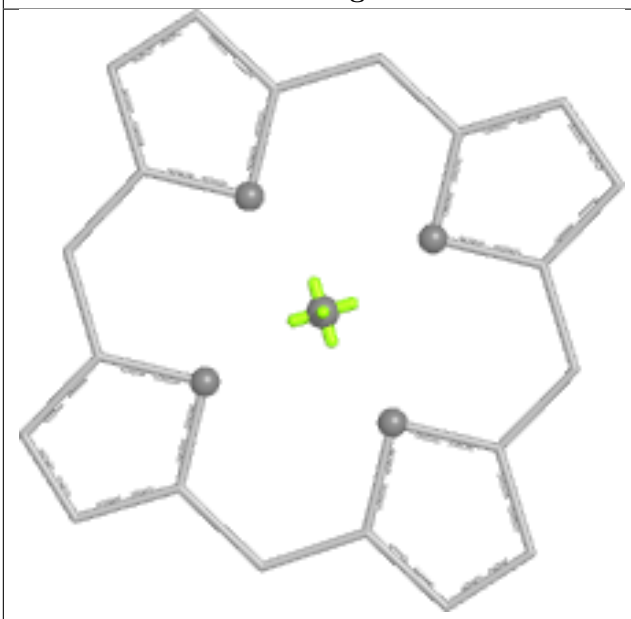


Bond angles



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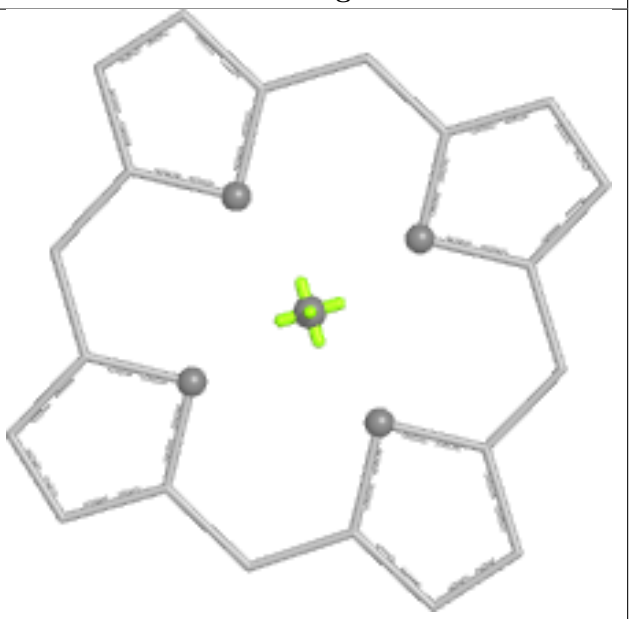
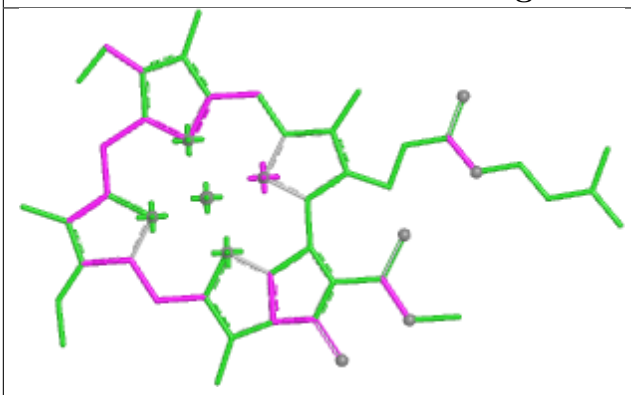


Rings

Ligand CLA B 1202



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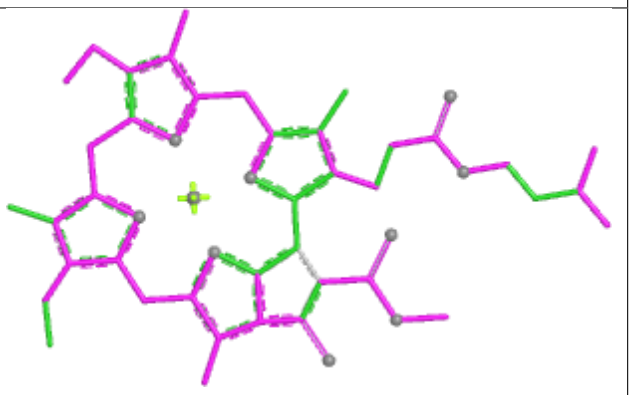
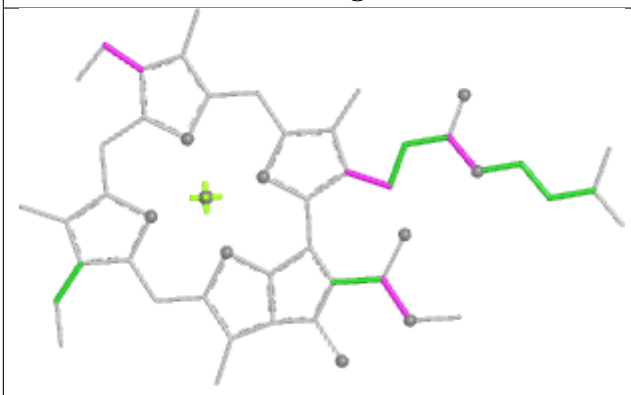


Bond angles



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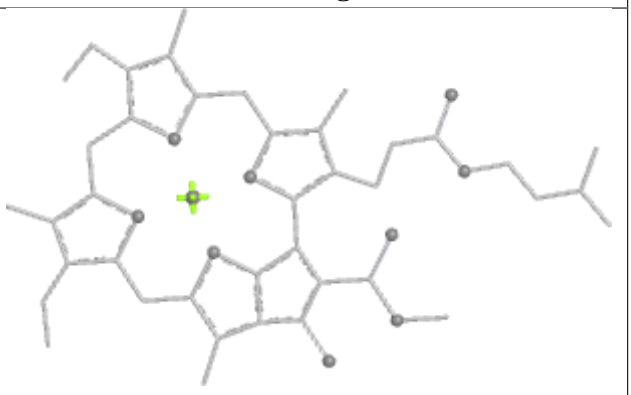
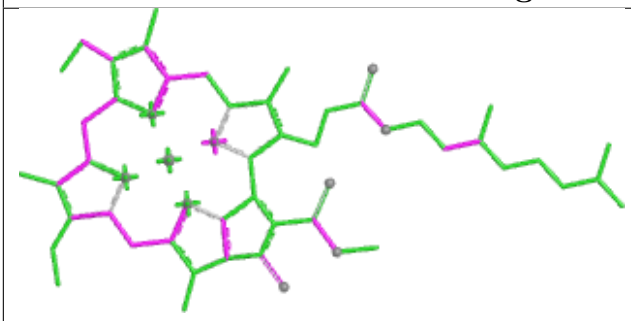


Rings

Ligand CLA B 1208



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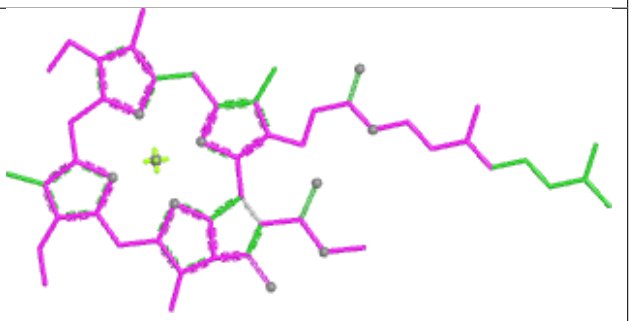
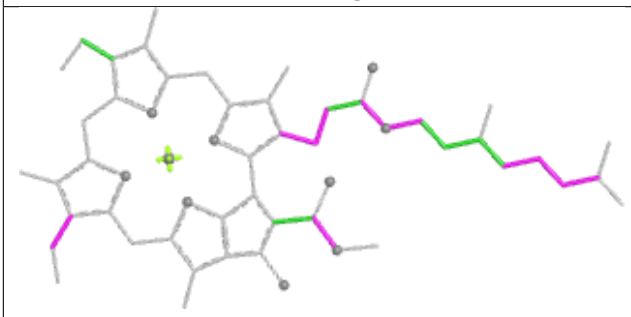


Bond angles



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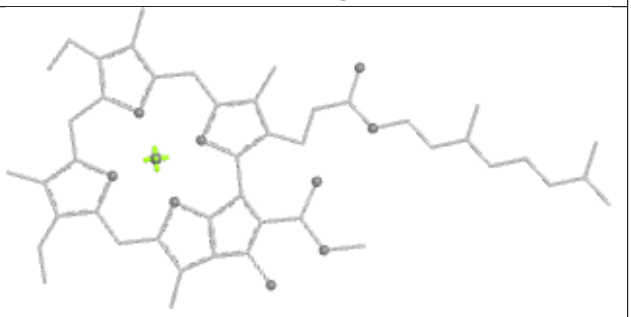

Rings

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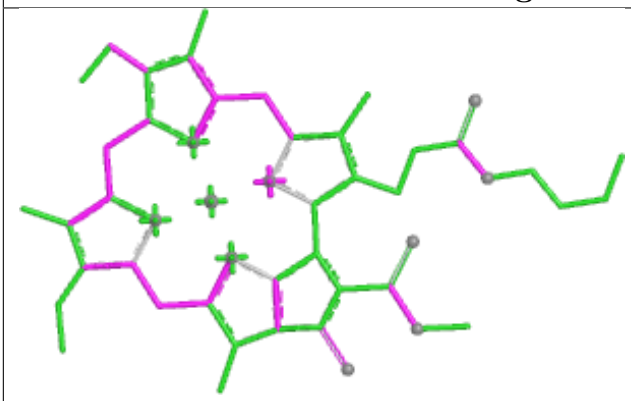
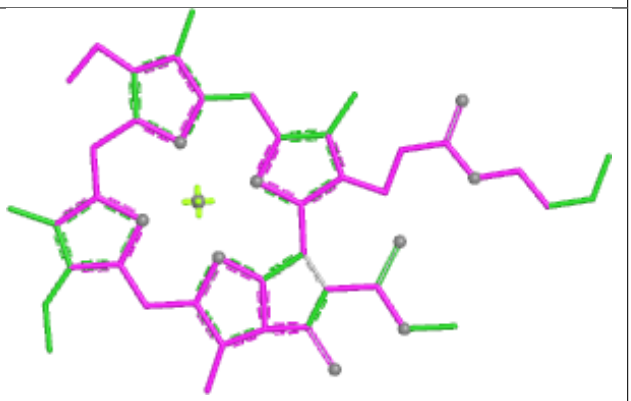
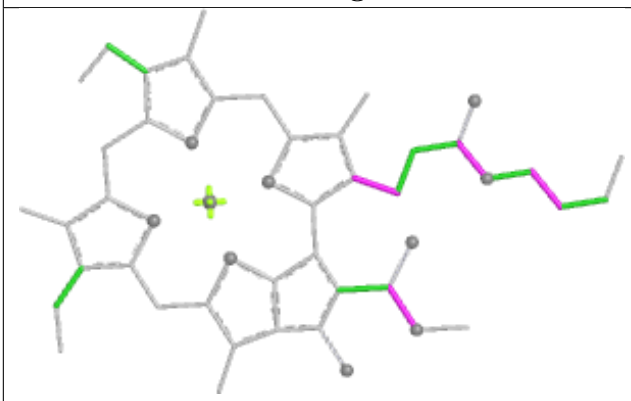
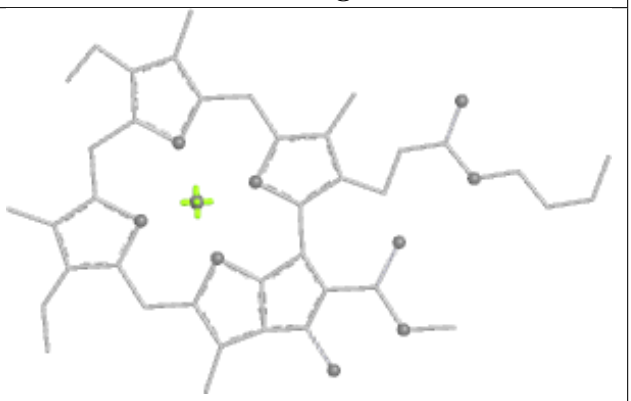
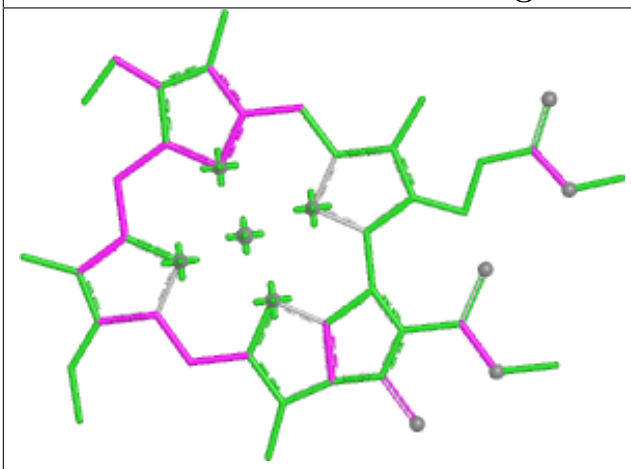
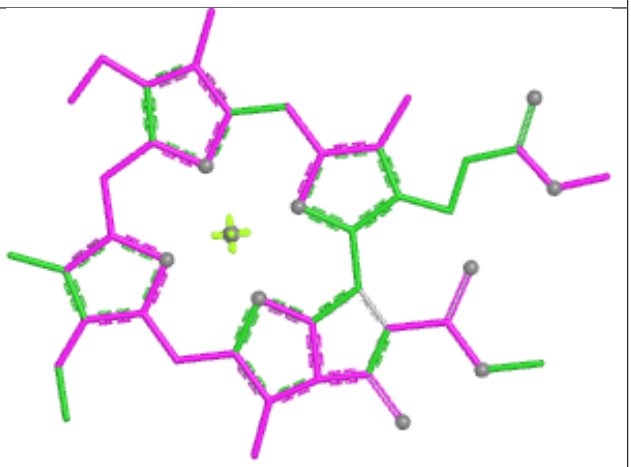
 Bond lengths	 Bond angles
 Torsions	 Rings

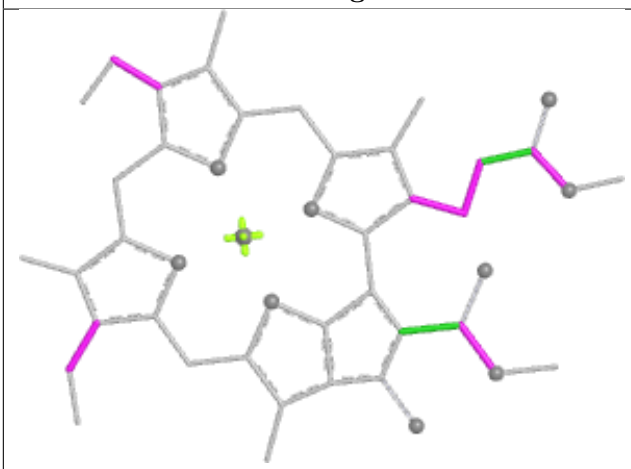
Ligand CLA B 1231



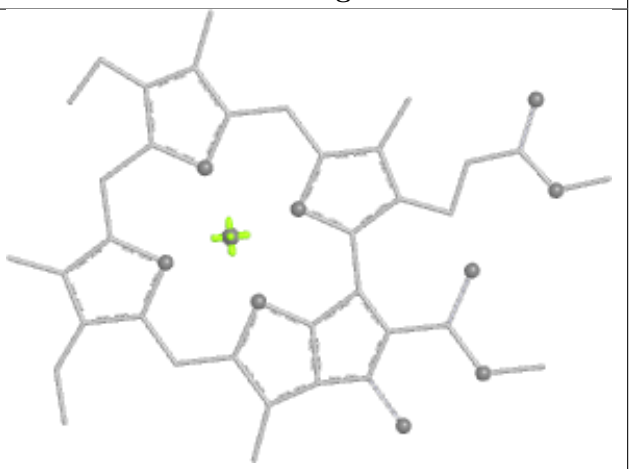
Bond lengths



Bond angles

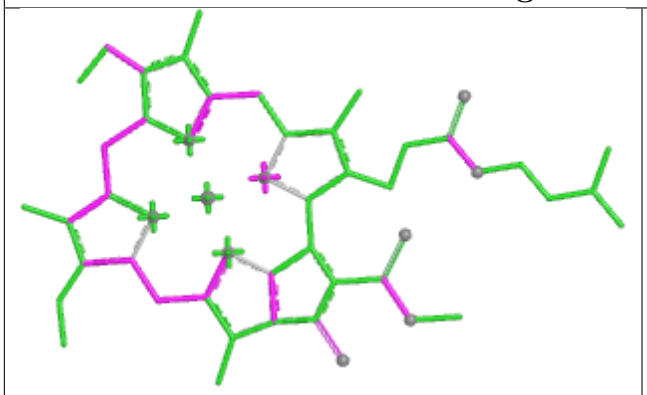


Torsions

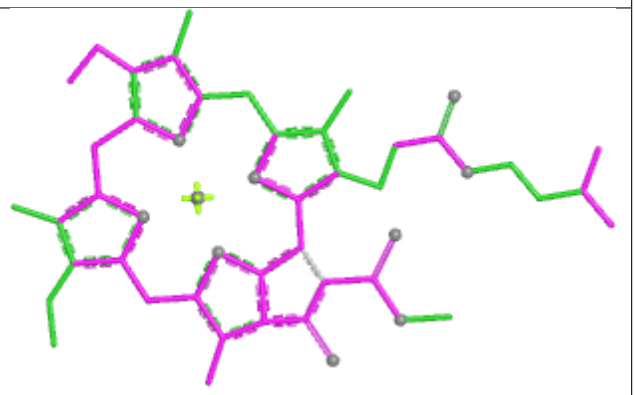


Rings

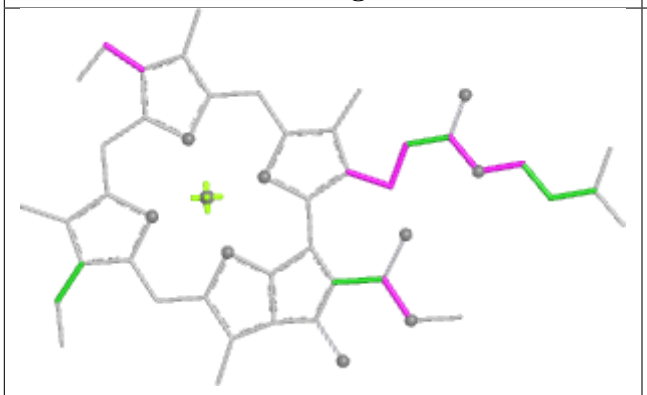
Ligand CLA B 1234



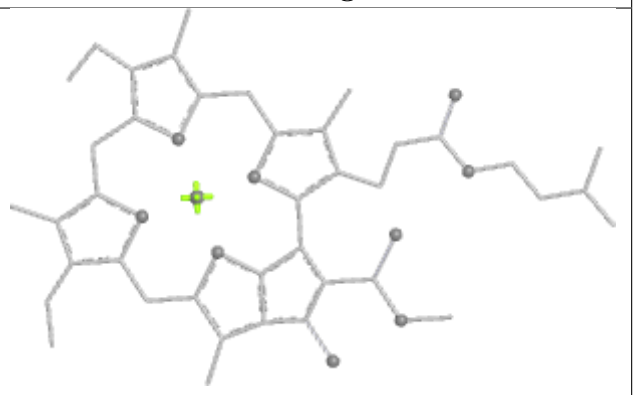
Bond lengths



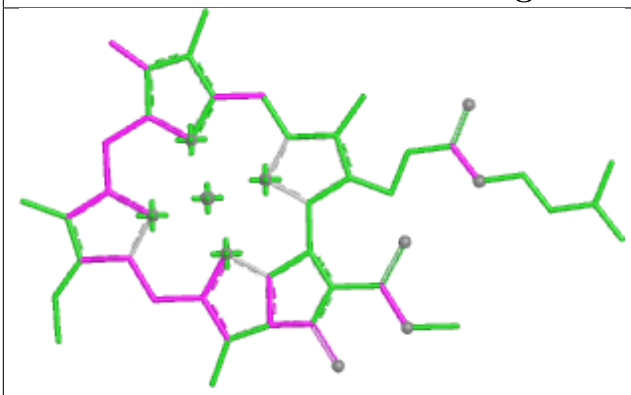
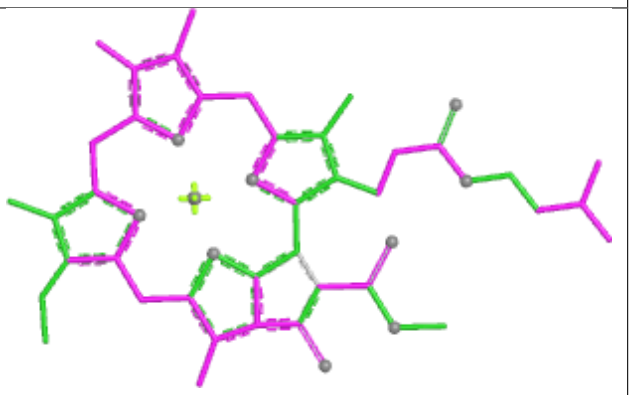
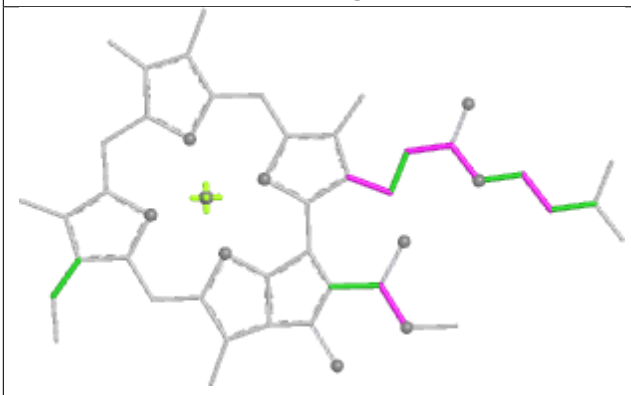
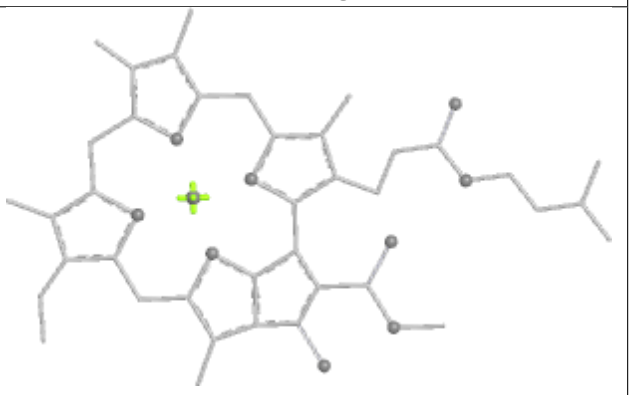
Bond angles



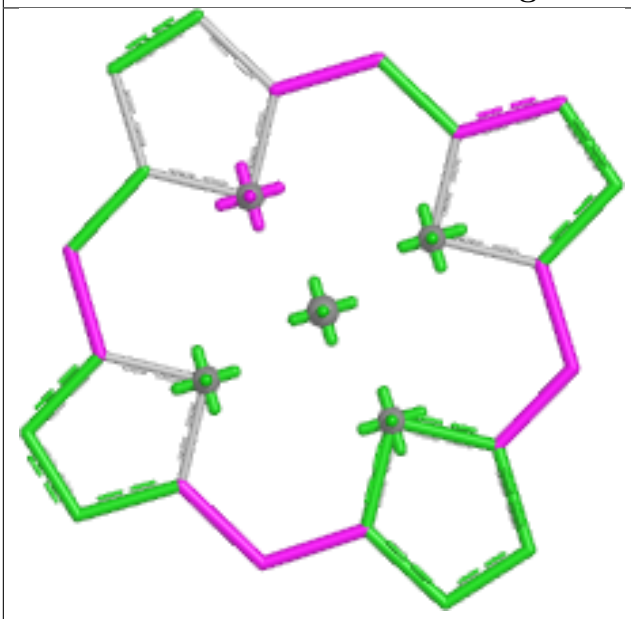
Torsions



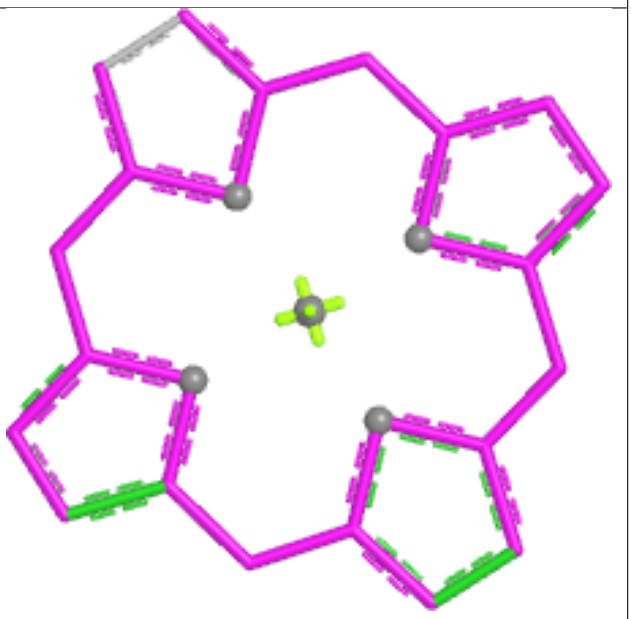
Rings

Ligand CLA B 1229	
 Bond lengths	 Bond angles
 Torsions	 Rings

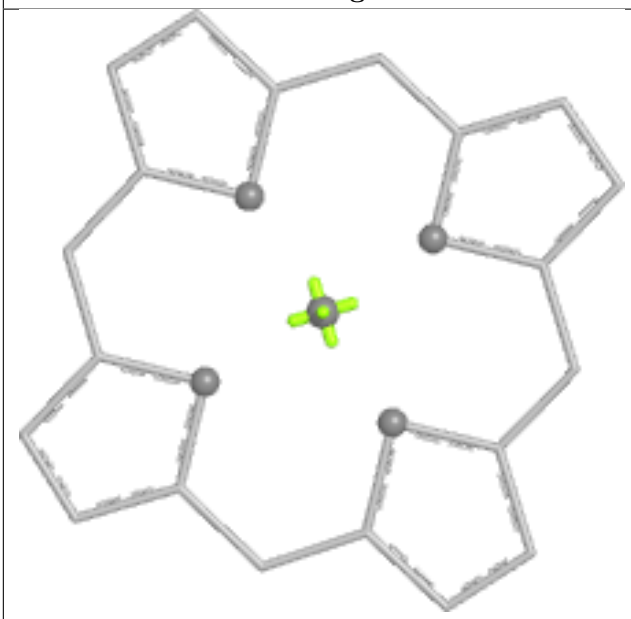
Ligand CLA 4 4005



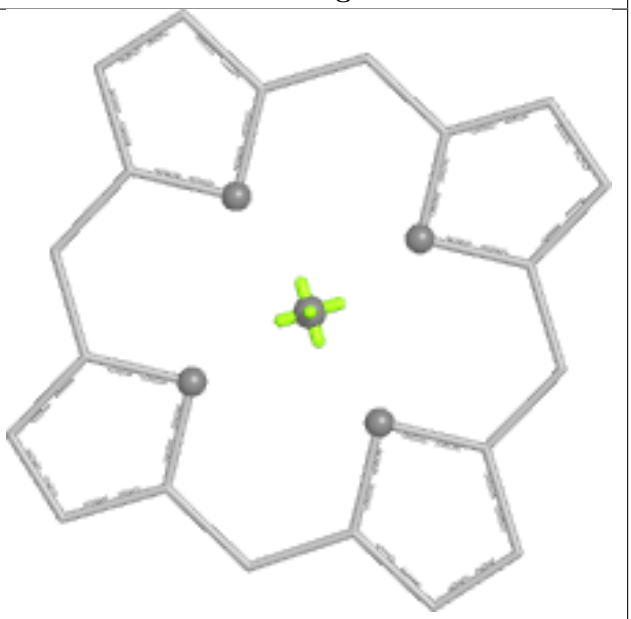
Bond lengths



Bond angles

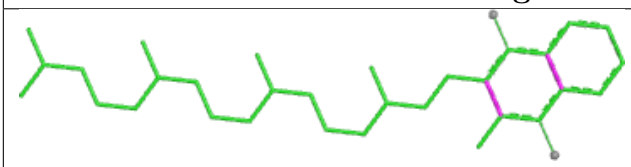


Torsions

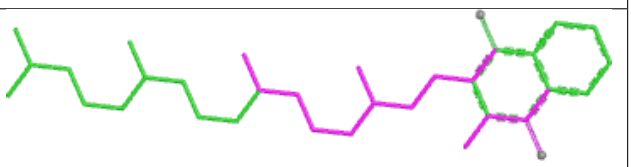


Rings

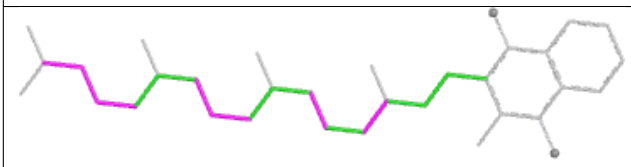
Ligand PQN B 5002



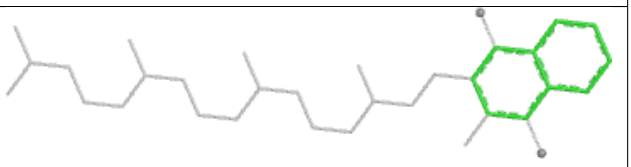
Bond lengths



Bond angles

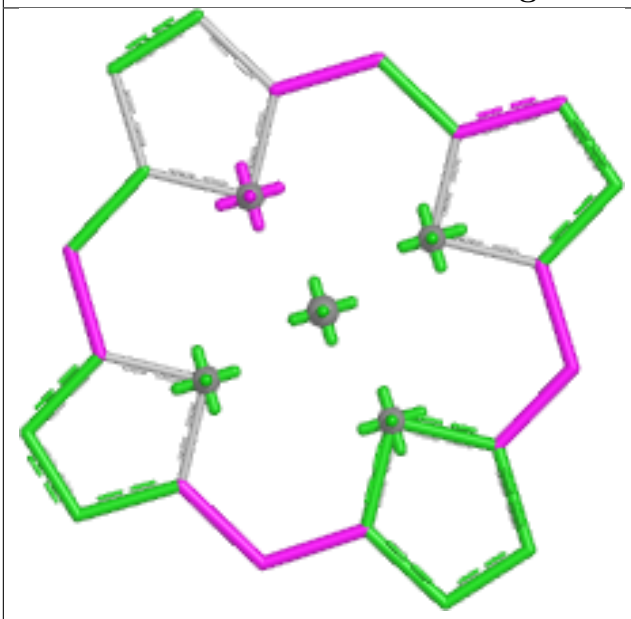


Torsions

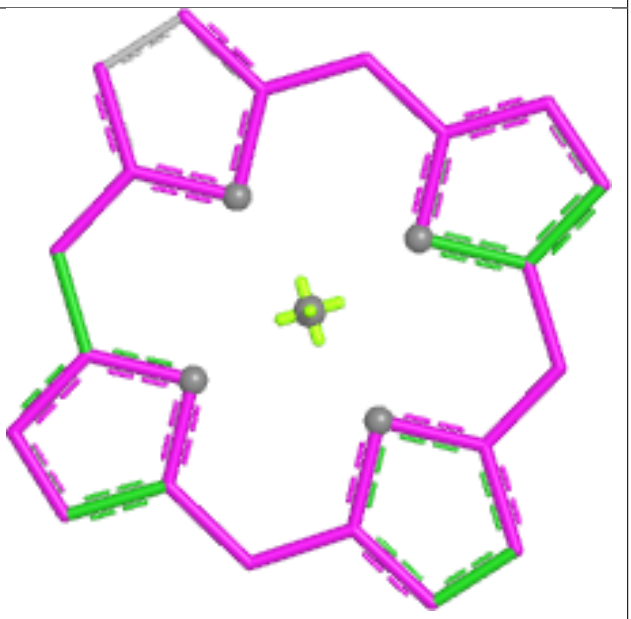


Rings

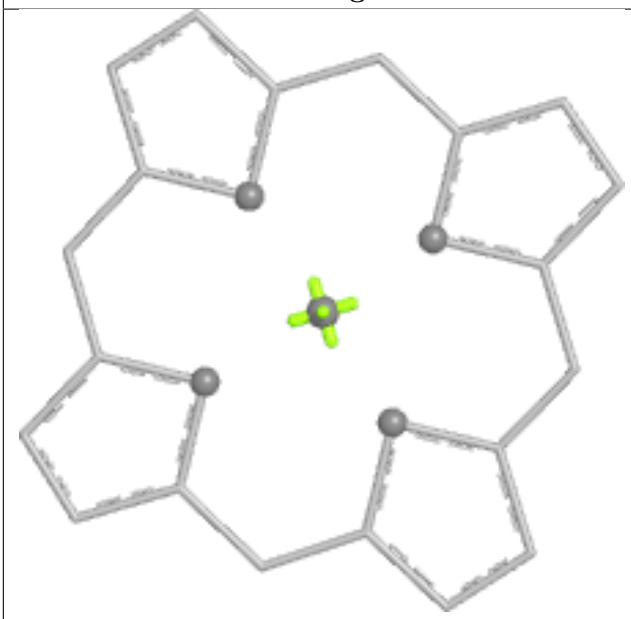
Ligand CLA 3 3011



Bond lengths



Bond angles



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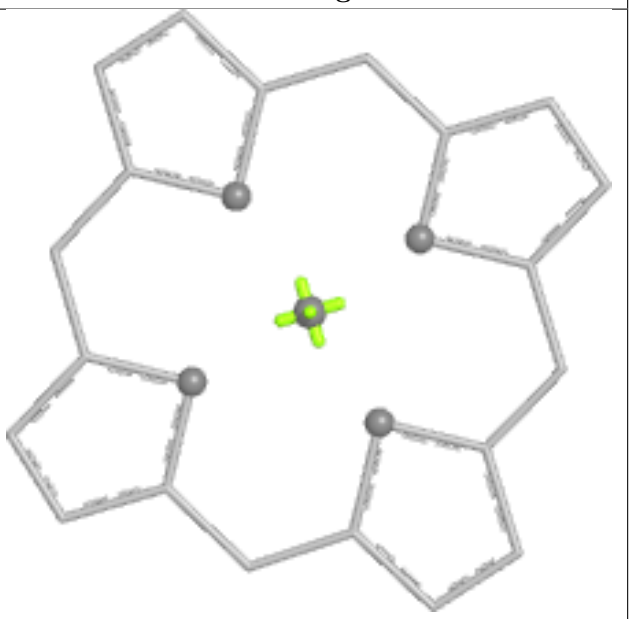
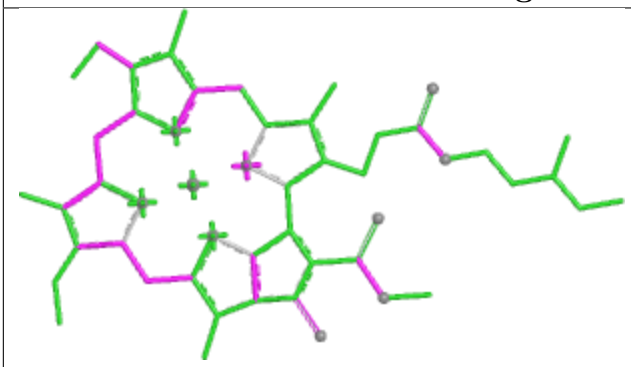
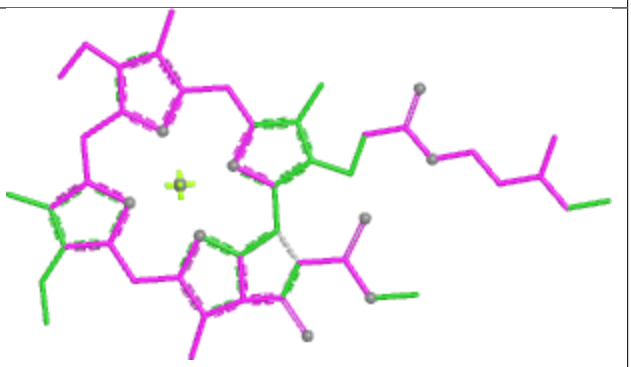


Rings

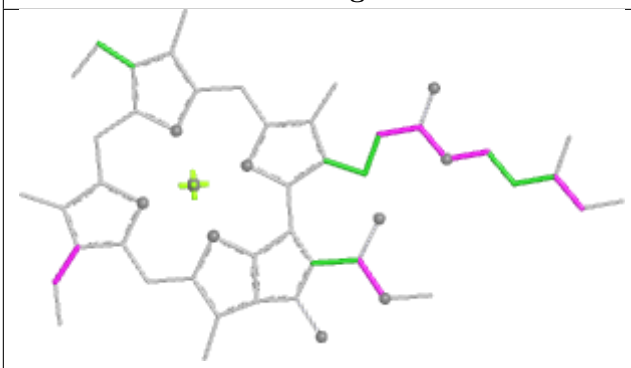
Ligand CLA B 1237



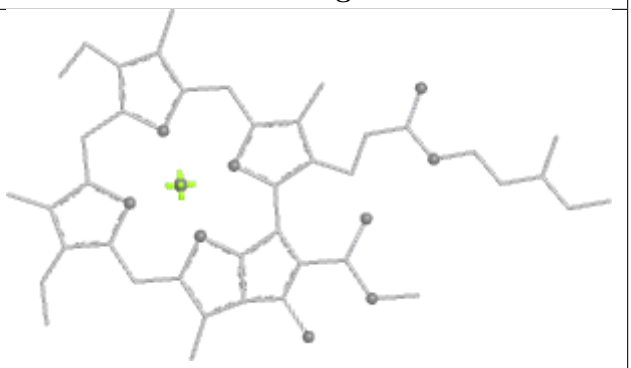
Bond lengths



Bond angles

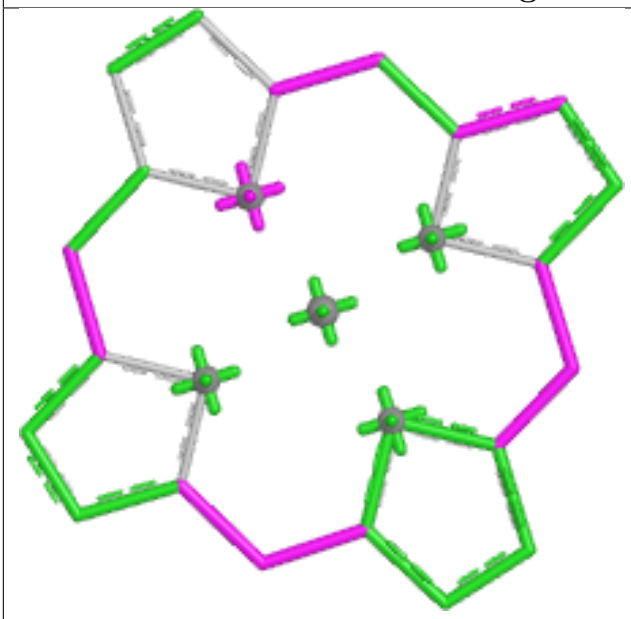


Torsions

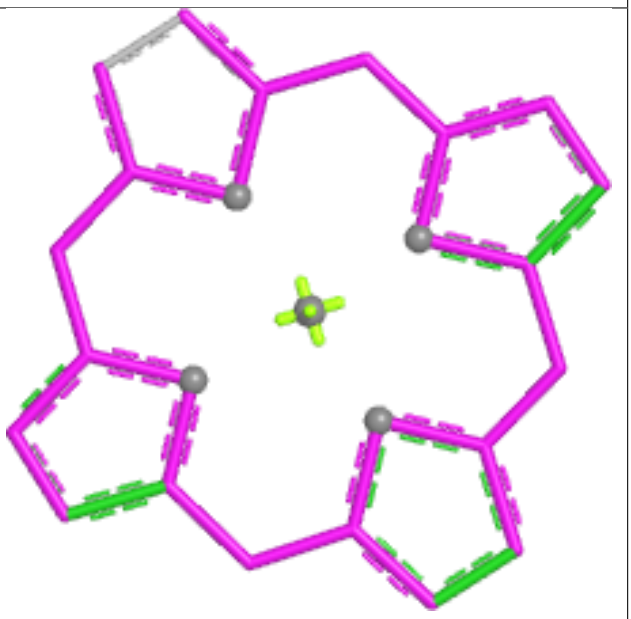


Rings

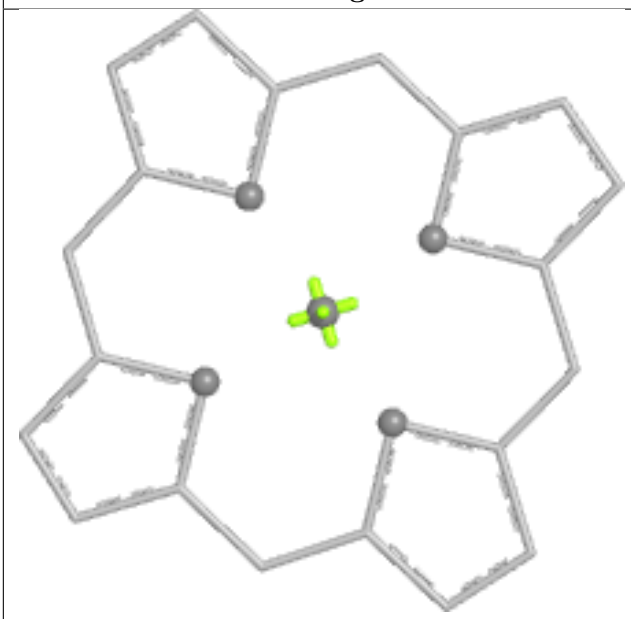
Ligand CLA 1 1014



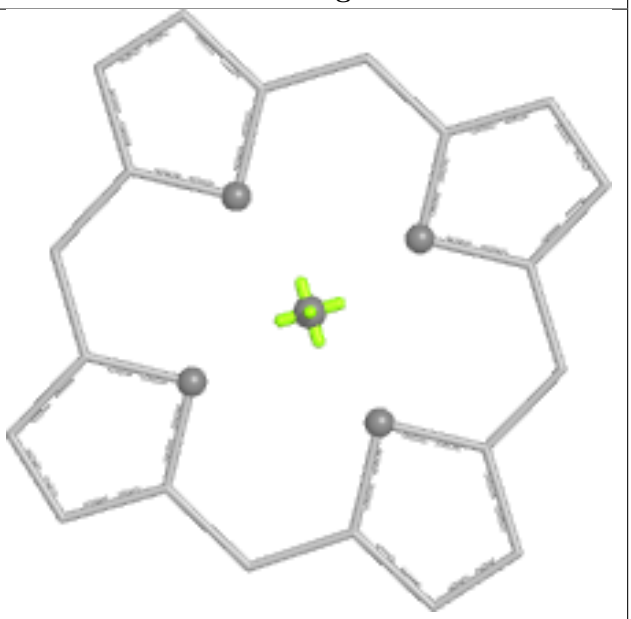
Bond lengths



Bond angles

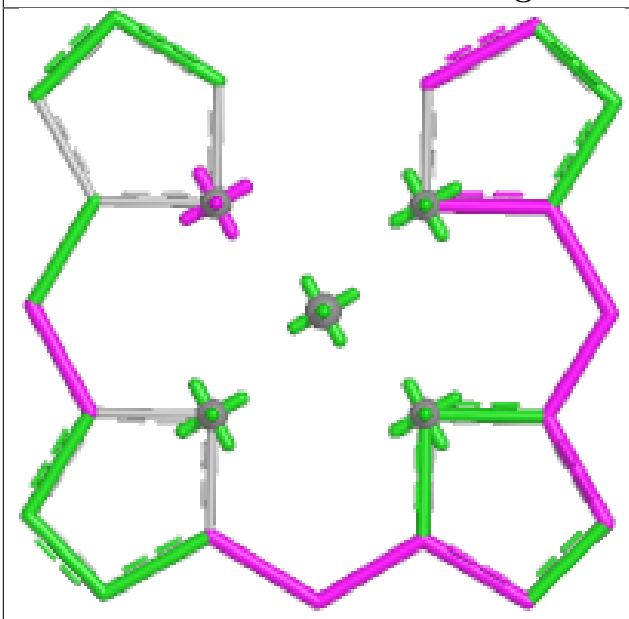


Torsions

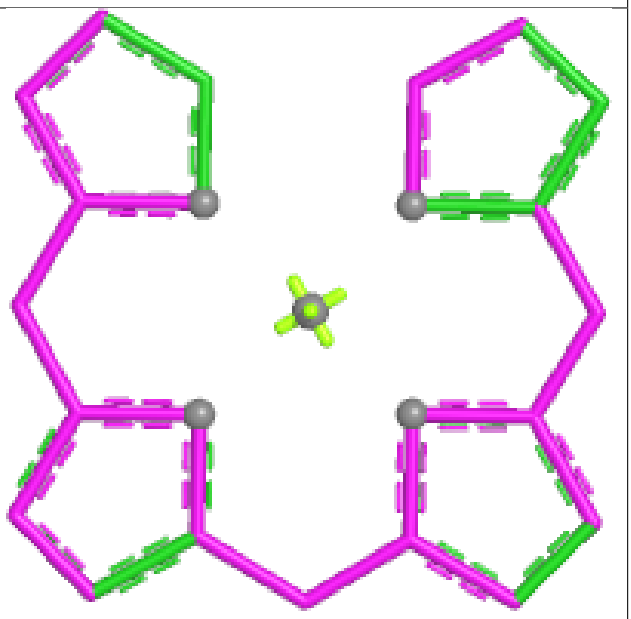


Rings

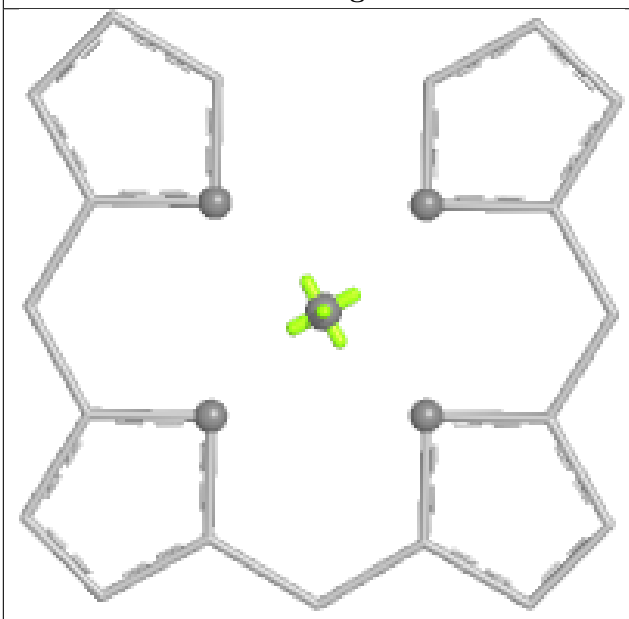
Ligand CLA A 1109



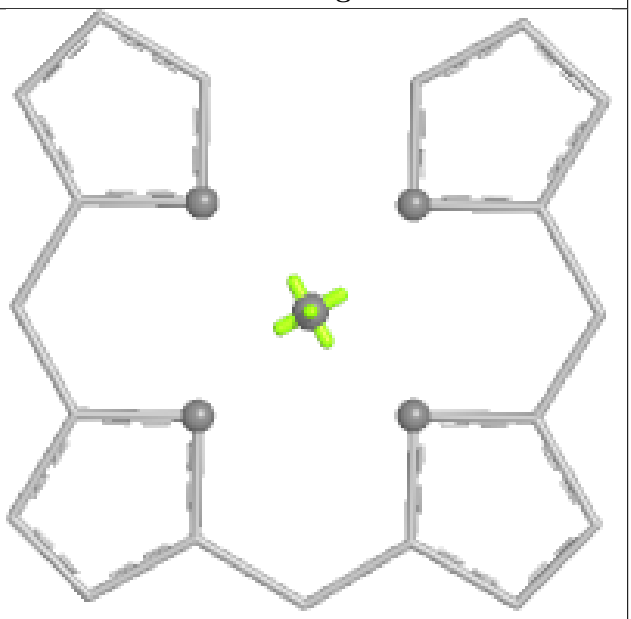
Bond lengths



Bond angles

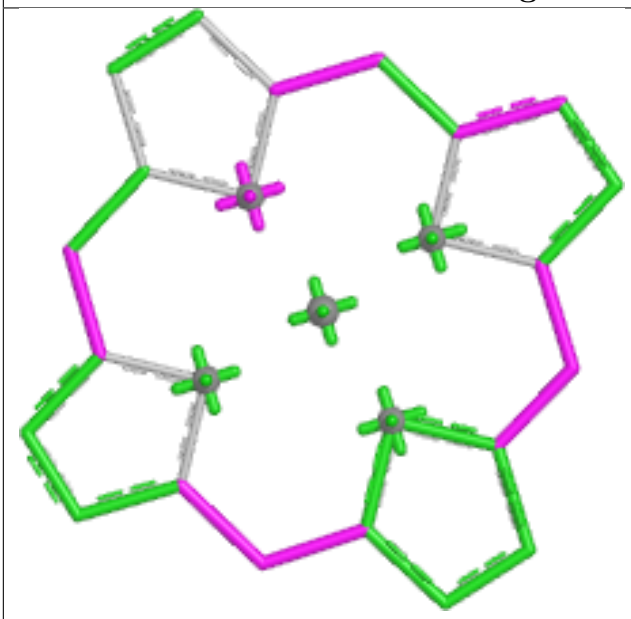


Torsions

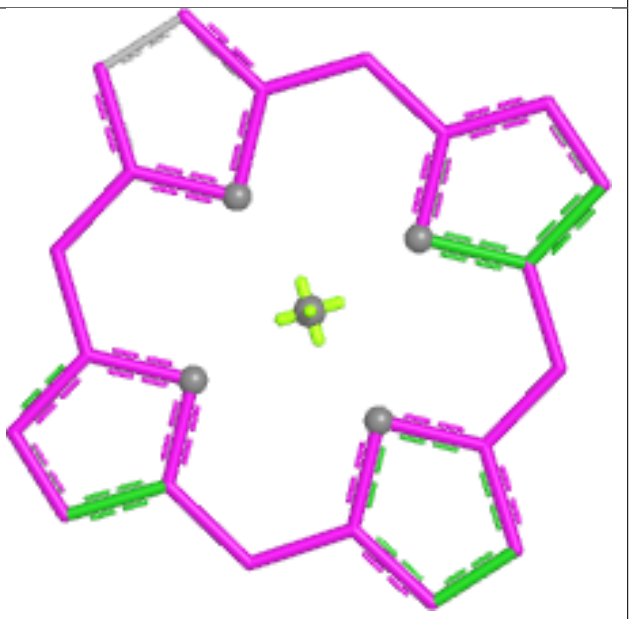


Rings

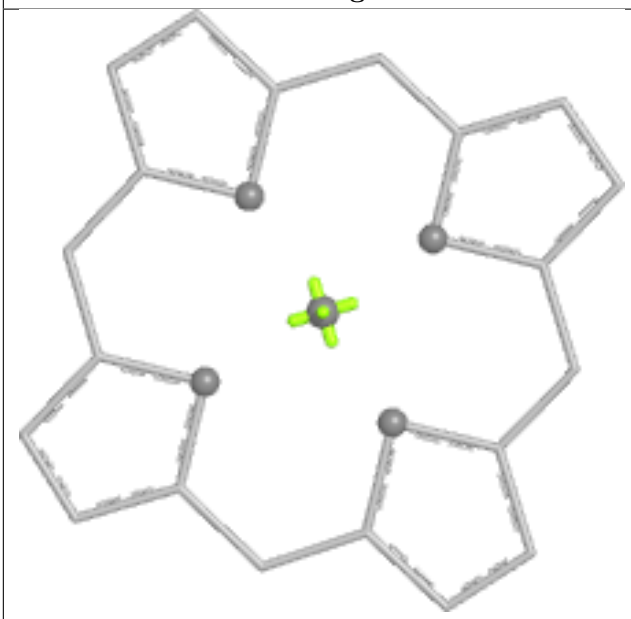
Ligand CLA 2 2013



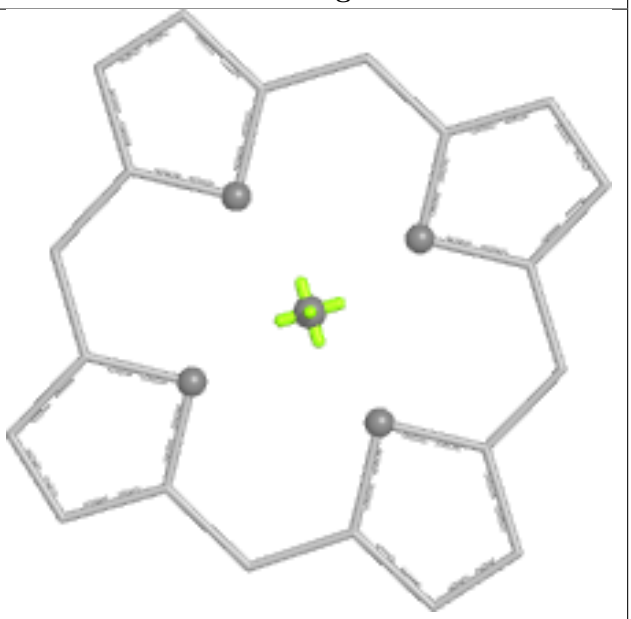
Bond lengths



Bond angles

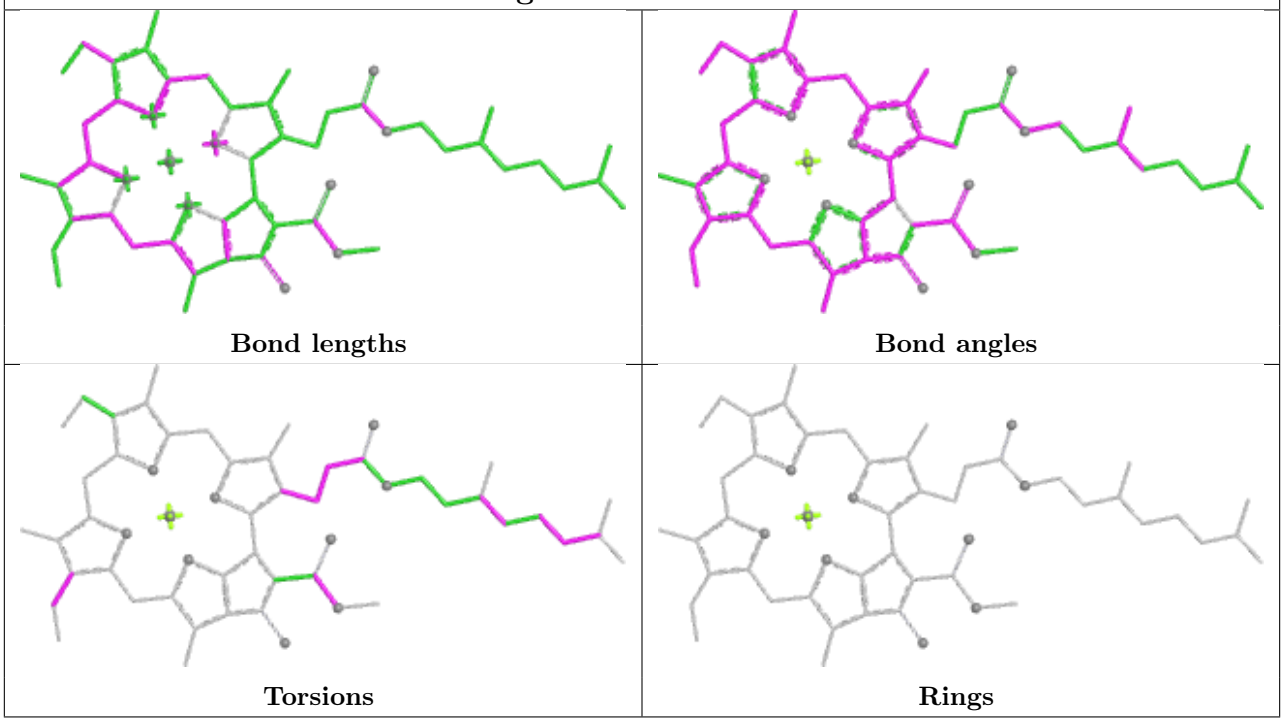


Torsions



Rings

Ligand CLA B 1207



5.7 Other polymers (i)

There are no such residues in this entry.

5.8 Polymer linkage issues (i)

There are no chain breaks in this entry.

6 Fit of model and data (i)

6.1 Protein, DNA and RNA chains (i)

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%)	-0.45	18 (2%)	58	43	12, 39, 59, 72	0
2	B	732/732 (100%)	-0.53	9 (1%)	76	63	13, 39, 58, 64	0
3	C	80/80 (100%)	-0.49	0	100	100	32, 38, 46, 48	0
4	D	138/138 (100%)	-0.55	3 (2%)	62	47	25, 45, 53, 55	0
5	E	62/62 (100%)	-0.67	1 (1%)	70	56	41, 52, 59, 59	0
6	F	154/154 (100%)	-0.62	0	100	100	25, 47, 60, 62	0
7	G	95/95 (100%)	-0.41	2 (2%)	63	48	50, 61, 68, 73	0
8	H	75/75 (100%)	-0.73	0	100	100	43, 56, 75, 83	0
9	I	30/30 (100%)	-0.61	1 (3%)	49	36	39, 46, 55, 58	0
10	J	42/42 (100%)	-0.73	0	100	100	28, 55, 65, 67	0
11	K	0/38	-	-			-	-
12	L	164/164 (100%)	-0.45	4 (2%)	59	45	24, 49, 62, 69	0
13	N	85/85 (100%)	-0.64	0	100	100	25, 70, 87, 90	0
14	1	175/187 (93%)	-0.48	5 (2%)	53	39	28, 71, 84, 87	0
15	2	166/186 (89%)	-0.66	2 (1%)	76	63	25, 71, 86, 91	0
16	3	115/165 (69%)	-0.50	2 (1%)	69	54	57, 79, 88, 89	0
17	4	165/165 (100%)	-0.39	6 (3%)	46	33	23, 65, 72, 75	0
All	All	3006/3152 (95%)	-0.52	53 (1%)	67	53	12, 47, 78, 91	0

All (53) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
14	1	32	VAL	6.5
4	D	60	MET	5.8
1	A	502	THR	5.6
15	2	61	GLY	4.9

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Mol	Chain	Res	Type	RSRZ
1	A	35	ALA	4.6
12	L	116	PRO	4.4
14	1	49	TRP	4.2
14	1	33	PRO	4.2
17	4	37	LEU	4.1
1	A	319	THR	4.0
17	4	131	VAL	3.9
1	A	570	PRO	3.8
4	D	75	LEU	3.8
17	4	130	GLU	3.5
1	A	574	ASN	3.5
4	D	129	GLY	3.5
2	B	450	GLU	3.4
16	3	193	LEU	3.4
17	4	36	ASN	3.4
12	L	82	ALA	3.3
7	G	14	LEU	3.3
2	B	234	ALA	3.0
2	B	107	GLY	3.0
1	A	249	ILE	3.0
2	B	451	LYS	3.0
12	L	45	THR	3.0
1	A	539	PHE	2.9
1	A	224	HIS	2.8
14	1	30	GLY	2.8
2	B	256	THR	2.8
1	A	151	GLN	2.7
9	I	2	ILE	2.7
14	1	79	GLY	2.7
15	2	112	ASP	2.7
1	A	750	PHE	2.6
17	4	86	SER	2.6
7	G	36	PRO	2.6
2	B	645	VAL	2.6
2	B	137	THR	2.6
17	4	122	LYS	2.5
1	A	194	ALA	2.5
1	A	146	THR	2.5
1	A	290	LEU	2.5
1	A	646	SER	2.5
2	B	136	TYR	2.5
16	3	89	THR	2.4

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Mol	Chain	Res	Type	RSRZ
1	A	33	GLN	2.4
1	A	225	VAL	2.3
12	L	127	PRO	2.3
5	E	48	ASN	2.1
2	B	182	LEU	2.1
1	A	127	VAL	2.1
1	A	540	LEU	2.0

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

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

6.3 Carbohydrates (i)

There are no oligosaccharides in this entry.

