Full wwPDB X-ray Structure Validation Report ⓘ

Dec 19, 2023 – 03:27 PM EST

PDB ID	:	1IZL
Title	:	Crystal Structure of Photosystem II
Authors	:	Kamiya, N.; Shen, J.-R.
Deposited on	:	2002-10-04
Resolution	:	3.70 Å(reported)

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

We welcome your comments at *validation@mail.wwpdb.org*
A user guide is available at
https://www.wwpdb.org/validation/2017/XrayValidationReportHelp
with specific help available everywhere you see the ⓘ symbol.

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

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

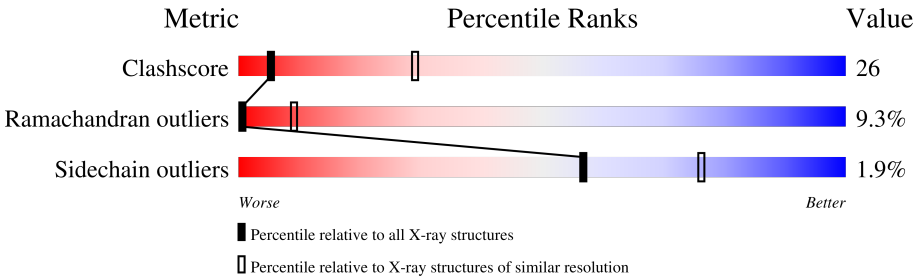
MolProbity	:	4.02b-467
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	NOT EXECUTED
EDS	:	NOT EXECUTED
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.36

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 3.70 Å.

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



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
Clashscore	141614	1027 (3.86-3.54)
Ramachandran outliers	138981	1069 (3.88-3.52)
Sidechain outliers	138945	1065 (3.88-3.52)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments of the lower bar indicate the fraction of residues that contain outliers for >=3, 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions <=5%

Note EDS was not executed.

Mol	Chain	Length	Quality of chain
1	A	360	67% 16% • 17%
1	J	360	67% 15% • 17%
2	B	472	77% 13% 10%
2	L	472	75% 15% 10%
3	C	473	60% 13% 26%
3	M	473	60% 13% • 27%
4	D	352	63% 14% • 21%
4	N	352	65% 13% • 21%

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Mol	Chain	Length	Quality of chain
5	E	83	35% 6% 58%
5	P	83	19% 80%
6	F	44	57% 11% 32%
6	Q	44	57% 41%
7	G	220	99%
7	R	220	98%
8	H	33	97%
8	S	33	94%
9	I	26	88% 12%
9	T	26	88% 8%
10	K	37	62% 8% 27%
10	W	37	62% 8% 27%
11	O	205	93% 7%
11	Y	205	88% 5% 6%
12	U	97	97%
12	Z	97	94% 5%
13	0	137	75% 9% 16%
13	V	137	84% 10% 6%
14	1	25	88% 12%
14	X	25	92% 8%

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
16	CLA	A	365	X	-	-	-
16	CLA	A	366	X	-	-	-
16	CLA	A	368	X	-	X	-

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Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
16	CLA	A	369	X	-	-	-
16	CLA	B	1107	X	-	-	-
16	CLA	B	1108	X	-	-	-
16	CLA	B	1109	X	-	-	-
16	CLA	B	1110	X	-	-	-
16	CLA	B	1111	X	-	-	-
16	CLA	B	1112	X	-	-	-
16	CLA	B	1113	X	-	-	-
16	CLA	B	1114	X	-	-	-
16	CLA	B	1115	X	-	-	-
16	CLA	B	1116	X	-	-	-
16	CLA	B	1117	X	-	-	-
16	CLA	B	1118	X	-	-	-
16	CLA	B	1119	X	-	-	-
16	CLA	B	1120	X	-	-	-
16	CLA	B	1121	X	-	-	-
16	CLA	B	1122	X	-	-	-
16	CLA	C	1078	X	-	-	-
16	CLA	C	1079	X	-	-	-
16	CLA	C	1080	X	-	-	-
16	CLA	C	1081	X	-	-	-
16	CLA	C	1082	X	-	-	-
16	CLA	C	1083	X	-	-	-
16	CLA	C	1084	X	-	-	-
16	CLA	C	1085	X	-	-	-
16	CLA	C	1086	X	-	-	-
16	CLA	C	1087	X	-	-	-
16	CLA	C	1088	X	-	-	-
16	CLA	C	1089	X	-	X	-
16	CLA	D	354	X	-	-	-
16	CLA	D	355	X	-	-	-
16	CLA	D	357	X	-	-	-
16	CLA	G	221	X	-	-	-
16	CLA	J	365	X	-	-	-
16	CLA	J	367	X	-	X	-
16	CLA	J	368	X	-	-	-
16	CLA	L	1107	X	-	-	-
16	CLA	L	1108	X	-	-	-
16	CLA	L	1109	X	-	-	-
16	CLA	L	1110	X	-	-	-
16	CLA	L	1111	X	-	-	-
16	CLA	L	1112	X	-	-	-

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Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
16	CLA	L	1113	X	-	-	-
16	CLA	L	1114	X	-	-	-
16	CLA	L	1115	X	-	-	-
16	CLA	L	1116	X	-	-	-
16	CLA	L	1117	X	-	-	-
16	CLA	L	1118	X	-	-	-
16	CLA	L	1119	X	-	X	-
16	CLA	L	1120	X	-	X	-
16	CLA	L	1121	X	-	-	-
16	CLA	L	1122	X	-	-	-
16	CLA	M	1078	X	-	-	-
16	CLA	M	1079	X	-	-	-
16	CLA	M	1080	X	-	-	-
16	CLA	M	1081	X	-	-	-
16	CLA	M	1082	X	-	-	-
16	CLA	M	1083	X	-	-	-
16	CLA	M	1084	X	-	-	-
16	CLA	M	1085	X	-	-	-
16	CLA	M	1086	X	-	-	-
16	CLA	M	1087	X	-	-	-
16	CLA	M	1088	X	-	-	-
16	CLA	N	354	X	-	-	-
16	CLA	N	355	X	-	-	-
16	CLA	N	356	X	-	-	-
16	CLA	N	358	X	-	-	-
16	CLA	R	221	X	-	-	-
16	CLA	W	64	X	-	-	-
17	PHO	N	357	-	-	X	-
19	PLA	N	359	-	X	-	-

2 Entry composition (i)

There are 21 unique types of molecules in this entry. The entry contains 22804 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 II: Subunit PsbA.

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
1	A	299	Total	C	N	O	0	0	0
			1595	975	310	310			
1	J	299	Total	C	N	O	0	0	0
			1602	984	308	310			

- Molecule 2 is a protein called Photosystem II: Subunit PsbB.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B	427	Total	C	N	O	S	0	0	48
			2004	1238	386	379	1			
2	L	424	Total	C	N	O		0	0	48
			2001	1242	383	376				

- Molecule 3 is a protein called Photosystem II: Subunit PsbC.

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
3	C	349	Total	C	N	O	0	0	0
			1792	1082	358	352			
3	M	347	Total	C	N	O	0	0	0
			1759	1057	354	348			

- Molecule 4 is a protein called Photosystem II: Subunit PsbD.

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
4	D	277	Total	C	N	O	0	0	0
			1460	899	282	279			
4	N	277	Total	C	N	O	0	0	0
			1451	888	284	279			

- Molecule 5 is a protein called Photosystem II: Subunit PsbE.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf	Trace
5	E	35	Total C N O 175 105 35 35	0	0	0
5	P	17	Total C N O 83 49 17 17	0	0	0

- Molecule 6 is a protein called Photosystem II: Subunit PsbF.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf	Trace
6	F	30	Total C N O 166 105 31 30	0	0	0
6	Q	26	Total C N O 129 77 26 26	0	0	0

- Molecule 7 is a protein called Photosystem II: Subunit PsbG.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf	Trace
7	G	220	Total C 220 220	0	0	220
7	R	220	Total C 220 220	0	0	220

- Molecule 8 is a protein called Photosystem II: Subunit PsbH.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf	Trace
8	H	33	Total C N O 165 99 33 33	0	0	0
8	S	32	Total C N O 160 96 32 32	0	0	0

- Molecule 9 is a protein called Photosystem II: Subunit PsbI.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf	Trace
9	I	26	Total C N O 130 78 26 26	0	0	0
9	T	25	Total C N O 125 75 25 25	0	0	0

- Molecule 10 is a protein called Photosystem II: Subunit PsbK.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf	Trace
10	K	27	Total C N O 137 83 27 27	0	0	0

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Mol	Chain	Residues	Atoms	ZeroOcc	AltConf	Trace
10	W	27	Total C N O 137 83 27 27	0	0	0

- Molecule 11 is a protein called Photosystem II: Subunit PsbO.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf	Trace
11	O	205	Total C N O 1025 615 205 205	0	0	0
11	Y	192	Total C N O 960 576 192 192	0	0	0

- Molecule 12 is a protein called Photosystem II: Subunit PsbU.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf	Trace
12	U	97	Total C N O 485 291 97 97	0	0	0
12	Z	92	Total C N O 460 276 92 92	0	0	0

- Molecule 13 is a protein called Photosystem II: Subunit PsbV.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf	Trace
13	V	129	Total C N O 676 410 136 130	0	0	0
13	0	115	Total C N O 597 360 121 116	0	0	0

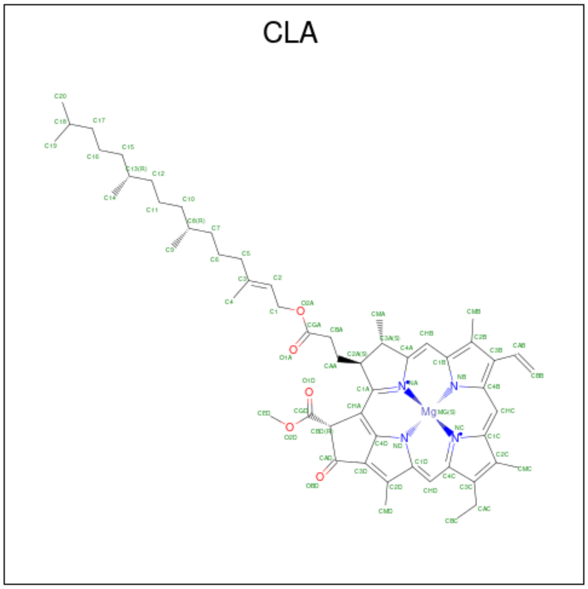
- Molecule 14 is a protein called Photosystem II: Subunit PsbX.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf	Trace
14	X	25	Total C N O 125 75 25 25	0	0	0
14	1	25	Total C N O 125 75 25 25	0	0	0

- Molecule 15 is MANGANESE (II) ION (three-letter code: MN) (formula: Mn).

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
15	A	4	Total Mn 4 4	0	0
15	J	4	Total Mn 4 4	0	0

- Molecule 16 is CHLOROPHYLL A (three-letter code: CLA) (formula: $C_{55}H_{72}MgN_4O_5$).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
			Total	C	Mg	N	O		
16	A	1	35	29	1	4	1	0	0
16	A	1	35	29	1	4	1	0	0
16	A	1	35	29	1	4	1	0	0
16	A	1	35	29	1	4	1	0	0
16	B	1	35	29	1	4	1	0	0
16	B	1	35	29	1	4	1	0	0
16	B	1	35	29	1	4	1	0	0
16	B	1	35	29	1	4	1	0	0
16	B	1	35	29	1	4	1	0	0
16	B	1	35	29	1	4	1	0	0
16	B	1	35	29	1	4	1	0	0
16	B	1	35	29	1	4	1	0	0
16	B	1	35	29	1	4	1	0	0

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Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
16	B	1	Total C Mg N O 35 29 1 4 1	0	0
16	B	1	Total C Mg N O 35 29 1 4 1	0	0
16	B	1	Total C Mg N O 35 29 1 4 1	0	0
16	B	1	Total C Mg N O 35 29 1 4 1	0	0
16	B	1	Total C Mg N O 35 29 1 4 1	0	0
16	B	1	Total C Mg N O 35 29 1 4 1	0	0
16	B	1	Total C Mg N O 35 29 1 4 1	0	0
16	C	1	Total C Mg N O 35 29 1 4 1	0	0
16	C	1	Total C Mg N O 35 29 1 4 1	0	0
16	C	1	Total C Mg N O 35 29 1 4 1	0	0
16	C	1	Total C Mg N O 35 29 1 4 1	0	0
16	C	1	Total C Mg N O 35 29 1 4 1	0	0
16	C	1	Total C Mg N O 35 29 1 4 1	0	0
16	C	1	Total C Mg N O 35 29 1 4 1	0	0
16	C	1	Total C Mg N O 35 29 1 4 1	0	0
16	C	1	Total C Mg N O 35 29 1 4 1	0	0
16	C	1	Total C Mg N O 35 29 1 4 1	0	0
16	C	1	Total C Mg N O 35 29 1 4 1	0	0
16	C	1	Total C Mg N O 35 29 1 4 1	0	0
16	D	1	Total C Mg N O 35 29 1 4 1	0	0
16	D	1	Total C Mg N O 35 29 1 4 1	0	0

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Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
16	D	1	Total 35	C 29	Mg 1	N 4	O 1	0	0
16	G	1	Total 35	C 29	Mg 1	N 4	O 1	0	0
16	J	1	Total 35	C 29	Mg 1	N 4	O 1	0	0
16	J	1	Total 35	C 29	Mg 1	N 4	O 1	0	0
16	J	1	Total 35	C 29	Mg 1	N 4	O 1	0	0
16	L	1	Total 35	C 29	Mg 1	N 4	O 1	0	0
16	L	1	Total 35	C 29	Mg 1	N 4	O 1	0	0
16	L	1	Total 35	C 29	Mg 1	N 4	O 1	0	0
16	L	1	Total 35	C 29	Mg 1	N 4	O 1	0	0
16	L	1	Total 35	C 29	Mg 1	N 4	O 1	0	0
16	L	1	Total 35	C 29	Mg 1	N 4	O 1	0	0
16	L	1	Total 35	C 29	Mg 1	N 4	O 1	0	0
16	L	1	Total 35	C 29	Mg 1	N 4	O 1	0	0
16	L	1	Total 35	C 29	Mg 1	N 4	O 1	0	0
16	L	1	Total 35	C 29	Mg 1	N 4	O 1	0	0
16	L	1	Total 35	C 29	Mg 1	N 4	O 1	0	0
16	L	1	Total 35	C 29	Mg 1	N 4	O 1	0	0
16	L	1	Total 35	C 29	Mg 1	N 4	O 1	0	0
16	L	1	Total 35	C 29	Mg 1	N 4	O 1	0	0
16	L	1	Total 35	C 29	Mg 1	N 4	O 1	0	0
16	L	1	Total 35	C 29	Mg 1	N 4	O 1	0	0

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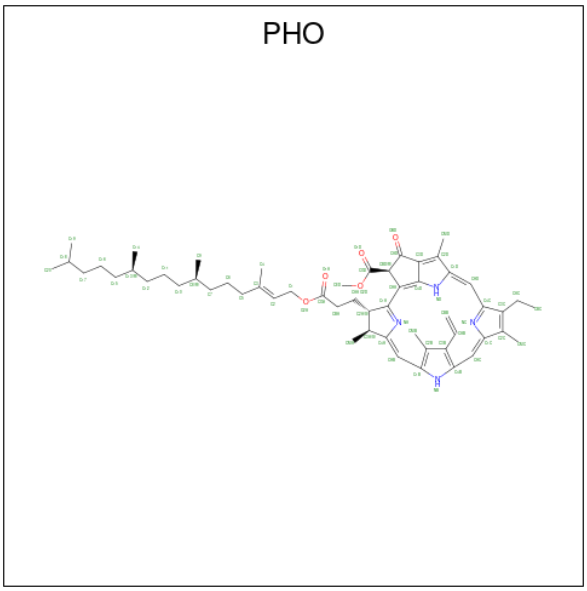
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
16	M	1	Total C Mg N O 35 29 1 4 1	0	0
16	M	1	Total C Mg N O 35 29 1 4 1	0	0
16	M	1	Total C Mg N O 35 29 1 4 1	0	0
16	M	1	Total C Mg N O 35 29 1 4 1	0	0
16	M	1	Total C Mg N O 35 29 1 4 1	0	0
16	M	1	Total C Mg N O 35 29 1 4 1	0	0
16	M	1	Total C Mg N O 35 29 1 4 1	0	0
16	M	1	Total C Mg N O 35 29 1 4 1	0	0
16	M	1	Total C Mg N O 35 29 1 4 1	0	0
16	M	1	Total C Mg N O 35 29 1 4 1	0	0
16	M	1	Total C Mg N O 35 29 1 4 1	0	0
16	N	1	Total C Mg N O 35 29 1 4 1	0	0
16	N	1	Total C Mg N O 35 29 1 4 1	0	0
16	N	1	Total C Mg N O 35 29 1 4 1	0	0
16	N	1	Total C Mg N O 35 29 1 4 1	0	0
16	R	1	Total C Mg N O 35 29 1 4 1	0	0
16	W	1	Total C Mg N O 35 29 1 4 1	0	0

- Molecule 17 is PHEOPHYTIN A (three-letter code: PHO) (formula: $C_{55}H_{74}N_4O_5$).

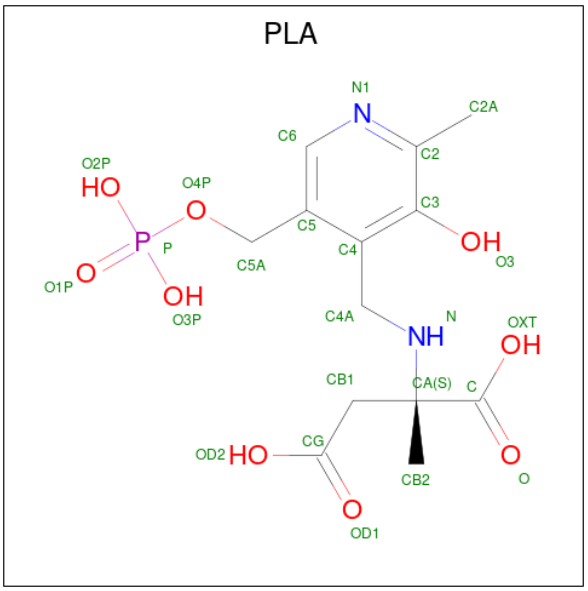


Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
17	A	1	Total C N O 34 29 4 1	0	0
17	D	1	Total C N O 34 29 4 1	0	0
17	J	1	Total C N O 34 29 4 1	0	0
17	N	1	Total C N O 34 29 4 1	0	0

- Molecule 18 is FE (III) ION (three-letter code: FE) (formula: Fe).

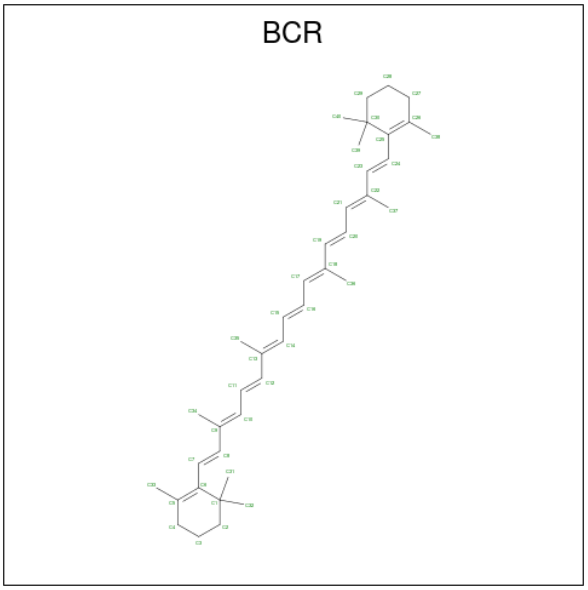
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
18	D	1	Total Fe 1 1	0	0
18	N	1	Total Fe 1 1	0	0

- Molecule 19 is 2-[(3-HYDROXY-2-METHYL-5-PHOSPHONOOXYMETHYL-PYRIDIN-4-YLMETHYL)-AMINO]-2-METHYL-SUCCINIC ACID (three-letter code: PLA) (formula: $C_{13}H_{19}N_2O_9P$).



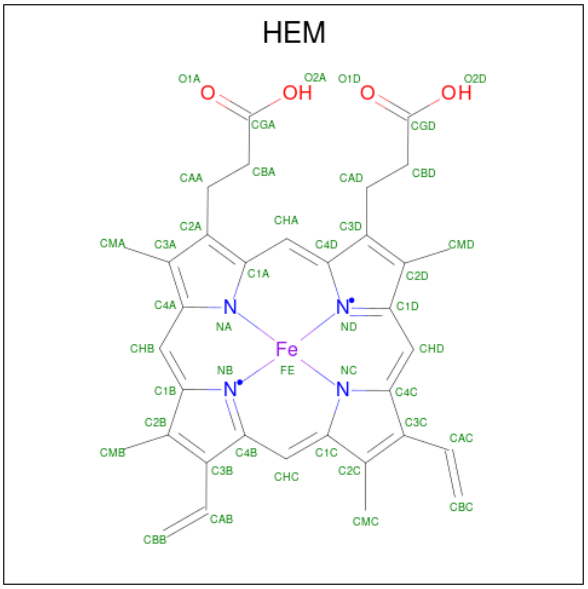
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
19	D	1	Total C N 6 5 1	0	0
19	N	1	Total C N 6 5 1	0	0

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



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
20	D	1	Total C 40 40	0	0
20	K	1	Total C 22 22	0	0

- Molecule 21 is PROTOPORPHYRIN IX CONTAINING FE (three-letter code: HEM) (formula: $C_{34}H_{32}FeN_4O_4$).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
21	E	1	Total	C	Fe	N	0	0
			25	20	1	4		
21	V	1	Total	C	Fe	N	0	0
			25	20	1	4		
21	P	1	Total	C	Fe	N	0	0
			25	20	1	4		
21	0	1	Total	C	Fe	N	0	0
			25	20	1	4		

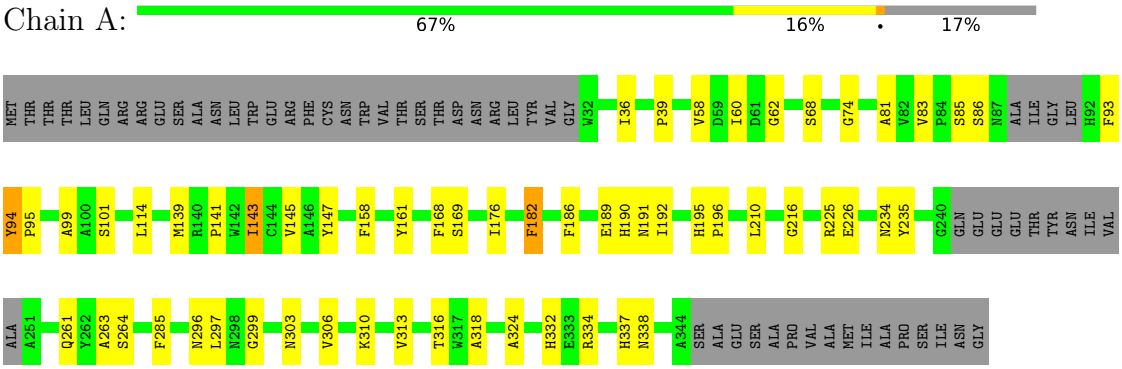
3 Residue-property plots (i)

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

Note EDS was not executed.

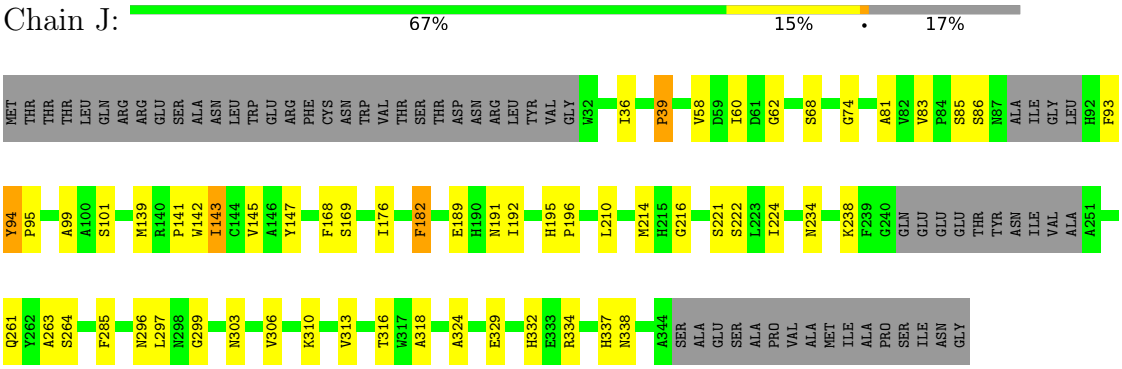
• Molecule 1: Photosystem II: Subunit PsbA

Chain A:



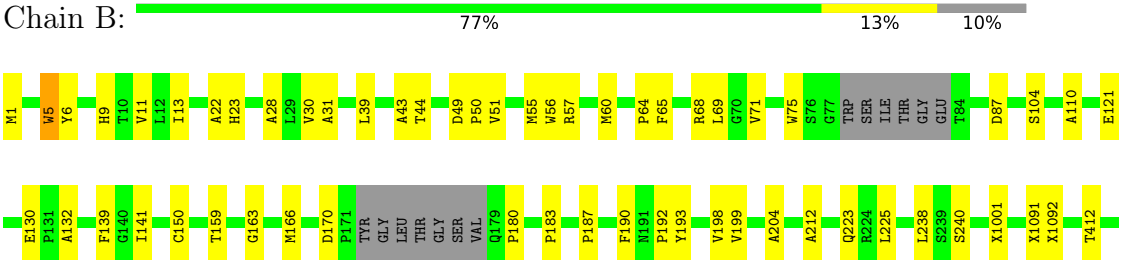
• Molecule 1: Photosystem II: Subunit PsbA

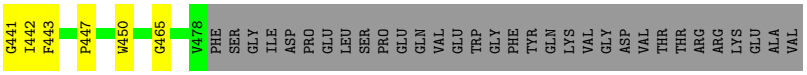
Chain J:



• Molecule 2: Photosystem II: Subunit PsbB

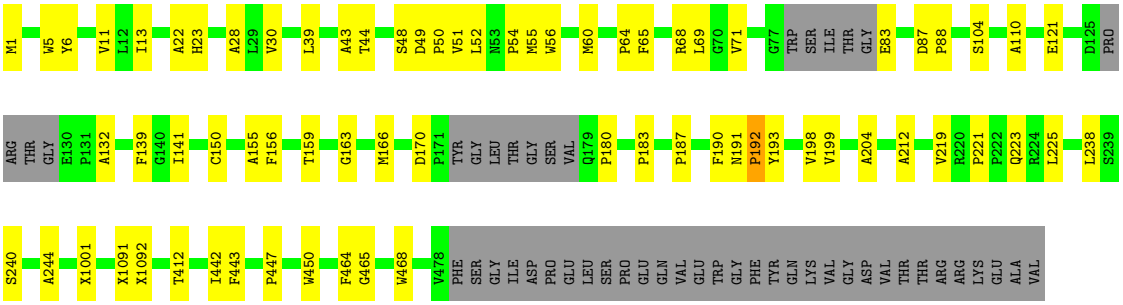
Chain B:





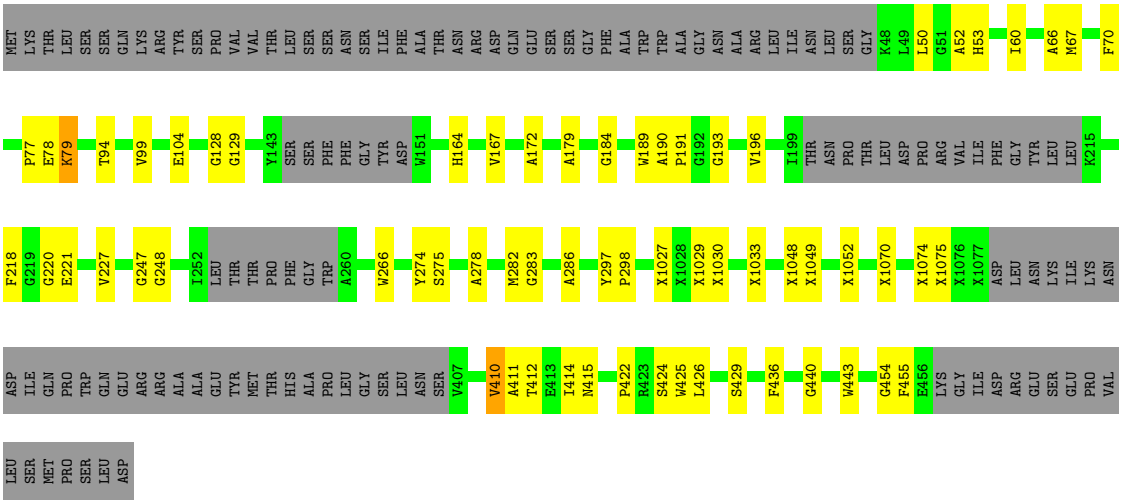
• Molecule 2: Photosystem II: Subunit PsbB

Chain L:



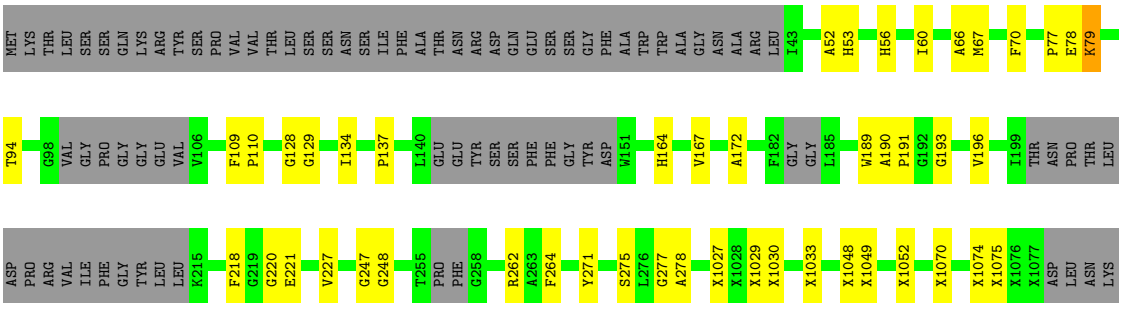
• Molecule 3: Photosystem II: Subunit PsbC

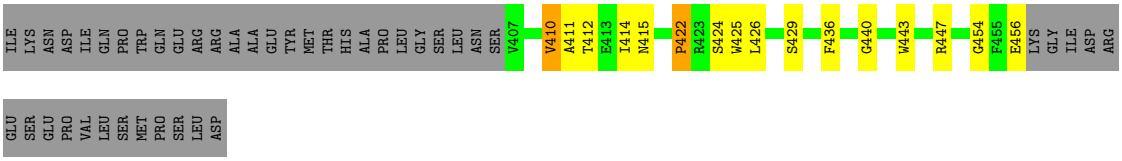
Chain C:



• Molecule 3: Photosystem II: Subunit PsbC

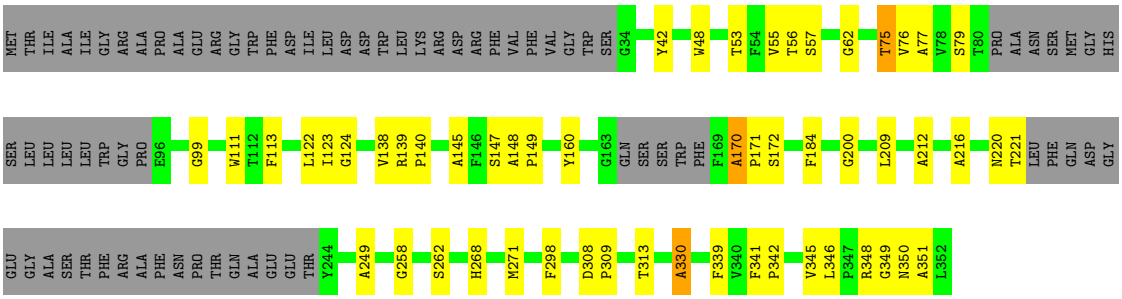
Chain M:





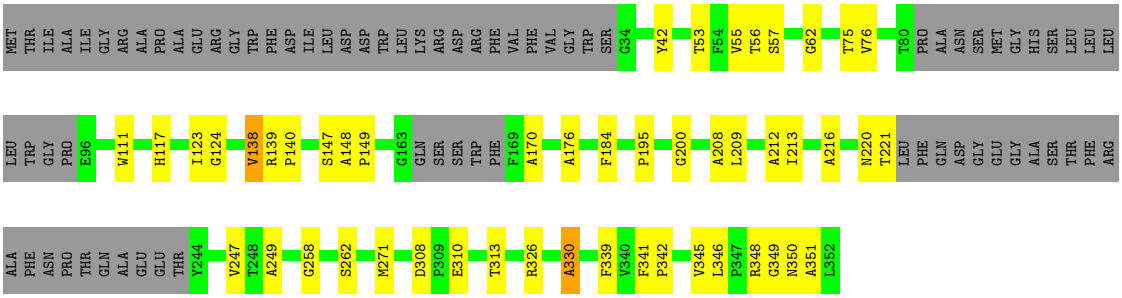
• Molecule 4: Photosystem II: Subunit PsbD

Chain D:



• Molecule 4: Photosystem II: Subunit PsbD

Chain N:

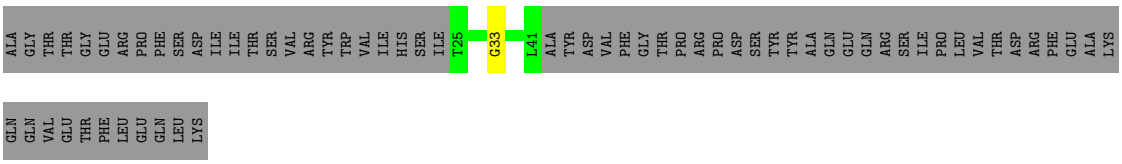


• Molecule 5: Photosystem II: Subunit PsbE

Chain E:

• Molecule 5: Photosystem II: Subunit PsbE

Chain P:

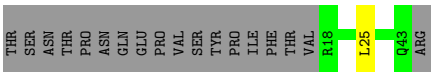


• Molecule 6: Photosystem II: Subunit PsbF

Chain F:

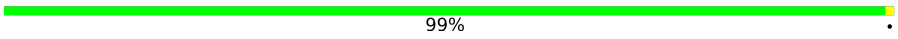
• Molecule 6: Photosystem II: Subunit PsbF

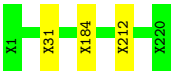
Chain Q:



• Molecule 7: Photosystem II: Subunit PsbG

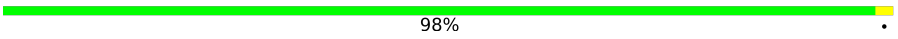
Chain G:

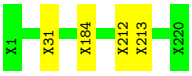




• Molecule 7: Photosystem II: Subunit PsbG

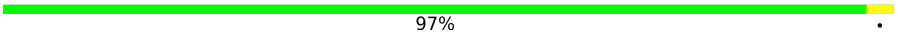
Chain R:





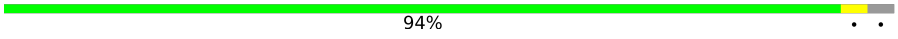
• Molecule 8: Photosystem II: Subunit PsbH

Chain H:



• Molecule 8: Photosystem II: Subunit PsbH

Chain S:

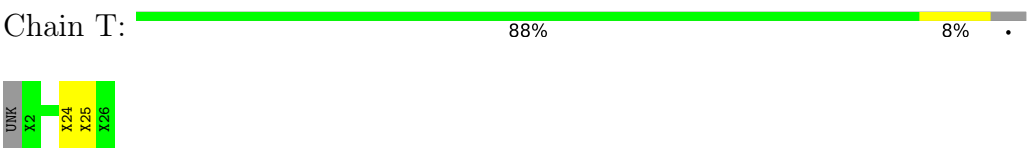


• Molecule 9: Photosystem II: Subunit PsbI

Chain I:

• Molecule 9: Photosystem II: Subunit PsbI

Chain T:



• Molecule 10: Photosystem II: Subunit PsbK

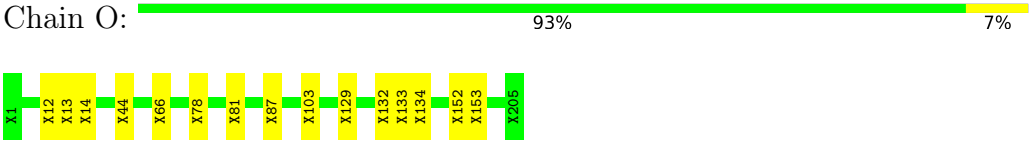
Chain K:

• Molecule 10: Photosystem II: Subunit PsbK

Chain W:

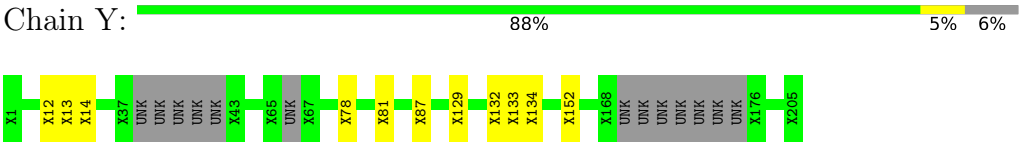
• Molecule 11: Photosystem II: Subunit PsbO

Chain O:



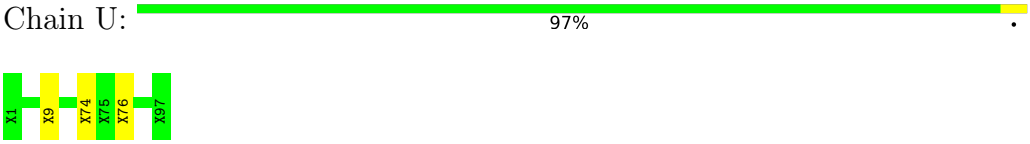
• Molecule 11: Photosystem II: Subunit PsbO

Chain Y:



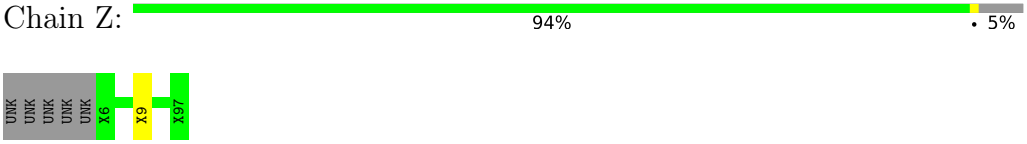
• Molecule 12: Photosystem II: Subunit PsbU

Chain U:



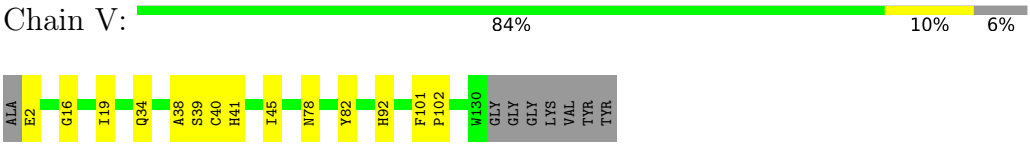
• Molecule 12: Photosystem II: Subunit PsbU

Chain Z:



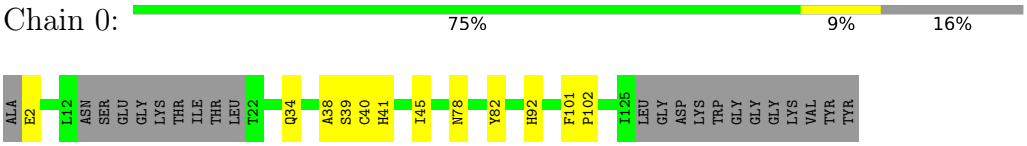
• Molecule 13: Photosystem II: Subunit PsbV

Chain V:



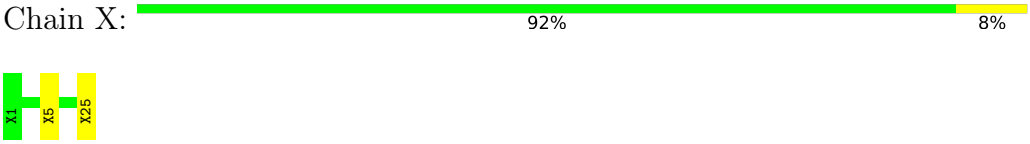
• Molecule 13: Photosystem II: Subunit PsbV

Chain 0:



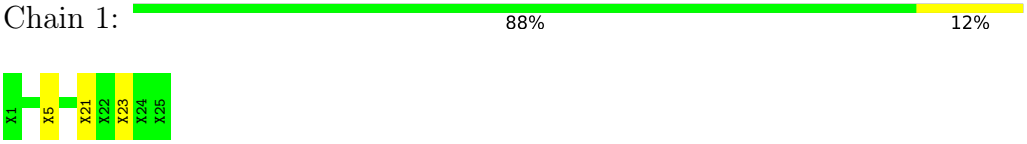
• Molecule 14: Photosystem II: Subunit PsbX

Chain X:



• Molecule 14: Photosystem II: Subunit PsbX

Chain 1:



4 Data and refinement statistics (i)

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

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α, β, γ	129.38Å 225.19Å 308.67Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	25.00 – 3.70	Depositor
% Data completeness (in resolution range)	100.0 (25.00-3.70)	Depositor
R_{merge}	0.07	Depositor
R_{sym}	(Not available)	Depositor
Refinement program		Depositor
R, R_{free}	0.530 , (Not available)	Depositor
Estimated twinning fraction	No twinning to report.	Xtriage
Total number of atoms	22804	wwPDB-VP
Average B, all atoms (Å^2)	47.0	wwPDB-VP

5 Model quality

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: BCR, HEM, CLA, MN, PLA, PHO, FE

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	0.25	0/1613	0.40	0/2229
1	J	0.26	0/1621	0.40	0/2239
2	B	0.24	0/1685	0.41	0/2331
2	L	0.26	0/1682	0.40	0/2323
3	C	0.24	0/1421	0.40	0/1961
3	M	0.25	0/1379	0.40	0/1898
4	D	0.27	0/1475	0.40	0/2037
4	N	0.27	0/1464	0.39	0/2022
5	E	0.24	0/175	0.46	0/243
5	P	0.31	0/82	0.42	0/112
6	F	0.28	0/169	0.47	0/234
6	Q	0.26	0/128	0.40	0/177
10	K	0.25	0/137	0.45	0/191
10	W	0.25	0/137	0.45	0/191
13	0	0.24	0/600	0.37	0/831
13	V	0.23	0/683	0.38	0/949
All	All	0.25	0/14451	0.40	0/19968

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	1595	0	834	95	0
1	J	1602	0	843	82	0
2	B	2004	0	968	147	0
2	L	2001	0	961	141	0
3	C	1792	0	842	126	0
3	M	1759	0	793	114	0
4	D	1460	0	761	71	0
4	N	1451	0	746	68	0
5	E	175	0	81	6	0
5	P	83	0	40	2	0
6	F	166	0	95	4	0
6	Q	129	0	66	4	0
7	G	220	0	0	8	0
7	R	220	0	0	10	0
8	H	165	0	36	1	0
8	S	160	0	35	2	0
9	I	130	0	30	2	0
9	T	125	0	29	1	0
10	K	137	0	68	11	0
10	W	137	0	68	11	0
11	O	1025	0	279	37	0
11	Y	960	0	265	34	0
12	U	485	0	112	5	0
12	Z	460	0	106	1	0
13	0	597	0	278	15	0
13	V	676	0	323	16	0
14	1	125	0	28	3	0
14	X	125	0	29	6	0
15	A	4	0	0	0	0
15	J	4	0	0	0	0
16	A	140	0	68	37	0
16	B	560	0	272	119	0
16	C	420	0	204	99	0
16	D	105	0	48	13	0
16	G	35	0	17	0	0
16	J	105	0	50	25	0
16	L	560	0	272	128	0
16	M	385	0	187	77	0
16	N	140	0	68	11	0
16	R	35	0	17	0	0
16	W	35	0	17	15	0
17	A	34	0	19	20	0
17	D	34	0	19	9	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
17	J	34	0	19	19	0
17	N	34	0	19	28	0
18	D	1	0	0	0	0
18	N	1	0	0	0	0
19	D	6	0	1	0	0
19	N	6	0	1	0	0
20	D	40	0	56	9	0
20	K	22	0	24	1	0
21	0	25	0	4	8	0
21	E	25	0	4	0	0
21	P	25	0	4	0	0
21	V	25	0	4	8	0
All	All	22804	0	10110	868	0

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 26.

All (868) 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)
2:B:450:TRP:HB3	16:B:1110:CLA:CMB	1.26	1.64
2:B:30:VAL:CB	16:B:1108:CLA:CAA	1.76	1.63
3:M:52:ALA:HB1	16:M:1081:CLA:CAB	1.27	1.62
2:B:465:GLY:CA	16:B:1119:CLA:HMA1	1.22	1.60
2:B:1:MET:HA	7:G:31:UNK:CA	1.20	1.60
1:A:95:PRO:HA	16:A:368:CLA:C3A	1.32	1.59
4:D:212:ALA:CB	17:D:356:PHO:CAC	1.79	1.59
1:A:235:TYR:CE2	2:B:5:TRP:HA	1.11	1.58
2:L:204:ALA:CB	16:L:1117:CLA:HHC	1.16	1.57
11:O:152:UNK:CB	12:U:9:UNK:CB	1.77	1.57
2:B:204:ALA:CB	16:B:1117:CLA:HHC	1.16	1.56
3:C:52:ALA:HB1	16:C:1082:CLA:CAB	1.28	1.55
2:L:1:MET:HA	7:R:31:UNK:CA	1.21	1.54
2:L:223:GLN:CB	7:R:184:UNK:CA	1.78	1.53
1:J:95:PRO:CA	16:J:367:CLA:C3A	1.79	1.53
2:B:465:GLY:CA	16:B:1119:CLA:CMA	1.85	1.52
11:Y:152:UNK:CB	12:Z:9:UNK:CB	1.85	1.51
17:A:367:PHO:CMC	4:D:148:ALA:HB1	1.37	1.51
2:L:223:GLN:H	7:R:184:UNK:CA	1.25	1.50
2:B:450:TRP:CB	16:B:1110:CLA:HMB2	1.41	1.50
4:D:212:ALA:HB3	17:D:356:PHO:CAC	1.37	1.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:L:450:TRP:HB3	16:L:1110:CLA:CMB	1.40	1.49
3:C:167:VAL:CB	16:C:1086:CLA:HMD2	1.40	1.47
2:L:1:MET:CA	7:R:31:UNK:CA	1.93	1.47
1:A:95:PRO:CA	16:A:368:CLA:C3A	1.88	1.47
1:A:95:PRO:CA	16:A:368:CLA:H3A	0.99	1.45
1:J:95:PRO:HA	16:J:367:CLA:C3A	0.98	1.45
2:B:223:GLN:H	7:G:184:UNK:CA	1.28	1.44
2:B:1:MET:CA	7:G:31:UNK:CA	1.93	1.44
16:M:1081:CLA:CMA	16:W:64:CLA:HMD2	1.46	1.43
2:L:450:TRP:CB	16:L:1110:CLA:HMB2	1.47	1.42
1:A:143:ILE:CB	4:D:216:ALA:O	1.64	1.42
1:J:143:ILE:CB	4:N:216:ALA:O	1.64	1.41
1:A:235:TYR:CE2	2:B:5:TRP:CA	2.02	1.39
2:B:223:GLN:CB	7:G:184:UNK:CA	2.01	1.37
3:C:52:ALA:CB	16:C:1082:CLA:CAB	2.01	1.37
3:M:425:TRP:CD2	16:M:1079:CLA:CAB	2.08	1.37
1:A:297:LEU:CA	3:C:1074:UNK:O	1.64	1.36
1:A:310:LYS:CB	13:V:2:GLU:C	1.86	1.36
2:L:223:GLN:N	7:R:184:UNK:CA	1.87	1.36
3:M:129:GLY:CA	16:M:1087:CLA:HMB1	1.44	1.36
2:B:22:ALA:CB	16:B:1109:CLA:CAB	2.04	1.35
5:E:33:GLY:HA2	14:X:5:UNK:CB	1.54	1.35
2:L:23:HIS:CB	16:L:1118:CLA:CMC	2.05	1.35
5:E:8:PRO:HG3	14:X:25:UNK:CB	1.55	1.34
1:A:95:PRO:N	16:A:368:CLA:H3A	1.38	1.34
3:C:425:TRP:CD2	16:C:1079:CLA:CAB	2.08	1.33
5:P:33:GLY:HA2	14:1:5:UNK:CB	1.55	1.33
2:L:204:ALA:CB	16:L:1117:CLA:CHC	2.04	1.33
2:L:22:ALA:CB	16:L:1109:CLA:CAB	2.07	1.32
2:B:204:ALA:CB	16:B:1117:CLA:CHC	2.05	1.31
16:B:1108:CLA:CAC	16:B:1119:CLA:CAD	2.06	1.31
3:M:79:LYS:CB	13:0:102:PRO:CB	2.09	1.31
1:J:210:LEU:CB	17:J:366:PHO:C2C	2.07	1.30
3:C:79:LYS:CB	13:V:102:PRO:CB	2.07	1.30
2:B:9:HIS:HE1	16:B:1116:CLA:ND	1.28	1.30
2:B:23:HIS:CB	16:B:1118:CLA:CMC	2.09	1.30
2:L:465:GLY:HA2	16:L:1119:CLA:CMA	1.61	1.30
2:L:1092:UNK:CA	11:Y:132:UNK:O	1.80	1.29
3:C:129:GLY:O	16:C:1088:CLA:CAB	1.80	1.28
3:C:53:HIS:CB	16:C:1086:CLA:CAB	2.12	1.28
3:M:53:HIS:CB	16:M:1085:CLA:CAB	2.10	1.28

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:465:GLY:HA2	16:B:1119:CLA:CMA	1.53	1.28
11:O:87:UNK:CB	2:L:87:ASP:CB	2.11	1.27
1:J:297:LEU:CA	3:M:1074:UNK:O	1.64	1.27
16:C:1080:CLA:CAB	10:K:21:VAL:CB	2.12	1.27
2:B:223:GLN:N	7:G:184:UNK:CA	1.96	1.27
2:B:1092:UNK:CA	11:O:132:UNK:O	1.80	1.27
20:D:359:BCR:H343	20:D:359:BCR:C31	1.63	1.27
17:A:367:PHO:C2C	4:D:148:ALA:HB1	1.65	1.25
2:L:30:VAL:CB	16:L:1108:CLA:CAA	2.13	1.25
3:M:79:LYS:CB	13:0:102:PRO:O	1.84	1.25
3:C:79:LYS:CB	13:V:102:PRO:C	2.05	1.25
4:D:200:GLY:O	16:D:354:CLA:HMA1	1.35	1.25
3:M:79:LYS:CB	13:0:102:PRO:C	2.04	1.24
1:J:297:LEU:HA	3:M:1074:UNK:O	1.19	1.24
16:M:1081:CLA:HMA2	16:W:64:CLA:CMD	1.69	1.23
1:A:95:PRO:HA	16:A:368:CLA:C2A	1.68	1.23
3:C:79:LYS:CB	13:V:102:PRO:O	1.86	1.23
2:L:223:GLN:CA	7:R:184:UNK:CA	2.17	1.23
1:A:216:GLY:O	4:D:271:MET:CB	1.88	1.22
3:M:456:GLU:O	4:N:247:VAL:CB	1.86	1.22
10:W:21:VAL:CB	16:W:64:CLA:CAB	2.17	1.21
2:B:87:ASP:CB	11:Y:87:UNK:CB	2.18	1.21
3:M:52:ALA:CB	16:M:1081:CLA:CAB	2.16	1.21
2:B:465:GLY:HA3	16:B:1119:CLA:HMA2	1.21	1.21
3:C:425:TRP:CE3	16:C:1079:CLA:CAB	2.24	1.21
3:M:425:TRP:O	16:M:1079:CLA:CMC	1.89	1.21
1:J:216:GLY:O	4:N:271:MET:CB	1.90	1.20
2:L:238:LEU:HA	16:L:1109:CLA:HMD3	1.20	1.20
4:N:209:LEU:HA	17:N:357:PHO:C3C	1.72	1.19
2:L:212:ALA:CB	16:L:1107:CLA:HMD3	1.73	1.18
2:B:22:ALA:O	16:B:1109:CLA:CMB	1.90	1.18
3:C:425:TRP:O	16:C:1079:CLA:CMC	1.88	1.18
1:J:324:ALA:O	4:N:330:ALA:CB	1.90	1.18
2:B:87:ASP:CB	11:Y:87:UNK:CA	2.22	1.18
3:M:425:TRP:CE3	16:M:1079:CLA:CAB	2.27	1.18
1:A:235:TYR:CZ	2:B:5:TRP:HA	1.79	1.18
1:A:324:ALA:O	4:D:330:ALA:CB	1.91	1.18
2:L:22:ALA:HB1	16:L:1109:CLA:HMB1	1.22	1.17
3:C:275:SER:CA	16:C:1089:CLA:HMA3	1.74	1.17
3:M:1027:UNK:CB	11:Y:78:UNK:CB	2.22	1.17
4:N:184:PHE:O	16:N:354:CLA:CAC	1.93	1.17

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:316:THR:CB	4:D:62:GLY:O	1.93	1.16
2:B:23:HIS:CB	16:B:1118:CLA:HMC1	1.70	1.16
3:M:129:GLY:CA	16:M:1087:CLA:CMB	2.19	1.16
3:M:129:GLY:C	16:M:1087:CLA:HMB1	1.65	1.16
3:C:1027:UNK:CB	11:O:78:UNK:CB	2.22	1.16
2:B:1:MET:CB	7:G:31:UNK:CA	2.24	1.16
2:L:1:MET:CB	7:R:31:UNK:CA	2.23	1.16
3:M:1052:UNK:CB	11:Y:12:UNK:CB	2.24	1.16
2:B:22:ALA:HB3	16:B:1109:CLA:CAB	1.72	1.15
2:L:22:ALA:O	16:L:1109:CLA:HMB2	1.00	1.15
1:J:316:THR:CB	4:N:62:GLY:O	1.93	1.15
2:L:22:ALA:HB3	16:L:1109:CLA:CAB	1.74	1.15
3:M:167:VAL:CB	16:M:1085:CLA:HMD2	1.76	1.15
4:N:212:ALA:CB	17:N:357:PHO:CAC	2.23	1.15
3:M:425:TRP:CE2	16:M:1079:CLA:CAB	2.29	1.15
2:B:87:ASP:CB	11:Y:87:UNK:HA	1.77	1.15
16:C:1080:CLA:HMD2	16:C:1082:CLA:CMA	1.77	1.14
16:M:1081:CLA:CMA	16:W:64:CLA:CMD	2.24	1.14
2:B:238:LEU:HA	16:B:1109:CLA:HMD3	1.20	1.14
3:C:275:SER:O	16:C:1089:CLA:CMA	1.96	1.14
2:L:22:ALA:O	16:L:1109:CLA:CMB	1.94	1.14
3:C:275:SER:HA	16:C:1089:CLA:HMA3	1.26	1.14
17:J:366:PHO:C2C	4:N:148:ALA:HB1	1.78	1.13
3:C:425:TRP:CE2	16:C:1079:CLA:CAB	2.31	1.13
1:A:297:LEU:HA	3:C:1074:UNK:O	1.19	1.13
3:C:167:VAL:CB	16:C:1086:CLA:CMD	2.27	1.13
16:M:1081:CLA:HMA3	16:W:64:CLA:HMD2	1.19	1.12
7:G:212:UNK:CA	8:H:3:UNK:CB	2.27	1.12
2:L:23:HIS:CB	16:L:1118:CLA:HMC1	1.70	1.12
2:L:465:GLY:HA2	16:L:1119:CLA:HMA3	1.26	1.12
3:C:425:TRP:O	16:C:1079:CLA:HMC2	1.48	1.12
2:L:465:GLY:CA	16:L:1119:CLA:CMA	2.27	1.12
2:B:22:ALA:HB1	16:B:1109:CLA:HMB1	1.23	1.11
3:M:128:GLY:O	16:M:1087:CLA:HMB3	1.48	1.11
2:B:9:HIS:CE1	16:B:1116:CLA:ND	2.17	1.11
2:B:22:ALA:O	16:B:1109:CLA:HMB2	0.95	1.11
3:M:425:TRP:O	16:M:1079:CLA:HMC2	1.49	1.11
1:A:296:ASN:HA	3:C:1074:UNK:CB	1.80	1.10
17:A:367:PHO:CMC	4:D:148:ALA:CB	2.29	1.10
1:J:210:LEU:CB	17:J:366:PHO:C1C	2.28	1.10
16:C:1080:CLA:HMD2	16:C:1082:CLA:HMA3	1.18	1.09

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:212:ALA:CB	16:B:1107:CLA:HMD3	1.81	1.09
1:J:296:ASN:CA	3:M:1074:UNK:CB	2.27	1.09
1:J:296:ASN:HA	3:M:1074:UNK:CB	1.81	1.09
4:N:212:ALA:HB2	17:N:357:PHO:CAC	1.81	1.09
1:A:210:LEU:CB	17:A:367:PHO:C2C	2.31	1.09
2:B:22:ALA:HB1	16:B:1109:CLA:CAB	1.82	1.09
2:B:1092:UNK:HA	11:O:132:UNK:O	1.51	1.09
3:C:275:SER:C	16:C:1089:CLA:HMA3	1.73	1.09
16:A:369:CLA:CAB	16:C:1081:CLA:HMC2	1.82	1.08
2:B:204:ALA:HB1	16:B:1117:CLA:CHC	1.78	1.08
7:R:213:UNK:CA	8:S:3:UNK:CB	2.31	1.08
3:C:278:ALA:HB3	16:C:1089:CLA:HMA2	1.31	1.08
1:A:296:ASN:CA	3:C:1074:UNK:CB	2.27	1.07
1:A:95:PRO:HA	16:A:368:CLA:CAA	1.83	1.07
4:D:200:GLY:O	16:D:354:CLA:CMA	2.01	1.07
2:L:244:ALA:HB1	16:L:1120:CLA:HMD3	1.18	1.07
16:L:1111:CLA:H3A	16:L:1114:CLA:HMD2	1.11	1.07
2:B:465:GLY:HA3	16:B:1119:CLA:CMA	1.68	1.07
1:J:210:LEU:CB	17:J:366:PHO:C3C	2.32	1.07
2:L:1092:UNK:HA	11:Y:132:UNK:O	1.51	1.06
2:B:212:ALA:HB2	16:B:1107:CLA:CMD	1.85	1.06
2:L:212:ALA:HB2	16:L:1107:CLA:CMD	1.85	1.06
2:L:468:TRP:CH2	16:L:1119:CLA:CHC	2.38	1.06
3:M:128:GLY:O	16:M:1087:CLA:CMB	2.04	1.05
17:A:367:PHO:HMC1	4:D:148:ALA:HB1	1.34	1.05
1:J:94:TYR:O	16:J:367:CLA:CMA	2.03	1.05
1:A:310:LYS:CB	13:V:2:GLU:O	2.02	1.05
2:B:204:ALA:HB3	16:B:1117:CLA:CHC	1.79	1.05
1:J:94:TYR:C	16:J:367:CLA:HMA1	1.77	1.05
2:L:68:ARG:CB	16:L:1111:CLA:HMA1	1.87	1.05
20:D:359:BCR:H311	20:D:359:BCR:C34	1.88	1.04
3:C:128:GLY:O	16:C:1088:CLA:HMB3	1.57	1.04
2:L:212:ALA:CB	16:L:1107:CLA:CMD	2.35	1.04
2:B:223:GLN:CA	7:G:184:UNK:CA	2.36	1.04
16:B:1111:CLA:H3A	16:B:1114:CLA:HMD2	1.11	1.04
16:B:1108:CLA:CAC	16:B:1119:CLA:CBD	2.35	1.03
3:C:129:GLY:HA2	16:C:1088:CLA:CMB	1.88	1.03
16:L:1111:CLA:C3A	16:L:1114:CLA:HMD2	1.87	1.03
2:B:212:ALA:CB	16:B:1107:CLA:CMD	2.36	1.03
4:N:200:GLY:O	16:N:354:CLA:HMA1	1.59	1.03
2:L:204:ALA:HB3	16:L:1117:CLA:CHC	1.79	1.03

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:M:275:SER:O	16:M:1088:CLA:HMA3	1.58	1.03
2:B:68:ARG:CB	16:B:1111:CLA:HMA1	1.89	1.03
16:B:1111:CLA:C3A	16:B:1114:CLA:HMD2	1.87	1.03
3:C:275:SER:O	16:C:1089:CLA:HMA3	1.57	1.02
3:C:1048:UNK:N	11:O:14:UNK:CB	2.19	1.02
2:B:1092:UNK:C	11:O:132:UNK:O	2.07	1.02
2:L:1092:UNK:C	11:Y:132:UNK:O	2.07	1.02
5:E:33:GLY:CA	14:X:5:UNK:CB	2.36	1.01
16:L:1108:CLA:HHD	16:L:1119:CLA:OBD	1.58	1.01
16:M:1081:CLA:HMA2	16:W:64:CLA:HMD2	1.23	1.01
5:E:8:PRO:CG	14:X:25:UNK:CB	2.38	1.01
2:L:139:PHE:HB2	16:L:1120:CLA:CMB	1.91	1.01
2:L:1092:UNK:CB	11:Y:132:UNK:O	2.08	1.01
2:B:1092:UNK:CB	11:O:132:UNK:O	2.08	1.01
3:C:70:PHE:CB	10:K:10:ASP:HA	1.90	1.01
16:C:1080:CLA:CAC	16:C:1087:CLA:CAC	2.38	1.01
1:J:95:PRO:HA	16:J:367:CLA:C2A	1.90	1.01
16:M:1086:CLA:CAC	16:W:64:CLA:CAC	2.38	1.01
3:C:172:ALA:HB2	16:C:1083:CLA:OBD	1.60	1.01
16:C:1086:CLA:HMA3	16:C:1088:CLA:CAC	1.90	1.01
4:D:113:PHE:CE1	16:D:357:CLA:C1A	2.42	1.00
2:B:69:LEU:N	16:B:1111:CLA:HMA2	1.76	1.00
20:D:359:BCR:C31	20:D:359:BCR:C34	2.38	1.00
2:L:139:PHE:HB2	16:L:1120:CLA:HMB2	1.01	1.00
3:M:70:PHE:CB	10:W:10:ASP:HA	1.90	1.00
3:M:1049:UNK:CB	11:Y:14:UNK:HA	1.85	1.00
1:A:297:LEU:CB	3:C:424:SER:CB	2.40	0.99
2:L:22:ALA:HB1	16:L:1109:CLA:CAB	1.86	0.99
2:L:1092:UNK:HA	11:Y:132:UNK:C	1.92	0.99
1:A:210:LEU:CB	17:A:367:PHO:C1C	2.41	0.99
17:J:366:PHO:CMC	4:N:148:ALA:HB1	1.93	0.99
4:D:212:ALA:HB1	17:D:356:PHO:CAC	1.90	0.99
3:M:172:ALA:HB2	16:M:1082:CLA:OBD	1.63	0.99
2:B:1092:UNK:HA	11:O:132:UNK:C	1.92	0.98
20:D:359:BCR:H343	20:D:359:BCR:H311	1.00	0.98
1:J:85:SER:CB	3:M:221:GLU:O	2.11	0.98
3:M:1048:UNK:N	11:Y:14:UNK:CB	2.17	0.98
3:C:1052:UNK:CB	11:O:12:UNK:CB	2.41	0.98
2:L:204:ALA:HB1	16:L:1117:CLA:CHC	1.77	0.98
3:C:129:GLY:CA	16:C:1088:CLA:HMB1	1.94	0.97
4:D:212:ALA:HB2	17:D:356:PHO:CAC	1.92	0.97

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:94:TYR:C	16:A:368:CLA:CMA	2.33	0.97
1:J:324:ALA:O	4:N:330:ALA:HB3	1.64	0.97
16:A:365:CLA:HMB2	16:D:354:CLA:HMB2	1.44	0.97
17:A:367:PHO:CAC	4:D:148:ALA:HB3	1.94	0.96
2:L:204:ALA:HB2	16:L:1117:CLA:HHC	1.46	0.96
1:A:324:ALA:O	4:D:330:ALA:HB3	1.65	0.96
17:A:367:PHO:HMC2	4:D:148:ALA:HB1	1.45	0.96
3:C:50:LEU:HA	16:C:1086:CLA:HMB3	1.45	0.96
1:A:85:SER:CB	3:C:221:GLU:O	2.13	0.95
11:O:44:UNK:O	2:L:83:GLU:CB	2.14	0.95
1:A:296:ASN:CB	3:C:1074:UNK:HA	1.84	0.95
2:L:244:ALA:CB	16:L:1120:CLA:HMD3	1.95	0.95
11:O:87:UNK:CA	2:L:87:ASP:CB	2.44	0.95
4:N:42:TYR:HE1	6:Q:25:LEU:CB	1.79	0.94
4:N:42:TYR:CE1	6:Q:25:LEU:CB	2.49	0.94
2:B:22:ALA:C	16:B:1109:CLA:HMB2	1.88	0.94
1:A:94:TYR:O	16:A:368:CLA:HMA2	1.66	0.94
16:L:1108:CLA:CAC	16:L:1119:CLA:CAD	2.46	0.94
11:O:87:UNK:HA	2:L:87:ASP:CB	1.97	0.94
2:L:22:ALA:HB1	16:L:1109:CLA:CMB	1.97	0.94
2:L:204:ALA:HB1	16:L:1117:CLA:HHC	0.94	0.94
17:A:367:PHO:C2C	4:D:148:ALA:CB	2.46	0.93
4:N:212:ALA:HB3	17:N:357:PHO:CAC	1.94	0.93
1:J:297:LEU:CB	3:M:424:SER:CB	2.47	0.93
5:P:33:GLY:CA	14:1:5:UNK:CB	2.47	0.93
16:B:1108:CLA:CAC	16:B:1119:CLA:OBD	2.16	0.93
3:C:129:GLY:C	16:C:1088:CLA:HMB1	1.88	0.93
1:A:139:MET:O	4:D:221:THR:O	1.86	0.93
2:B:204:ALA:HB1	16:B:1117:CLA:HHC	0.94	0.93
1:A:95:PRO:N	16:A:368:CLA:C3A	2.19	0.93
1:J:296:ASN:CB	3:M:1074:UNK:HA	1.85	0.92
2:B:204:ALA:HB2	16:B:1117:CLA:HHC	1.47	0.92
3:C:1049:UNK:CB	11:O:14:UNK:HA	1.85	0.92
1:J:214:MET:CB	17:J:366:PHO:HMD3	1.99	0.92
16:C:1080:CLA:CMD	16:C:1082:CLA:CMA	2.47	0.92
2:L:65:PHE:HA	16:L:1114:CLA:CAC	2.00	0.92
1:A:235:TYR:HE2	2:B:5:TRP:CA	1.60	0.92
3:C:129:GLY:HA2	16:C:1088:CLA:HMB1	1.50	0.92
1:J:139:MET:O	4:N:221:THR:O	1.86	0.92
2:B:238:LEU:HA	16:B:1109:CLA:CMD	2.01	0.91
2:B:22:ALA:HB1	16:B:1109:CLA:CMB	1.99	0.91

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:64:PRO:CB	16:B:1114:CLA:HMC2	2.00	0.91
2:L:69:LEU:N	16:L:1111:CLA:HMA2	1.84	0.91
3:C:1049:UNK:CB	11:O:13:UNK:O	2.19	0.91
2:L:22:ALA:C	16:L:1109:CLA:HMB2	1.91	0.91
3:C:52:ALA:O	16:C:1082:CLA:HMB2	1.71	0.90
20:D:359:BCR:H21C	20:K:47:BCR:H373	1.53	0.90
17:J:366:PHO:C3C	4:N:148:ALA:HB1	2.01	0.90
2:L:238:LEU:HA	16:L:1109:CLA:CMD	2.01	0.90
3:C:79:LYS:CB	13:V:102:PRO:CA	2.49	0.90
2:L:30:VAL:CB	16:L:1108:CLA:H3A	2.02	0.90
2:B:465:GLY:C	16:B:1119:CLA:CMA	2.40	0.90
1:A:94:TYR:C	16:A:368:CLA:HMA1	1.92	0.90
3:M:79:LYS:CB	13:0:102:PRO:CA	2.50	0.90
1:A:95:PRO:CB	16:A:368:CLA:H3A	2.01	0.90
2:B:204:ALA:HB3	16:B:1117:CLA:HHC	1.31	0.90
1:A:94:TYR:O	16:A:368:CLA:CMA	2.19	0.89
17:A:367:PHO:CAC	4:D:148:ALA:CB	2.50	0.89
4:D:113:PHE:HE1	16:D:357:CLA:C1A	1.77	0.89
2:L:139:PHE:CB	16:L:1120:CLA:HMB2	1.97	0.89
16:B:1108:CLA:CMA	16:B:1112:CLA:CAB	2.50	0.89
16:L:1108:CLA:CMA	16:L:1112:CLA:CAB	2.50	0.89
2:B:450:TRP:CB	16:B:1110:CLA:CMB	2.18	0.89
2:B:465:GLY:C	16:B:1119:CLA:HMA1	1.91	0.89
2:L:240:SER:CB	16:L:1120:CLA:C1C	2.50	0.89
3:M:1049:UNK:CB	11:Y:13:UNK:O	2.19	0.89
2:L:1092:UNK:C	11:Y:132:UNK:C	2.44	0.89
16:M:1081:CLA:HMA2	16:W:64:CLA:C2D	2.03	0.89
2:L:68:ARG:CB	16:L:1111:CLA:CMA	2.52	0.88
2:L:1092:UNK:HA	11:Y:133:UNK:C	2.03	0.88
2:L:465:GLY:CA	16:L:1119:CLA:HMA2	2.02	0.88
2:B:68:ARG:C	16:B:1111:CLA:CMA	2.42	0.88
2:L:68:ARG:C	16:L:1111:CLA:CMA	2.42	0.88
2:B:1092:UNK:C	11:O:132:UNK:C	2.44	0.88
1:A:95:PRO:CA	16:A:368:CLA:CAA	2.50	0.88
3:C:425:TRP:CZ3	16:C:1079:CLA:CAB	2.57	0.88
2:B:1092:UNK:CA	11:O:132:UNK:C	2.51	0.87
11:O:152:UNK:CA	12:U:9:UNK:CB	2.52	0.87
3:C:172:ALA:CB	16:C:1083:CLA:CAD	2.52	0.87
2:L:1092:UNK:CA	11:Y:132:UNK:C	2.51	0.87
3:M:70:PHE:CB	10:W:10:ASP:CA	2.53	0.87
2:B:68:ARG:CB	16:B:1111:CLA:CMA	2.52	0.87

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
16:L:1111:CLA:H3A	16:L:1114:CLA:CMD	2.04	0.87
2:B:1092:UNK:HA	11:O:133:UNK:C	2.04	0.87
2:B:212:ALA:HB1	16:B:1107:CLA:C2D	2.04	0.86
1:A:235:TYR:CD2	2:B:5:TRP:O	2.29	0.86
16:B:1108:CLA:HMA2	16:B:1112:CLA:CAB	2.05	0.86
16:J:365:CLA:HMB2	16:N:354:CLA:HMB2	1.53	0.86
2:L:60:MET:CB	16:L:1110:CLA:HMA3	2.05	0.86
16:L:1108:CLA:HMA2	16:L:1112:CLA:CAB	2.05	0.86
17:A:367:PHO:C3C	4:D:148:ALA:CB	2.53	0.86
3:C:70:PHE:CB	10:K:10:ASP:CA	2.53	0.86
1:J:94:TYR:O	16:J:367:CLA:HMA2	1.74	0.86
2:L:1092:UNK:O	11:Y:132:UNK:O	1.88	0.86
3:M:66:ALA:C	10:W:13:VAL:CB	2.44	0.86
3:C:66:ALA:C	10:K:13:VAL:CB	2.44	0.86
3:M:172:ALA:CB	16:M:1082:CLA:CAD	2.54	0.86
2:L:23:HIS:CB	16:L:1118:CLA:HMC2	2.06	0.85
2:L:65:PHE:CB	16:L:1114:CLA:CAC	2.54	0.85
1:A:296:ASN:CB	3:C:1074:UNK:CA	2.54	0.85
1:J:94:TYR:C	16:J:367:CLA:CMA	2.43	0.85
4:N:209:LEU:HA	17:N:357:PHO:C4C	2.06	0.85
3:C:425:TRP:O	16:C:1079:CLA:HMC3	1.76	0.85
2:L:240:SER:CB	16:L:1120:CLA:C2C	2.54	0.85
3:C:278:ALA:HB3	16:C:1089:CLA:CMA	2.06	0.85
4:D:48:TRP:HZ3	20:D:359:BCR:H332	1.41	0.85
2:L:465:GLY:CA	16:L:1119:CLA:HMA3	2.02	0.85
2:B:68:ARG:C	16:B:1111:CLA:HMA2	1.95	0.85
3:C:429:SER:CB	16:C:1079:CLA:HMC2	2.06	0.85
1:J:296:ASN:CB	3:M:1074:UNK:CA	2.54	0.85
3:M:129:GLY:C	16:M:1087:CLA:CMB	2.41	0.85
1:A:337:HIS:CB	4:D:351:ALA:HB2	2.07	0.84
2:B:238:LEU:CA	16:B:1109:CLA:HMD3	2.06	0.84
3:M:429:SER:CB	16:M:1079:CLA:HMC2	2.06	0.84
2:L:212:ALA:HB1	16:L:1107:CLA:HMD3	1.59	0.84
2:B:1092:UNK:HA	11:O:133:UNK:O	1.78	0.83
3:M:425:TRP:CZ3	16:M:1079:CLA:CAB	2.61	0.83
3:C:266:TRP:HZ2	16:C:1078:CLA:CAC	1.91	0.83
2:L:1092:UNK:HA	11:Y:133:UNK:O	1.77	0.83
17:A:367:PHO:HMC1	4:D:148:ALA:CB	1.99	0.83
1:J:337:HIS:CB	4:N:351:ALA:HB2	2.07	0.83
2:L:65:PHE:CA	16:L:1114:CLA:CAC	2.56	0.83
2:L:238:LEU:CA	16:L:1109:CLA:HMD3	2.06	0.83

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
16:C:1078:CLA:HMD1	16:C:1089:CLA:C3D	2.09	0.83
16:B:1111:CLA:H3A	16:B:1114:CLA:CMD	2.04	0.83
1:J:95:PRO:CB	16:J:367:CLA:C4A	2.56	0.83
16:M:1081:CLA:CMA	16:W:64:CLA:C2D	2.57	0.83
1:A:161:TYR:OH	1:A:190:HIS:CB	2.27	0.83
3:C:275:SER:HA	16:C:1089:CLA:CMA	2.07	0.82
3:M:425:TRP:O	16:M:1079:CLA:HMC3	1.77	0.82
1:J:94:TYR:O	16:J:367:CLA:HMA1	1.72	0.82
2:L:139:PHE:HD1	16:L:1120:CLA:CHB	1.93	0.82
4:N:209:LEU:CA	17:N:357:PHO:C3C	2.57	0.82
3:C:429:SER:CB	16:C:1079:CLA:CMC	2.58	0.82
1:A:95:PRO:CB	16:A:368:CLA:C3A	2.58	0.82
2:L:141:ILE:O	16:L:1118:CLA:HMA2	1.80	0.81
2:L:139:PHE:CD1	16:L:1120:CLA:CHB	2.62	0.81
1:J:182:PHE:O	16:J:365:CLA:HMD2	1.80	0.81
1:J:95:PRO:N	16:J:367:CLA:C3A	2.42	0.81
1:A:158:PHE:HZ	16:A:366:CLA:HMC3	1.45	0.81
3:M:278:ALA:HB3	16:M:1088:CLA:H2A	1.63	0.81
1:J:324:ALA:O	4:N:330:ALA:HB1	1.80	0.81
3:C:172:ALA:HB1	16:C:1083:CLA:CAD	2.12	0.80
3:M:275:SER:O	16:M:1088:CLA:CMA	2.27	0.80
2:L:68:ARG:C	16:L:1111:CLA:HMA2	2.01	0.80
3:C:172:ALA:CB	16:C:1083:CLA:OBD	2.30	0.80
1:J:95:PRO:CA	16:J:367:CLA:C4A	2.58	0.80
3:M:429:SER:CB	16:M:1079:CLA:CMC	2.59	0.80
16:C:1080:CLA:CMD	16:C:1082:CLA:HMA2	2.09	0.80
13:0:41:HIS:NE2	21:0:138:HEM:NB	2.30	0.80
17:A:367:PHO:C3C	4:D:148:ALA:HB3	2.11	0.80
13:V:41:HIS:CD2	21:V:138:HEM:C4B	2.70	0.80
3:C:128:GLY:O	16:C:1088:CLA:CMB	2.30	0.80
17:J:366:PHO:C3C	4:N:148:ALA:CB	2.60	0.79
1:J:95:PRO:CB	16:J:367:CLA:C3A	2.59	0.79
20:D:359:BCR:C34	20:D:359:BCR:H312	2.10	0.79
2:L:23:HIS:CB	16:L:1118:CLA:HMC3	2.11	0.79
13:0:41:HIS:CD2	21:0:138:HEM:C4B	2.70	0.79
1:A:235:TYR:OH	2:B:5:TRP:N	2.16	0.78
16:B:1111:CLA:CAA	16:B:1114:CLA:HMD3	2.12	0.78
16:C:1080:CLA:C2D	16:C:1082:CLA:HMA2	2.14	0.78
16:L:1111:CLA:CAA	16:L:1114:CLA:HMD3	2.12	0.78
4:N:208:ALA:HB3	17:N:357:PHO:HMC3	1.66	0.78
3:M:1048:UNK:C	11:Y:14:UNK:N	2.44	0.77

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:324:ALA:O	4:D:330:ALA:HB1	1.81	0.77
16:B:1111:CLA:CAA	16:B:1114:CLA:CMD	2.62	0.77
2:L:110:ALA:CB	16:L:1121:CLA:HMB2	2.14	0.77
2:B:204:ALA:O	16:B:1117:CLA:HMC3	1.85	0.77
16:L:1111:CLA:CAA	16:L:1114:CLA:CMD	2.62	0.77
3:M:425:TRP:CZ2	16:M:1079:CLA:CAB	2.68	0.77
16:C:1080:CLA:C2D	16:C:1082:CLA:CMA	2.63	0.77
2:L:212:ALA:HB2	16:L:1107:CLA:HMD1	1.66	0.77
2:L:212:ALA:HB1	16:L:1107:CLA:C2D	2.15	0.77
17:A:367:PHO:C3C	4:D:148:ALA:HB1	2.14	0.77
2:B:9:HIS:HE1	16:B:1116:CLA:C4D	1.97	0.77
3:M:277:GLY:HA3	16:M:1080:CLA:CAC	2.15	0.77
3:M:278:ALA:HB3	16:M:1088:CLA:HMA2	1.64	0.77
1:A:297:LEU:C	3:C:1074:UNK:O	2.22	0.76
3:C:275:SER:O	16:C:1089:CLA:HMA1	1.83	0.76
2:L:69:LEU:CB	16:L:1111:CLA:H2A	2.14	0.76
1:A:235:TYR:CZ	2:B:5:TRP:CA	2.53	0.76
2:B:22:ALA:CB	16:B:1109:CLA:HMB1	2.12	0.76
16:B:1108:CLA:HMA3	16:B:1112:CLA:CAB	2.15	0.76
1:J:310:LYS:CB	13:0:2:GLU:O	2.13	0.76
2:L:204:ALA:O	16:L:1117:CLA:HMC3	1.85	0.76
3:C:266:TRP:CZ2	16:C:1078:CLA:CAC	2.68	0.76
1:J:297:LEU:C	3:M:1074:UNK:O	2.23	0.76
4:N:208:ALA:O	17:N:357:PHO:CAC	2.34	0.76
16:L:1115:CLA:HMA2	16:L:1120:CLA:HMC1	1.67	0.76
16:L:1108:CLA:HMA3	16:L:1112:CLA:CAB	2.15	0.76
4:N:209:LEU:CB	17:N:357:PHO:C1C	2.64	0.76
2:B:23:HIS:CB	16:B:1118:CLA:HMC2	2.12	0.76
1:J:210:LEU:CB	17:J:366:PHO:C4C	2.64	0.76
3:C:1048:UNK:C	11:O:14:UNK:N	2.45	0.76
2:L:212:ALA:HB1	16:L:1107:CLA:CMD	2.13	0.76
3:M:172:ALA:HB1	16:M:1082:CLA:CAD	2.15	0.76
2:B:212:ALA:HB2	16:B:1107:CLA:HMD1	1.66	0.75
3:M:172:ALA:CB	16:M:1082:CLA:OBD	2.34	0.75
2:B:23:HIS:CB	16:B:1118:CLA:HMC3	2.15	0.75
4:N:209:LEU:CB	17:N:357:PHO:NC	2.50	0.75
3:C:425:TRP:CZ2	16:C:1079:CLA:CAB	2.69	0.75
2:L:450:TRP:CB	16:L:1110:CLA:CMB	2.29	0.75
3:C:129:GLY:C	16:C:1088:CLA:CAB	2.54	0.75
3:M:425:TRP:HB3	16:M:1079:CLA:HHC	1.69	0.75
2:B:110:ALA:CB	16:B:1121:CLA:HMB2	2.18	0.73

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:450:TRP:CG	16:B:1110:CLA:HMB2	2.24	0.73
9:T:24:UNK:O	9:T:25:UNK:CB	2.37	0.73
3:C:66:ALA:CB	10:K:13:VAL:CB	2.67	0.73
17:J:366:PHO:CAC	4:N:148:ALA:CB	2.66	0.73
3:M:66:ALA:CB	10:W:13:VAL:CB	2.67	0.73
16:C:1078:CLA:HMD1	16:C:1089:CLA:CAD	2.19	0.73
1:A:235:TYR:CE2	2:B:5:TRP:C	2.61	0.72
2:L:468:TRP:CZ2	16:L:1119:CLA:CHC	2.72	0.72
3:M:248:GLY:HA2	16:M:1078:CLA:HMA3	1.70	0.72
9:I:24:UNK:O	9:I:25:UNK:CB	2.37	0.72
2:B:212:ALA:CB	16:B:1107:CLA:C2D	2.65	0.72
16:M:1079:CLA:HMD3	16:M:1084:CLA:CAC	2.19	0.72
2:L:150:CYS:HA	16:L:1113:CLA:HMB2	1.72	0.72
3:C:425:TRP:HB3	16:C:1079:CLA:HHC	1.72	0.72
1:A:158:PHE:HZ	16:A:366:CLA:CMC	2.02	0.71
1:A:94:TYR:C	16:A:368:CLA:H3A	2.09	0.71
1:A:95:PRO:HA	16:A:368:CLA:H3A	0.86	0.71
3:M:164:HIS:HB2	16:M:1088:CLA:CAB	2.20	0.71
2:B:64:PRO:CB	16:B:1114:CLA:CMC	2.68	0.71
13:V:41:HIS:NE2	21:V:138:HEM:NB	2.38	0.71
2:L:139:PHE:HD1	16:L:1120:CLA:C4A	2.03	0.71
3:M:129:GLY:N	16:M:1087:CLA:HMB1	2.04	0.71
1:A:95:PRO:CB	16:A:368:CLA:C4A	2.69	0.70
3:M:271:TYR:CB	16:M:1088:CLA:HHD	2.20	0.70
2:B:150:CYS:HA	16:B:1113:CLA:HMB2	1.73	0.70
2:B:465:GLY:O	16:B:1119:CLA:CMA	2.39	0.70
2:L:22:ALA:CB	16:L:1109:CLA:HMB1	2.12	0.70
3:M:128:GLY:O	16:M:1087:CLA:HMB1	1.91	0.70
2:L:141:ILE:O	16:L:1118:CLA:CMA	2.39	0.70
3:M:271:TYR:CB	16:M:1088:CLA:CHD	2.70	0.70
1:J:95:PRO:N	16:J:367:CLA:HHB	2.07	0.70
4:D:113:PHE:CE1	16:D:357:CLA:NA	2.56	0.69
2:B:465:GLY:CA	16:B:1119:CLA:HMA2	1.82	0.69
1:A:182:PHE:O	16:A:365:CLA:HMD2	1.92	0.69
1:A:296:ASN:CB	3:C:1074:UNK:CB	2.70	0.69
1:J:296:ASN:CB	3:M:1074:UNK:CB	2.70	0.69
4:N:212:ALA:HB3	17:N:357:PHO:HHD	1.73	0.69
2:B:39:LEU:HA	2:B:43:ALA:HB3	1.75	0.68
2:B:212:ALA:HB1	16:B:1107:CLA:CMD	2.19	0.68
2:L:465:GLY:HA3	16:L:1119:CLA:HMA2	1.75	0.68
2:L:465:GLY:HA2	16:L:1119:CLA:HMA1	1.69	0.68