6.4 Ligands (i)

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	1303	25/65	0.94	0.08	76,77,77,77	0
18	CLA	1	1007	25/65	0.94	0.09	68,68,69,69	0
18	CLA	2	2001	25/65	0.94	0.08	61,63,65,65	0
18	CLA	2	2015	25/65	0.94	0.07	92,93,93,93	0
18	CLA	3	3009	25/65	0.94	0.10	94,94,94,95	0
18	CLA	3	3012	25/65	0.94	0.07	77,79,81,81	0
20	BCR	F	6016	40/40	0.94	0.09	28,33,39,40	0
18	CLA	1	1005	25/65	0.95	0.10	77,78,78,78	0
18	CLA	A	1309	25/65	0.95	0.10	112,112,112,112	0
18	CLA	1	1008	25/65	0.95	0.07	79,79,79,80	0
18	CLA	2	2005	25/65	0.95	0.07	64,65,66,66	0
18	CLA	F	1305	25/65	0.95	0.07	78,79,79,79	0
18	CLA	2	2011	25/65	0.95	0.08	93,94,94,94	0
18	CLA	F	1306	25/65	0.95	0.07	87,88,89,89	0
18	CLA	G	1233	51/65	0.95	0.06	61,66,67,67	0
18	CLA	J	1307	25/65	0.95	0.07	77,78,78,79	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
18	CLA	4	4005	25/65	0.95	0.09	60,62,63,63	0
18	CLA	4	4001	25/65	0.95	0.11	82,83,83,84	0
18	CLA	L	1504	55/65	0.95	0.11	32,67,68,71	0
18	CLA	K	1141	25/65	0.96	0.06	78,79,79,80	0
18	CLA	K	1150	25/65	0.96	0.07	88,90,90,90	0
18	CLA	L	1125	25/65	0.96	0.07	80,80,82,82	0
18	CLA	A	1151	25/65	0.96	0.06	73,76,77,77	0
18	CLA	A	1118	25/65	0.96	0.07	89,90,91,91	0
18	CLA	1	1013	25/65	0.96	0.07	86,87,88,88	0
18	CLA	1	1011	25/65	0.96	0.06	94,95,95,96	0
18	CLA	1	1001	25/65	0.96	0.08	63,64,65,66	0
18	CLA	B	1201	25/65	0.96	0.09	50,51,53,53	0
18	CLA	1	1002	25/65	0.96	0.08	86,86,87,88	0
18	CLA	B	1232	55/65	0.96	0.08	74,91,93,93	0
18	CLA	B	1301	25/65	0.96	0.06	73,74,75,75	0
18	CLA	2	2006	25/65	0.96	0.08	81,82,82,83	0
18	CLA	2	2010	25/65	0.96	0.07	90,90,91,91	0
18	CLA	A	1119	55/65	0.96	0.11	60,66,68,69	0
18	CLA	A	1127	25/65	0.96	0.10	58,59,60,60	0
18	CLA	2	2012	25/65	0.96	0.09	99,100,100,100	0
18	CLA	A	1144	25/65	0.96	0.08	101,101,101,102	0
18	CLA	F	4015	25/65	0.96	0.09	132,133,133,133	0
18	CLA	A	1147	25/65	0.96	0.07	66,67,68,69	0
18	CLA	3	3001	25/65	0.96	0.11	137,137,138,138	0
18	CLA	3	3002	25/65	0.96	0.05	68,70,70,70	0
18	CLA	3	3015	25/65	0.96	0.06	72,73,74,75	0
18	CLA	4	1009	25/65	0.96	0.08	78,79,79,79	0
18	CLA	4	4009	25/65	0.96	0.07	80,81,82,82	0
18	CLA	4	4004	25/65	0.96	0.07	71,72,74,74	0
18	CLA	H	1505	25/65	0.96	0.09	84,85,86,86	0
18	CLA	4	4006	25/65	0.96	0.09	82,83,84,85	0
18	CLA	A	1148	25/65	0.96	0.09	93,94,95,95	0
18	CLA	4	4007	25/65	0.96	0.08	89,91,91,91	0
18	CLA	4	4002	25/65	0.96	0.06	65,66,67,67	0
18	CLA	4	4003	25/65	0.96	0.07	80,81,81,81	0
20	BCR	A	6011	40/40	0.96	0.08	9,12,19,21	0
18	CLA	J	1308	25/65	0.96	0.07	106,107,107,108	0
20	BCR	I	6018	40/40	0.96	0.09	6,19,26,28	0
18	CLA	B	1236	46/65	0.97	0.08	34,44,46,47	0
18	CLA	B	1239	55/65	0.97	0.08	27,52,53,55	0
18	CLA	B	1242	47/65	0.97	0.10	85,91,92,94	0
18	CLA	A	1102	25/65	0.97	0.08	72,73,75,75	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
18	CLA	F	1139	44/65	0.97	0.08	36,40,42,43	0
18	CLA	F	1302	55/65	0.97	0.10	19,75,77,79	0
18	CLA	A	1104	25/65	0.97	0.06	40,42,43,44	0
18	CLA	A	1120	25/65	0.97	0.07	76,78,79,80	0
18	CLA	A	1122	55/65	0.97	0.07	18,39,41,43	0
18	CLA	A	1123	55/65	0.97	0.08	37,46,49,50	0
18	CLA	A	1124	25/65	0.97	0.06	48,51,52,53	0
18	CLA	G	1248	25/65	0.97	0.07	109,110,111,111	0
18	CLA	H	1501	55/65	0.97	0.08	49,68,70,73	0
18	CLA	A	1126	55/65	0.97	0.08	15,40,42,44	0
18	CLA	I	1204	55/65	0.97	0.08	40,44,51,52	0
18	CLA	A	1106	41/65	0.97	0.09	16,20,22,24	0
18	CLA	A	1128	55/65	0.97	0.07	20,37,39,40	0
18	CLA	J	2107	61/65	0.97	0.07	40,62,63,63	0
18	CLA	A	1129	55/65	0.97	0.08	35,58,60,61	0
18	CLA	A	1131	44/65	0.97	0.08	35,39,42,44	0
18	CLA	K	1153	25/65	0.97	0.06	54,55,56,56	0
18	CLA	A	1133	25/65	0.97	0.06	44,46,47,48	0
18	CLA	L	1130	50/65	0.97	0.09	57,66,69,70	0
18	CLA	L	1502	51/65	0.97	0.08	36,63,65,65	0
18	CLA	A	1134	25/65	0.97	0.07	49,51,52,52	0
18	CLA	A	1135	45/65	0.97	0.09	39,54,55,56	0
18	CLA	1	1006	25/65	0.97	0.05	60,62,63,63	0
18	CLA	A	1137	55/65	0.97	0.08	20,28,30,32	0
18	CLA	1	1010	25/65	0.97	0.08	81,81,82,82	0
18	CLA	A	1140	55/65	0.97	0.10	12,39,41,43	0
18	CLA	A	1142	25/65	0.97	0.07	88,89,90,91	0
18	CLA	A	1143	25/65	0.97	0.09	116,118,118,118	0
18	CLA	A	1108	50/65	0.97	0.06	52,74,76,76	0
18	CLA	1	1003	25/65	0.97	0.07	84,85,86,86	0
18	CLA	A	1146	25/65	0.97	0.06	70,72,73,73	0
18	CLA	1	1014	25/65	0.97	0.05	67,68,70,70	0
18	CLA	A	1110	25/65	0.97	0.05	70,71,72,72	0
18	CLA	A	1111	25/65	0.97	0.08	65,66,68,68	0
18	CLA	A	1113	50/65	0.97	0.08	41,60,62,63	0
18	CLA	A	1152	25/65	0.97	0.08	68,69,70,71	0
18	CLA	A	9011	55/65	0.97	0.09	2,26,28,29	0
18	CLA	A	9013	46/65	0.97	0.10	11,17,21,24	0
18	CLA	A	1115	47/65	0.97	0.07	40,44,48,50	0
18	CLA	2	2007	25/65	0.97	0.05	79,80,81,81	0
18	CLA	2	2002	25/65	0.97	0.08	103,103,104,104	0
18	CLA	2	2003	25/65	0.97	0.06	114,114,115,115	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
18	CLA	3	2009	25/65	0.97	0.06	94,94,95,95	0
18	CLA	B	9010	47/65	0.97	0.09	23,37,40,41	0
18	CLA	3	3004	25/65	0.97	0.07	76,77,78,78	0
18	CLA	3	3005	25/65	0.97	0.06	95,96,97,97	0
18	CLA	B	9012	55/65	0.97	0.11	16,47,50,52	0
18	CLA	3	3006	25/65	0.97	0.07	112,113,113,114	0
18	CLA	3	3013	25/65	0.97	0.07	77,78,78,78	0
18	CLA	3	3010	25/65	0.97	0.07	92,93,93,93	0
18	CLA	A	1116	25/65	0.97	0.09	81,82,83,83	0
18	CLA	3	3011	25/65	0.97	0.07	107,107,108,108	0
18	CLA	B	1205	55/65	0.97	0.08	17,41,43,46	0
18	CLA	B	1208	55/65	0.97	0.07	36,39,41,42	0
18	CLA	3	3003	25/65	0.97	0.04	67,68,70,70	0
18	CLA	3	3008	25/65	0.97	0.07	90,90,91,91	0
18	CLA	4	1304	55/65	0.97	0.08	40,77,78,79	0
18	CLA	B	1210	25/65	0.97	0.10	75,76,76,77	0
18	CLA	B	1212	60/65	0.97	0.10	59,73,75,77	0
18	CLA	B	1216	56/65	0.97	0.10	66,72,73,73	0
18	CLA	B	1217	50/65	0.97	0.08	60,66,68,68	0
18	CLA	B	1219	51/65	0.97	0.07	27,47,48,49	0
18	CLA	4	4013	25/65	0.97	0.06	86,86,87,87	0
18	CLA	4	4010	25/65	0.97	0.10	99,99,99,99	0
18	CLA	4	4011	25/65	0.97	0.07	51,52,53,54	0
18	CLA	4	4012	25/65	0.97	0.08	63,65,66,67	0
18	CLA	B	1220	60/65	0.97	0.08	31,39,50,53	0
18	CLA	B	1221	48/65	0.97	0.08	20,31,38,42	0
18	CLA	B	1222	65/65	0.97	0.09	46,69,70,73	0
18	CLA	B	1228	55/65	0.97	0.08	42,46,47,49	0
18	CLA	4	4008	25/65	0.97	0.09	72,74,74,74	0
19	PQN	A	5001	33/33	0.97	0.08	15,23,34,36	0
19	PQN	B	5002	33/33	0.97	0.08	8,18,21,21	0
18	CLA	B	1229	49/65	0.97	0.09	35,48,50,51	0
20	BCR	B	6017	40/40	0.97	0.09	27,33,46,47	0
18	CLA	A	1117	25/65	0.97	0.06	47,48,49,49	0
18	CLA	B	1235	55/65	0.97	0.09	31,40,42,44	0
20	BCR	L	6020	40/40	0.97	0.08	11,24,35,38	0
18	CLA	B	9022	54/65	0.98	0.08	28,31,41,41	0
18	CLA	2	2008	25/65	0.98	0.05	60,61,62,63	0
18	CLA	B	9023	47/65	0.98	0.08	36,40,41,43	0
18	CLA	A	1103	47/65	0.98	0.09	67,77,78,79	0
18	CLA	B	1223	25/65	0.98	0.06	46,48,49,50	0
18	CLA	B	1224	51/65	0.98	0.09	47,55,56,57	0

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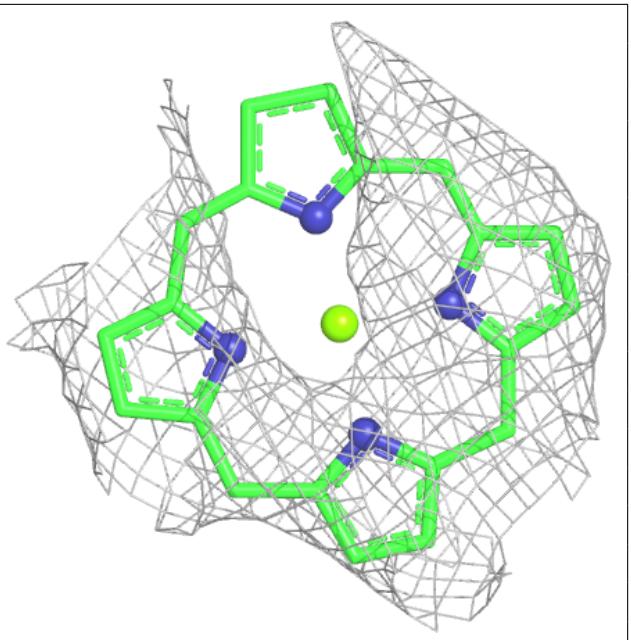
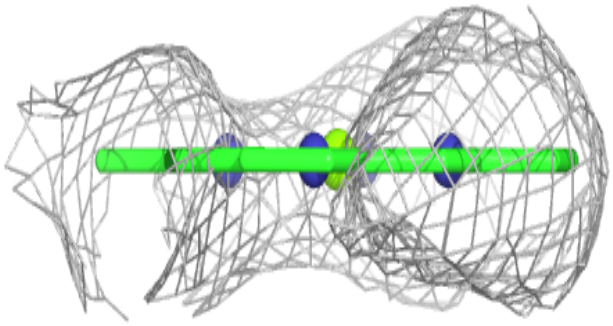
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
18	CLA	B	1225	45/65	0.98	0.07	34,50,52,52	0
18	CLA	B	1226	25/65	0.98	0.07	50,53,54,54	0
18	CLA	B	1227	50/65	0.98	0.06	34,41,44,45	0
18	CLA	B	1202	50/65	0.98	0.08	23,37,39,42	0
18	CLA	B	1203	48/65	0.98	0.06	2,23,24,26	0
18	CLA	B	1230	25/65	0.98	0.09	73,75,76,76	0
18	CLA	L	1503	46/65	0.98	0.06	19,22,25,28	0
18	CLA	3	3007	25/65	0.98	0.05	80,81,82,83	0
18	CLA	B	1231	46/65	0.98	0.07	36,46,49,51	0
18	CLA	1	1004	25/65	0.98	0.09	88,89,89,90	0
18	CLA	A	1132	25/65	0.98	0.06	27,29,31,32	0
18	CLA	B	1234	50/65	0.98	0.08	35,53,55,56	0
18	CLA	B	1206	25/65	0.98	0.08	50,54,55,56	0
18	CLA	B	1207	55/65	0.98	0.07	19,30,35,37	0
18	CLA	B	1237	51/65	0.98	0.08	29,59,62,62	0
18	CLA	1	1012	25/65	0.98	0.06	76,77,77,77	0
18	CLA	B	1238	54/65	0.98	0.08	13,27,32,33	0
18	CLA	A	1107	57/65	0.98	0.06	21,26,30,33	0
18	CLA	B	1241	25/65	0.98	0.09	103,104,104,104	0
18	CLA	B	1209	55/65	0.98	0.06	32,50,53,54	0
18	CLA	A	1101	25/65	0.98	0.07	61,63,64,64	0
18	CLA	B	1211	25/65	0.98	0.07	52,54,55,55	0
18	CLA	2	2004	25/65	0.98	0.07	83,84,84,85	0
18	CLA	F	1240	25/65	0.98	0.04	43,44,45,46	0
18	CLA	A	1109	24/65	0.98	0.07	48,49,50,51	0
18	CLA	B	1213	25/65	0.98	0.08	79,81,82,82	0
18	CLA	2	2013	25/65	0.98	0.07	81,82,84,84	0
18	CLA	B	1214	49/65	0.98	0.07	51,69,70,71	0
18	CLA	B	1215	52/65	0.98	0.06	11,16,27,30	0
18	CLA	B	1138	56/65	0.98	0.06	18,47,50,53	0
18	CLA	A	1136	55/65	0.98	0.06	40,45,57,58	0
18	CLA	B	1218	51/65	0.98	0.05	20,47,50,51	0
18	CLA	A	1105	25/65	0.98	0.08	83,83,84,84	0
21	SF4	B	3101	8/8	1.00	0.02	14,21,22,25	0
21	SF4	C	3102	8/8	1.00	0.03	19,21,24,26	0
21	SF4	C	3103	8/8	1.00	0.03	10,12,15,15	0

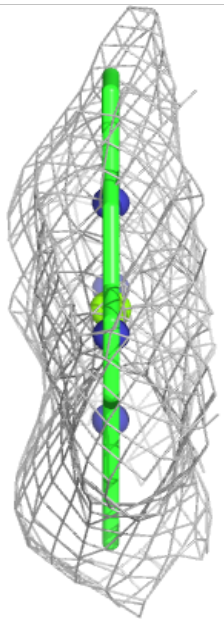
The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation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

Electron density around CLA F 1303:

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

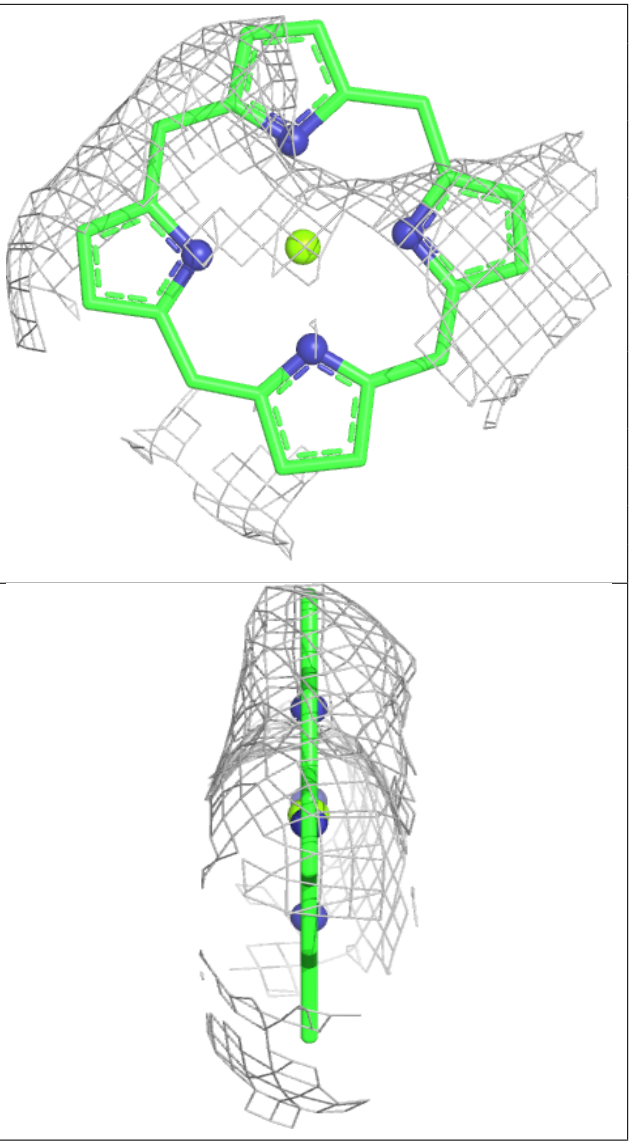






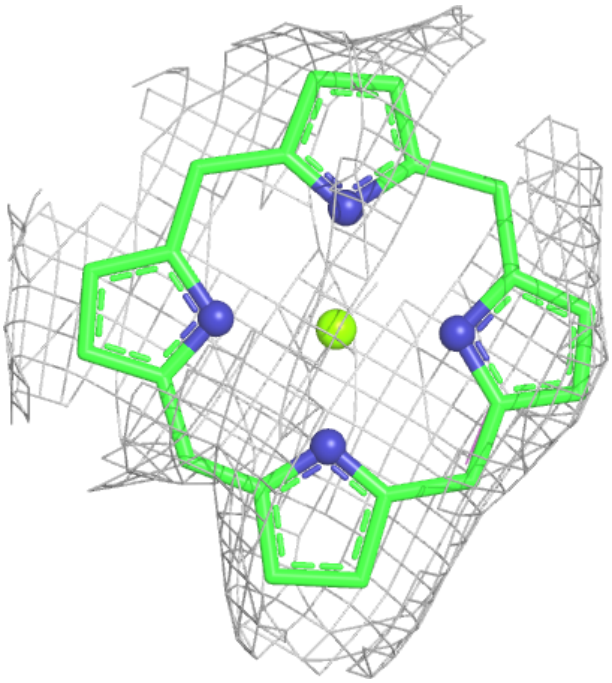
Electron density around CLA 1 1007:

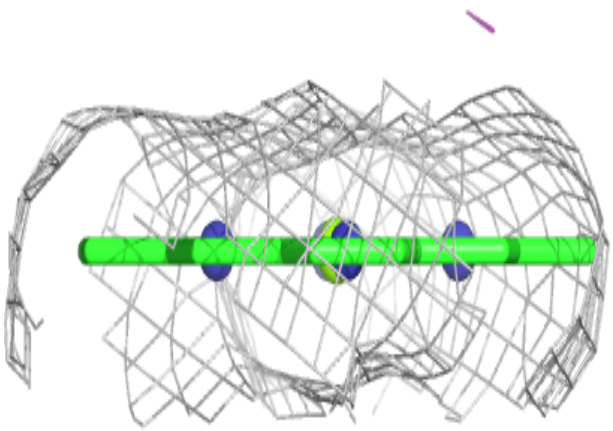
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

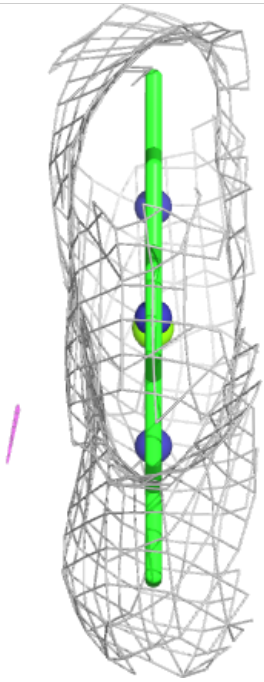


Electron density around CLA 2 2001:

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

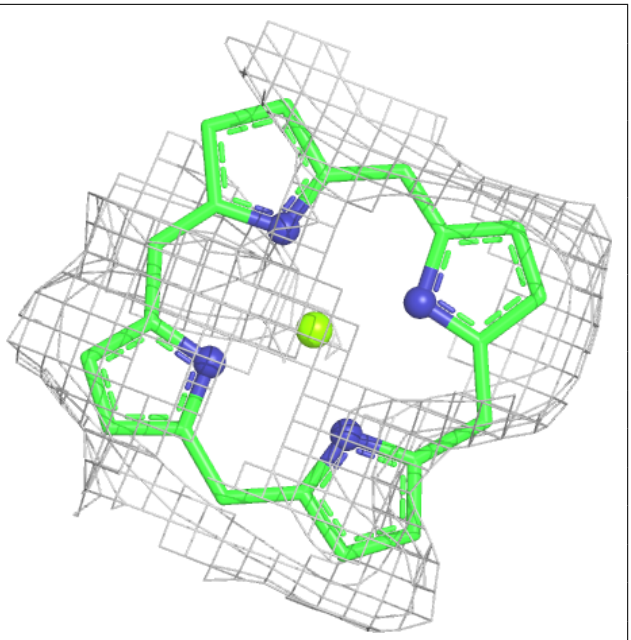


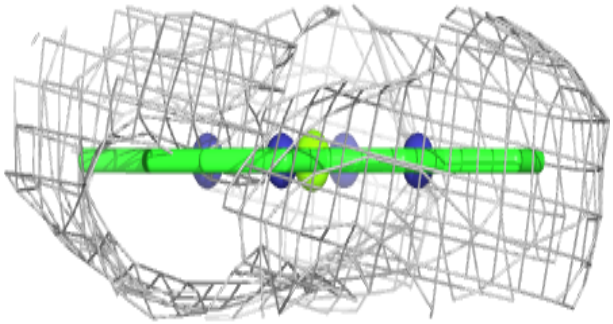


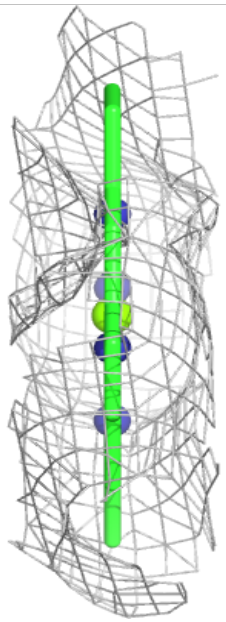


Electron density around CLA 2 2015:

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

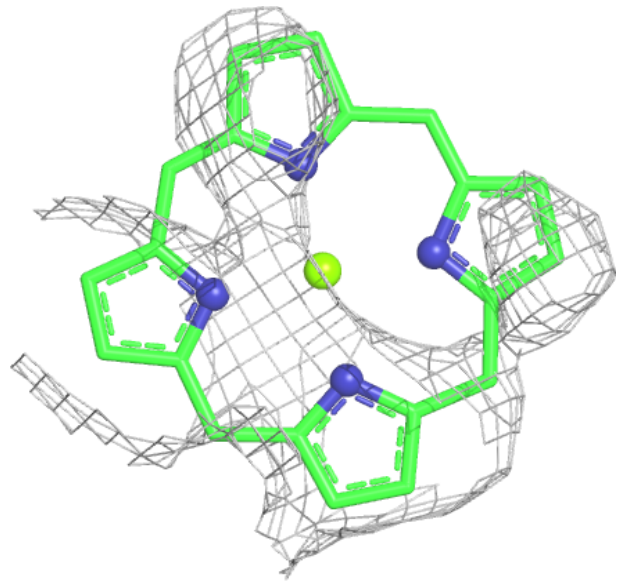


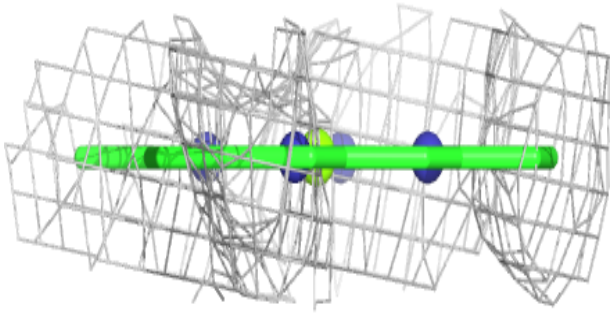


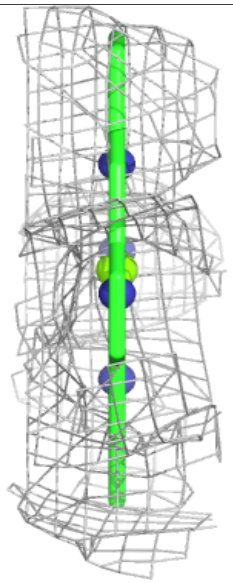


Electron density around CLA 3 3009:

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

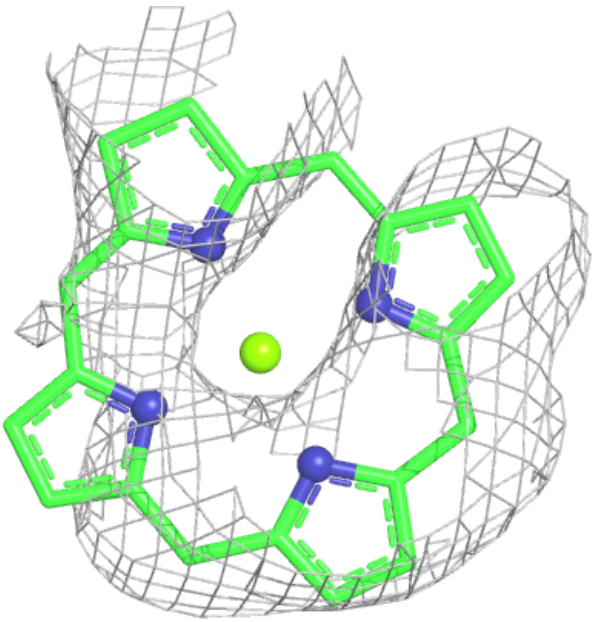


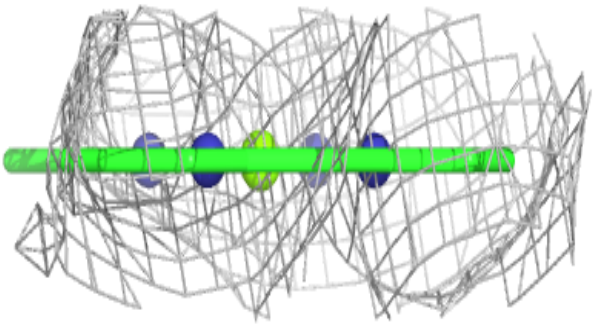


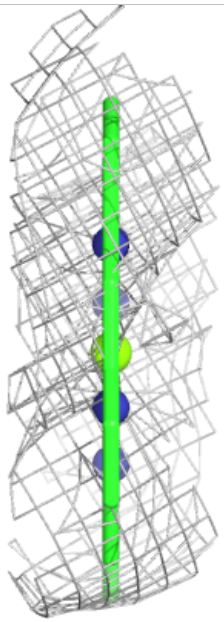


Electron density around CLA 3 3012:

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

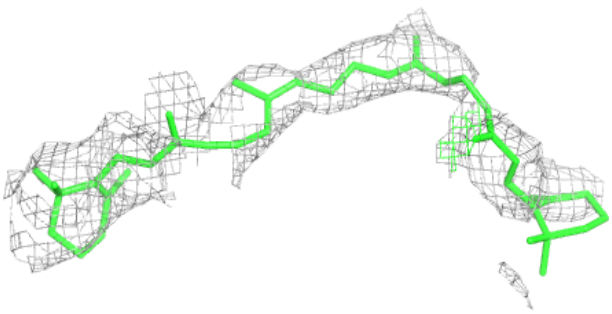


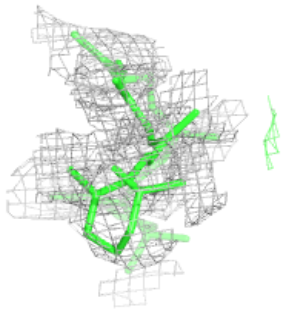




Electron density around BCR F 6016:

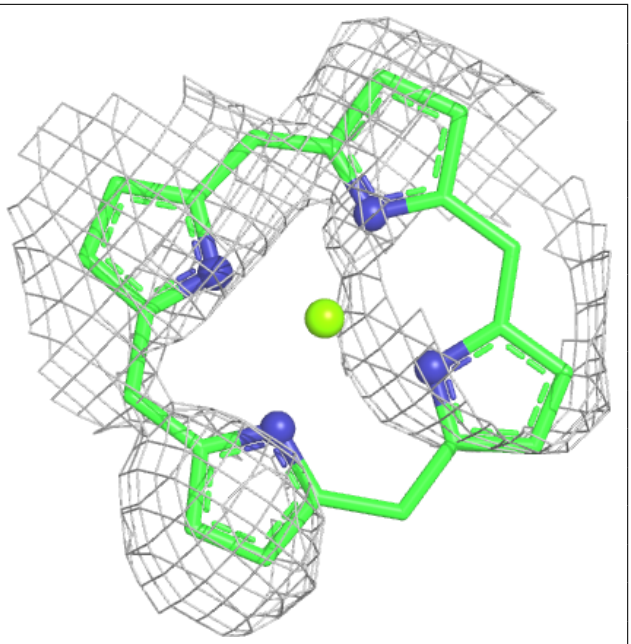
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

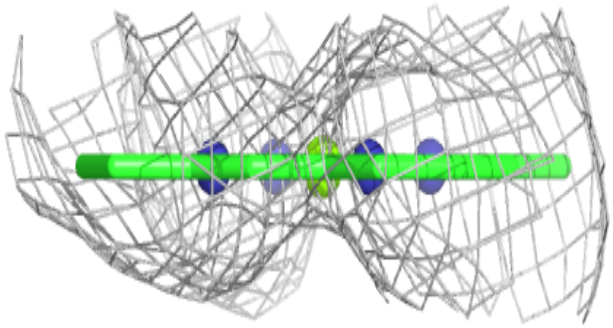


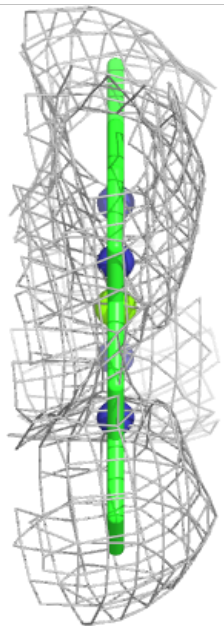


Electron density around CLA 1 1005:

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

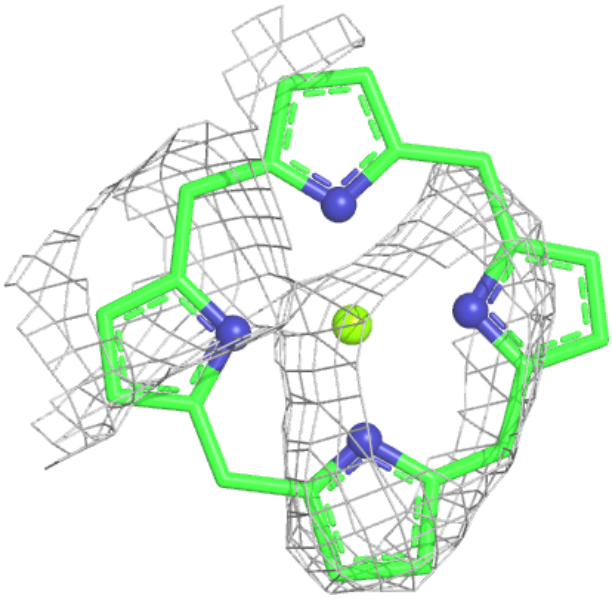


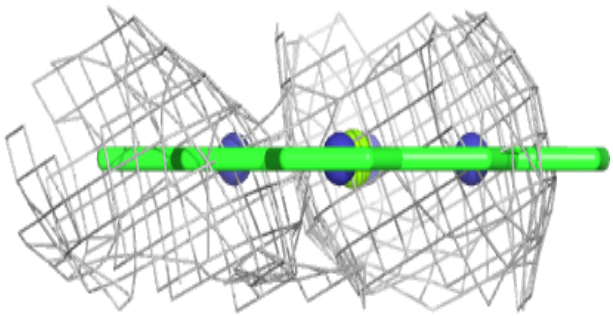


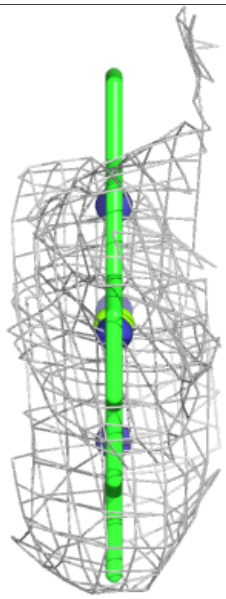


Electron density around CLA A 1309:

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

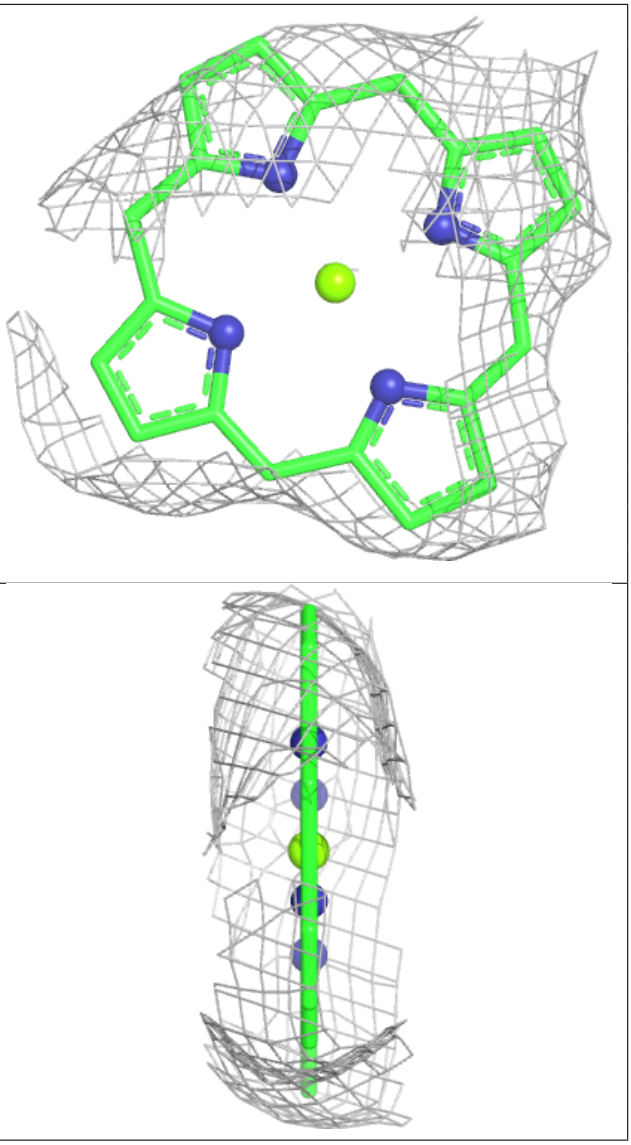






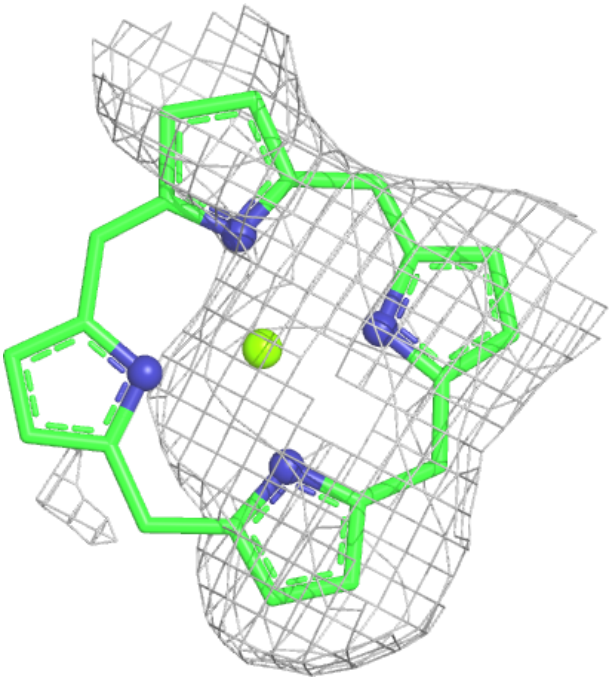
Electron density around CLA 1 1008:

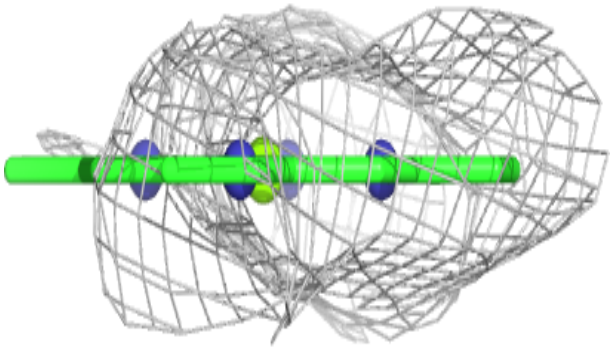
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

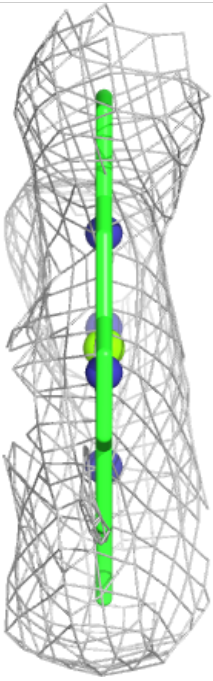


Electron density around CLA 2 2005:

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

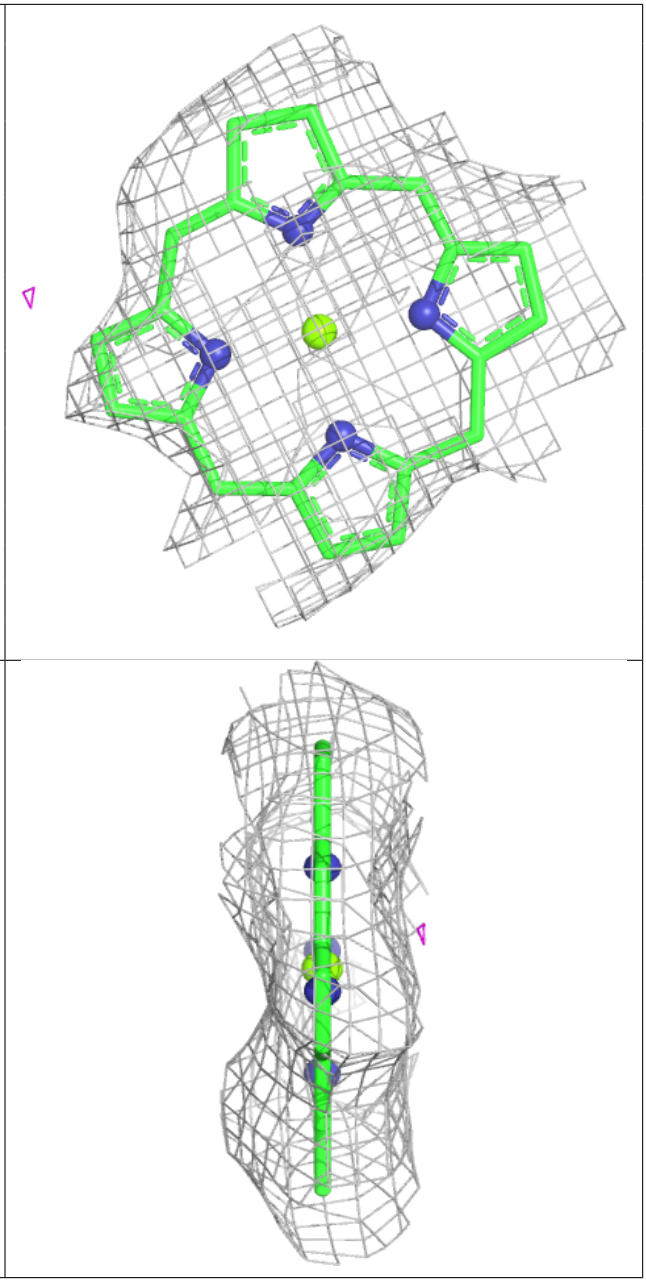






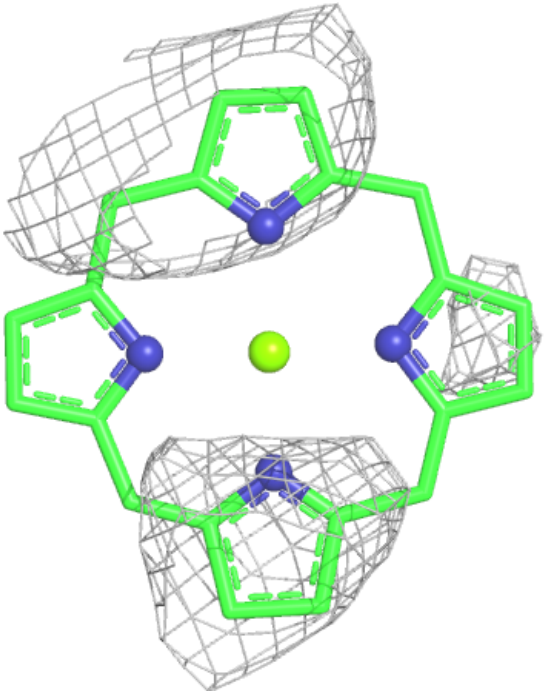
Electron density around CLA F 1305:

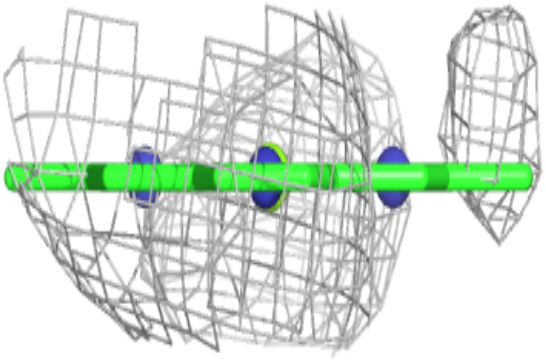
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

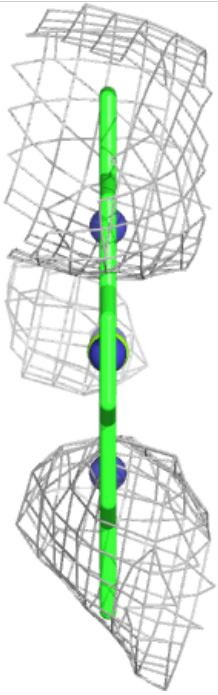


Electron density around CLA 2 2011:

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

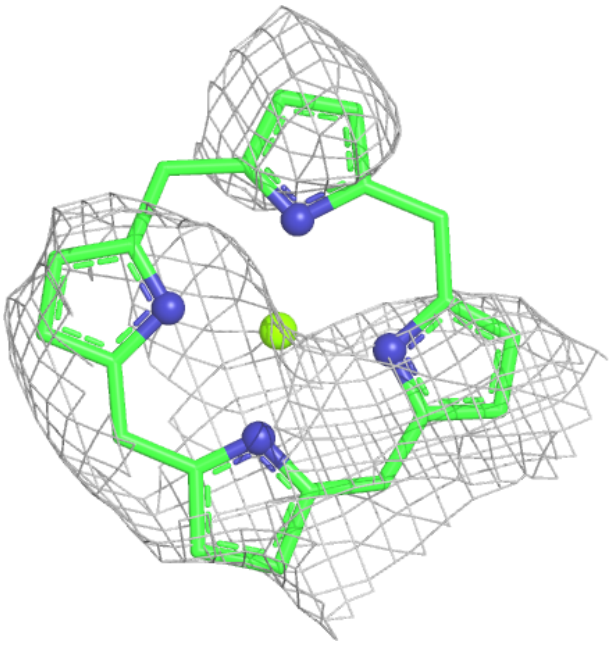


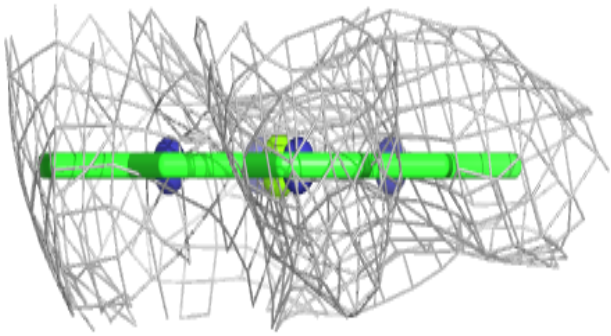


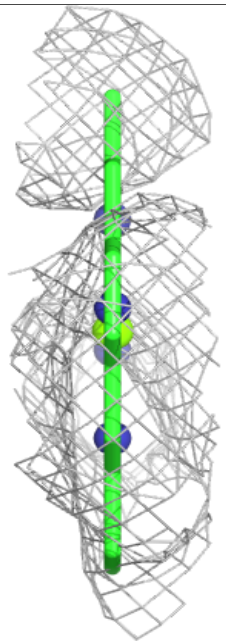


Electron density around CLA F 1306:

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

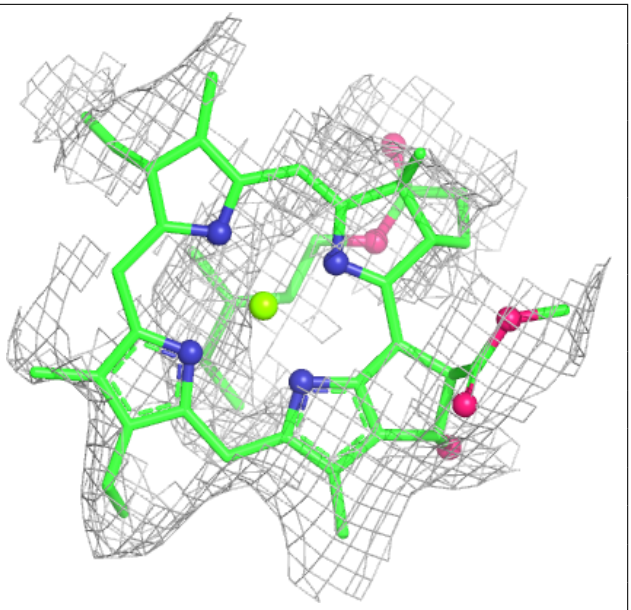


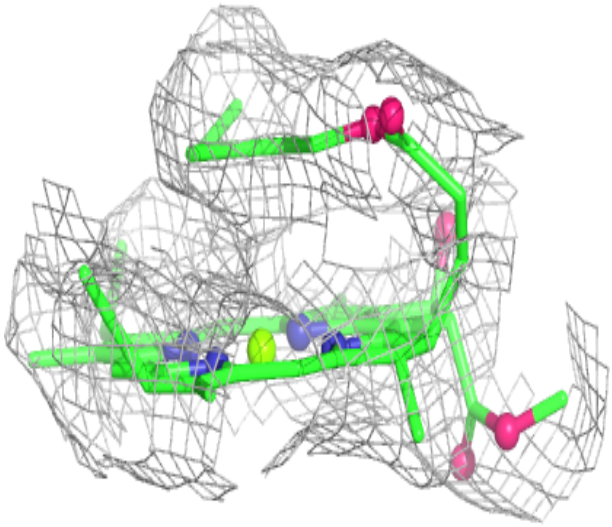


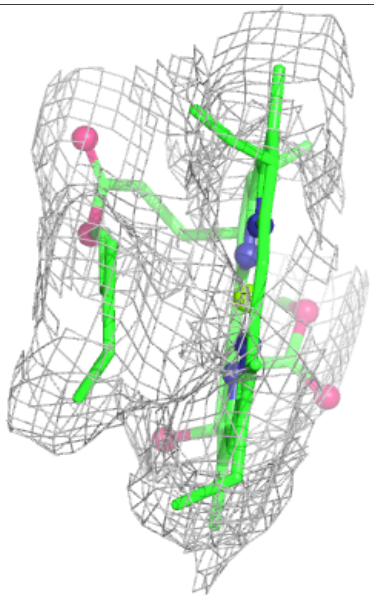


Electron density around CLA G 1233:

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

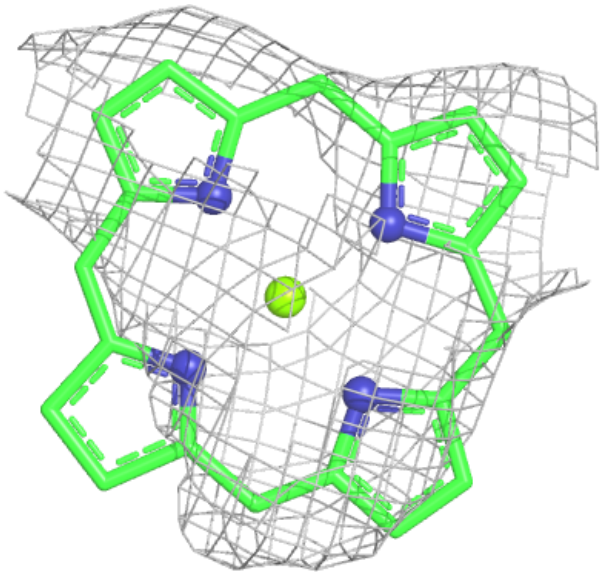


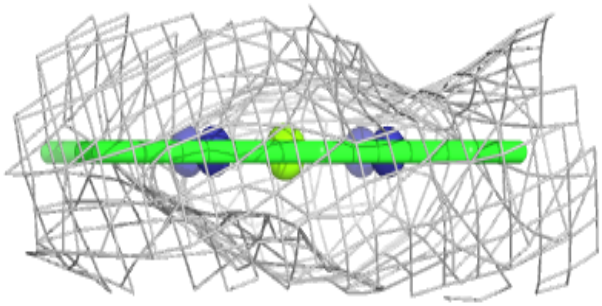


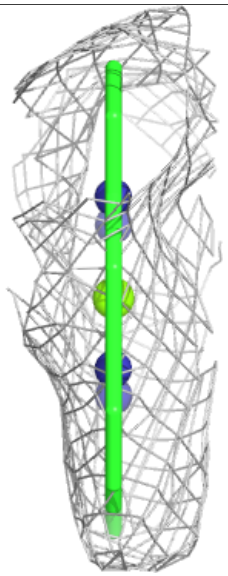


Electron density around CLA J 1307:

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

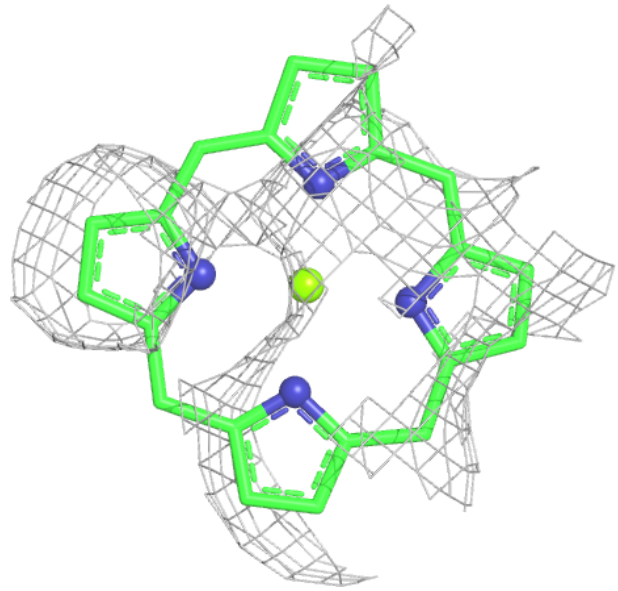


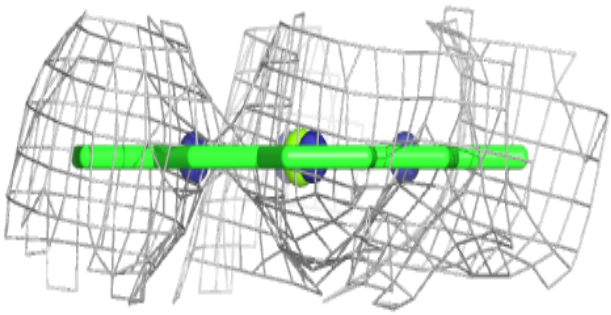


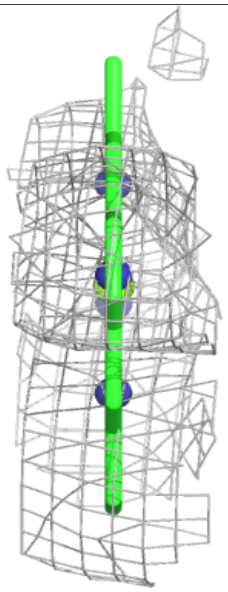


Electron density around CLA 4 4005:

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

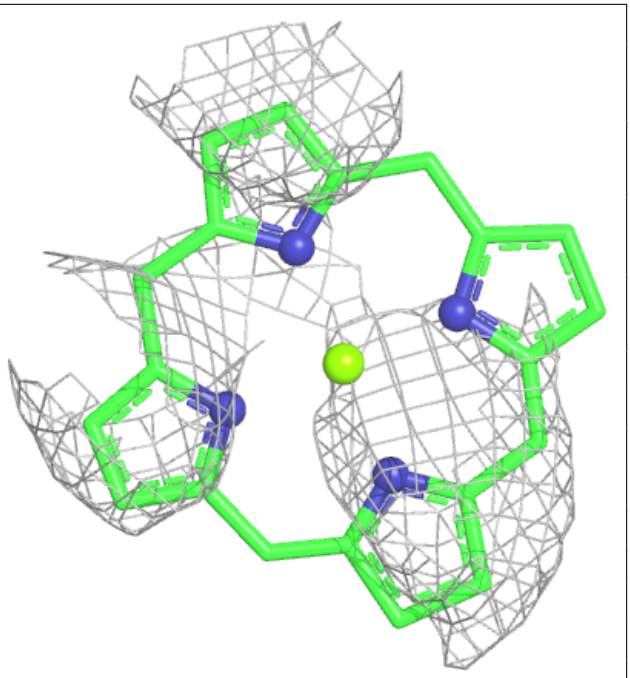


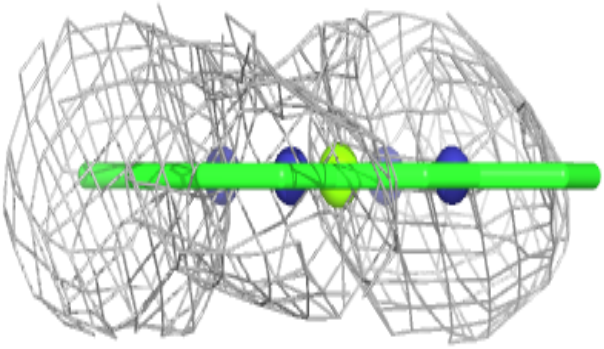


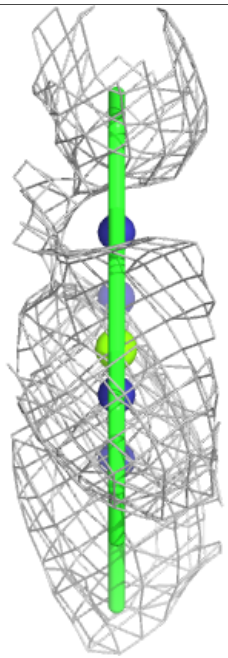


Electron density around CLA 4 4001:

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

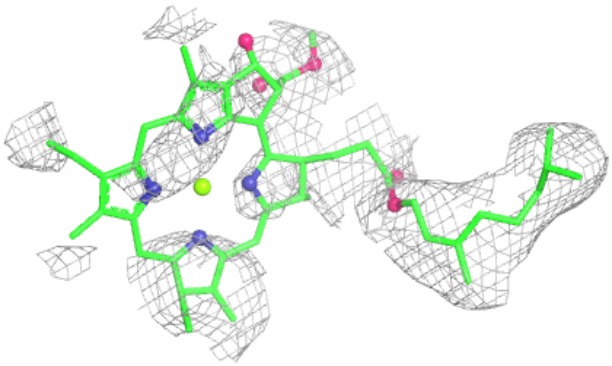


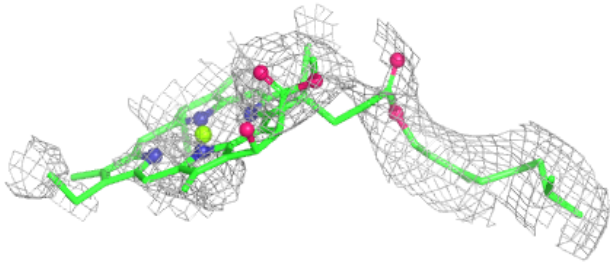


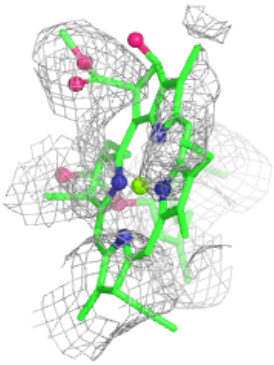


Electron density around CLA L 1504:

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

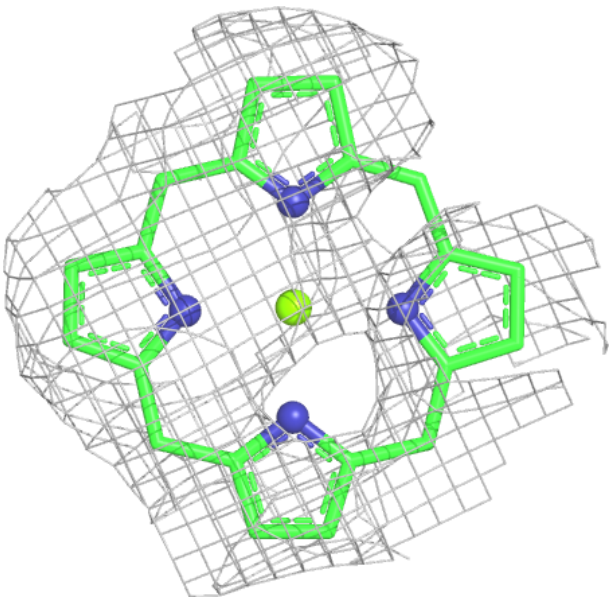


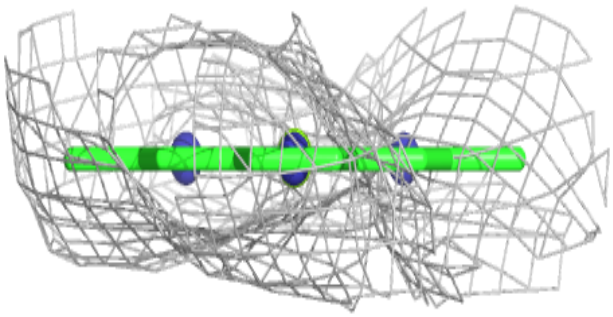


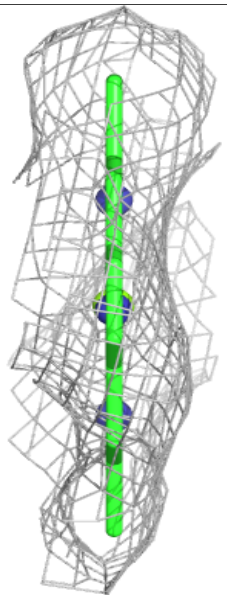


Electron density around CLA K 1141:

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

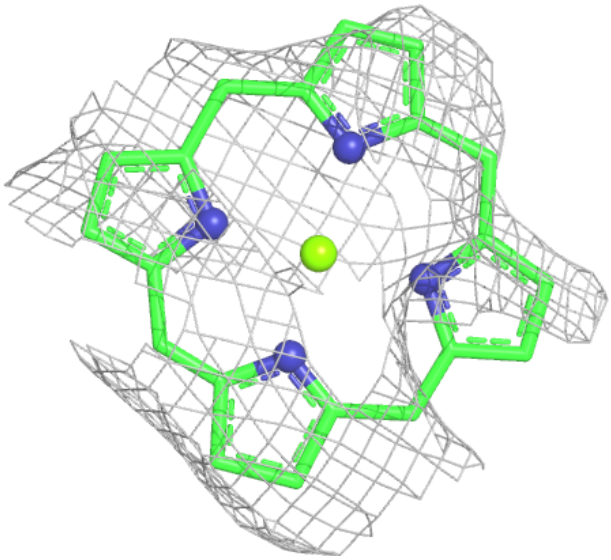


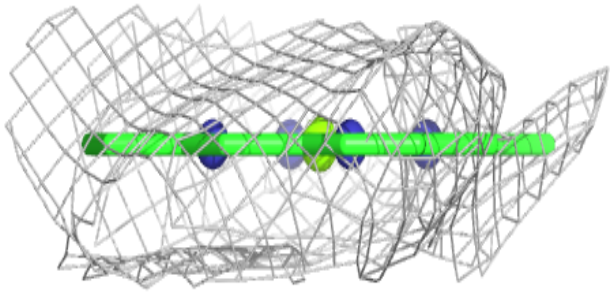


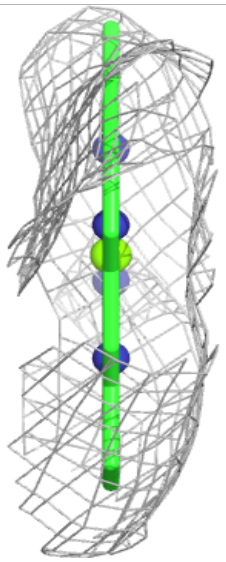


Electron density around CLA K 1150:

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

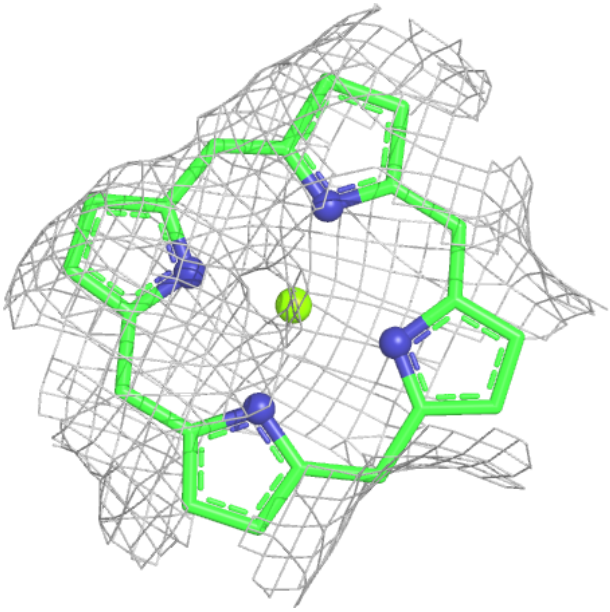


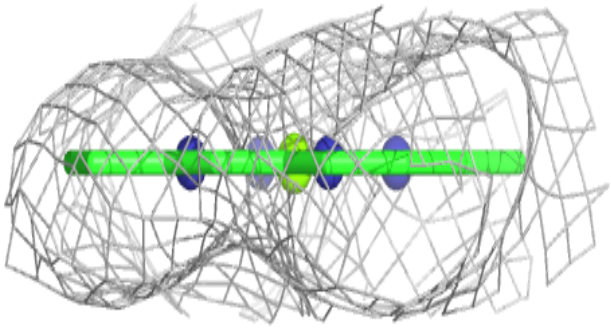


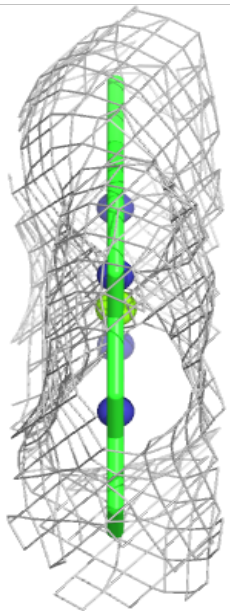


Electron density around CLA L 1125:

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

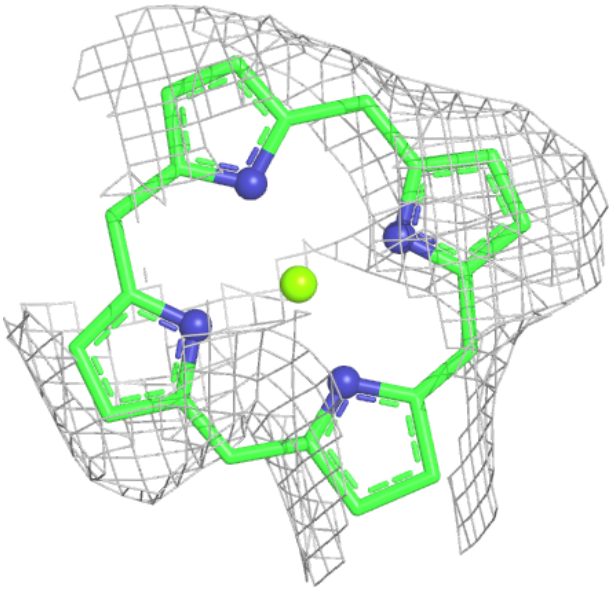


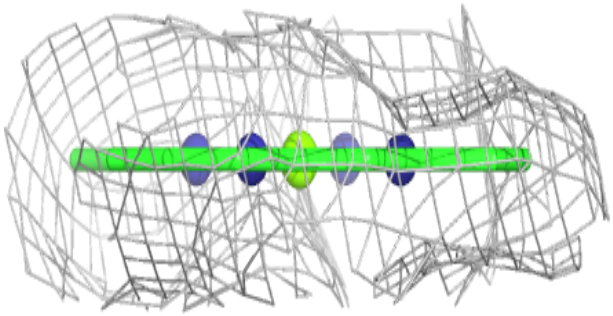


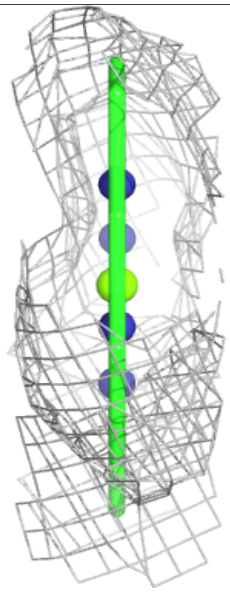


Electron density around CLA A 1151:

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

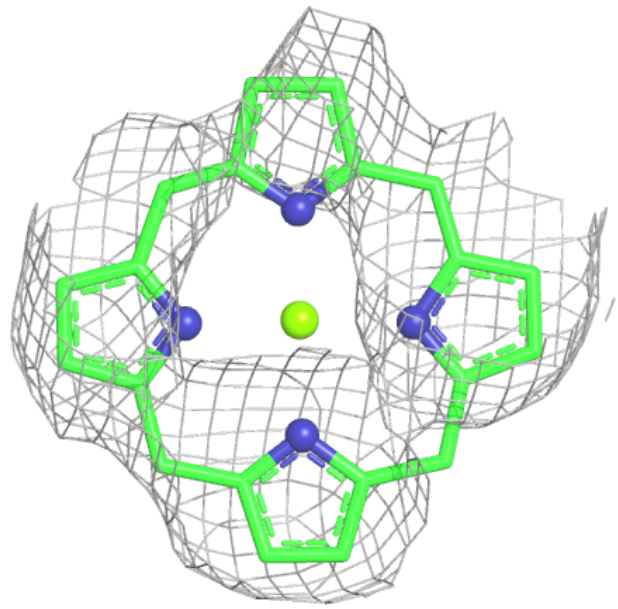


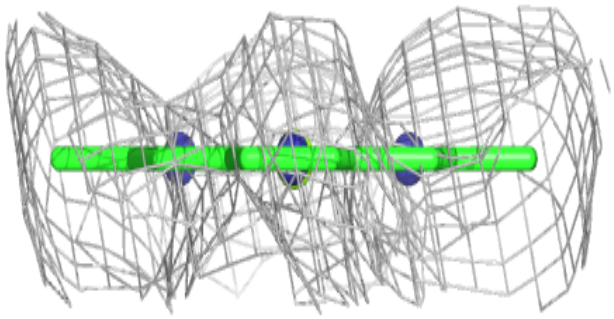


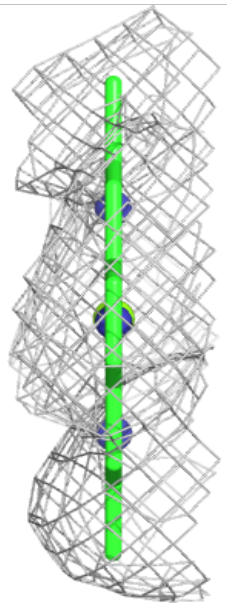


Electron density around CLA A 1118:

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

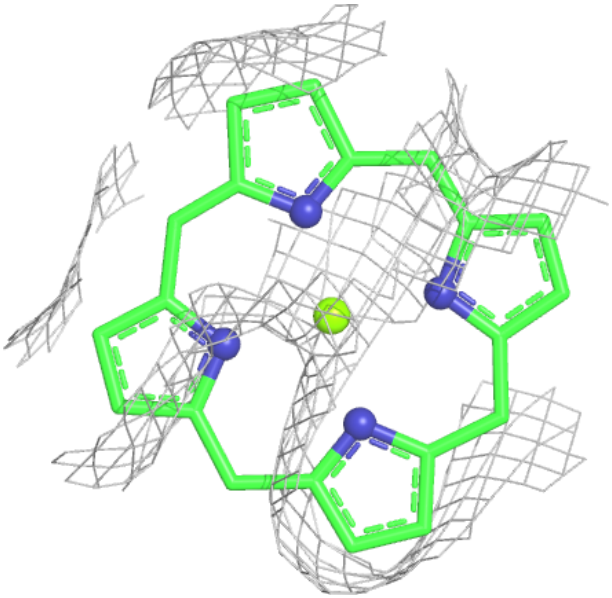


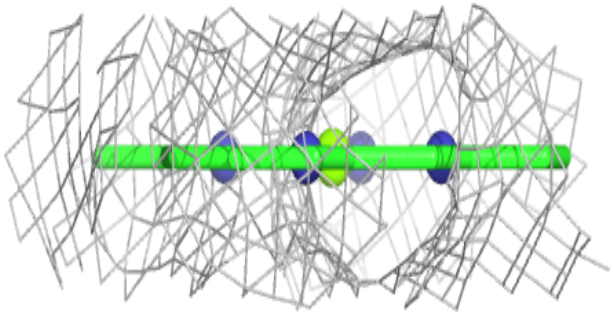


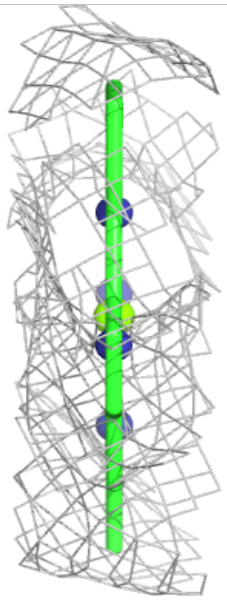


Electron density around CLA 1 1013:

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

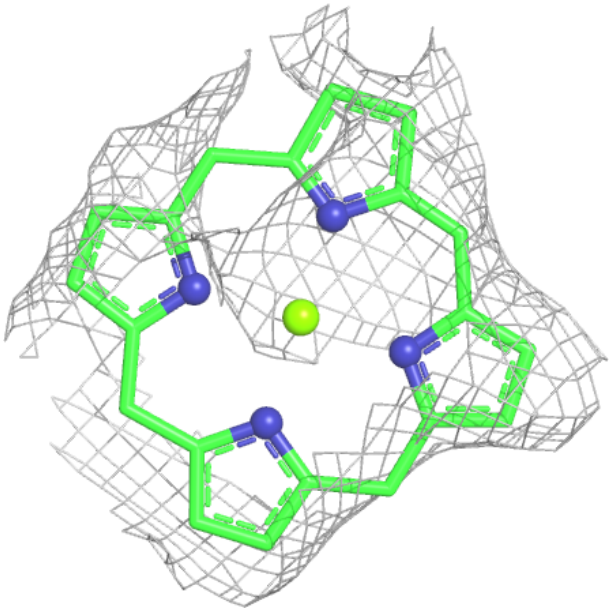


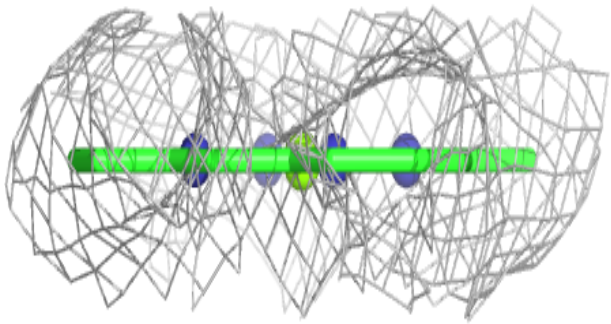


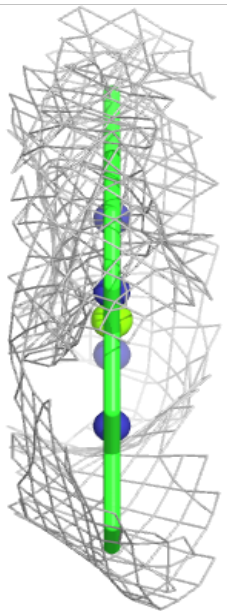


Electron density around CLA 1 1011:

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

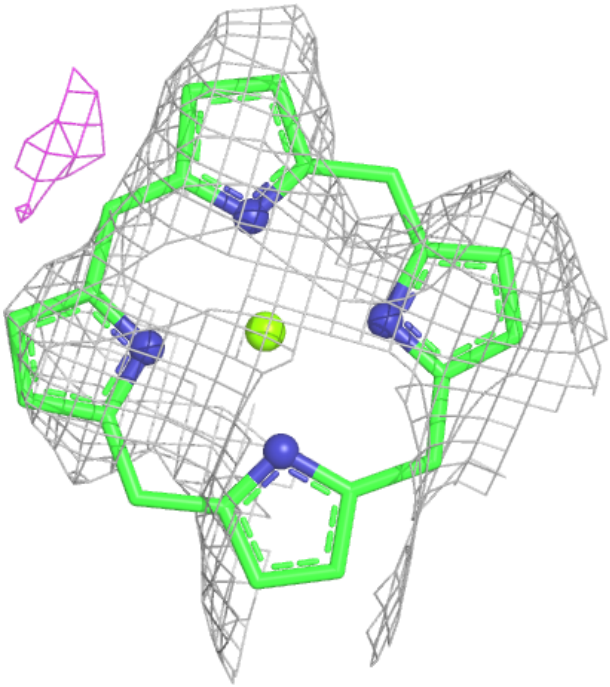


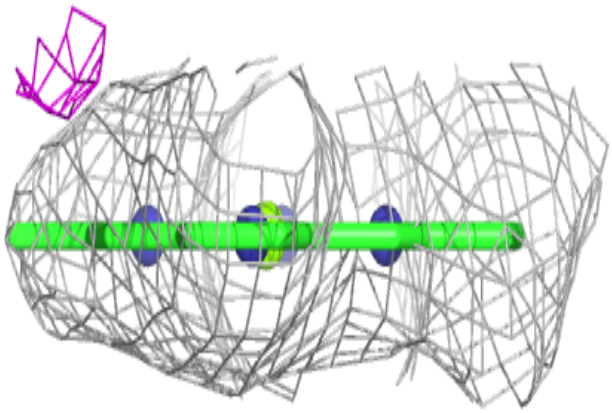


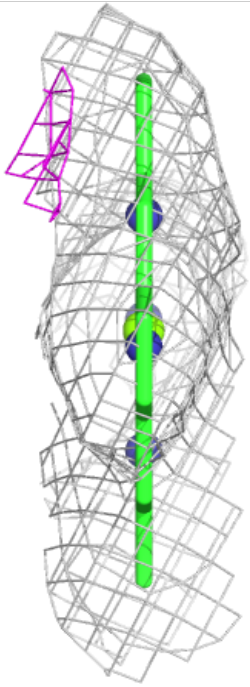


Electron density around CLA 1 1001:

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

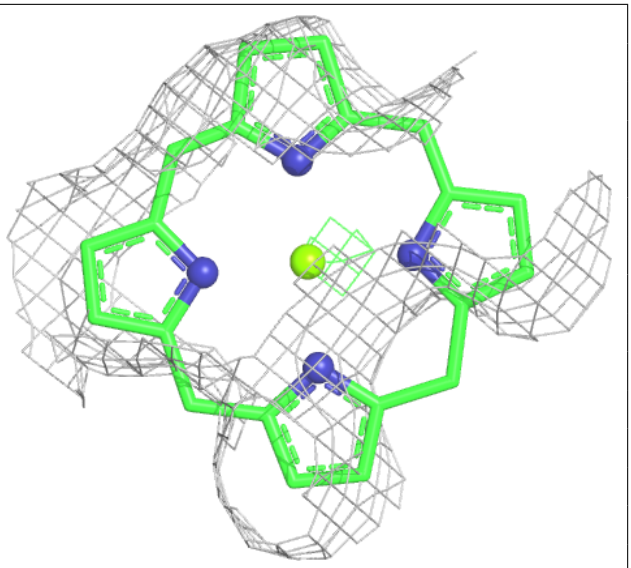


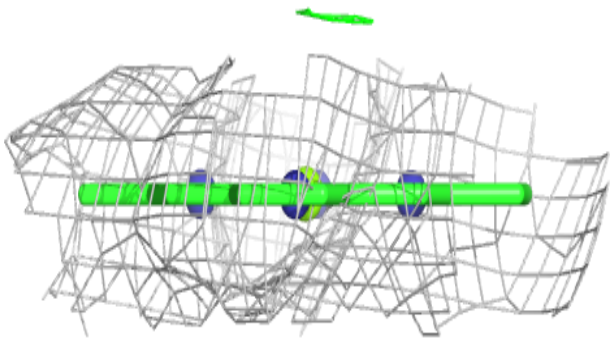


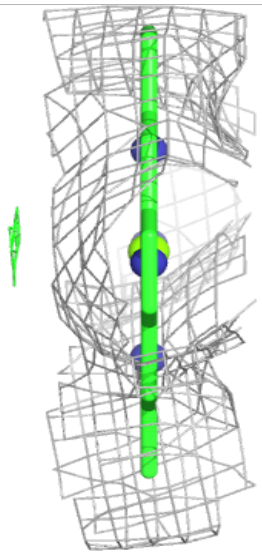


Electron density around CLA B 1201:

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

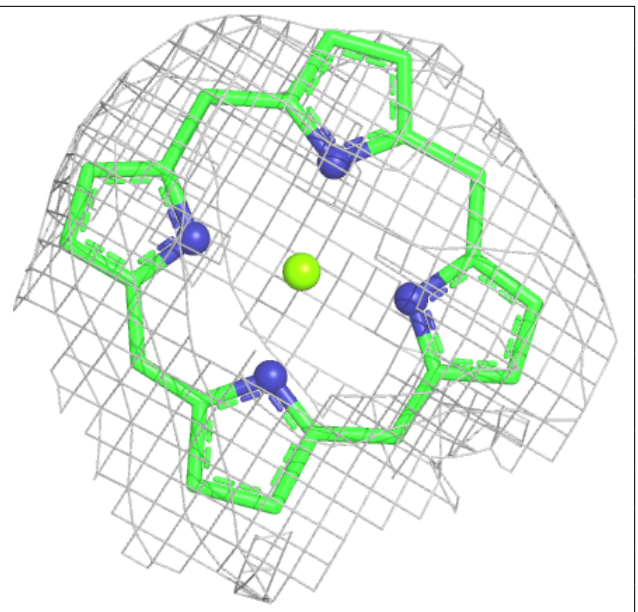


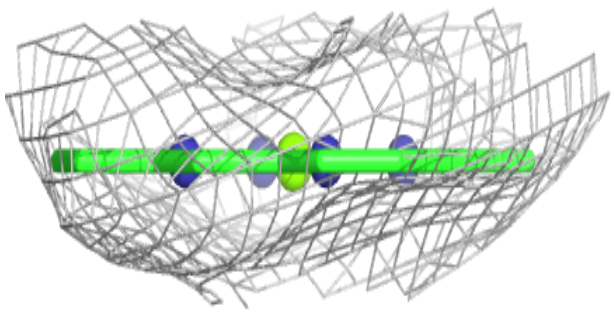


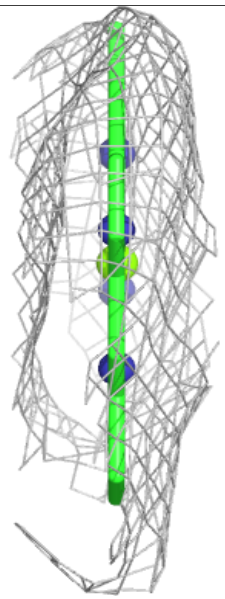


Electron density around CLA 1 1002:

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

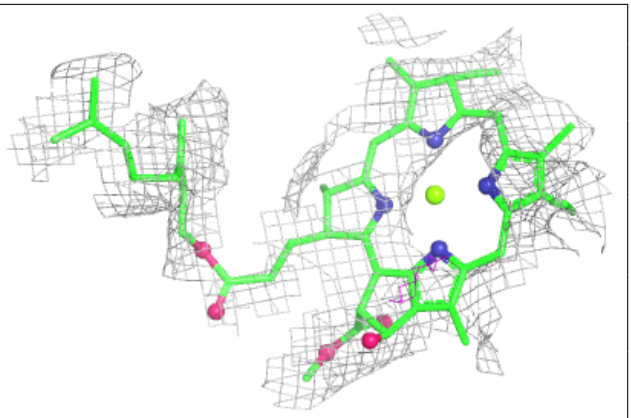


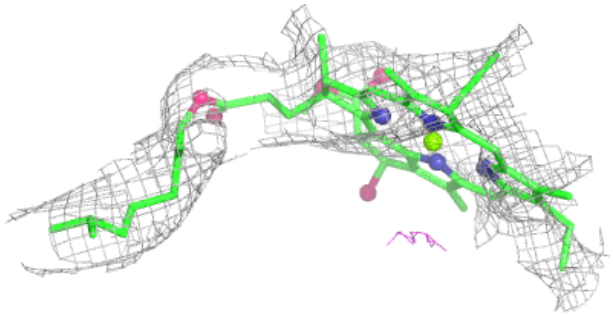


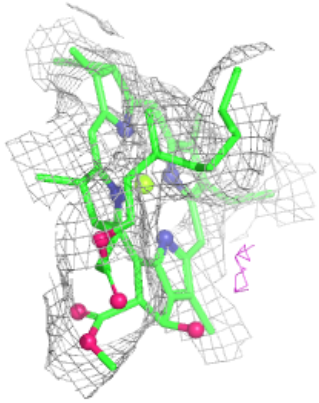


Electron density around CLA B 1232:

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

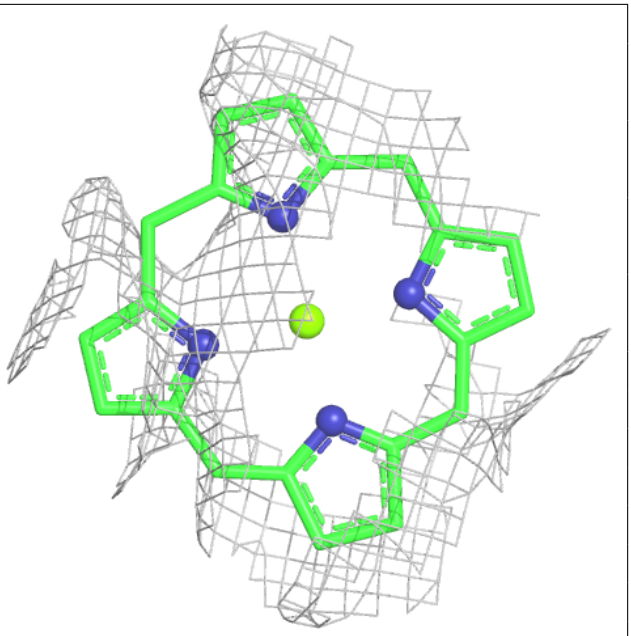


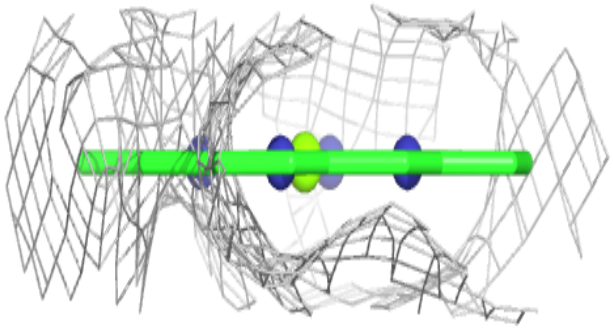


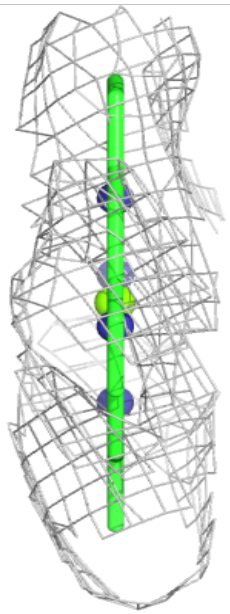


Electron density around CLA B 1301:

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

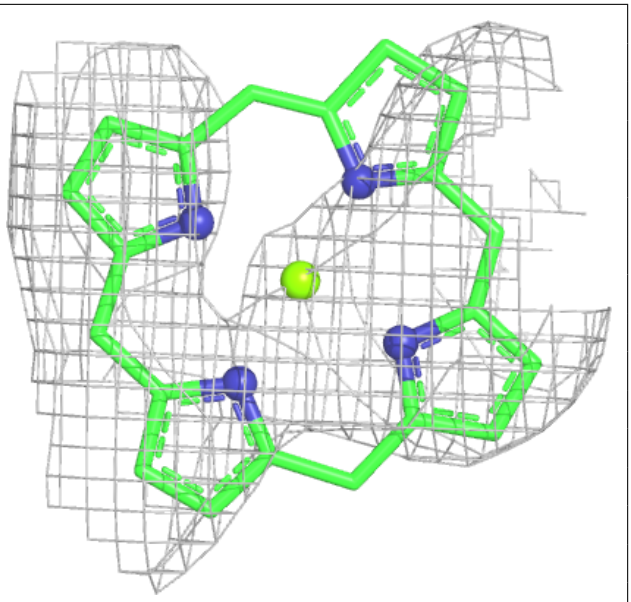


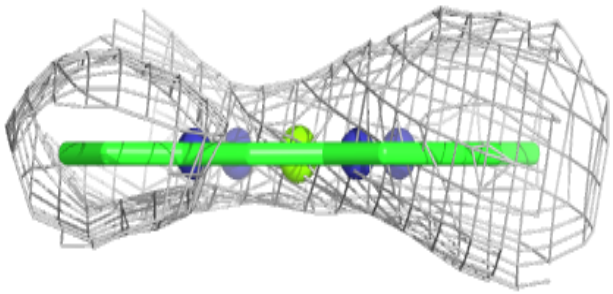


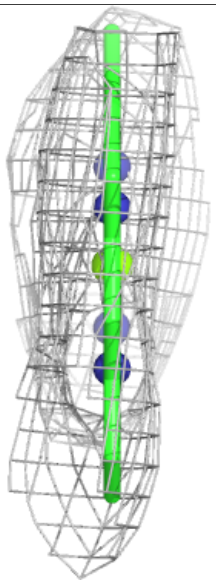


Electron density around CLA 2 2006:

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

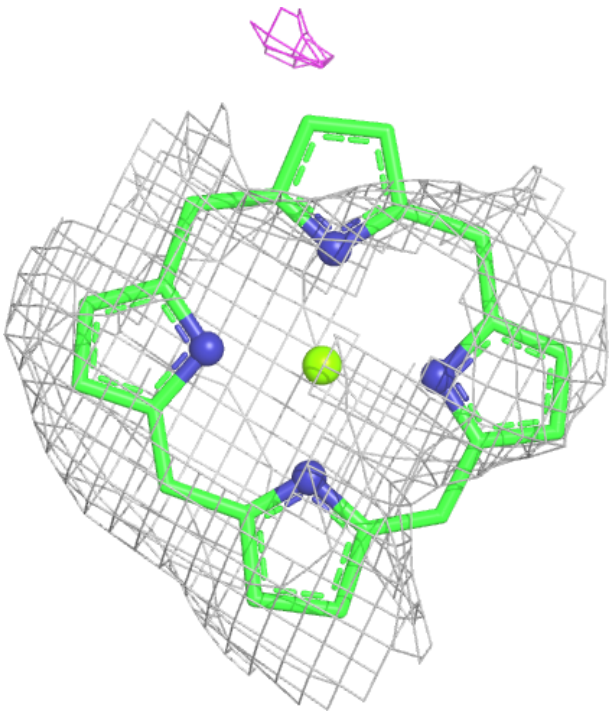


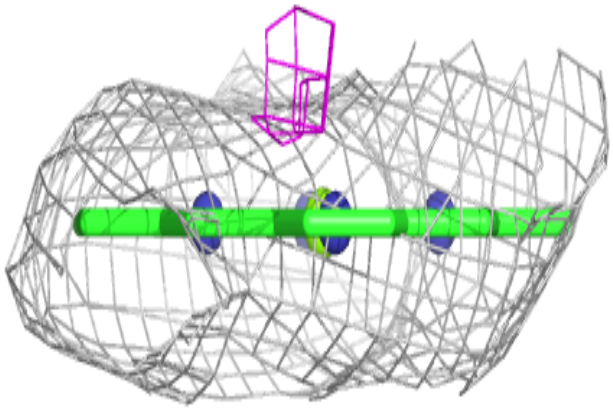


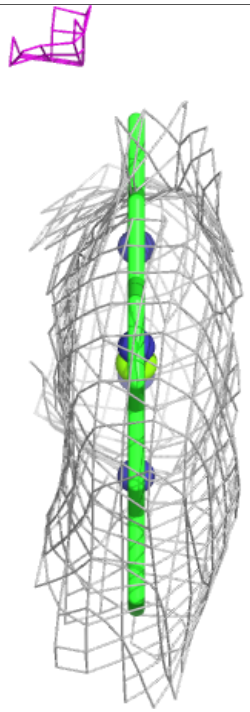


Electron density around CLA 2 2010:

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

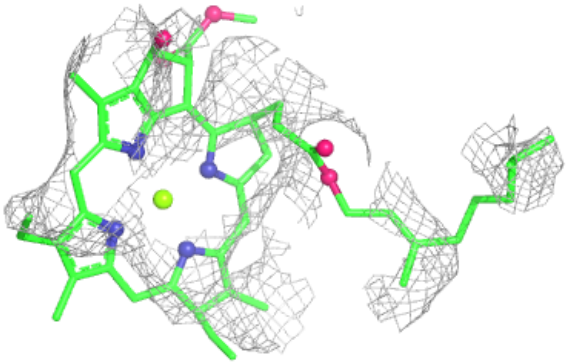


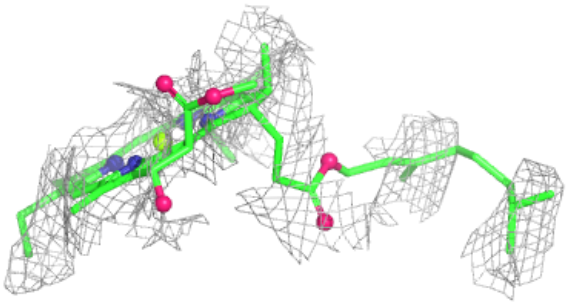


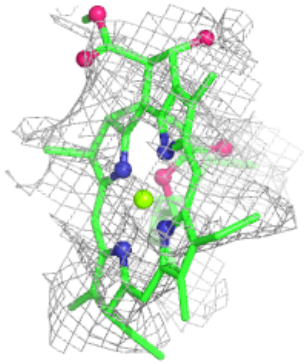


Electron density around CLA A 1119:

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

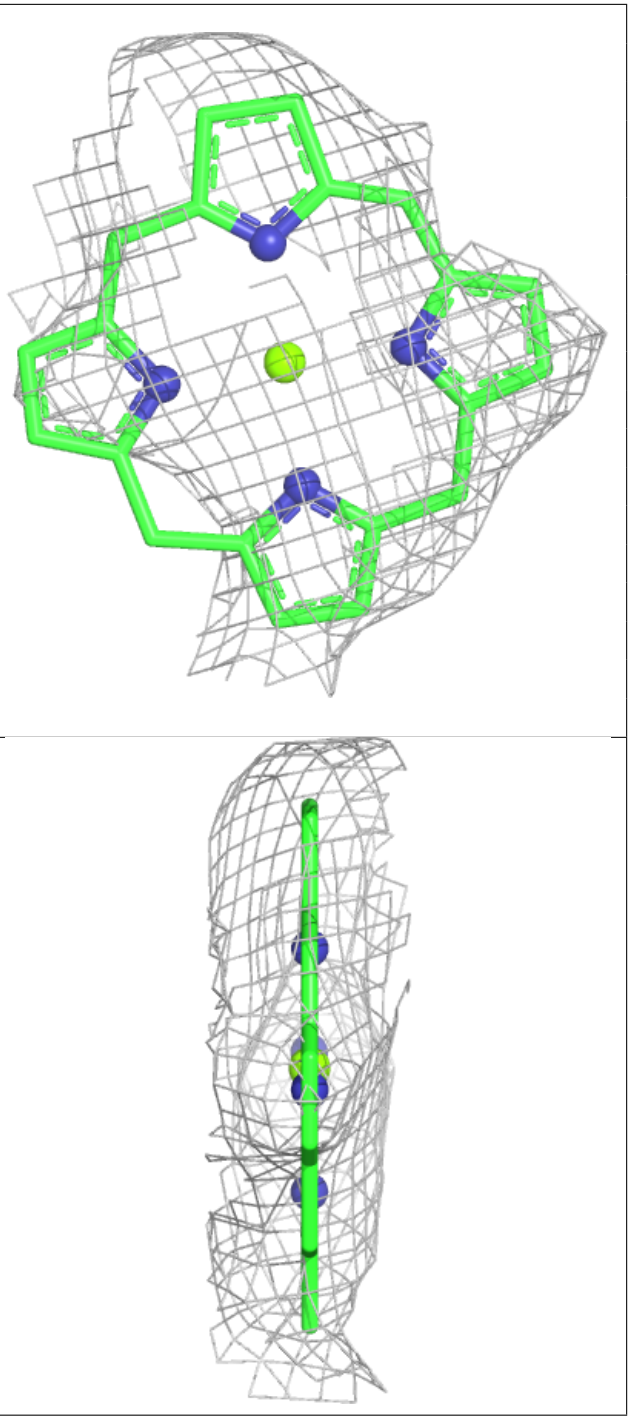






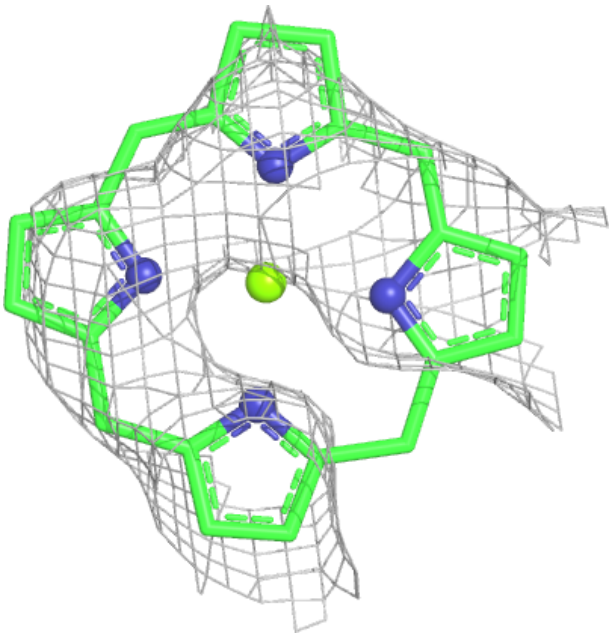
Electron density around CLA A 1127:

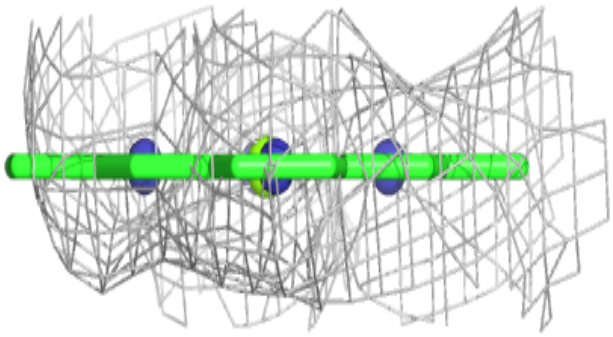
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

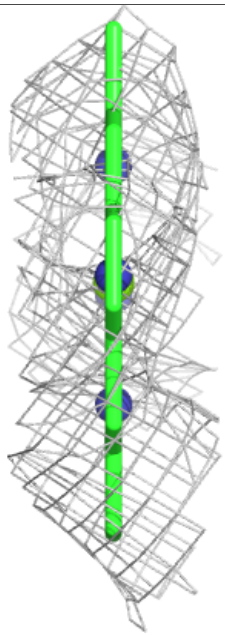


Electron density around CLA 2 2012:

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

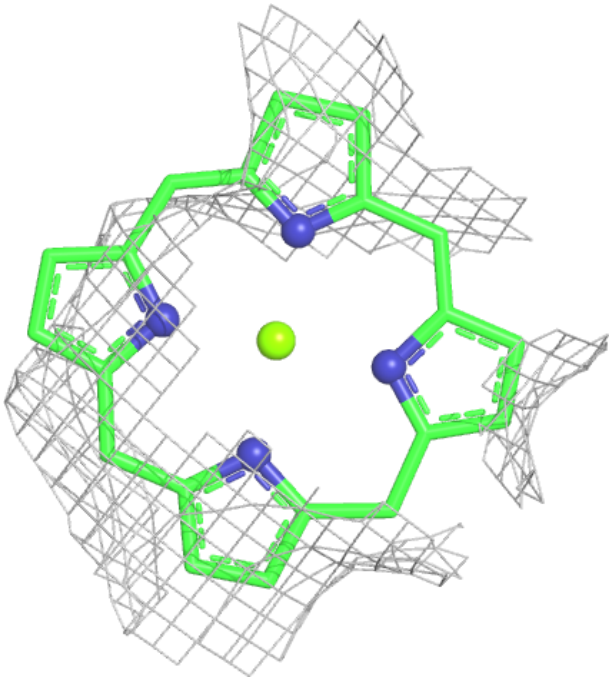


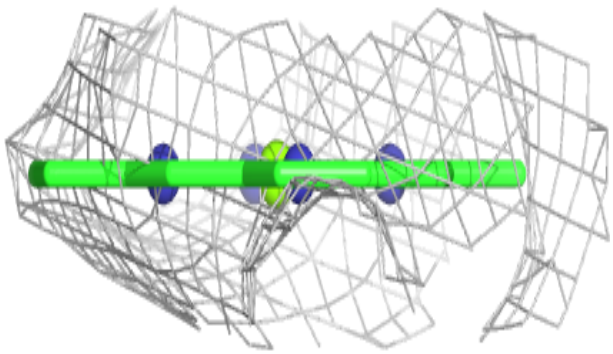


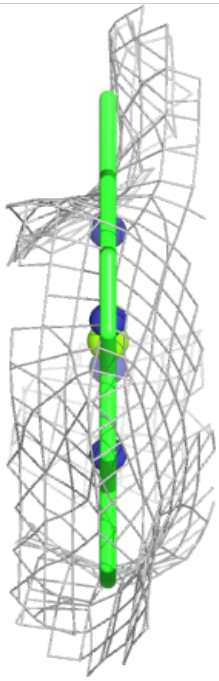


Electron density around CLA A 1144:

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

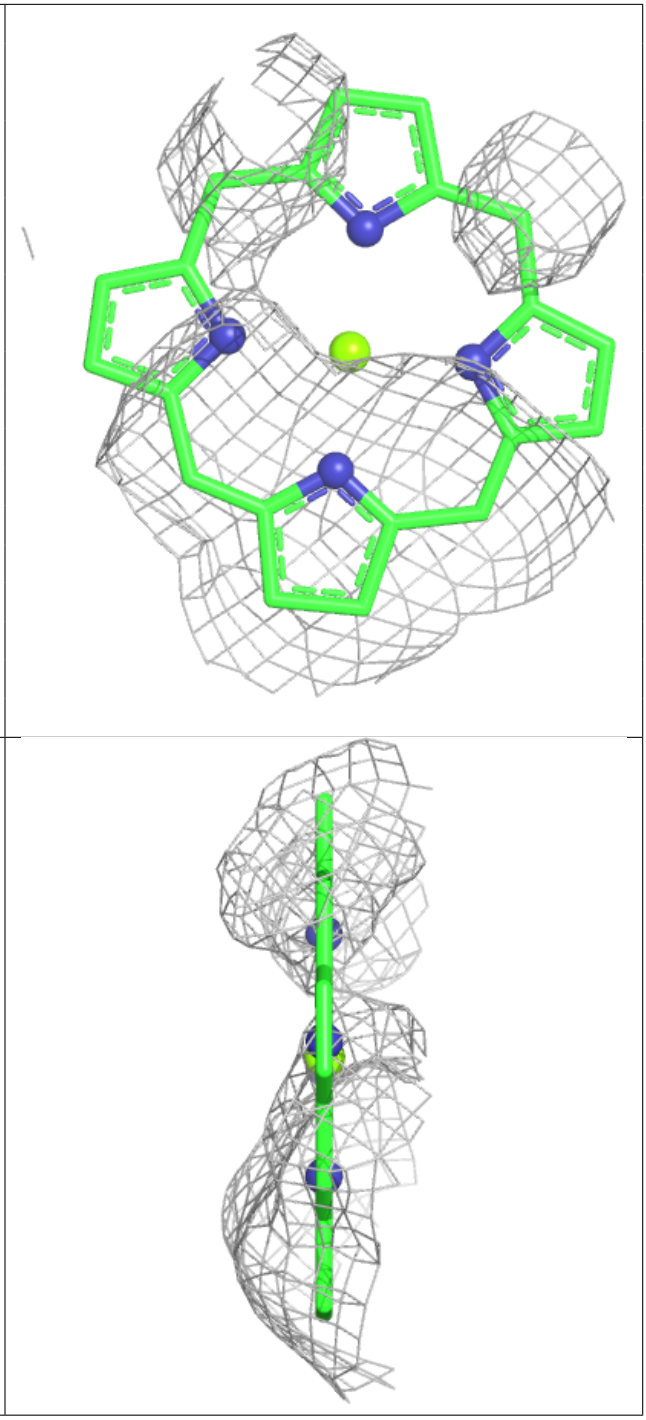






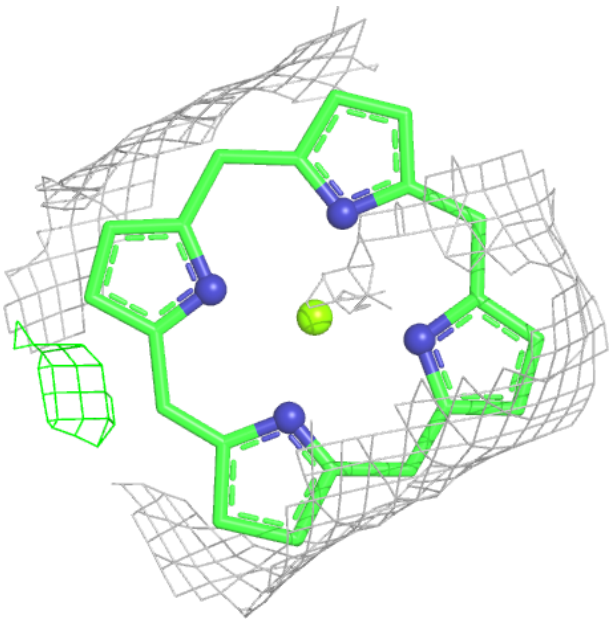
Electron density around CLA F 4015:

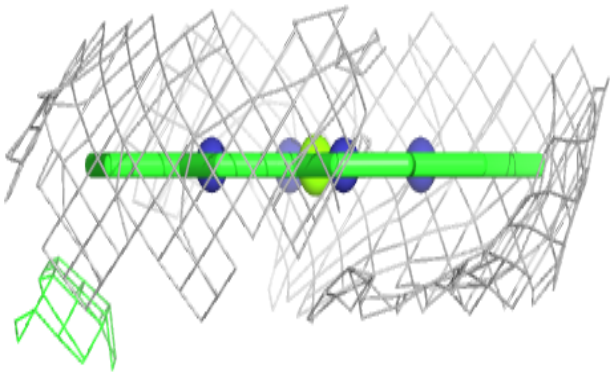
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

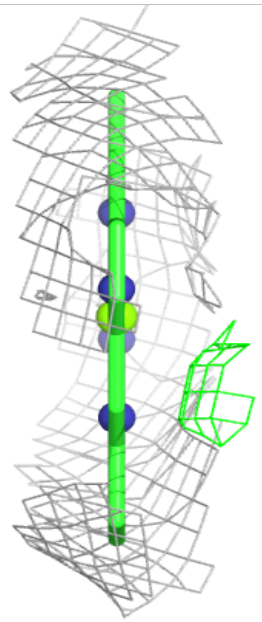


Electron density around CLA A 1147:

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

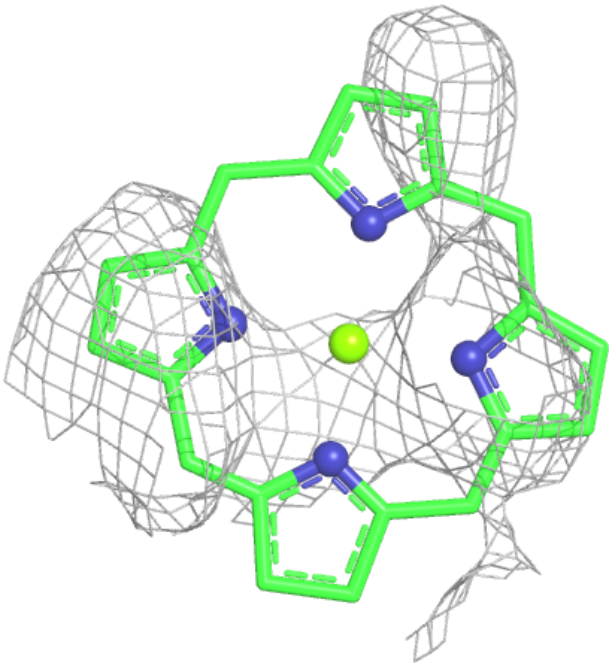


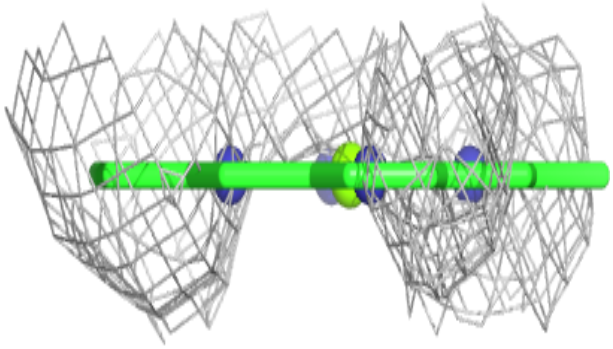


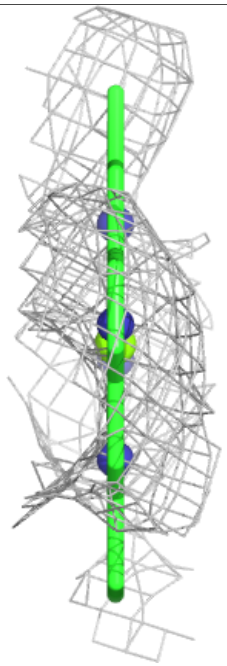


Electron density around CLA 3 3001:

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

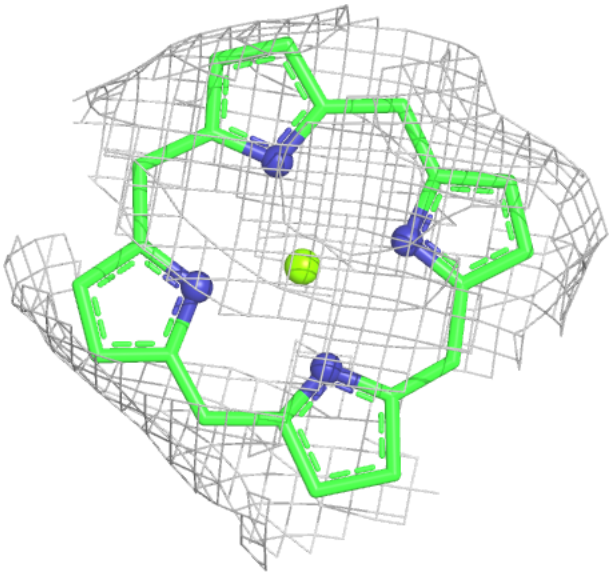


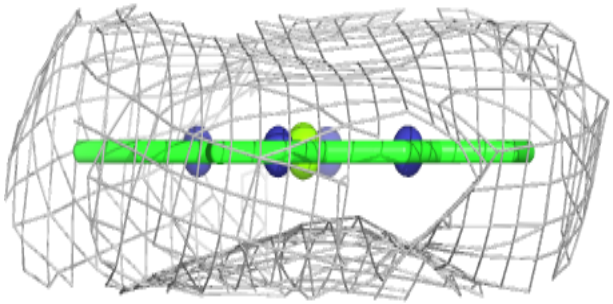


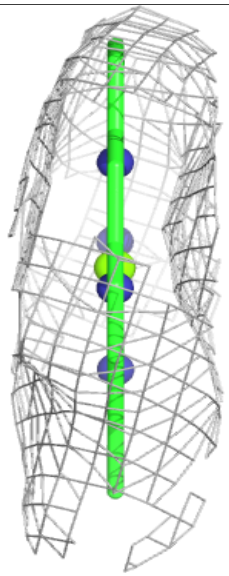


Electron density around CLA 3 3002:

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

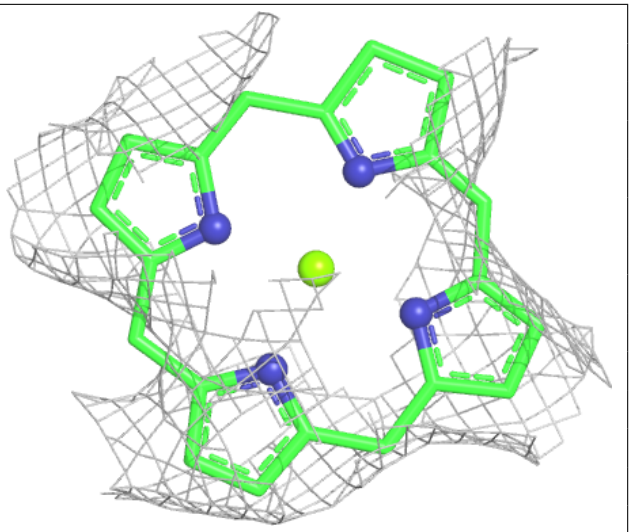


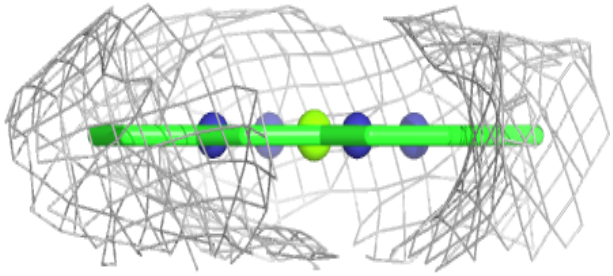


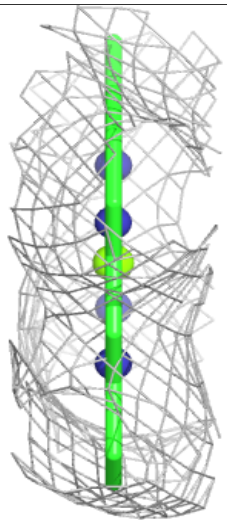


Electron density around CLA 3 3015:

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

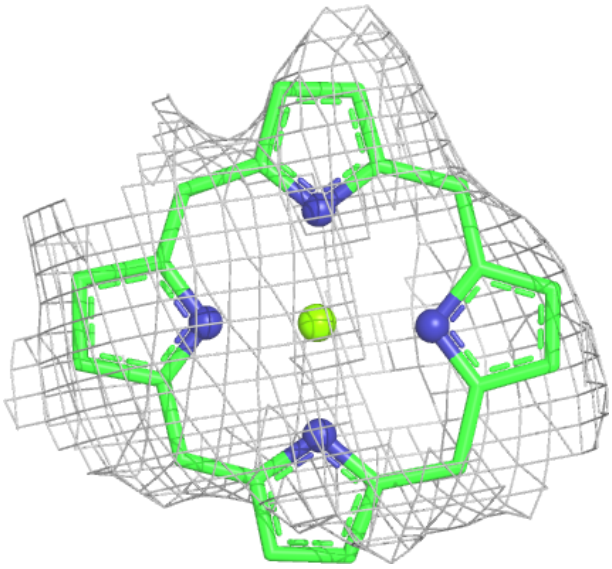


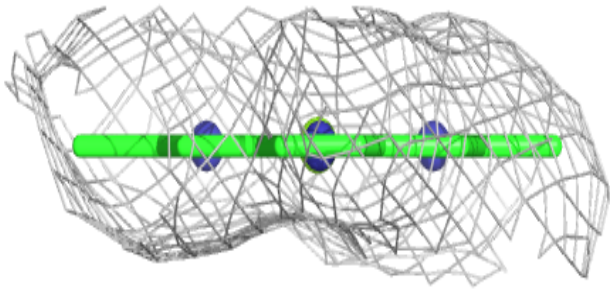


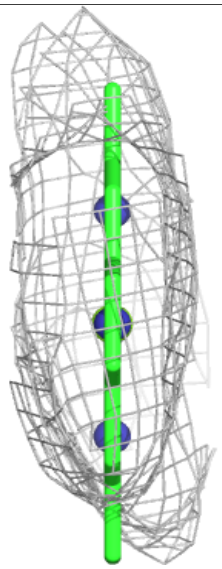


Electron density around CLA 4 1009:

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

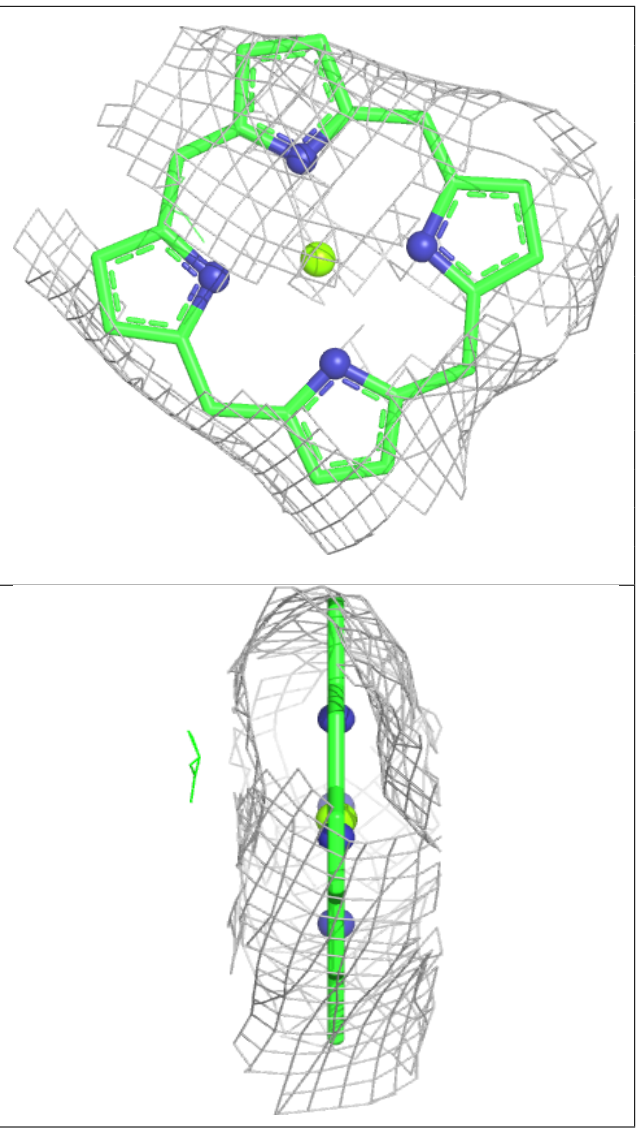






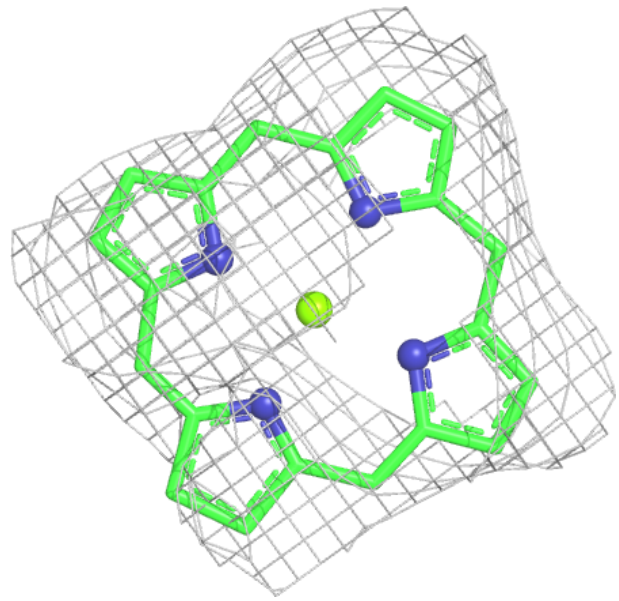
Electron density around CLA 4 4009:

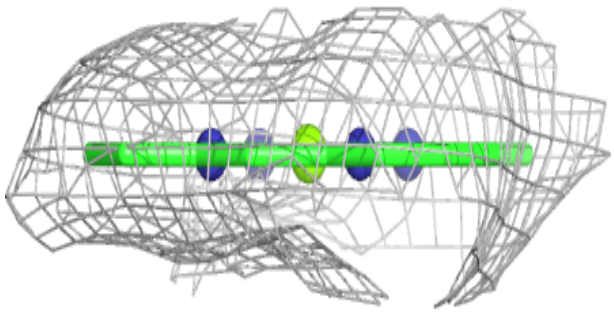
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

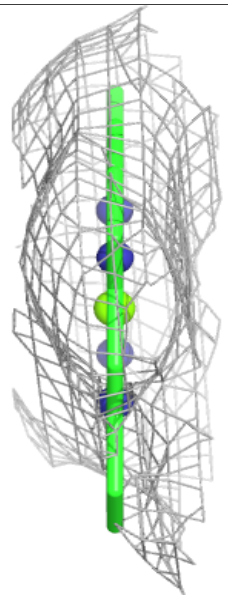


Electron density around CLA 4 4004:

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

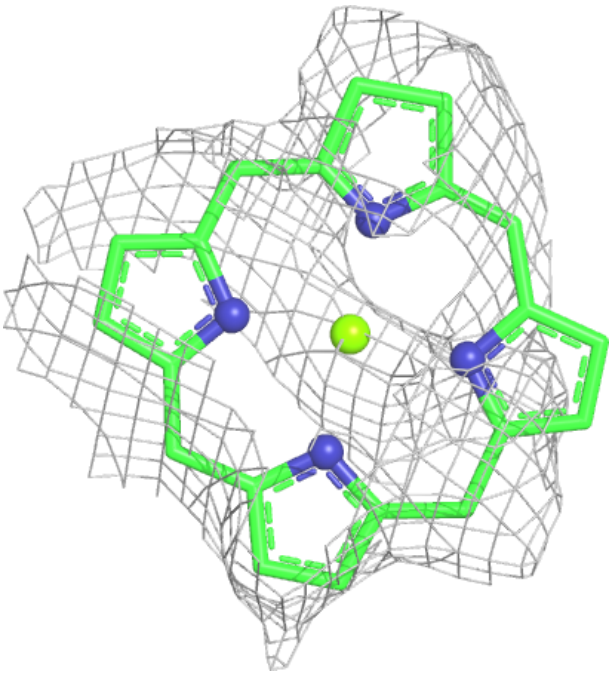


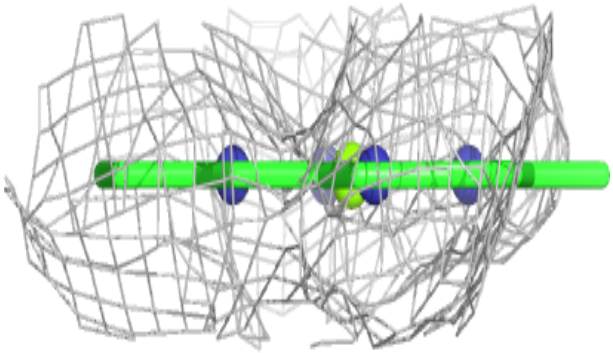


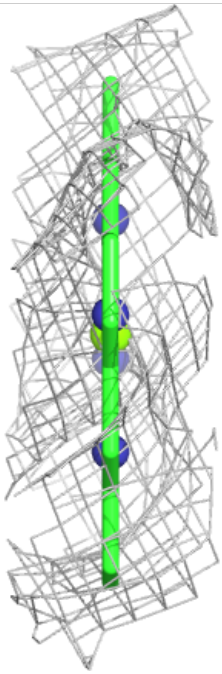


Electron density around CLA H 1505:

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

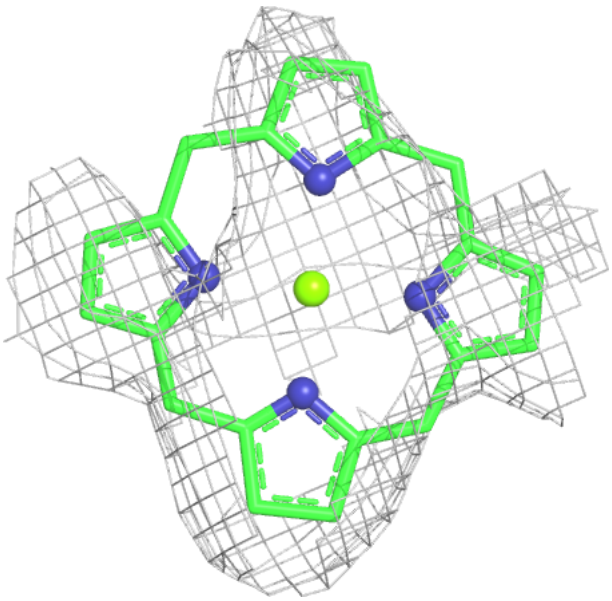


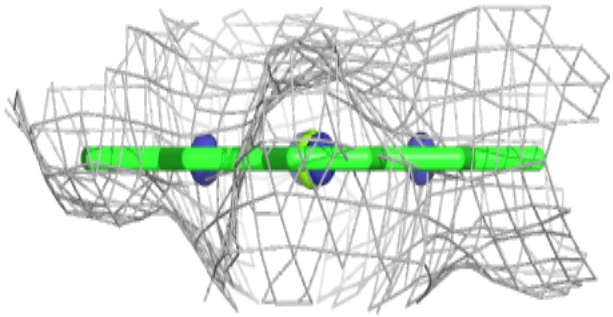


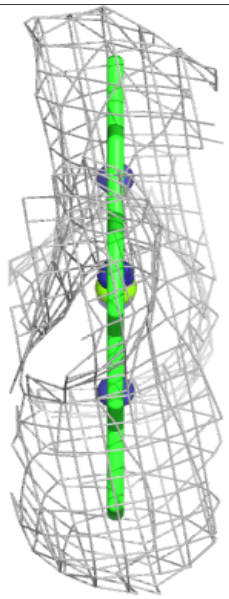


Electron density around CLA 4 4006:

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

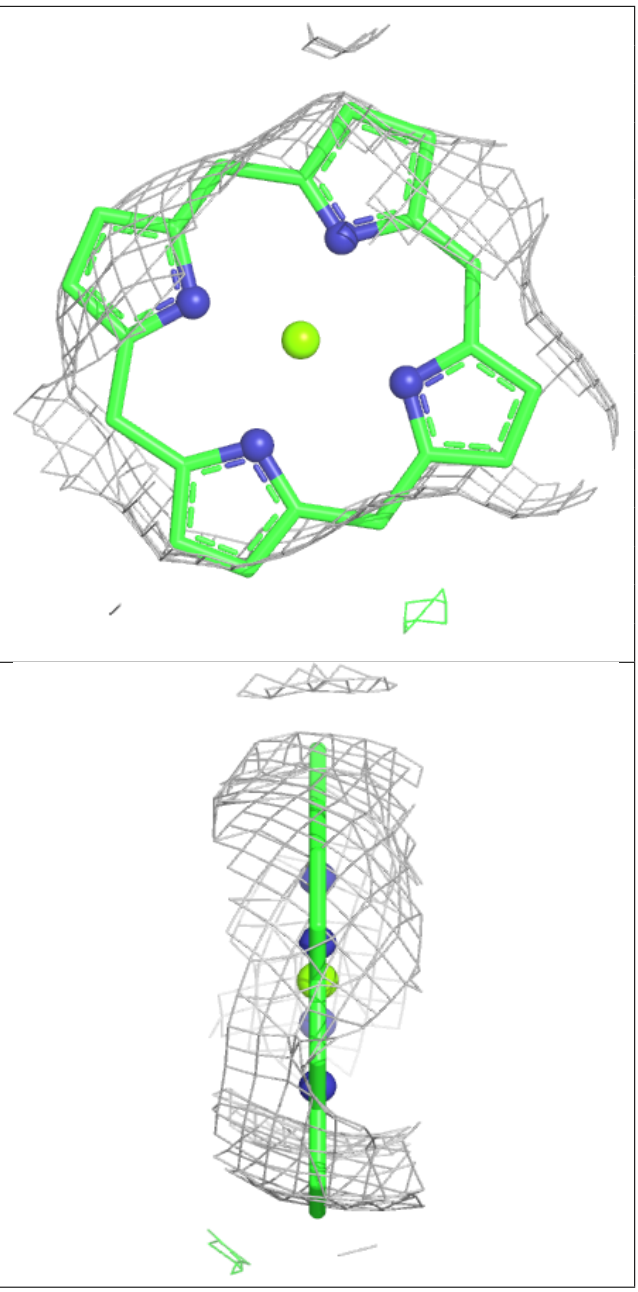






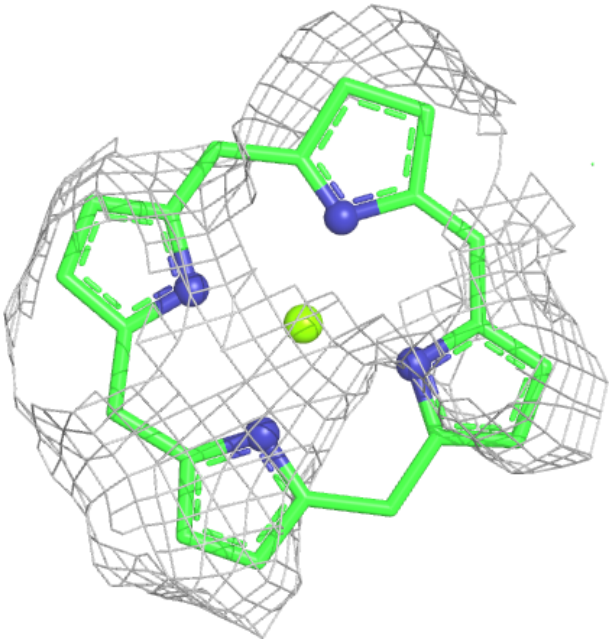
Electron density around CLA A 1148:

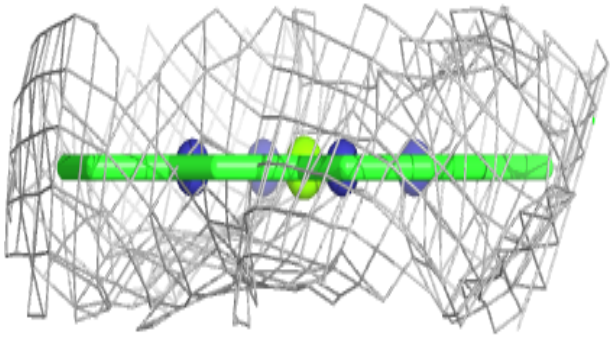
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

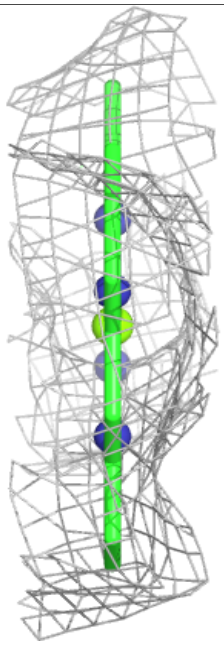


Electron density around CLA 4 4007:

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

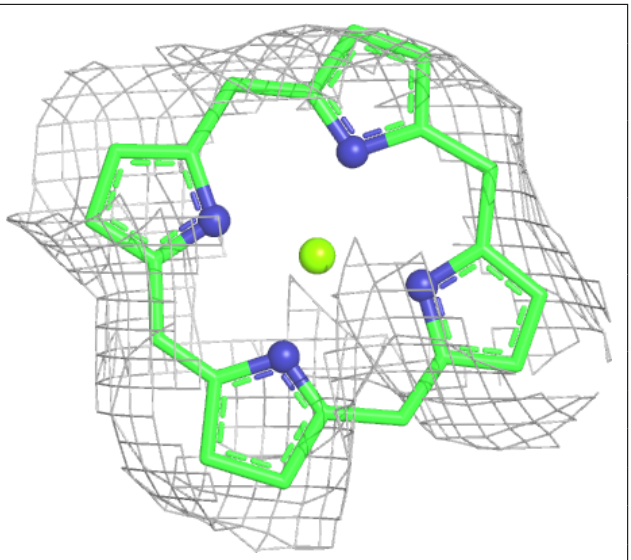


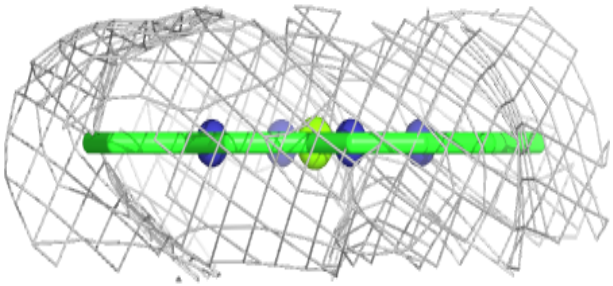


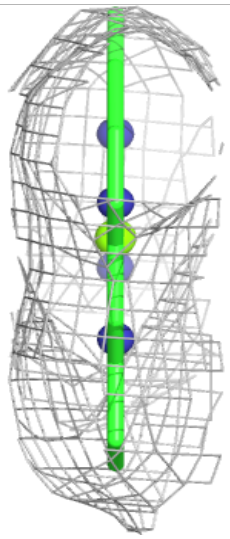


Electron density around CLA 4 4002:

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

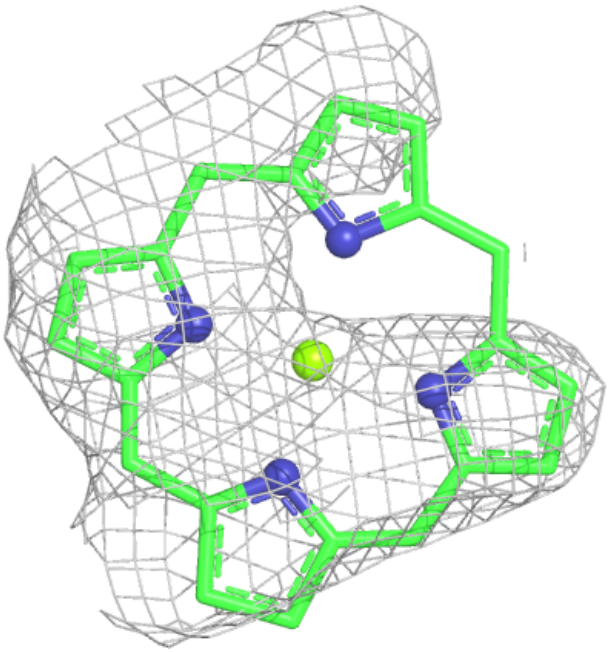


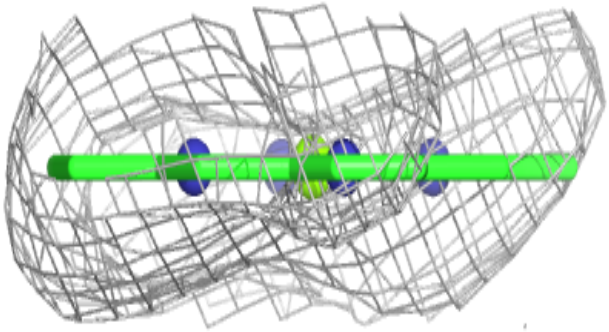


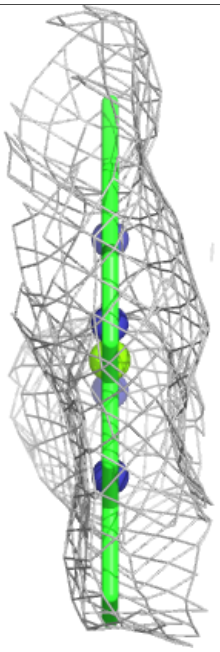


Electron density around CLA 4 4003:

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

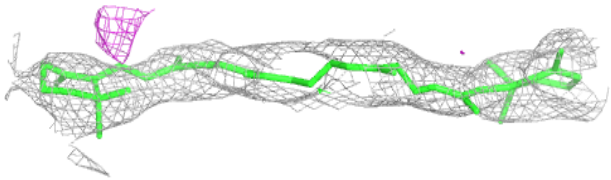


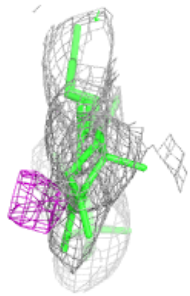




Electron density around BCR A 6011:

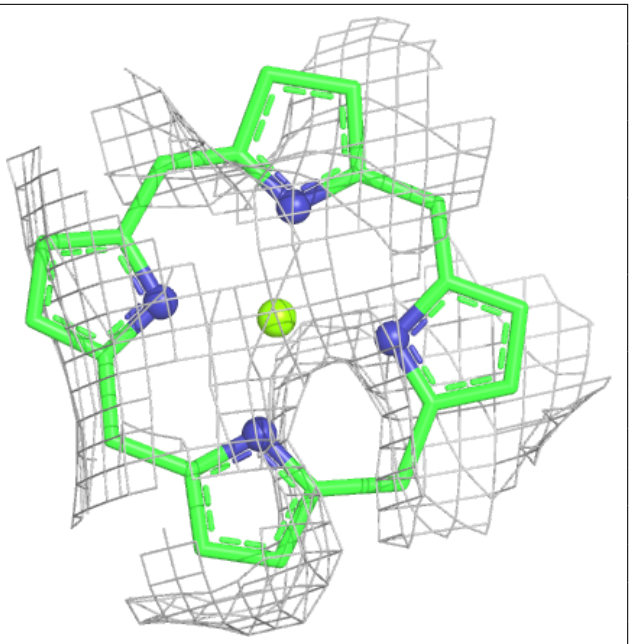
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

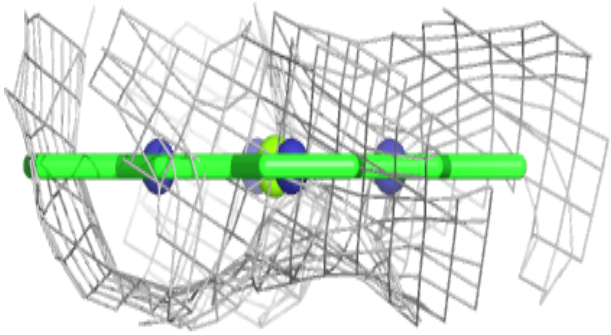


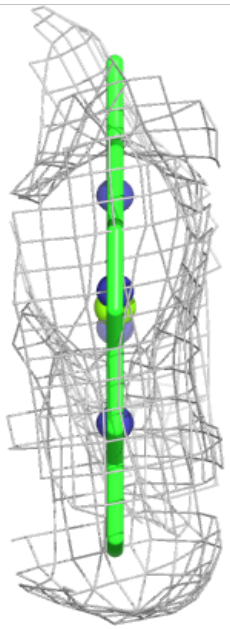


Electron density around CLA J 1308:

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

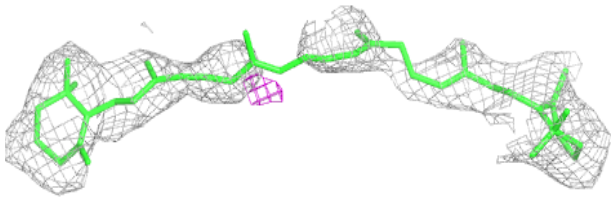


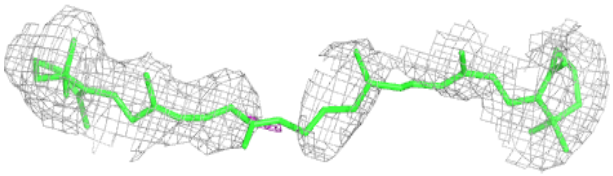


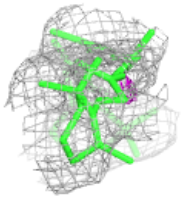


Electron density around BCR I 6018:

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

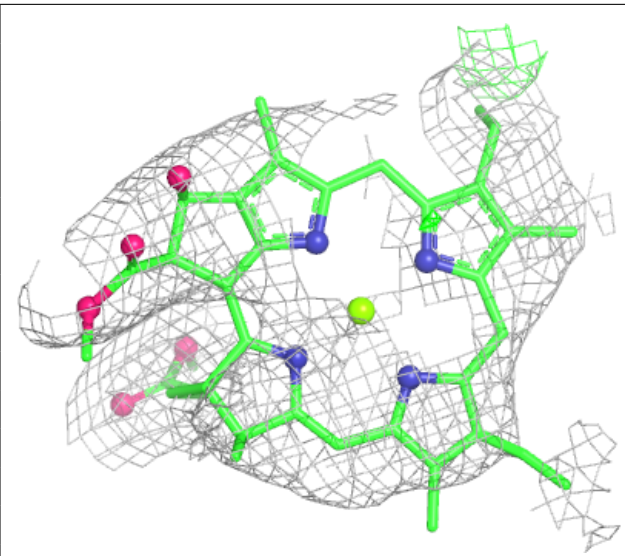


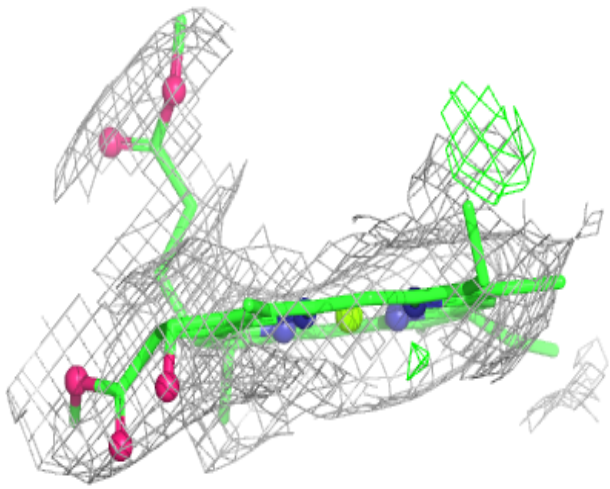


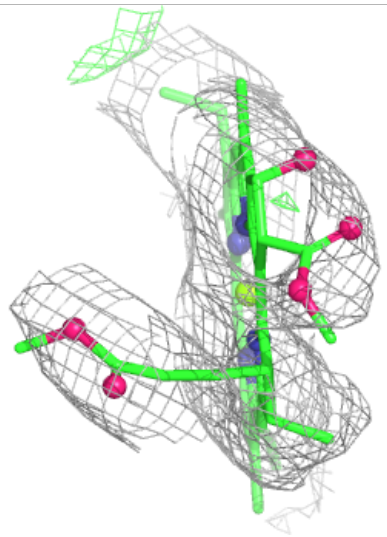


Electron density around CLA B 1236:

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

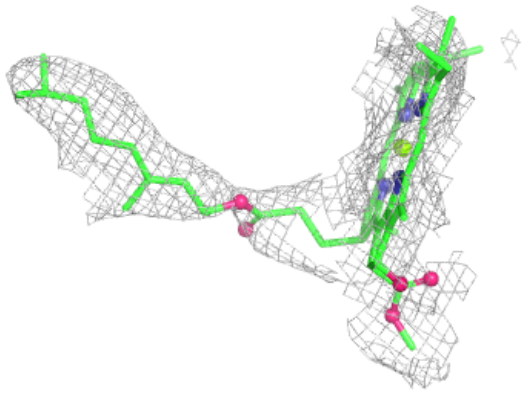


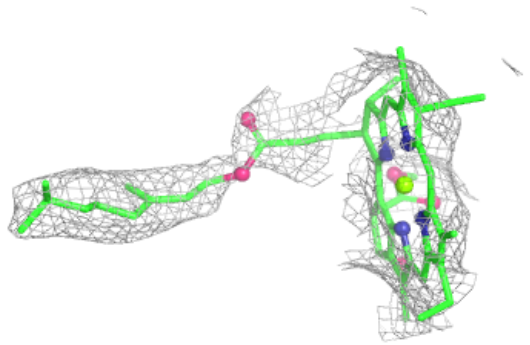


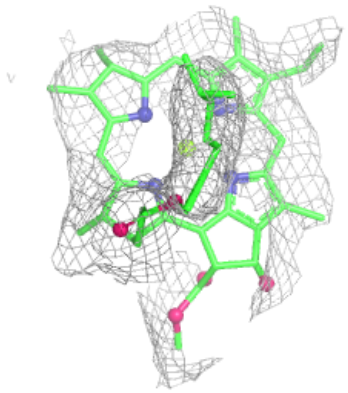


Electron density around CLA B 1239:

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

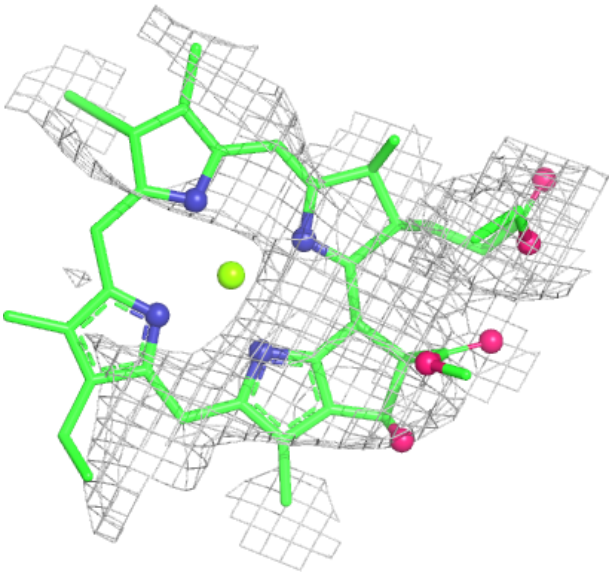


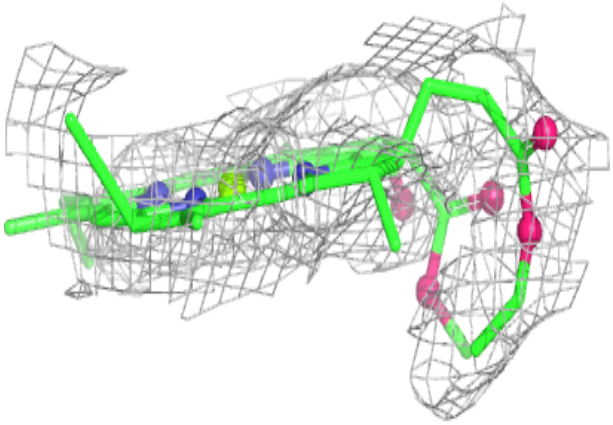


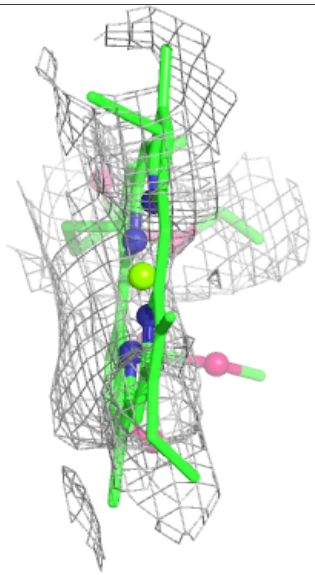


Electron density around CLA B 1242:

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

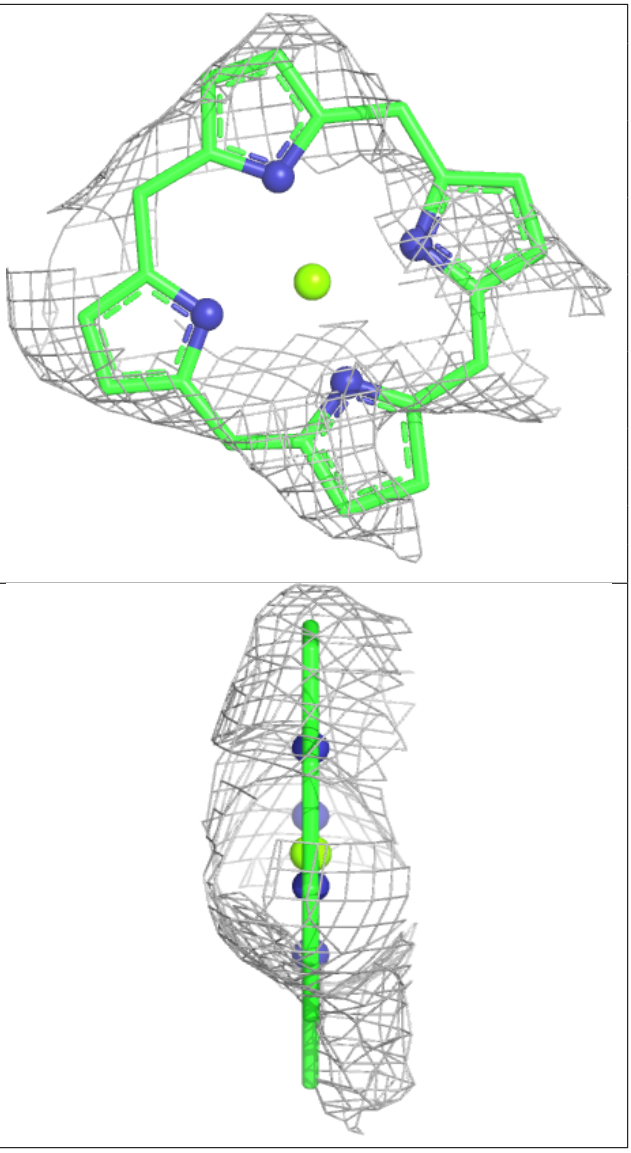






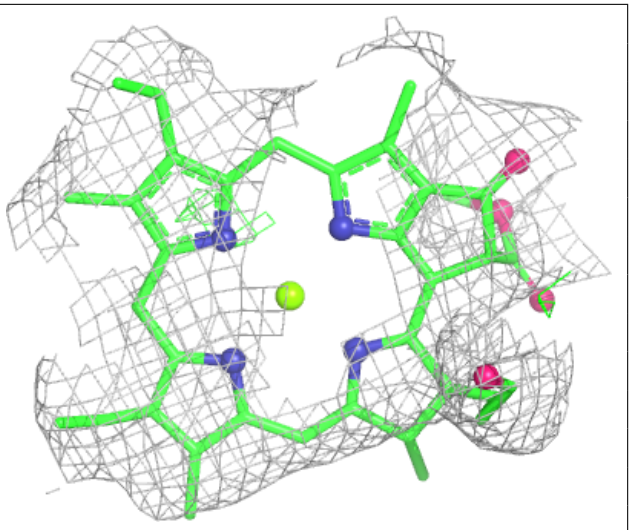
Electron density around CLA A 1102:

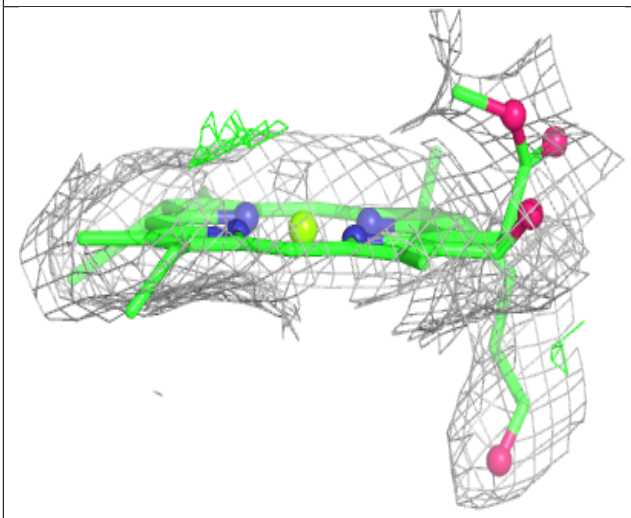
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)



Electron density around CLA F 1139:

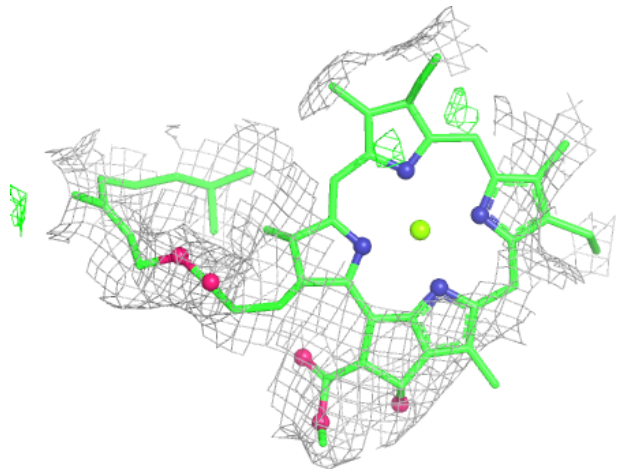
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

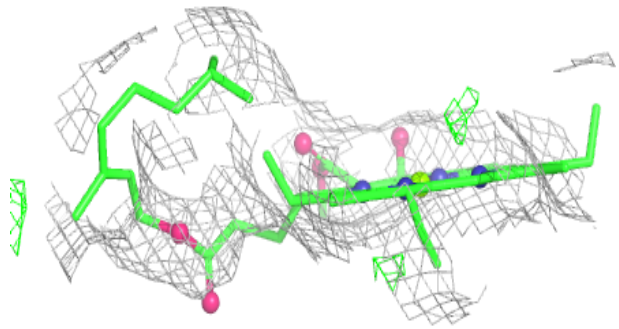


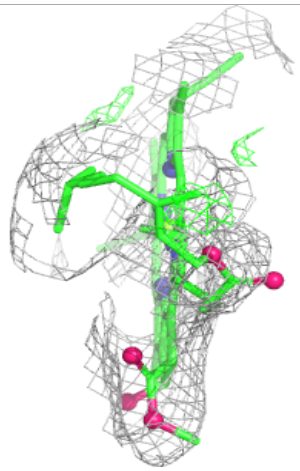


Electron density around CLA F 1302:

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

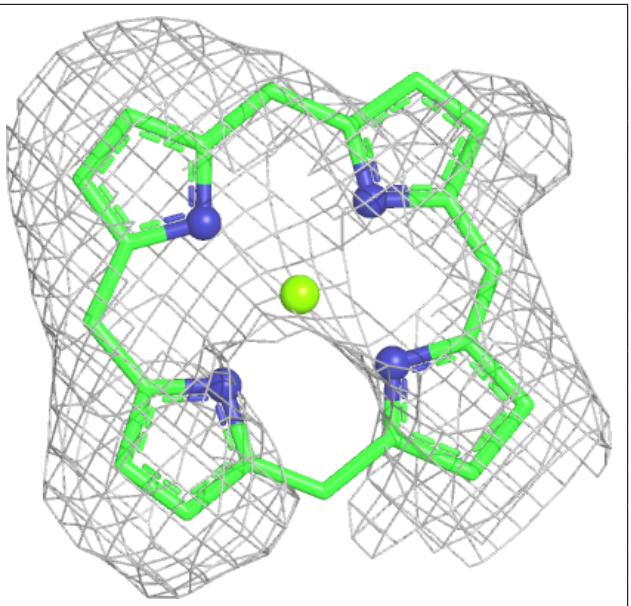


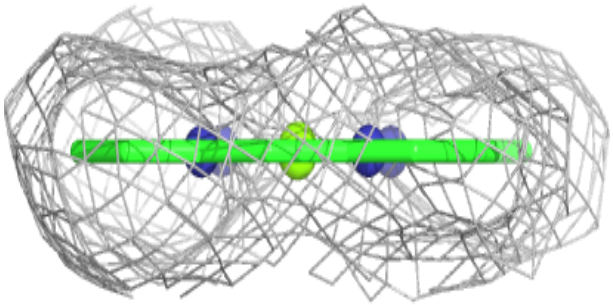


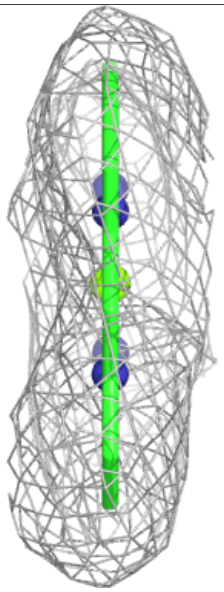


Electron density around CLA A 1104:

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

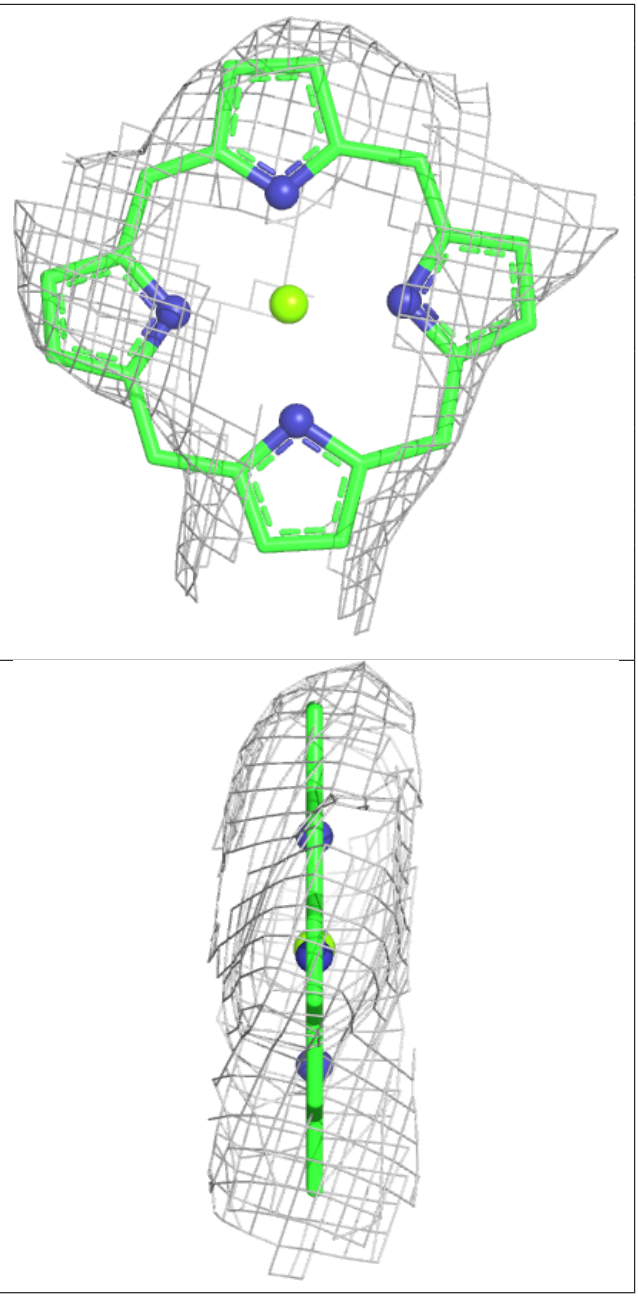






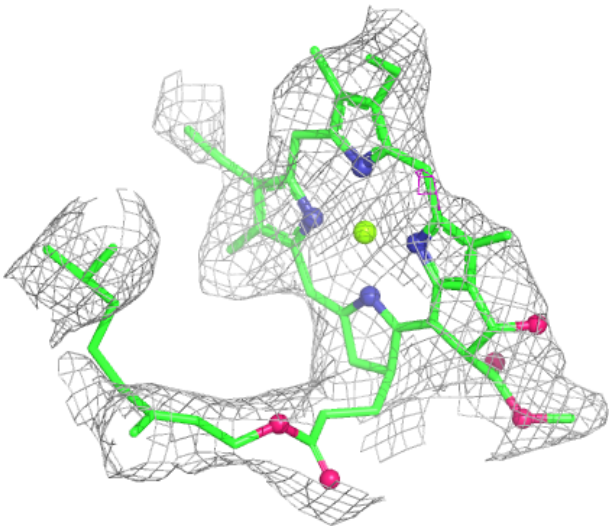
Electron density around CLA A 1120:

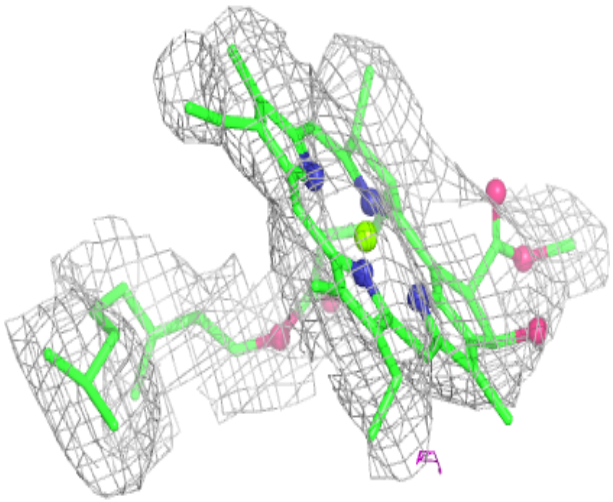
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

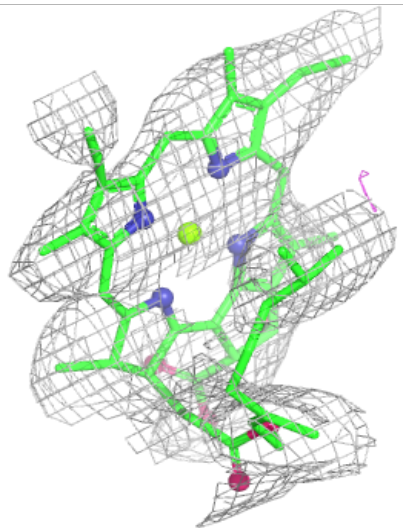


Electron density around CLA A 1122:

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

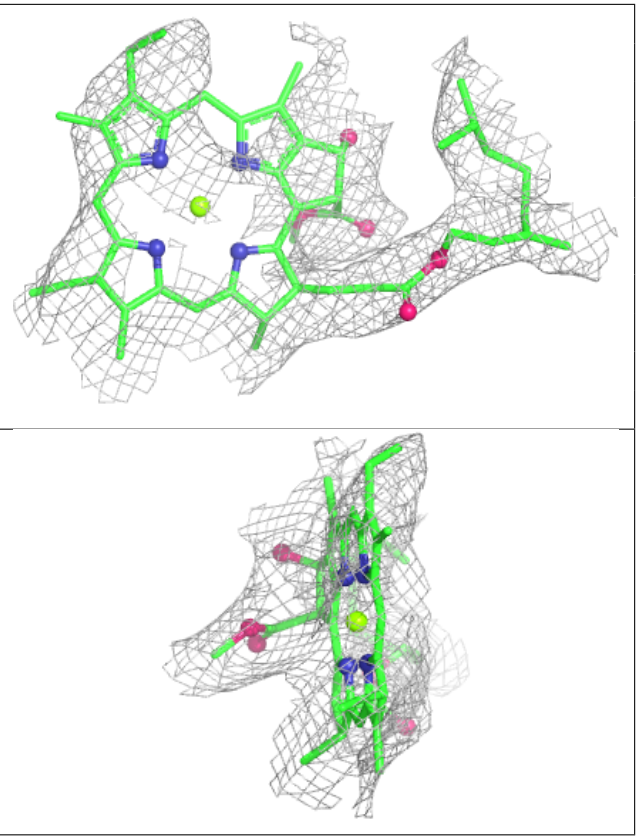






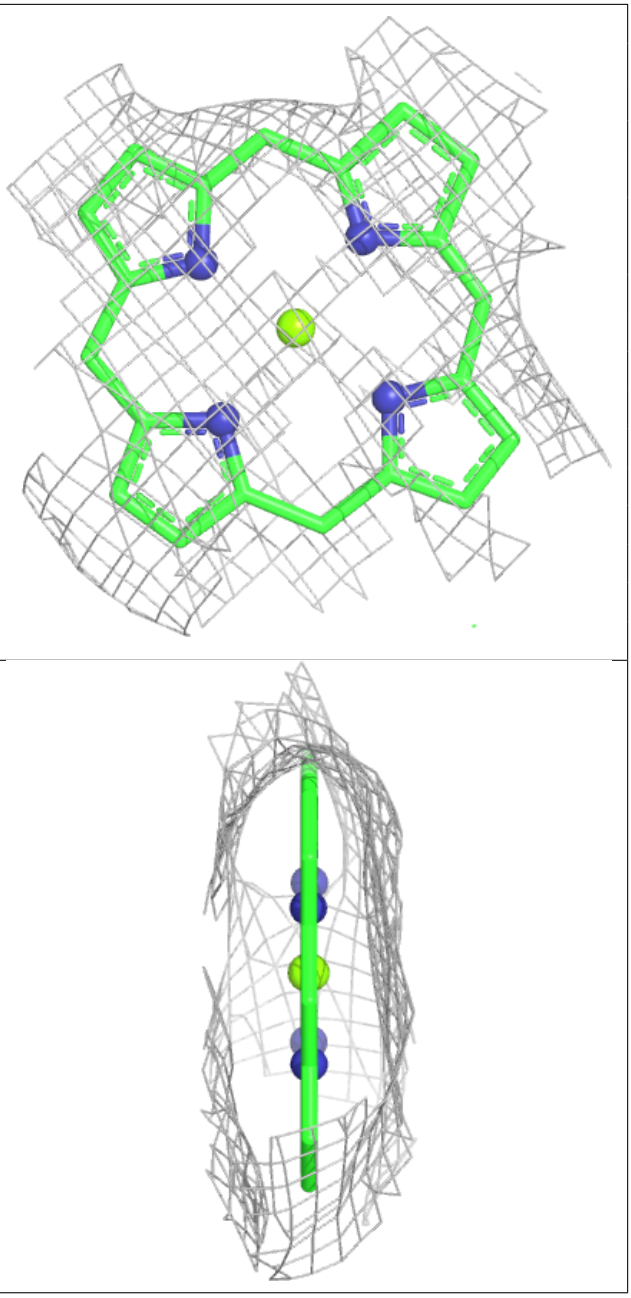
Electron density around CLA A 1123:

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



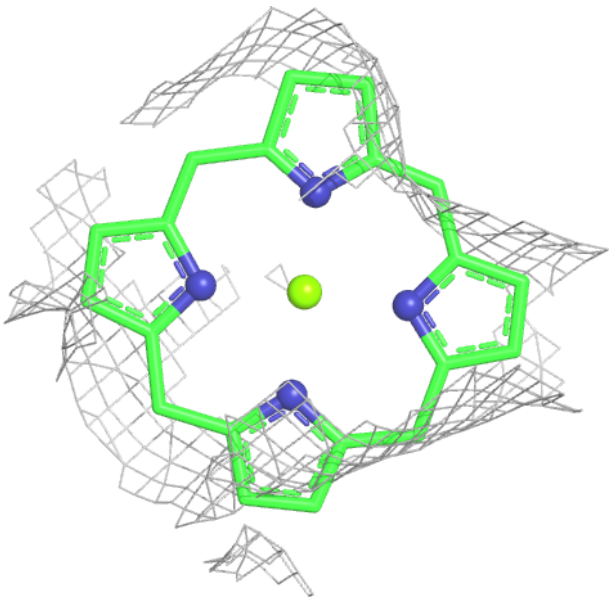
Electron density around CLA A 1124:

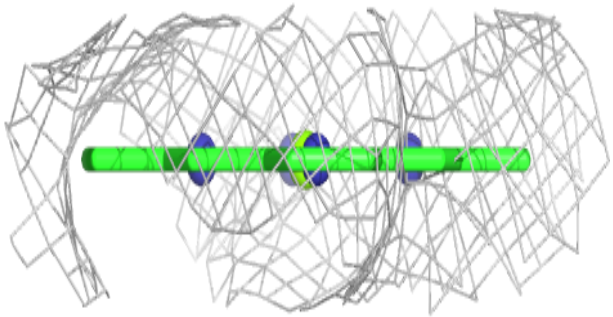
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

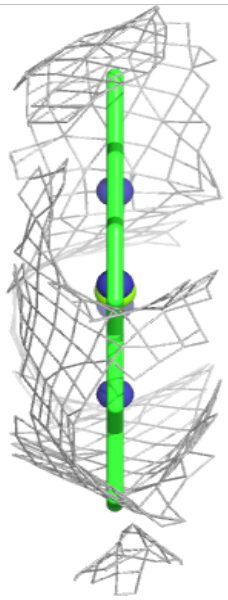


Electron density around CLA G 1248:

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

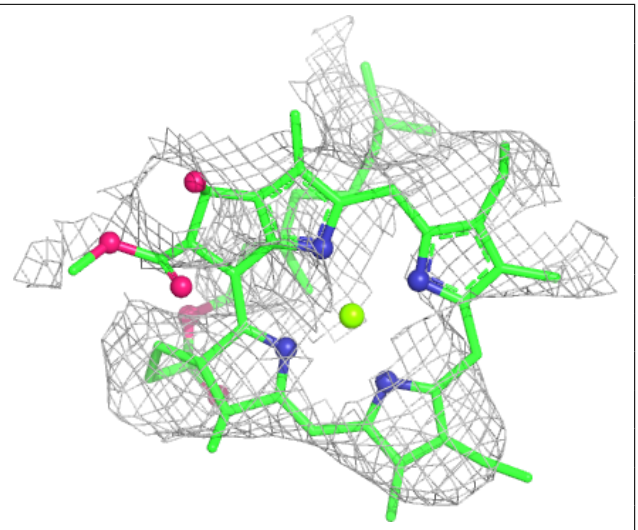


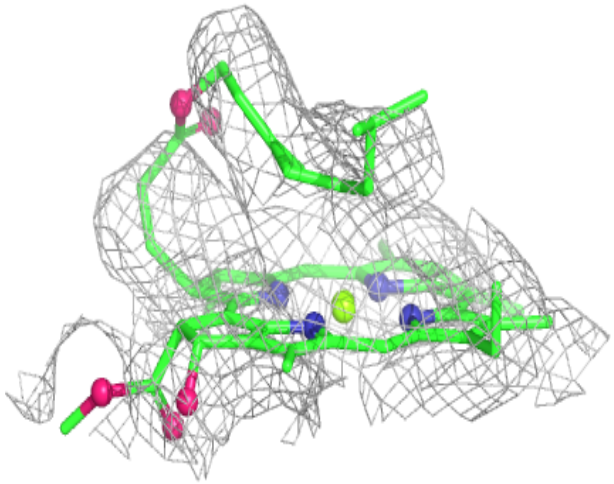


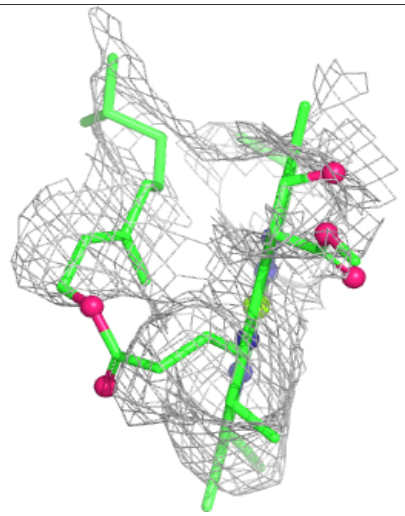


Electron density around CLA H 1501:

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

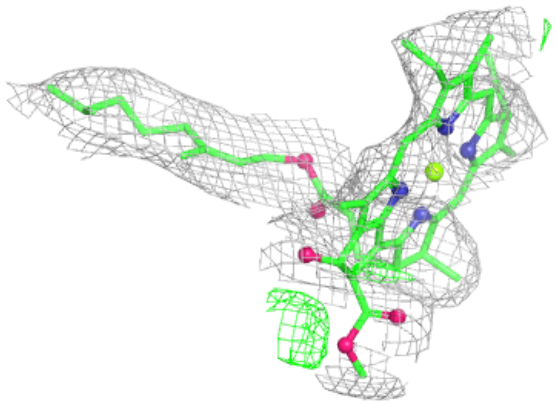


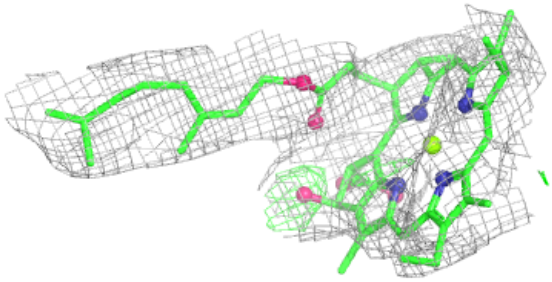


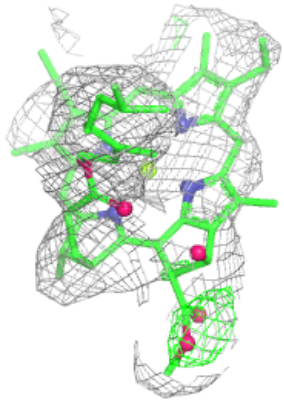


Electron density around CLA A 1126:

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

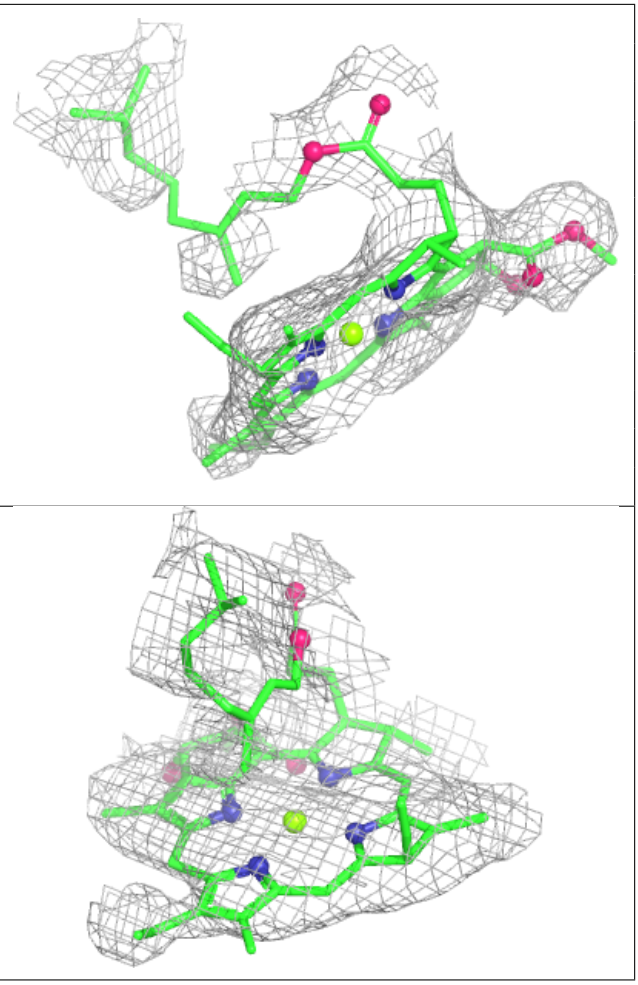






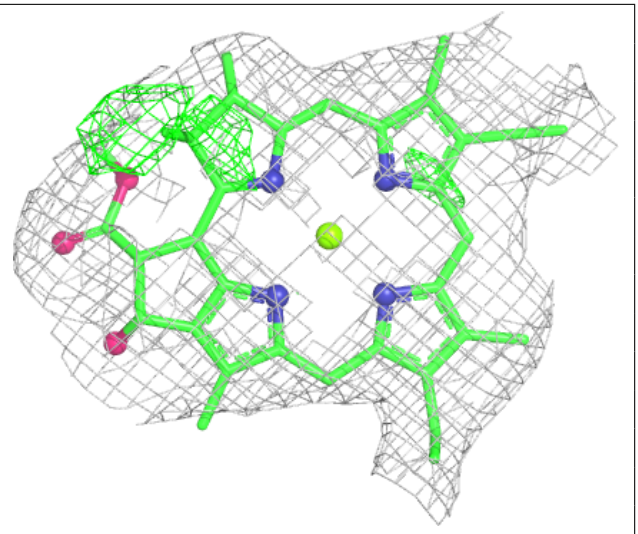
Electron density around CLA I 1204:

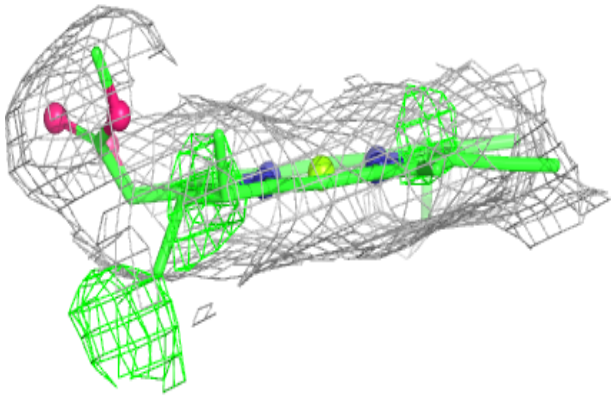
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

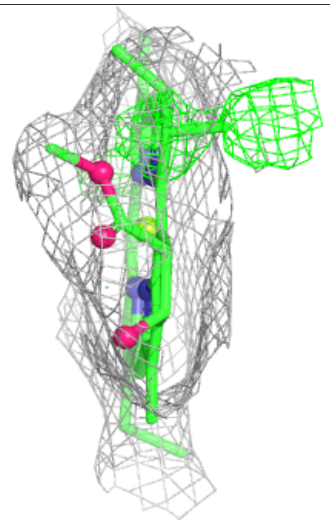


Electron density around CLA A 1106:

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

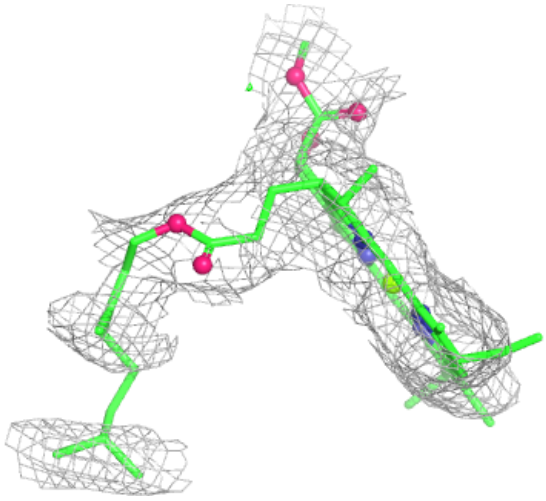


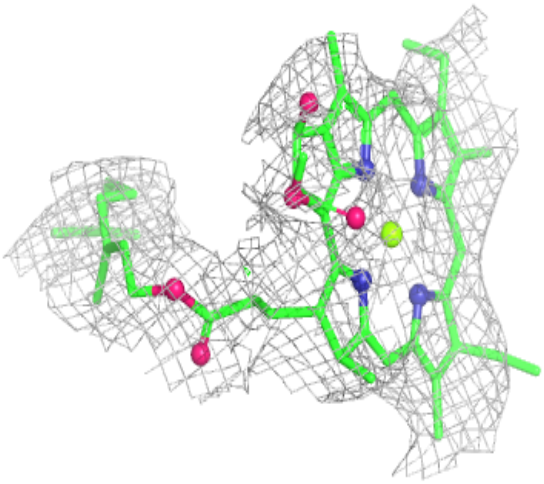


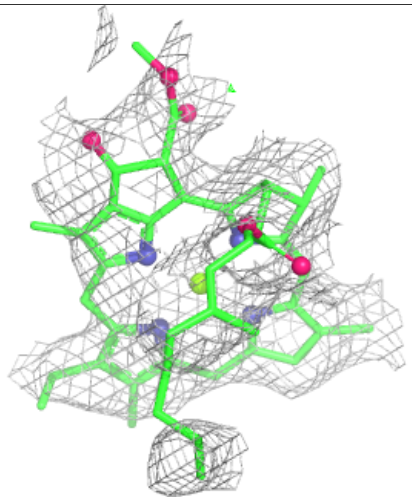


Electron density around CLA A 1128:

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

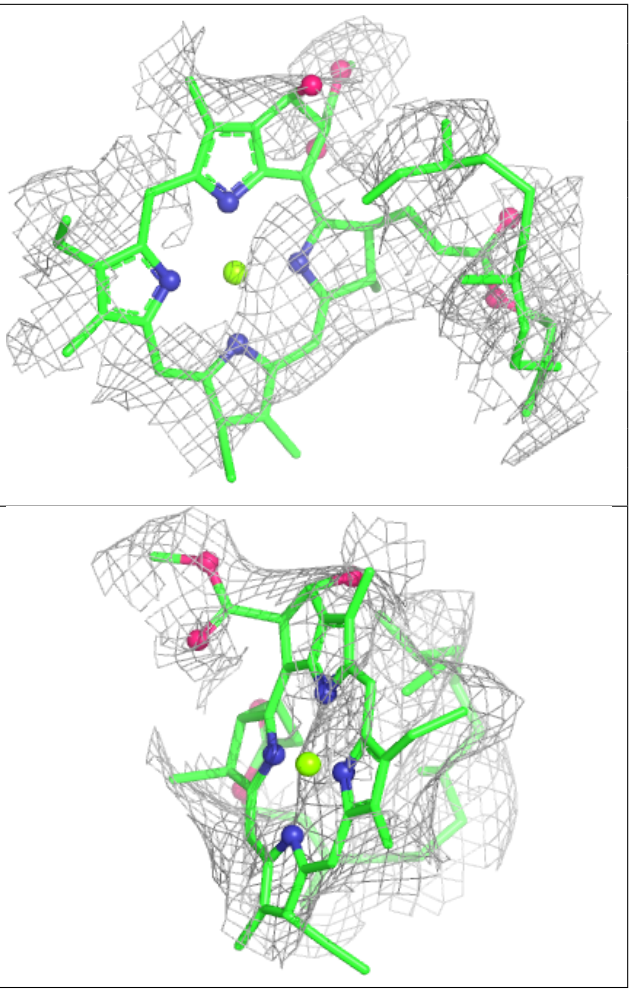






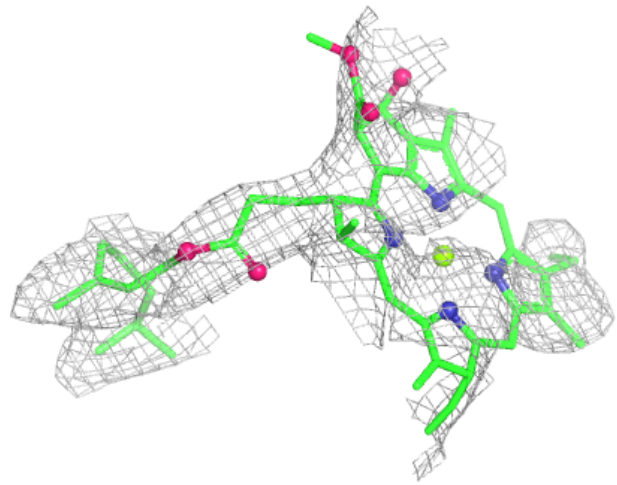
Electron density around CLA J 2107:

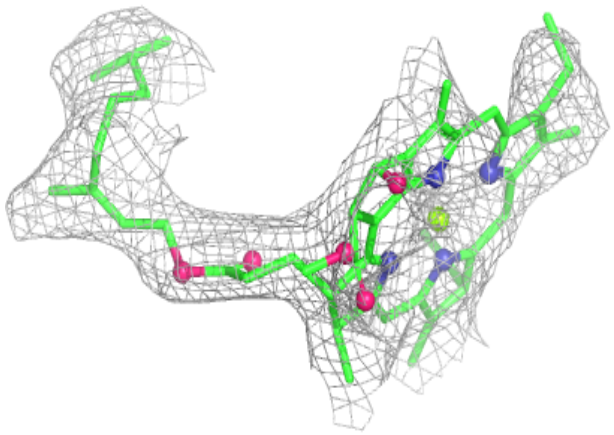
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

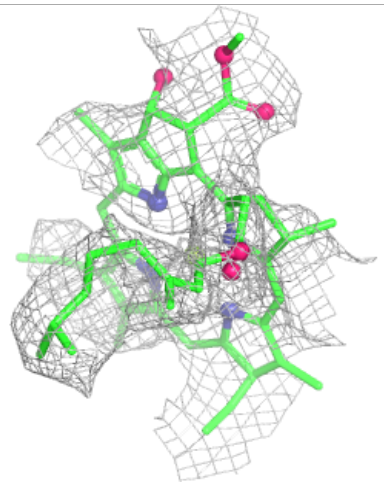


Electron density around CLA A 1129:

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

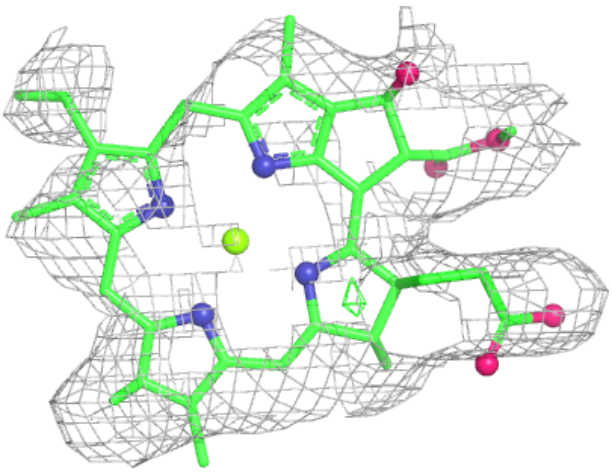


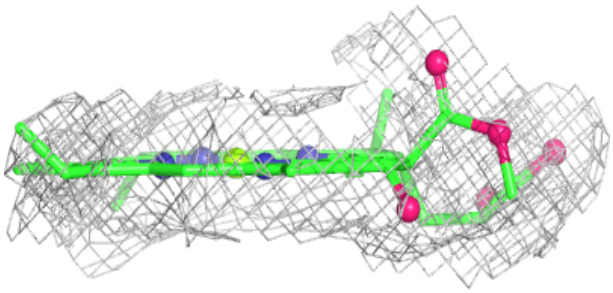


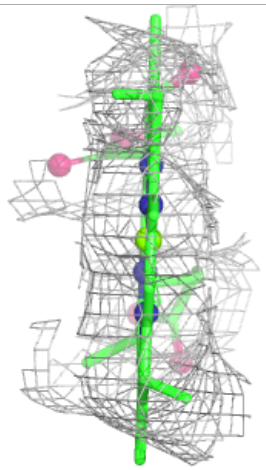


Electron density around CLA A 1131:

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

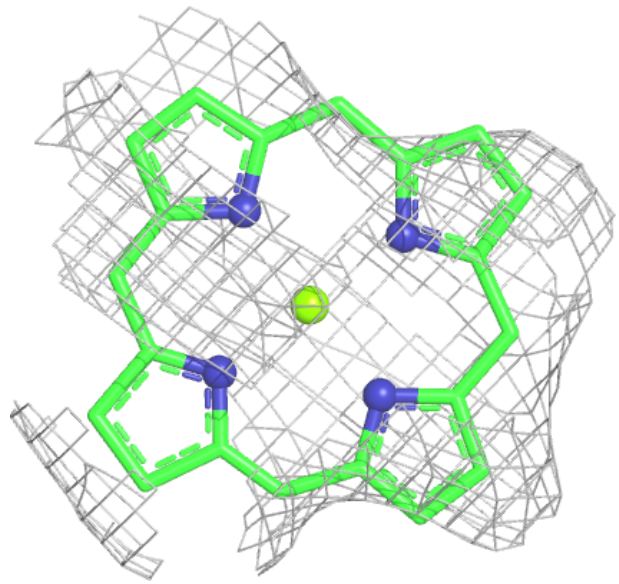


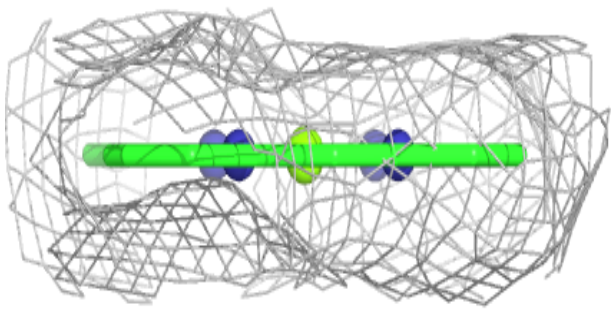


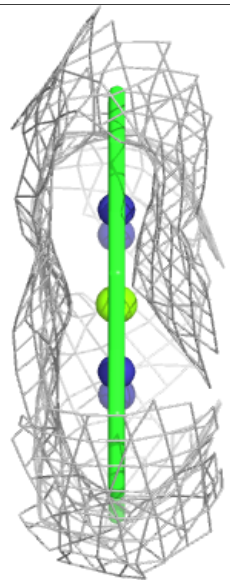


Electron density around CLA K 1153:

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

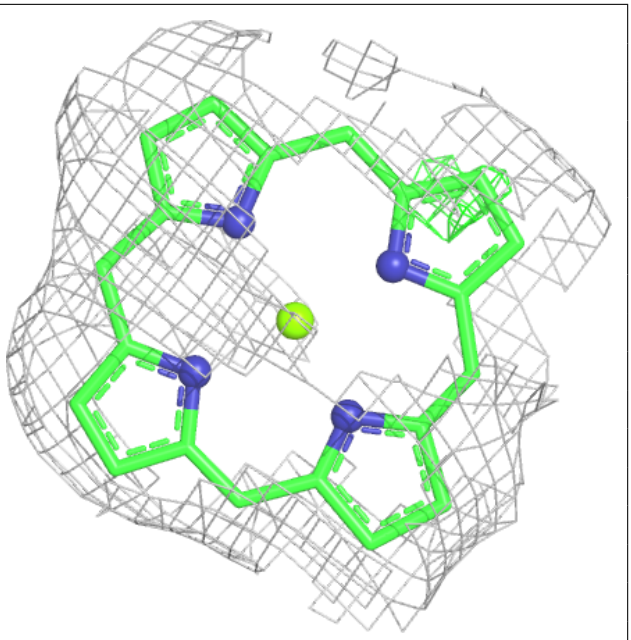


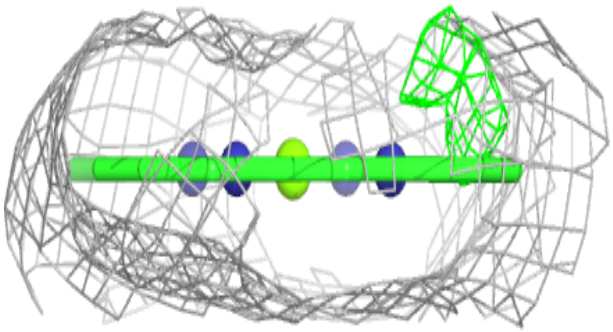


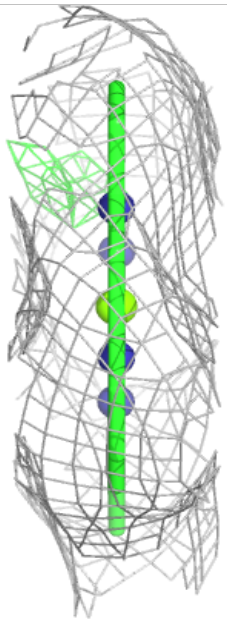


Electron density around CLA A 1133:

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

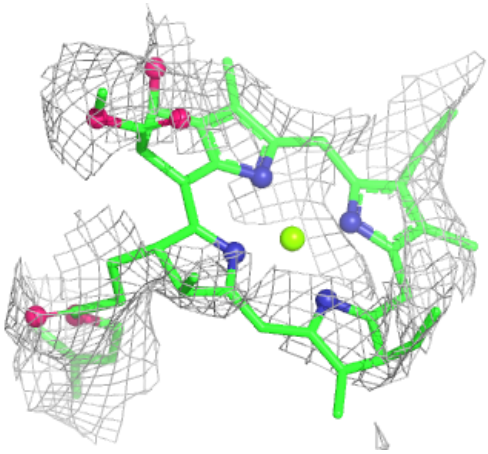


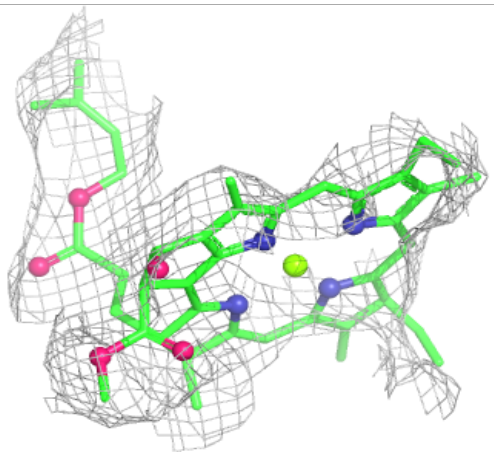


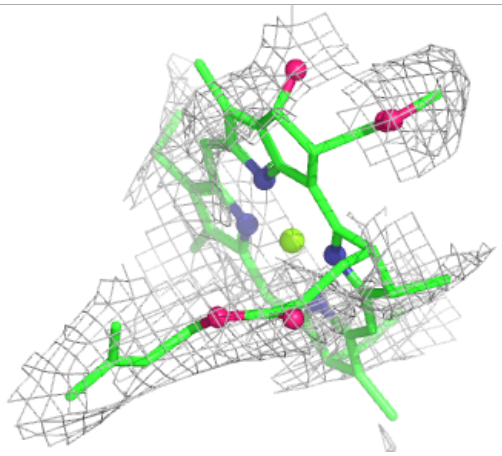


Electron density around CLA L 1130:

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

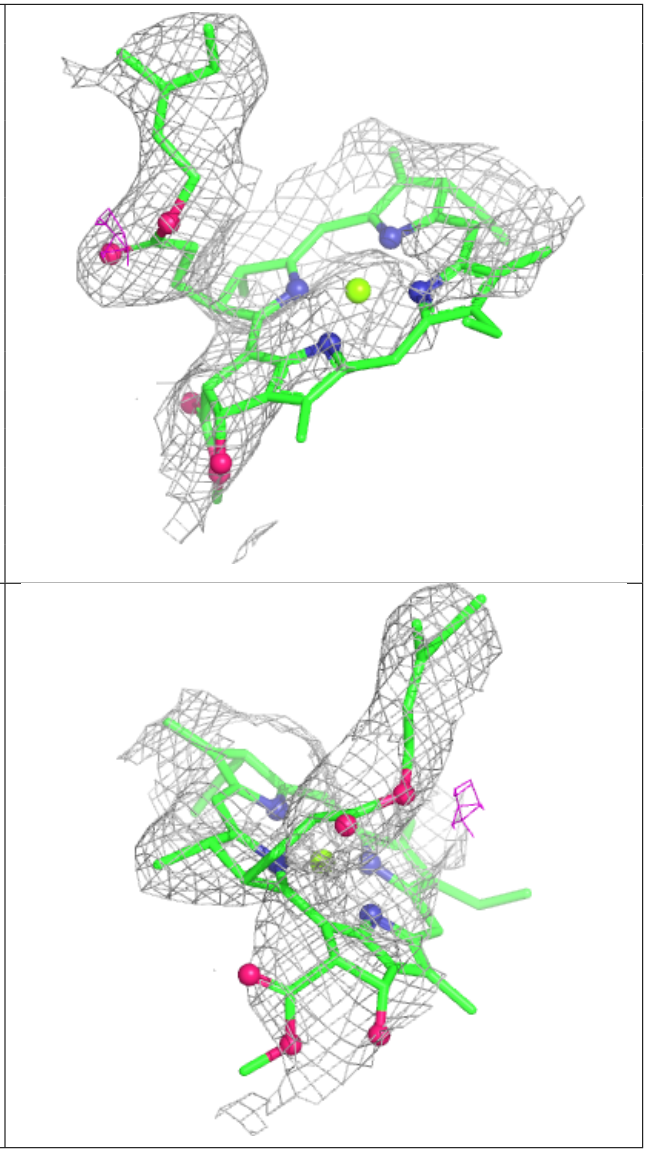






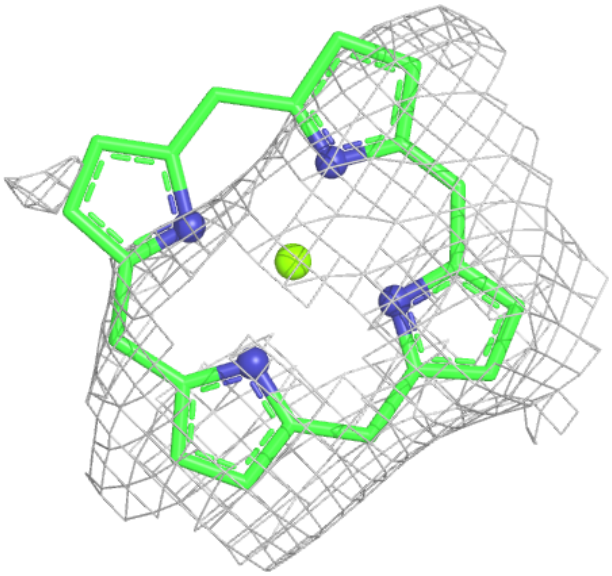
Electron density around CLA L 1502:

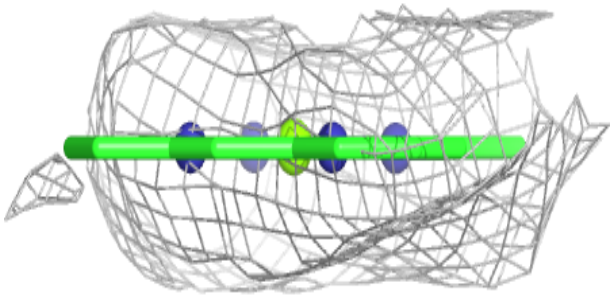
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

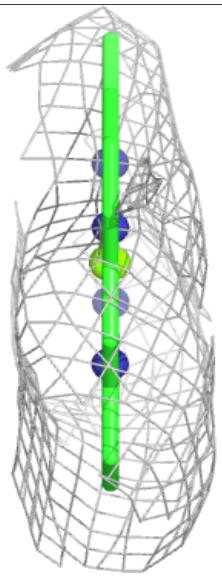


Electron density around CLA A 1134:

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

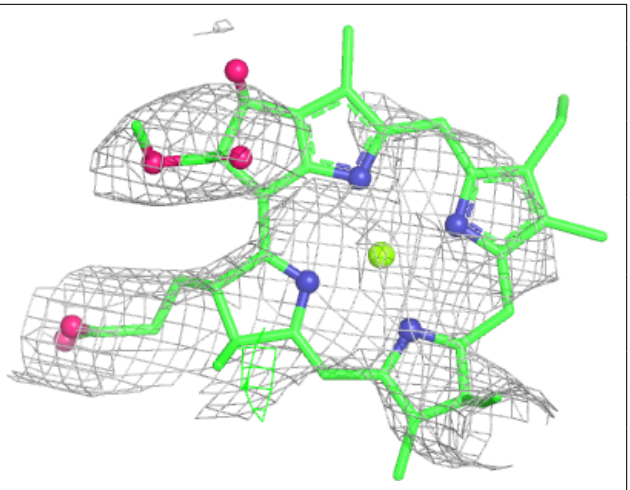


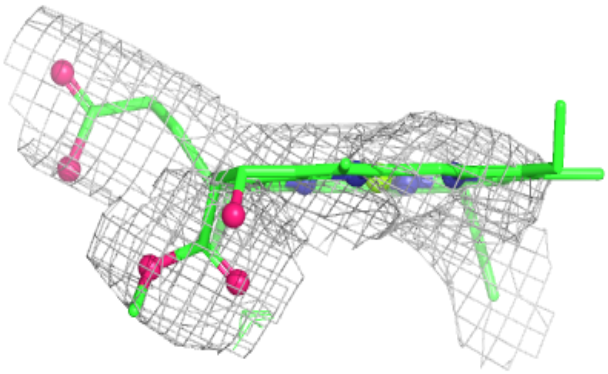


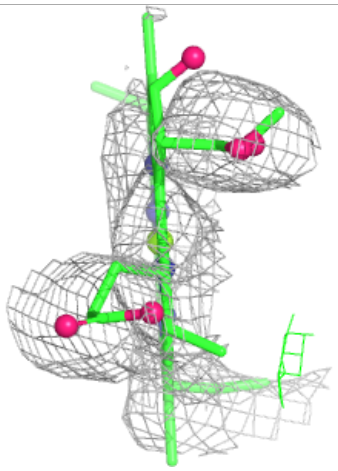


Electron density around CLA A 1135:

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

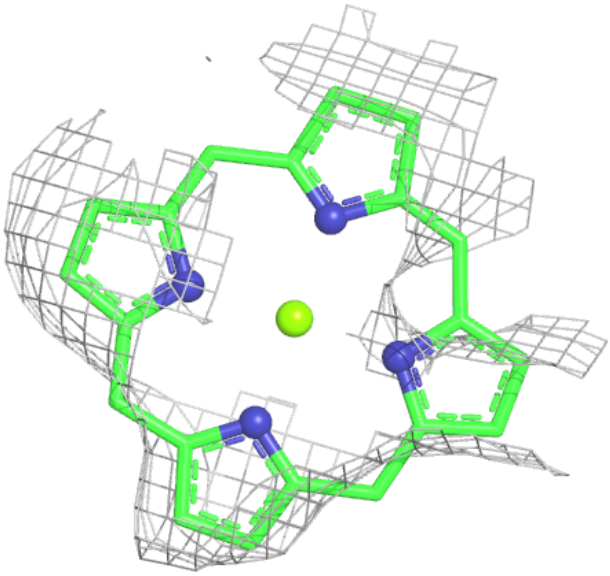


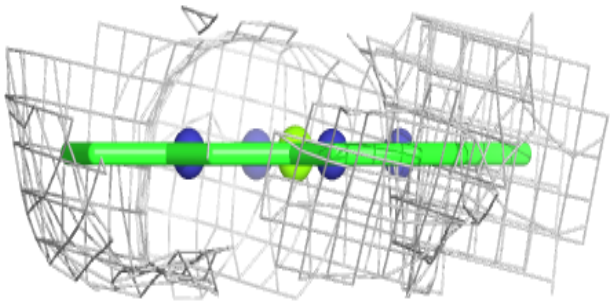


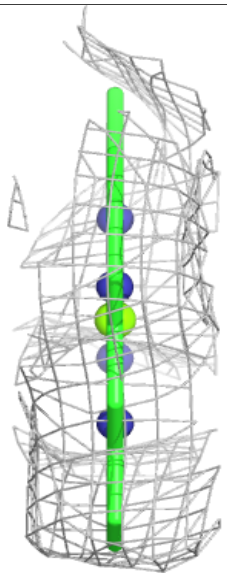


Electron density around CLA 1 1006:

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

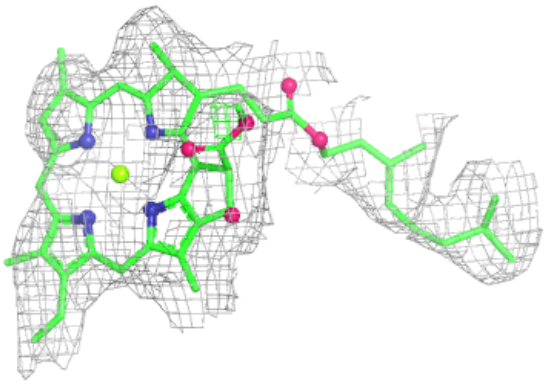


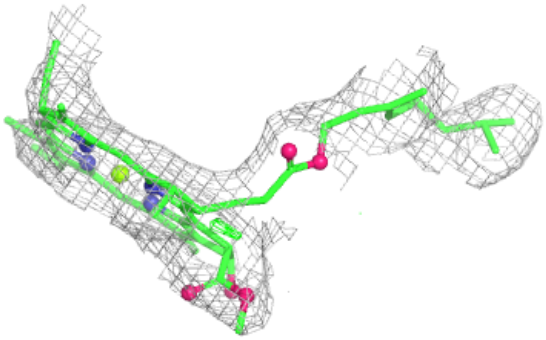


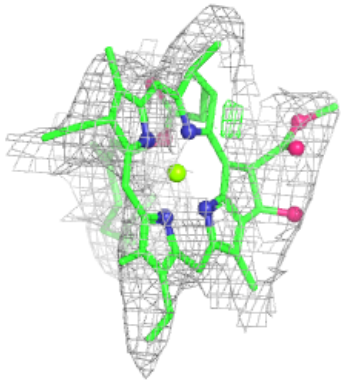


Electron density around CLA A 1137:

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

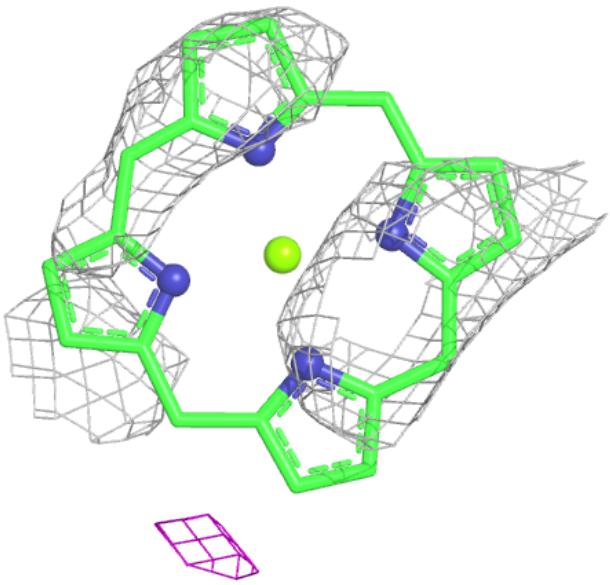


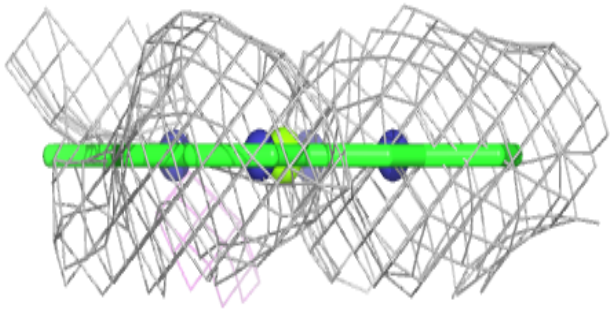


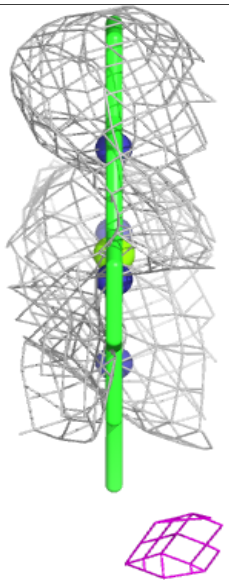


Electron density around CLA 1 1010:

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

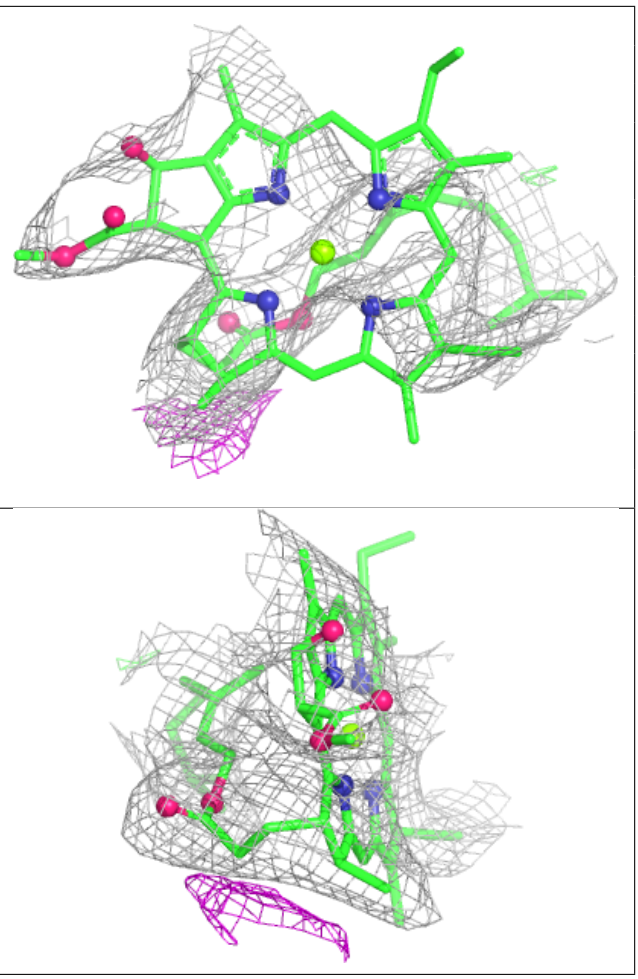






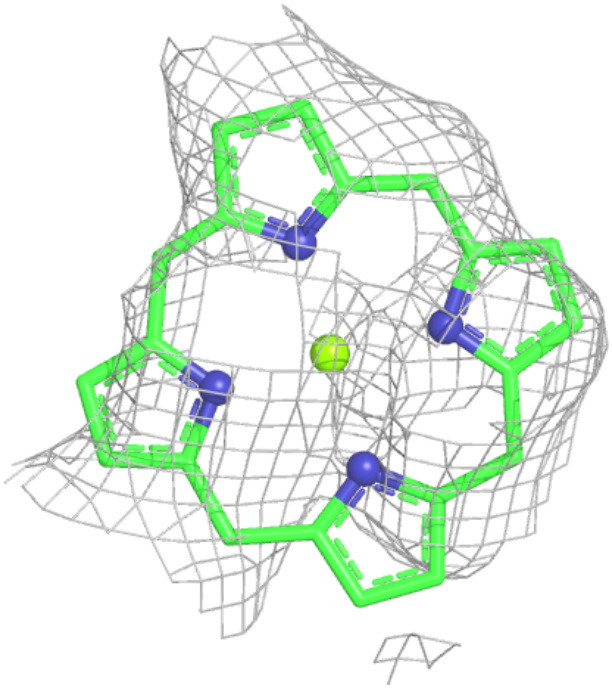
Electron density around CLA A 1140:

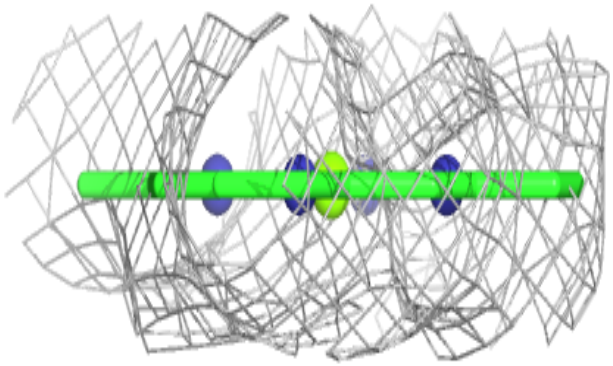
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

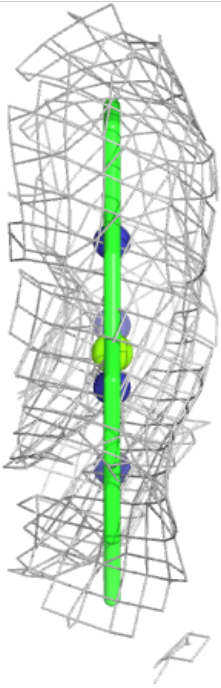


Electron density around CLA A 1142:

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

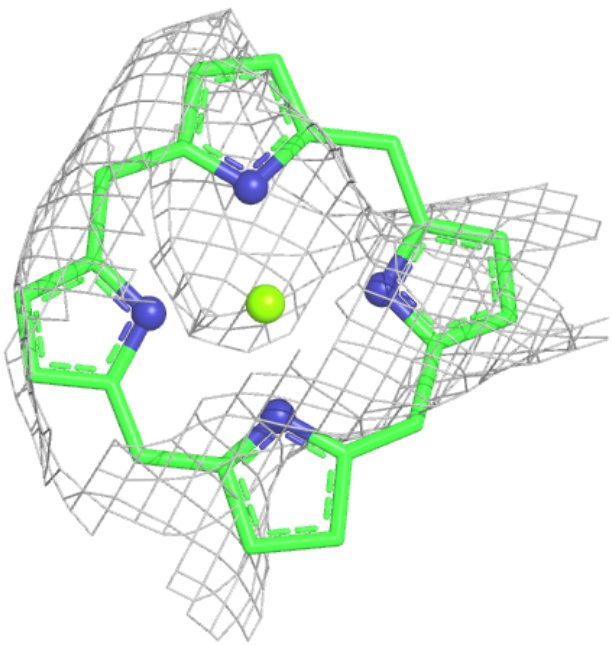


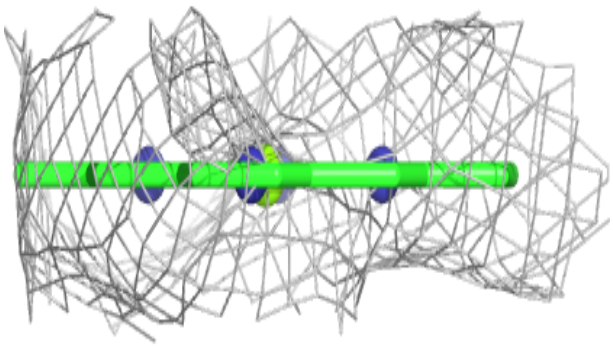


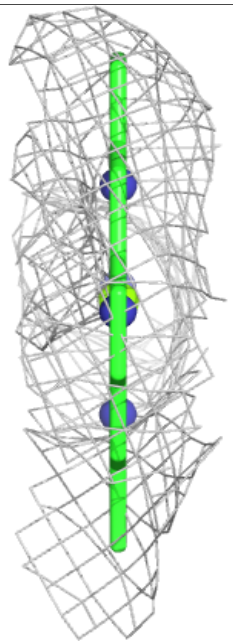


Electron density around CLA A 1143:

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

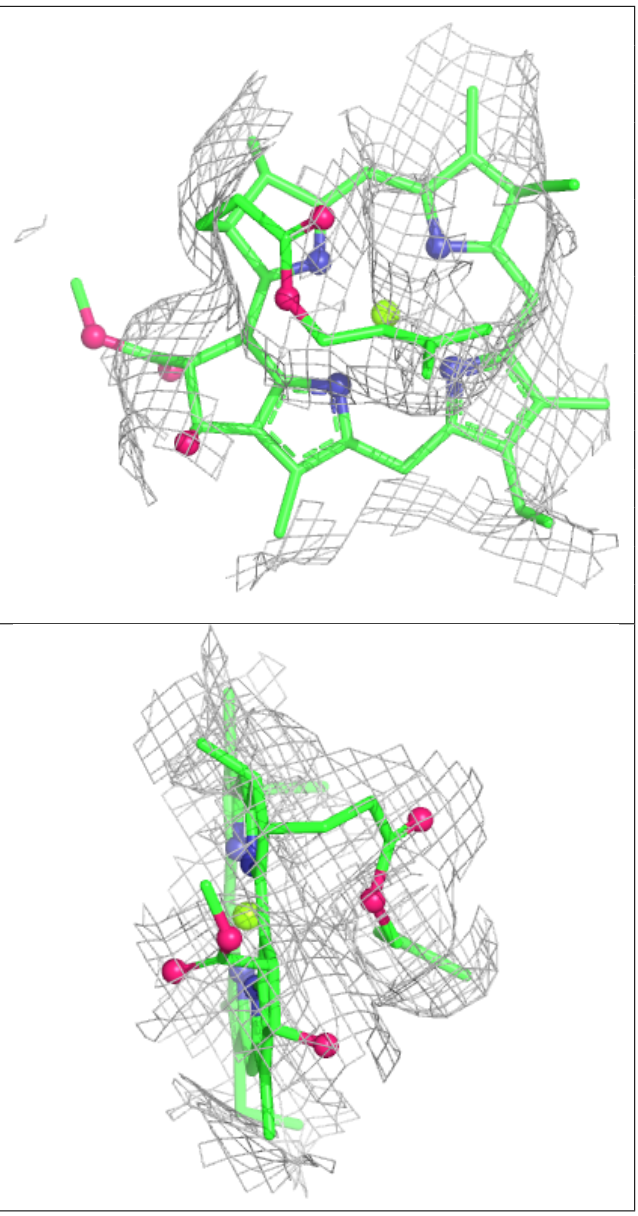






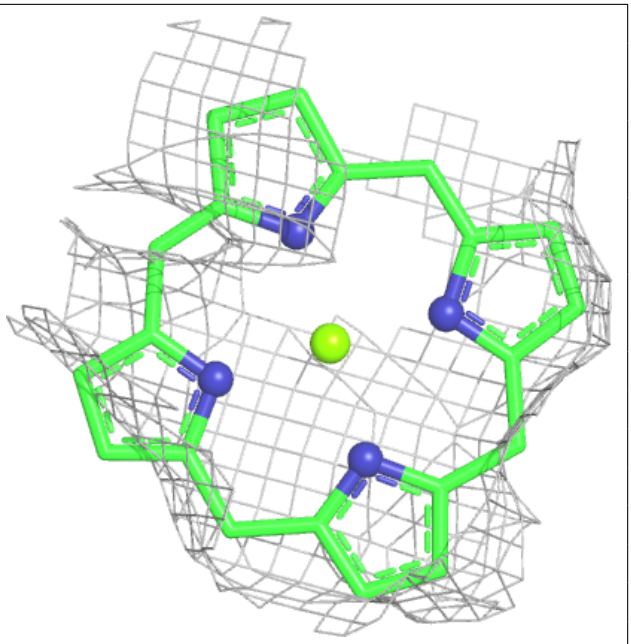
Electron density around CLA A 1108:

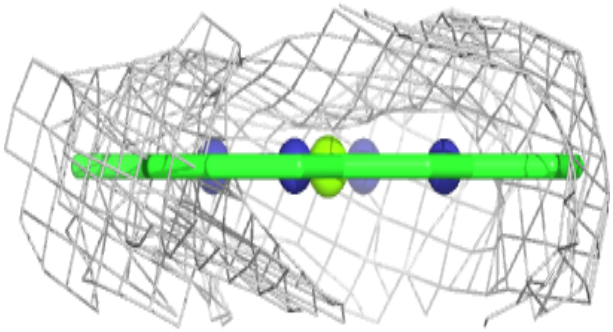
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

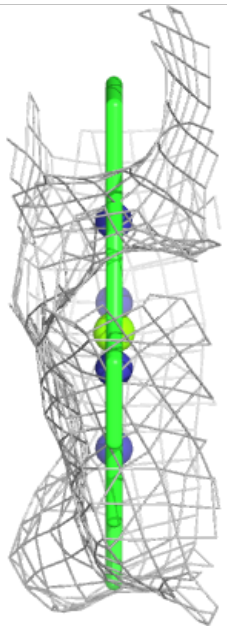


Electron density around CLA 1 1003:

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

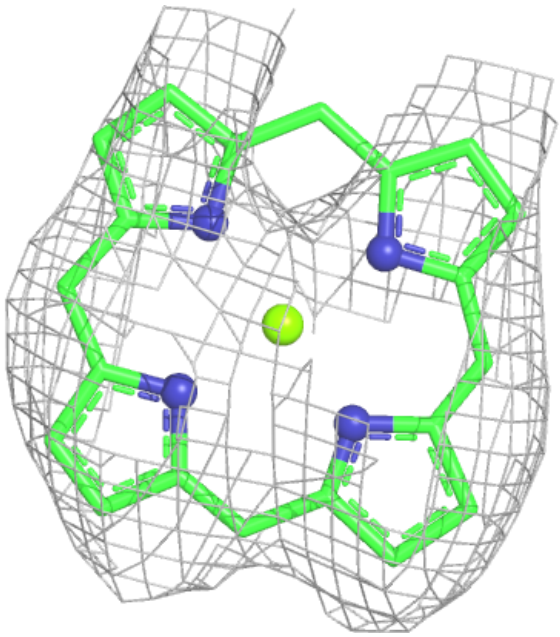


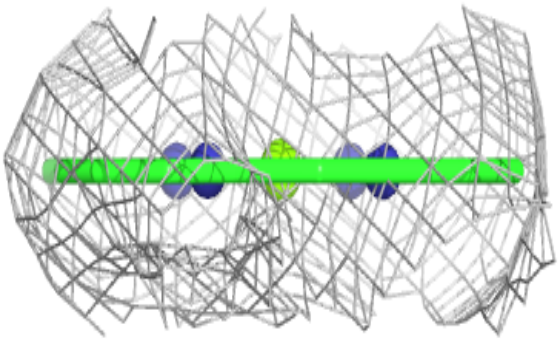


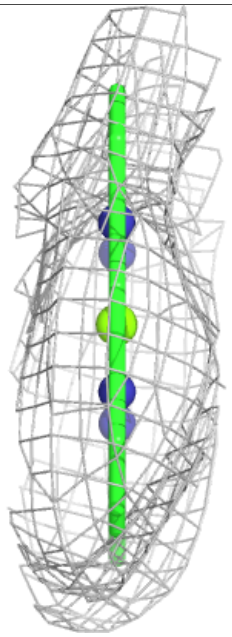


Electron density around CLA A 1146:

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

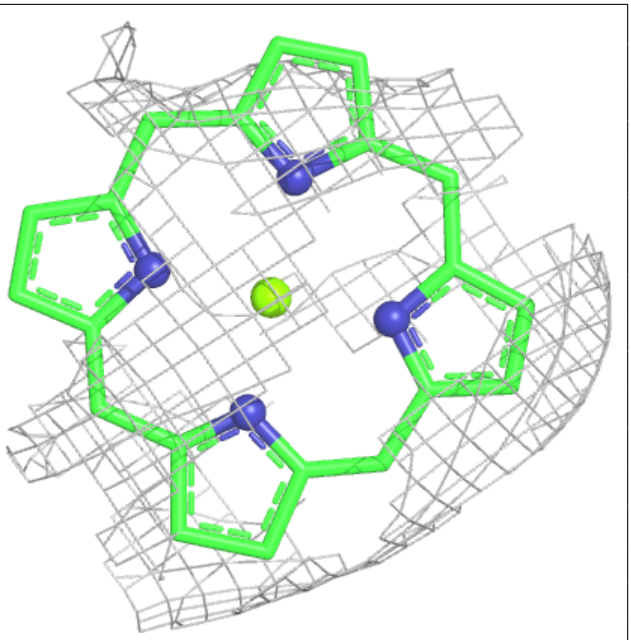


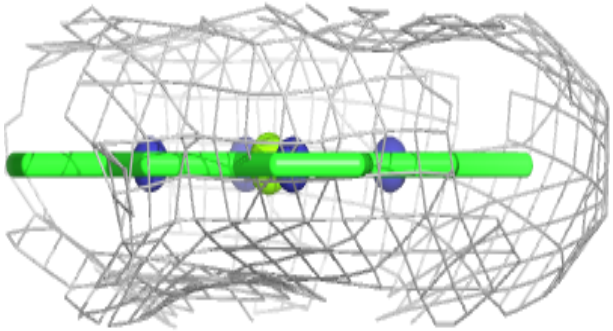


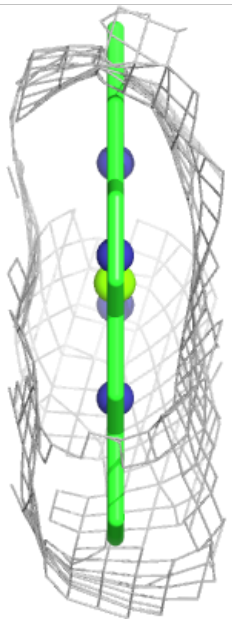


Electron density around CLA 1 1014:

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

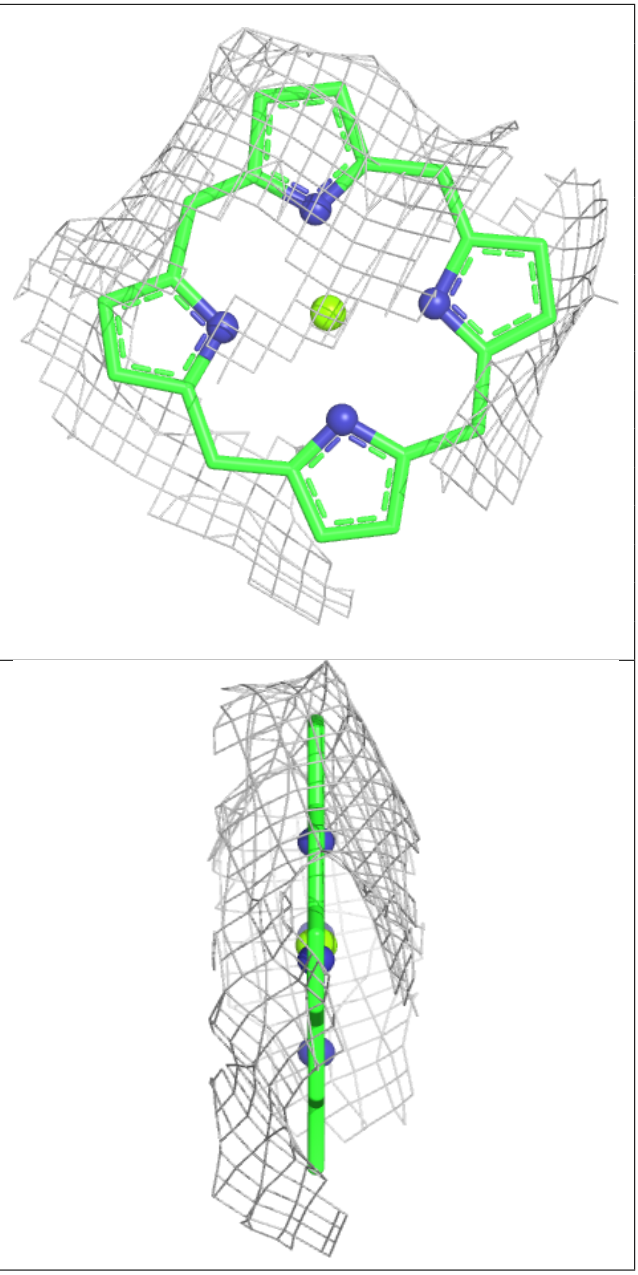






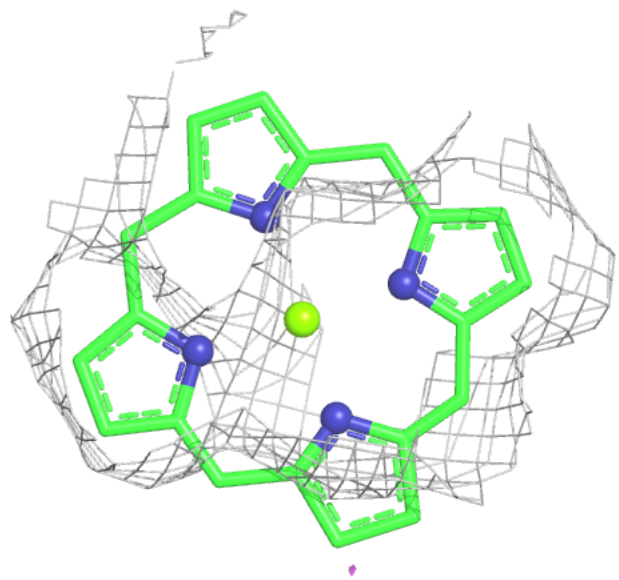
Electron density around CLA A 1110:

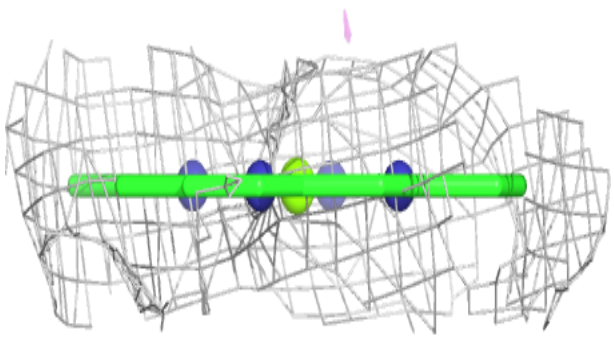
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

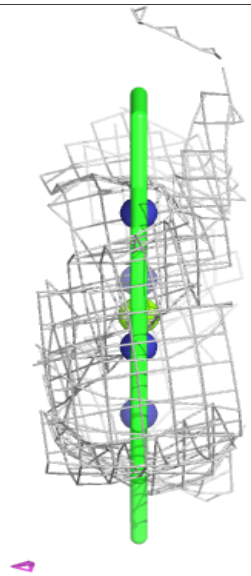


Electron density around CLA A 1111:

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

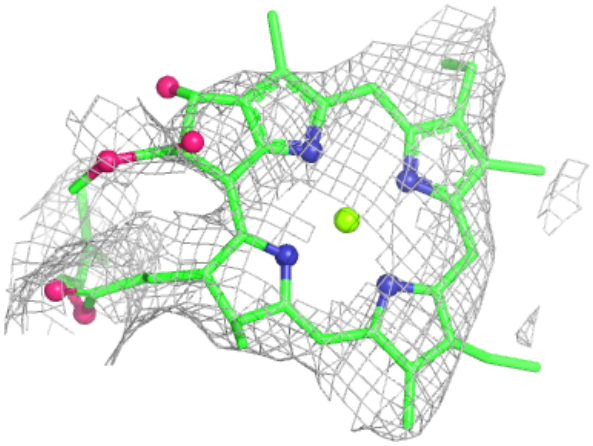


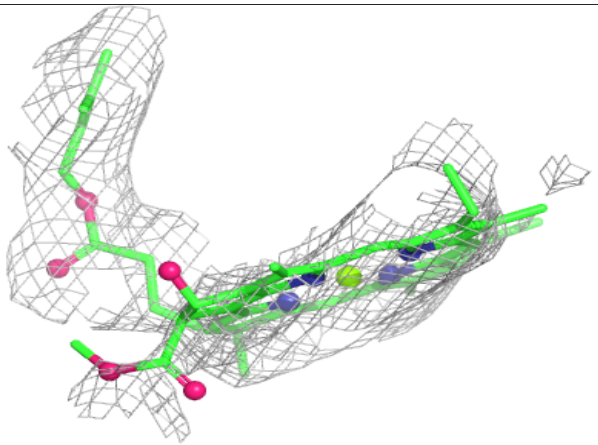


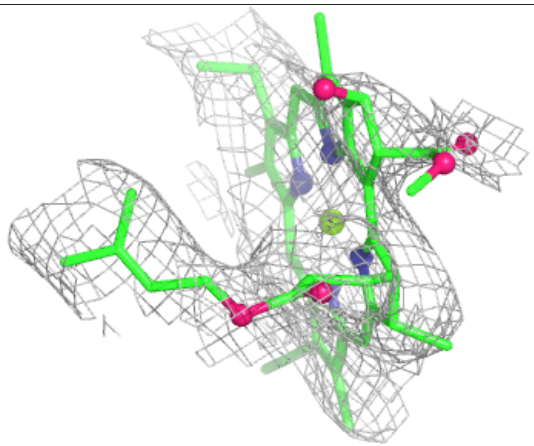


Electron density around CLA A 1113:

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

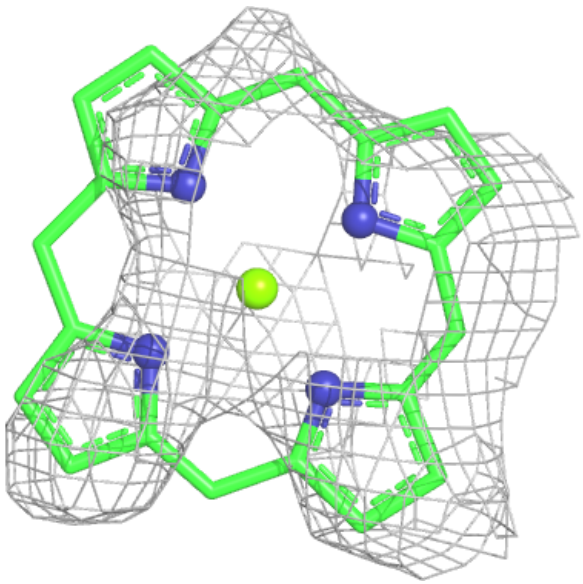


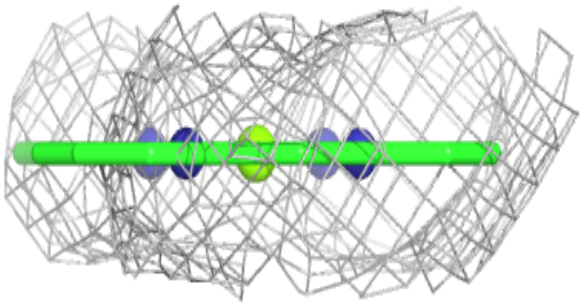


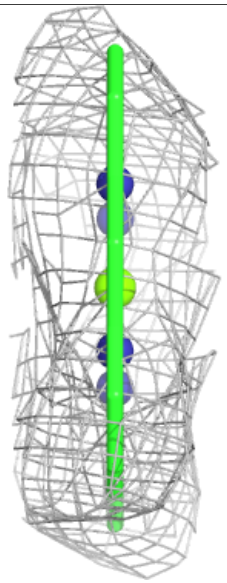


Electron density around CLA A 1152:

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

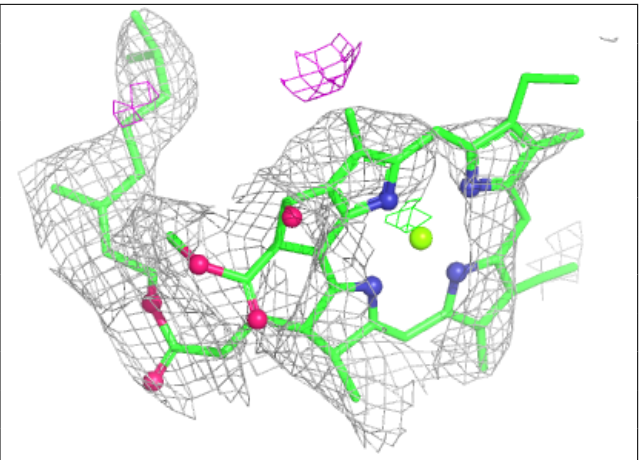


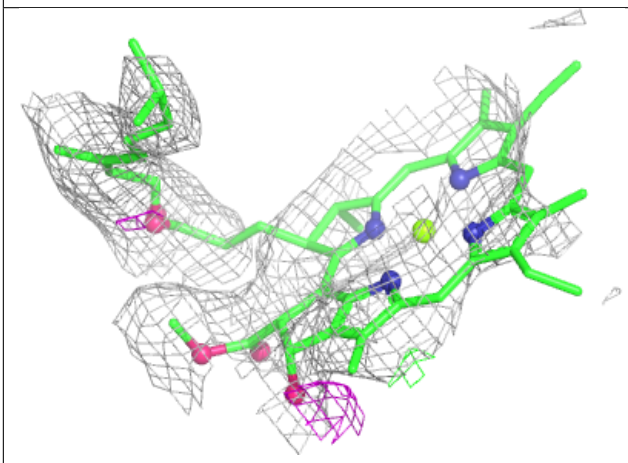


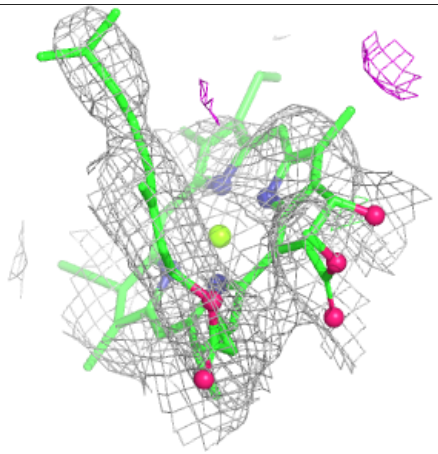


Electron density around CLA A 9011:

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

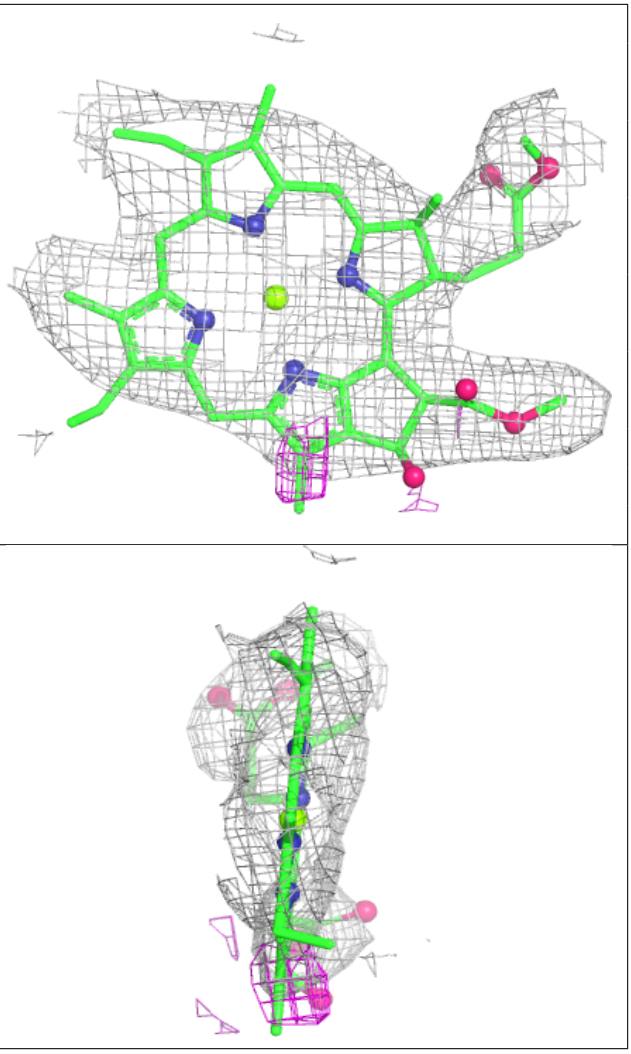






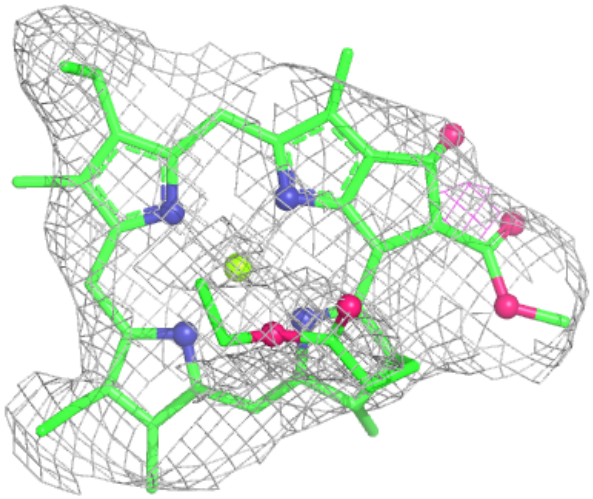
Electron density around CLA A 9013:

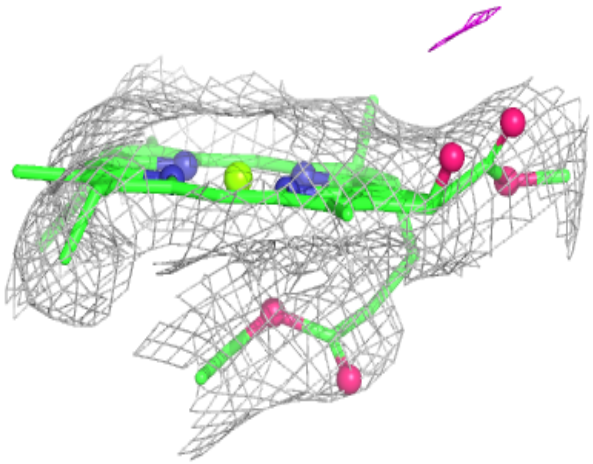
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

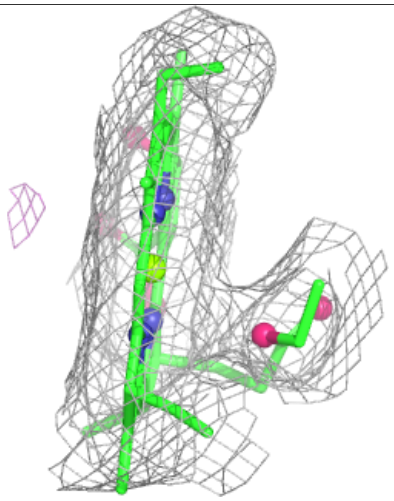


Electron density around CLA A 1115:

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

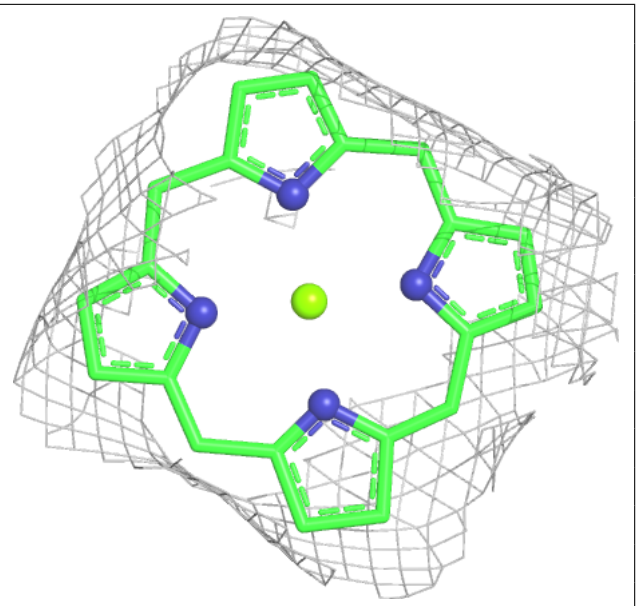


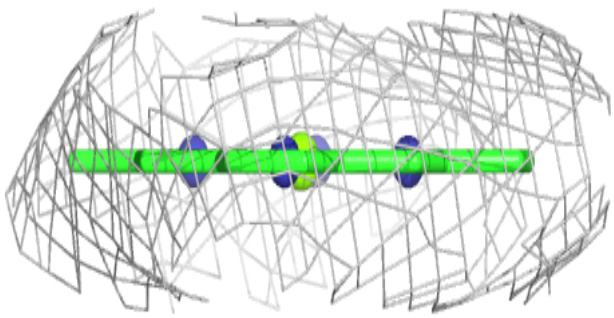


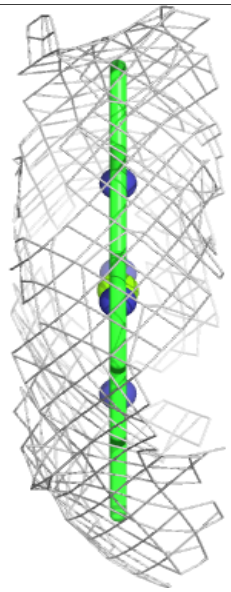


Electron density around CLA 2 2007:

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

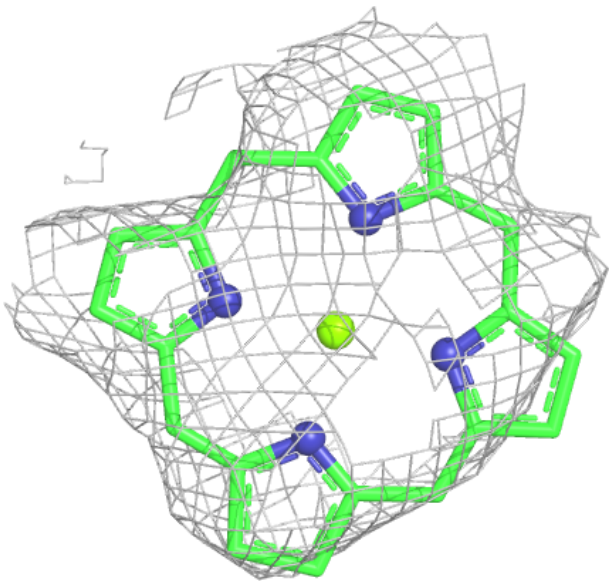


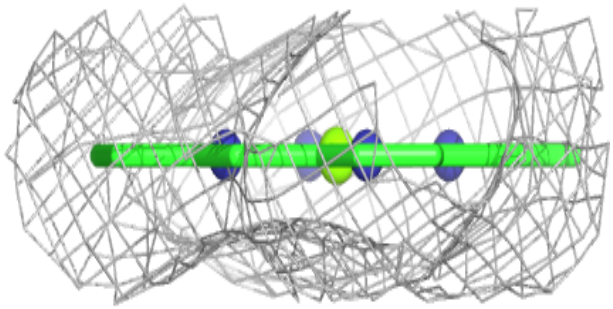


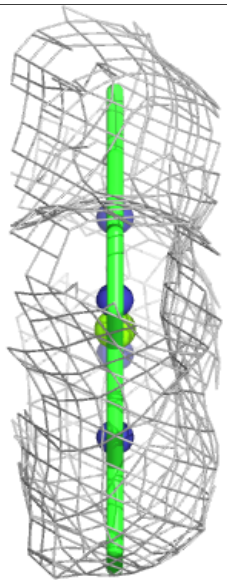


Electron density around CLA 2 2002:

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

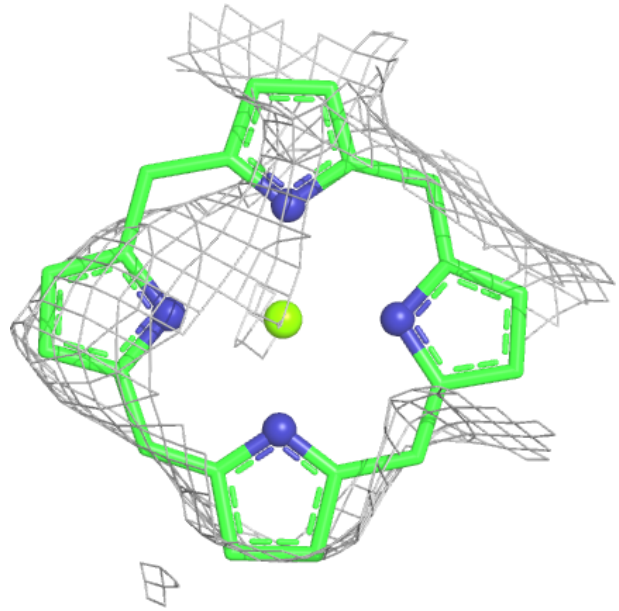


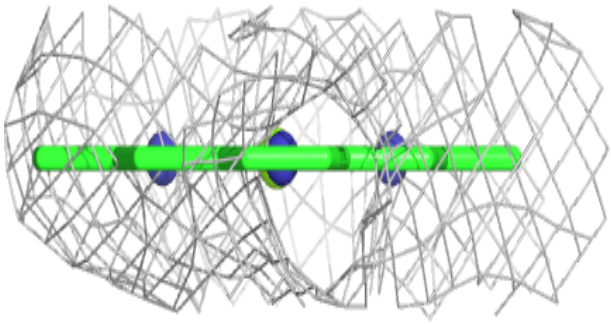


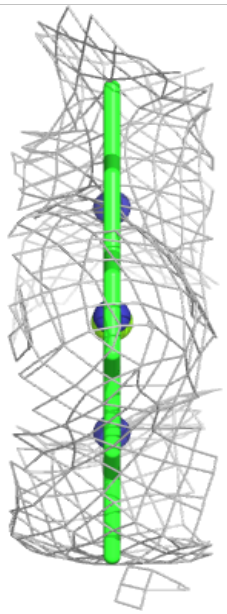


Electron density around CLA 2 2003:

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

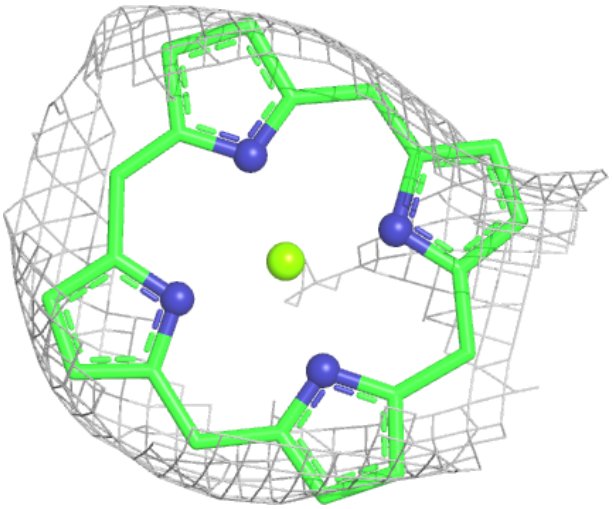


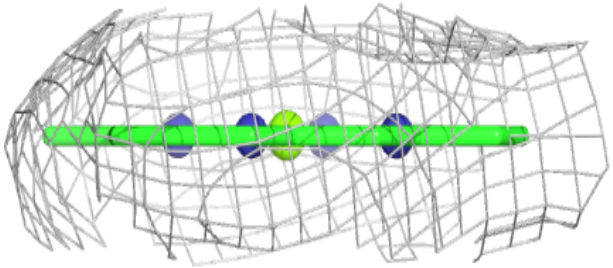


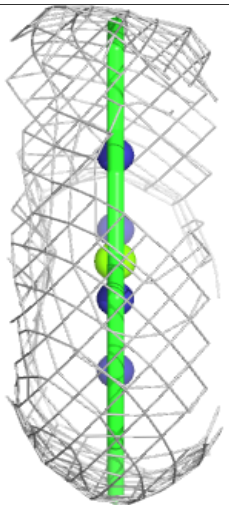


Electron density around CLA 3 2009:

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

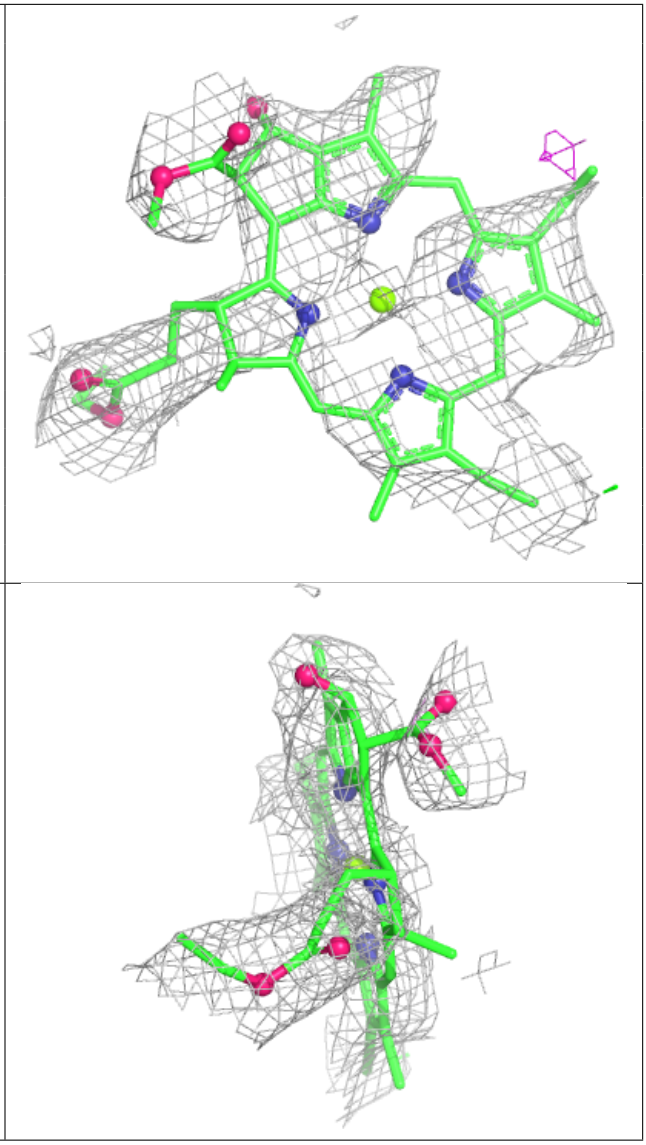






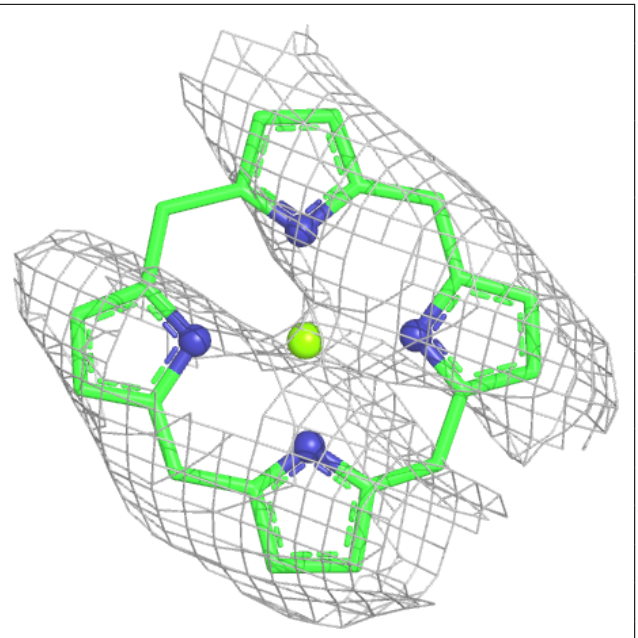
Electron density around CLA B 9010:

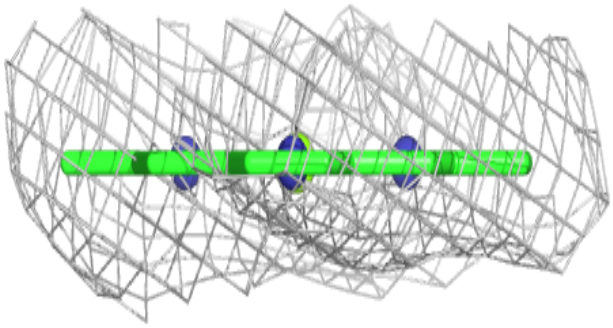
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

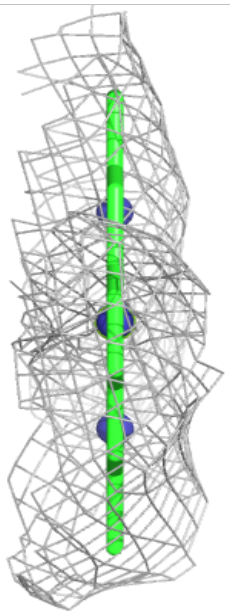


Electron density around CLA 3 3004:

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

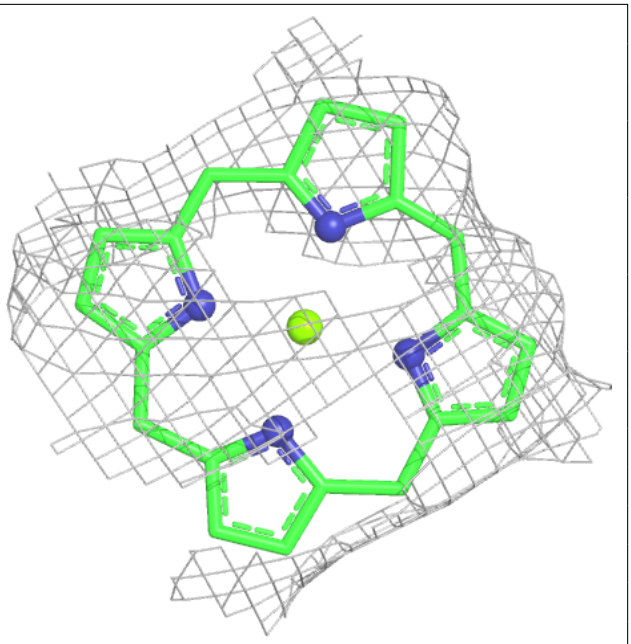


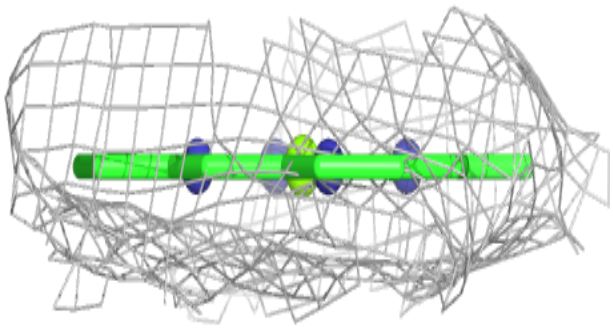


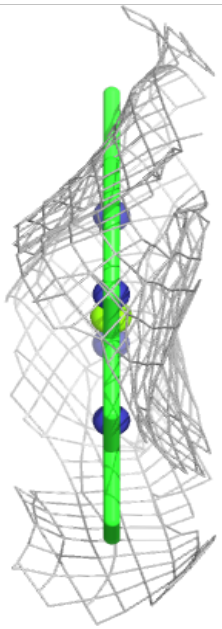


Electron density around CLA 3 3005:

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

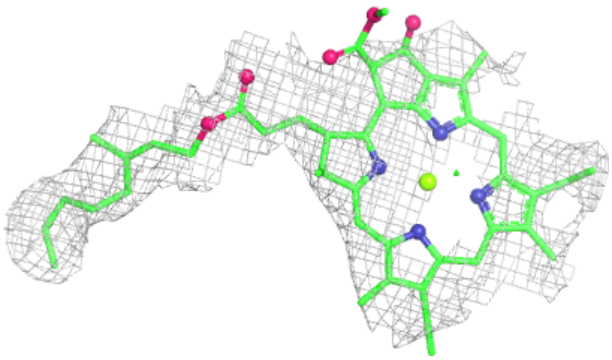


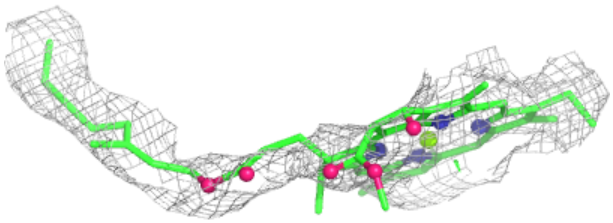


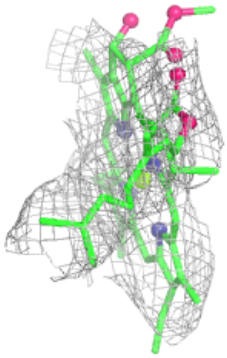


Electron density around CLA B 9012:

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

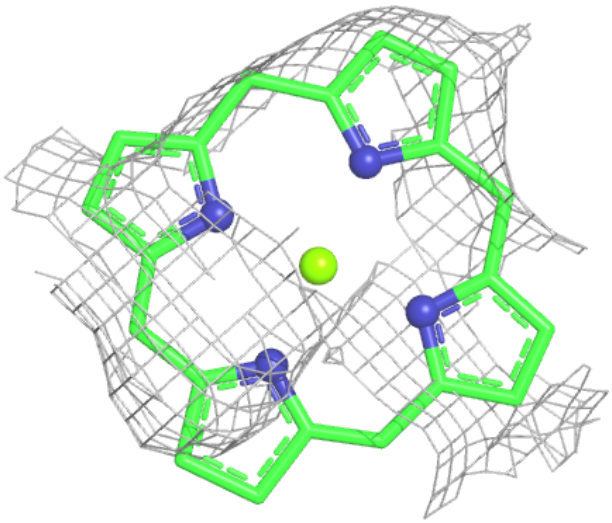


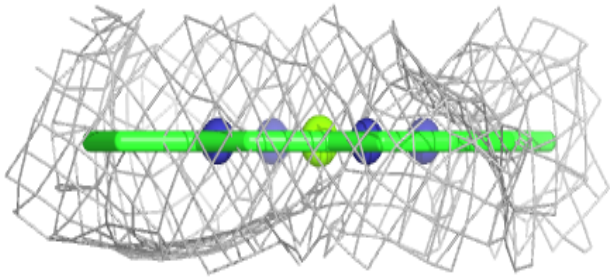


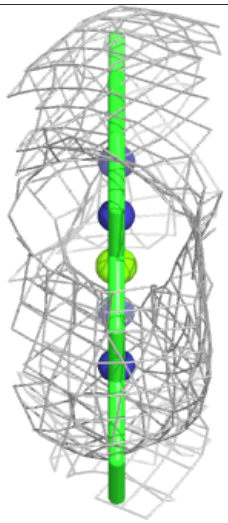


Electron density around CLA 3 3006:

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

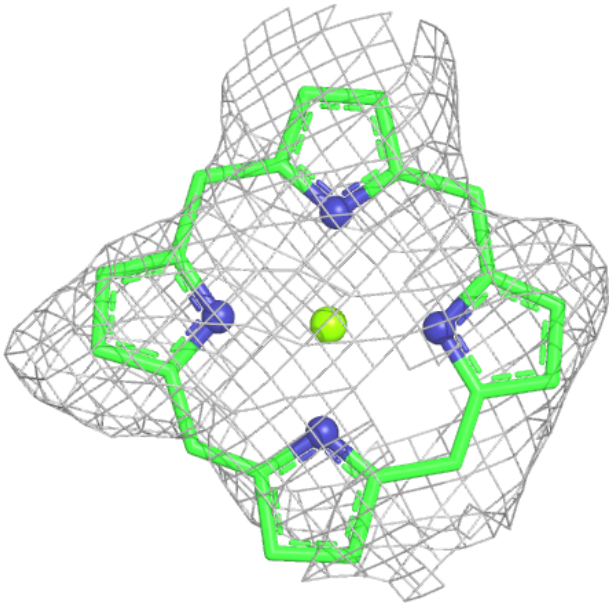


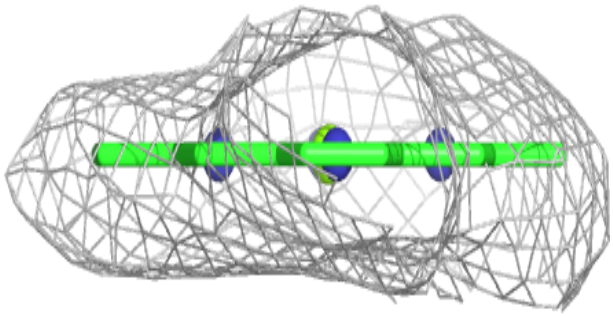


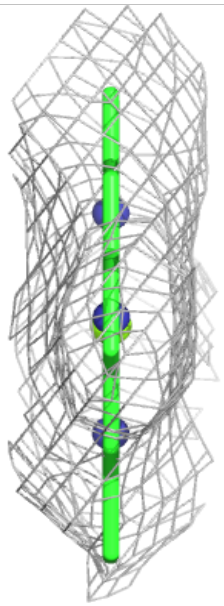


Electron density around CLA 3 3013:

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

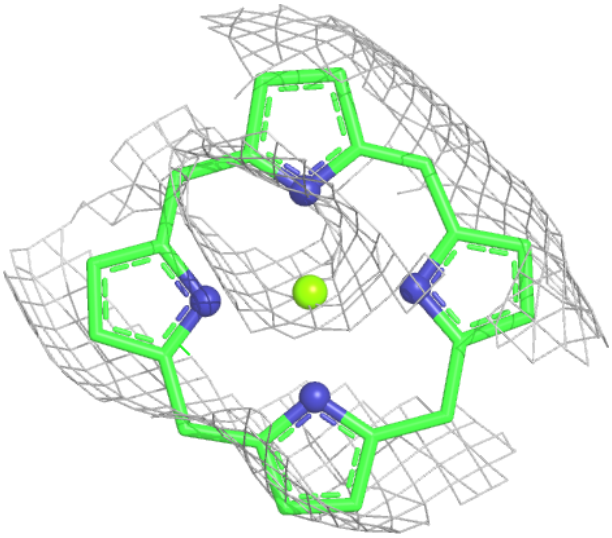


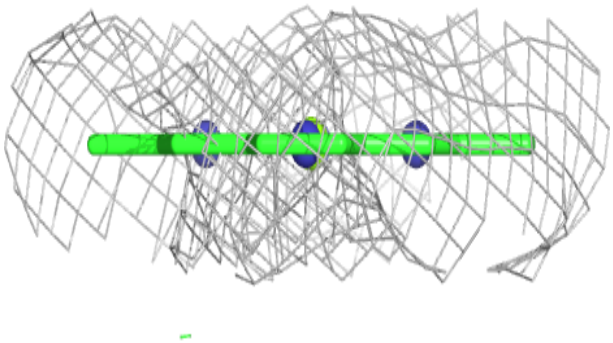


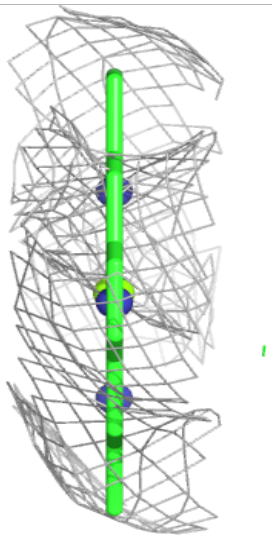


Electron density around CLA 3 3010:

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

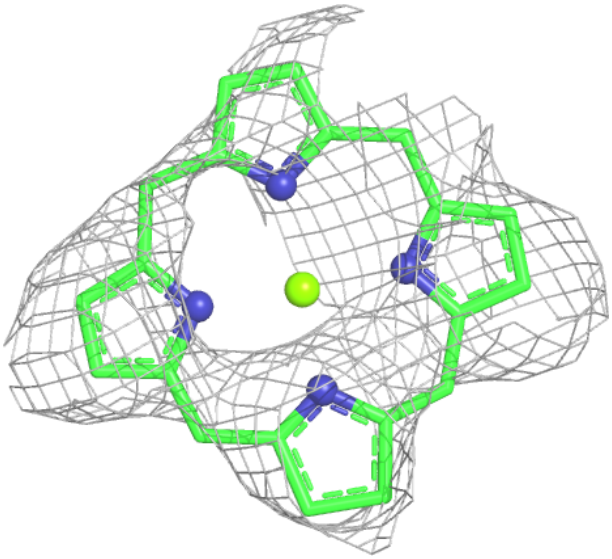


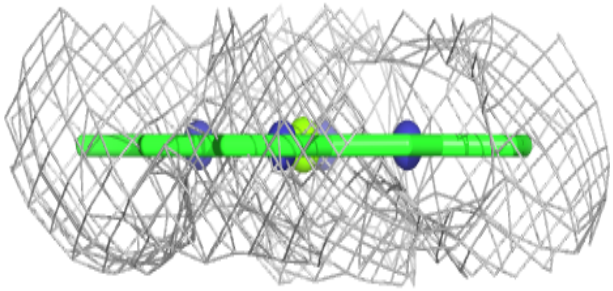


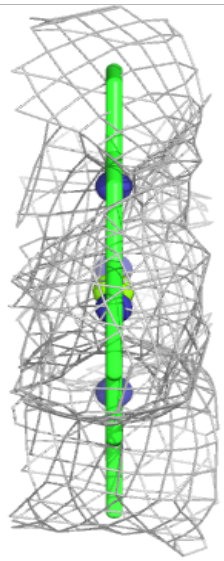


Electron density around CLA A 1116:

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

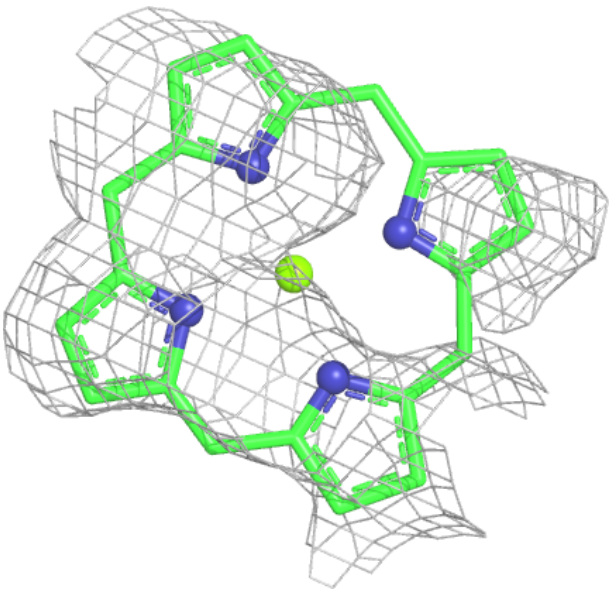


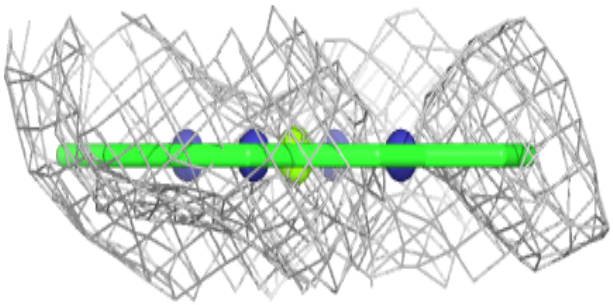


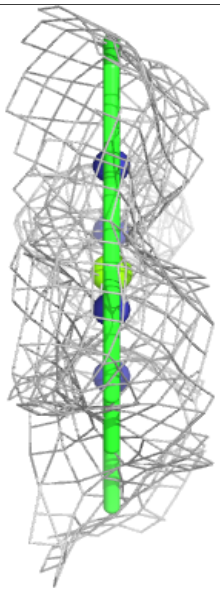


Electron density around CLA 3 3011:

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

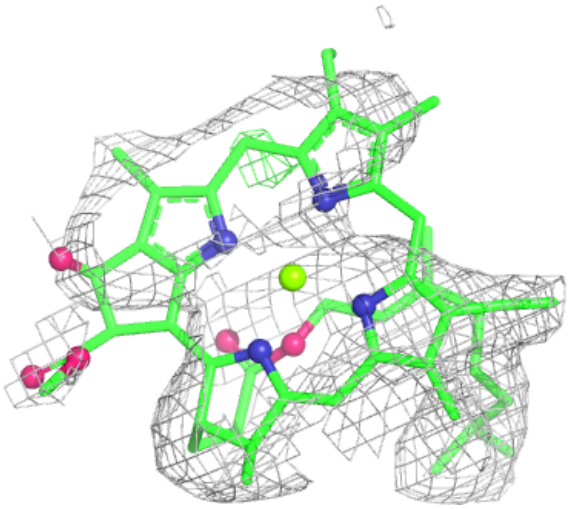


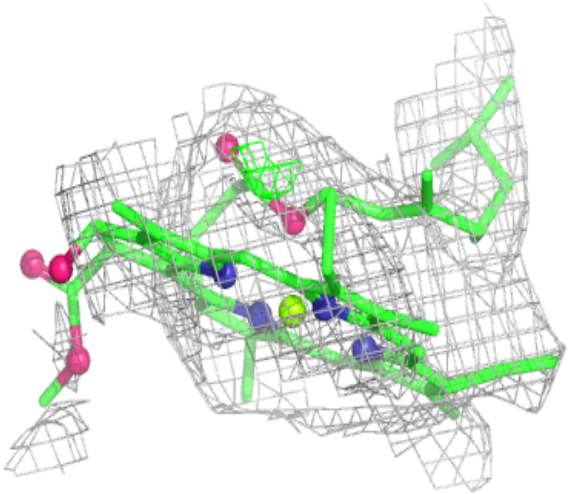


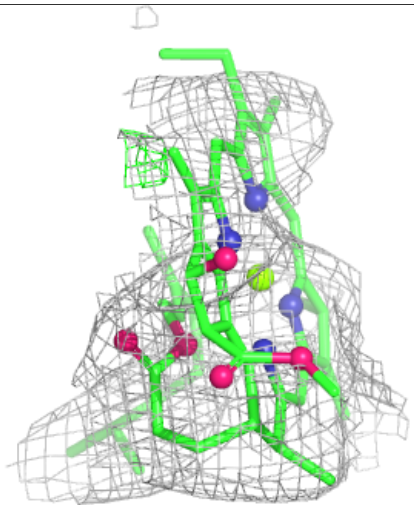


Electron density around CLA B 1205:

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

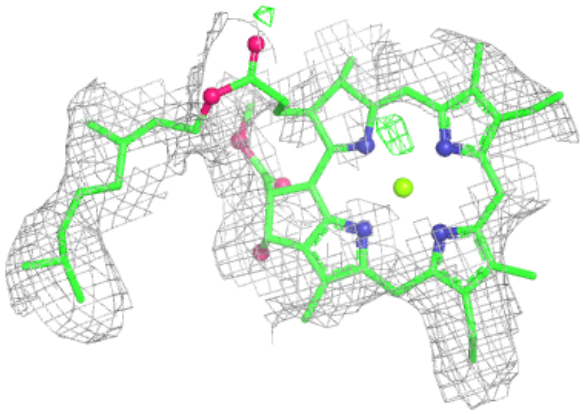


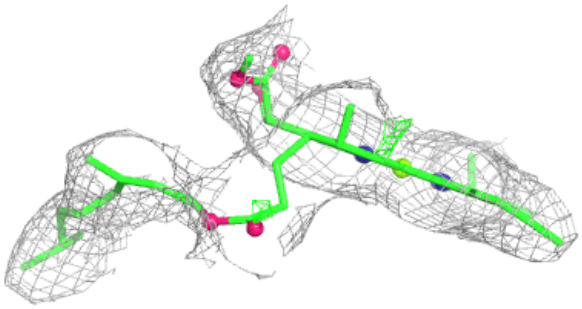


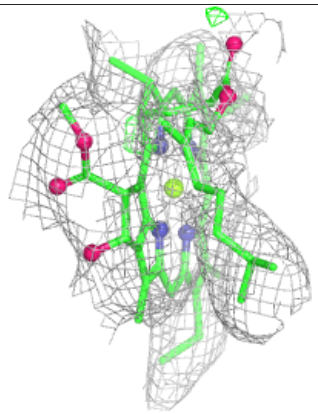


Electron density around CLA B 1208:

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

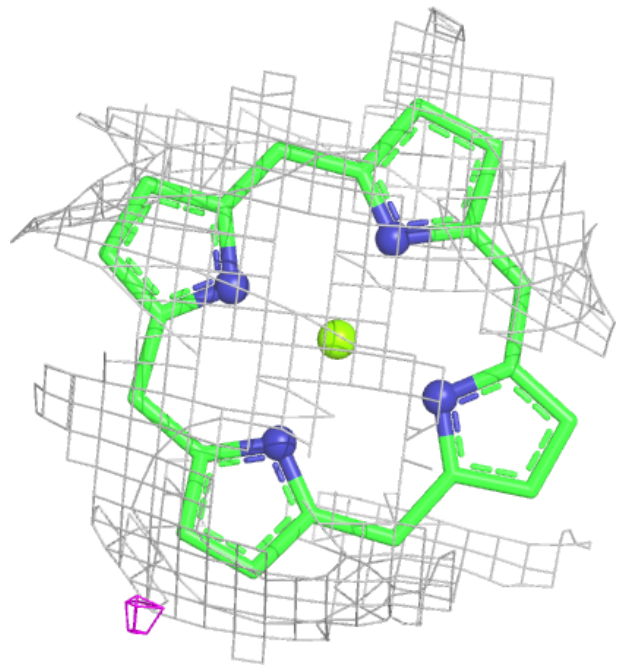


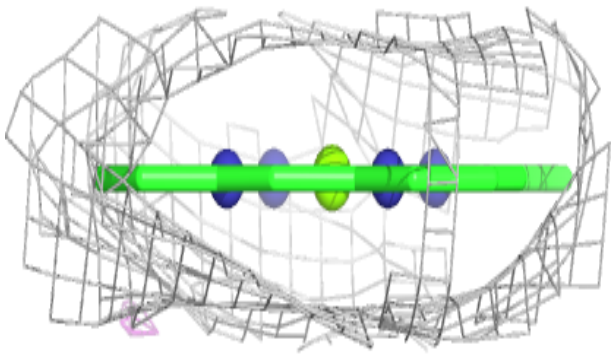


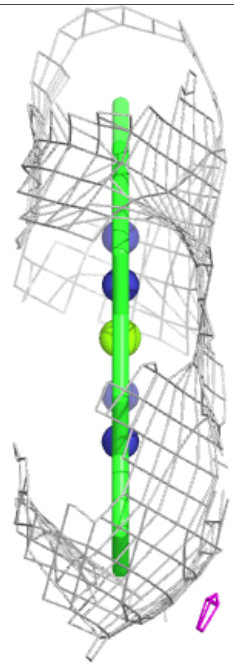


Electron density around CLA 3 3003:

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

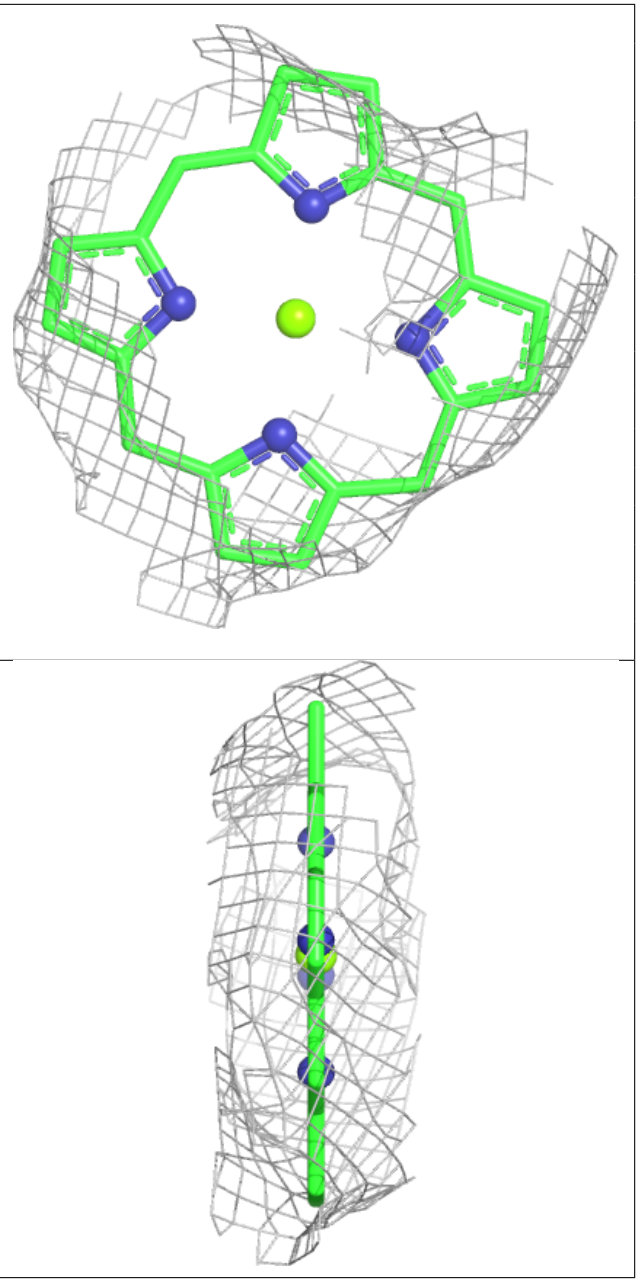






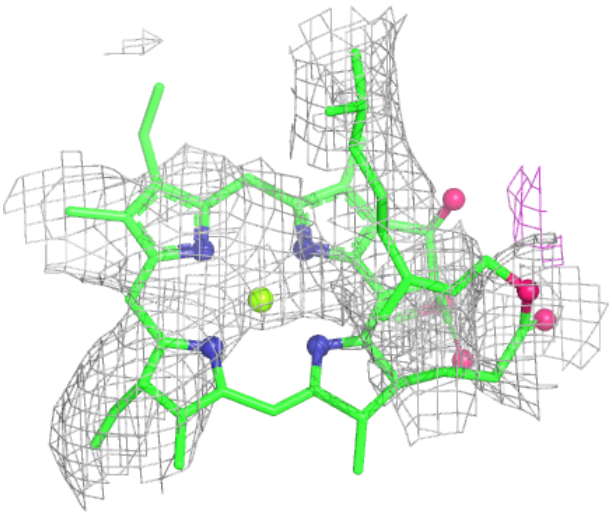
Electron density around CLA 3 3008:

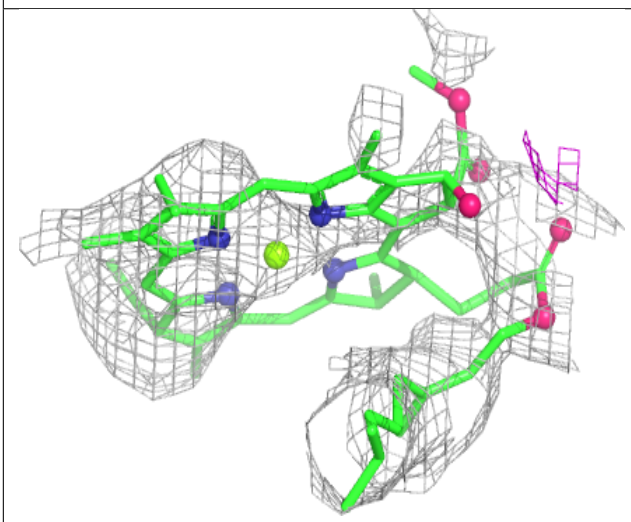
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

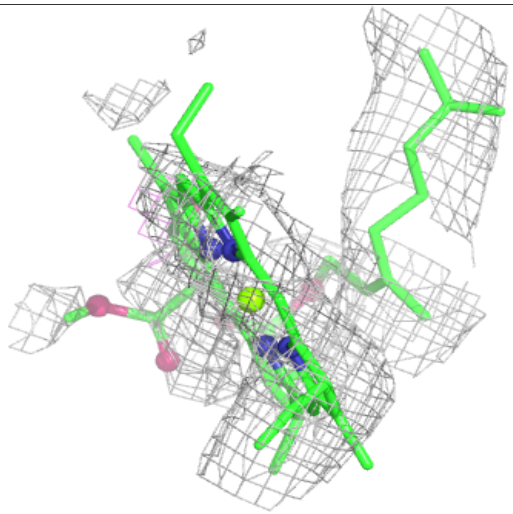


Electron density around CLA 4 1304:

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

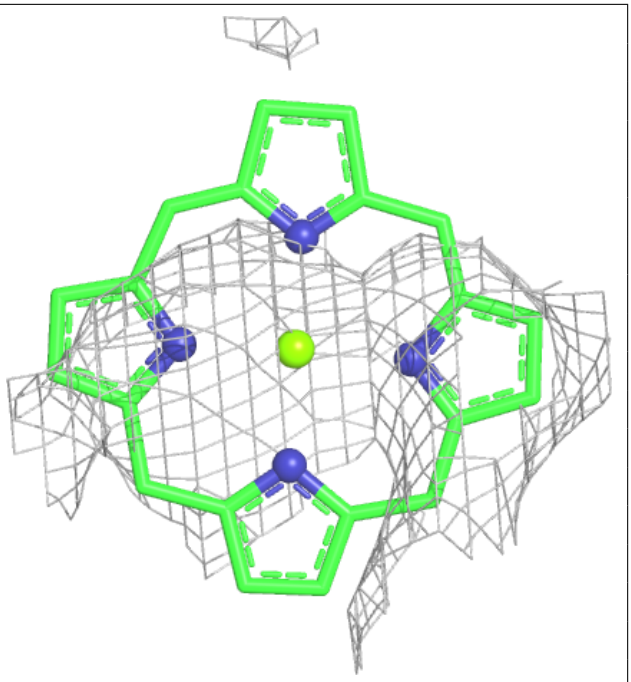


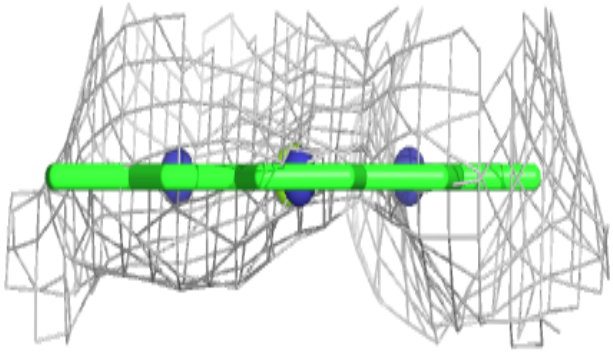


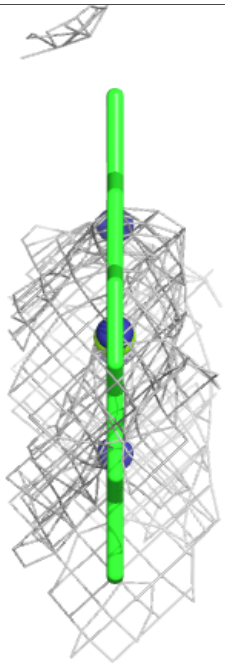


Electron density around CLA B 1210:

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

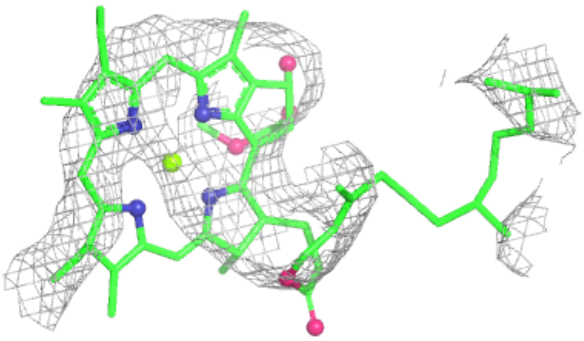


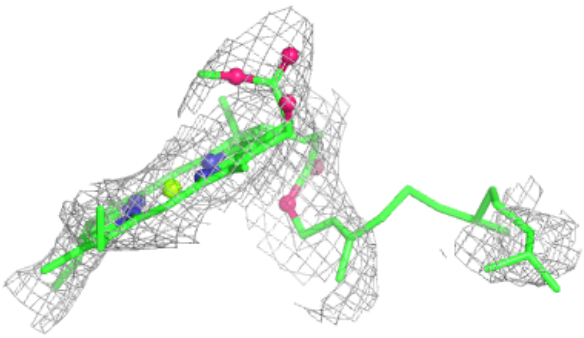


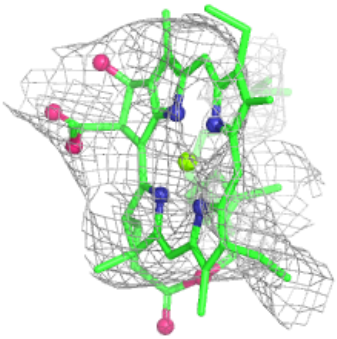


Electron density around CLA B 1212:

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

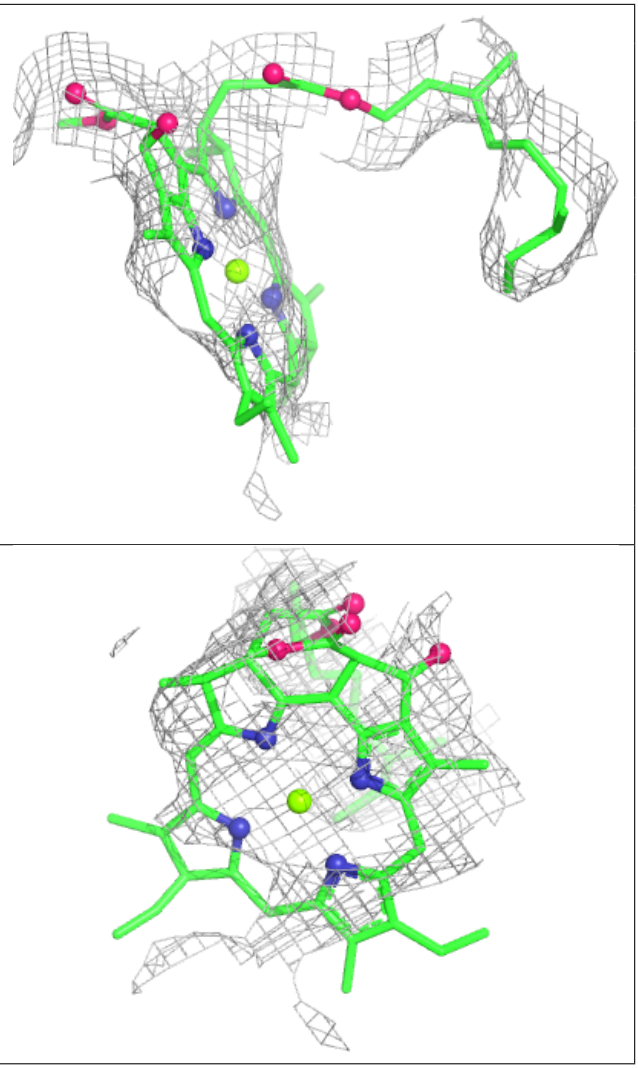






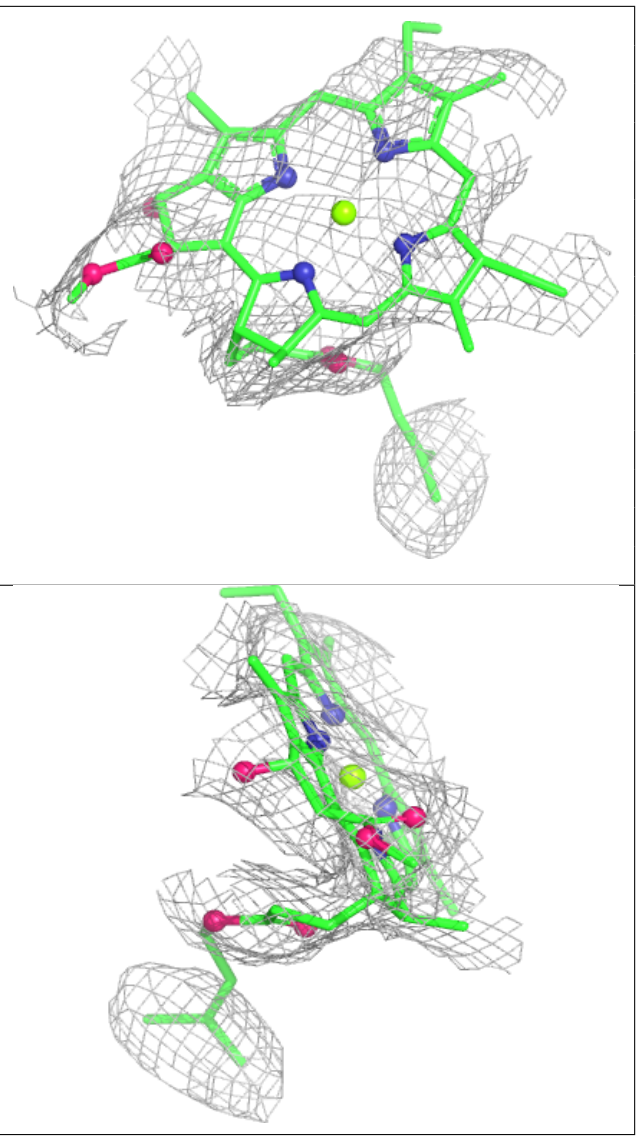
Electron density around CLA B 1216:

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



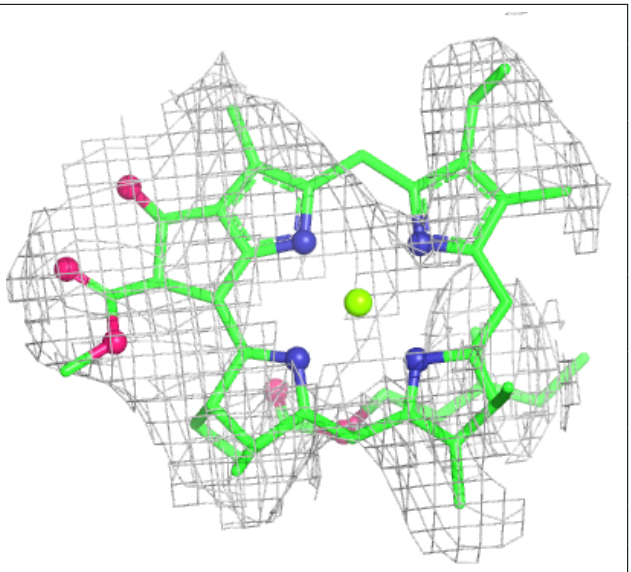
Electron density around CLA B 1217:

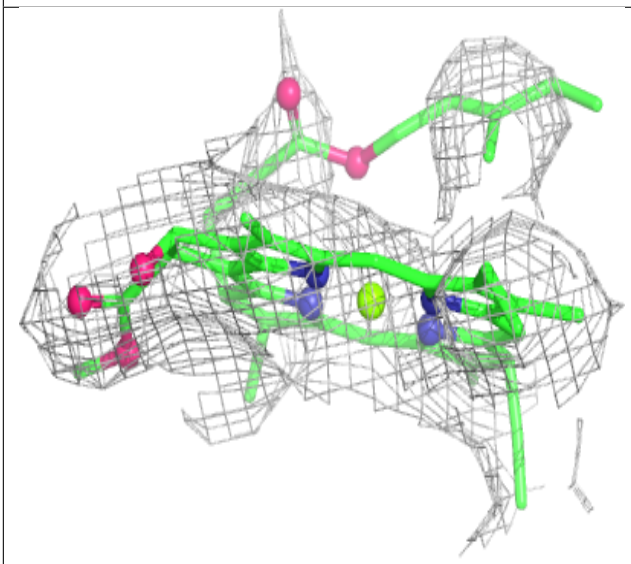
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)



Electron density around CLA B 1219:

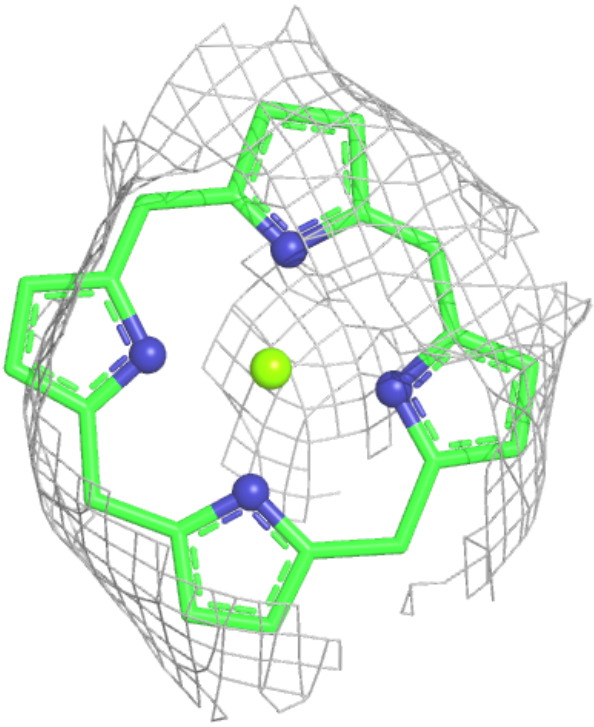
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

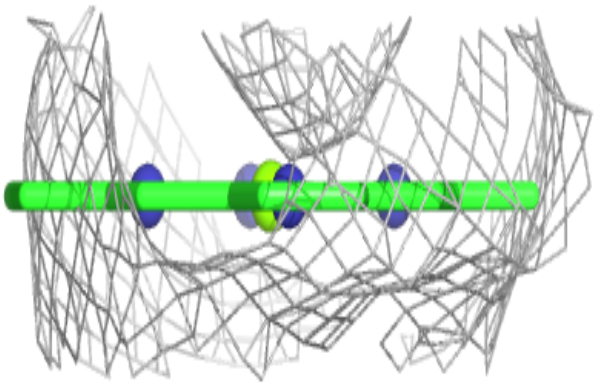


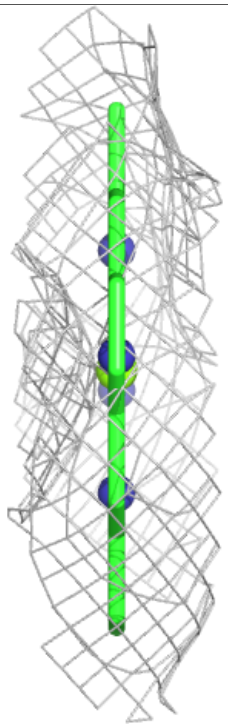


Electron density around CLA 4 4013:

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

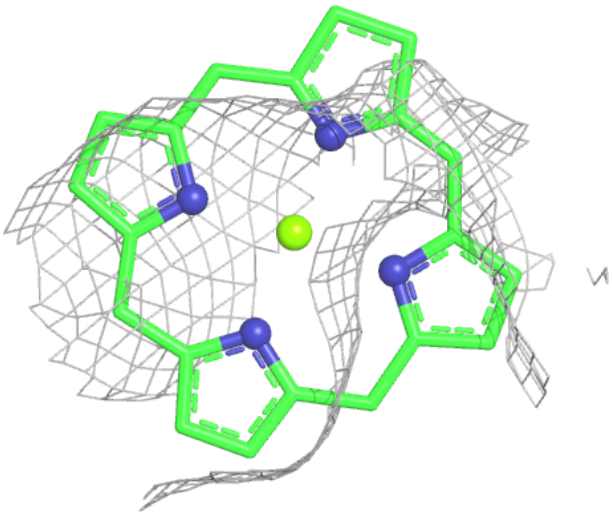


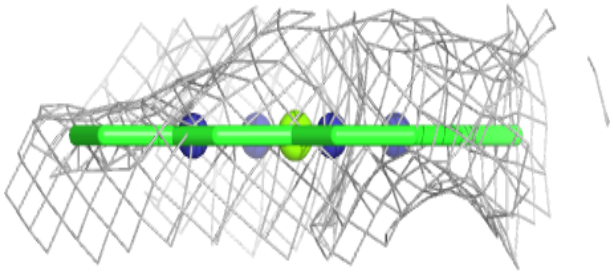


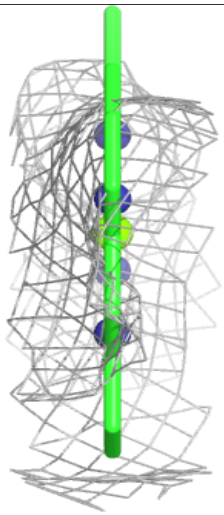


Electron density around CLA 4 4010:

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

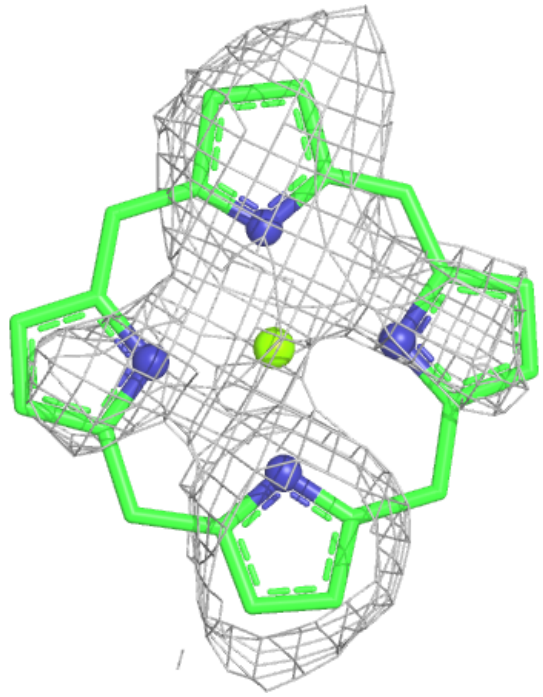


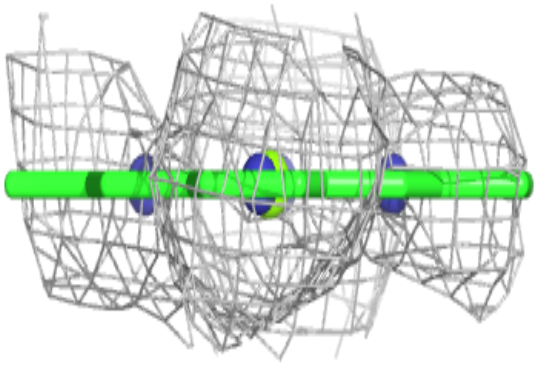


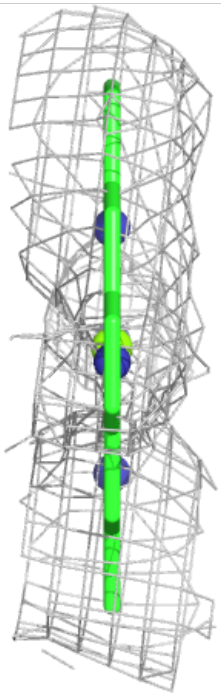


Electron density around CLA 4 4011:

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

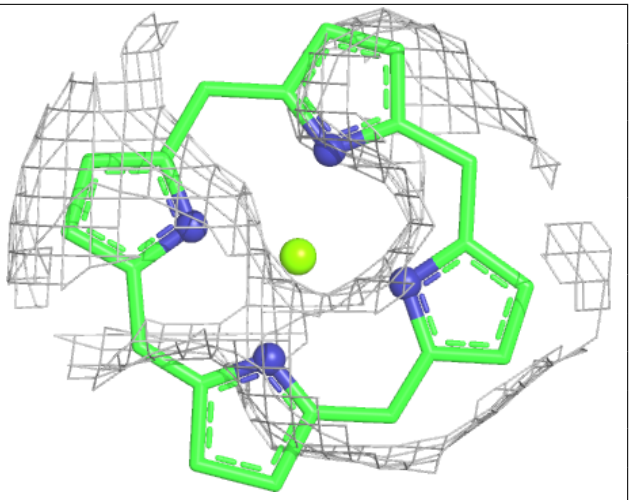


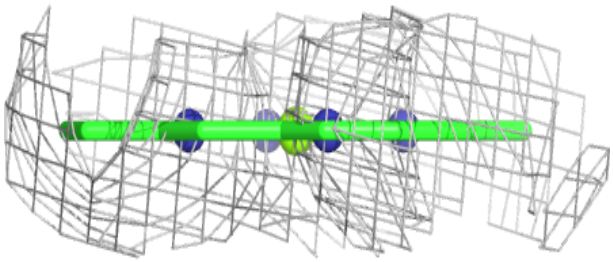


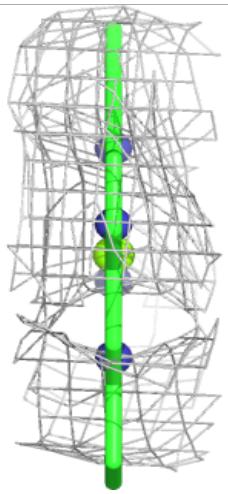


Electron density around CLA 4 4012:

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

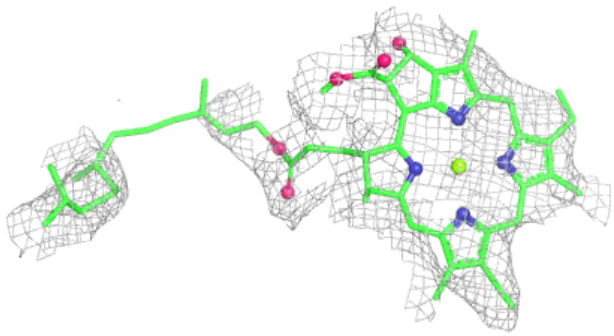


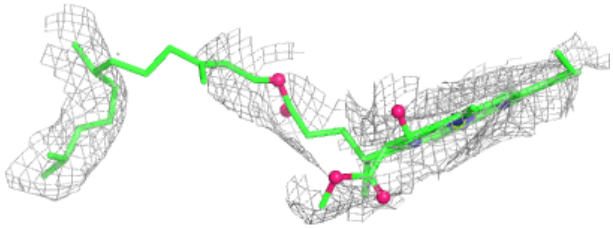




Electron density around CLA B 1220:

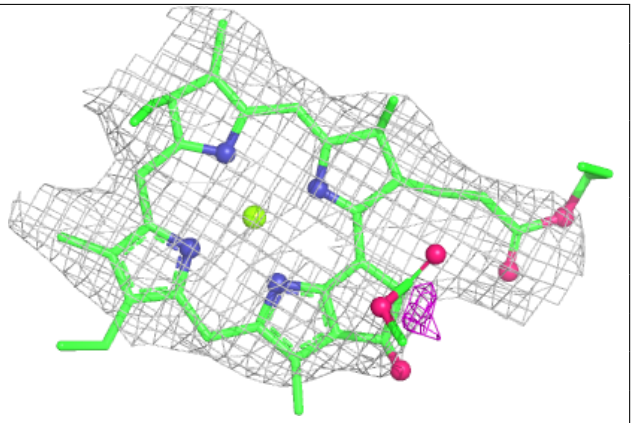
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

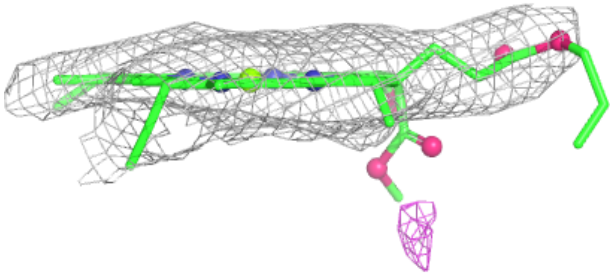


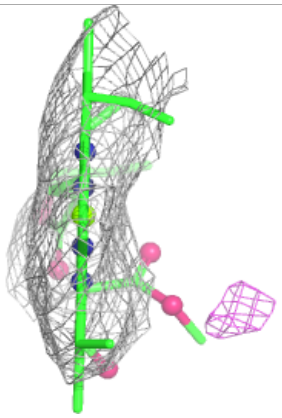


Electron density around CLA B 1221:

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

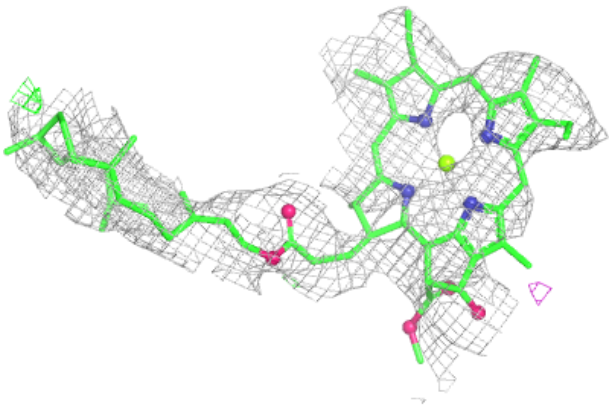


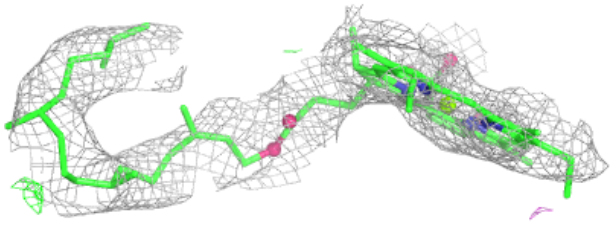


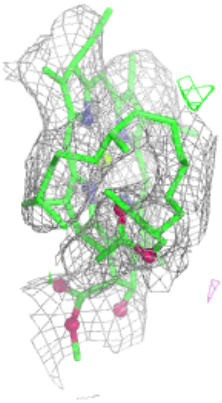


Electron density around CLA B 1222:

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

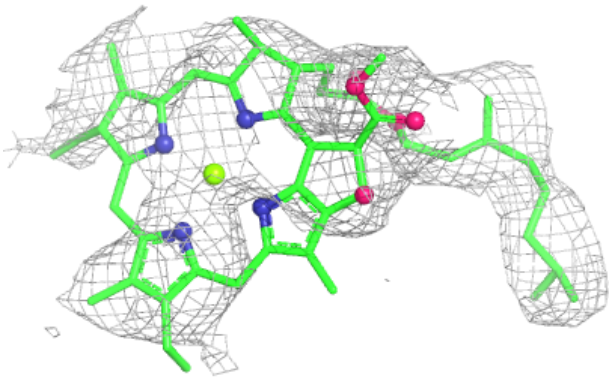


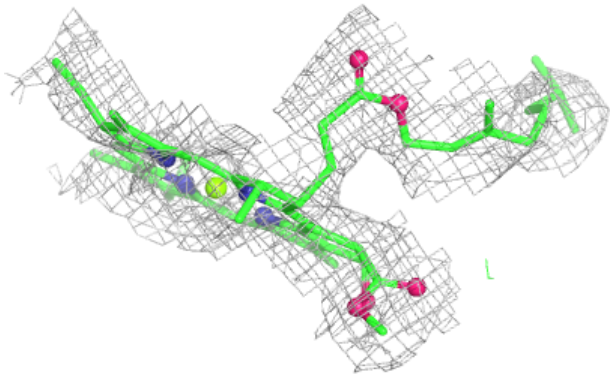


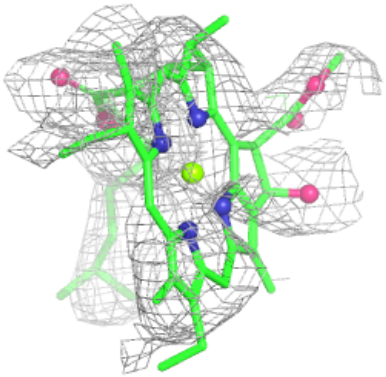


Electron density around CLA B 1228:

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

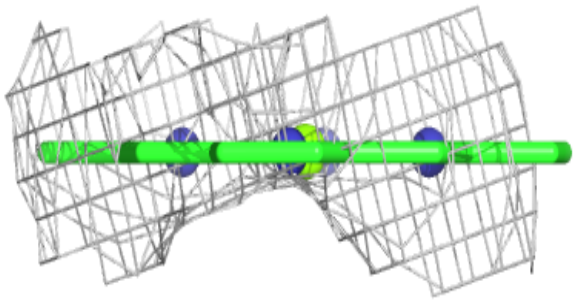


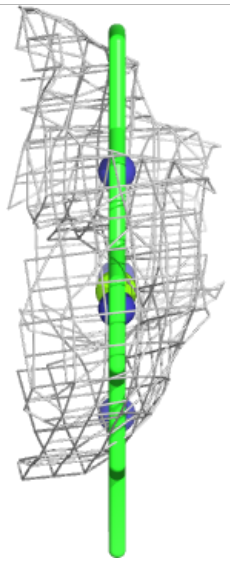




Electron density around CLA 4 4008:

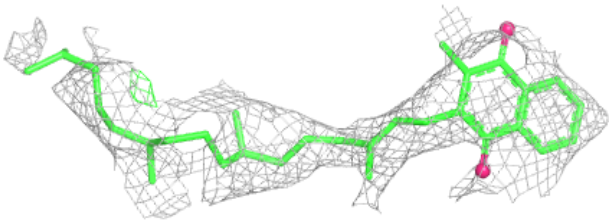
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

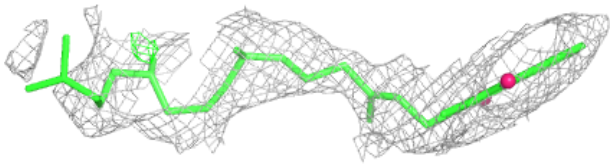


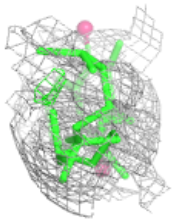


Electron density around PQN A 5001:

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

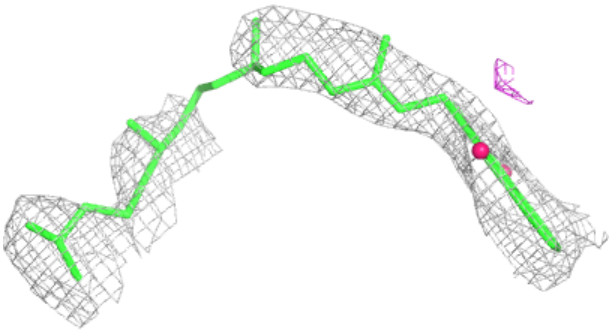


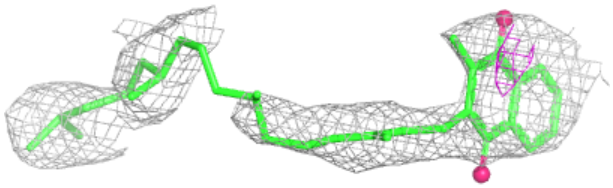




Electron density around PQN B 5002:

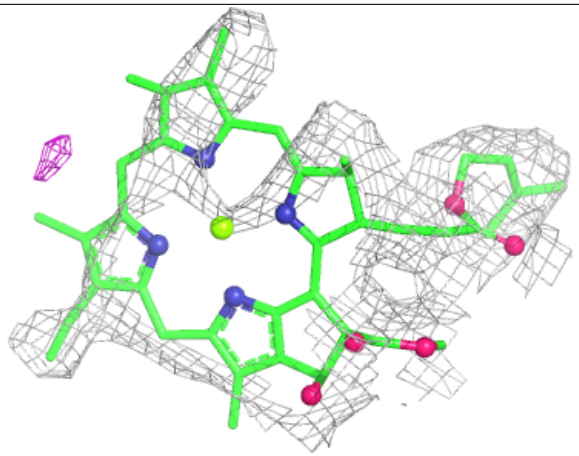
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

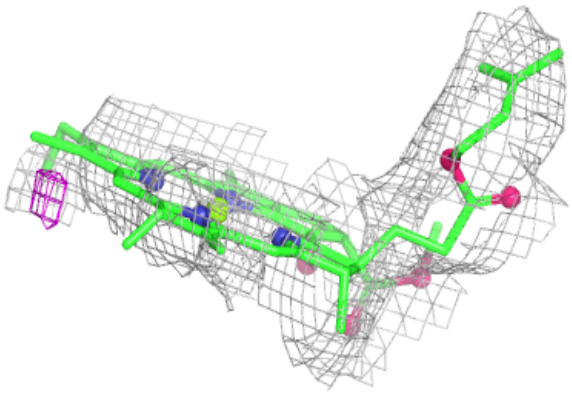


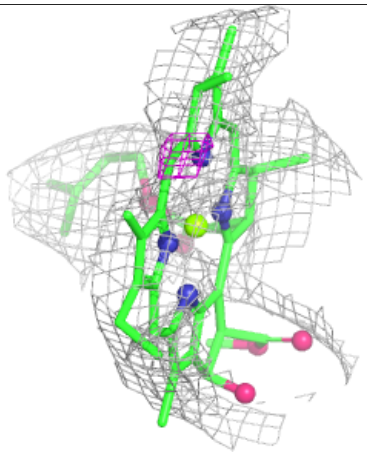


Electron density around CLA B 1229:

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

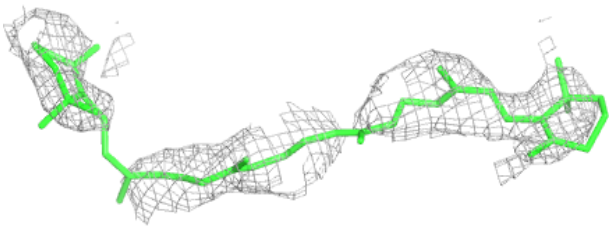


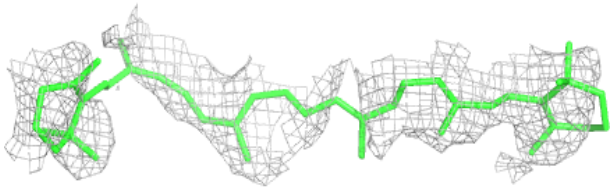


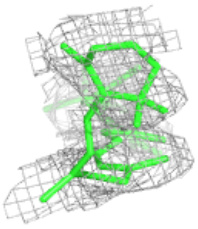


Electron density around BCR B 6017:

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

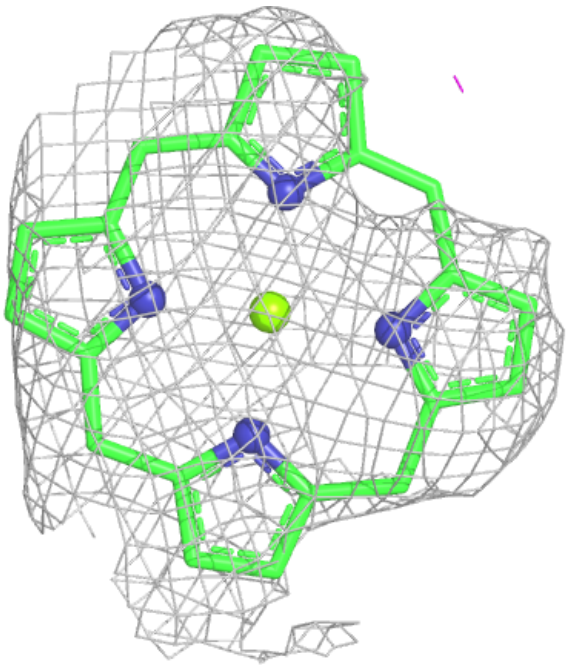


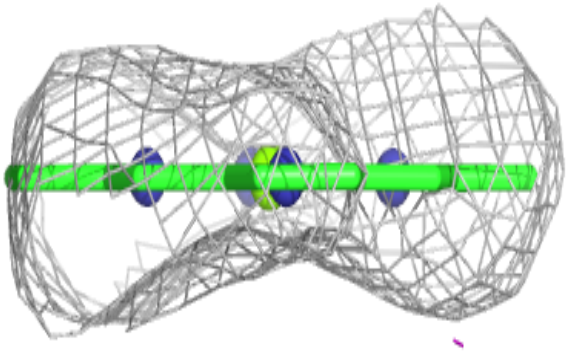


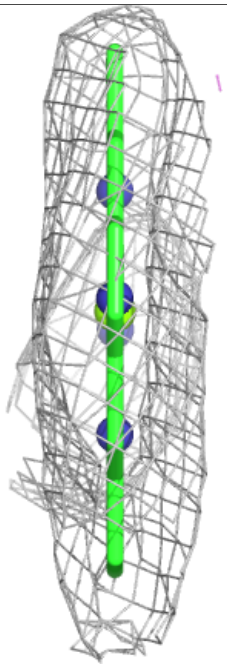


Electron density around CLA A 1117:

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

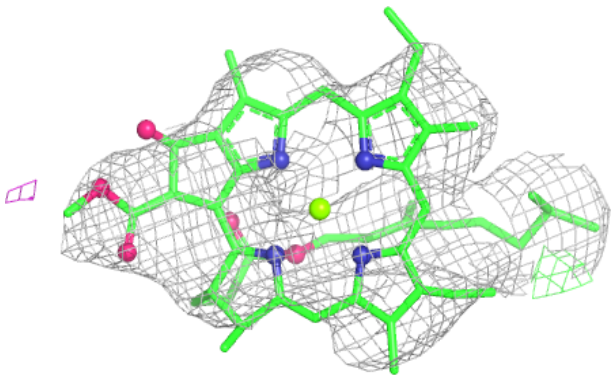


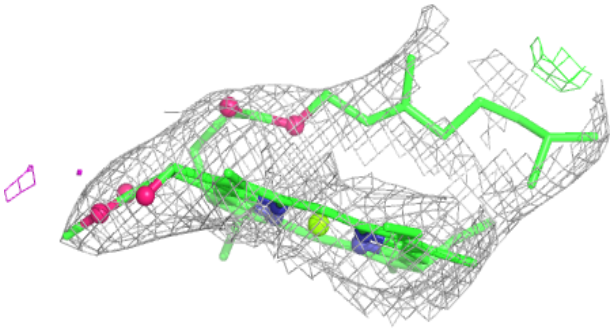


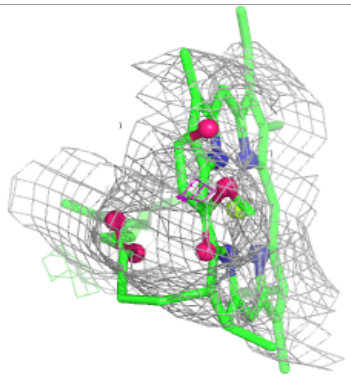


Electron density around CLA B 1235:

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

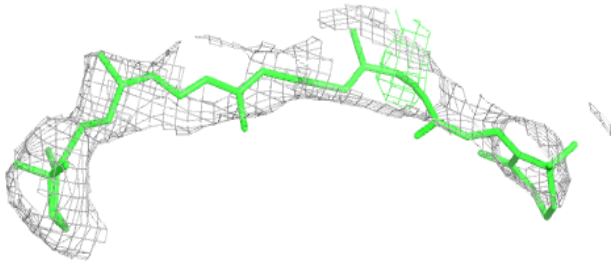






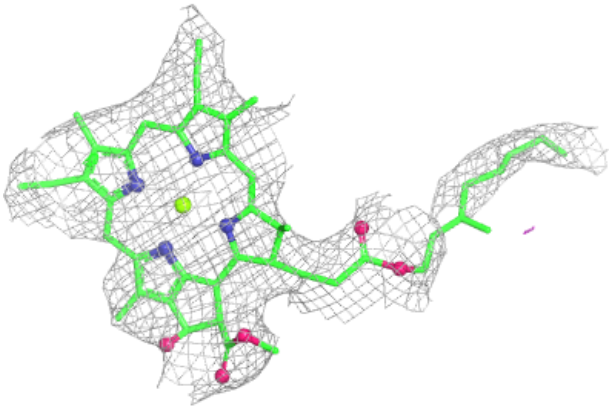
Electron density around BCR L 6020:

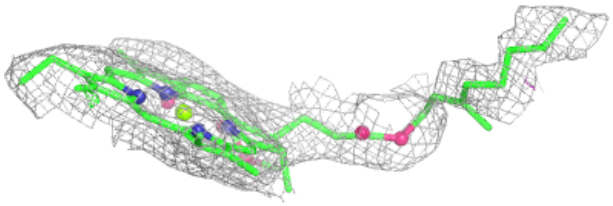
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

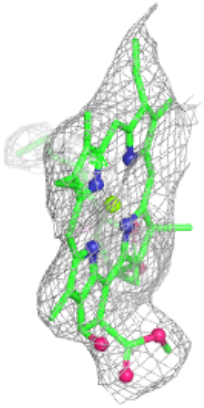


Electron density around CLA B 9022:

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

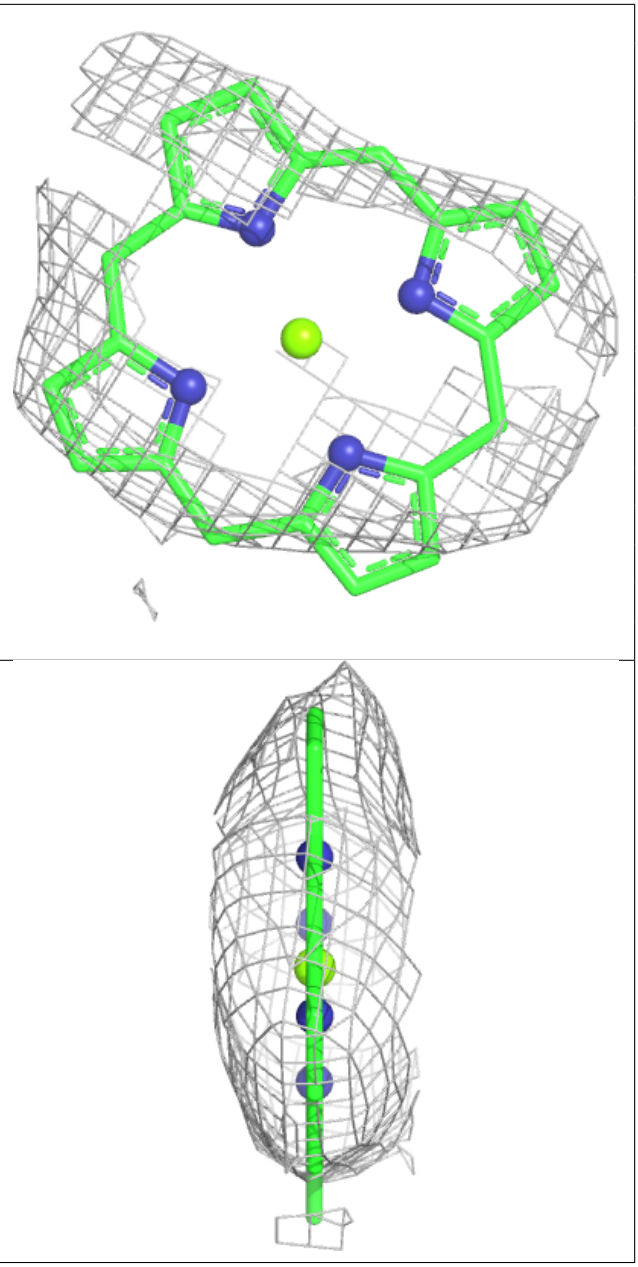






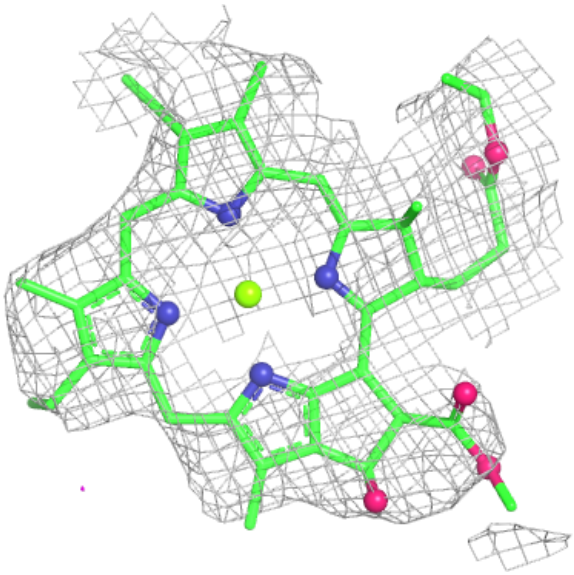
Electron density around CLA 2 2008:

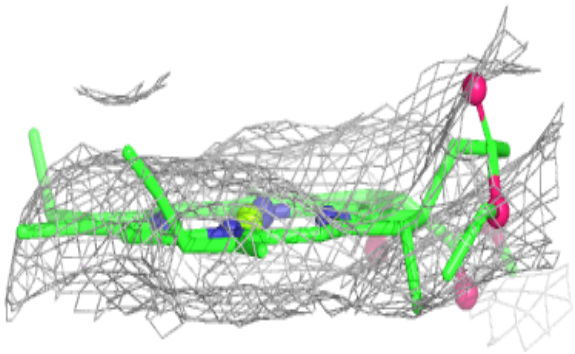
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

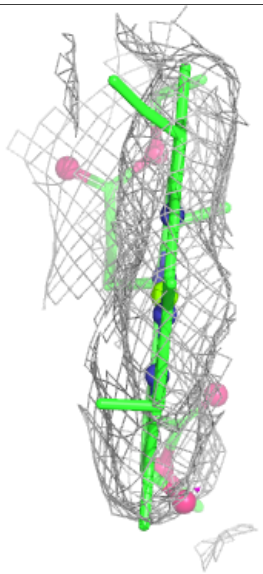


Electron density around CLA B 9023:

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

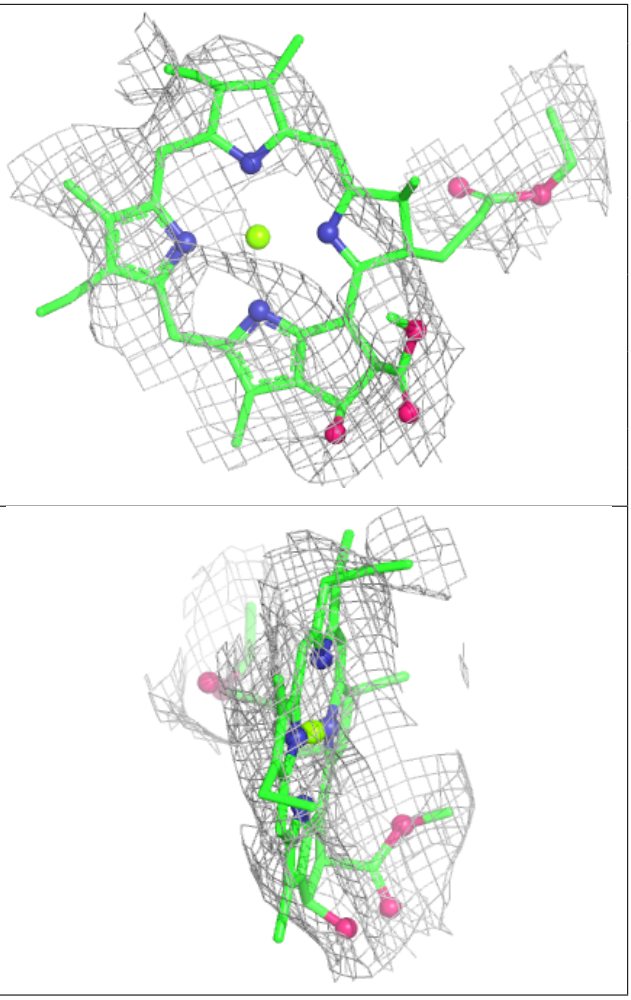






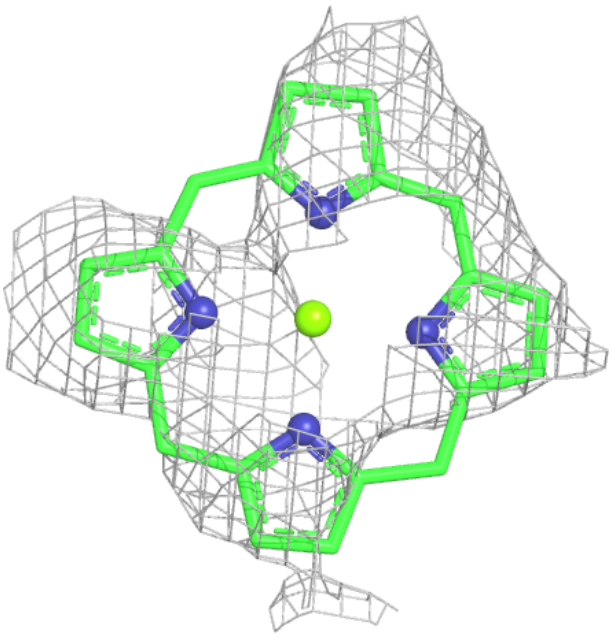
Electron density around CLA A 1103:

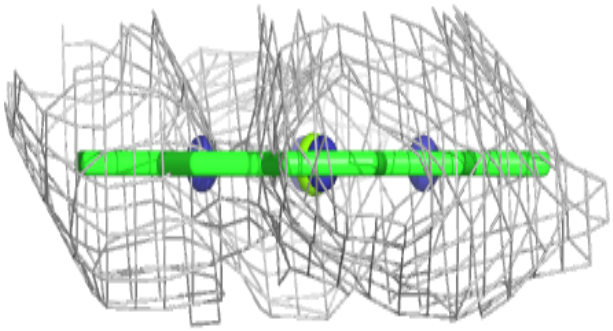
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

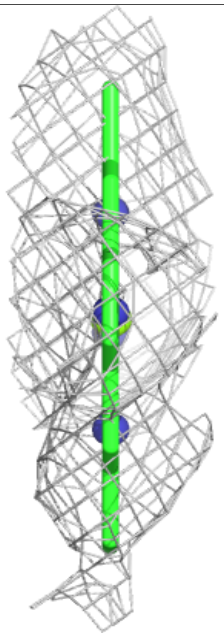


Electron density around CLA B 1223:

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

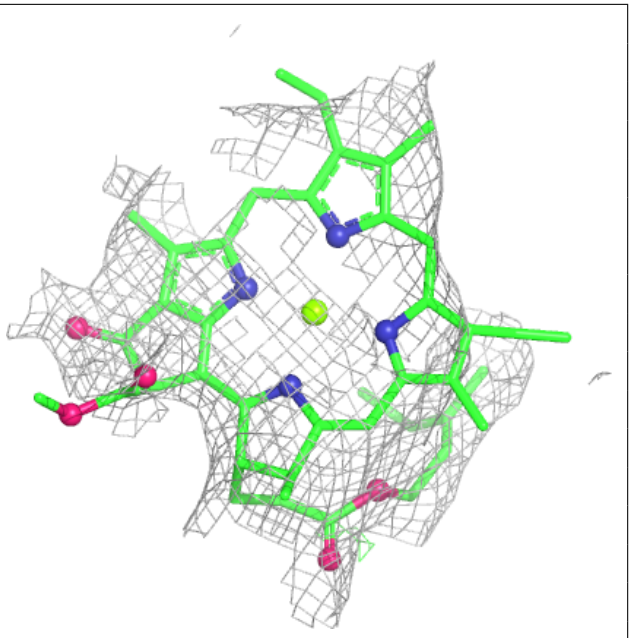


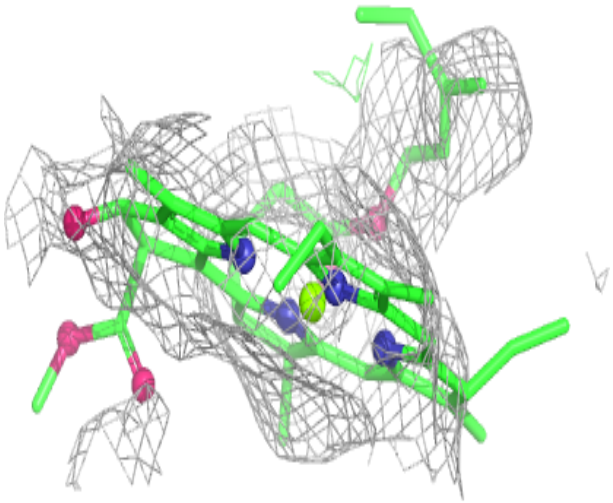


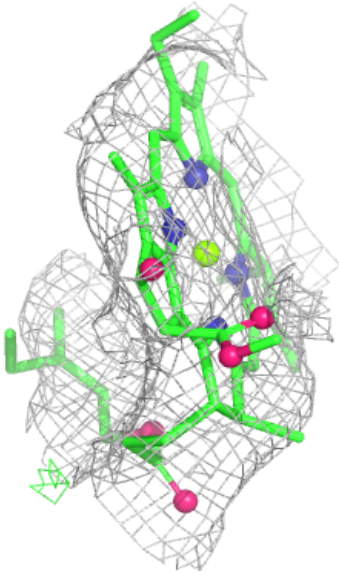


Electron density around CLA B 1224:

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

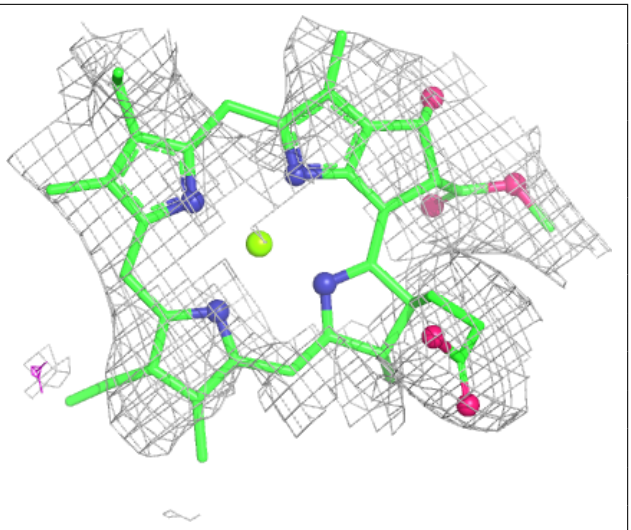


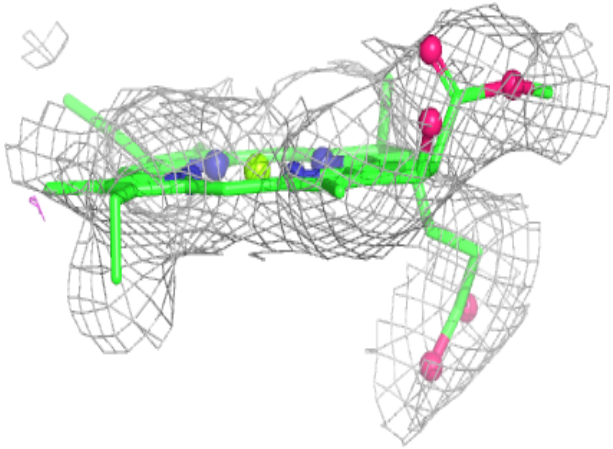


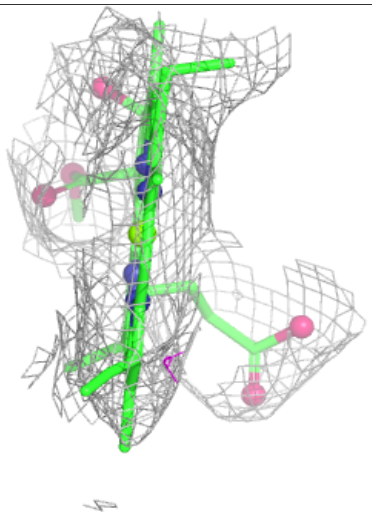


Electron density around CLA B 1225:

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

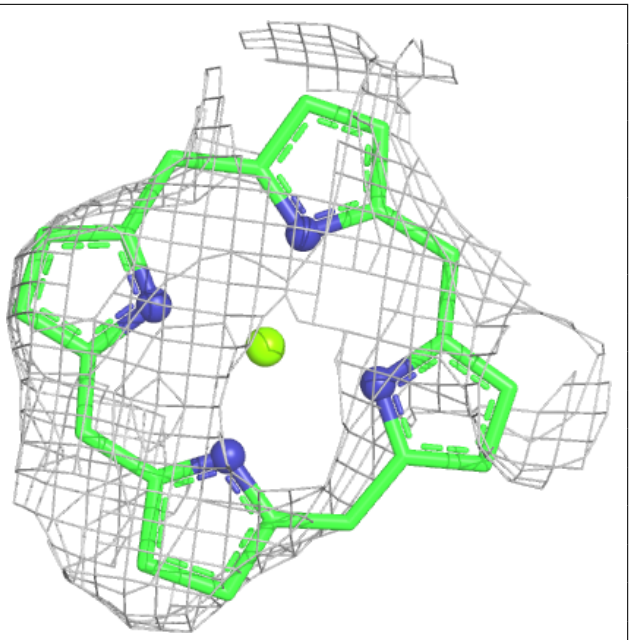


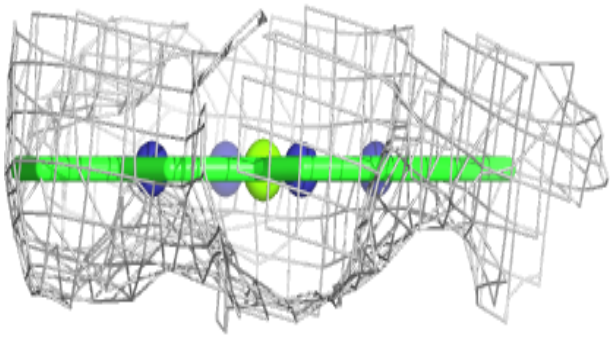


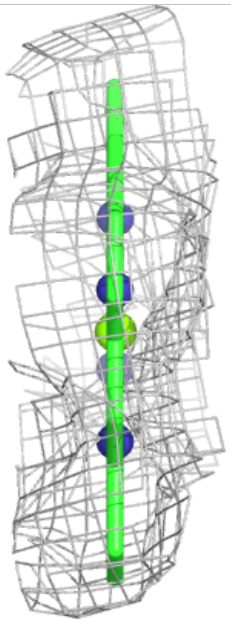


Electron density around CLA B 1226:

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

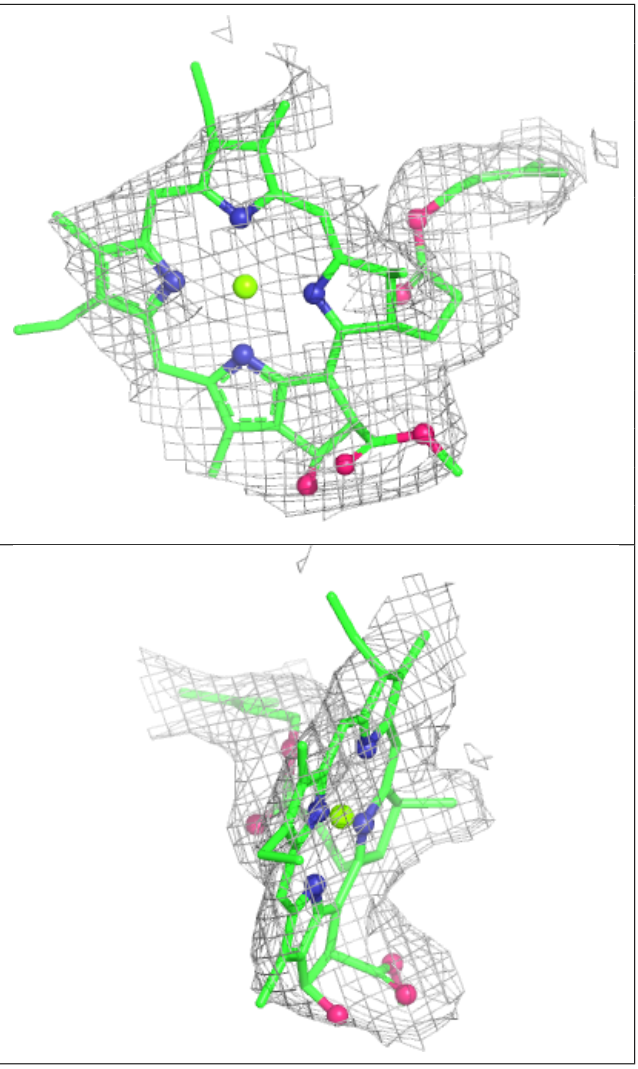






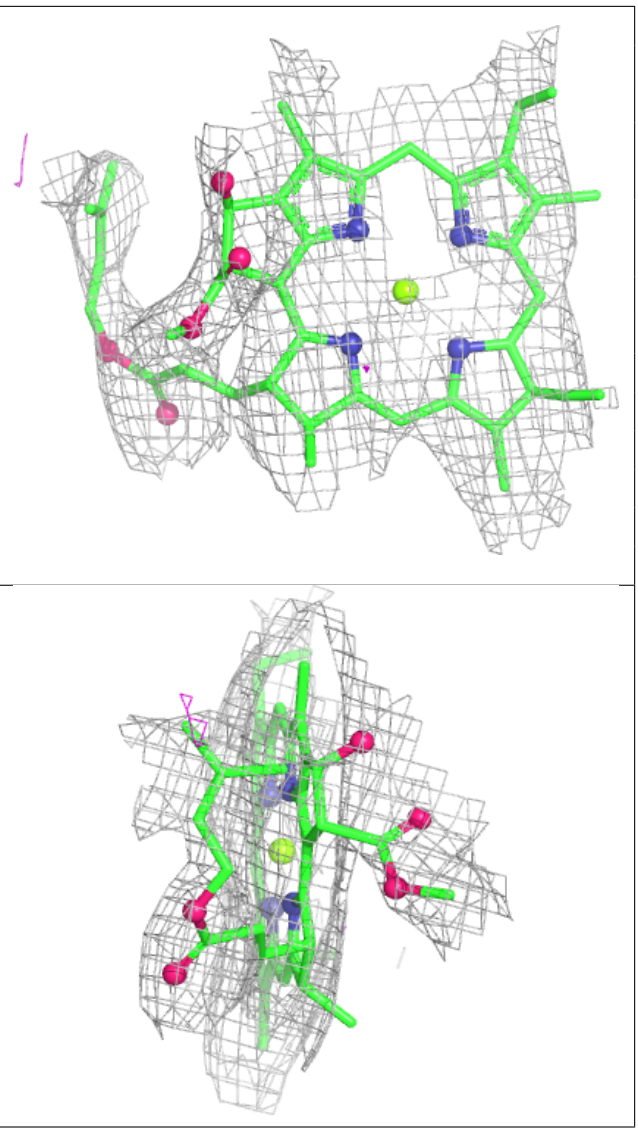
Electron density around CLA B 1227:

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



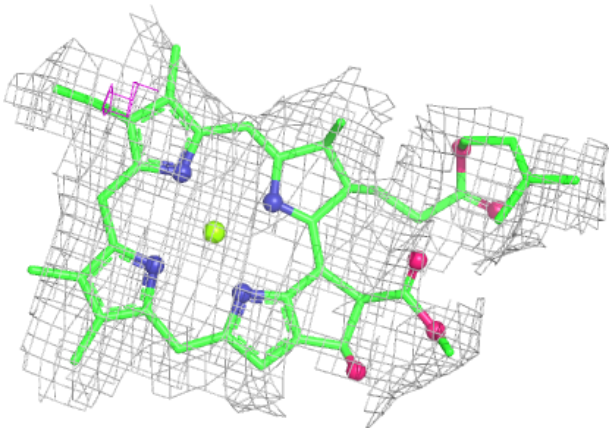
Electron density around CLA B 1202:

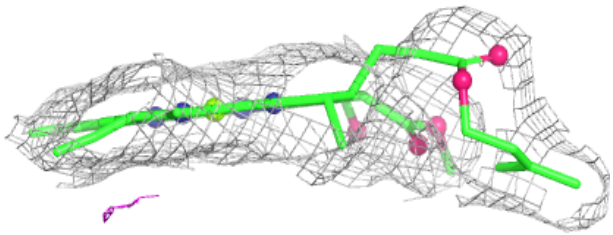
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

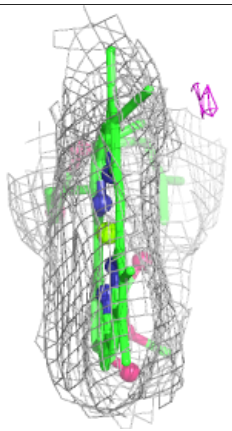


Electron density around CLA B 1203:

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

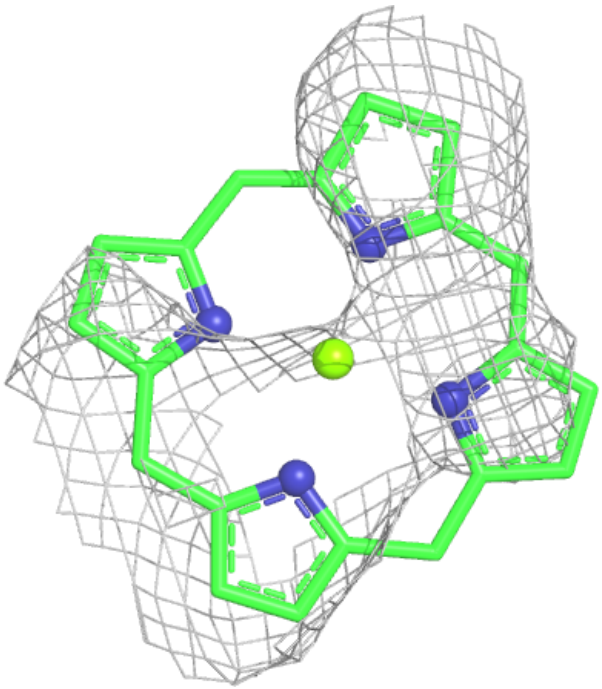


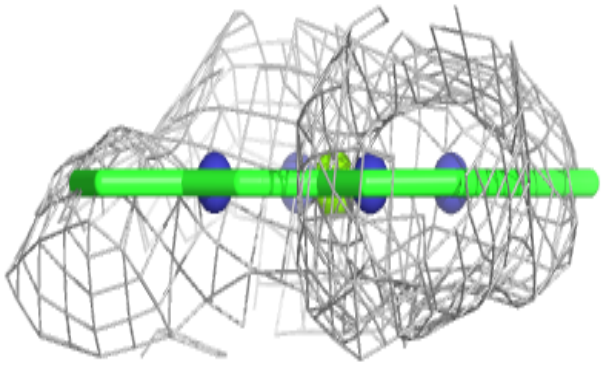


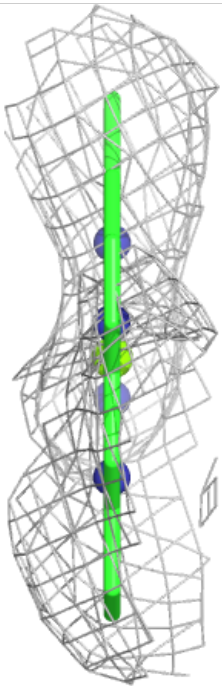


Electron density around CLA B 1230:

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

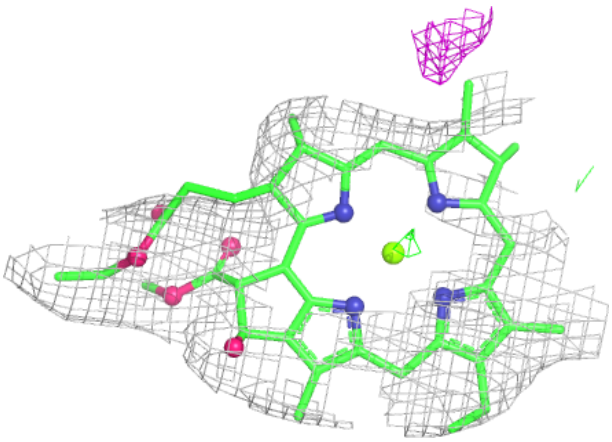


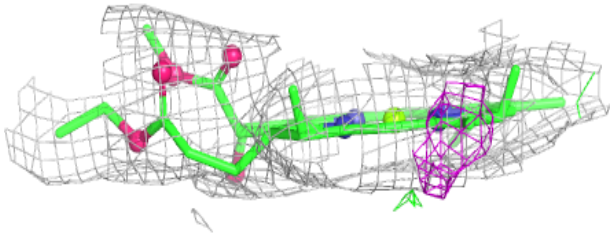


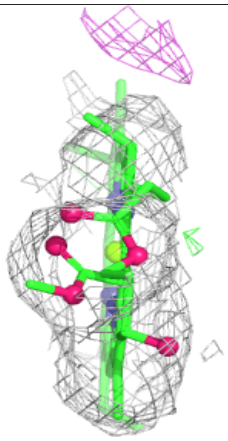


Electron density around CLA L 1503:

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

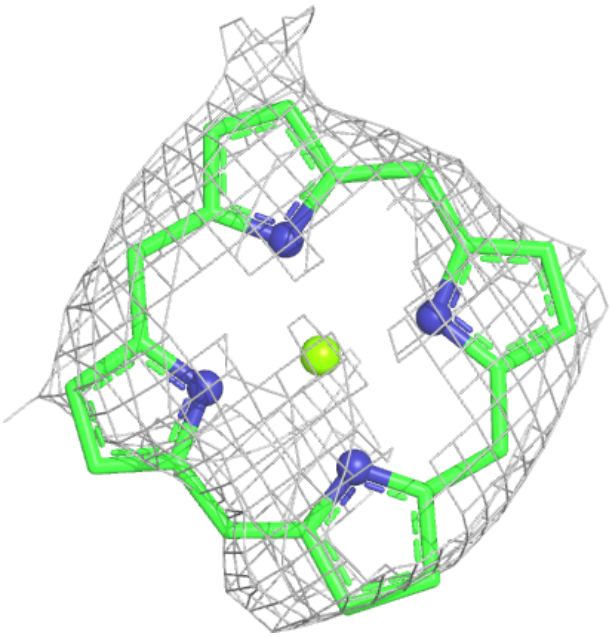


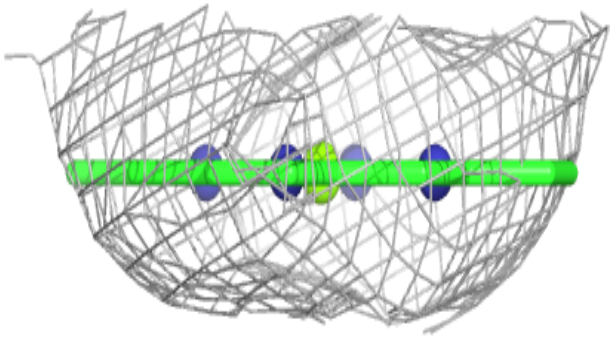


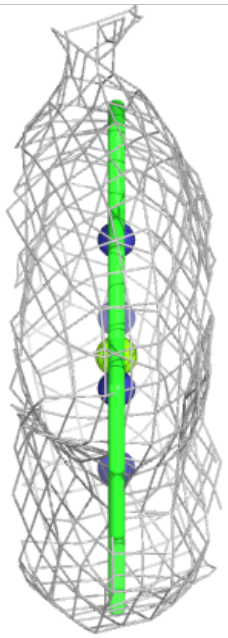


Electron density around CLA 3 3007:

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

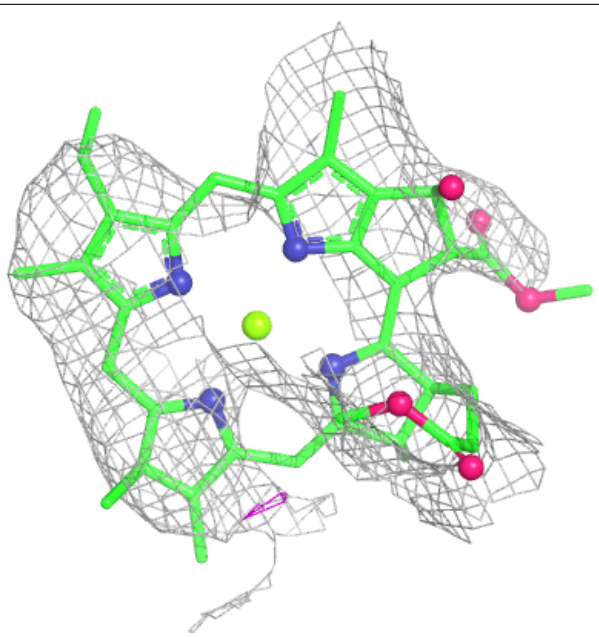


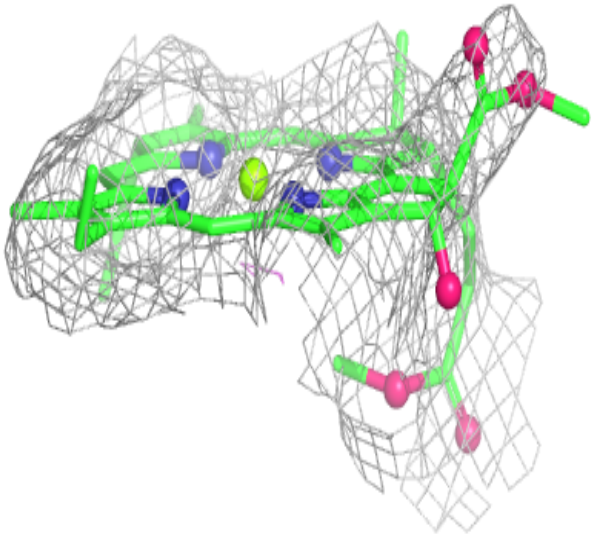


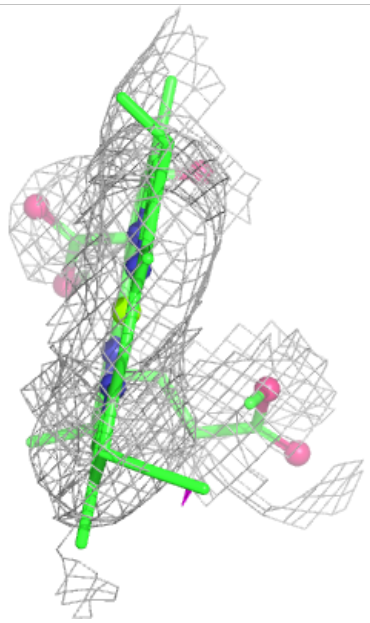


Electron density around CLA B 1231:

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

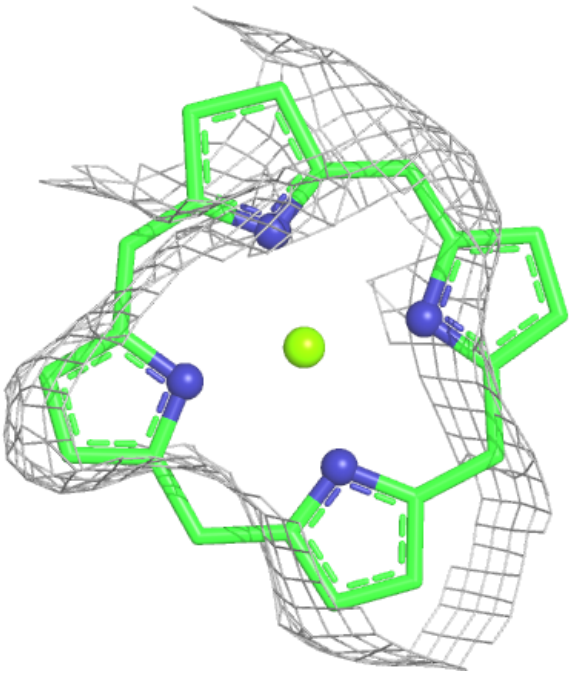


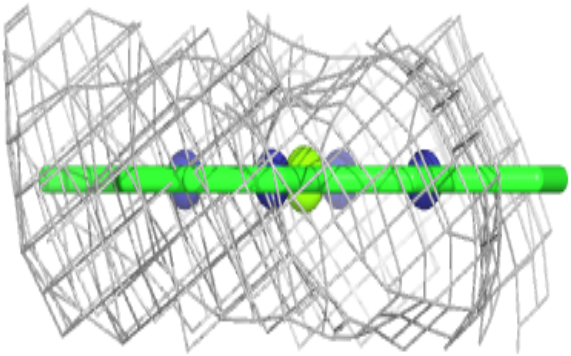


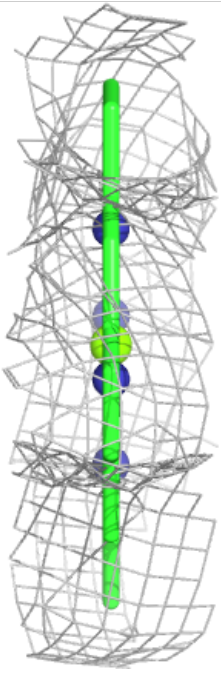


Electron density around CLA 1 1004:

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

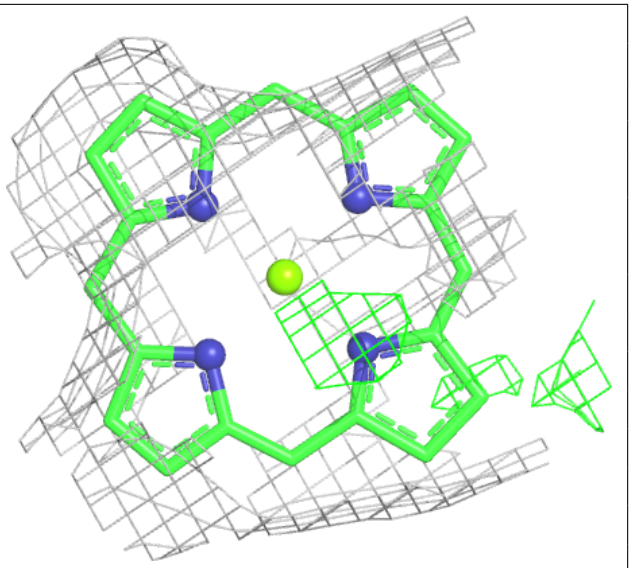


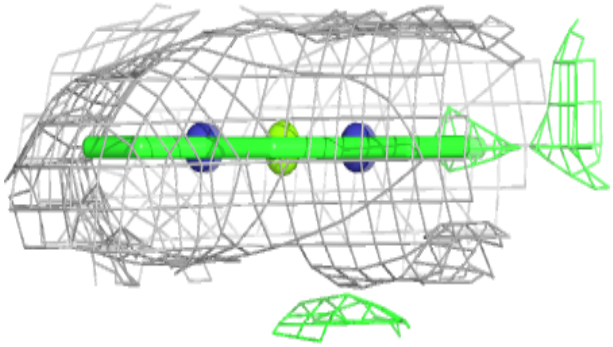


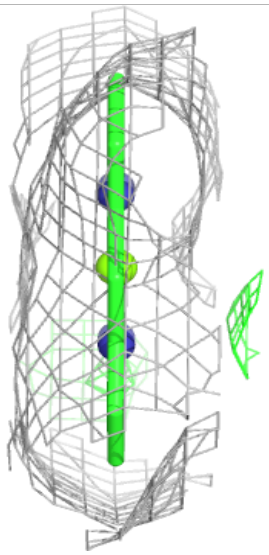


Electron density around CLA A 1132:

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

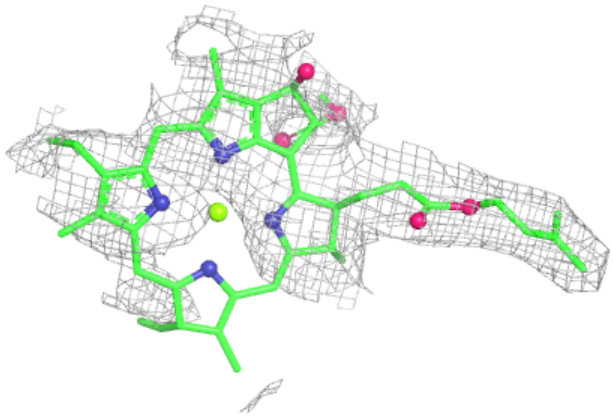


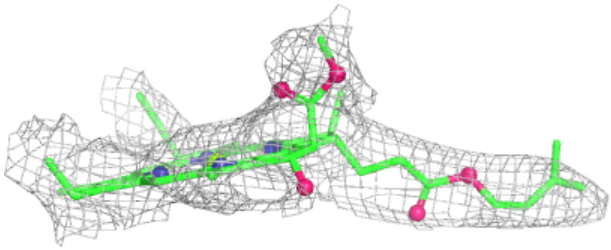


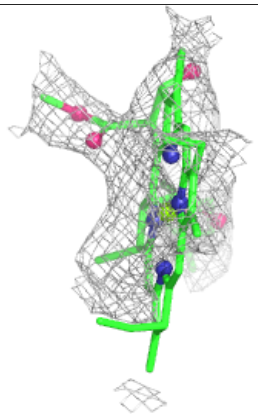


Electron density around CLA B 1234:

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

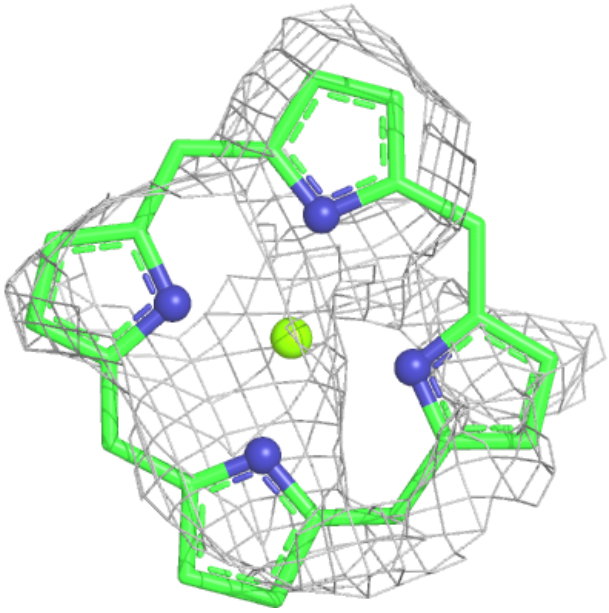


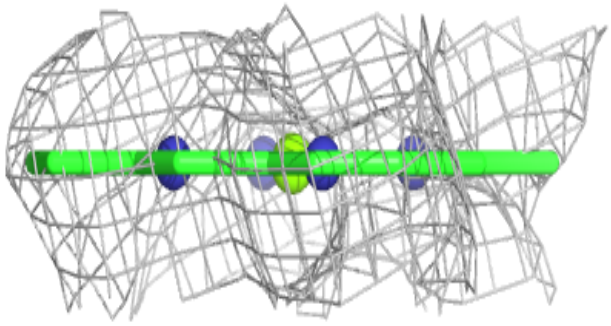


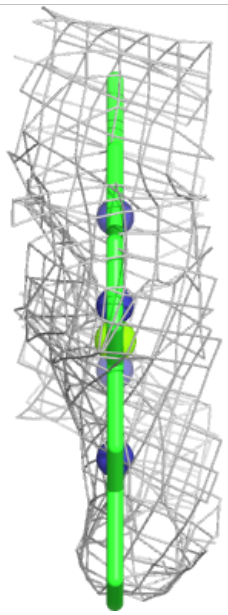


Electron density around CLA B 1206:

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

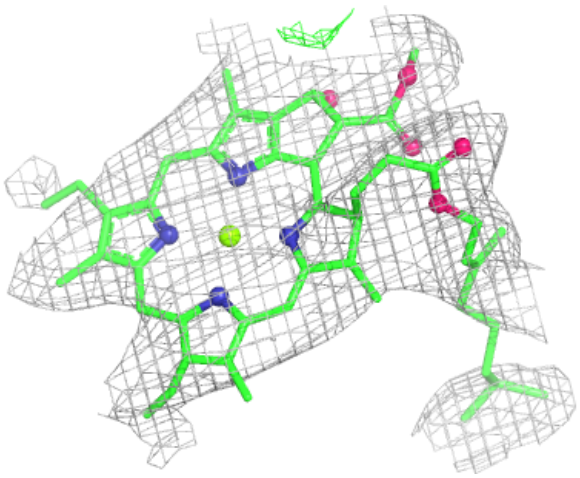


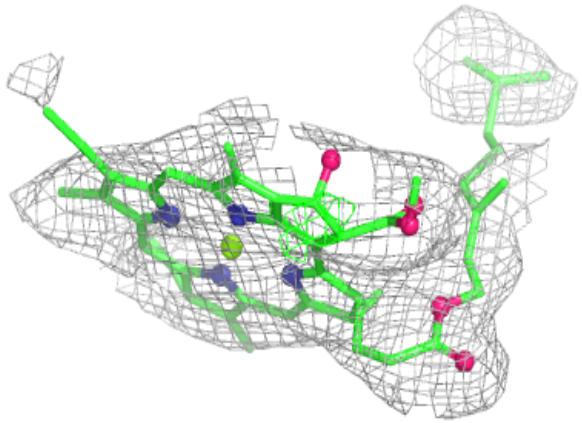


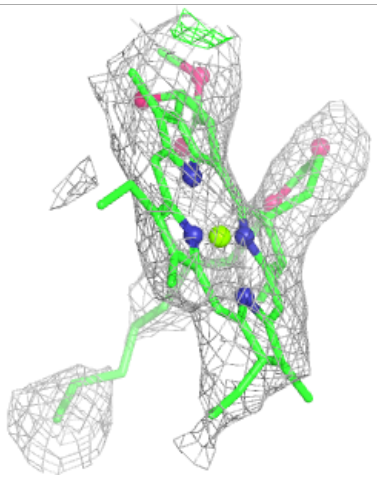


Electron density around CLA B 1207:

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

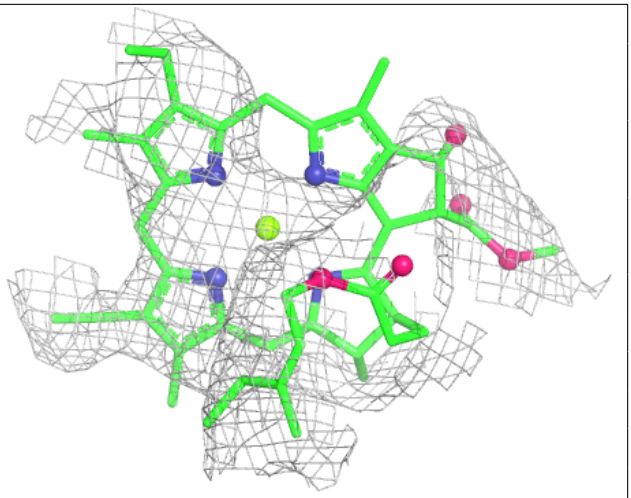


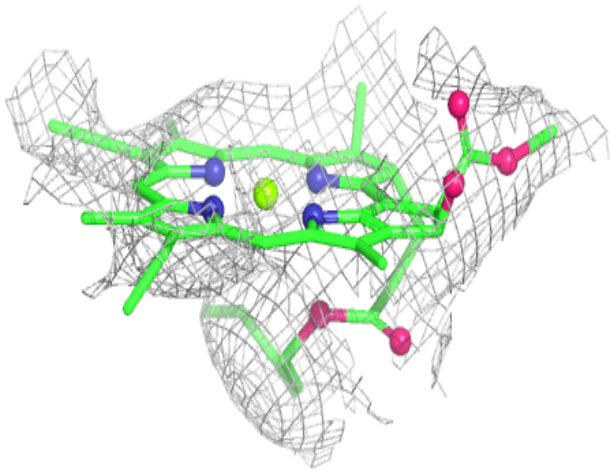


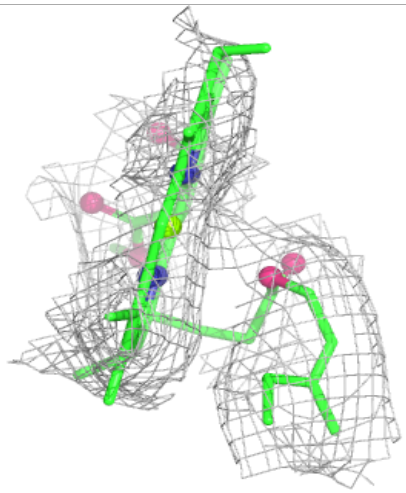


Electron density around CLA B 1237:

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

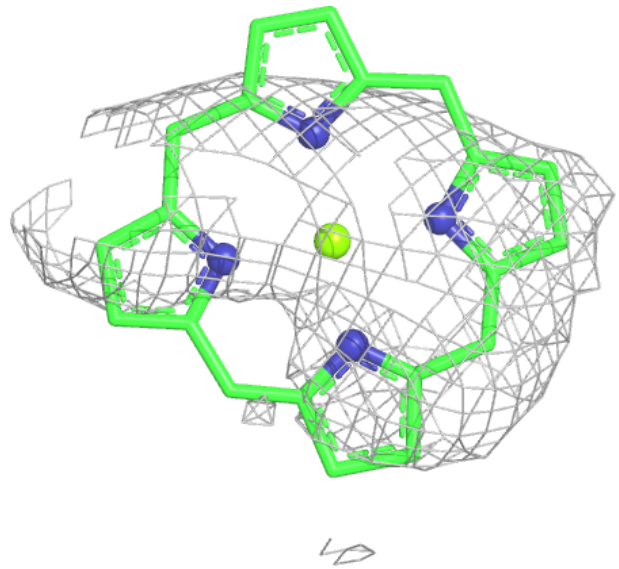


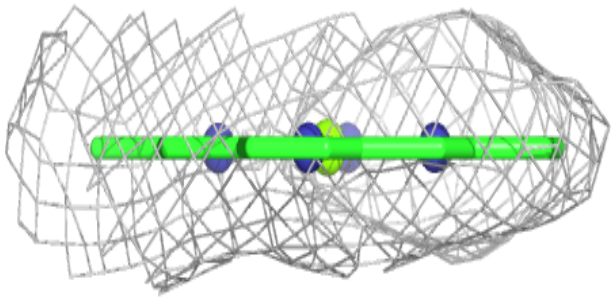


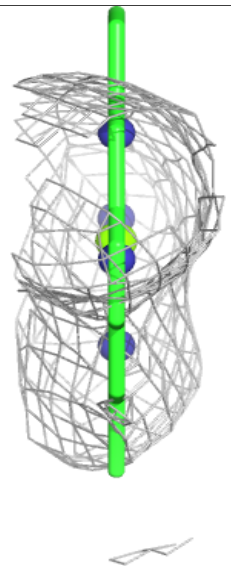


Electron density around CLA 1 1012:

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

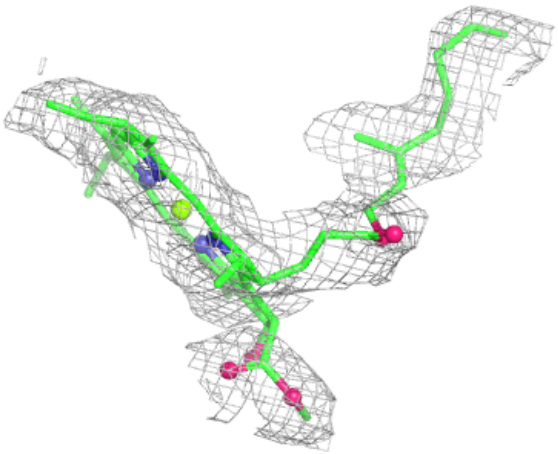


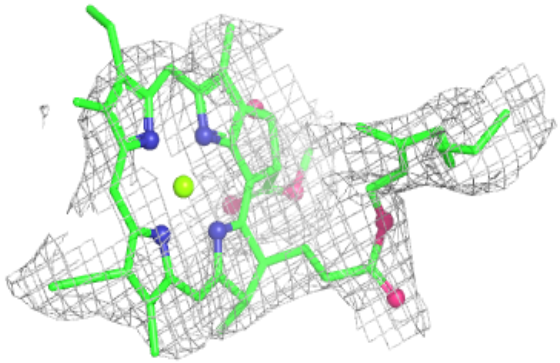


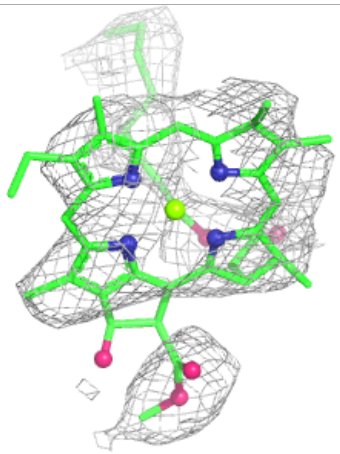


Electron density around CLA B 1238:

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

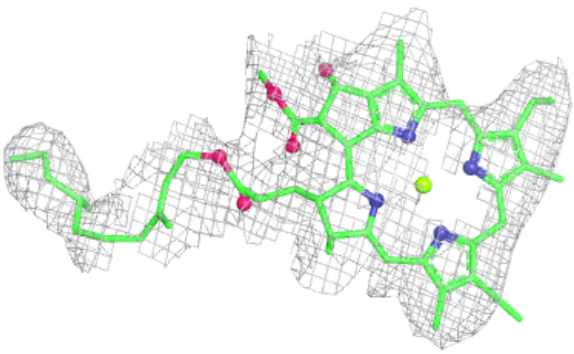


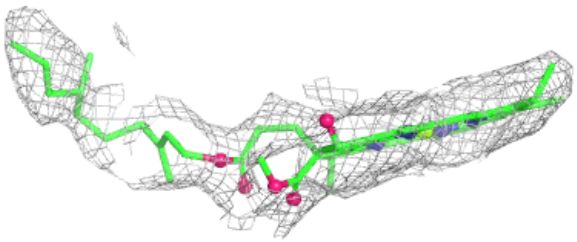


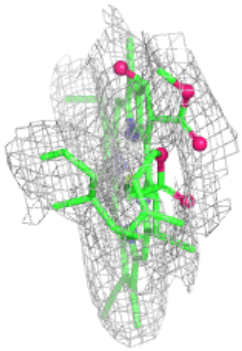


Electron density around CLA A 1107:

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

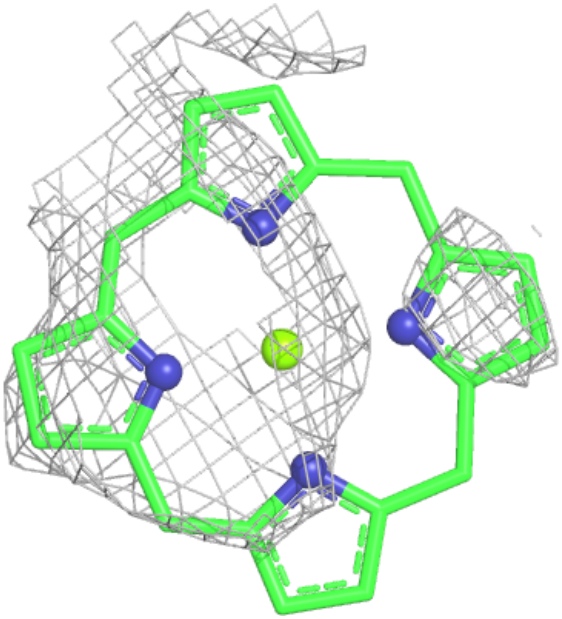


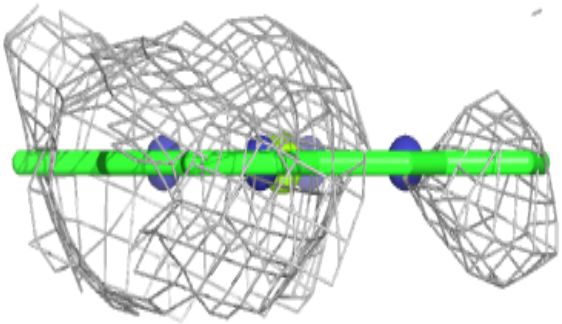


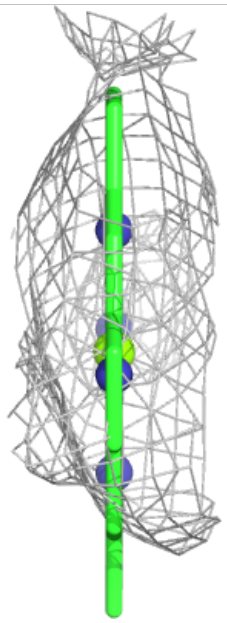


Electron density around CLA B 1241:

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

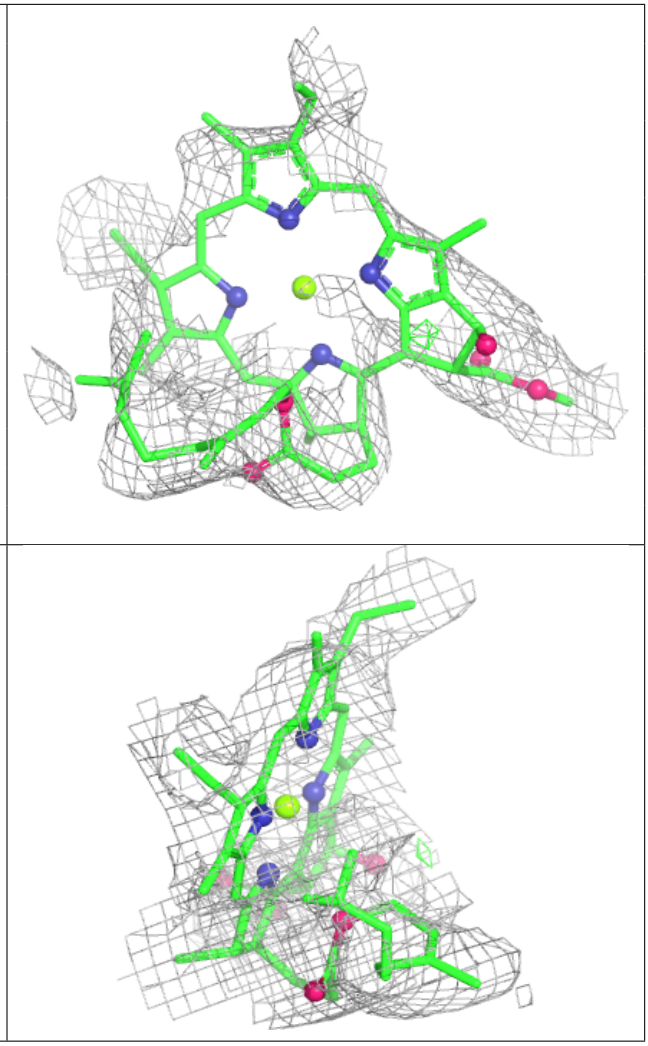






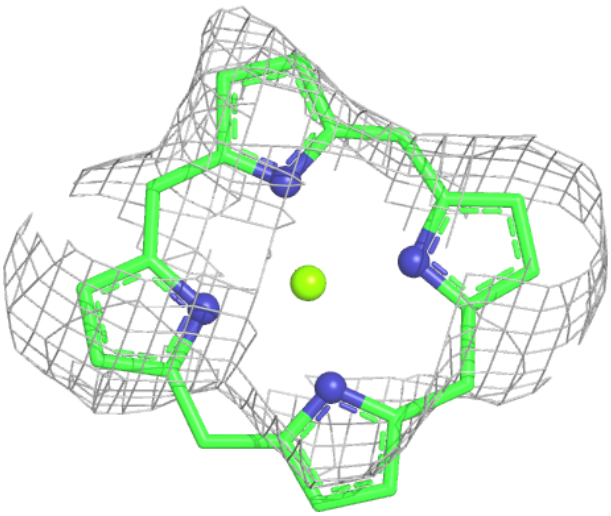
Electron density around CLA B 1209:

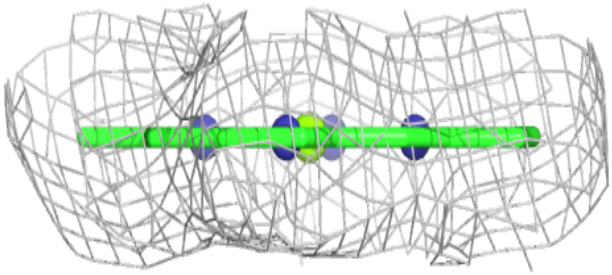
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

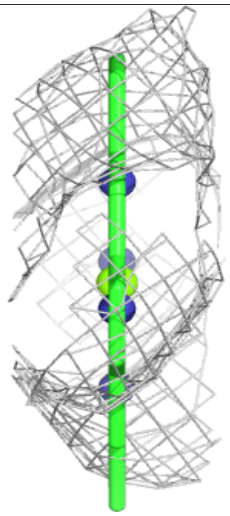


Electron density around CLA A 1101:

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

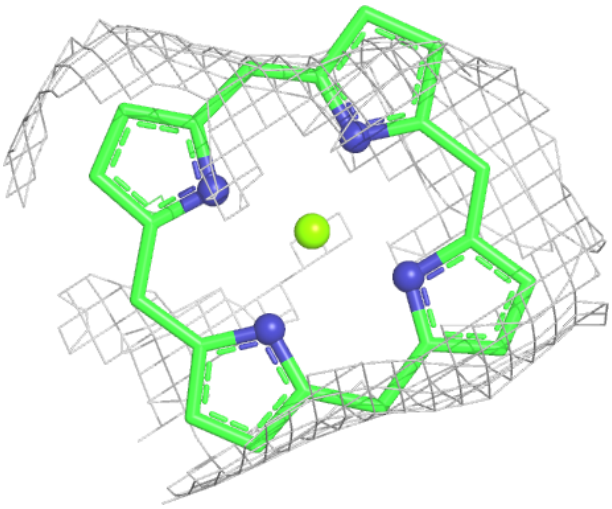


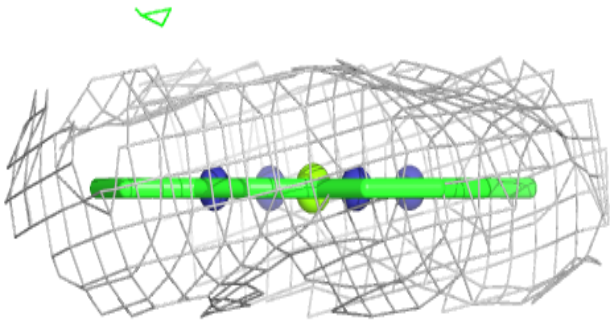


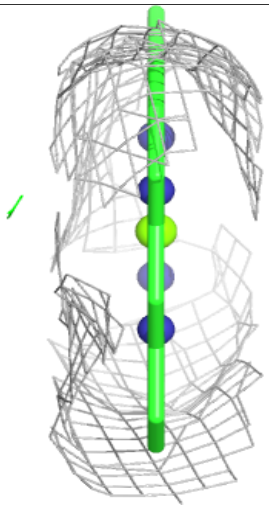


Electron density around CLA B 1211:

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

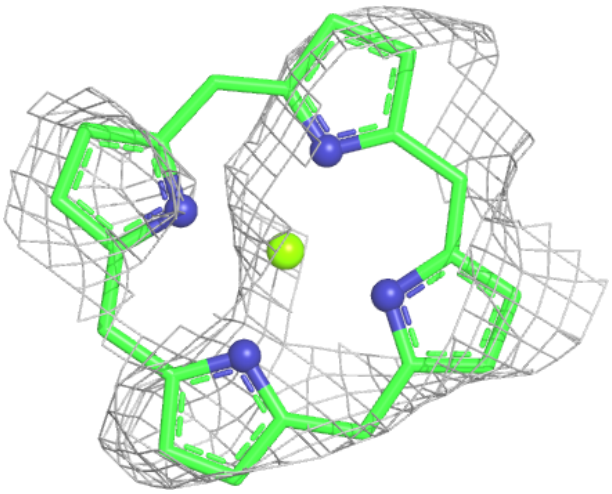


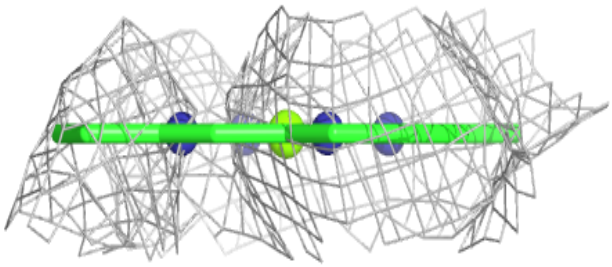


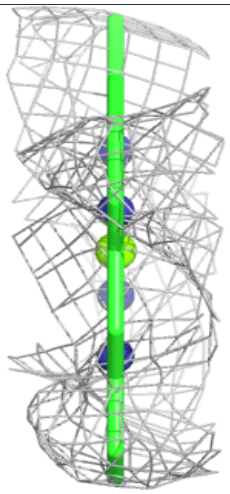


Electron density around CLA 2 2004:

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

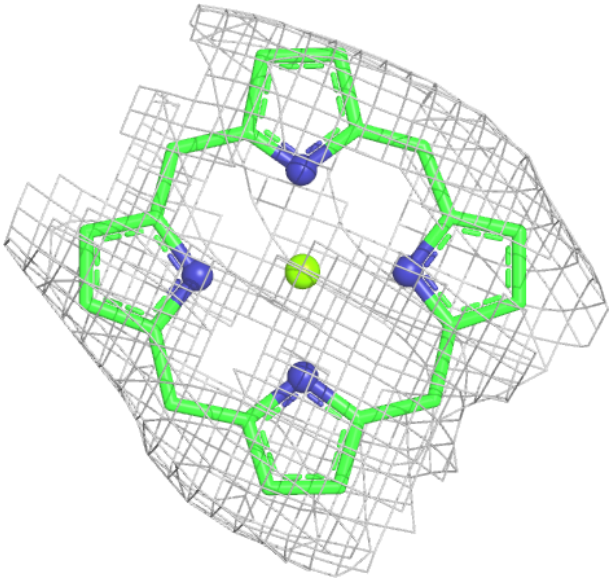


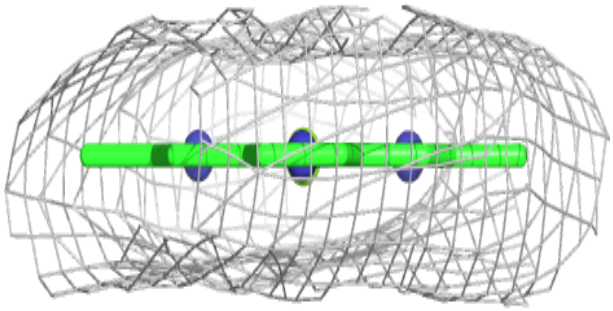


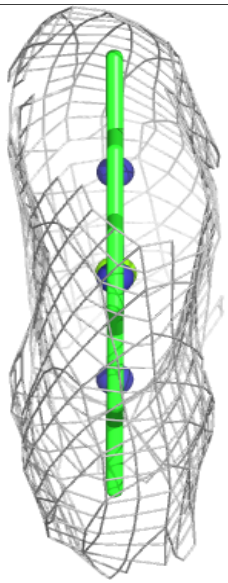


Electron density around CLA F 1240:

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

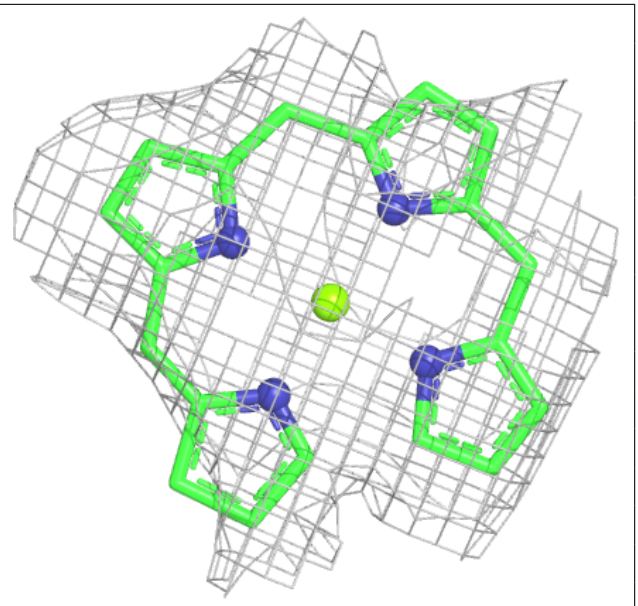


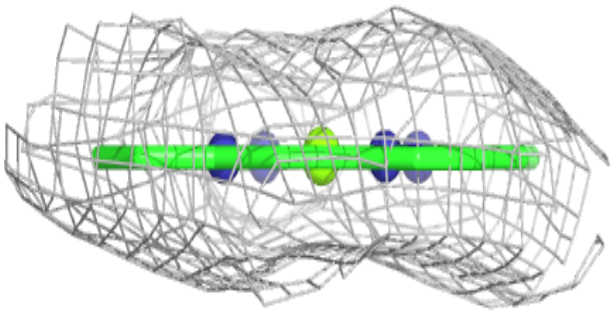


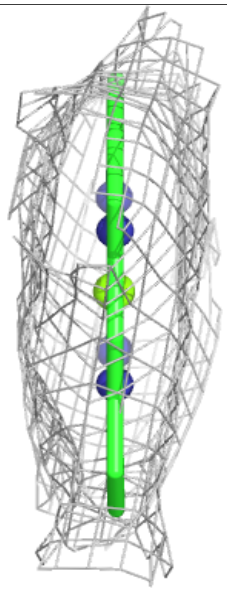


Electron density around CLA A 1109:

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

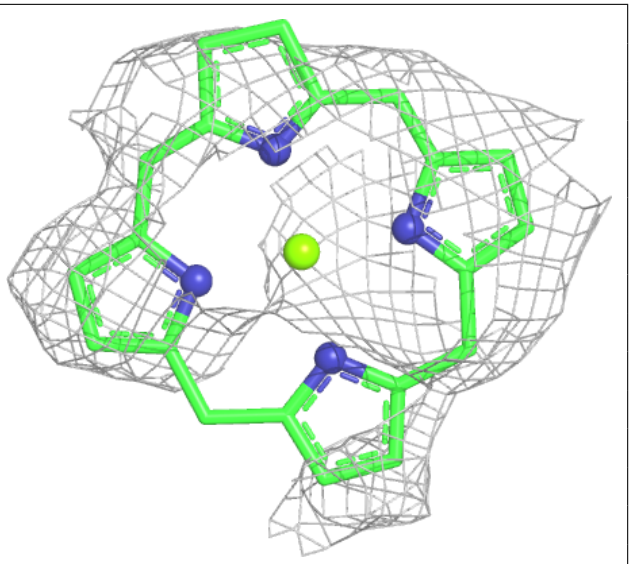


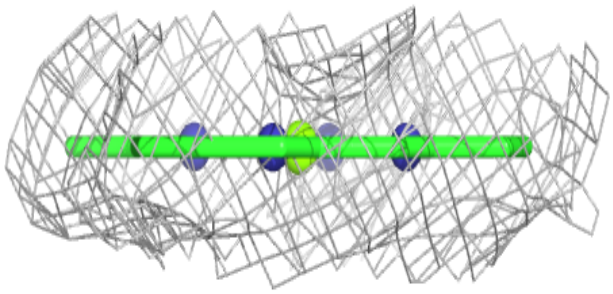


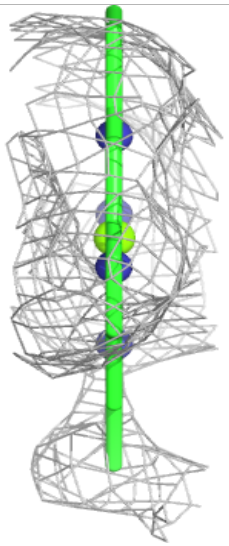


Electron density around CLA B 1213:

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

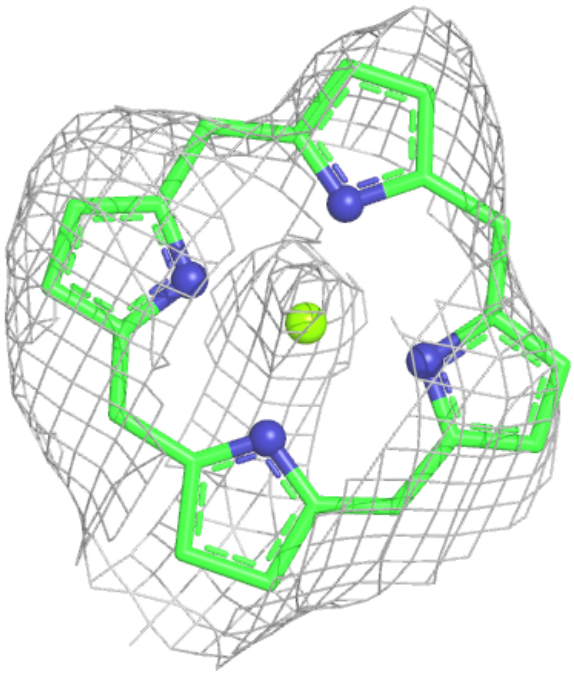


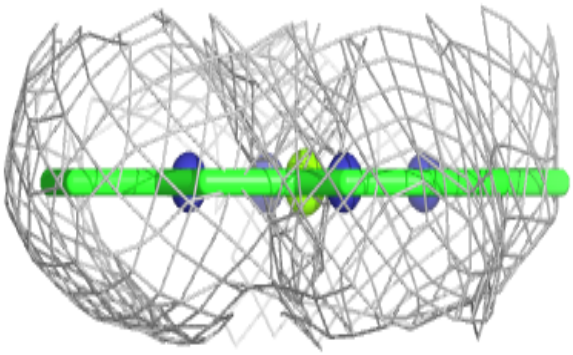


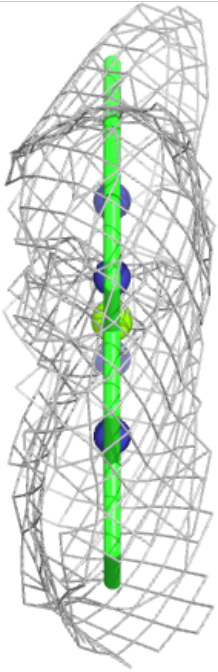


Electron density around CLA 2 2013:

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

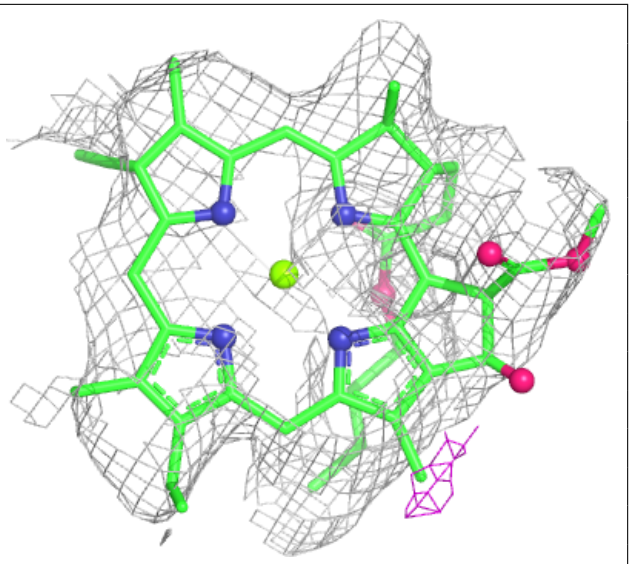


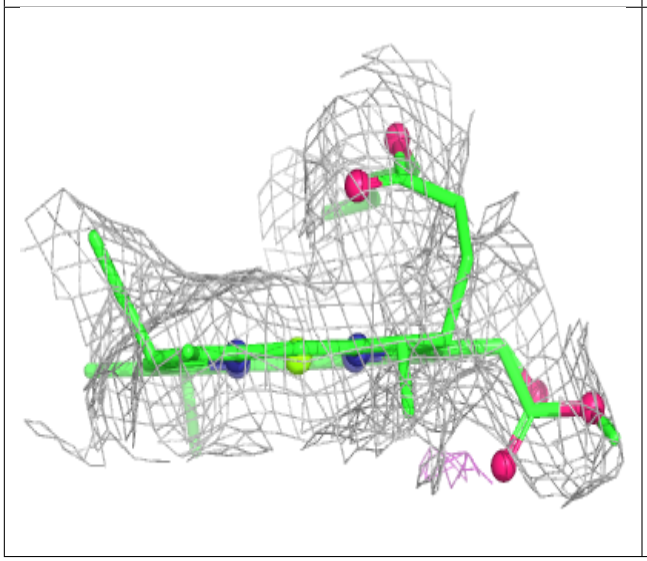


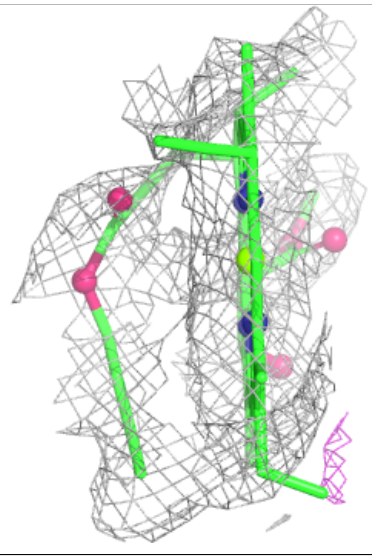


Electron density around CLA B 1214:

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

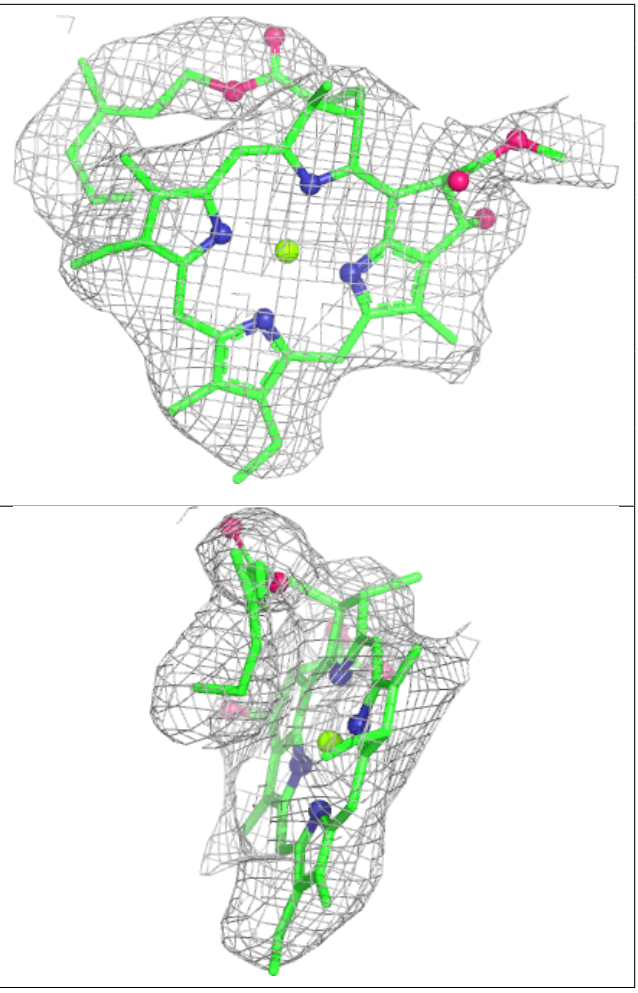






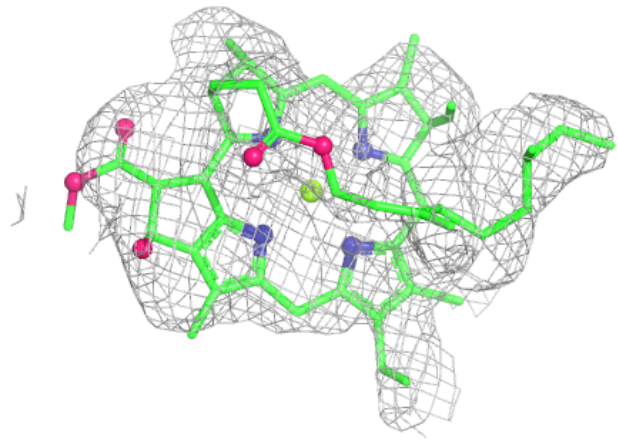
Electron density around CLA B 1215:

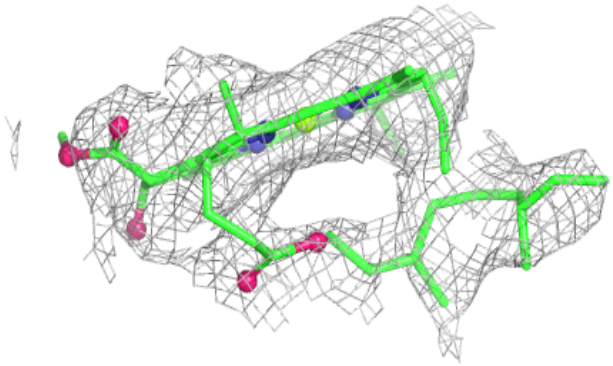
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

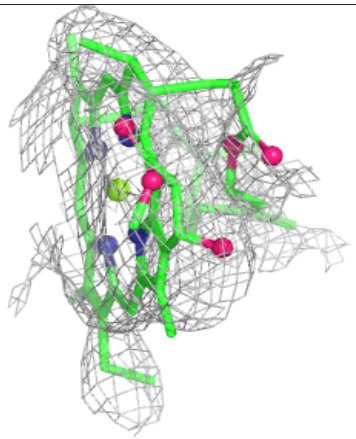


Electron density around CLA B 1138:

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

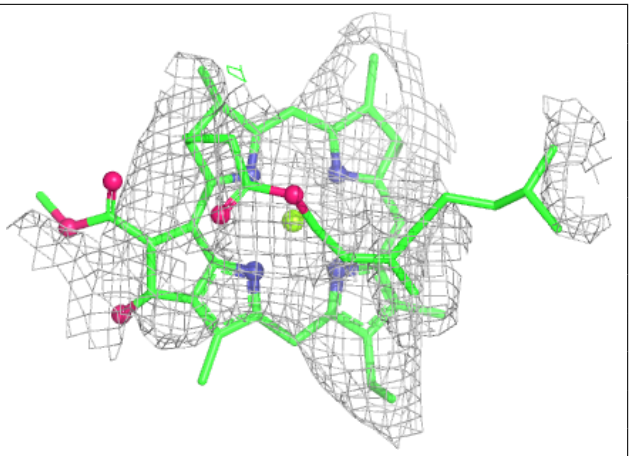


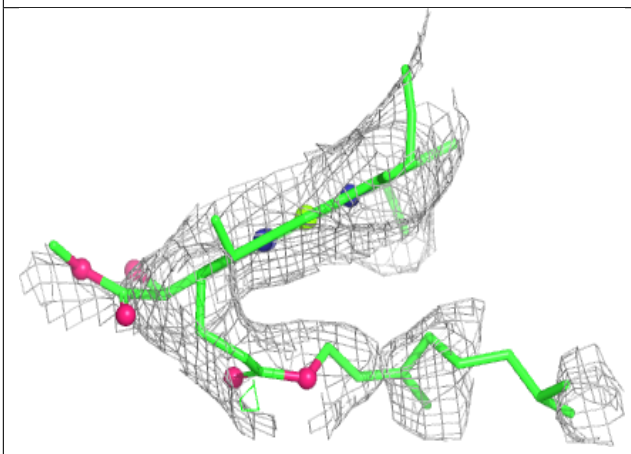


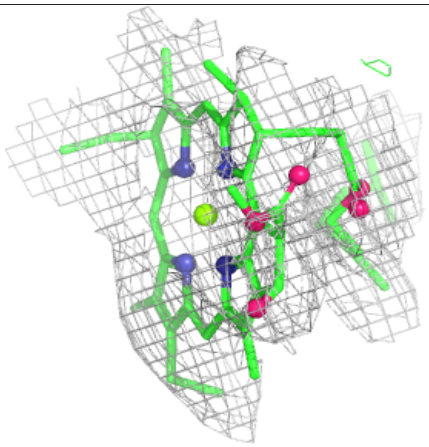


Electron density around CLA A 1136:

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

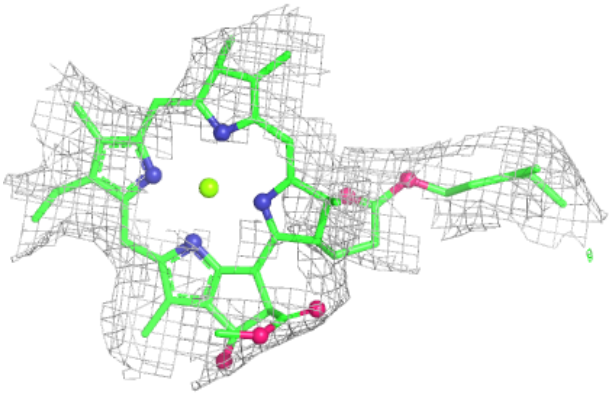


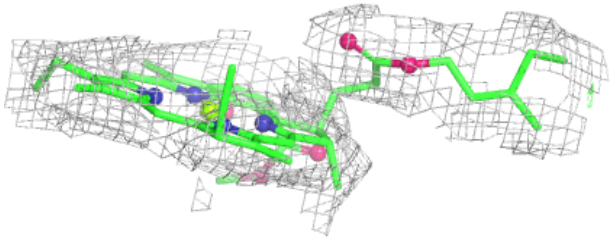


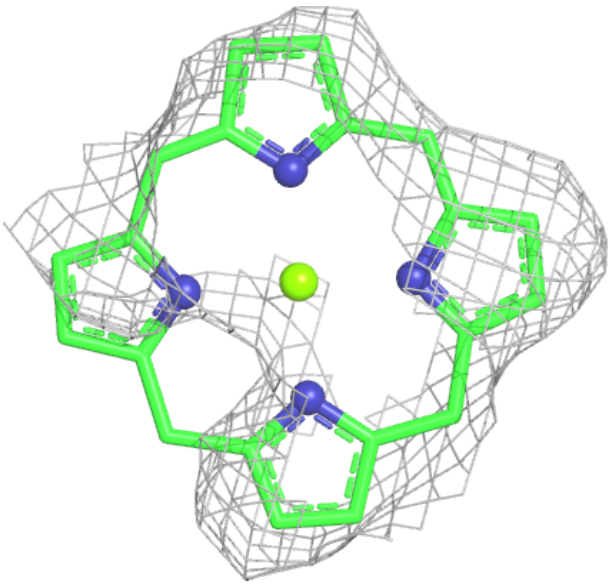
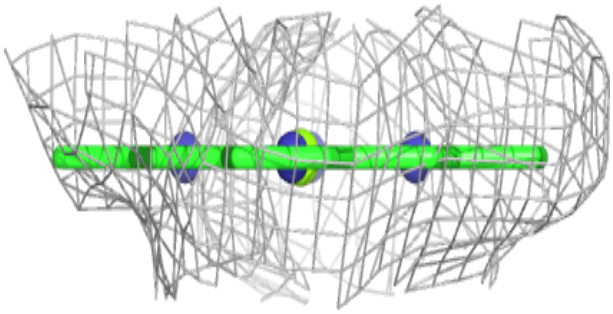
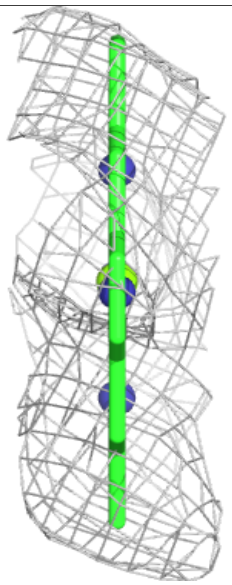


Electron density around CLA B 1218:

$2mF_o$-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 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)	
	

6.5 Other polymers (i)

There are no such residues in this entry.