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:C:53:HIS:CB	16:C:1086:CLA:C3B	2.71	0.68
1:A:225:ARG:CB	4:D:268:HIS:CB	2.72	0.68
1:J:94:TYR:CB	16:J:367:CLA:HMB3	2.23	0.68
2:L:60:MET:CB	16:L:1110:CLA:CMA	2.71	0.67
2:B:65:PHE:HA	16:B:1114:CLA:CAC	2.23	0.67
3:C:129:GLY:HA2	16:C:1088:CLA:C2B	2.24	0.67
2:L:244:ALA:HB1	16:L:1120:CLA:CMD	2.12	0.67
16:L:1108:CLA:CHD	16:L:1119:CLA:OBD	2.39	0.67
3:C:172:ALA:HB1	16:C:1083:CLA:C3D	2.24	0.67
1:A:337:HIS:CB	4:D:351:ALA:CB	2.73	0.67
3:C:425:TRP:CH2	16:C:1079:CLA:CAB	2.78	0.67
16:L:1111:CLA:C3A	16:L:1114:CLA:CMD	2.68	0.67
1:A:95:PRO:O	16:A:368:CLA:CAA	2.43	0.67
2:L:139:PHE:CD1	16:L:1120:CLA:C4A	2.78	0.67
17:A:367:PHO:HMD2	4:D:145:ALA:HB2	1.77	0.67
16:B:1111:CLA:C3A	16:B:1114:CLA:CMD	2.68	0.67
2:B:1092:UNK:O	11:O:132:UNK:O	1.88	0.66
3:C:425:TRP:C	16:C:1079:CLA:HMC3	2.16	0.66
4:D:209:LEU:HA	17:D:356:PHO:C3C	2.24	0.66
2:L:64:PRO:CB	16:L:1114:CLA:HMC2	2.24	0.66
2:L:204:ALA:HB1	16:L:1117:CLA:CMC	2.25	0.66
1:A:94:TYR:C	16:A:368:CLA:C3A	2.61	0.66
1:J:210:LEU:CB	17:J:366:PHO:NC	2.58	0.66
1:J:337:HIS:CB	4:N:351:ALA:CB	2.73	0.66
3:M:172:ALA:HB2	16:M:1082:CLA:CAD	2.23	0.66
16:L:1108:CLA:CAC	16:L:1119:CLA:CBD	2.74	0.66
1:A:235:TYR:CZ	2:B:5:TRP:N	2.64	0.66
4:N:209:LEU:HA	17:N:357:PHO:CAC	2.26	0.66
2:B:204:ALA:HB1	16:B:1117:CLA:CMC	2.26	0.66
2:B:465:GLY:HA2	16:B:1119:CLA:HMA1	0.67	0.66
3:M:425:TRP:CH2	16:M:1079:CLA:CAB	2.79	0.66
2:B:60:MET:CB	16:B:1110:CLA:HMA1	2.26	0.66
3:M:425:TRP:C	16:M:1079:CLA:HMC3	2.15	0.66
1:A:235:TYR:CE2	2:B:5:TRP:O	2.49	0.65
20:D:359:BCR:H312	20:D:359:BCR:H342	1.77	0.65
2:B:139:PHE:CB	16:B:1120:CLA:HMB2	2.26	0.65
1:J:147:TYR:CB	17:N:357:PHO:CMD	2.74	0.65
4:D:42:TYR:CE1	6:F:25:LEU:CB	2.80	0.65
16:L:1108:CLA:CAC	16:L:1119:CLA:C3D	2.75	0.65
13:0:41:HIS:NE2	21:0:138:HEM:C4B	2.64	0.65
3:M:278:ALA:CB	16:M:1088:CLA:H2A	2.26	0.65

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:316:THR:CA	4:D:62:GLY:O	2.45	0.65
3:C:172:ALA:HB2	16:C:1083:CLA:CAD	2.23	0.65
3:C:52:ALA:HB3	16:C:1082:CLA:CAB	2.22	0.64
2:B:9:HIS:HE1	16:B:1116:CLA:C1D	2.08	0.64
2:B:65:PHE:CA	16:B:1114:CLA:CAC	2.75	0.64
1:J:316:THR:CA	4:N:62:GLY:O	2.45	0.64
2:L:30:VAL:CB	16:L:1108:CLA:C3A	2.75	0.64
13:V:41:HIS:CD2	21:V:138:HEM:CHC	2.80	0.64
2:L:110:ALA:HB2	16:L:1121:CLA:HMB2	1.78	0.64
3:C:129:GLY:CA	16:C:1088:CLA:CAB	2.76	0.64
2:L:212:ALA:HB2	16:L:1107:CLA:HMD3	1.52	0.64
3:C:129:GLY:O	16:C:1088:CLA:HMB1	1.97	0.64
1:J:210:LEU:CA	17:J:366:PHO:C3C	2.77	0.64
2:L:1092:UNK:CA	11:Y:133:UNK:O	2.38	0.64
4:D:42:TYR:HE1	6:F:25:LEU:CB	2.11	0.63
2:B:60:MET:H	16:B:1110:CLA:HMA3	1.63	0.63
1:J:95:PRO:CB	16:J:367:CLA:CHB	2.76	0.63
13:0:41:HIS:CD2	21:0:138:HEM:CHC	2.82	0.63
2:L:22:ALA:CB	16:L:1109:CLA:CMB	2.76	0.63
2:B:141:ILE:O	16:B:1118:CLA:HMA2	1.98	0.62
1:A:158:PHE:CZ	16:A:366:CLA:HMC3	2.31	0.62
16:C:1080:CLA:CMD	16:C:1082:CLA:HMA3	2.09	0.62
1:J:95:PRO:HA	16:J:367:CLA:CMA	2.15	0.62
2:L:465:GLY:HA3	16:L:1119:CLA:CMA	2.27	0.62
3:M:172:ALA:HB1	16:M:1082:CLA:C3D	2.28	0.62
4:D:48:TRP:CZ3	20:D:359:BCR:H332	2.29	0.62
16:L:1108:CLA:HHD	16:L:1119:CLA:CAD	2.30	0.62
3:C:52:ALA:O	16:C:1082:CLA:CMB	2.45	0.62
3:M:128:GLY:C	16:M:1087:CLA:HMB1	2.20	0.62
1:A:145:VAL:CB	3:C:443:TRP:CB	2.77	0.62
16:N:355:CLA:HMB2	17:N:357:PHO:CMB	2.30	0.61
1:J:337:HIS:O	4:N:350:ASN:O	2.19	0.61
3:M:248:GLY:HA2	16:M:1078:CLA:CMA	2.31	0.61
1:A:337:HIS:O	4:D:350:ASN:O	2.19	0.61
1:J:147:TYR:CB	17:N:357:PHO:HMD1	2.31	0.61
3:M:53:HIS:CB	16:M:1085:CLA:C3B	2.79	0.61
2:L:68:ARG:O	16:L:1111:CLA:HMA3	2.01	0.61
3:C:1049:UNK:CB	11:O:13:UNK:C	2.79	0.60
5:E:8:PRO:CD	14:X:25:UNK:CB	2.79	0.60
2:B:240:SER:CB	16:B:1120:CLA:C1C	2.79	0.60
2:L:68:ARG:C	16:L:1111:CLA:HMA3	2.22	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:M:66:ALA:HB3	10:W:13:VAL:CB	2.32	0.60
2:L:139:PHE:CD1	16:L:1120:CLA:C1B	2.85	0.60
4:N:42:TYR:CD1	6:Q:25:LEU:CB	2.84	0.60
4:N:208:ALA:HB3	17:N:357:PHO:CMC	2.30	0.60
2:B:60:MET:CB	16:B:1110:CLA:CMA	2.80	0.60
1:J:221:SER:CB	4:N:138:VAL:CB	2.80	0.60
2:L:468:TRP:CH2	16:L:1119:CLA:HHC	2.32	0.60
2:B:204:ALA:C	16:B:1117:CLA:HMC3	2.22	0.60
2:B:190:PHE:CB	2:B:1001:UNK:CA	2.80	0.60
1:J:210:LEU:HA	17:J:366:PHO:CAC	2.31	0.60
2:B:9:HIS:CE1	16:B:1116:CLA:C1D	2.83	0.60
1:J:95:PRO:O	16:J:367:CLA:CAA	2.50	0.60
3:M:275:SER:C	16:M:1088:CLA:HMA3	2.21	0.60
1:A:216:GLY:C	4:D:271:MET:CB	2.69	0.59
4:D:200:GLY:C	16:D:354:CLA:HMA1	2.21	0.59
3:C:274:TYR:HD1	16:C:1081:CLA:HHD	1.67	0.59
2:L:212:ALA:CB	16:L:1107:CLA:C2D	2.78	0.59
2:B:22:ALA:CB	16:B:1109:CLA:CMB	2.76	0.59
2:B:204:ALA:HB3	16:B:1117:CLA:C4B	2.32	0.59
3:C:66:ALA:HB3	10:K:13:VAL:CB	2.32	0.59
2:L:204:ALA:C	16:L:1117:CLA:HMC3	2.22	0.59
2:B:87:ASP:CB	11:Y:87:UNK:C	2.81	0.59
1:J:145:VAL:CB	3:M:443:TRP:CB	2.81	0.59
1:A:86:SER:CB	3:C:218:PHE:CB	2.81	0.59
1:A:216:GLY:O	4:D:271:MET:CA	2.51	0.59
3:C:274:TYR:O	16:C:1089:CLA:H2A	2.02	0.59
2:L:150:CYS:CB	16:L:1113:CLA:CAB	2.81	0.59
2:B:212:ALA:HB2	16:B:1107:CLA:HMD3	1.60	0.59
2:L:190:PHE:CB	2:L:1001:UNK:CA	2.81	0.59
1:J:86:SER:CB	3:M:218:PHE:CB	2.81	0.58
2:L:240:SER:CB	16:L:1120:CLA:CHC	2.81	0.58
3:M:1049:UNK:CB	11:Y:13:UNK:C	2.80	0.58
2:B:110:ALA:HB2	16:B:1121:CLA:HMB2	1.85	0.58
1:J:39:PRO:CB	16:J:367:CLA:CAC	2.80	0.58
2:B:150:CYS:CB	16:B:1113:CLA:CAB	2.82	0.58
2:L:204:ALA:HB3	16:L:1117:CLA:C4B	2.32	0.58
3:M:52:ALA:O	16:M:1081:CLA:HMB2	2.03	0.58
3:M:70:PHE:CB	10:W:10:ASP:CB	2.82	0.58
3:C:60:ILE:CB	16:C:1080:CLA:CAA	2.81	0.58
3:C:1049:UNK:CB	11:O:14:UNK:CA	2.72	0.58
2:L:39:LEU:HA	2:L:43:ALA:HB3	1.83	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:L:468:TRP:CH2	16:L:1119:CLA:C1C	2.87	0.58
3:M:60:ILE:CB	16:W:64:CLA:CAA	2.82	0.57
2:L:110:ALA:HB1	16:L:1121:CLA:HMB2	1.86	0.57
4:N:200:GLY:C	16:N:354:CLA:HMA1	2.23	0.57
4:D:113:PHE:CZ	16:D:357:CLA:C1A	2.87	0.57
17:J:366:PHO:HMB2	16:N:356:CLA:CAB	2.34	0.57
13:V:41:HIS:HD2	21:V:138:HEM:CHC	2.16	0.57
4:N:209:LEU:CA	17:N:357:PHO:C4C	2.79	0.57
1:J:95:PRO:HA	16:J:367:CLA:CAA	2.35	0.57
2:L:150:CYS:HA	16:L:1113:CLA:CMB	2.34	0.57
1:J:216:GLY:C	4:N:271:MET:CB	2.69	0.57
1:A:235:TYR:HE2	2:B:5:TRP:HA	0.77	0.57
3:C:70:PHE:CB	10:K:10:ASP:CB	2.82	0.56
2:L:468:TRP:CZ2	16:L:1119:CLA:HHC	2.40	0.56
2:B:150:CYS:HA	16:B:1113:CLA:CMB	2.36	0.56
4:D:200:GLY:C	16:D:354:CLA:CMA	2.73	0.56
13:V:41:HIS:NE2	21:V:138:HEM:C4B	2.72	0.56
1:J:147:TYR:CB	17:N:357:PHO:HMD2	2.36	0.56
2:B:68:ARG:C	16:B:1111:CLA:HMA3	2.26	0.56
3:C:275:SER:C	16:C:1089:CLA:CMA	2.52	0.55
3:M:1049:UNK:CB	11:Y:14:UNK:CA	2.73	0.55
4:N:209:LEU:CB	17:N:357:PHO:C4C	2.84	0.55
2:B:69:LEU:HA	16:B:1111:CLA:H2A	1.88	0.55
3:C:278:ALA:HB3	16:C:1089:CLA:C3A	2.35	0.55
2:B:65:PHE:CB	16:B:1114:CLA:CAC	2.73	0.55
2:B:110:ALA:HB1	16:B:1121:CLA:HMB2	1.88	0.55
2:B:450:TRP:CB	16:B:1110:CLA:HMB3	2.27	0.55
3:C:129:GLY:CA	16:C:1088:CLA:CMB	2.62	0.55
3:C:282:MET:O	16:C:1085:CLA:CAA	2.54	0.54
2:B:68:ARG:O	16:B:1111:CLA:HMA3	2.07	0.54
3:M:67:MET:N	10:W:13:VAL:CB	2.69	0.54
3:M:275:SER:CA	16:M:1088:CLA:HMA3	2.38	0.54
16:N:355:CLA:CMB	17:N:357:PHO:HMB2	2.38	0.54
1:A:216:GLY:O	4:D:271:MET:C	2.45	0.54
3:C:67:MET:N	10:K:13:VAL:CB	2.70	0.54
2:L:28:ALA:HB1	2:L:104:SER:HA	1.89	0.54
4:D:160:TYR:HE2	4:D:171:PRO:O	1.91	0.54
3:M:167:VAL:CB	16:M:1085:CLA:CMD	2.68	0.53
7:R:212:UNK:CA	8:S:3:UNK:CB	2.86	0.53
1:A:297:LEU:O	3:C:1075:UNK:CB	2.57	0.53
3:C:248:GLY:HA2	16:C:1078:CLA:HMA3	1.90	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:J:324:ALA:O	4:N:330:ALA:HB2	2.02	0.53
2:B:465:GLY:O	16:B:1119:CLA:HMA3	2.09	0.53
2:B:465:GLY:HA2	16:B:1119:CLA:C3A	2.32	0.53
11:O:153:UNK:H	12:U:9:UNK:CB	2.21	0.53
3:M:275:SER:HA	16:M:1088:CLA:HMA3	1.91	0.53
1:A:210:LEU:CB	17:A:367:PHO:CMC	2.87	0.52
1:J:297:LEU:O	3:M:1075:UNK:CB	2.57	0.52
2:B:212:ALA:HB1	16:B:1107:CLA:HMD3	1.75	0.52
3:M:278:ALA:HB3	16:M:1088:CLA:C2A	2.37	0.52
13:0:41:HIS:HD2	21:0:138:HEM:CHC	2.22	0.52
4:N:209:LEU:CA	17:N:357:PHO:C2C	2.87	0.52
1:A:158:PHE:CZ	16:A:366:CLA:CMC	2.89	0.52
3:M:164:HIS:CB	16:M:1088:CLA:CAB	2.88	0.52
13:V:40:CYS:CB	21:V:138:HEM:C2B	2.93	0.52
16:A:369:CLA:CAB	16:C:1081:CLA:CMC	2.74	0.52
2:L:468:TRP:CZ2	16:L:1119:CLA:C4B	2.92	0.52
3:C:286:ALA:HB3	16:C:1085:CLA:CAA	2.40	0.52
4:N:208:ALA:CB	17:N:357:PHO:CMC	2.88	0.51
16:A:365:CLA:CMB	16:D:354:CLA:HMB2	2.31	0.51
3:M:1029:UNK:O	11:Y:129:UNK:CB	2.59	0.51
2:L:240:SER:CB	16:L:1120:CLA:HMC3	2.41	0.51
3:C:1029:UNK:O	11:O:129:UNK:CB	2.58	0.51
2:B:69:LEU:CB	16:B:1111:CLA:H2A	2.41	0.51
3:C:66:ALA:O	10:K:13:VAL:CB	2.57	0.51
3:C:297:TYR:N	3:C:298:PRO:HD2	2.25	0.51
3:M:275:SER:HA	16:M:1088:CLA:C1A	2.40	0.51
1:A:85:SER:O	3:C:220:GLY:HA3	2.10	0.51
16:C:1078:CLA:CMD	16:C:1089:CLA:CAD	2.88	0.51
4:N:42:TYR:HE1	6:Q:25:LEU:CA	2.24	0.51
1:A:210:LEU:CB	17:A:367:PHO:C3C	2.89	0.51
3:C:66:ALA:HB1	10:K:13:VAL:CB	2.41	0.51
2:B:65:PHE:CZ	16:B:1114:CLA:CMC	2.90	0.51
16:B:1107:CLA:CMC	16:B:1120:CLA:C4C	2.88	0.51
4:D:113:PHE:HE1	16:D:357:CLA:NA	1.66	0.51
2:B:240:SER:CB	16:B:1120:CLA:C2C	2.88	0.51
3:M:278:ALA:HB3	16:M:1088:CLA:CMA	2.36	0.51
16:C:1080:CLA:CAC	16:C:1087:CLA:C3C	2.89	0.51
16:M:1086:CLA:C3C	16:W:64:CLA:CAC	2.89	0.51
1:A:147:TYR:CB	17:D:356:PHO:HMD2	2.41	0.50
1:J:95:PRO:CA	16:J:367:CLA:CMA	2.81	0.50
1:A:316:THR:HA	4:D:62:GLY:O	2.12	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:C:266:TRP:HZ3	16:C:1089:CLA:HMD1	1.77	0.50
16:C:1086:CLA:CMA	16:C:1088:CLA:CAC	2.79	0.50
3:M:66:ALA:HB1	10:W:13:VAL:CB	2.41	0.50
1:A:186:PHE:CB	16:A:365:CLA:HMD3	2.42	0.50
4:N:184:PHE:O	16:N:354:CLA:C3C	2.56	0.50
3:C:278:ALA:CB	16:C:1089:CLA:HMA2	2.21	0.50
3:M:66:ALA:O	10:W:13:VAL:CB	2.59	0.50
17:A:367:PHO:HMC2	4:D:148:ALA:CB	2.24	0.49
1:J:85:SER:O	3:M:220:GLY:HA3	2.12	0.49
1:J:324:ALA:C	4:N:330:ALA:HB1	2.33	0.49
2:L:464:PHE:CE2	16:L:1119:CLA:HMB3	2.47	0.49
1:A:94:TYR:CA	16:A:368:CLA:HMA1	2.43	0.49
4:N:117:HIS:CE1	16:N:358:CLA:NC	2.80	0.49
1:J:142:TRP:NE1	3:M:447:ARG:CB	2.75	0.49
13:0:92:HIS:NE2	21:0:138:HEM:NB	2.60	0.49
1:A:216:GLY:O	4:D:271:MET:O	2.30	0.49
2:B:30:VAL:HA	16:B:1108:CLA:H3A	1.94	0.49
3:C:440:GLY:HA3	16:C:1087:CLA:CAD	2.43	0.49
4:D:75:THR:HA	4:D:111:TRP:HB2	1.93	0.49
3:M:440:GLY:HA3	16:M:1086:CLA:CAD	2.42	0.49
4:D:160:TYR:CD2	4:D:172:SER:HA	2.48	0.49
1:J:316:THR:HA	4:N:62:GLY:O	2.12	0.49
2:L:240:SER:O	16:L:1120:CLA:C4C	2.61	0.48
3:C:1030:UNK:HA	11:O:129:UNK:CB	2.43	0.48
13:V:92:HIS:NE2	21:V:138:HEM:NB	2.60	0.48
13:0:41:HIS:HD2	21:0:138:HEM:C4B	2.30	0.48
3:C:266:TRP:HZ3	16:C:1089:CLA:CMD	2.26	0.48
1:J:216:GLY:O	4:N:271:MET:C	2.51	0.48
11:O:66:UNK:O	11:O:103:UNK:HA	2.14	0.48
3:C:164:HIS:CE1	16:C:1086:CLA:C1D	2.80	0.48
4:D:77:ALA:HB3	4:D:171:PRO:HA	1.96	0.48
2:L:204:ALA:HB1	16:L:1117:CLA:C1C	2.40	0.48
2:L:244:ALA:HB2	16:L:1120:CLA:HHD	1.96	0.48
1:A:39:PRO:CB	16:A:368:CLA:CAC	2.92	0.48
16:A:366:CLA:CAB	17:D:356:PHO:HMB2	2.44	0.48
2:B:69:LEU:CA	16:B:1111:CLA:H2A	2.44	0.48
3:M:1030:UNK:HA	11:Y:129:UNK:CB	2.44	0.48
3:M:129:GLY:O	16:M:1087:CLA:CMB	2.60	0.48
2:B:65:PHE:CG	16:B:1114:CLA:CAC	1.99	0.48
1:J:95:PRO:N	16:J:367:CLA:CHB	2.77	0.47
2:L:204:ALA:CB	16:L:1117:CLA:C4B	2.85	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
11:O:152:UNK:HA	12:U:9:UNK:CB	2.40	0.47
3:M:52:ALA:O	16:M:1081:CLA:CMB	2.63	0.47
1:A:143:ILE:HA	4:D:216:ALA:HB1	1.97	0.47
2:B:22:ALA:C	16:B:1109:CLA:CMB	2.65	0.47
1:A:235:TYR:HE2	2:B:5:TRP:CB	2.24	0.47
3:C:66:ALA:HB3	10:K:13:VAL:HA	1.97	0.47
1:J:210:LEU:HA	17:J:366:PHO:C3C	2.45	0.47
1:J:324:ALA:HB1	4:N:330:ALA:HB1	1.97	0.47
2:L:240:SER:CB	16:L:1120:CLA:CMC	2.92	0.47
2:L:468:TRP:CH2	16:L:1119:CLA:C4B	2.95	0.47
1:A:141:PRO:O	4:D:220:ASN:CB	2.63	0.47
1:A:95:PRO:C	16:A:368:CLA:CAA	2.83	0.47
1:A:324:ALA:O	4:D:330:ALA:HB2	2.03	0.47
2:B:204:ALA:HB1	16:B:1117:CLA:C1C	2.41	0.47
2:L:30:VAL:CB	16:L:1108:CLA:C2A	2.91	0.47
4:N:213:ILE:HA	17:N:357:PHO:HMD3	1.97	0.46
1:J:216:GLY:CA	4:N:271:MET:CB	2.92	0.46
2:L:221:PRO:O	7:R:184:UNK:CA	2.64	0.46
4:N:208:ALA:CB	17:N:357:PHO:HMC1	2.44	0.46
1:A:324:ALA:C	4:D:330:ALA:HB1	2.34	0.46
3:C:278:ALA:HB3	16:C:1089:CLA:C2A	2.45	0.46
1:J:141:PRO:O	4:N:220:ASN:CB	2.63	0.46
2:B:87:ASP:CB	11:Y:87:UNK:O	2.63	0.46
1:J:95:PRO:N	16:J:367:CLA:CMA	2.77	0.46
17:J:366:PHO:C3C	4:N:148:ALA:HB3	2.43	0.46
17:J:366:PHO:HMC2	4:N:148:ALA:HB1	1.92	0.46
16:M:1084:CLA:HMC3	16:W:64:CLA:H2A	1.96	0.46
2:B:141:ILE:O	16:B:1118:CLA:CMA	2.61	0.46
2:L:1092:UNK:CA	11:Y:133:UNK:C	2.84	0.46
16:L:1115:CLA:HMA2	16:L:1120:CLA:CMC	2.42	0.46
4:N:75:THR:HA	4:N:111:TRP:HB2	1.98	0.46
3:M:1048:UNK:HA	11:Y:14:UNK:N	2.30	0.46
4:N:208:ALA:HB1	17:N:357:PHO:HMC1	1.98	0.46
13:0:40:CYS:CB	21:0:138:HEM:C2B	2.99	0.46
13:0:34:GLN:HA	13:0:38:ALA:HB2	1.97	0.46
3:C:274:TYR:CD1	16:C:1081:CLA:HHD	2.49	0.46
1:J:143:ILE:HA	4:N:216:ALA:HB1	1.97	0.46
3:M:1033:UNK:CB	11:Y:81:UNK:CB	2.94	0.46
16:C:1078:CLA:HMD1	16:C:1089:CLA:C2D	2.45	0.46
2:L:68:ARG:CB	16:L:1111:CLA:HMA2	2.43	0.46
1:A:332:HIS:NE2	4:D:349:GLY:N	2.64	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:J:189:GLU:HB3	3:M:412:THR:CB	2.46	0.45
1:A:189:GLU:HB3	3:C:412:THR:CB	2.47	0.45
4:D:258:GLY:HA2	4:D:262:SER:O	2.16	0.45
3:C:1052:UNK:CB	11:O:12:UNK:CA	2.95	0.45
2:L:464:PHE:CZ	16:L:1119:CLA:HMB3	2.51	0.45
3:M:66:ALA:HB3	10:W:13:VAL:HA	1.97	0.45
17:J:366:PHO:CAC	4:N:148:ALA:HB3	2.45	0.45
1:A:216:GLY:CA	4:D:271:MET:CB	2.95	0.45
2:B:1092:UNK:CA	11:O:133:UNK:C	2.84	0.45
3:C:1033:UNK:CB	11:O:81:UNK:CB	2.94	0.45
4:D:79:SER:HA	4:D:170:ALA:CB	2.47	0.45
1:J:216:GLY:O	4:N:271:MET:CA	2.58	0.45
1:J:332:HIS:NE2	4:N:349:GLY:N	2.64	0.45
4:N:258:GLY:HA2	4:N:262:SER:O	2.16	0.45
1:A:114:LEU:CB	16:A:368:CLA:HMA3	2.47	0.45
2:B:204:ALA:CB	16:B:1117:CLA:C4B	2.85	0.45
1:A:324:ALA:HB1	4:D:330:ALA:HB1	1.97	0.45
3:C:1048:UNK:HA	11:O:14:UNK:N	2.32	0.45
3:M:128:GLY:C	16:M:1087:CLA:CMB	2.75	0.45
1:J:329:GLU:C	4:N:326:ARG:CB	2.55	0.44
2:L:1091:UNK:C	11:Y:134:UNK:HA	2.47	0.44
16:M:1081:CLA:HMA1	16:W:64:CLA:C1D	2.47	0.44
16:N:355:CLA:CMB	17:N:357:PHO:CMB	2.94	0.44
2:B:60:MET:CB	16:B:1110:CLA:CHB	2.95	0.44
2:B:68:ARG:CB	16:B:1111:CLA:HMA2	2.42	0.44
3:M:1052:UNK:CB	11:Y:12:UNK:CA	2.93	0.44
3:C:410:VAL:HA	3:C:415:ASN:HA	2.00	0.44
1:J:142:TRP:HE1	3:M:447:ARG:CB	2.30	0.44
2:B:1091:UNK:C	11:O:134:UNK:HA	2.47	0.44
4:D:200:GLY:O	16:D:354:CLA:HMA2	2.08	0.44
3:M:247:GLY:O	16:M:1078:CLA:HMA1	2.17	0.44
4:N:212:ALA:CB	17:N:357:PHO:HHD	2.46	0.44
2:B:30:VAL:CB	16:B:1108:CLA:H3A	2.48	0.44
5:E:8:PRO:HD3	14:X:25:UNK:CB	2.48	0.44
2:B:1092:UNK:CA	11:O:133:UNK:O	2.38	0.44
3:C:247:GLY:C	16:C:1078:CLA:CMA	2.86	0.44
16:C:1078:CLA:HMD3	16:C:1089:CLA:CMD	2.48	0.44
6:F:40:GLN:HA	9:I:26:UNK:CB	2.47	0.44
13:V:34:GLN:HA	13:V:38:ALA:HB2	1.99	0.44
3:M:1070:UNK:CB	13:0:39:SER:O	2.65	0.44
16:N:355:CLA:HMB2	17:N:357:PHO:HMB2	1.97	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:C:275:SER:HA	16:C:1089:CLA:C2A	2.48	0.43
1:J:143:ILE:CA	4:N:216:ALA:HB1	2.48	0.43
3:C:283:GLY:HA2	16:C:1085:CLA:CAA	2.48	0.43
13:V:41:HIS:HD2	21:V:138:HEM:C4B	2.25	0.43
1:A:143:ILE:CA	4:D:216:ALA:HB1	2.49	0.43
2:B:69:LEU:CA	16:B:1111:CLA:HMA2	2.48	0.43
2:L:22:ALA:C	16:L:1109:CLA:CMB	2.68	0.43
3:C:179:ALA:HB1	3:C:184:GLY:HA2	2.01	0.43
3:M:410:VAL:HA	3:M:415:ASN:HA	1.99	0.43
2:B:450:TRP:HB3	16:B:1110:CLA:HMB2	0.47	0.43
3:M:425:TRP:CG	16:M:1079:CLA:CAB	2.92	0.43
16:M:1084:CLA:CMC	16:W:64:CLA:H2A	2.49	0.43
2:B:22:ALA:HB1	16:B:1109:CLA:C2B	2.48	0.43
2:L:1092:UNK:HA	11:Y:133:UNK:CA	2.48	0.43
3:M:429:SER:CB	16:M:1079:CLA:HMC1	2.48	0.43
2:L:204:ALA:HB1	16:L:1117:CLA:HMC3	1.99	0.43
2:L:450:TRP:O	16:L:1110:CLA:HMB1	2.19	0.42
1:A:285:PHE:CD1	3:C:436:PHE:HD1	2.37	0.42
3:C:275:SER:HA	16:C:1089:CLA:C3A	2.49	0.42
16:L:1111:CLA:C4A	16:L:1114:CLA:HMD2	2.47	0.42
2:B:9:HIS:CE1	16:B:1116:CLA:C4D	2.85	0.42
3:C:429:SER:CB	16:C:1079:CLA:HMC1	2.47	0.42
4:D:79:SER:HA	4:D:170:ALA:HB2	2.01	0.42
2:B:9:HIS:NE2	16:B:1116:CLA:NC	2.67	0.42
2:B:1092:UNK:HA	11:O:133:UNK:CA	2.48	0.42
16:B:1107:CLA:CMC	16:B:1120:CLA:C3C	2.98	0.42
4:D:184:PHE:O	16:D:354:CLA:CAC	2.68	0.42
1:J:216:GLY:O	4:N:271:MET:O	2.37	0.42
3:C:1070:UNK:CB	13:V:39:SER:O	2.68	0.42
3:C:426:LEU:HA	16:C:1079:CLA:CMC	2.50	0.42
3:M:129:GLY:HA2	16:M:1087:CLA:CMB	1.56	0.42
17:A:367:PHO:HMC1	4:D:148:ALA:HB2	1.94	0.42
1:J:285:PHE:CD1	3:M:436:PHE:HD1	2.37	0.42
17:J:366:PHO:CMC	4:N:148:ALA:CB	2.83	0.42
3:C:129:GLY:HA2	16:C:1088:CLA:C3B	2.49	0.41
2:L:139:PHE:CE1	16:L:1120:CLA:NA	2.88	0.41
2:L:155:ALA:O	2:L:156:PHE:HB3	2.19	0.41
1:A:186:PHE:CB	16:A:365:CLA:CMD	2.99	0.41
4:D:209:LEU:HA	17:D:356:PHO:C2C	2.49	0.41
4:D:308:ASP:N	4:D:309:PRO:HD3	2.35	0.41
2:L:191:ASN:HA	2:L:192:PRO:HD3	1.84	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:L:240:SER:O	16:L:1120:CLA:C3C	2.68	0.41
1:J:85:SER:CB	3:M:221:GLU:C	2.86	0.41
1:A:210:LEU:CB	17:A:367:PHO:HMC3	2.50	0.41
2:B:31:ALA:HB2	16:B:1114:CLA:CHB	2.51	0.41
1:A:235:TYR:OH	2:B:5:TRP:CA	2.64	0.41
3:C:274:TYR:CD1	16:C:1081:CLA:HMD3	2.56	0.41
1:J:95:PRO:CA	16:J:367:CLA:CAA	2.98	0.41
1:A:95:PRO:CB	16:A:368:CLA:CAA	2.99	0.41
16:M:1081:CLA:HMA1	16:W:64:CLA:C2D	2.46	0.41
3:M:56:HIS:CB	16:M:1081:CLA:HMB2	2.51	0.41
2:B:28:ALA:HB1	2:B:104:SER:HA	2.03	0.41
3:C:275:SER:HA	16:C:1089:CLA:C1A	2.51	0.41
12:U:74:UNK:C	12:U:76:UNK:H	2.33	0.41
4:D:42:TYR:CD1	6:F:25:LEU:CB	3.04	0.41
4:D:209:LEU:CB	17:D:356:PHO:C1C	2.99	0.41
3:M:1048:UNK:CA	11:Y:14:UNK:N	2.82	0.41
16:C:1078:CLA:HMD2	16:C:1089:CLA:OBD	2.21	0.41
2:L:150:CYS:CA	16:L:1113:CLA:CMB	2.99	0.41
3:C:164:HIS:ND1	16:C:1086:CLA:C1D	2.84	0.40
3:C:266:TRP:HH2	16:C:1078:CLA:HHD	1.86	0.40
3:M:426:LEU:HA	16:M:1079:CLA:CMC	2.51	0.40
1:A:94:TYR:CB	16:A:368:CLA:HHB	2.51	0.40
2:L:64:PRO:CB	16:L:1114:CLA:CMC	2.97	0.40
14:1:21:UNK:C	14:1:23:UNK:H	2.33	0.40
2:B:1092:UNK:HA	11:O:133:UNK:N	2.32	0.40
16:B:1111:CLA:C4A	16:B:1114:CLA:HMD2	2.47	0.40
3:C:425:TRP:CG	16:C:1079:CLA:CAB	2.94	0.40

There are no symmetry-related clashes.

5.3 Torsion angles (i)

5.3.1 Protein backbone (i)

In the following table, the Percentiles column shows the percent Ramachandran outliers of the chain as a percentile score with respect to all 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	293/360 (81%)	195 (67%)	66 (22%)	32 (11%)	0 6
1	J	293/360 (81%)	199 (68%)	59 (20%)	35 (12%)	0 5
2	B	314/472 (66%)	219 (70%)	62 (20%)	33 (10%)	0 6
2	L	309/472 (66%)	215 (70%)	60 (19%)	34 (11%)	0 6
3	C	263/473 (56%)	198 (75%)	47 (18%)	18 (7%)	1 16
3	M	257/473 (54%)	189 (74%)	47 (18%)	21 (8%)	1 11
4	D	269/352 (76%)	187 (70%)	56 (21%)	26 (10%)	0 8
4	N	269/352 (76%)	184 (68%)	59 (22%)	26 (10%)	0 8
5	E	33/83 (40%)	23 (70%)	5 (15%)	5 (15%)	0 3
5	P	15/83 (18%)	11 (73%)	4 (27%)	0	100 100
6	F	28/44 (64%)	22 (79%)	3 (11%)	3 (11%)	0 6
6	Q	24/44 (54%)	22 (92%)	2 (8%)	0	100 100
10	K	25/37 (68%)	14 (56%)	9 (36%)	2 (8%)	1 12
10	W	25/37 (68%)	15 (60%)	8 (32%)	2 (8%)	1 12
13	0	111/137 (81%)	90 (81%)	17 (15%)	4 (4%)	3 29
13	V	127/137 (93%)	102 (80%)	19 (15%)	6 (5%)	2 23
All	All	2655/3916 (68%)	1885 (71%)	523 (20%)	247 (9%)	0 9

All (247) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	94	TYR
1	A	101	SER
1	A	168	PHE
1	A	191	ASN
1	A	192	ILE
1	A	195	HIS
1	A	196	PRO
1	A	306	VAL
1	A	313	VAL
2	B	49	ASP
2	B	130	GLU
2	B	170	ASP
2	B	183	PRO
2	B	447	PRO
3	C	190	ALA
3	C	191	PRO

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Mol	Chain	Res	Type
3	C	196	VAL
3	C	410	VAL
3	C	422	PRO
4	D	56	THR
4	D	57	SER
4	D	122	LEU
4	D	139	ARG
4	D	149	PRO
4	D	330	ALA
6	F	17	VAL
10	K	17	PRO
1	J	94	TYR
1	J	101	SER
1	J	168	PHE
1	J	191	ASN
1	J	192	ILE
1	J	195	HIS
1	J	196	PRO
1	J	222	SER
1	J	306	VAL
1	J	313	VAL
2	L	56	TRP
2	L	170	ASP
2	L	183	PRO
2	L	442	ILE
2	L	447	PRO
3	M	79	LYS
3	M	110	PRO
3	M	190	ALA
3	M	191	PRO
3	M	196	VAL
3	M	410	VAL
4	N	56	THR
4	N	57	SER
4	N	139	ARG
4	N	149	PRO
4	N	308	ASP
4	N	330	ALA
10	W	17	PRO
13	0	45	ILE
1	A	36	ILE
1	A	58	VAL

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Mol	Chain	Res	Type
1	A	143	ILE
1	A	169	SER
1	A	226	GLU
1	A	234	ASN
1	A	261	GLN
1	A	264	SER
1	A	334	ARG
2	B	50	PRO
2	B	159	THR
2	B	180	PRO
2	B	198	VAL
3	C	78	GLU
3	C	79	LYS
3	C	99	VAL
3	C	189	TRP
3	C	227	VAL
4	D	76	VAL
4	D	249	ALA
4	D	341	PHE
4	D	342	PRO
5	E	8	PRO
5	E	20	VAL
1	J	36	ILE
1	J	58	VAL
1	J	143	ILE
1	J	169	SER
1	J	261	GLN
1	J	264	SER
1	J	334	ARG
2	L	6	TYR
2	L	49	ASP
2	L	50	PRO
2	L	51	VAL
2	L	159	THR
2	L	180	PRO
2	L	187	PRO
2	L	198	VAL
3	M	78	GLU
3	M	189	TRP
3	M	227	VAL
3	M	262	ARG
3	M	422	PRO

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Mol	Chain	Res	Type
3	M	454	GLY
4	N	76	VAL
4	N	249	ALA
4	N	341	PHE
4	N	342	PRO
1	A	68	SER
1	A	263	ALA
1	A	318	ALA
2	B	6	TYR
2	B	13	ILE
2	B	75	TRP
2	B	121	GLU
2	B	163	GLY
2	B	187	PRO
2	B	193	TYR
2	B	441	GLY
3	C	94	THR
3	C	411	ALA
3	C	454	GLY
4	D	53	THR
4	D	147	SER
5	E	13	ILE
6	F	18	ARG
13	V	82	TYR
1	J	68	SER
1	J	263	ALA
1	J	318	ALA
2	L	13	ILE
2	L	44	THR
2	L	48	SER
2	L	54	PRO
2	L	55	MET
2	L	132	ALA
3	M	94	THR
3	M	137	PRO
3	M	411	ALA
4	N	53	THR
4	N	123	ILE
4	N	147	SER
4	N	195	PRO
13	0	82	TYR
1	A	93	PHE

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Mol	Chain	Res	Type
1	A	303	ASN
1	A	338	ASN
2	B	132	ALA
2	B	199	VAL
2	B	412	THR
2	B	442	ILE
3	C	77	PRO
3	C	104	GLU
4	D	123	ILE
4	D	313	THR
4	D	345	VAL
5	E	14	THR
6	F	14	ILE
1	J	93	PHE
1	J	303	ASN
1	J	338	ASN
2	L	52	LEU
2	L	88	PRO
2	L	121	GLU
2	L	163	GLY
2	L	193	TYR
2	L	199	VAL
2	L	412	THR
3	M	77	PRO
4	N	313	THR
4	N	345	VAL
1	A	74	GLY
1	A	81	ALA
1	A	99	ALA
1	A	176	ILE
2	B	5	TRP
2	B	11	VAL
2	B	55	MET
2	B	56	TRP
2	B	57	ARG
2	B	166	MET
2	B	192	PRO
2	B	225	LEU
2	B	443	PHE
3	C	455	PHE
4	D	55	VAL
4	D	140	PRO

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Mol	Chain	Res	Type
4	D	170	ALA
4	D	298	PHE
4	D	339	PHE
4	D	348	ARG
13	V	16	GLY
13	V	78	ASN
1	J	74	GLY
1	J	81	ALA
1	J	99	ALA
1	J	176	ILE
1	J	234	ASN
1	J	238	LYS
2	L	5	TRP
2	L	11	VAL
2	L	166	MET
2	L	225	LEU
2	L	443	PHE
3	M	264	PHE
4	N	55	VAL
4	N	170	ALA
4	N	176	ALA
4	N	310	GLU
4	N	339	PHE
4	N	348	ARG
13	0	78	ASN
1	A	62	GLY
1	A	83	VAL
1	A	299	GLY
2	B	44	THR
3	C	193	GLY
3	C	414	ILE
4	D	75	THR
1	J	62	GLY
1	J	83	VAL
1	J	299	GLY
2	L	192	PRO
3	M	109	PHE
3	M	414	ILE
4	N	124	GLY
4	N	140	PRO
2	B	51	VAL
4	D	138	VAL

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Mol	Chain	Res	Type
4	D	346	LEU
13	V	19	ILE
2	L	219	VAL
3	M	193	GLY
4	N	138	VAL
4	N	346	LEU
10	W	21	VAL
10	K	21	VAL
1	J	224	ILE
3	M	134	ILE
2	B	71	VAL
4	D	99	GLY
4	D	124	GLY
5	E	40	GLY
1	A	60	ILE
13	V	45	ILE
13	V	101	PHE
1	J	60	ILE
13	0	101	PHE
1	J	39	PRO
2	L	71	VAL

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	21/290 (7%)	20 (95%)	1 (5%)	25 56
1	J	22/290 (8%)	21 (96%)	1 (4%)	27 57
2	B	21/290 (7%)	21 (100%)	0	100 100
2	L	21/290 (7%)	21 (100%)	0	100 100
3	C	16/315 (5%)	16 (100%)	0	100 100
3	M	10/315 (3%)	9 (90%)	1 (10%)	7 32
4	D	16/283 (6%)	16 (100%)	0	100 100
4	N	14/283 (5%)	14 (100%)	0	100 100

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
5	E	1/72 (1%)	1 (100%)	0	100 100
6	F	3/38 (8%)	3 (100%)	0	100 100
10	K	1/30 (3%)	1 (100%)	0	100 100
10	W	1/30 (3%)	1 (100%)	0	100 100
13	0	5/117 (4%)	5 (100%)	0	100 100
13	V	7/117 (6%)	7 (100%)	0	100 100
All	All	159/2760 (6%)	156 (98%)	3 (2%)	57 76

All (3) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	182	PHE
1	J	182	PHE
3	M	422	PRO

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (6) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	332	HIS
2	B	9	HIS
3	C	164	HIS
1	J	332	HIS
3	M	164	HIS
4	N	117	HIS

5.3.3 RNA (i)

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates (i)

There are no monosaccharides in this entry.

5.6 Ligand geometry (i)

Of 94 ligands modelled in this entry, 10 are monoatomic - leaving 84 for Mogul analysis.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\| > 2$	Counts	RMSZ	$\#\|Z\| > 2$
21	HEM	E	84	-	22,32,50	2.71	7 (31%)	25,54,82	3.06	13 (52%)
17	PHO	A	367	-	22,39,69	1.38	4 (18%)	17,62,99	2.52	7 (41%)
16	CLA	L	1110	-	36,43,73	1.99	9 (25%)	45,76,113	2.24	9 (20%)
16	CLA	A	368	-	36,43,73	2.01	7 (19%)	45,76,113	2.19	8 (17%)
16	CLA	J	367	-	36,43,73	2.01	8 (22%)	45,76,113	2.19	8 (17%)
16	CLA	L	1108	-	36,43,73	1.99	8 (22%)	45,76,113	2.19	8 (17%)
16	CLA	M	1084	-	36,43,73	2.00	8 (22%)	45,76,113	2.21	7 (15%)
16	CLA	M	1083	-	36,43,73	1.99	8 (22%)	45,76,113	2.22	9 (20%)
16	CLA	R	221	-	36,43,73	1.93	11 (30%)	45,76,113	2.19	10 (22%)
16	CLA	L	1114	-	36,43,73	2.01	7 (19%)	45,76,113	2.24	10 (22%)
16	CLA	C	1082	-	36,43,73	2.00	8 (22%)	45,76,113	2.21	8 (17%)
16	CLA	D	354	4	36,43,73	1.85	9 (25%)	45,76,113	2.24	9 (20%)
17	PHO	J	366	-	22,39,69	1.37	3 (13%)	17,62,99	2.53	7 (41%)
16	CLA	J	368	-	36,43,73	1.99	8 (22%)	45,76,113	2.23	9 (20%)
16	CLA	M	1078	-	36,43,73	2.03	8 (22%)	45,76,113	2.20	7 (15%)
16	CLA	L	1111	-	36,43,73	2.01	8 (22%)	45,76,113	2.19	8 (17%)
16	CLA	N	355	-	36,43,73	1.90	11 (30%)	45,76,113	2.20	8 (17%)
16	CLA	B	1111	-	36,43,73	2.01	7 (19%)	45,76,113	2.21	8 (17%)
16	CLA	L	1122	-	36,43,73	2.00	7 (19%)	45,76,113	2.21	8 (17%)
16	CLA	L	1118	-	36,43,73	2.00	8 (22%)	45,76,113	2.22	8 (17%)
16	CLA	L	1109	-	36,43,73	1.99	7 (19%)	45,76,113	2.19	9 (20%)
16	CLA	M	1079	-	36,43,73	2.00	7 (19%)	45,76,113	2.23	9 (20%)
16	CLA	L	1113	-	36,43,73	2.00	7 (19%)	45,76,113	2.22	8 (17%)
16	CLA	B	1113	-	36,43,73	1.99	7 (19%)	45,76,113	2.23	9 (20%)
16	CLA	C	1081	-	36,43,73	1.99	8 (22%)	45,76,113	2.22	8 (17%)
16	CLA	D	357	-	36,43,73	2.01	8 (22%)	45,76,113	2.25	9 (20%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
16	CLA	B	1110	-	36,43,73	1.99	9 (25%)	45,76,113	2.24	9 (20%)
16	CLA	L	1120	-	36,43,73	2.00	9 (25%)	45,76,113	2.20	9 (20%)
21	HEM	P	92	-	22,32,50	2.70	7 (31%)	25,54,82	3.07	13 (52%)
16	CLA	B	1109	-	36,43,73	1.98	7 (19%)	45,76,113	2.20	8 (17%)
16	CLA	B	1117	-	36,43,73	2.01	8 (22%)	45,76,113	2.20	10 (22%)
21	HEM	V	138	13	22,32,50	2.71	7 (31%)	25,54,82	3.05	13 (52%)
16	CLA	M	1082	-	36,43,73	1.99	7 (19%)	45,76,113	2.21	8 (17%)
17	PHO	D	356	-	22,39,69	1.34	3 (13%)	17,62,99	2.50	7 (41%)
16	CLA	M	1087	3	36,43,73	2.00	8 (22%)	45,76,113	2.21	8 (17%)
16	CLA	L	1121	-	36,43,73	1.98	7 (19%)	45,76,113	2.23	10 (22%)
16	CLA	G	221	-	36,43,73	1.93	11 (30%)	45,76,113	2.17	10 (22%)
16	CLA	J	365	-	36,43,73	1.86	8 (22%)	45,76,113	2.68	14 (31%)
16	CLA	B	1112	-	36,43,73	1.99	9 (25%)	45,76,113	2.22	10 (22%)
16	CLA	B	1107	-	36,43,73	1.99	7 (19%)	45,76,113	2.20	8 (17%)
21	HEM	0	138	13	22,32,50	2.71	7 (31%)	25,54,82	3.06	13 (52%)
16	CLA	M	1086	-	36,43,73	2.00	8 (22%)	45,76,113	2.20	8 (17%)
16	CLA	B	1116	-	36,43,73	1.98	9 (25%)	45,76,113	2.20	8 (17%)
16	CLA	B	1108	-	36,43,73	1.99	7 (19%)	45,76,113	2.19	8 (17%)
16	CLA	D	355	-	36,43,73	1.91	7 (19%)	45,76,113	2.15	10 (22%)
16	CLA	C	1086	-	36,43,73	2.00	7 (19%)	45,76,113	2.23	9 (20%)
16	CLA	B	1115	-	36,43,73	1.99	8 (22%)	45,76,113	2.23	8 (17%)
16	CLA	C	1084	-	36,43,73	1.98	8 (22%)	45,76,113	2.21	9 (20%)
19	PLA	N	359	-	6,6,25	2.92	6 (100%)	6,6,37	0.89	0
16	CLA	C	1079	-	36,43,73	2.01	7 (19%)	45,76,113	2.22	9 (20%)
16	CLA	B	1114	2	36,43,73	2.00	7 (19%)	45,76,113	2.22	10 (22%)
16	CLA	A	369	-	36,43,73	2.02	8 (22%)	45,76,113	2.24	10 (22%)
16	CLA	A	365	-	36,43,73	1.98	9 (25%)	45,76,113	2.49	13 (28%)
16	CLA	B	1119	-	36,43,73	2.00	9 (25%)	45,76,113	2.21	9 (20%)
16	CLA	C	1089	3	36,43,73	2.01	8 (22%)	45,76,113	2.25	9 (20%)
20	BCR	D	359	-	41,41,41	1.27	4 (9%)	56,56,56	1.74	17 (30%)
20	BCR	K	47	-	21,21,41	1.02	1 (4%)	24,24,56	1.49	4 (16%)
16	CLA	C	1085	-	36,43,73	2.01	7 (19%)	45,76,113	2.19	8 (17%)
16	CLA	M	1085	-	36,43,73	2.00	7 (19%)	45,76,113	2.23	9 (20%)
16	CLA	C	1087	-	36,43,73	2.01	7 (19%)	45,76,113	2.21	8 (17%)
16	CLA	A	366	-	36,43,73	1.89	11 (30%)	45,76,113	2.18	8 (17%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
17	PHO	N	357	-	22,39,69	1.35	3 (13%)	17,62,99	2.51	7 (41%)
16	CLA	B	1120	-	36,43,73	2.00	7 (19%)	45,76,113	2.20	9 (20%)
16	CLA	M	1088	-	36,43,73	2.01	9 (25%)	45,76,113	2.22	9 (20%)
16	CLA	C	1078	-	36,43,73	2.03	8 (22%)	45,76,113	2.20	6 (13%)
19	PLA	D	358	-	6,6,25	2.92	5 (83%)	6,6,37	0.89	0
16	CLA	L	1112	-	36,43,73	1.99	8 (22%)	45,76,113	2.24	10 (22%)
16	CLA	L	1107	-	36,43,73	2.00	8 (22%)	45,76,113	2.21	8 (17%)
16	CLA	L	1116	-	36,43,73	2.00	8 (22%)	45,76,113	2.19	9 (20%)
16	CLA	B	1122	-	36,43,73	2.01	7 (19%)	45,76,113	2.20	8 (17%)
16	CLA	C	1088	-	36,43,73	2.00	9 (25%)	45,76,113	2.20	9 (20%)
16	CLA	L	1119	-	36,43,73	2.01	8 (22%)	45,76,113	2.22	9 (20%)
16	CLA	N	354	4	36,43,73	1.84	9 (25%)	45,76,113	2.24	9 (20%)
16	CLA	M	1081	-	36,43,73	2.00	7 (19%)	45,76,113	2.21	7 (15%)
16	CLA	N	356	-	36,43,73	1.91	7 (19%)	45,76,113	2.16	10 (22%)
16	CLA	W	64	-	36,43,73	2.01	9 (25%)	45,76,113	2.20	9 (20%)
16	CLA	L	1115	-	36,43,73	2.01	8 (22%)	45,76,113	2.21	9 (20%)
16	CLA	B	1118	-	36,43,73	2.01	9 (25%)	45,76,113	2.21	8 (17%)
16	CLA	C	1080	-	36,43,73	2.00	9 (25%)	45,76,113	2.22	10 (22%)
16	CLA	M	1080	-	36,43,73	1.99	7 (19%)	45,76,113	2.23	8 (17%)
16	CLA	N	358	-	36,43,73	2.00	8 (22%)	45,76,113	2.25	9 (20%)
16	CLA	B	1121	-	36,43,73	1.98	7 (19%)	45,76,113	2.21	9 (20%)
16	CLA	L	1117	-	36,43,73	2.01	8 (22%)	45,76,113	2.20	9 (20%)
16	CLA	C	1083	-	36,43,73	1.99	7 (19%)	45,76,113	2.21	8 (17%)

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
17	PHO	A	367	-	-	0/0/60/103	0/5/6/6
16	CLA	L	1110	-	1/1/8/20	-	-
16	CLA	A	368	-	1/1/8/20	-	-
16	CLA	J	367	-	1/1/8/20	-	-
16	CLA	L	1108	-	1/1/8/20	-	-
16	CLA	M	1084	-	1/1/8/20	-	-
16	CLA	M	1083	-	1/1/8/20	-	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
16	CLA	R	221	-	1/1/8/20	-	-
16	CLA	L	1114	-	1/1/8/20	-	-
16	CLA	C	1082	-	1/1/8/20	-	-
16	CLA	D	354	4	1/1/8/20	-	-
17	PHO	J	366	-	-	0/0/60/103	0/5/6/6
16	CLA	J	368	-	1/1/8/20	-	-
16	CLA	M	1078	-	1/1/8/20	-	-
16	CLA	L	1111	-	1/1/8/20	-	-
16	CLA	N	355	-	1/1/8/20	-	-
16	CLA	B	1111	-	1/1/8/20	-	-
16	CLA	L	1122	-	1/1/8/20	-	-
16	CLA	L	1118	-	1/1/8/20	-	-
16	CLA	L	1109	-	1/1/8/20	-	-
16	CLA	M	1079	-	1/1/8/20	-	-
16	CLA	L	1113	-	1/1/8/20	-	-
16	CLA	B	1113	-	1/1/8/20	-	-
16	CLA	C	1081	-	1/1/8/20	-	-
16	CLA	D	357	-	1/1/8/20	-	-
16	CLA	B	1110	-	1/1/8/20	-	-
16	CLA	L	1120	-	1/1/8/20	-	-
16	CLA	B	1109	-	1/1/8/20	-	-
16	CLA	B	1117	-	1/1/8/20	-	-
16	CLA	M	1082	-	1/1/8/20	-	-
17	PHO	D	356	-	-	0/0/60/103	0/5/6/6
16	CLA	M	1087	3	1/1/8/20	-	-
16	CLA	L	1121	-	1/1/8/20	-	-
16	CLA	G	221	-	1/1/8/20	-	-
16	CLA	J	365	-	1/1/8/20	-	-
16	CLA	B	1112	-	1/1/8/20	-	-
16	CLA	B	1107	-	1/1/8/20	-	-
16	CLA	M	1086	-	1/1/8/20	-	-
16	CLA	B	1116	-	1/1/8/20	-	-
16	CLA	B	1108	-	1/1/8/20	-	-
16	CLA	D	355	-	1/1/8/20	-	-
16	CLA	C	1086	-	1/1/8/20	-	-
16	CLA	B	1115	-	1/1/8/20	-	-
16	CLA	C	1084	-	1/1/8/20	-	-
19	PLA	N	359	-	-	-	0/1/1/1
16	CLA	C	1079	-	1/1/8/20	-	-
16	CLA	B	1114	2	1/1/8/20	-	-
16	CLA	A	369	-	1/1/8/20	-	-
16	CLA	A	365	-	1/1/8/20	-	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
16	CLA	B	1119	-	1/1/8/20	-	-
16	CLA	C	1089	3	2/2/8/20	-	-
20	BCR	D	359	-	-	3/29/63/63	0/2/2/2
20	BCR	K	47	-	-	1/23/23/63	-
16	CLA	C	1085	-	1/1/8/20	-	-
16	CLA	M	1085	-	1/1/8/20	-	-
16	CLA	C	1087	-	1/1/8/20	-	-
16	CLA	A	366	-	1/1/8/20	-	-
17	PHO	N	357	-	-	0/0/60/103	0/5/6/6
16	CLA	B	1120	-	1/1/8/20	-	-
16	CLA	M	1088	-	1/1/8/20	-	-
16	CLA	C	1078	-	1/1/8/20	-	-
16	CLA	L	1112	-	1/1/8/20	-	-
19	PLA	D	358	-	-	-	0/1/1/1
16	CLA	L	1107	-	1/1/8/20	-	-
16	CLA	L	1116	-	1/1/8/20	-	-
16	CLA	B	1122	-	1/1/8/20	-	-
16	CLA	C	1088	-	1/1/8/20	-	-
16	CLA	L	1119	-	1/1/8/20	-	-
16	CLA	N	354	4	1/1/8/20	-	-
16	CLA	M	1081	-	1/1/8/20	-	-
16	CLA	N	356	-	1/1/8/20	-	-
16	CLA	W	64	-	1/1/8/20	-	-
16	CLA	L	1115	-	1/1/8/20	-	-
16	CLA	B	1118	-	1/1/8/20	-	-
16	CLA	C	1080	-	1/1/8/20	-	-
16	CLA	M	1080	-	1/1/8/20	-	-
16	CLA	N	358	-	1/1/8/20	-	-
16	CLA	B	1121	-	1/1/8/20	-	-
16	CLA	L	1117	-	1/1/8/20	-	-
16	CLA	C	1083	-	1/1/8/20	-	-

All (632) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
21	E	84	HEM	C2A-C1A	7.38	1.52	1.39
21	0	138	HEM	C2A-C1A	7.34	1.52	1.39
21	V	138	HEM	C2A-C1A	7.31	1.52	1.39
21	P	92	HEM	C2A-C1A	7.29	1.52	1.39
21	V	138	HEM	C3A-C4A	6.78	1.51	1.39
21	P	92	HEM	C3A-C4A	6.77	1.51	1.39
21	E	84	HEM	C3A-C4A	6.77	1.51	1.39

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
21	0	138	HEM	C3A-C4A	6.75	1.51	1.39
16	D	355	CLA	MG-NA	5.92	2.20	2.06
16	N	356	CLA	MG-NA	5.89	2.20	2.06
16	M	1078	CLA	MG-ND	5.80	2.17	2.05
16	C	1078	CLA	MG-ND	5.77	2.17	2.05
16	M	1084	CLA	MG-ND	5.74	2.17	2.05
16	C	1085	CLA	MG-ND	5.72	2.17	2.05
16	J	367	CLA	MG-ND	5.70	2.17	2.05
16	M	1086	CLA	MG-ND	5.69	2.17	2.05
16	A	368	CLA	MG-ND	5.68	2.17	2.05
16	C	1087	CLA	MG-ND	5.67	2.17	2.05
16	L	1119	CLA	MG-ND	5.67	2.17	2.05
16	L	1115	CLA	MG-ND	5.65	2.17	2.05
16	M	1079	CLA	MG-ND	5.64	2.17	2.05
16	C	1079	CLA	MG-ND	5.64	2.17	2.05
16	B	1111	CLA	MG-ND	5.63	2.16	2.05
16	B	1118	CLA	MG-ND	5.62	2.16	2.05
16	B	1119	CLA	MG-ND	5.62	2.16	2.05
16	M	1082	CLA	MG-ND	5.61	2.16	2.05
16	C	1082	CLA	MG-ND	5.60	2.16	2.05
16	B	1115	CLA	MG-ND	5.60	2.16	2.05
16	L	1111	CLA	MG-ND	5.60	2.16	2.05
16	L	1116	CLA	MG-ND	5.59	2.16	2.05
16	B	1108	CLA	MG-ND	5.59	2.16	2.05
16	M	1081	CLA	MG-ND	5.59	2.16	2.05
16	L	1108	CLA	MG-ND	5.58	2.16	2.05
16	B	1116	CLA	MG-ND	5.57	2.16	2.05
16	C	1083	CLA	MG-ND	5.57	2.16	2.05
16	B	1122	CLA	MG-ND	5.56	2.16	2.05
16	L	1118	CLA	MG-ND	5.56	2.16	2.05
16	L	1122	CLA	MG-ND	5.56	2.16	2.05
16	B	1109	CLA	MG-ND	5.55	2.16	2.05
16	L	1107	CLA	MG-ND	5.55	2.16	2.05
16	L	1109	CLA	MG-ND	5.55	2.16	2.05
16	A	369	CLA	MG-ND	5.54	2.16	2.05
16	C	1088	CLA	MG-ND	5.53	2.16	2.05
16	M	1088	CLA	MG-ND	5.53	2.16	2.05
16	C	1086	CLA	MG-ND	5.52	2.16	2.05
16	L	1114	CLA	MG-ND	5.51	2.16	2.05
16	L	1113	CLA	MG-ND	5.51	2.16	2.05
16	C	1089	CLA	MG-ND	5.50	2.16	2.05
16	M	1087	CLA	MG-ND	5.50	2.16	2.05

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
16	B	1113	CLA	MG-ND	5.50	2.16	2.05
16	B	1117	CLA	MG-ND	5.50	2.16	2.05
16	B	1114	CLA	MG-ND	5.49	2.16	2.05
16	B	1120	CLA	MG-ND	5.49	2.16	2.05
16	B	1121	CLA	MG-ND	5.49	2.16	2.05
16	J	368	CLA	MG-ND	5.49	2.16	2.05
16	M	1085	CLA	MG-ND	5.49	2.16	2.05
16	B	1110	CLA	MG-ND	5.48	2.16	2.05
16	L	1117	CLA	MG-ND	5.47	2.16	2.05
16	L	1110	CLA	MG-ND	5.47	2.16	2.05
16	N	358	CLA	MG-ND	5.46	2.16	2.05
16	C	1081	CLA	MG-ND	5.46	2.16	2.05
16	D	357	CLA	MG-ND	5.45	2.16	2.05
16	B	1112	CLA	MG-ND	5.45	2.16	2.05
16	W	64	CLA	MG-ND	5.45	2.16	2.05
16	C	1084	CLA	MG-ND	5.45	2.16	2.05
16	L	1120	CLA	MG-ND	5.45	2.16	2.05
16	M	1083	CLA	MG-ND	5.45	2.16	2.05
16	B	1107	CLA	MG-ND	5.44	2.16	2.05
16	L	1121	CLA	MG-ND	5.43	2.16	2.05
16	C	1080	CLA	MG-ND	5.43	2.16	2.05
16	M	1080	CLA	MG-ND	5.42	2.16	2.05
16	L	1112	CLA	MG-ND	5.41	2.16	2.05
16	J	365	CLA	MG-NA	5.41	2.19	2.06
16	N	354	CLA	MG-NA	5.36	2.19	2.06
16	A	365	CLA	MG-NA	5.36	2.19	2.06
16	D	354	CLA	MG-NA	5.34	2.19	2.06
16	B	1122	CLA	C4B-NB	5.32	1.40	1.35
16	A	369	CLA	C4B-NB	5.25	1.39	1.35
16	L	1122	CLA	C4B-NB	5.22	1.39	1.35
16	B	1117	CLA	C4B-NB	5.20	1.39	1.35
16	L	1114	CLA	C4B-NB	5.20	1.39	1.35
16	L	1115	CLA	C4B-NB	5.18	1.39	1.35
16	J	365	CLA	C4B-NB	5.17	1.39	1.35
16	L	1117	CLA	C4B-NB	5.17	1.39	1.35
16	L	1120	CLA	C4B-NB	5.17	1.39	1.35
16	W	64	CLA	C4B-NB	5.16	1.39	1.35
16	M	1081	CLA	C4B-NB	5.16	1.39	1.35
16	M	1085	CLA	C4B-NB	5.16	1.39	1.35
16	C	1078	CLA	C4B-NB	5.16	1.39	1.35
16	B	1114	CLA	C4B-NB	5.15	1.39	1.35
16	J	367	CLA	C4B-NB	5.15	1.39	1.35

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
16	L	1113	CLA	C4B-NB	5.15	1.39	1.35
16	B	1111	CLA	C4B-NB	5.15	1.39	1.35
16	M	1080	CLA	C4B-NB	5.15	1.39	1.35
16	C	1082	CLA	C4B-NB	5.14	1.39	1.35
16	D	357	CLA	C4B-NB	5.14	1.39	1.35
16	M	1087	CLA	C4B-NB	5.14	1.39	1.35
16	A	365	CLA	C4B-NB	5.14	1.39	1.35
16	C	1080	CLA	C4B-NB	5.13	1.39	1.35
16	B	1118	CLA	C4B-NB	5.12	1.39	1.35
16	L	1112	CLA	C4B-NB	5.12	1.39	1.35
16	M	1088	CLA	C4B-NB	5.12	1.39	1.35
16	B	1112	CLA	C4B-NB	5.11	1.39	1.35
16	B	1107	CLA	C4B-NB	5.10	1.39	1.35
16	C	1086	CLA	C4B-NB	5.10	1.39	1.35
16	M	1078	CLA	C4B-NB	5.10	1.39	1.35
16	N	358	CLA	C4B-NB	5.10	1.39	1.35
16	C	1079	CLA	C4B-NB	5.10	1.39	1.35
16	L	1111	CLA	C4B-NB	5.09	1.39	1.35
16	A	368	CLA	C4B-NB	5.09	1.39	1.35
16	B	1120	CLA	C4B-NB	5.08	1.39	1.35
16	M	1084	CLA	C4B-NB	5.08	1.39	1.35
16	C	1089	CLA	C4B-NB	5.08	1.39	1.35
16	C	1085	CLA	C4B-NB	5.07	1.39	1.35
16	N	355	CLA	MG-NA	5.07	2.18	2.06
16	B	1121	CLA	C4B-NB	5.07	1.39	1.35
16	A	366	CLA	MG-NA	5.07	2.18	2.06
16	C	1088	CLA	C4B-NB	5.07	1.39	1.35
16	M	1082	CLA	C4B-NB	5.06	1.39	1.35
16	L	1107	CLA	C4B-NB	5.06	1.39	1.35
16	C	1081	CLA	C4B-NB	5.05	1.39	1.35
16	L	1116	CLA	C4B-NB	5.05	1.39	1.35
16	M	1083	CLA	C4B-NB	5.05	1.39	1.35
16	L	1119	CLA	C4B-NB	5.04	1.39	1.35
16	C	1087	CLA	C4B-NB	5.04	1.39	1.35
16	B	1110	CLA	C4B-NB	5.04	1.39	1.35
16	L	1118	CLA	C4B-NB	5.04	1.39	1.35
16	L	1121	CLA	C4B-NB	5.04	1.39	1.35
16	B	1119	CLA	C4B-NB	5.02	1.39	1.35
16	B	1113	CLA	C4B-NB	5.02	1.39	1.35
16	M	1079	CLA	C4B-NB	5.02	1.39	1.35
16	J	368	CLA	C4B-NB	5.00	1.39	1.35
16	C	1084	CLA	C4B-NB	4.99	1.39	1.35

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
16	L	1109	CLA	C4B-NB	4.99	1.39	1.35
16	B	1109	CLA	C4B-NB	4.98	1.39	1.35
16	B	1115	CLA	C4B-NB	4.98	1.39	1.35
16	C	1083	CLA	C4B-NB	4.97	1.39	1.35
16	G	221	CLA	MG-NA	4.97	2.18	2.06
16	R	221	CLA	MG-NA	4.96	2.18	2.06
16	L	1108	CLA	C4B-NB	4.95	1.39	1.35
16	B	1108	CLA	C4B-NB	4.95	1.39	1.35
16	B	1116	CLA	C4B-NB	4.95	1.39	1.35
16	L	1110	CLA	C4B-NB	4.94	1.39	1.35
16	M	1086	CLA	C4B-NB	4.92	1.39	1.35
16	G	221	CLA	C3A-C2A	-4.84	1.50	1.54
16	R	221	CLA	C3A-C2A	-4.80	1.50	1.54
16	N	356	CLA	C4B-NB	4.77	1.39	1.35
16	D	355	CLA	C4B-NB	4.67	1.39	1.35
16	N	355	CLA	C4B-NB	4.66	1.39	1.35
16	A	366	CLA	C4B-NB	4.55	1.39	1.35
16	M	1084	CLA	MG-NA	4.49	2.16	2.06
16	D	357	CLA	MG-NA	4.48	2.16	2.06
16	A	369	CLA	MG-NA	4.46	2.16	2.06
16	C	1085	CLA	MG-NA	4.46	2.16	2.06
16	M	1081	CLA	MG-NA	4.46	2.16	2.06
16	B	1115	CLA	MG-NA	4.46	2.16	2.06
16	N	358	CLA	MG-NA	4.46	2.16	2.06
16	L	1119	CLA	MG-NA	4.45	2.16	2.06
16	C	1089	CLA	MG-NA	4.45	2.16	2.06
16	B	1118	CLA	MG-NA	4.45	2.16	2.06
16	L	1118	CLA	MG-NA	4.45	2.16	2.06
16	M	1079	CLA	MG-NA	4.45	2.16	2.06
16	L	1115	CLA	MG-NA	4.44	2.16	2.06
16	B	1122	CLA	MG-NA	4.44	2.16	2.06
16	L	1108	CLA	MG-NA	4.43	2.16	2.06
16	B	1108	CLA	MG-NA	4.43	2.16	2.06
16	M	1078	CLA	MG-NA	4.43	2.16	2.06
16	B	1116	CLA	MG-NA	4.43	2.16	2.06
16	C	1078	CLA	MG-NA	4.43	2.16	2.06
16	M	1086	CLA	MG-NA	4.43	2.16	2.06
16	C	1082	CLA	MG-NA	4.43	2.16	2.06
16	C	1087	CLA	MG-NA	4.43	2.16	2.06
16	B	1111	CLA	MG-NA	4.42	2.16	2.06
16	C	1079	CLA	MG-NA	4.42	2.16	2.06
16	L	1122	CLA	MG-NA	4.42	2.16	2.06

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
16	J	367	CLA	MG-NA	4.41	2.16	2.06
16	A	368	CLA	MG-NA	4.40	2.16	2.06
16	C	1083	CLA	MG-NA	4.40	2.16	2.06
16	J	368	CLA	MG-NA	4.40	2.16	2.06
16	B	1113	CLA	MG-NA	4.40	2.16	2.06
16	L	1113	CLA	MG-NA	4.39	2.16	2.06
16	C	1081	CLA	MG-NA	4.39	2.16	2.06
16	L	1111	CLA	MG-NA	4.39	2.16	2.06
16	M	1088	CLA	MG-NA	4.38	2.16	2.06
16	L	1116	CLA	MG-NA	4.38	2.16	2.06
16	M	1082	CLA	MG-NA	4.38	2.16	2.06
16	L	1121	CLA	MG-NA	4.38	2.16	2.06
16	L	1114	CLA	MG-NA	4.38	2.16	2.06
16	B	1110	CLA	MG-NA	4.37	2.16	2.06
16	M	1087	CLA	MG-NA	4.37	2.16	2.06
16	B	1119	CLA	MG-NA	4.37	2.16	2.06
16	M	1080	CLA	MG-NA	4.36	2.16	2.06
16	M	1085	CLA	MG-NA	4.36	2.16	2.06
16	B	1121	CLA	MG-NA	4.36	2.16	2.06
16	B	1117	CLA	MG-NA	4.36	2.16	2.06
16	L	1110	CLA	MG-NA	4.35	2.16	2.06
16	N	354	CLA	C4B-NB	4.35	1.39	1.35
16	C	1080	CLA	MG-NA	4.34	2.16	2.06
16	B	1109	CLA	MG-NA	4.34	2.16	2.06
16	W	64	CLA	MG-NA	4.34	2.16	2.06
16	C	1088	CLA	MG-NA	4.34	2.16	2.06
16	L	1109	CLA	MG-NA	4.34	2.16	2.06
16	C	1086	CLA	MG-NA	4.33	2.16	2.06
16	B	1114	CLA	MG-NA	4.33	2.16	2.06
16	B	1112	CLA	MG-NA	4.33	2.16	2.06
16	L	1112	CLA	MG-NA	4.33	2.16	2.06
16	L	1107	CLA	MG-NA	4.32	2.16	2.06
16	C	1084	CLA	MG-NA	4.31	2.16	2.06
16	M	1083	CLA	MG-NA	4.31	2.16	2.06
16	L	1117	CLA	MG-NA	4.30	2.16	2.06
16	B	1107	CLA	MG-NA	4.29	2.16	2.06
16	B	1120	CLA	MG-NA	4.28	2.16	2.06
16	D	354	CLA	C4B-NB	4.27	1.39	1.35
16	L	1120	CLA	MG-NA	4.26	2.16	2.06
16	A	365	CLA	CBD-CAD	-4.14	1.42	1.51
16	M	1080	CLA	CHC-C1C	3.82	1.44	1.35
16	L	1114	CLA	CHC-C1C	3.80	1.44	1.35

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
16	A	369	CLA	CHC-C1C	3.78	1.44	1.35
16	B	1114	CLA	CHC-C1C	3.78	1.44	1.35
16	W	64	CLA	CHC-C1C	3.78	1.44	1.35
16	C	1089	CLA	CHC-C1C	3.77	1.44	1.35
16	C	1081	CLA	CHC-C1C	3.77	1.44	1.35
16	J	368	CLA	CHC-C1C	3.76	1.44	1.35
16	M	1084	CLA	CHC-C1C	3.76	1.44	1.35
16	B	1112	CLA	CHC-C1C	3.76	1.44	1.35
16	C	1080	CLA	CHC-C1C	3.76	1.44	1.35
16	L	1112	CLA	CHC-C1C	3.75	1.44	1.35
16	B	1120	CLA	CHC-C1C	3.75	1.44	1.35
16	B	1113	CLA	CHC-C1C	3.74	1.44	1.35
16	M	1078	CLA	CHC-C1C	3.74	1.44	1.35
16	L	1110	CLA	CHC-C1C	3.74	1.44	1.35
16	C	1087	CLA	CHC-C1C	3.74	1.44	1.35
16	L	1116	CLA	CHC-C1C	3.74	1.44	1.35
16	M	1087	CLA	CHC-C1C	3.74	1.44	1.35
16	M	1086	CLA	CHC-C1C	3.74	1.44	1.35
16	L	1117	CLA	CHC-C1C	3.74	1.44	1.35
16	B	1117	CLA	CHC-C1C	3.74	1.44	1.35
16	L	1108	CLA	CHC-C1C	3.74	1.44	1.35
16	C	1085	CLA	CHC-C1C	3.73	1.44	1.35
16	L	1113	CLA	CHC-C1C	3.73	1.44	1.35
16	B	1122	CLA	CHC-C1C	3.73	1.44	1.35
16	L	1107	CLA	CHC-C1C	3.72	1.44	1.35
16	N	358	CLA	CHC-C1C	3.72	1.44	1.35
16	B	1110	CLA	CHC-C1C	3.72	1.44	1.35
16	L	1120	CLA	CHC-C1C	3.72	1.44	1.35
16	B	1119	CLA	CHC-C1C	3.72	1.44	1.35
16	C	1088	CLA	CHC-C1C	3.72	1.44	1.35
16	L	1115	CLA	CHC-C1C	3.72	1.44	1.35
16	C	1083	CLA	CHC-C1C	3.72	1.44	1.35
16	B	1108	CLA	CHC-C1C	3.72	1.44	1.35
16	C	1086	CLA	CHC-C1C	3.71	1.44	1.35
16	M	1079	CLA	CHC-C1C	3.71	1.44	1.35
16	D	357	CLA	CHC-C1C	3.71	1.44	1.35
16	B	1109	CLA	CHC-C1C	3.71	1.44	1.35
16	M	1088	CLA	CHC-C1C	3.71	1.44	1.35
16	L	1111	CLA	CHC-C1C	3.71	1.44	1.35
16	B	1107	CLA	CHC-C1C	3.71	1.44	1.35
16	C	1078	CLA	CHC-C1C	3.70	1.44	1.35
16	C	1079	CLA	CHC-C1C	3.70	1.44	1.35

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
16	M	1082	CLA	CHC-C1C	3.70	1.44	1.35
16	L	1122	CLA	CHC-C1C	3.70	1.44	1.35
16	M	1081	CLA	CHC-C1C	3.70	1.44	1.35
16	B	1111	CLA	CHC-C1C	3.70	1.44	1.35
16	B	1115	CLA	CHC-C1C	3.70	1.44	1.35
16	L	1119	CLA	CHC-C1C	3.70	1.44	1.35
16	C	1082	CLA	CHC-C1C	3.69	1.44	1.35
16	A	368	CLA	CHC-C1C	3.69	1.44	1.35
16	B	1116	CLA	CHC-C1C	3.69	1.44	1.35
16	C	1084	CLA	CHC-C1C	3.69	1.44	1.35
16	L	1121	CLA	CHC-C1C	3.69	1.44	1.35
16	J	367	CLA	CHC-C1C	3.69	1.44	1.35
16	L	1118	CLA	CHC-C1C	3.69	1.44	1.35
16	L	1109	CLA	CHC-C1C	3.68	1.44	1.35
19	N	359	PLA	C6-N1	3.68	1.44	1.33
16	M	1085	CLA	CHC-C1C	3.67	1.44	1.35
16	B	1118	CLA	CHC-C1C	3.67	1.44	1.35
19	D	358	PLA	C6-N1	3.65	1.44	1.33
16	M	1083	CLA	CHC-C1C	3.65	1.44	1.35
16	B	1121	CLA	CHC-C1C	3.63	1.44	1.35
19	D	358	PLA	C2-N1	3.51	1.44	1.33
19	N	359	PLA	C2-N1	3.50	1.44	1.33
16	D	355	CLA	CHC-C1C	3.50	1.43	1.35
16	N	356	CLA	CHC-C1C	3.41	1.43	1.35
21	0	138	HEM	FE-NB	3.33	2.13	1.96
21	V	138	HEM	FE-NB	3.32	2.13	1.96
21	P	92	HEM	FE-NB	3.32	2.13	1.96
21	E	84	HEM	FE-NB	3.32	2.13	1.96
17	A	367	PHO	CAA-C2A	3.29	1.59	1.53
17	J	366	PHO	CAA-C2A	3.29	1.59	1.53
16	N	355	CLA	CHC-C1C	3.27	1.43	1.35
17	N	357	PHO	CAA-C2A	3.27	1.59	1.53
16	R	221	CLA	CBD-CAD	3.25	1.59	1.51
16	A	366	CLA	CHC-C1C	3.24	1.43	1.35
16	G	221	CLA	C4B-NB	3.23	1.38	1.35
17	D	356	PHO	CAA-C2A	3.21	1.59	1.53
16	D	355	CLA	MG-NC	3.20	2.13	2.06
16	R	221	CLA	C4B-NB	3.19	1.38	1.35
16	G	221	CLA	CBD-CAD	3.18	1.59	1.51
16	N	356	CLA	MG-NC	3.18	2.13	2.06
20	D	359	BCR	C2-C1	3.14	1.61	1.54
16	A	366	CLA	MG-NC	3.11	2.13	2.06

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
16	N	355	CLA	MG-NC	3.10	2.13	2.06
16	G	221	CLA	CHC-C1C	3.07	1.42	1.35
21	P	92	HEM	C3B-C2B	3.07	1.42	1.35
16	R	221	CLA	CHC-C1C	3.06	1.42	1.35
21	E	84	HEM	C3B-C2B	3.05	1.42	1.35
16	A	366	CLA	C3A-C2A	-3.04	1.51	1.54
16	J	365	CLA	CHC-C1C	3.04	1.42	1.35
21	V	138	HEM	C3B-C2B	3.04	1.42	1.35
16	A	365	CLA	CHC-C1C	3.02	1.42	1.35
21	0	138	HEM	C3B-C2B	2.98	1.42	1.35
16	D	354	CLA	MG-NC	2.98	2.13	2.06
16	L	1118	CLA	CAA-C2A	2.97	1.59	1.53
20	K	47	BCR	C23-C22	-2.97	1.40	1.46
16	C	1078	CLA	CAA-C2A	2.97	1.59	1.53
16	W	64	CLA	CAA-C2A	2.97	1.59	1.53
16	L	1114	CLA	CAA-C2A	2.97	1.59	1.53
16	M	1078	CLA	CAA-C2A	2.95	1.59	1.53
16	M	1085	CLA	CAA-C2A	2.95	1.59	1.53
16	C	1086	CLA	CAA-C2A	2.95	1.59	1.53
16	N	355	CLA	C3A-C2A	-2.95	1.51	1.54
16	L	1109	CLA	CAA-C2A	2.94	1.59	1.53
16	N	354	CLA	MG-NC	2.94	2.13	2.06
19	D	358	PLA	C5-C6	2.94	1.46	1.37
16	C	1079	CLA	CAA-C2A	2.94	1.59	1.53
16	C	1080	CLA	CAA-C2A	2.94	1.59	1.53
19	N	359	PLA	C5-C6	2.94	1.46	1.37
16	M	1087	CLA	CAA-C2A	2.94	1.59	1.53
16	M	1088	CLA	CAA-C2A	2.93	1.59	1.53
16	A	368	CLA	CAA-C2A	2.93	1.59	1.53
16	L	1117	CLA	CAA-C2A	2.93	1.59	1.53
16	L	1113	CLA	CAA-C2A	2.93	1.59	1.53
16	D	357	CLA	CAA-C2A	2.93	1.59	1.53
16	C	1087	CLA	CAA-C2A	2.93	1.59	1.53
16	A	369	CLA	CAA-C2A	2.93	1.59	1.53
16	L	1122	CLA	CAA-C2A	2.92	1.59	1.53
16	L	1116	CLA	CAA-C2A	2.92	1.59	1.53
16	B	1118	CLA	CAA-C2A	2.92	1.59	1.53
16	C	1085	CLA	CAA-C2A	2.92	1.59	1.53
16	M	1080	CLA	CAA-C2A	2.92	1.59	1.53
16	B	1119	CLA	CAA-C2A	2.92	1.59	1.53
16	B	1120	CLA	CAA-C2A	2.92	1.59	1.53
16	M	1086	CLA	CAA-C2A	2.92	1.59	1.53

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
16	B	1111	CLA	CAA-C2A	2.92	1.59	1.53
16	C	1084	CLA	CAA-C2A	2.91	1.59	1.53
16	B	1109	CLA	CAA-C2A	2.91	1.59	1.53
16	B	1122	CLA	CAA-C2A	2.91	1.59	1.53
16	B	1115	CLA	CAA-C2A	2.91	1.59	1.53
16	B	1117	CLA	CAA-C2A	2.91	1.59	1.53
16	B	1112	CLA	CAA-C2A	2.90	1.59	1.53
16	L	1110	CLA	CAA-C2A	2.90	1.59	1.53
16	B	1114	CLA	CAA-C2A	2.90	1.59	1.53
16	C	1081	CLA	CAA-C2A	2.90	1.59	1.53
16	C	1088	CLA	CAA-C2A	2.90	1.59	1.53
16	J	367	CLA	CAA-C2A	2.90	1.59	1.53
16	L	1120	CLA	CAA-C2A	2.89	1.59	1.53
16	L	1121	CLA	CAA-C2A	2.89	1.59	1.53
20	D	359	BCR	C30-C25	2.89	1.57	1.53
16	L	1119	CLA	CAA-C2A	2.89	1.59	1.53
16	B	1121	CLA	CAA-C2A	2.88	1.59	1.53
20	D	359	BCR	C29-C30	2.88	1.60	1.54
16	C	1089	CLA	CAA-C2A	2.88	1.59	1.53
16	N	358	CLA	CAA-C2A	2.88	1.59	1.53
16	J	368	CLA	CAA-C2A	2.88	1.59	1.53
16	L	1112	CLA	CAA-C2A	2.88	1.59	1.53
16	B	1107	CLA	CAA-C2A	2.88	1.59	1.53
16	B	1110	CLA	CAA-C2A	2.88	1.59	1.53
16	B	1116	CLA	CAA-C2A	2.88	1.59	1.53
16	M	1083	CLA	CAA-C2A	2.87	1.59	1.53
16	L	1111	CLA	CAA-C2A	2.87	1.59	1.53
16	A	365	CLA	CAB-C3B	-2.87	1.45	1.51
16	L	1115	CLA	CAA-C2A	2.87	1.59	1.53
21	V	138	HEM	C3D-C2D	2.87	1.41	1.35
16	B	1113	CLA	CAA-C2A	2.87	1.59	1.53
16	J	365	CLA	CAB-C3B	-2.86	1.45	1.51
16	G	221	CLA	C1B-CHB	-2.86	1.33	1.41
16	M	1081	CLA	CAA-C2A	2.86	1.59	1.53
21	0	138	HEM	C3D-C2D	2.86	1.41	1.35
16	M	1079	CLA	CAA-C2A	2.86	1.59	1.53
16	D	355	CLA	C1D-ND	-2.86	1.34	1.37
21	E	84	HEM	C3D-C2D	2.85	1.41	1.35
16	M	1084	CLA	CAA-C2A	2.85	1.59	1.53
16	L	1107	CLA	CAA-C2A	2.85	1.59	1.53
16	R	221	CLA	C1B-CHB	-2.85	1.33	1.41
16	C	1082	CLA	CAA-C2A	2.85	1.59	1.53

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
16	C	1083	CLA	CAA-C2A	2.84	1.59	1.53
16	M	1082	CLA	CAA-C2A	2.81	1.59	1.53
21	P	92	HEM	C3D-C2D	2.81	1.41	1.35
16	N	356	CLA	C1D-ND	-2.80	1.34	1.37
16	B	1108	CLA	CAA-C2A	2.79	1.59	1.53
16	L	1108	CLA	CAA-C2A	2.77	1.59	1.53
16	R	221	CLA	C1D-ND	-2.76	1.34	1.37
16	G	221	CLA	C1D-ND	-2.71	1.34	1.37
17	J	366	PHO	OBD-CAD	2.71	1.26	1.22
19	D	358	PLA	C5-C4	2.70	1.45	1.38
19	N	359	PLA	C5-C4	2.68	1.45	1.38
16	N	354	CLA	C1B-CHB	-2.66	1.33	1.41
16	D	354	CLA	C1B-CHB	-2.66	1.33	1.41
16	D	354	CLA	C1B-NB	2.66	1.37	1.35
16	R	221	CLA	CAA-C2A	2.64	1.58	1.53
17	A	367	PHO	OBD-CAD	2.64	1.26	1.22
21	0	138	HEM	C4D-ND	-2.63	1.34	1.40
16	G	221	CLA	CAA-C2A	2.62	1.58	1.53
17	N	357	PHO	OBD-CAD	2.61	1.26	1.22
16	M	1078	CLA	C1D-ND	-2.61	1.34	1.37
21	P	92	HEM	C4D-ND	-2.60	1.35	1.40
21	V	138	HEM	C4D-ND	-2.60	1.35	1.40
21	E	84	HEM	C4D-ND	-2.59	1.35	1.40
16	D	354	CLA	CHC-C1C	2.58	1.41	1.35
16	N	355	CLA	MG-ND	-2.58	2.00	2.05
16	C	1078	CLA	C1D-ND	-2.57	1.34	1.37
17	D	356	PHO	OBD-CAD	2.56	1.26	1.22
16	N	354	CLA	CHC-C1C	2.55	1.41	1.35
16	A	366	CLA	MG-ND	-2.54	2.00	2.05
16	M	1084	CLA	C1D-ND	-2.54	1.34	1.37
16	D	354	CLA	CBD-CAD	2.53	1.57	1.51
16	N	354	CLA	C1B-NB	2.52	1.37	1.35
16	C	1085	CLA	C1D-ND	-2.52	1.34	1.37
16	M	1087	CLA	C1D-ND	-2.51	1.34	1.37
16	N	354	CLA	CBD-CAD	2.51	1.57	1.51
16	B	1115	CLA	C1D-ND	-2.50	1.34	1.37
16	C	1088	CLA	C1D-ND	-2.48	1.34	1.37
16	L	1109	CLA	C1D-ND	-2.47	1.34	1.37
16	B	1108	CLA	C1D-ND	-2.46	1.34	1.37
16	L	1119	CLA	C1D-ND	-2.46	1.34	1.37
16	M	1088	CLA	C1D-ND	-2.46	1.34	1.37
16	B	1109	CLA	C1D-ND	-2.45	1.34	1.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
16	A	365	CLA	CBD-CHA	-2.45	1.45	1.52
16	L	1108	CLA	C1D-ND	-2.45	1.34	1.37
16	C	1083	CLA	CMD-C2D	2.45	1.56	1.50
16	M	1082	CLA	CMD-C2D	2.44	1.56	1.50
16	N	355	CLA	C1B-CHB	-2.44	1.34	1.41
16	B	1111	CLA	C1D-ND	-2.43	1.34	1.37
16	L	1107	CLA	C1D-ND	-2.43	1.34	1.37
16	J	368	CLA	C1D-ND	-2.43	1.34	1.37
16	D	357	CLA	CMD-C2D	2.43	1.55	1.50
16	A	366	CLA	C1B-CHB	-2.42	1.34	1.41
16	B	1118	CLA	C1D-ND	-2.42	1.34	1.37
16	B	1119	CLA	C1D-ND	-2.42	1.34	1.37
16	M	1085	CLA	C1D-ND	-2.41	1.34	1.37
16	R	221	CLA	CMD-C2D	2.41	1.55	1.50
16	L	1118	CLA	C1D-ND	-2.41	1.34	1.37
16	L	1117	CLA	CMD-C2D	2.41	1.55	1.50
16	L	1111	CLA	C1D-ND	-2.41	1.34	1.37
16	W	64	CLA	C1D-ND	-2.41	1.34	1.37
16	G	221	CLA	CMD-C2D	2.41	1.55	1.50
16	A	368	CLA	C1D-ND	-2.40	1.34	1.37
16	L	1115	CLA	C1D-ND	-2.40	1.34	1.37
16	M	1079	CLA	C1D-ND	-2.40	1.34	1.37
16	B	1117	CLA	CMD-C2D	2.40	1.55	1.50
16	B	1112	CLA	C1D-ND	-2.39	1.34	1.37
16	M	1083	CLA	C1D-ND	-2.39	1.34	1.37
16	B	1114	CLA	CMD-C2D	2.39	1.55	1.50
16	C	1089	CLA	C1D-ND	-2.39	1.34	1.37
16	B	1108	CLA	CMD-C2D	2.39	1.55	1.50
16	C	1080	CLA	C1D-ND	-2.39	1.34	1.37
16	L	1110	CLA	C1D-ND	-2.39	1.34	1.37
16	B	1107	CLA	CMD-C2D	2.39	1.55	1.50
16	A	369	CLA	C1D-ND	-2.38	1.34	1.37
16	M	1086	CLA	C1D-ND	-2.38	1.34	1.37
16	C	1088	CLA	CMD-C2D	2.38	1.55	1.50
16	L	1119	CLA	CMD-C2D	2.38	1.55	1.50
16	J	367	CLA	C1D-ND	-2.38	1.34	1.37
16	L	1108	CLA	CMD-C2D	2.38	1.55	1.50
16	N	358	CLA	CMD-C2D	2.38	1.55	1.50
16	M	1082	CLA	C1D-ND	-2.38	1.34	1.37
16	C	1087	CLA	CMD-C2D	2.38	1.55	1.50
16	C	1082	CLA	C1D-ND	-2.38	1.34	1.37
16	L	1114	CLA	CMD-C2D	2.38	1.55	1.50

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
20	D	359	BCR	C23-C22	-2.38	1.40	1.45
16	L	1116	CLA	C1D-ND	-2.38	1.34	1.37
16	M	1086	CLA	CMD-C2D	2.38	1.55	1.50
16	L	1112	CLA	C1D-ND	-2.37	1.34	1.37
16	C	1084	CLA	CMD-C2D	2.37	1.55	1.50
16	M	1078	CLA	CMD-C2D	2.37	1.55	1.50
16	B	1107	CLA	C1D-ND	-2.37	1.34	1.37
17	J	366	PHO	CBD-CAD	2.37	1.55	1.51
16	C	1086	CLA	CMD-C2D	2.37	1.55	1.50
16	M	1087	CLA	CMD-C2D	2.36	1.55	1.50
16	B	1120	CLA	CMD-C2D	2.36	1.55	1.50
19	D	358	PLA	C4-C3	2.35	1.44	1.38
16	A	368	CLA	CMD-C2D	2.35	1.55	1.50
16	L	1107	CLA	CMD-C2D	2.35	1.55	1.50
16	B	1121	CLA	C1D-ND	-2.35	1.34	1.37
16	M	1080	CLA	CMD-C2D	2.35	1.55	1.50
16	L	1120	CLA	CMD-C2D	2.35	1.55	1.50
16	C	1087	CLA	C1D-ND	-2.35	1.34	1.37
16	C	1089	CLA	CMD-C2D	2.35	1.55	1.50
16	C	1086	CLA	C1D-ND	-2.35	1.34	1.37
16	L	1113	CLA	C1D-ND	-2.35	1.34	1.37
16	M	1085	CLA	CMD-C2D	2.34	1.55	1.50
16	J	367	CLA	CMD-C2D	2.34	1.55	1.50
16	L	1115	CLA	CMD-C2D	2.34	1.55	1.50
16	M	1081	CLA	C1D-ND	-2.34	1.34	1.37
16	C	1079	CLA	C1D-ND	-2.34	1.34	1.37
16	M	1081	CLA	CMD-C2D	2.34	1.55	1.50
16	C	1083	CLA	C1D-ND	-2.34	1.34	1.37
16	B	1110	CLA	CMD-C2D	2.34	1.55	1.50
19	N	359	PLA	C4-C3	2.33	1.44	1.38
16	C	1080	CLA	CMD-C2D	2.33	1.55	1.50
17	A	367	PHO	CBD-CAD	2.33	1.55	1.51
16	L	1111	CLA	CMD-C2D	2.33	1.55	1.50
16	C	1078	CLA	CMD-C2D	2.33	1.55	1.50
17	D	356	PHO	CBD-CAD	2.33	1.55	1.51
16	B	1121	CLA	CMD-C2D	2.33	1.55	1.50
16	L	1122	CLA	C1D-ND	-2.33	1.34	1.37
16	B	1113	CLA	C1D-ND	-2.33	1.34	1.37
16	B	1111	CLA	CMD-C2D	2.33	1.55	1.50
16	D	357	CLA	C1D-ND	-2.32	1.34	1.37
16	B	1122	CLA	C1D-ND	-2.32	1.34	1.37
16	L	1121	CLA	CMD-C2D	2.32	1.55	1.50

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
16	C	1081	CLA	CMD-C2D	2.32	1.55	1.50
16	B	1113	CLA	CMD-C2D	2.32	1.55	1.50
16	A	369	CLA	CMD-C2D	2.32	1.55	1.50
16	B	1110	CLA	C1D-ND	-2.31	1.34	1.37
16	L	1117	CLA	C1D-ND	-2.31	1.34	1.37
16	B	1115	CLA	CMD-C2D	2.31	1.55	1.50
16	J	368	CLA	CMD-C2D	2.31	1.55	1.50
16	L	1116	CLA	CMD-C2D	2.31	1.55	1.50
16	B	1116	CLA	CMD-C2D	2.31	1.55	1.50
16	B	1117	CLA	C1D-ND	-2.31	1.34	1.37
16	B	1116	CLA	C1D-ND	-2.31	1.34	1.37
16	M	1079	CLA	CMD-C2D	2.31	1.55	1.50
16	C	1079	CLA	CMD-C2D	2.31	1.55	1.50
16	W	64	CLA	CMD-C2D	2.31	1.55	1.50
16	M	1088	CLA	CMD-C2D	2.31	1.55	1.50
16	B	1122	CLA	CMD-C2D	2.30	1.55	1.50
16	B	1114	CLA	C1D-ND	-2.30	1.35	1.37
16	L	1121	CLA	C1D-ND	-2.30	1.35	1.37
16	L	1110	CLA	CMD-C2D	2.30	1.55	1.50
16	L	1112	CLA	CMD-C2D	2.30	1.55	1.50
16	D	355	CLA	CMD-C2D	2.30	1.55	1.50
16	C	1082	CLA	CMD-C2D	2.30	1.55	1.50
16	L	1118	CLA	CMD-C2D	2.30	1.55	1.50
17	N	357	PHO	CBD-CAD	2.30	1.55	1.51
16	L	1113	CLA	CMD-C2D	2.30	1.55	1.50
16	L	1122	CLA	CMD-C2D	2.30	1.55	1.50
16	C	1084	CLA	C1D-ND	-2.29	1.35	1.37
16	B	1119	CLA	CMD-C2D	2.29	1.55	1.50
16	B	1118	CLA	CMD-C2D	2.29	1.55	1.50
16	B	1120	CLA	C1D-ND	-2.29	1.35	1.37
16	C	1085	CLA	CMD-C2D	2.29	1.55	1.50
16	M	1080	CLA	C1D-ND	-2.28	1.35	1.37
16	M	1083	CLA	CMD-C2D	2.27	1.55	1.50
16	B	1109	CLA	CMD-C2D	2.27	1.55	1.50
16	L	1114	CLA	C1D-ND	-2.26	1.35	1.37
16	L	1120	CLA	C1D-ND	-2.26	1.35	1.37
16	L	1109	CLA	CMD-C2D	2.26	1.55	1.50
16	B	1112	CLA	CMD-C2D	2.26	1.55	1.50
16	M	1084	CLA	CMD-C2D	2.25	1.55	1.50
16	C	1081	CLA	C1D-ND	-2.24	1.35	1.37
16	N	356	CLA	CMD-C2D	2.24	1.55	1.50
16	A	366	CLA	CHD-C1D	2.23	1.42	1.38

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
16	J	365	CLA	MG-ND	-2.23	2.01	2.05
16	A	365	CLA	MG-NC	2.23	2.11	2.06
16	N	358	CLA	C1D-ND	-2.21	1.35	1.37
16	A	366	CLA	CBD-CAD	2.20	1.56	1.51
16	N	355	CLA	CBD-CAD	2.19	1.56	1.51
16	N	355	CLA	CHD-C1D	2.19	1.42	1.38
16	J	365	CLA	MG-NC	2.19	2.11	2.06
16	R	221	CLA	MG-NC	2.19	2.11	2.06
16	M	1088	CLA	C1B-NB	2.18	1.37	1.35
16	C	1089	CLA	C1B-NB	2.17	1.37	1.35
16	L	1112	CLA	C1B-NB	2.16	1.37	1.35
16	R	221	CLA	CHD-C1D	2.16	1.42	1.38
16	J	365	CLA	CBD-CHA	2.15	1.58	1.52
21	P	92	HEM	C2D-C1D	-2.15	1.38	1.43
16	A	365	CLA	MG-ND	-2.15	2.01	2.05
16	D	354	CLA	C3A-C2A	-2.15	1.52	1.54
16	C	1080	CLA	C1B-NB	2.14	1.37	1.35
16	W	64	CLA	C1B-NB	2.14	1.37	1.35
16	B	1112	CLA	C1B-NB	2.13	1.37	1.35
21	0	138	HEM	C2D-C1D	-2.13	1.38	1.43
16	A	369	CLA	C1B-NB	2.12	1.37	1.35
16	M	1083	CLA	C1B-NB	2.11	1.37	1.35
16	N	355	CLA	C1D-ND	-2.11	1.35	1.37
16	J	365	CLA	C1B-CHB	-2.11	1.35	1.41
16	L	1107	CLA	C1B-NB	2.11	1.37	1.35
16	M	1086	CLA	C1B-NB	2.11	1.37	1.35
16	A	365	CLA	C1B-CHB	-2.10	1.35	1.41
21	V	138	HEM	C2D-C1D	-2.10	1.38	1.43
16	A	366	CLA	C1D-ND	-2.10	1.35	1.37
16	L	1116	CLA	C1B-NB	2.10	1.37	1.35
16	G	221	CLA	MG-NC	2.09	2.11	2.06
16	G	221	CLA	CHD-C1D	2.09	1.42	1.38
16	L	1111	CLA	C1B-NB	2.09	1.37	1.35
16	N	354	CLA	CAA-C2A	2.09	1.57	1.53
16	L	1115	CLA	C1B-NB	2.08	1.37	1.35
16	D	357	CLA	C1B-NB	2.08	1.37	1.35
16	C	1088	CLA	C1B-NB	2.08	1.37	1.35
16	N	354	CLA	C3A-C2A	-2.07	1.52	1.54
16	L	1117	CLA	C1B-NB	2.07	1.37	1.35
16	B	1116	CLA	C1B-NB	2.07	1.37	1.35
21	E	84	HEM	C2D-C1D	-2.07	1.38	1.43
16	L	1119	CLA	C1B-CHB	-2.06	1.35	1.41

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
16	N	355	CLA	C1D-C2D	-2.06	1.41	1.45
16	B	1110	CLA	C1B-NB	2.06	1.37	1.35
16	J	368	CLA	C1B-NB	2.06	1.37	1.35
16	M	1078	CLA	C1B-NB	2.06	1.37	1.35
16	L	1110	CLA	C1B-NB	2.05	1.37	1.35
16	C	1081	CLA	C1B-NB	2.05	1.37	1.35
16	B	1115	CLA	C1B-NB	2.05	1.37	1.35
16	A	366	CLA	C1D-C2D	-2.05	1.41	1.45
16	L	1120	CLA	C1B-CHB	-2.04	1.35	1.41
17	A	367	PHO	C2A-C3A	-2.04	1.52	1.54
16	M	1087	CLA	C1B-CHB	-2.03	1.35	1.41
16	C	1088	CLA	C1B-CHB	-2.03	1.35	1.41
16	B	1118	CLA	C1B-NB	2.03	1.37	1.35
16	L	1120	CLA	C1B-NB	2.03	1.37	1.35
16	L	1118	CLA	C1B-CHB	-2.03	1.35	1.41
16	B	1112	CLA	C1B-CHB	-2.03	1.35	1.41
16	N	356	CLA	CAA-C2A	2.02	1.57	1.53
16	B	1119	CLA	C1B-CHB	-2.02	1.35	1.41
16	C	1078	CLA	C1B-NB	2.01	1.37	1.35
16	B	1118	CLA	C1B-CHB	-2.01	1.35	1.41
16	L	1110	CLA	C1B-CHB	-2.01	1.35	1.41
16	C	1080	CLA	C1B-CHB	-2.01	1.35	1.41
16	J	367	CLA	C1B-CHB	-2.01	1.35	1.41
16	L	1108	CLA	C1B-CHB	-2.01	1.35	1.41
16	D	355	CLA	CAA-C2A	2.01	1.57	1.53
16	B	1110	CLA	C1B-CHB	-2.01	1.35	1.41
16	N	358	CLA	C1B-NB	2.01	1.37	1.35
16	M	1088	CLA	C1B-CHB	-2.01	1.35	1.41
16	B	1117	CLA	C1B-NB	2.01	1.37	1.35
16	W	64	CLA	C1B-CHB	-2.01	1.35	1.41
16	D	354	CLA	CAA-C2A	2.01	1.57	1.53
16	C	1082	CLA	C1B-CHB	-2.00	1.35	1.41
16	B	1119	CLA	C1B-NB	2.00	1.37	1.35
16	C	1084	CLA	C1B-NB	2.00	1.37	1.35
16	B	1116	CLA	C1B-CHB	-2.00	1.35	1.41
16	M	1084	CLA	C1B-CHB	-2.00	1.35	1.41
19	N	359	PLA	C3-C2	2.00	1.43	1.37

All (734) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
16	N	354	CLA	C4A-NA-C1A	10.53	111.44	106.71

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
16	D	354	CLA	C4A-NA-C1A	10.52	111.44	106.71
16	C	1089	CLA	C4A-NA-C1A	10.43	111.39	106.71
16	D	357	CLA	C4A-NA-C1A	10.37	111.37	106.71
16	N	358	CLA	C4A-NA-C1A	10.30	111.34	106.71
16	L	1119	CLA	C4A-NA-C1A	10.25	111.31	106.71
16	B	1115	CLA	C4A-NA-C1A	10.23	111.31	106.71
16	M	1081	CLA	C4A-NA-C1A	10.23	111.31	106.71
16	C	1087	CLA	C4A-NA-C1A	10.23	111.31	106.71
16	L	1114	CLA	C4A-NA-C1A	10.22	111.30	106.71
16	B	1110	CLA	C4A-NA-C1A	10.22	111.30	106.71
16	M	1080	CLA	C4A-NA-C1A	10.21	111.30	106.71
16	A	369	CLA	C4A-NA-C1A	10.21	111.29	106.71
16	M	1079	CLA	C4A-NA-C1A	10.20	111.29	106.71
16	L	1118	CLA	C4A-NA-C1A	10.19	111.29	106.71
16	L	1110	CLA	C4A-NA-C1A	10.19	111.29	106.71
16	J	368	CLA	C4A-NA-C1A	10.18	111.28	106.71
16	M	1085	CLA	C4A-NA-C1A	10.18	111.28	106.71
16	C	1082	CLA	C4A-NA-C1A	10.17	111.28	106.71
16	C	1078	CLA	C4A-NA-C1A	10.17	111.28	106.71
16	L	1122	CLA	C4A-NA-C1A	10.17	111.28	106.71
16	M	1084	CLA	C4A-NA-C1A	10.17	111.28	106.71
16	C	1079	CLA	C4A-NA-C1A	10.16	111.27	106.71
16	M	1088	CLA	C4A-NA-C1A	10.15	111.27	106.71
16	B	1114	CLA	C4A-NA-C1A	10.15	111.27	106.71
16	C	1081	CLA	C4A-NA-C1A	10.15	111.27	106.71
16	B	1118	CLA	C4A-NA-C1A	10.14	111.27	106.71
16	B	1119	CLA	C4A-NA-C1A	10.14	111.27	106.71
16	M	1086	CLA	C4A-NA-C1A	10.12	111.26	106.71
16	L	1112	CLA	C4A-NA-C1A	10.12	111.25	106.71
16	L	1115	CLA	C4A-NA-C1A	10.11	111.25	106.71
16	B	1113	CLA	C4A-NA-C1A	10.11	111.25	106.71
16	M	1082	CLA	C4A-NA-C1A	10.11	111.25	106.71
16	L	1121	CLA	C4A-NA-C1A	10.10	111.25	106.71
16	B	1111	CLA	C4A-NA-C1A	10.10	111.25	106.71
16	C	1083	CLA	C4A-NA-C1A	10.09	111.24	106.71
16	M	1078	CLA	C4A-NA-C1A	10.08	111.24	106.71
16	B	1116	CLA	C4A-NA-C1A	10.08	111.24	106.71
16	C	1086	CLA	C4A-NA-C1A	10.07	111.23	106.71
16	B	1122	CLA	C4A-NA-C1A	10.06	111.23	106.71
16	M	1083	CLA	C4A-NA-C1A	10.05	111.22	106.71
16	C	1080	CLA	C4A-NA-C1A	10.03	111.22	106.71
16	B	1112	CLA	C4A-NA-C1A	10.03	111.22	106.71

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
16	M	1087	CLA	C4A-NA-C1A	10.02	111.21	106.71
16	L	1113	CLA	C4A-NA-C1A	10.02	111.21	106.71
16	B	1121	CLA	C4A-NA-C1A	10.01	111.21	106.71
16	B	1109	CLA	C4A-NA-C1A	10.01	111.20	106.71
16	C	1085	CLA	C4A-NA-C1A	9.99	111.20	106.71
16	C	1088	CLA	C4A-NA-C1A	9.97	111.19	106.71
16	L	1107	CLA	C4A-NA-C1A	9.96	111.18	106.71
16	J	367	CLA	C4A-NA-C1A	9.95	111.18	106.71
16	L	1111	CLA	C4A-NA-C1A	9.94	111.18	106.71
16	C	1084	CLA	C4A-NA-C1A	9.94	111.17	106.71
16	B	1108	CLA	C4A-NA-C1A	9.94	111.17	106.71
16	A	368	CLA	C4A-NA-C1A	9.93	111.17	106.71
16	L	1109	CLA	C4A-NA-C1A	9.92	111.17	106.71
16	W	64	CLA	C4A-NA-C1A	9.92	111.16	106.71
16	B	1117	CLA	C4A-NA-C1A	9.90	111.16	106.71
16	L	1108	CLA	C4A-NA-C1A	9.88	111.15	106.71
16	L	1116	CLA	C4A-NA-C1A	9.86	111.14	106.71
16	L	1117	CLA	C4A-NA-C1A	9.86	111.14	106.71
16	B	1107	CLA	C4A-NA-C1A	9.86	111.14	106.71
16	B	1120	CLA	C4A-NA-C1A	9.77	111.10	106.71
16	L	1120	CLA	C4A-NA-C1A	9.73	111.08	106.71
16	R	221	CLA	C4A-NA-C1A	9.72	111.07	106.71
16	G	221	CLA	C4A-NA-C1A	9.52	110.98	106.71
16	N	356	CLA	C4A-NA-C1A	9.51	110.98	106.71
16	D	355	CLA	C4A-NA-C1A	9.40	110.93	106.71
16	N	355	CLA	C4A-NA-C1A	9.29	110.88	106.71
16	A	366	CLA	C4A-NA-C1A	9.02	110.76	106.71
16	A	365	CLA	C4A-NA-C1A	8.89	110.70	106.71
16	J	365	CLA	C4A-NA-C1A	8.81	110.67	106.71
16	J	365	CLA	OBD-CAD-CBD	-8.25	109.14	125.97
21	P	92	HEM	C3D-C4D-ND	7.94	116.18	109.48
21	0	138	HEM	C3D-C4D-ND	7.93	116.17	109.48
21	V	138	HEM	C3D-C4D-ND	7.88	116.12	109.48
21	E	84	HEM	C3D-C4D-ND	7.87	116.12	109.48
21	P	92	HEM	C2D-C3D-C4D	-7.02	98.80	107.21
21	0	138	HEM	C2D-C3D-C4D	-7.01	98.81	107.21
21	E	84	HEM	C2D-C3D-C4D	-6.97	98.86	107.21
21	V	138	HEM	C2D-C3D-C4D	-6.96	98.87	107.21
16	A	365	CLA	CAD-CBD-CHA	6.40	112.34	105.14
16	J	365	CLA	CBD-CAD-C3D	5.36	115.21	107.37
16	M	1079	CLA	CAB-C3B-C4B	5.18	136.43	128.46
16	N	355	CLA	CAB-C3B-C4B	5.16	136.39	128.46

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
17	J	366	PHO	OBD-CAD-C3D	5.15	132.15	127.22
16	B	1115	CLA	CAB-C3B-C4B	5.13	136.35	128.46
16	A	366	CLA	CAB-C3B-C4B	5.13	136.35	128.46
16	L	1115	CLA	CAB-C3B-C4B	5.12	136.33	128.46
16	C	1079	CLA	CAB-C3B-C4B	5.10	136.31	128.46
16	J	368	CLA	CAB-C3B-C4B	5.10	136.31	128.46
16	N	358	CLA	CAB-C3B-C4B	5.09	136.29	128.46
16	A	365	CLA	OBD-CAD-CBD	-5.09	115.58	125.97
16	B	1108	CLA	CAB-C3B-C4B	5.09	136.28	128.46
16	J	367	CLA	CAB-C3B-C4B	5.08	136.27	128.46
16	A	369	CLA	CAB-C3B-C4B	5.08	136.27	128.46
16	M	1082	CLA	CAB-C3B-C4B	5.08	136.27	128.46
16	M	1086	CLA	CAB-C3B-C4B	5.08	136.27	128.46
16	L	1113	CLA	CAB-C3B-C4B	5.07	136.26	128.46
16	M	1078	CLA	CAB-C3B-C4B	5.07	136.26	128.46
16	C	1084	CLA	CAB-C3B-C4B	5.07	136.26	128.46
16	L	1116	CLA	CAB-C3B-C4B	5.07	136.25	128.46
16	B	1113	CLA	CAB-C3B-C4B	5.07	136.25	128.46
16	B	1118	CLA	CAB-C3B-C4B	5.07	136.25	128.46
16	C	1086	CLA	CAB-C3B-C4B	5.06	136.25	128.46
16	M	1084	CLA	CAB-C3B-C4B	5.06	136.25	128.46
16	B	1122	CLA	CAB-C3B-C4B	5.06	136.24	128.46
16	C	1083	CLA	CAB-C3B-C4B	5.06	136.24	128.46
16	L	1108	CLA	CAB-C3B-C4B	5.06	136.24	128.46
16	B	1116	CLA	CAB-C3B-C4B	5.06	136.24	128.46
16	L	1110	CLA	CAB-C3B-C4B	5.05	136.23	128.46
16	C	1087	CLA	CAB-C3B-C4B	5.05	136.23	128.46
16	A	368	CLA	CAB-C3B-C4B	5.05	136.22	128.46
16	L	1118	CLA	CAB-C3B-C4B	5.05	136.22	128.46
16	B	1109	CLA	CAB-C3B-C4B	5.04	136.22	128.46
16	L	1114	CLA	CAB-C3B-C4B	5.04	136.22	128.46
16	C	1078	CLA	CAB-C3B-C4B	5.04	136.21	128.46
16	L	1112	CLA	CAB-C3B-C4B	5.04	136.21	128.46
17	A	367	PHO	OBD-CAD-C3D	5.04	132.05	127.22
16	B	1121	CLA	CAB-C3B-C4B	5.03	136.20	128.46
16	C	1080	CLA	CAB-C3B-C4B	5.03	136.20	128.46
16	C	1089	CLA	CAB-C3B-C4B	5.03	136.20	128.46
16	L	1119	CLA	CAB-C3B-C4B	5.03	136.20	128.46
16	C	1085	CLA	CAB-C3B-C4B	5.03	136.20	128.46
16	L	1122	CLA	CAB-C3B-C4B	5.03	136.20	128.46
16	B	1119	CLA	CAB-C3B-C4B	5.03	136.20	128.46
16	B	1107	CLA	CAB-C3B-C4B	5.03	136.19	128.46

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
16	C	1082	CLA	CAB-C3B-C4B	5.03	136.19	128.46
16	L	1107	CLA	CAB-C3B-C4B	5.03	136.19	128.46
16	M	1080	CLA	CAB-C3B-C4B	5.03	136.19	128.46
16	B	1117	CLA	CAB-C3B-C4B	5.03	136.19	128.46
16	B	1120	CLA	CAB-C3B-C4B	5.03	136.19	128.46
16	M	1085	CLA	CAB-C3B-C4B	5.02	136.19	128.46
16	L	1117	CLA	CAB-C3B-C4B	5.02	136.19	128.46
16	M	1087	CLA	CAB-C3B-C4B	5.02	136.19	128.46
16	C	1081	CLA	CAB-C3B-C4B	5.02	136.18	128.46
16	W	64	CLA	CAB-C3B-C4B	5.02	136.18	128.46
16	B	1111	CLA	CAB-C3B-C4B	5.02	136.18	128.46
16	M	1081	CLA	CAB-C3B-C4B	5.02	136.18	128.46
17	D	356	PHO	OBD-CAD-C3D	5.02	132.03	127.22
16	L	1121	CLA	CAB-C3B-C4B	5.01	136.17	128.46
16	B	1112	CLA	CAB-C3B-C4B	5.01	136.17	128.46
16	B	1114	CLA	CAB-C3B-C4B	5.01	136.16	128.46
16	B	1110	CLA	CAB-C3B-C4B	5.01	136.16	128.46
16	L	1109	CLA	CAB-C3B-C4B	5.01	136.16	128.46
16	D	357	CLA	CAB-C3B-C4B	5.01	136.16	128.46
16	M	1083	CLA	CAB-C3B-C4B	5.00	136.15	128.46
16	L	1120	CLA	CAB-C3B-C4B	5.00	136.14	128.46
16	C	1088	CLA	CAB-C3B-C4B	4.99	136.14	128.46
16	L	1111	CLA	CAB-C3B-C4B	4.99	136.13	128.46
17	N	357	PHO	OBD-CAD-C3D	4.98	132.00	127.22
16	N	355	CLA	CAB-C3B-C2B	-4.95	114.99	124.69
16	M	1088	CLA	CAB-C3B-C4B	4.95	136.07	128.46
16	A	366	CLA	CAB-C3B-C2B	-4.94	115.00	124.69
16	A	369	CLA	CAB-C3B-C2B	-4.83	115.22	124.69
16	J	368	CLA	CAB-C3B-C2B	-4.82	115.25	124.69
17	J	366	PHO	CAB-C3B-C2B	-4.82	115.25	124.69
17	N	357	PHO	CAB-C3B-C2B	-4.81	115.27	124.69
16	B	1113	CLA	CAB-C3B-C2B	-4.80	115.28	124.69
16	L	1120	CLA	CAB-C3B-C2B	-4.80	115.28	124.69
16	N	358	CLA	CAB-C3B-C2B	-4.80	115.28	124.69
16	C	1089	CLA	CAB-C3B-C2B	-4.80	115.28	124.69
16	M	1087	CLA	CAB-C3B-C2B	-4.79	115.29	124.69
16	B	1107	CLA	CAB-C3B-C2B	-4.79	115.30	124.69
16	M	1083	CLA	CAB-C3B-C2B	-4.79	115.30	124.69
16	C	1086	CLA	CAB-C3B-C2B	-4.79	115.30	124.69
17	D	356	PHO	CAB-C3B-C2B	-4.79	115.30	124.69
16	M	1085	CLA	CAB-C3B-C2B	-4.79	115.31	124.69
16	J	367	CLA	CAB-C3B-C2B	-4.79	115.31	124.69

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
16	L	1113	CLA	CAB-C3B-C2B	-4.79	115.31	124.69
16	C	1079	CLA	CAB-C3B-C2B	-4.78	115.31	124.69
16	C	1084	CLA	CAB-C3B-C2B	-4.78	115.31	124.69
16	C	1082	CLA	CAB-C3B-C2B	-4.78	115.32	124.69
16	C	1080	CLA	CAB-C3B-C2B	-4.78	115.33	124.69
16	A	368	CLA	CAB-C3B-C2B	-4.78	115.33	124.69
16	L	1121	CLA	CAB-C3B-C2B	-4.77	115.34	124.69
16	M	1079	CLA	CAB-C3B-C2B	-4.77	115.34	124.69
16	L	1107	CLA	CAB-C3B-C2B	-4.77	115.34	124.69
16	B	1115	CLA	CAB-C3B-C2B	-4.77	115.34	124.69
16	B	1120	CLA	CAB-C3B-C2B	-4.77	115.34	124.69
16	B	1108	CLA	CAB-C3B-C2B	-4.77	115.34	124.69
16	W	64	CLA	CAB-C3B-C2B	-4.77	115.34	124.69
16	C	1088	CLA	CAB-C3B-C2B	-4.77	115.35	124.69
16	M	1088	CLA	CAB-C3B-C2B	-4.77	115.35	124.69
16	B	1114	CLA	CAB-C3B-C2B	-4.77	115.35	124.69
16	M	1080	CLA	CAB-C3B-C2B	-4.77	115.35	124.69
16	L	1110	CLA	CAB-C3B-C2B	-4.76	115.35	124.69
16	L	1112	CLA	CAB-C3B-C2B	-4.76	115.36	124.69
16	D	357	CLA	CAB-C3B-C2B	-4.76	115.36	124.69
16	M	1084	CLA	CAB-C3B-C2B	-4.76	115.37	124.69
16	L	1114	CLA	CAB-C3B-C2B	-4.76	115.37	124.69
17	A	367	PHO	CAB-C3B-C2B	-4.75	115.38	124.69
16	C	1078	CLA	CAB-C3B-C2B	-4.75	115.38	124.69
16	M	1078	CLA	CAB-C3B-C2B	-4.75	115.39	124.69
16	B	1119	CLA	CAB-C3B-C2B	-4.75	115.39	124.69
16	C	1081	CLA	CAB-C3B-C2B	-4.74	115.39	124.69
16	M	1082	CLA	CAB-C3B-C2B	-4.74	115.40	124.69
16	B	1121	CLA	CAB-C3B-C2B	-4.74	115.40	124.69
16	B	1117	CLA	CAB-C3B-C2B	-4.73	115.41	124.69
16	B	1110	CLA	CAB-C3B-C2B	-4.73	115.41	124.69
16	L	1116	CLA	CAB-C3B-C2B	-4.73	115.42	124.69
16	M	1086	CLA	CAB-C3B-C2B	-4.73	115.42	124.69
16	L	1119	CLA	CAB-C3B-C2B	-4.73	115.42	124.69
16	L	1108	CLA	CAB-C3B-C2B	-4.73	115.42	124.69
16	C	1085	CLA	CAB-C3B-C2B	-4.73	115.42	124.69
16	L	1117	CLA	CAB-C3B-C2B	-4.73	115.43	124.69
16	L	1115	CLA	CAB-C3B-C2B	-4.72	115.43	124.69
16	B	1111	CLA	CAB-C3B-C2B	-4.72	115.43	124.69
16	B	1122	CLA	CAB-C3B-C2B	-4.72	115.43	124.69
16	B	1109	CLA	CAB-C3B-C2B	-4.72	115.43	124.69
16	L	1118	CLA	CAB-C3B-C2B	-4.72	115.44	124.69

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
16	L	1111	CLA	CAB-C3B-C2B	-4.72	115.44	124.69
16	B	1116	CLA	CAB-C3B-C2B	-4.71	115.45	124.69
16	M	1081	CLA	CAB-C3B-C2B	-4.71	115.45	124.69
16	B	1112	CLA	CAB-C3B-C2B	-4.71	115.46	124.69
16	C	1087	CLA	CAB-C3B-C2B	-4.71	115.46	124.69
16	L	1109	CLA	CAB-C3B-C2B	-4.71	115.47	124.69
16	B	1118	CLA	CAB-C3B-C2B	-4.71	115.47	124.69
16	L	1122	CLA	CAB-C3B-C2B	-4.70	115.48	124.69
16	C	1083	CLA	CAB-C3B-C2B	-4.70	115.48	124.69
21	P	92	HEM	C2C-C1C-NC	4.66	111.95	108.27
21	E	84	HEM	C2C-C1C-NC	4.65	111.94	108.27
21	0	138	HEM	C2C-C1C-NC	4.59	111.90	108.27
21	V	138	HEM	C2C-C1C-NC	4.59	111.90	108.27
16	D	355	CLA	CAB-C3B-C4B	4.57	135.48	128.46
16	N	356	CLA	CAB-C3B-C4B	4.52	135.40	128.46
16	J	365	CLA	CMA-C3A-C2A	-4.42	105.79	116.10
16	A	365	CLA	CMA-C3A-C2A	-4.42	105.80	116.10
16	R	221	CLA	CMA-C3A-C2A	-4.34	105.98	116.10
16	G	221	CLA	CMA-C3A-C2A	-4.32	106.02	116.10
16	N	354	CLA	CMA-C3A-C2A	-4.28	106.11	116.10
16	D	354	CLA	CMA-C3A-C2A	-4.26	106.17	116.10
16	D	354	CLA	CAB-C3B-C4B	4.23	134.97	128.46
16	N	354	CLA	CAB-C3B-C4B	4.22	134.95	128.46
16	N	354	CLA	CAA-C2A-C3A	-4.21	106.27	116.10
16	D	354	CLA	CAA-C2A-C3A	-4.19	106.31	116.10
16	D	355	CLA	CAB-C3B-C2B	-4.12	116.61	124.69
16	R	221	CLA	CAA-C2A-C3A	-4.12	106.48	116.10
16	N	356	CLA	CAB-C3B-C2B	-4.11	116.64	124.69
16	G	221	CLA	CAA-C2A-C3A	-4.09	106.56	116.10
16	J	365	CLA	CAA-C2A-C3A	-4.07	106.59	116.10
16	A	365	CLA	CAA-C2A-C3A	-4.05	106.65	116.10
20	D	359	BCR	C38-C26-C25	3.97	128.98	124.53
16	A	365	CLA	CAB-C3B-C4B	3.97	134.56	128.46
16	J	365	CLA	CAB-C3B-C4B	3.94	134.52	128.46
20	D	359	BCR	C33-C5-C6	3.90	128.90	124.53
20	K	47	BCR	C7-C8-C9	3.87	130.69	126.59
16	J	365	CLA	CAD-CBD-CHA	-3.79	100.87	105.14
21	E	84	HEM	CHC-C4B-NB	-3.70	120.38	124.44
21	V	138	HEM	C3C-C4C-NC	3.69	111.19	108.27
21	P	92	HEM	CHC-C4B-NB	-3.67	120.41	124.44
21	0	138	HEM	C3C-C4C-NC	3.67	111.17	108.27
21	0	138	HEM	C3D-C4D-CHA	-3.66	116.89	125.67

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
21	P	92	HEM	C3D-C4D-CHA	-3.65	116.93	125.67
21	E	84	HEM	C3C-C4C-NC	3.65	111.15	108.27
16	J	365	CLA	OBD-CAD-C3D	3.64	134.77	128.74
21	V	138	HEM	C3D-C4D-CHA	-3.63	116.98	125.67
21	V	138	HEM	CHC-C4B-NB	-3.62	120.46	124.44
21	E	84	HEM	C3D-C4D-CHA	-3.62	117.01	125.67
16	A	365	CLA	OBD-CAD-C3D	3.60	134.71	128.74
21	0	138	HEM	CHC-C4B-NB	-3.57	120.52	124.44
16	N	355	CLA	CAA-C2A-C3A	-3.56	107.80	116.10
21	P	92	HEM	C3C-C4C-NC	3.56	111.08	108.27
16	A	366	CLA	CAA-C2A-C3A	-3.54	107.84	116.10
21	0	138	HEM	C1C-NC-C4C	3.49	108.42	105.79
21	V	138	HEM	C1C-NC-C4C	3.48	108.41	105.79
21	P	92	HEM	C3D-C2D-C1D	3.48	111.38	107.21
21	P	92	HEM	C1C-NC-C4C	3.46	108.39	105.79
21	E	84	HEM	C1C-NC-C4C	3.44	108.38	105.79
16	D	354	CLA	CAB-C3B-C2B	-3.43	117.97	124.69
21	E	84	HEM	C3D-C2D-C1D	3.43	111.32	107.21
21	V	138	HEM	C3D-C2D-C1D	3.41	111.30	107.21
16	N	354	CLA	CAB-C3B-C2B	-3.41	118.00	124.69
21	0	138	HEM	C3D-C2D-C1D	3.41	111.30	107.21
16	N	356	CLA	CAA-C2A-C3A	-3.39	108.18	116.10
16	D	355	CLA	CAA-C2A-C3A	-3.37	108.22	116.10
16	A	365	CLA	CAB-C3B-C2B	-3.32	118.18	124.69
16	R	221	CLA	CHD-C1D-ND	-3.31	121.41	124.45
16	J	365	CLA	CAB-C3B-C2B	-3.28	118.25	124.69
16	G	221	CLA	CHD-C1D-ND	-3.27	121.44	124.45
17	A	367	PHO	C1A-C2A-C3A	3.26	103.97	101.74
20	D	359	BCR	C2-C1-C6	3.23	115.45	110.48
16	M	1080	CLA	CMA-C3A-C2A	-3.22	108.59	116.10
16	G	221	CLA	CMB-C2B-C1B	-3.19	123.56	128.46
16	L	1119	CLA	CMA-C3A-C2A	-3.18	108.67	116.10
16	M	1078	CLA	CMA-C3A-C2A	-3.18	108.68	116.10
16	J	365	CLA	C2D-C1D-ND	3.18	112.44	110.10
17	D	356	PHO	CMA-C3A-C2A	-3.18	108.69	116.10
16	B	1119	CLA	CMA-C3A-C2A	-3.17	108.69	116.10
16	B	1116	CLA	CMA-C3A-C2A	-3.17	108.70	116.10
16	B	1110	CLA	CMA-C3A-C2A	-3.17	108.70	116.10
16	C	1078	CLA	CMA-C3A-C2A	-3.17	108.70	116.10
16	C	1081	CLA	CMA-C3A-C2A	-3.17	108.70	116.10
16	L	1122	CLA	CMA-C3A-C2A	-3.17	108.70	116.10
16	L	1116	CLA	CMA-C3A-C2A	-3.17	108.71	116.10

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
16	J	367	CLA	CMA-C3A-C2A	-3.17	108.71	116.10
16	L	1115	CLA	CMA-C3A-C2A	-3.16	108.71	116.10
16	L	1114	CLA	CMA-C3A-C2A	-3.16	108.71	116.10
16	C	1085	CLA	CMA-C3A-C2A	-3.16	108.72	116.10
17	J	366	PHO	CMA-C3A-C2A	-3.16	108.72	116.10
16	C	1079	CLA	CMA-C3A-C2A	-3.16	108.72	116.10
16	L	1110	CLA	CMA-C3A-C2A	-3.16	108.72	116.10
16	C	1086	CLA	CMA-C3A-C2A	-3.16	108.72	116.10
16	G	221	CLA	CAB-C3B-C4B	3.16	133.32	128.46
17	N	357	PHO	CMA-C3A-C2A	-3.16	108.73	116.10
16	L	1108	CLA	CMA-C3A-C2A	-3.16	108.73	116.10
16	M	1082	CLA	CMA-C3A-C2A	-3.16	108.73	116.10
16	B	1115	CLA	CMA-C3A-C2A	-3.16	108.73	116.10
16	B	1108	CLA	CMA-C3A-C2A	-3.15	108.74	116.10
16	L	1111	CLA	CMA-C3A-C2A	-3.15	108.74	116.10
16	C	1087	CLA	CMA-C3A-C2A	-3.15	108.75	116.10
16	M	1084	CLA	CMA-C3A-C2A	-3.15	108.75	116.10
17	A	367	PHO	CMA-C3A-C2A	-3.15	108.76	116.10
16	B	1114	CLA	CMA-C3A-C2A	-3.15	108.76	116.10
16	L	1109	CLA	CMA-C3A-C2A	-3.15	108.76	116.10
16	R	221	CLA	CAB-C3B-C4B	3.15	133.30	128.46
16	M	1086	CLA	CMA-C3A-C2A	-3.14	108.76	116.10
16	B	1109	CLA	CMA-C3A-C2A	-3.14	108.76	116.10
16	M	1085	CLA	CMA-C3A-C2A	-3.14	108.76	116.10
16	L	1121	CLA	CMA-C3A-C2A	-3.14	108.76	116.10
16	M	1079	CLA	CMA-C3A-C2A	-3.14	108.77	116.10
16	B	1111	CLA	CMA-C3A-C2A	-3.14	108.77	116.10
16	B	1122	CLA	CMA-C3A-C2A	-3.14	108.77	116.10
16	C	1088	CLA	CMA-C3A-C2A	-3.14	108.78	116.10
16	A	368	CLA	CMA-C3A-C2A	-3.14	108.78	116.10
16	C	1082	CLA	CMA-C3A-C2A	-3.14	108.78	116.10
16	C	1080	CLA	CMA-C3A-C2A	-3.14	108.78	116.10
16	C	1089	CLA	CMA-C3A-C2A	-3.14	108.78	116.10
16	M	1087	CLA	CMA-C3A-C2A	-3.13	108.78	116.10
16	B	1107	CLA	CMA-C3A-C2A	-3.13	108.80	116.10
16	M	1081	CLA	CMA-C3A-C2A	-3.13	108.80	116.10
16	C	1083	CLA	CMA-C3A-C2A	-3.13	108.80	116.10
16	B	1118	CLA	CMA-C3A-C2A	-3.13	108.80	116.10
16	A	369	CLA	CMA-C3A-C2A	-3.13	108.80	116.10
16	C	1084	CLA	CMA-C3A-C2A	-3.13	108.80	116.10
16	L	1112	CLA	CMA-C3A-C2A	-3.13	108.81	116.10
16	B	1117	CLA	CMA-C3A-C2A	-3.12	108.81	116.10

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
16	M	1088	CLA	CMA-C3A-C2A	-3.12	108.81	116.10
16	L	1118	CLA	CMA-C3A-C2A	-3.12	108.81	116.10
16	L	1107	CLA	CMA-C3A-C2A	-3.12	108.82	116.10
16	W	64	CLA	CMA-C3A-C2A	-3.12	108.82	116.10
16	B	1121	CLA	CMA-C3A-C2A	-3.12	108.82	116.10
16	B	1112	CLA	CMA-C3A-C2A	-3.12	108.82	116.10
16	L	1117	CLA	CMA-C3A-C2A	-3.12	108.83	116.10
16	J	368	CLA	CMA-C3A-C2A	-3.12	108.83	116.10
16	R	221	CLA	CMB-C2B-C1B	-3.11	123.68	128.46
16	B	1120	CLA	CMA-C3A-C2A	-3.11	108.84	116.10
16	M	1083	CLA	CMA-C3A-C2A	-3.11	108.84	116.10
16	B	1113	CLA	CMA-C3A-C2A	-3.11	108.84	116.10
16	D	357	CLA	CMA-C3A-C2A	-3.11	108.84	116.10
16	L	1113	CLA	CMA-C3A-C2A	-3.11	108.85	116.10
16	L	1120	CLA	CMA-C3A-C2A	-3.10	108.86	116.10
16	N	358	CLA	CMA-C3A-C2A	-3.10	108.86	116.10
17	J	366	PHO	C1A-C2A-C3A	3.09	103.85	101.74
16	M	1088	CLA	CMB-C2B-C1B	-3.08	123.72	128.46
16	N	358	CLA	CMB-C2B-C1B	-3.08	123.74	128.46
16	M	1083	CLA	CMB-C2B-C1B	-3.07	123.74	128.46
16	L	1107	CLA	CMB-C2B-C1B	-3.07	123.75	128.46
16	L	1120	CLA	CMB-C2B-C1B	-3.07	123.75	128.46
16	D	357	CLA	CMB-C2B-C1B	-3.06	123.75	128.46
16	A	365	CLA	C2D-C1D-ND	3.06	112.36	110.10
16	L	1117	CLA	CMB-C2B-C1B	-3.06	123.76	128.46
16	L	1112	CLA	CMB-C2B-C1B	-3.05	123.77	128.46
16	B	1112	CLA	CMB-C2B-C1B	-3.05	123.78	128.46
16	B	1117	CLA	CMB-C2B-C1B	-3.05	123.78	128.46
16	C	1080	CLA	CMB-C2B-C1B	-3.04	123.79	128.46
16	W	64	CLA	CMB-C2B-C1B	-3.04	123.79	128.46
16	B	1113	CLA	CMB-C2B-C1B	-3.04	123.80	128.46
20	D	359	BCR	C38-C26-C27	-3.03	107.79	113.62
16	J	365	CLA	C2A-C3A-C4A	3.03	105.65	101.78
16	L	1110	CLA	CMB-C2B-C1B	-3.03	123.81	128.46
16	A	365	CLA	C2A-C3A-C4A	3.03	105.64	101.78
16	B	1120	CLA	CMB-C2B-C1B	-3.02	123.81	128.46
16	C	1086	CLA	CMB-C2B-C1B	-3.02	123.82	128.46
16	C	1084	CLA	CMB-C2B-C1B	-3.02	123.82	128.46
16	B	1107	CLA	CMB-C2B-C1B	-3.02	123.82	128.46
16	C	1081	CLA	CMB-C2B-C1B	-3.02	123.83	128.46
16	C	1082	CLA	CMB-C2B-C1B	-3.02	123.83	128.46
17	A	367	PHO	CMA-C3A-C4A	-3.01	107.79	114.38

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
20	D	359	BCR	C7-C8-C9	3.00	130.77	126.23
17	J	366	PHO	CMA-C3A-C4A	-3.00	107.80	114.38
16	L	1111	CLA	CMB-C2B-C1B	-3.00	123.85	128.46
16	L	1113	CLA	CMB-C2B-C1B	-3.00	123.85	128.46
16	L	1121	CLA	CMB-C2B-C1B	-3.00	123.86	128.46
16	M	1086	CLA	CMB-C2B-C1B	-3.00	123.86	128.46
16	B	1118	CLA	CMB-C2B-C1B	-2.99	123.86	128.46
16	L	1109	CLA	CMB-C2B-C1B	-2.99	123.86	128.46
16	M	1084	CLA	CMB-C2B-C1B	-2.99	123.86	128.46
16	M	1085	CLA	CMB-C2B-C1B	-2.99	123.86	128.46
16	C	1088	CLA	CMB-C2B-C1B	-2.99	123.86	128.46
16	M	1080	CLA	CMB-C2B-C1B	-2.99	123.87	128.46
17	N	357	PHO	C4A-C3A-C2A	2.99	103.78	101.74
16	B	1110	CLA	CMB-C2B-C1B	-2.99	123.87	128.46
16	B	1121	CLA	CMB-C2B-C1B	-2.99	123.87	128.46
16	L	1114	CLA	CMB-C2B-C1B	-2.99	123.87	128.46
16	B	1109	CLA	CMB-C2B-C1B	-2.99	123.87	128.46
16	B	1114	CLA	CMB-C2B-C1B	-2.99	123.87	128.46
16	C	1089	CLA	CMB-C2B-C1B	-2.99	123.87	128.46
16	A	369	CLA	CMB-C2B-C1B	-2.99	123.88	128.46
16	B	1111	CLA	CMB-C2B-C1B	-2.98	123.88	128.46
16	L	1108	CLA	CMB-C2B-C1B	-2.98	123.88	128.46
16	C	1079	CLA	CMB-C2B-C1B	-2.98	123.88	128.46
16	M	1079	CLA	CMB-C2B-C1B	-2.98	123.88	128.46
17	D	356	PHO	CMA-C3A-C4A	-2.98	107.86	114.38
20	K	47	BCR	C24-C23-C22	2.98	129.74	126.59
16	L	1118	CLA	CMB-C2B-C1B	-2.97	123.90	128.46
17	N	357	PHO	CAA-C2A-C1A	-2.97	107.27	114.23
16	C	1085	CLA	CMB-C2B-C1B	-2.96	123.91	128.46
16	C	1087	CLA	CMB-C2B-C1B	-2.96	123.91	128.46
16	L	1116	CLA	CMB-C2B-C1B	-2.96	123.91	128.46
16	J	368	CLA	CMB-C2B-C1B	-2.96	123.91	128.46
17	N	357	PHO	CMA-C3A-C4A	-2.96	107.89	114.38
16	B	1119	CLA	CMB-C2B-C1B	-2.96	123.91	128.46
16	L	1115	CLA	CMB-C2B-C1B	-2.96	123.91	128.46
16	B	1108	CLA	CMB-C2B-C1B	-2.96	123.92	128.46
16	B	1115	CLA	CMB-C2B-C1B	-2.96	123.92	128.46
16	J	367	CLA	CMB-C2B-C1B	-2.96	123.92	128.46
16	M	1087	CLA	CMB-C2B-C1B	-2.95	123.92	128.46
16	M	1078	CLA	CMB-C2B-C1B	-2.95	123.93	128.46
16	C	1083	CLA	CMB-C2B-C1B	-2.95	123.93	128.46
17	A	367	PHO	CAA-C2A-C1A	-2.95	107.32	114.23

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
17	J	366	PHO	CAA-C2A-C1A	-2.94	107.33	114.23
16	L	1119	CLA	CMB-C2B-C1B	-2.94	123.94	128.46
16	B	1122	CLA	CMB-C2B-C1B	-2.94	123.94	128.46
20	D	359	BCR	C29-C30-C25	2.94	115.01	110.48
16	B	1116	CLA	CMB-C2B-C1B	-2.94	123.95	128.46
16	C	1078	CLA	CMB-C2B-C1B	-2.94	123.95	128.46
16	A	368	CLA	CMB-C2B-C1B	-2.93	123.96	128.46
20	D	359	BCR	C33-C5-C4	-2.92	108.00	113.62
16	M	1081	CLA	CMB-C2B-C1B	-2.92	123.98	128.46
17	D	356	PHO	CAA-C2A-C1A	-2.91	107.40	114.23
16	N	356	CLA	CMB-C2B-C1B	-2.91	123.99	128.46
16	D	355	CLA	CMB-C2B-C1B	-2.91	124.00	128.46
16	M	1082	CLA	CMB-C2B-C1B	-2.91	124.00	128.46
16	L	1122	CLA	CMB-C2B-C1B	-2.90	124.01	128.46
17	D	356	PHO	C4A-C3A-C2A	2.88	103.70	101.74
16	A	366	CLA	CMB-C2B-C1B	-2.85	124.09	128.46
16	D	355	CLA	CMA-C3A-C2A	-2.85	109.45	116.10
16	N	355	CLA	CMB-C2B-C1B	-2.85	124.09	128.46
16	N	356	CLA	CMA-C3A-C2A	-2.84	109.47	116.10
17	D	356	PHO	C1A-C2A-C3A	2.83	103.67	101.74
17	N	357	PHO	C1A-C2A-C3A	2.81	103.66	101.74
16	D	355	CLA	OBD-CAD-CBD	-2.73	120.40	125.97
16	A	365	CLA	CMB-C2B-C1B	-2.72	124.28	128.46
16	J	365	CLA	CMB-C2B-C1B	-2.71	124.29	128.46
16	N	356	CLA	OBD-CAD-CBD	-2.71	120.43	125.97
16	R	221	CLA	C2A-C3A-C4A	2.68	105.20	101.78
16	G	221	CLA	C2A-C3A-C4A	2.66	105.18	101.78
20	D	359	BCR	C8-C9-C10	-2.64	114.89	118.94
16	A	366	CLA	OBD-CAD-CBD	-2.63	120.59	125.97
16	N	354	CLA	C2A-C3A-C4A	2.62	105.13	101.78
16	N	355	CLA	OBD-CAD-CBD	-2.62	120.62	125.97
17	J	366	PHO	C4A-C3A-C2A	2.60	103.52	101.74
17	A	367	PHO	C4A-C3A-C2A	2.59	103.51	101.74
16	N	356	CLA	C2A-C1A-CHA	2.58	128.35	123.85
16	D	354	CLA	C2A-C3A-C4A	2.56	105.06	101.78
16	N	355	CLA	CMA-C3A-C2A	-2.56	110.12	116.10
16	L	1112	CLA	C2D-C1D-ND	2.56	111.99	110.10
16	A	366	CLA	CMA-C3A-C2A	-2.55	110.15	116.10
16	G	221	CLA	CMB-C2B-C3B	2.55	129.67	124.69
16	L	1120	CLA	C2D-C1D-ND	2.54	111.98	110.10
21	P	92	HEM	C3C-C2C-C1C	-2.54	104.11	106.30
21	E	84	HEM	C3C-C2C-C1C	-2.54	104.12	106.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
16	R	221	CLA	CMB-C2B-C3B	2.53	129.64	124.69
21	0	138	HEM	C3C-C2C-C1C	-2.53	104.13	106.30
16	B	1112	CLA	C2D-C1D-ND	2.51	111.96	110.10
16	D	355	CLA	C2A-C1A-CHA	2.50	128.22	123.85
16	B	1120	CLA	C2D-C1D-ND	2.49	111.94	110.10
20	D	359	BCR	C34-C9-C8	2.48	121.99	118.08
16	L	1121	CLA	C2D-C1D-ND	2.47	111.93	110.10
21	V	138	HEM	C3C-C2C-C1C	-2.46	104.18	106.30
16	R	221	CLA	C2D-C1D-ND	2.45	111.91	110.10
16	L	1110	CLA	C2D-C1D-ND	2.44	111.90	110.10
16	L	1120	CLA	CHD-C1D-ND	-2.44	122.22	124.45
16	B	1110	CLA	C2D-C1D-ND	2.43	111.90	110.10
16	B	1120	CLA	CHD-C1D-ND	-2.43	122.22	124.45
16	L	1113	CLA	C2D-C1D-ND	2.43	111.89	110.10
16	J	368	CLA	C2D-C1D-ND	2.42	111.88	110.10
16	A	369	CLA	C2D-C1D-ND	2.41	111.88	110.10
16	A	365	CLA	C4D-C3D-CAD	-2.41	104.48	107.70
16	C	1080	CLA	C2D-C1D-ND	2.41	111.88	110.10
16	J	365	CLA	CHD-C1D-ND	-2.40	122.25	124.45
16	M	1083	CLA	C2D-C1D-ND	2.40	111.87	110.10
16	B	1107	CLA	C2D-C1D-ND	2.40	111.87	110.10
16	M	1087	CLA	C2D-C1D-ND	2.40	111.87	110.10
16	B	1113	CLA	C2D-C1D-ND	2.39	111.87	110.10
16	C	1088	CLA	C2D-C1D-ND	2.39	111.86	110.10
16	D	357	CLA	CHD-C1D-ND	-2.39	122.26	124.45
16	N	358	CLA	CHD-C1D-ND	-2.38	122.27	124.45
16	M	1085	CLA	C2D-C1D-ND	2.38	111.86	110.10
16	C	1086	CLA	C2D-C1D-ND	2.37	111.85	110.10
16	G	221	CLA	C2D-C1D-ND	2.37	111.85	110.10
16	L	1114	CLA	C2D-C1D-ND	2.37	111.85	110.10
16	B	1121	CLA	C2D-C1D-ND	2.36	111.84	110.10
16	W	64	CLA	C2D-C1D-ND	2.36	111.84	110.10
16	J	365	CLA	C4D-C3D-CAD	-2.36	104.56	107.70
16	B	1117	CLA	C2D-C1D-ND	2.36	111.84	110.10
16	C	1086	CLA	OBD-CAD-CBD	-2.36	121.16	125.97
16	L	1114	CLA	OBD-CAD-CBD	-2.35	121.18	125.97
16	A	366	CLA	C2A-C3A-C4A	2.35	104.78	101.78
16	L	1112	CLA	CHD-C1D-ND	-2.34	122.30	124.45
16	L	1107	CLA	C2D-C1D-ND	2.34	111.83	110.10
16	B	1110	CLA	CHD-C1D-ND	-2.34	122.31	124.45
16	L	1110	CLA	CHD-C1D-ND	-2.34	122.31	124.45
16	L	1117	CLA	OBD-CAD-CBD	-2.33	121.20	125.97

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
21	E	84	HEM	C4B-CHC-C1C	2.33	131.87	126.10
16	M	1085	CLA	OBD-CAD-CBD	-2.33	121.21	125.97
21	P	92	HEM	C4B-CHC-C1C	2.33	131.86	126.10
16	M	1088	CLA	OBD-CAD-CBD	-2.33	121.21	125.97
16	N	355	CLA	C2A-C3A-C4A	2.33	104.76	101.78
16	J	368	CLA	OBD-CAD-CBD	-2.33	121.21	125.97
16	L	1109	CLA	C2D-C1D-ND	2.33	111.82	110.10
16	B	1114	CLA	C2D-C1D-ND	2.33	111.82	110.10
16	B	1112	CLA	CHD-C1D-ND	-2.33	122.32	124.45
16	L	1113	CLA	CHD-C1D-ND	-2.32	122.32	124.45
16	B	1113	CLA	OBD-CAD-CBD	-2.32	121.23	125.97
16	L	1117	CLA	C2D-C1D-ND	2.32	111.81	110.10
16	L	1110	CLA	OBD-CAD-CBD	-2.32	121.24	125.97
16	M	1080	CLA	C2D-C1D-ND	2.31	111.81	110.10
16	L	1121	CLA	CHD-C1D-ND	-2.31	122.33	124.45
16	M	1082	CLA	OBD-CAD-CBD	-2.31	121.25	125.97
16	C	1081	CLA	OBD-CAD-CBD	-2.31	121.26	125.97
16	M	1088	CLA	C2D-C1D-ND	2.30	111.80	110.10
16	M	1083	CLA	OBD-CAD-CBD	-2.30	121.27	125.97
16	B	1117	CLA	OBD-CAD-CBD	-2.30	121.27	125.97
16	B	1120	CLA	OBD-CAD-CBD	-2.30	121.27	125.97
16	L	1112	CLA	OBD-CAD-CBD	-2.30	121.27	125.97
21	0	138	HEM	C3A-C2A-C1A	-2.30	104.32	106.29
20	D	359	BCR	C24-C23-C22	2.30	129.71	126.23
21	V	138	HEM	C2C-C3C-C4C	-2.30	104.32	106.30
16	B	1110	CLA	OBD-CAD-CBD	-2.30	121.28	125.97
16	L	1121	CLA	OBD-CAD-CBD	-2.30	121.28	125.97
16	D	357	CLA	C2D-C1D-ND	2.30	111.80	110.10
16	D	357	CLA	OBD-CAD-CBD	-2.30	121.28	125.97
16	C	1089	CLA	C2D-C1D-ND	2.30	111.80	110.10
21	0	138	HEM	C4B-CHC-C1C	2.30	131.78	126.10
16	W	64	CLA	OBD-CAD-CBD	-2.29	121.28	125.97
16	B	1107	CLA	CHD-C1D-ND	-2.29	122.35	124.45
21	V	138	HEM	C4B-CHC-C1C	2.29	131.77	126.10
16	M	1080	CLA	OBD-CAD-CBD	-2.29	121.29	125.97
21	E	84	HEM	C3A-C2A-C1A	-2.29	104.33	106.29
16	N	356	CLA	C2A-C3A-C4A	2.29	104.70	101.78
16	B	1109	CLA	C2D-C1D-ND	2.29	111.79	110.10
16	B	1112	CLA	OBD-CAD-CBD	-2.29	121.30	125.97
16	L	1120	CLA	OBD-CAD-CBD	-2.29	121.30	125.97
16	M	1079	CLA	C2D-C1D-ND	2.29	111.79	110.10
16	B	1114	CLA	OBD-CAD-CBD	-2.29	121.30	125.97

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
16	C	1084	CLA	OBD-CAD-CBD	-2.29	121.30	125.97
16	L	1107	CLA	OBD-CAD-CBD	-2.29	121.30	125.97
16	L	1119	CLA	OBD-CAD-CBD	-2.29	121.30	125.97
16	B	1107	CLA	OBD-CAD-CBD	-2.28	121.31	125.97
16	C	1081	CLA	C2D-C1D-ND	2.28	111.79	110.10
16	M	1080	CLA	CHD-C1D-ND	-2.28	122.36	124.45
16	A	369	CLA	OBD-CAD-CBD	-2.28	121.32	125.97
16	B	1113	CLA	CHD-C1D-ND	-2.27	122.36	124.45
16	L	1116	CLA	OBD-CAD-CBD	-2.27	121.33	125.97
16	C	1083	CLA	OBD-CAD-CBD	-2.27	121.33	125.97
16	L	1115	CLA	OBD-CAD-CBD	-2.27	121.33	125.97
16	J	368	CLA	CHD-C1D-ND	-2.27	122.37	124.45
16	M	1087	CLA	OBD-CAD-CBD	-2.27	121.34	125.97
16	C	1080	CLA	OBD-CAD-CBD	-2.27	121.34	125.97
16	C	1085	CLA	OBD-CAD-CBD	-2.27	121.34	125.97
16	L	1113	CLA	OBD-CAD-CBD	-2.27	121.34	125.97
16	C	1084	CLA	C2D-C1D-ND	2.26	111.77	110.10
16	C	1089	CLA	OBD-CAD-CBD	-2.26	121.34	125.97
16	M	1079	CLA	OBD-CAD-CBD	-2.26	121.34	125.97
21	P	92	HEM	C3A-C2A-C1A	-2.26	104.35	106.29
16	N	358	CLA	OBD-CAD-CBD	-2.26	121.35	125.97
16	C	1080	CLA	CHD-C1D-ND	-2.26	122.38	124.45
16	C	1086	CLA	CHD-C1D-ND	-2.26	122.38	124.45
16	B	1109	CLA	OBD-CAD-CBD	-2.26	121.36	125.97
16	B	1121	CLA	OBD-CAD-CBD	-2.26	121.36	125.97
20	D	359	BCR	C30-C25-C26	-2.26	119.43	122.61
16	C	1088	CLA	OBD-CAD-CBD	-2.25	121.37	125.97
16	B	1117	CLA	CHD-C1D-ND	-2.25	122.39	124.45
16	L	1114	CLA	CHD-C1D-ND	-2.25	122.39	124.45
16	B	1119	CLA	C2D-C1D-ND	2.25	111.76	110.10
16	J	367	CLA	OBD-CAD-CBD	-2.25	121.37	125.97
21	V	138	HEM	C3A-C2A-C1A	-2.25	104.36	106.29
16	B	1118	CLA	OBD-CAD-CBD	-2.25	121.38	125.97
20	D	359	BCR	C23-C24-C25	2.25	133.52	127.20
16	C	1089	CLA	CHD-C1D-ND	-2.25	122.39	124.45
16	N	354	CLA	C2D-C1D-ND	2.25	111.76	110.10
16	C	1079	CLA	OBD-CAD-CBD	-2.25	121.38	125.97
16	A	368	CLA	OBD-CAD-CBD	-2.25	121.38	125.97
16	C	1082	CLA	OBD-CAD-CBD	-2.25	121.38	125.97
16	M	1084	CLA	OBD-CAD-CBD	-2.25	121.38	125.97
16	L	1109	CLA	OBD-CAD-CBD	-2.24	121.39	125.97
16	B	1115	CLA	OBD-CAD-CBD	-2.24	121.39	125.97

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
16	B	1122	CLA	OBD-CAD-CBD	-2.24	121.39	125.97
20	D	359	BCR	C23-C22-C21	-2.24	115.50	118.94
16	B	1111	CLA	OBD-CAD-CBD	-2.24	121.39	125.97
16	A	369	CLA	CHD-C1D-ND	-2.24	122.40	124.45
16	M	1078	CLA	OBD-CAD-CBD	-2.24	121.40	125.97
16	C	1087	CLA	OBD-CAD-CBD	-2.24	121.40	125.97
16	C	1084	CLA	CHD-C1D-ND	-2.23	122.40	124.45
16	B	1116	CLA	OBD-CAD-CBD	-2.23	121.41	125.97
16	N	358	CLA	C2D-C1D-ND	2.23	111.75	110.10
16	L	1122	CLA	OBD-CAD-CBD	-2.23	121.41	125.97
16	L	1111	CLA	OBD-CAD-CBD	-2.23	121.42	125.97
16	B	1119	CLA	OBD-CAD-CBD	-2.23	121.42	125.97
16	L	1117	CLA	CHD-C1D-ND	-2.23	122.41	124.45
16	M	1085	CLA	CHD-C1D-ND	-2.23	122.41	124.45
16	D	355	CLA	C2A-C3A-C4A	2.23	104.63	101.78
16	M	1086	CLA	OBD-CAD-CBD	-2.23	121.42	125.97
16	L	1118	CLA	OBD-CAD-CBD	-2.22	121.43	125.97
21	0	138	HEM	C2C-C3C-C4C	-2.22	104.39	106.30
16	A	365	CLA	CHD-C1D-ND	-2.22	122.41	124.45
16	C	1078	CLA	OBD-CAD-CBD	-2.22	121.43	125.97
16	L	1108	CLA	C2D-C1D-ND	2.22	111.74	110.10
16	M	1083	CLA	CHD-C1D-ND	-2.22	122.42	124.45
16	D	354	CLA	CMB-C2B-C1B	-2.22	125.06	128.46
16	C	1079	CLA	C2D-C1D-ND	2.22	111.74	110.10
16	L	1118	CLA	C2D-C1D-ND	2.21	111.73	110.10
16	M	1087	CLA	CHD-C1D-ND	-2.21	122.42	124.45
16	D	354	CLA	C2D-C1D-ND	2.21	111.73	110.10
16	L	1108	CLA	OBD-CAD-CBD	-2.21	121.45	125.97
16	N	354	CLA	CMB-C2B-C1B	-2.21	125.06	128.46
16	B	1114	CLA	CHD-C1D-ND	-2.21	122.42	124.45
20	D	359	BCR	C15-C14-C13	2.21	130.46	127.31
16	L	1108	CLA	CHD-C1D-ND	-2.20	122.43	124.45
16	B	1121	CLA	CHD-C1D-ND	-2.20	122.43	124.45
16	L	1122	CLA	CHD-C1D-ND	-2.20	122.43	124.45
21	E	84	HEM	C2C-C3C-C4C	-2.20	104.41	106.30
16	M	1081	CLA	OBD-CAD-CBD	-2.20	121.48	125.97
16	B	1119	CLA	CHD-C1D-ND	-2.20	122.44	124.45
16	L	1115	CLA	CHD-C1D-ND	-2.20	122.44	124.45
20	K	47	BCR	C11-C10-C9	2.19	130.44	127.31
16	C	1088	CLA	CHD-C1D-ND	-2.19	122.44	124.45
16	L	1116	CLA	CHD-C1D-ND	-2.19	122.44	124.45
16	B	1108	CLA	OBD-CAD-CBD	-2.19	121.50	125.97

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
16	C	1081	CLA	CHD-C1D-ND	-2.19	122.44	124.45
16	B	1115	CLA	CHD-C1D-ND	-2.19	122.45	124.45
16	J	367	CLA	CHD-C1D-ND	-2.18	122.45	124.45
16	L	1122	CLA	C2D-C1D-ND	2.18	111.71	110.10
16	B	1108	CLA	C2D-C1D-ND	2.17	111.71	110.10
16	L	1111	CLA	C2D-C1D-ND	2.17	111.70	110.10
16	B	1122	CLA	CHD-C1D-ND	-2.17	122.46	124.45
20	K	47	BCR	C15-C14-C13	2.17	130.41	127.31
16	B	1109	CLA	CHD-C1D-ND	-2.17	122.46	124.45
16	L	1107	CLA	CHD-C1D-ND	-2.17	122.46	124.45
16	M	1088	CLA	CHD-C1D-ND	-2.16	122.47	124.45
21	P	92	HEM	C2B-C1B-NB	2.16	111.30	109.48
16	A	368	CLA	C2D-C1D-ND	2.16	111.70	110.10
16	M	1079	CLA	CHD-C1D-ND	-2.16	122.47	124.45
16	B	1122	CLA	C2D-C1D-ND	2.16	111.70	110.10
16	B	1108	CLA	CHD-C1D-ND	-2.16	122.47	124.45
20	D	359	BCR	C1-C6-C5	-2.16	119.57	122.61
16	L	1116	CLA	C2D-C1D-ND	2.15	111.69	110.10
16	A	368	CLA	CHD-C1D-ND	-2.15	122.48	124.45
16	B	1115	CLA	C2D-C1D-ND	2.15	111.69	110.10
16	L	1109	CLA	CHD-C1D-ND	-2.15	122.48	124.45
16	L	1118	CLA	CHD-C1D-ND	-2.15	122.48	124.45
16	B	1111	CLA	C2D-C1D-ND	2.14	111.68	110.10
16	M	1082	CLA	C2D-C1D-ND	2.14	111.68	110.10
21	P	92	HEM	C2C-C3C-C4C	-2.14	104.45	106.30
21	E	84	HEM	C2B-C1B-NB	2.14	111.28	109.48
16	C	1083	CLA	CHD-C1D-ND	-2.14	122.49	124.45
16	B	1118	CLA	C2D-C1D-ND	2.13	111.68	110.10
16	C	1083	CLA	C2D-C1D-ND	2.13	111.67	110.10
16	C	1085	CLA	C2D-C1D-ND	2.12	111.67	110.10
16	C	1086	CLA	OBD-CAD-C3D	2.12	132.25	128.74
16	J	367	CLA	C2D-C1D-ND	2.12	111.67	110.10
16	L	1111	CLA	CHD-C1D-ND	-2.12	122.51	124.45
21	0	138	HEM	C2B-C1B-NB	2.12	111.26	109.48
16	M	1082	CLA	CHD-C1D-ND	-2.11	122.51	124.45
16	L	1114	CLA	OBD-CAD-C3D	2.11	132.24	128.74
16	M	1088	CLA	OBD-CAD-C3D	2.11	132.24	128.74
16	M	1084	CLA	C2D-C1D-ND	2.11	111.66	110.10
21	V	138	HEM	C2B-C1B-NB	2.11	111.26	109.48
16	B	1116	CLA	CHD-C1D-ND	-2.11	122.52	124.45
16	L	1115	CLA	C2D-C1D-ND	2.11	111.66	110.10
20	D	359	BCR	C11-C10-C9	2.11	130.32	127.31

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
16	C	1079	CLA	CHD-C1D-ND	-2.11	122.52	124.45
16	L	1119	CLA	C2D-C1D-ND	2.09	111.65	110.10
16	L	1119	CLA	CHD-C1D-ND	-2.09	122.53	124.45
16	L	1121	CLA	OBD-CAD-C3D	2.09	132.20	128.74
16	W	64	CLA	CHD-C1D-ND	-2.09	122.54	124.45
16	B	1118	CLA	CHD-C1D-ND	-2.08	122.54	124.45
16	N	354	CLA	OBD-CAD-CBD	-2.08	121.72	125.97
16	B	1116	CLA	C2D-C1D-ND	2.08	111.64	110.10
16	C	1087	CLA	CHD-C1D-ND	-2.08	122.55	124.45
16	L	1110	CLA	OBD-CAD-C3D	2.07	132.18	128.74
16	R	221	CLA	C3C-C4C-NC	-2.07	108.31	110.57
16	B	1111	CLA	CHD-C1D-ND	-2.07	122.55	124.45
16	D	354	CLA	OBD-CAD-CBD	-2.07	121.75	125.97
16	N	356	CLA	CHA-C1A-NA	-2.07	121.67	126.40
16	C	1084	CLA	OBD-CAD-C3D	2.06	132.16	128.74
16	M	1085	CLA	OBD-CAD-C3D	2.06	132.15	128.74
16	C	1087	CLA	C2D-C1D-ND	2.06	111.62	110.10
16	L	1112	CLA	OBD-CAD-C3D	2.06	132.15	128.74
16	L	1120	CLA	OBD-CAD-C3D	2.06	132.15	128.74
16	B	1110	CLA	OBD-CAD-C3D	2.06	132.15	128.74
16	W	64	CLA	OBD-CAD-C3D	2.05	132.14	128.74
16	B	1113	CLA	OBD-CAD-C3D	2.05	132.14	128.74
16	M	1086	CLA	CHD-C1D-ND	-2.05	122.57	124.45
16	M	1083	CLA	OBD-CAD-C3D	2.05	132.13	128.74
16	L	1117	CLA	OBD-CAD-C3D	2.05	132.13	128.74
20	D	359	BCR	C30-C25-C24	2.04	121.56	115.78
16	B	1114	CLA	OBD-CAD-C3D	2.04	132.13	128.74
16	J	368	CLA	OBD-CAD-C3D	2.04	132.12	128.74
16	B	1121	CLA	OBD-CAD-C3D	2.04	132.12	128.74
16	M	1079	CLA	CMD-C2D-C1D	2.04	128.31	124.71
16	L	1112	CLA	CMD-C2D-C1D	2.03	128.30	124.71
16	B	1120	CLA	OBD-CAD-C3D	2.03	132.11	128.74
16	B	1117	CLA	OBD-CAD-C3D	2.03	132.11	128.74
16	D	355	CLA	CHA-C1A-NA	-2.03	121.75	126.40
16	B	1112	CLA	CMD-C2D-C1D	2.03	128.29	124.71
16	L	1109	CLA	CMD-C2D-C1D	2.03	128.29	124.71
16	A	369	CLA	OBD-CAD-C3D	2.03	132.10	128.74
16	C	1085	CLA	CMD-C2D-C1D	2.03	128.28	124.71
16	B	1112	CLA	OBD-CAD-C3D	2.03	132.10	128.74
16	B	1114	CLA	CMD-C2D-C1D	2.02	128.28	124.71
16	B	1117	CLA	CMD-C2D-C1D	2.02	128.28	124.71
16	A	369	CLA	CMD-C2D-C1D	2.02	128.28	124.71

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
16	L	1121	CLA	CMD-C2D-C1D	2.02	128.27	124.71
16	C	1080	CLA	OBD-CAD-C3D	2.02	132.09	128.74
16	B	1119	CLA	CMD-C2D-C1D	2.02	128.27	124.71
16	M	1086	CLA	C2D-C1D-ND	2.02	111.59	110.10
16	C	1082	CLA	C2D-C1D-ND	2.02	111.59	110.10
16	L	1115	CLA	OBD-CAD-C3D	2.01	132.07	128.74
16	C	1079	CLA	CMD-C2D-C1D	2.01	128.26	124.71
16	C	1088	CLA	CMD-C2D-C1D	2.01	128.26	124.71
16	N	358	CLA	OBD-CAD-C3D	2.01	132.07	128.74
16	L	1114	CLA	CMD-C2D-C1D	2.01	128.25	124.71
16	G	221	CLA	C3C-C4C-NC	-2.01	108.38	110.57
16	C	1080	CLA	CMD-C2D-C1D	2.01	128.25	124.71
16	L	1116	CLA	CMD-C2D-C1D	2.01	128.25	124.71
16	L	1119	CLA	CMD-C2D-C1D	2.00	128.24	124.71
16	C	1089	CLA	OBD-CAD-C3D	2.00	132.06	128.74
16	C	1082	CLA	CHD-C1D-ND	-2.00	122.61	124.45
16	D	357	CLA	OBD-CAD-C3D	2.00	132.05	128.74
16	M	1081	CLA	C2D-C1D-ND	2.00	111.58	110.10
16	M	1078	CLA	CHD-C1D-ND	-2.00	122.62	124.45

All (73) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
16	A	365	CLA	ND
16	A	366	CLA	ND
16	A	368	CLA	ND
16	A	369	CLA	ND
16	B	1107	CLA	ND
16	B	1108	CLA	ND
16	B	1109	CLA	ND
16	B	1110	CLA	ND
16	B	1111	CLA	ND
16	B	1112	CLA	ND
16	B	1113	CLA	ND
16	B	1114	CLA	ND
16	B	1115	CLA	ND
16	B	1116	CLA	ND
16	B	1117	CLA	ND
16	B	1118	CLA	ND
16	B	1119	CLA	ND
16	B	1120	CLA	ND
16	B	1121	CLA	ND

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Mol	Chain	Res	Type	Atom
16	B	1122	CLA	ND
16	C	1078	CLA	ND
16	C	1079	CLA	ND
16	C	1080	CLA	ND
16	C	1081	CLA	ND
16	C	1082	CLA	ND
16	C	1083	CLA	ND
16	C	1084	CLA	ND
16	C	1085	CLA	ND
16	C	1086	CLA	ND
16	C	1087	CLA	ND
16	C	1088	CLA	ND
16	C	1089	CLA	ND
16	C	1089	CLA	CBD
16	D	354	CLA	ND
16	D	355	CLA	ND
16	D	357	CLA	ND
16	G	221	CLA	ND
16	J	365	CLA	ND
16	J	367	CLA	ND
16	J	368	CLA	ND
16	L	1107	CLA	ND
16	L	1108	CLA	ND
16	L	1109	CLA	ND
16	L	1110	CLA	ND
16	L	1111	CLA	ND
16	L	1112	CLA	ND
16	L	1113	CLA	ND
16	L	1114	CLA	ND
16	L	1115	CLA	ND
16	L	1116	CLA	ND
16	L	1117	CLA	ND
16	L	1118	CLA	ND
16	L	1119	CLA	ND
16	L	1120	CLA	ND
16	L	1121	CLA	ND
16	L	1122	CLA	ND
16	M	1078	CLA	ND
16	M	1079	CLA	ND
16	M	1080	CLA	ND
16	M	1081	CLA	ND
16	M	1082	CLA	ND

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Mol	Chain	Res	Type	Atom
16	M	1083	CLA	ND
16	M	1084	CLA	ND
16	M	1085	CLA	ND
16	M	1086	CLA	ND
16	M	1087	CLA	ND
16	M	1088	CLA	ND
16	N	354	CLA	ND
16	N	355	CLA	ND
16	N	356	CLA	ND
16	N	358	CLA	ND
16	R	221	CLA	ND
16	W	64	CLA	ND

All (4) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
20	D	359	BCR	C6-C7-C8-C9
20	D	359	BCR	C1-C6-C7-C8
20	D	359	BCR	C5-C6-C7-C8
20	K	47	BCR	C14-C15-C16-C17

There are no ring outliers.

70 monomers are involved in 601 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
17	A	367	PHO	20	0
16	L	1110	CLA	6	0
16	A	368	CLA	25	0
16	J	367	CLA	23	0
16	L	1108	CLA	13	0
16	M	1084	CLA	3	0
16	L	1114	CLA	12	0
16	C	1082	CLA	12	0
16	D	354	CLA	8	0
17	J	366	PHO	19	0
16	M	1078	CLA	3	0
16	L	1111	CLA	16	0
16	N	355	CLA	4	0
16	B	1111	CLA	19	0
16	L	1118	CLA	6	0
16	L	1109	CLA	14	0
16	M	1079	CLA	17	0

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
16	L	1113	CLA	4	0
16	B	1113	CLA	3	0
16	C	1081	CLA	5	0
16	D	357	CLA	5	0
16	B	1110	CLA	10	0
16	L	1120	CLA	22	0
16	B	1109	CLA	15	0
16	B	1117	CLA	13	0
21	V	138	HEM	8	0
16	M	1082	CLA	6	0
17	D	356	PHO	9	0
16	M	1087	CLA	12	0
16	L	1121	CLA	3	0
16	J	365	CLA	2	0
16	B	1112	CLA	3	0
16	B	1107	CLA	11	0
21	0	138	HEM	8	0
16	M	1086	CLA	3	0
16	B	1116	CLA	7	0
16	B	1108	CLA	9	0
16	C	1086	CLA	9	0
16	C	1079	CLA	16	0
16	B	1114	CLA	15	0
16	A	369	CLA	2	0
16	A	365	CLA	5	0
16	B	1119	CLA	15	0
16	C	1089	CLA	25	0
20	D	359	BCR	9	0
20	K	47	BCR	1	0
16	C	1085	CLA	3	0
16	M	1085	CLA	4	0
16	C	1087	CLA	3	0
16	A	366	CLA	5	0
17	N	357	PHO	28	0
16	B	1120	CLA	5	0
16	M	1088	CLA	15	0
16	C	1078	CLA	11	0
16	L	1112	CLA	3	0
16	L	1107	CLA	9	0
16	C	1088	CLA	15	0
16	L	1119	CLA	23	0
16	N	354	CLA	5	0

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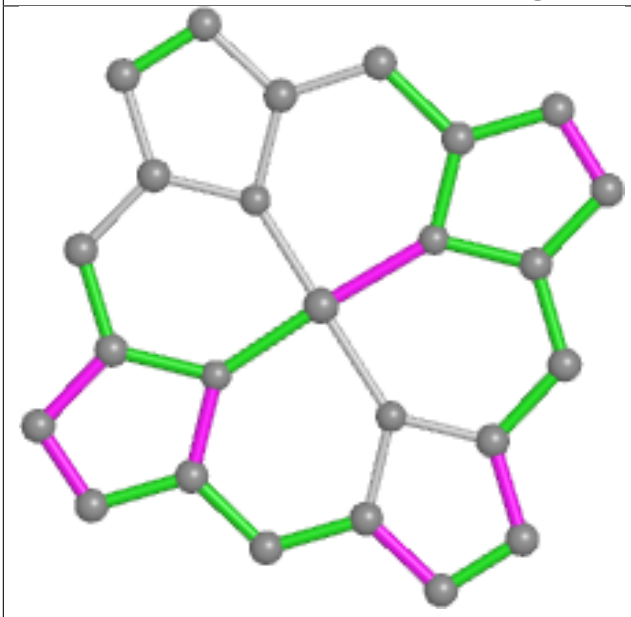
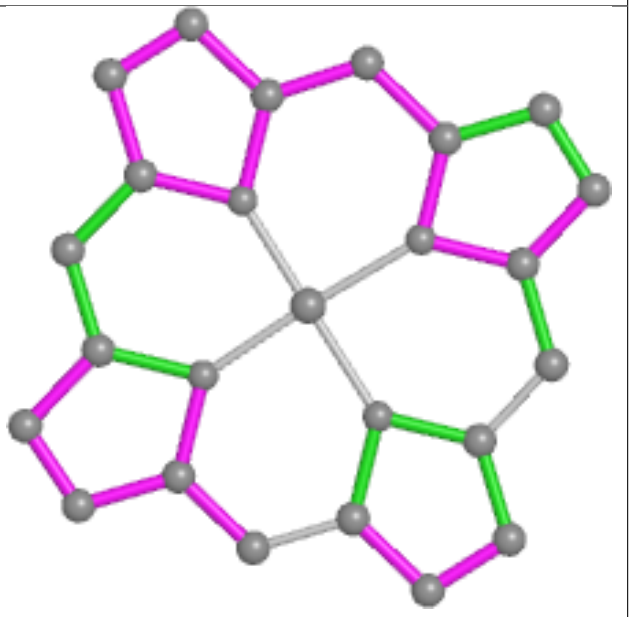
Mol	Chain	Res	Type	Clashes	Symm-Clashes
16	M	1081	CLA	14	0
16	N	356	CLA	1	0
16	W	64	CLA	15	0
16	L	1115	CLA	2	0
16	B	1118	CLA	6	0
16	C	1080	CLA	11	0
16	M	1080	CLA	1	0
16	N	358	CLA	1	0
16	B	1121	CLA	3	0
16	L	1117	CLA	13	0
16	C	1083	CLA	6	0

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.

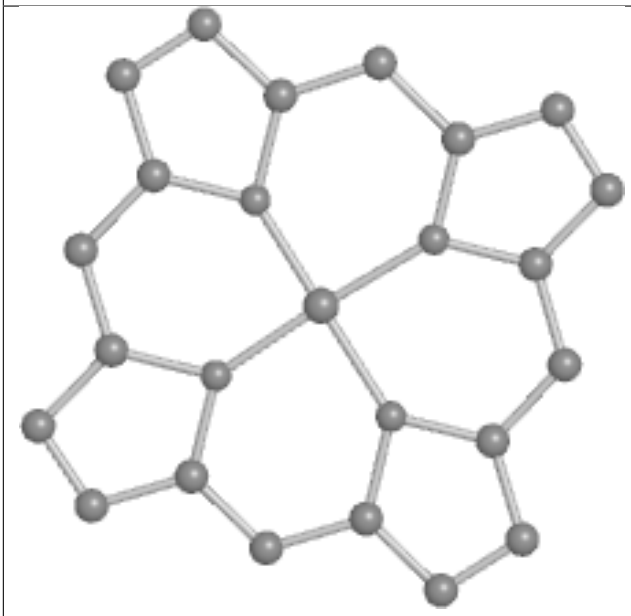
Ligand HEM E 84



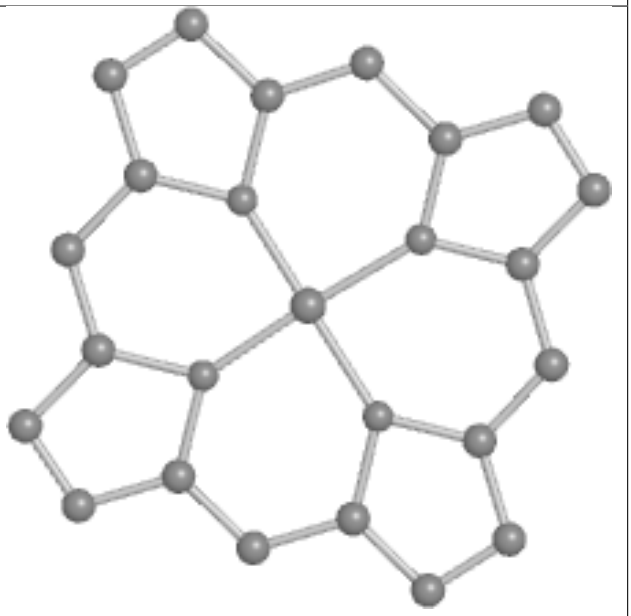
Bond lengths



Bond angles

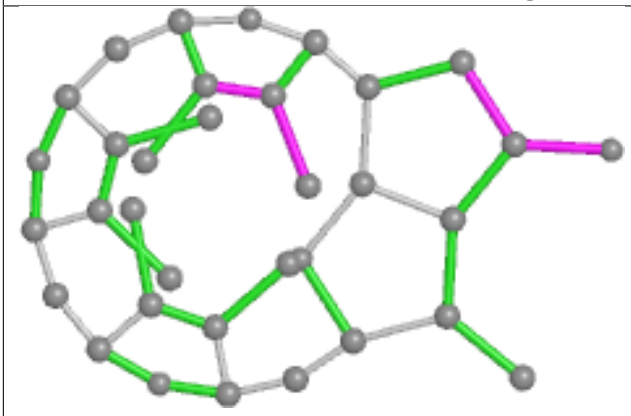


Torsions

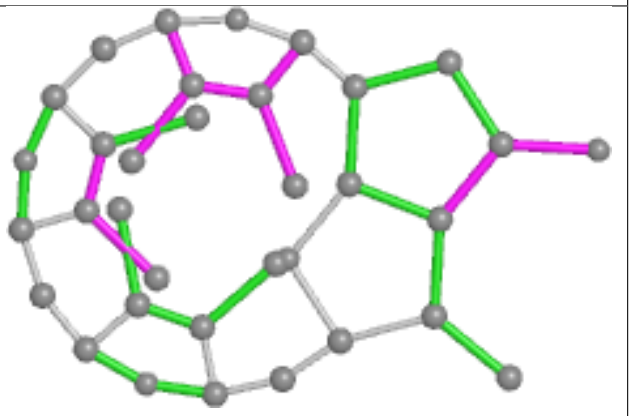


Rings

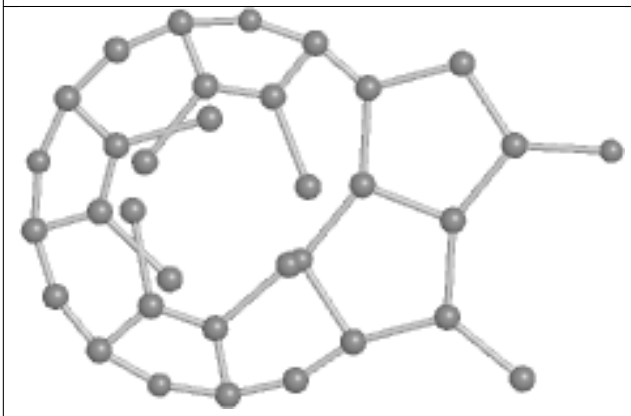
Ligand PHO A 367



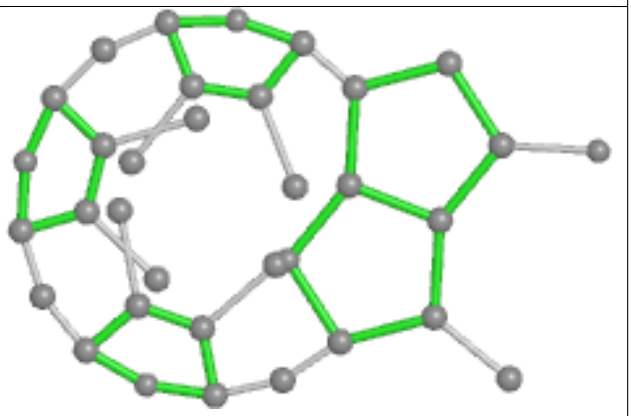
Bond lengths



Bond angles

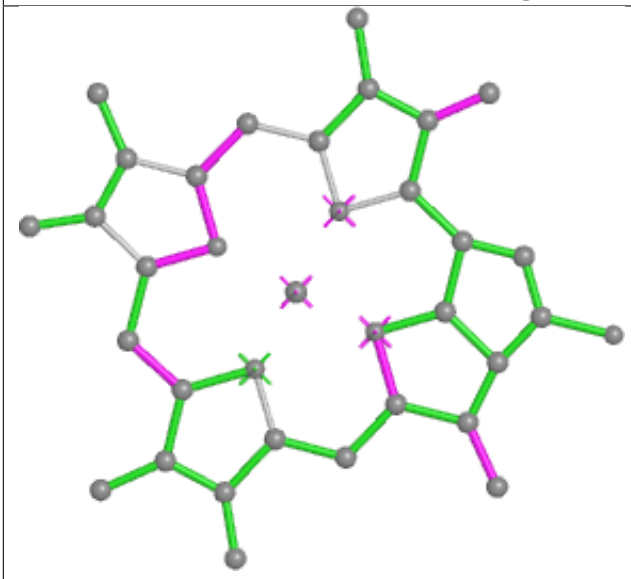


Torsions

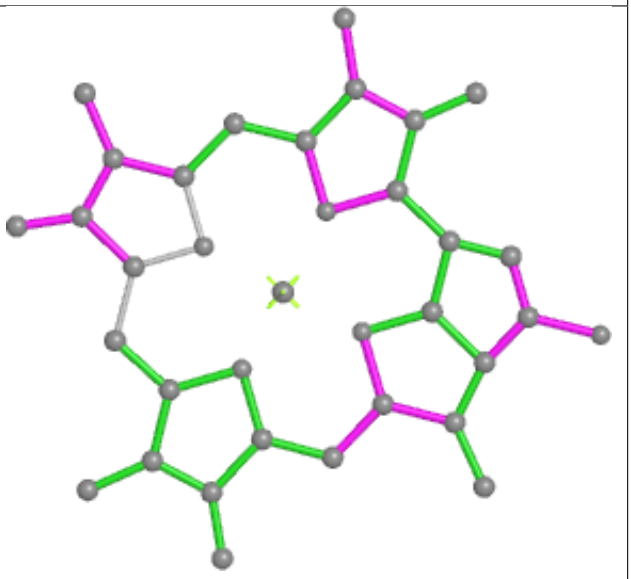


Rings

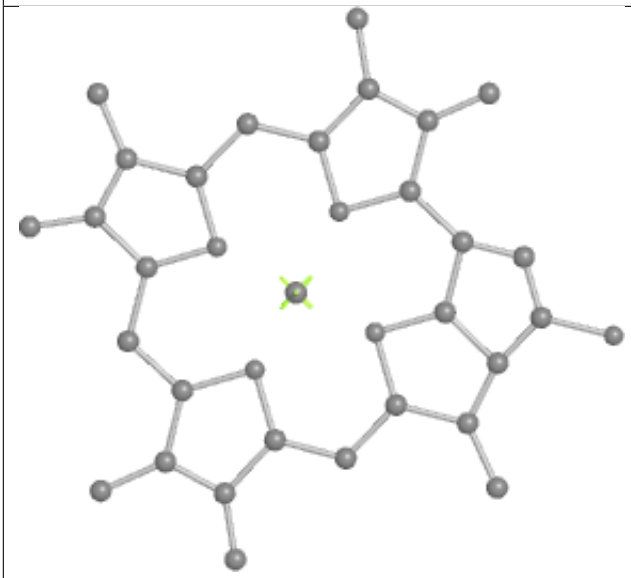
Ligand CLA L 1110



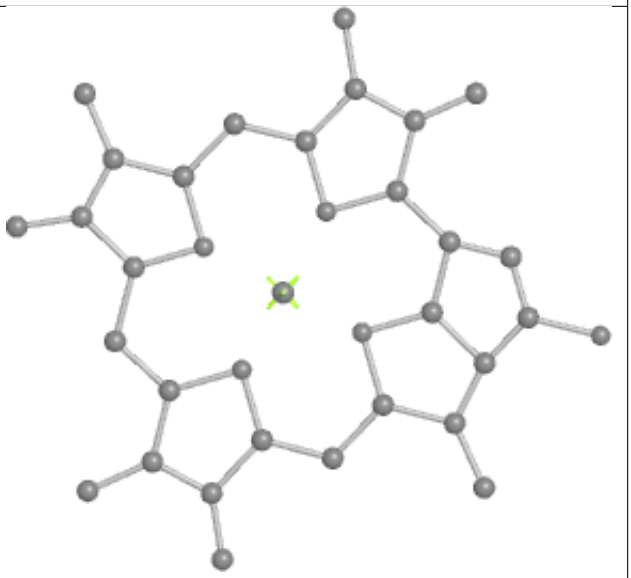
Bond lengths



Bond angles

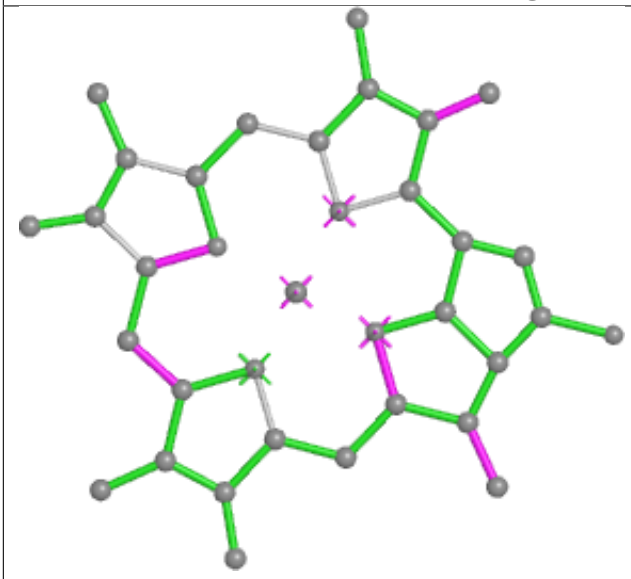


Torsions

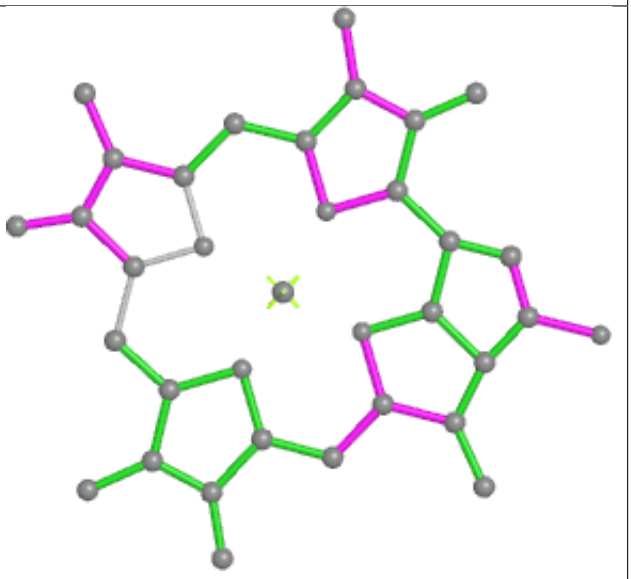


Rings

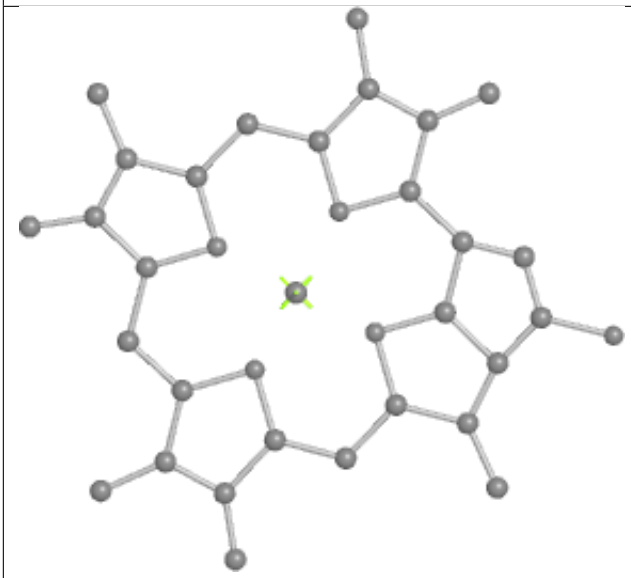
Ligand CLA A 368



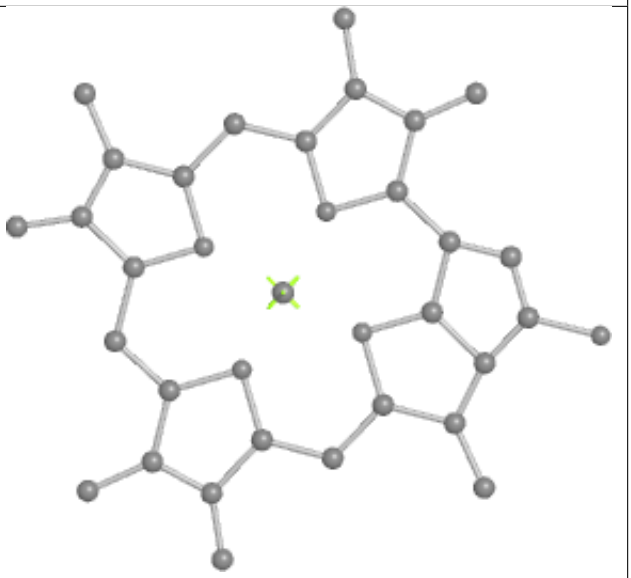
Bond lengths



Bond angles

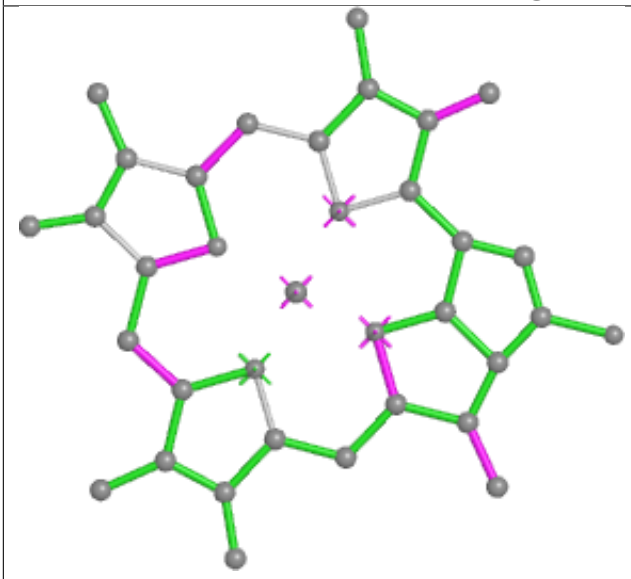


Torsions



Rings

Ligand CLA J 367



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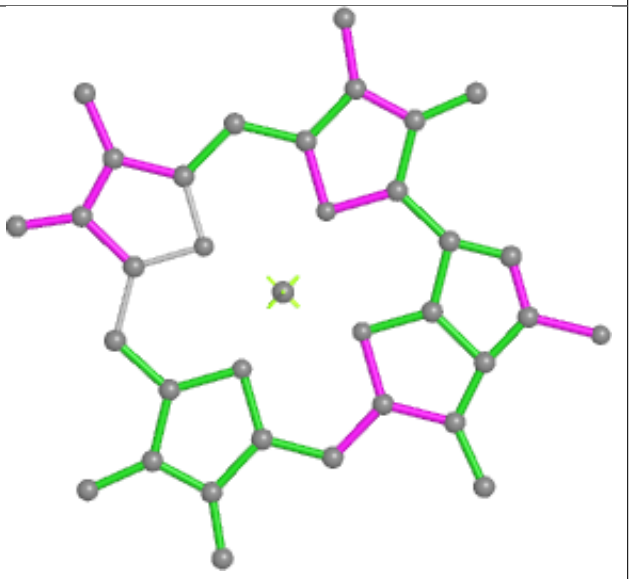
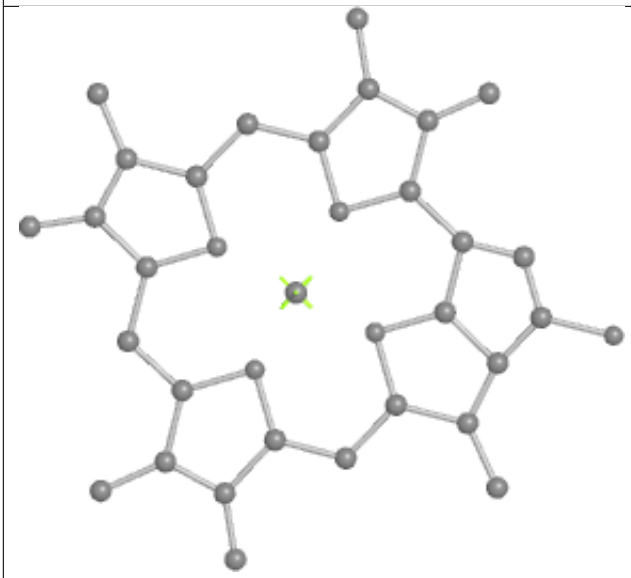
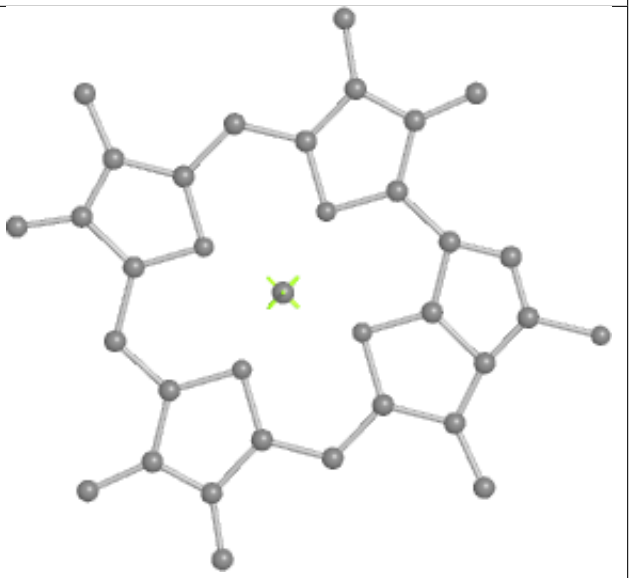


Bond angles

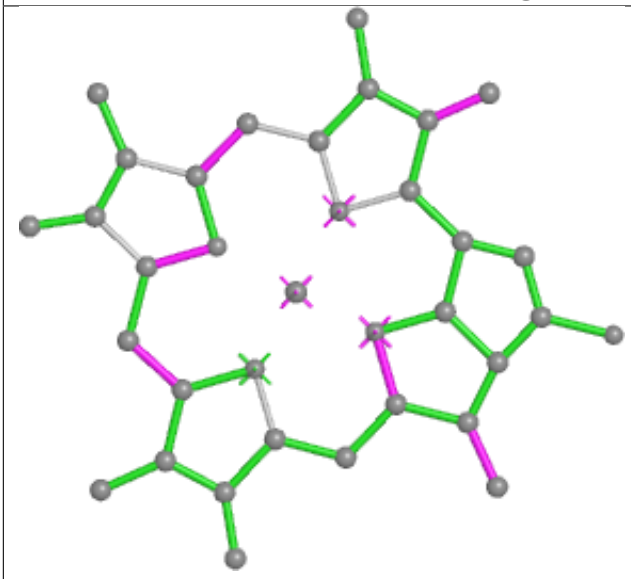


Torsions



Rings

Ligand CLA L 1108



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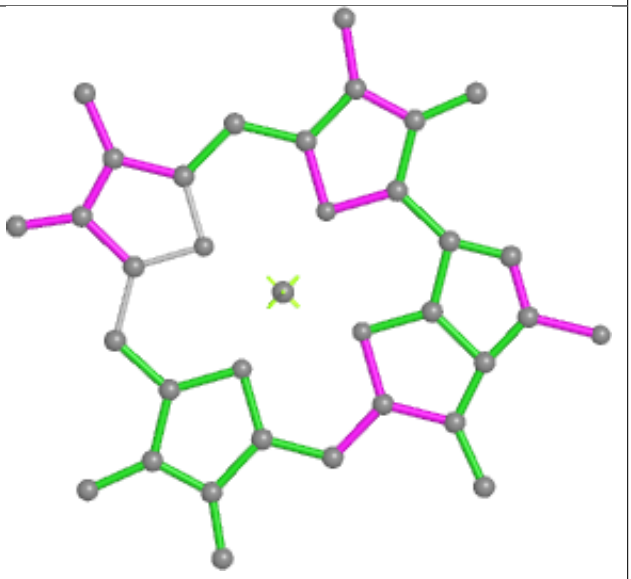
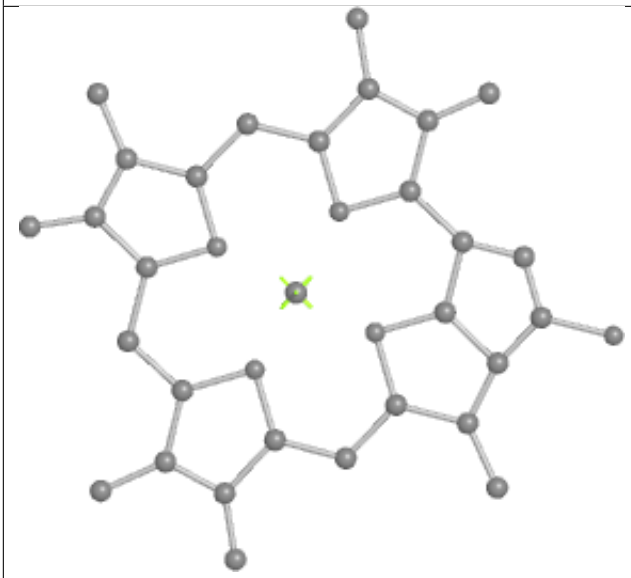
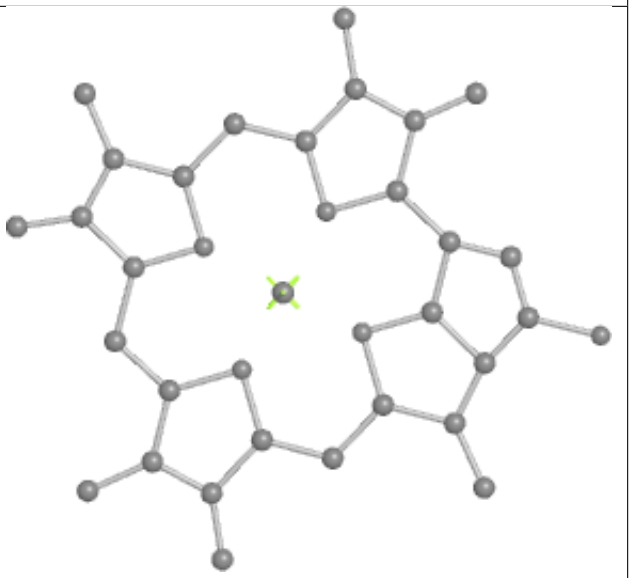


Bond angles

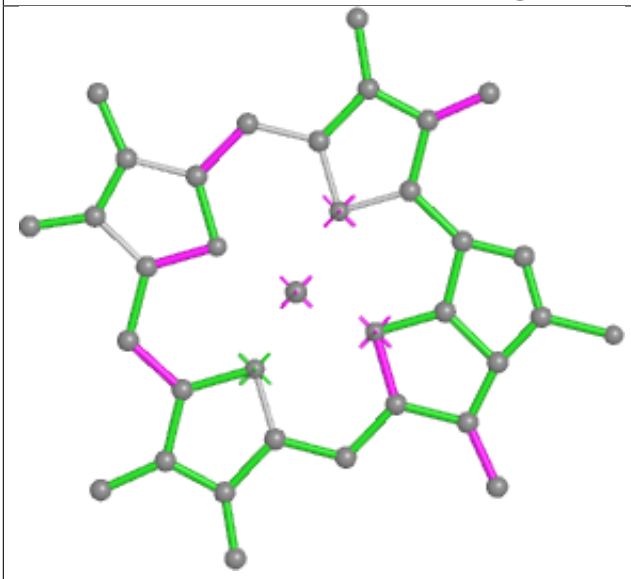


Torsions



Rings

Ligand CLA M 1084



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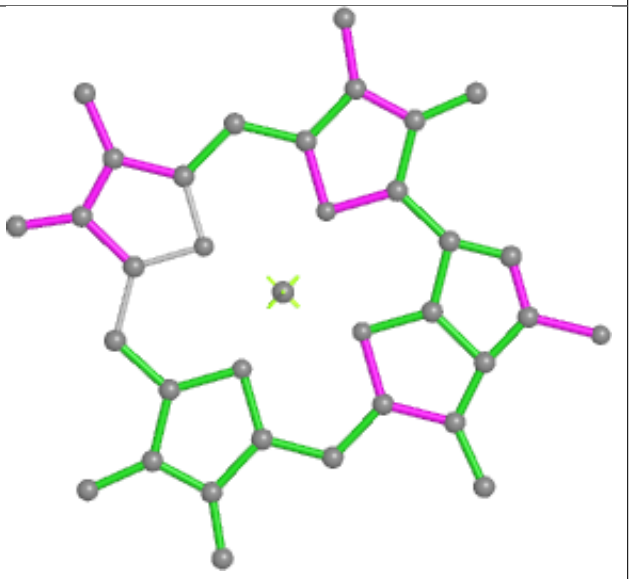

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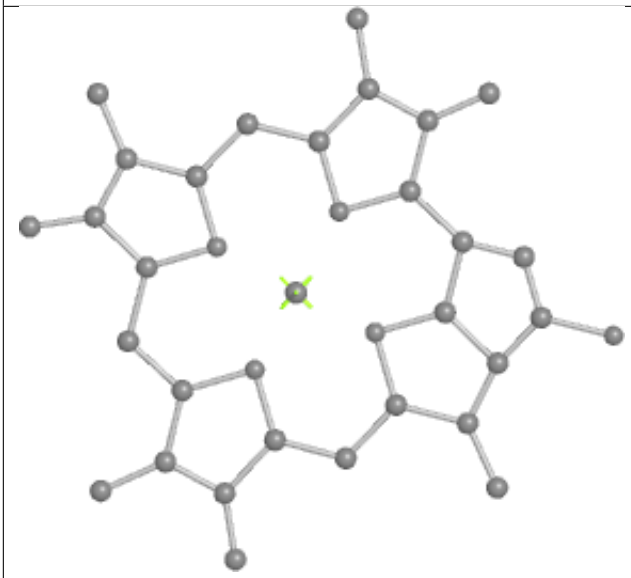

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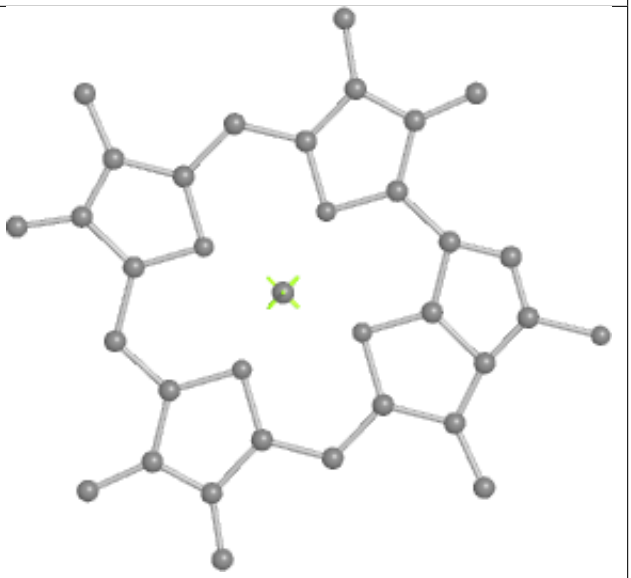
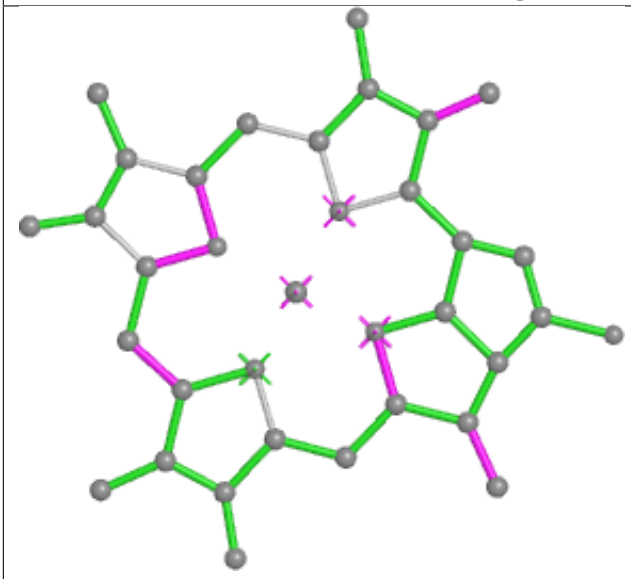


Rings

Ligand CLA M 1083



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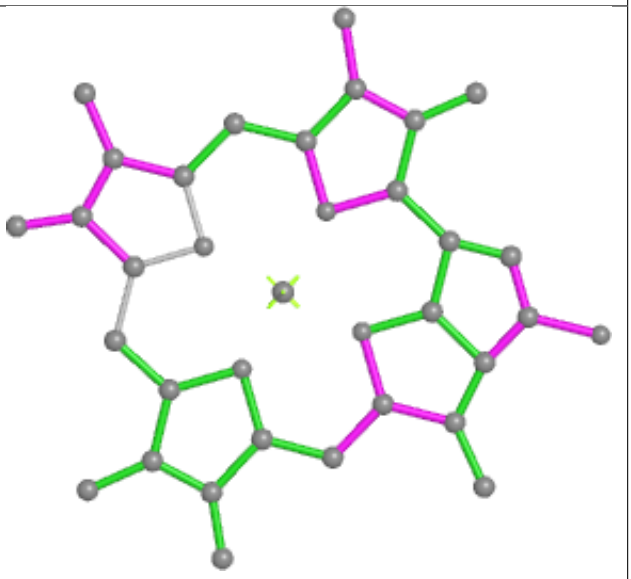
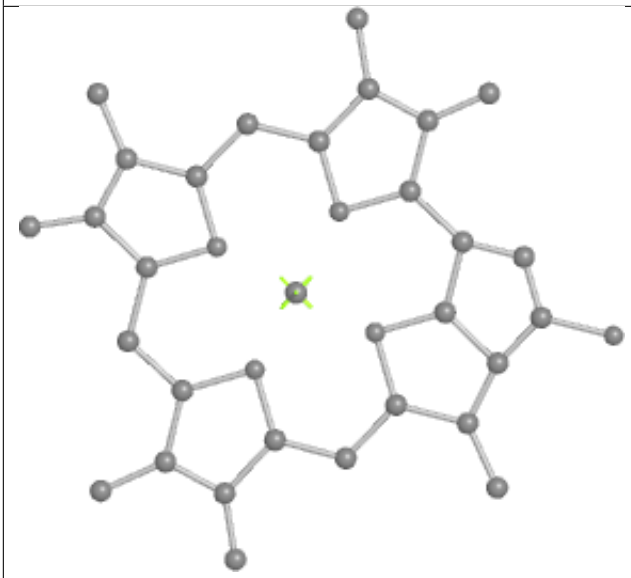
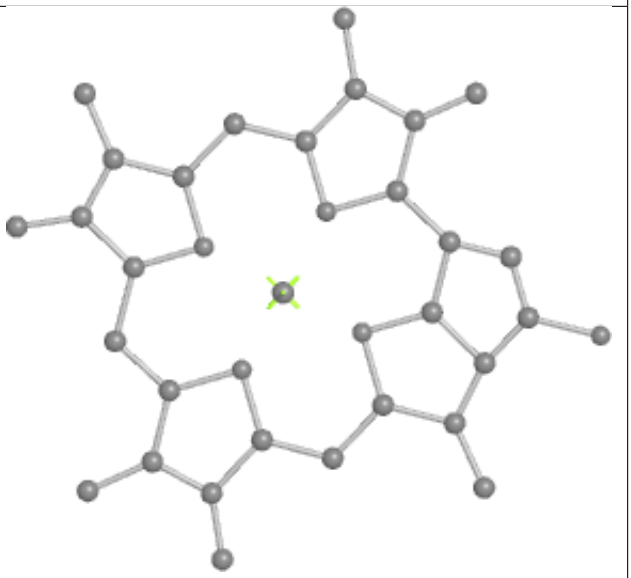


Bond angles

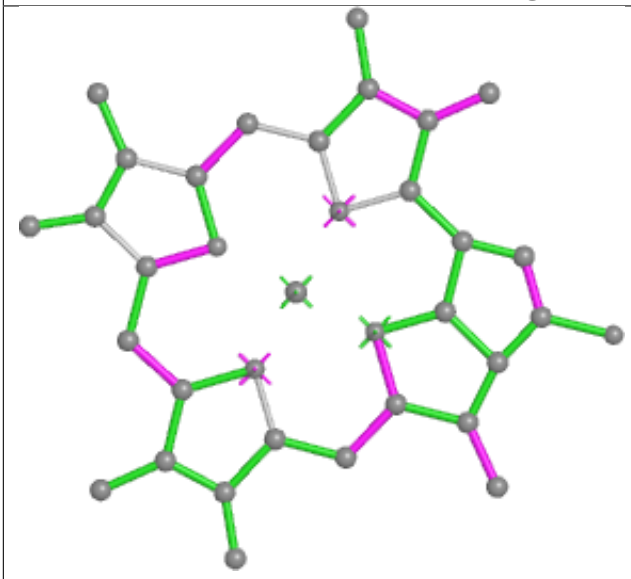


Torsions



Rings

Ligand CLA R 221



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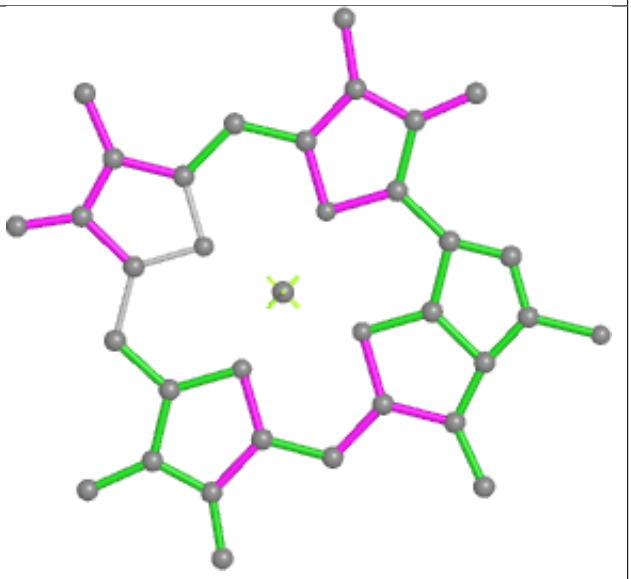
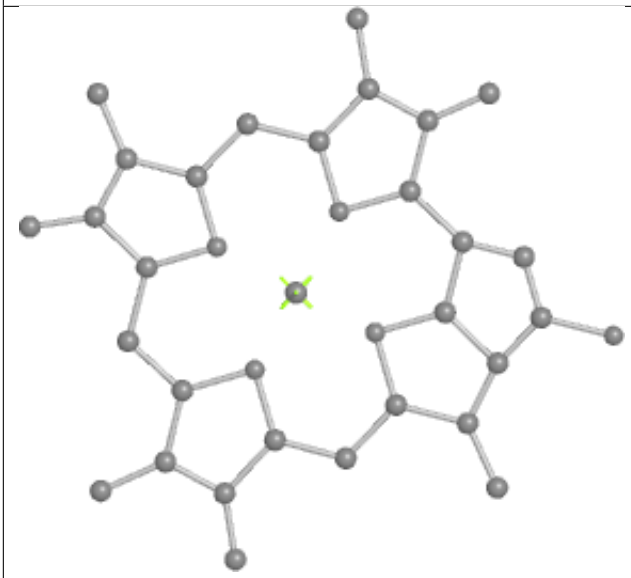
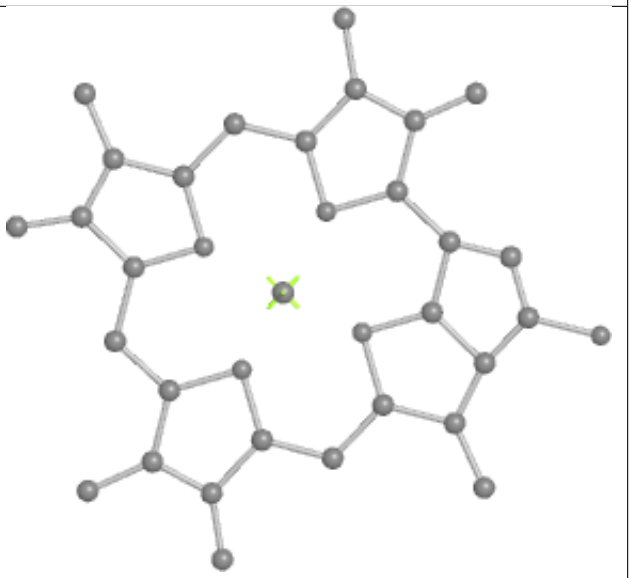


Bond angles

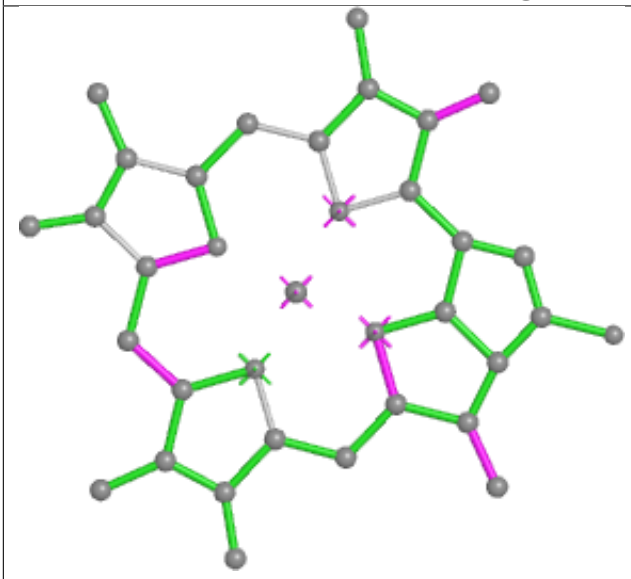


Torsions



Rings

Ligand CLA L 1114



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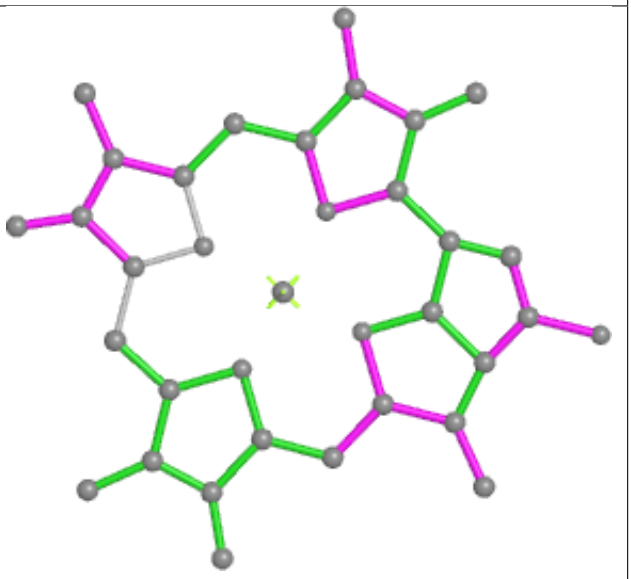
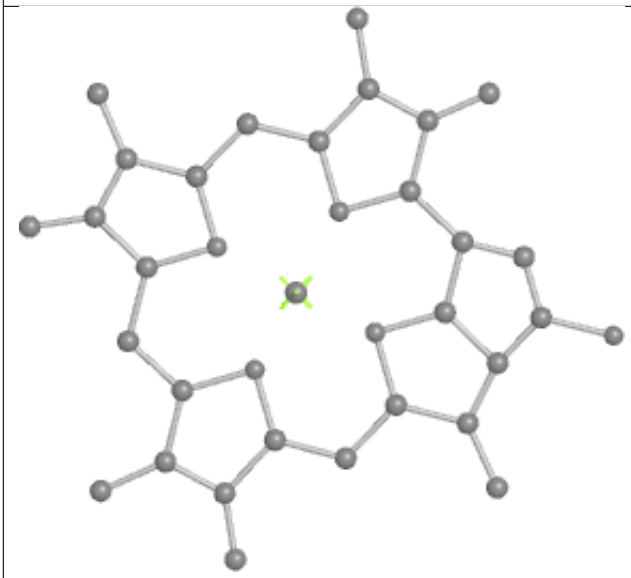
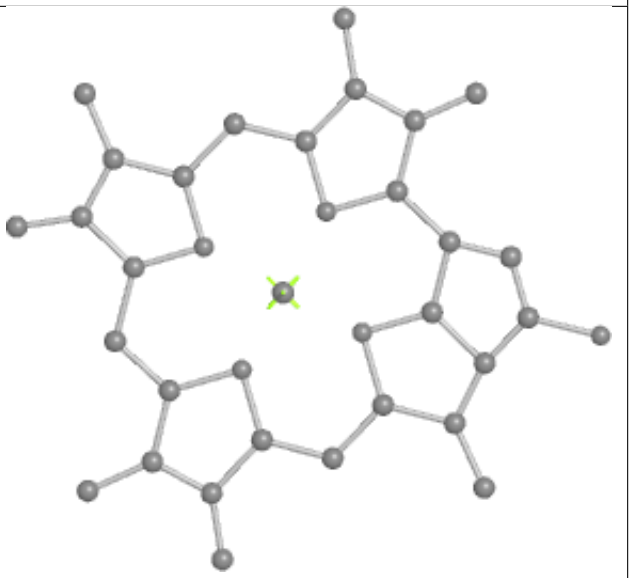


Bond angles

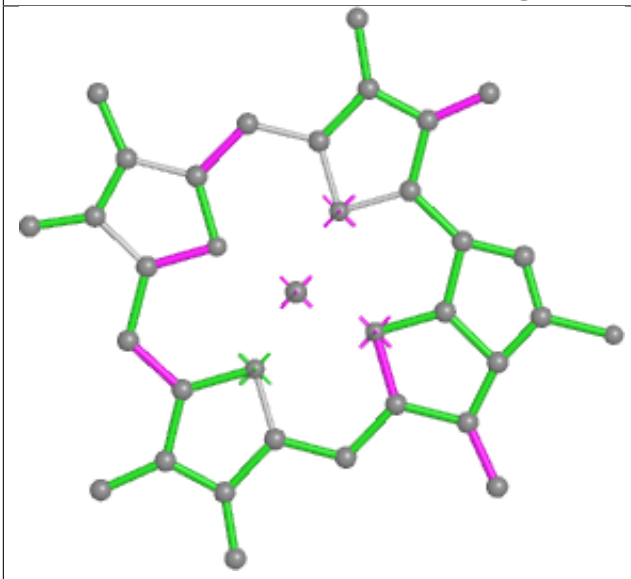


Torsions



Rings

Ligand CLA C 1082



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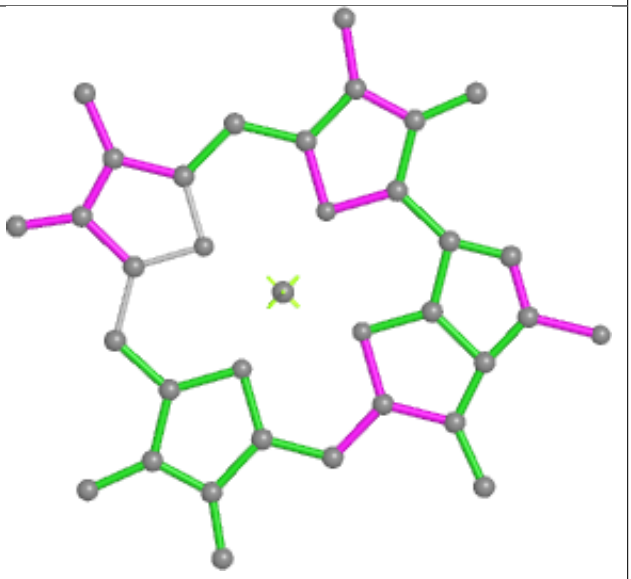
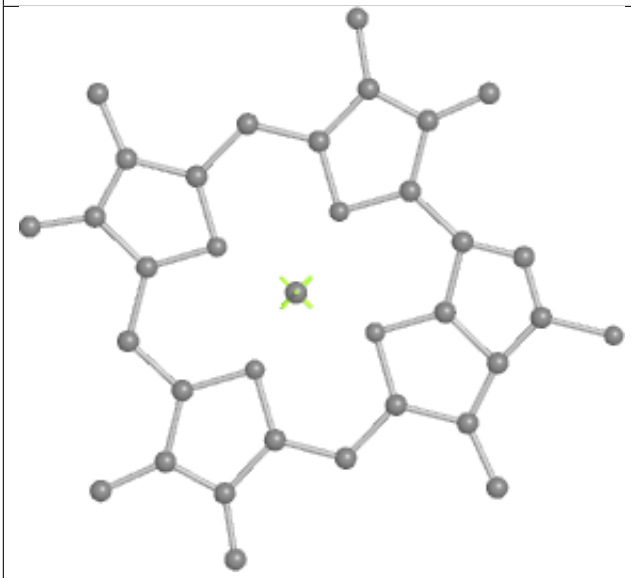
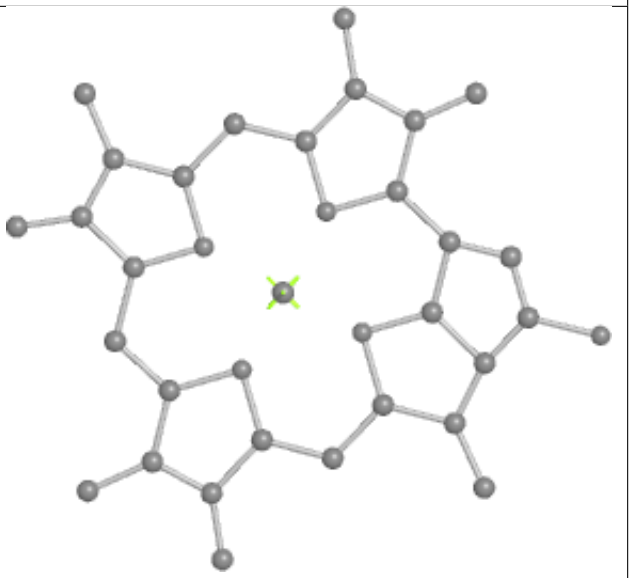


Bond angles

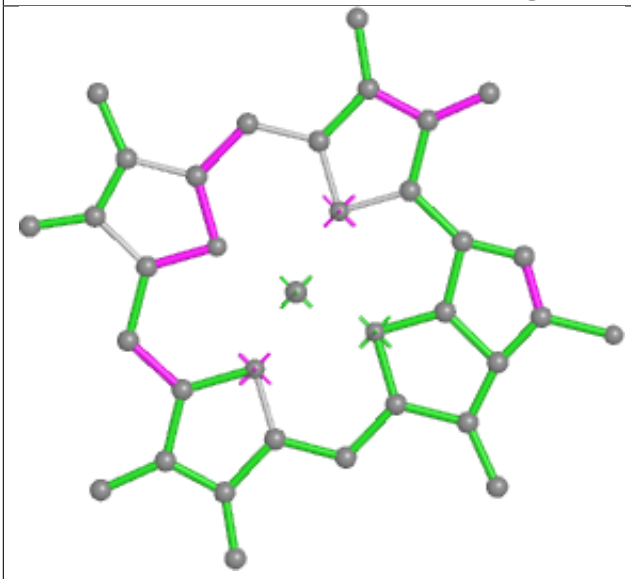


Torsions

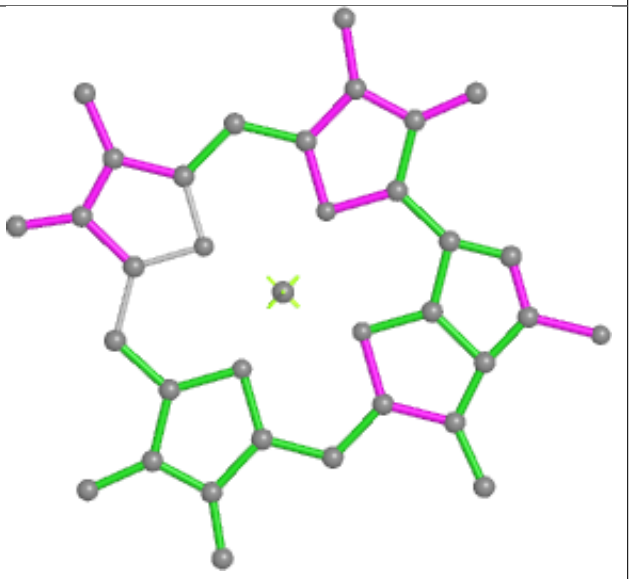


Rings

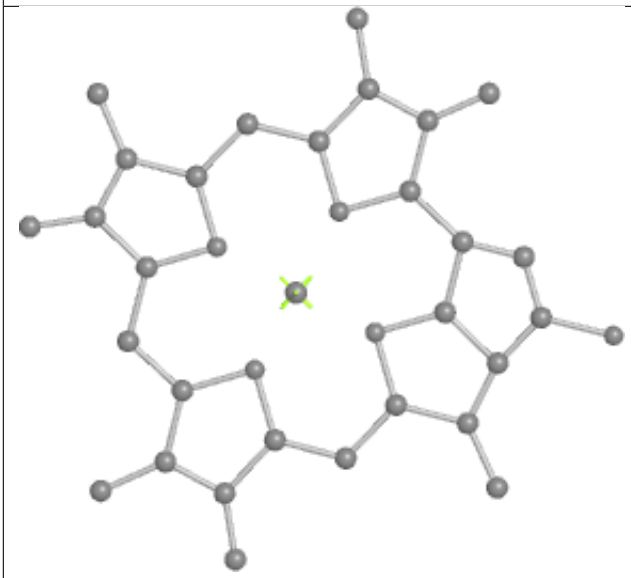
Ligand CLA D 354



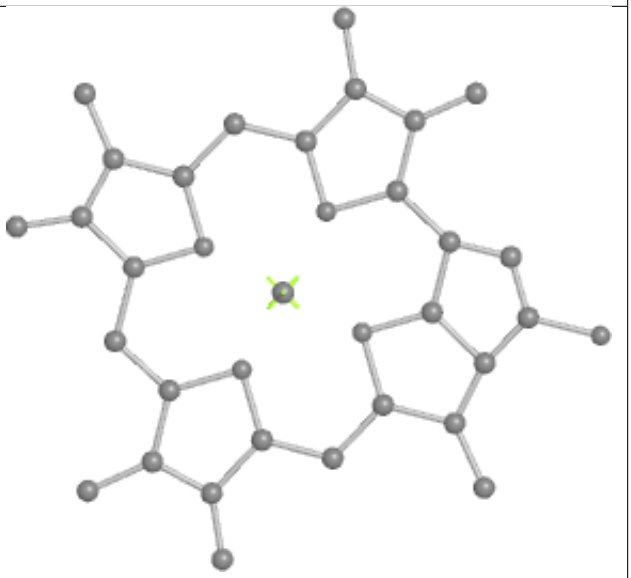
Bond lengths



Bond angles

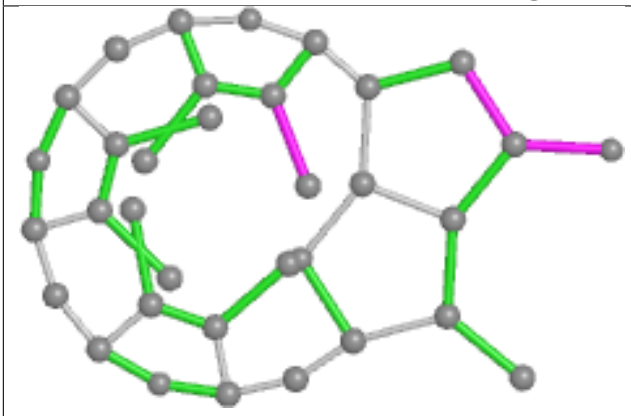


Torsions



Rings

Ligand PHO J 366



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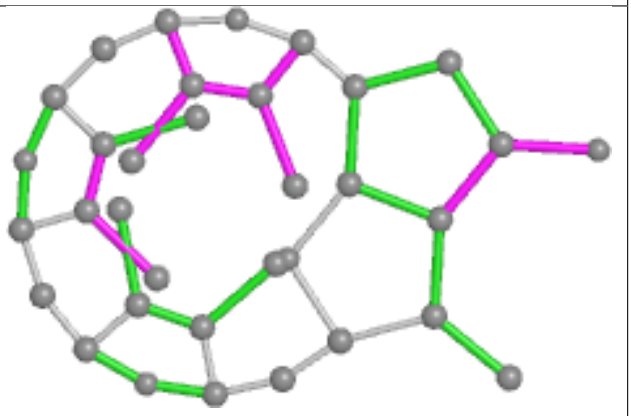
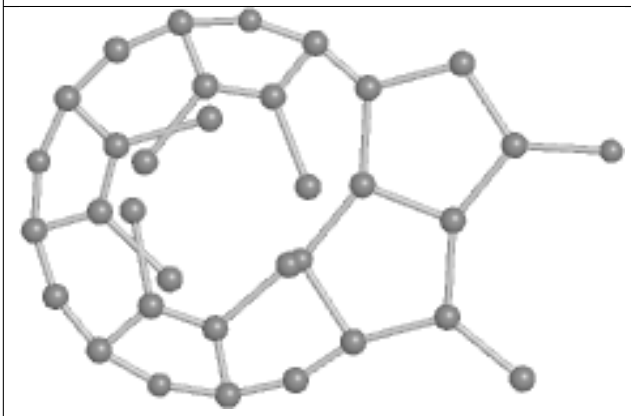


Bond angles



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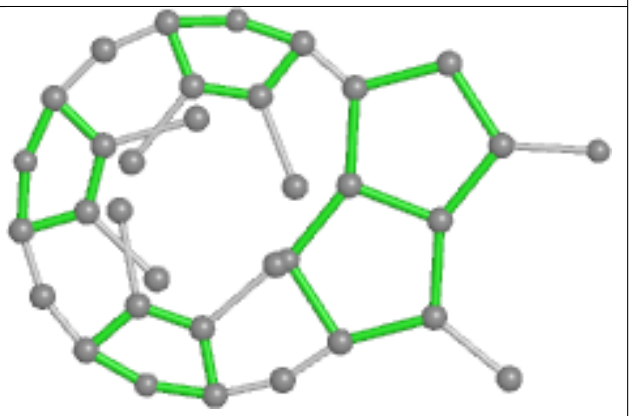
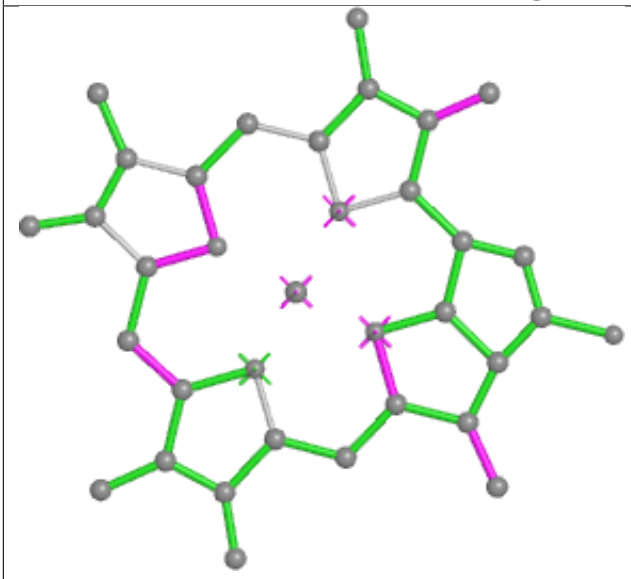


Rings

Ligand CLA J 368



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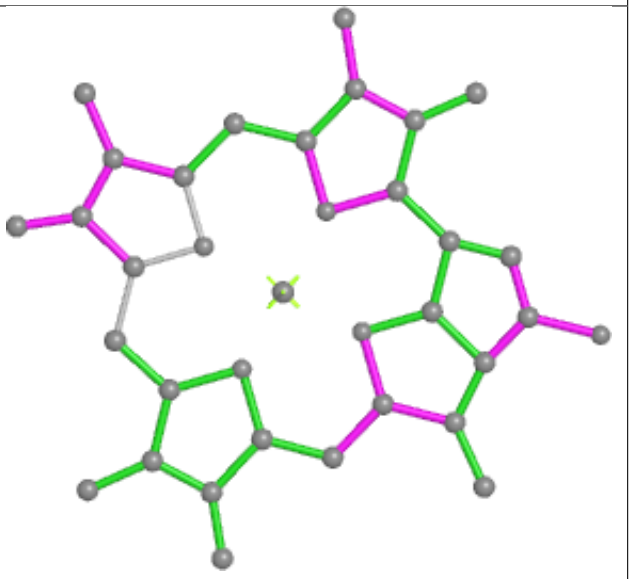
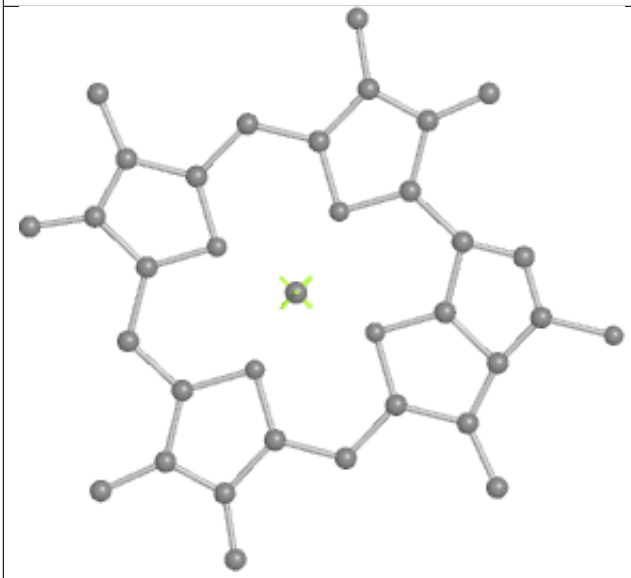
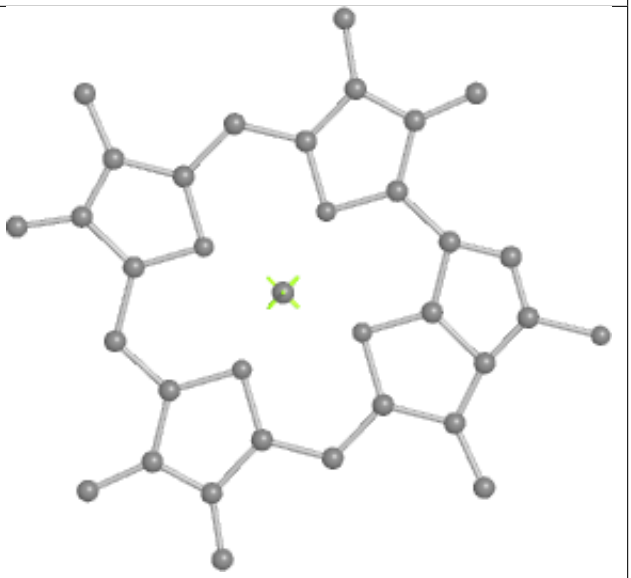


Bond angles

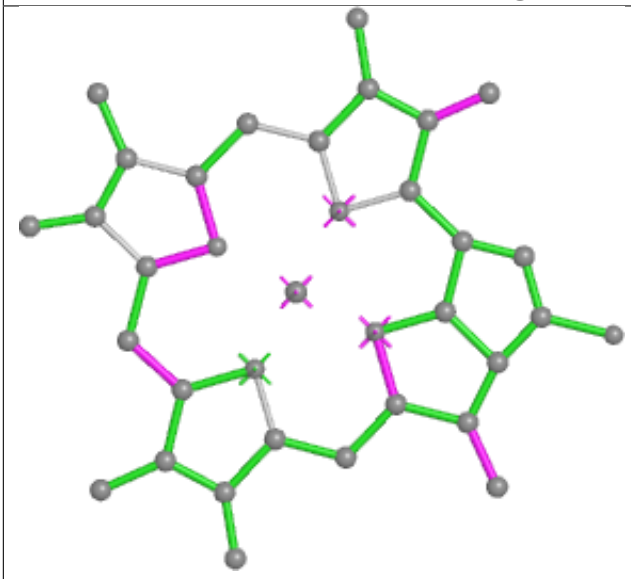


Torsions

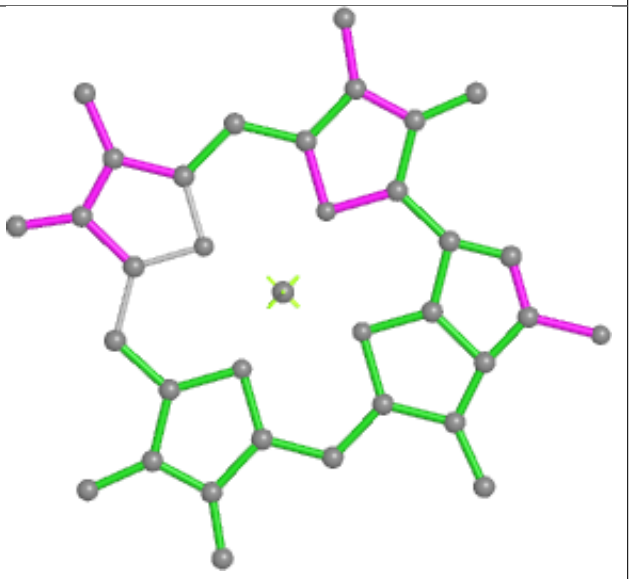


Rings

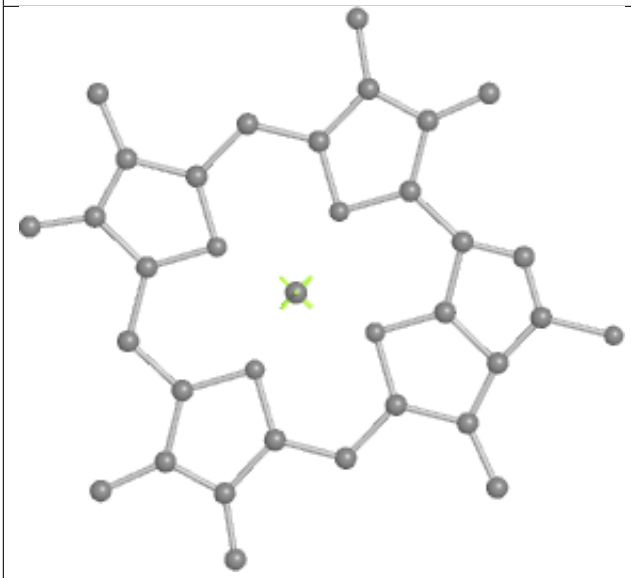
Ligand CLA M 1078



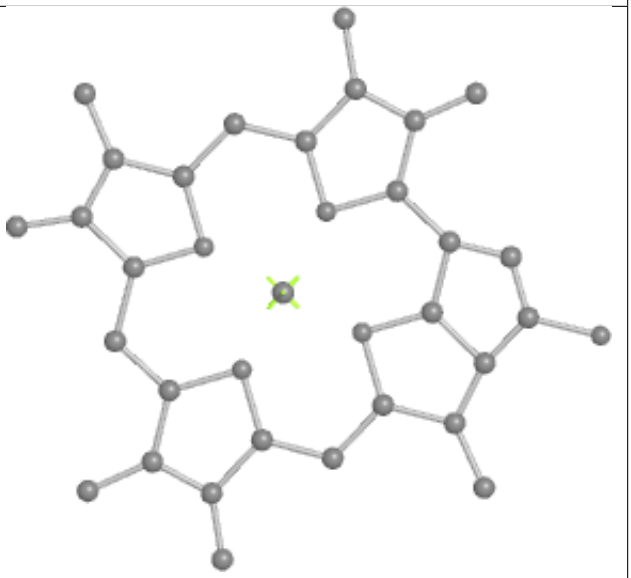
Bond lengths



Bond angles

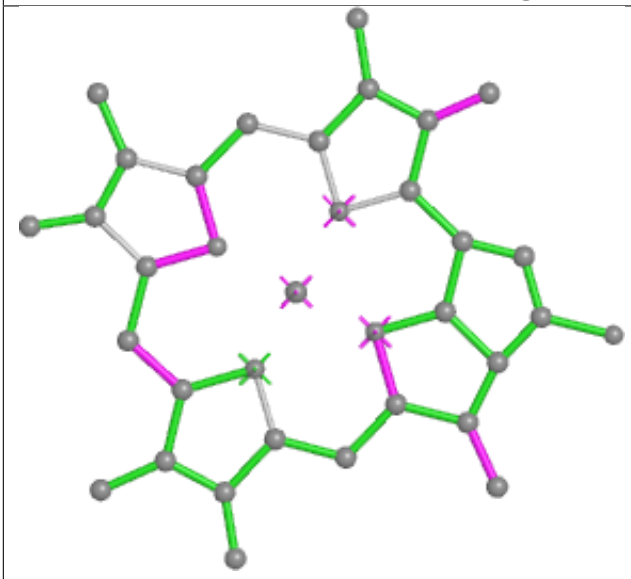


Torsions



Rings

Ligand CLA L 1111



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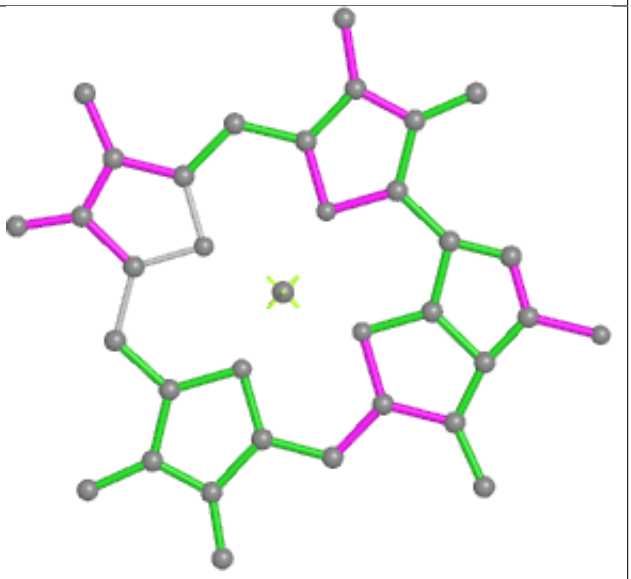

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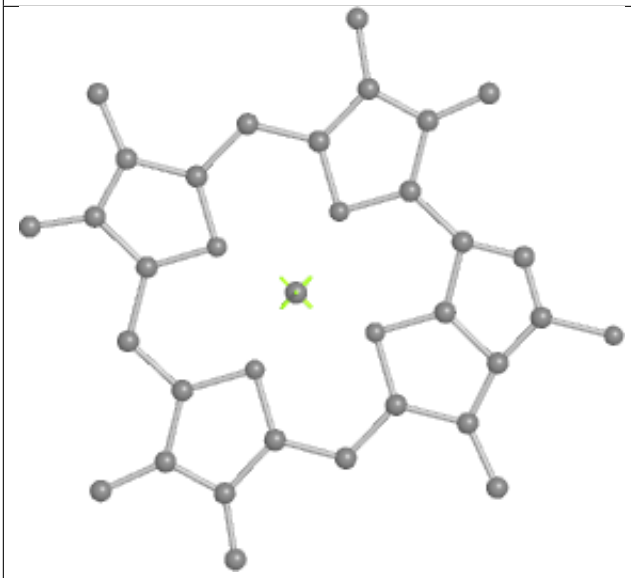

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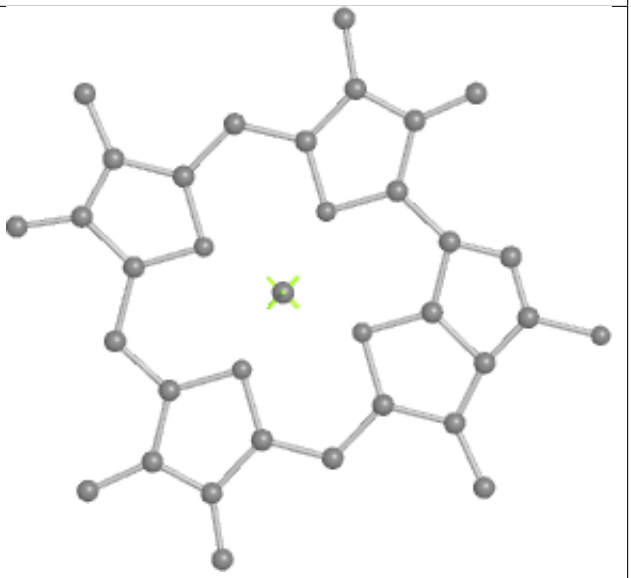
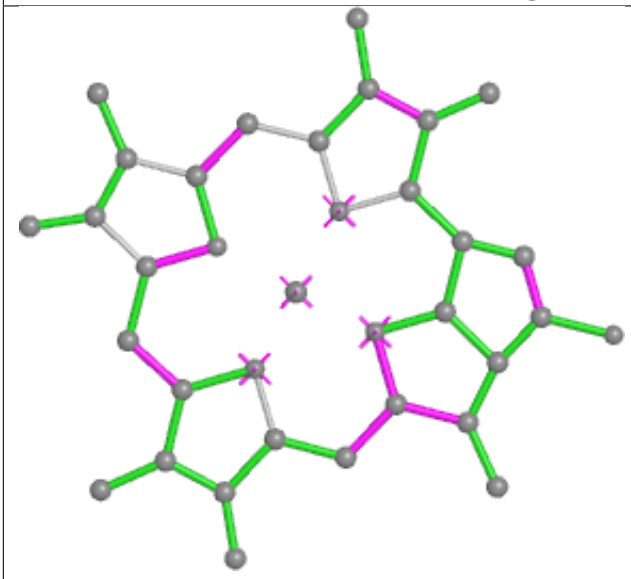


Rings

Ligand CLA N 355



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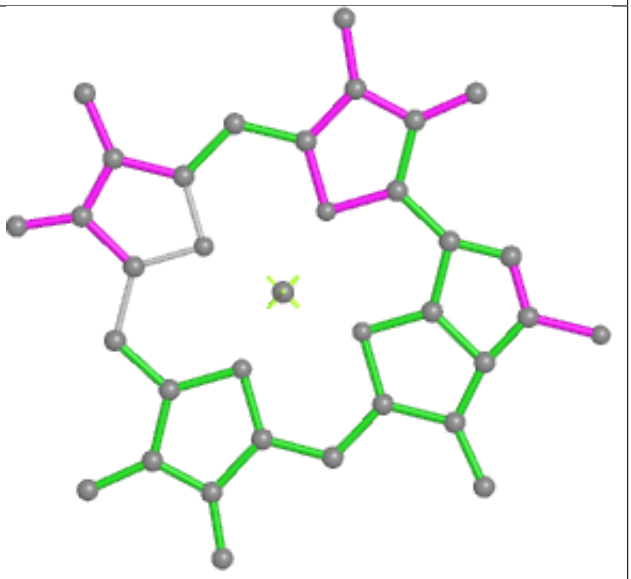
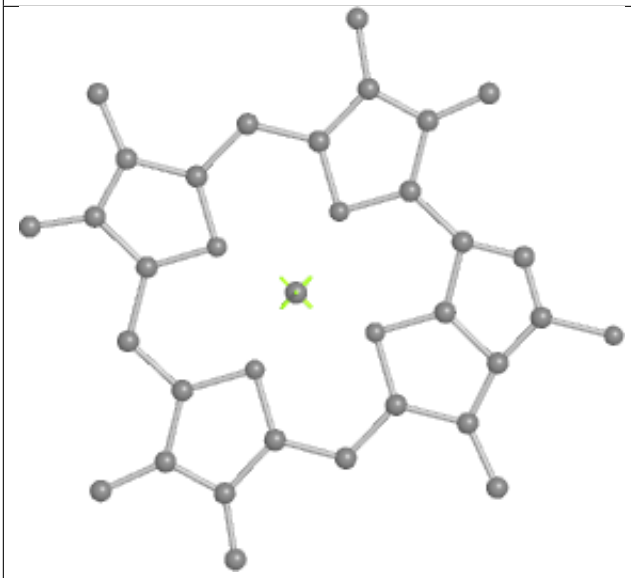
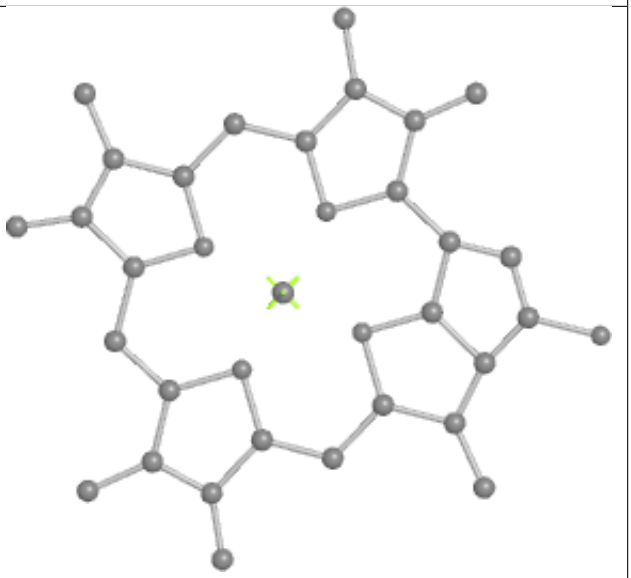


Bond angles

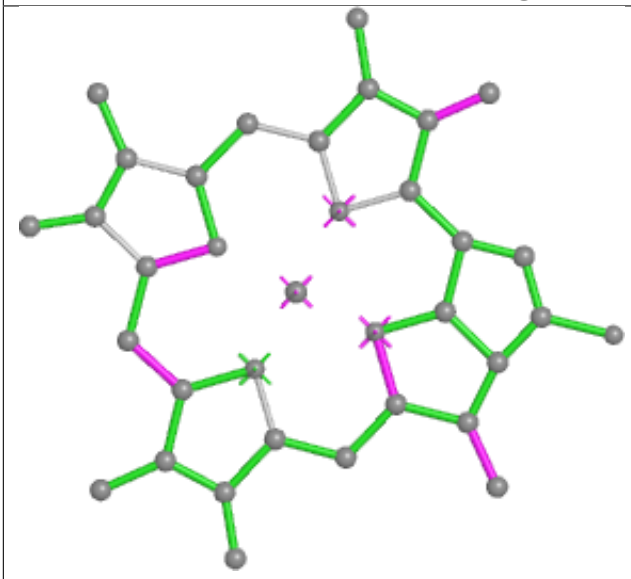


Torsions



Rings

Ligand CLA B 1111



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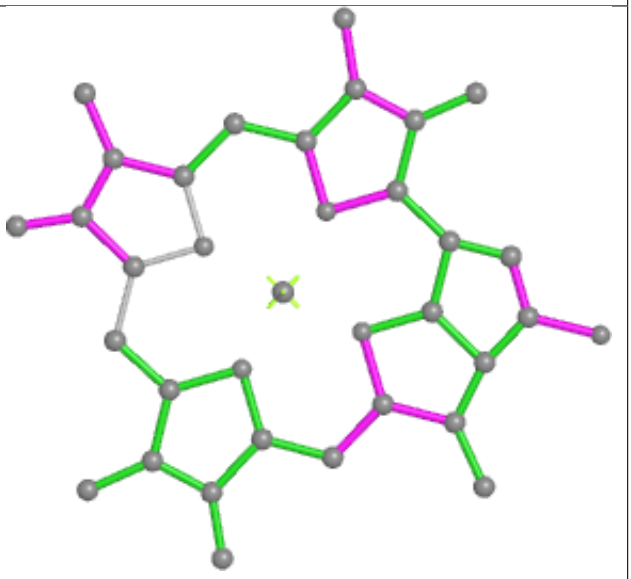
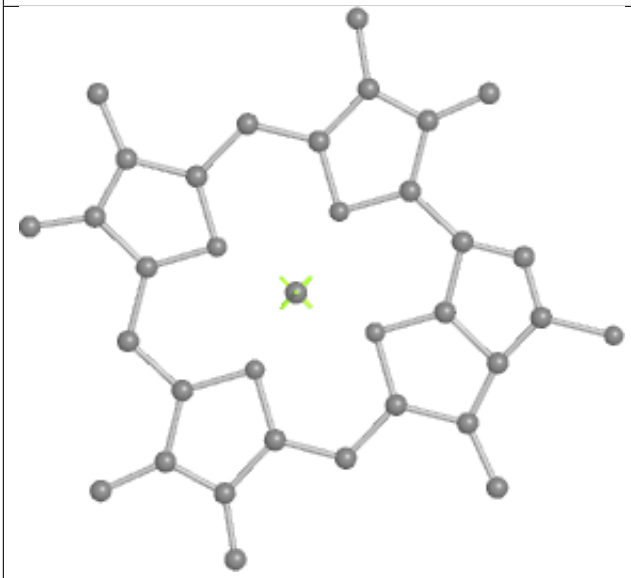


Bond angles



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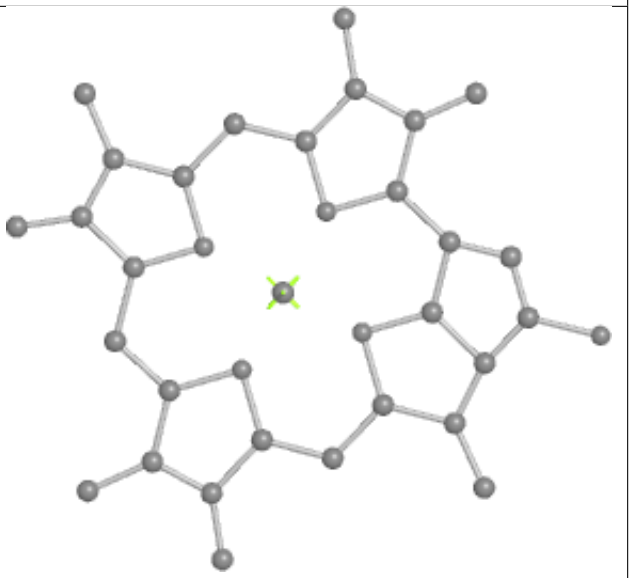
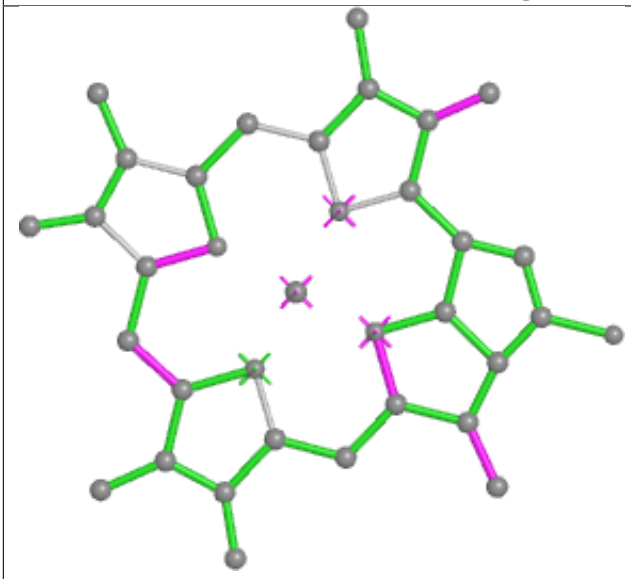
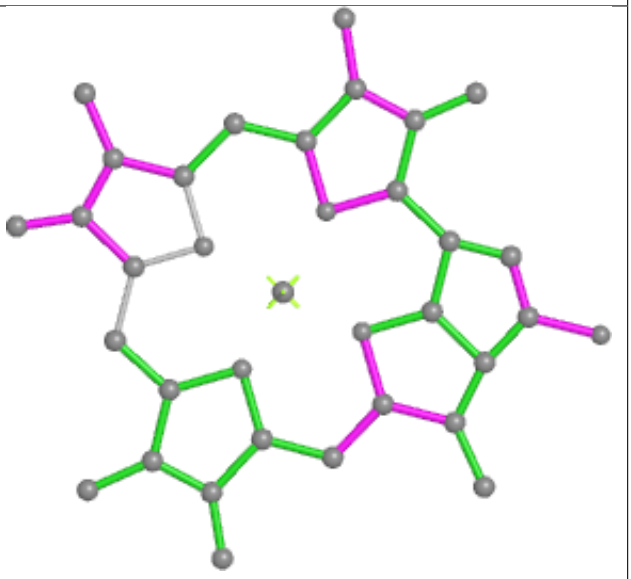


Rings

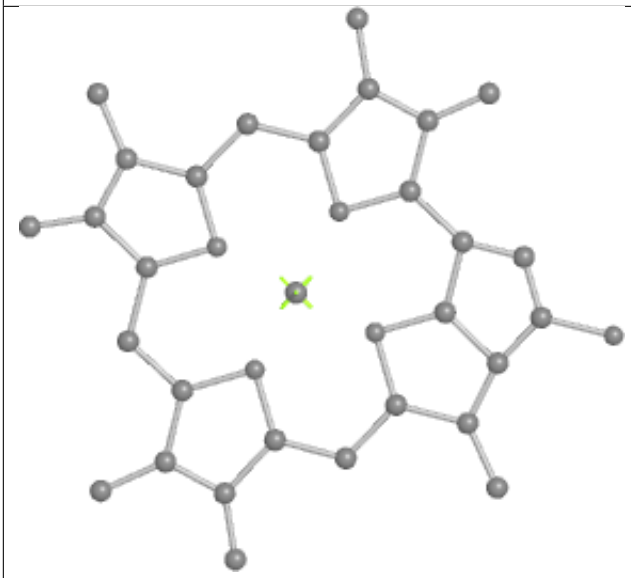
Ligand CLA L 1122



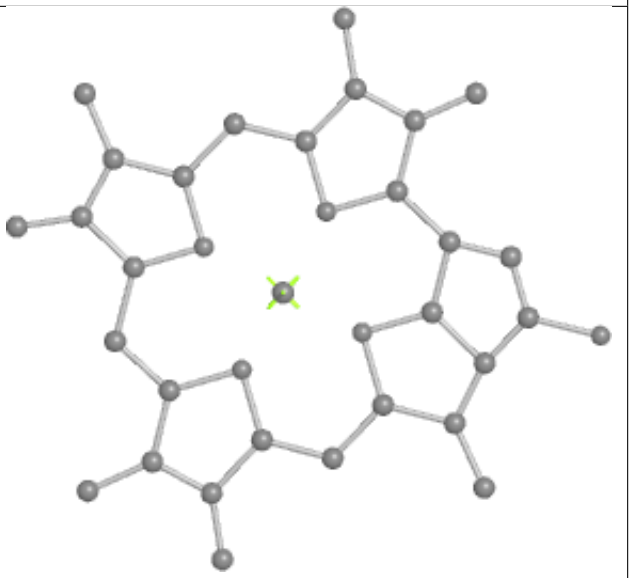
Bond lengths



Bond angles

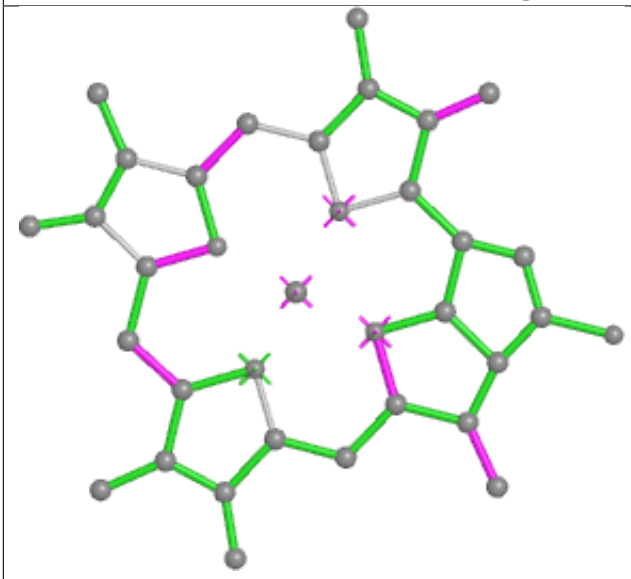


Torsions



Rings

Ligand CLA L 1118



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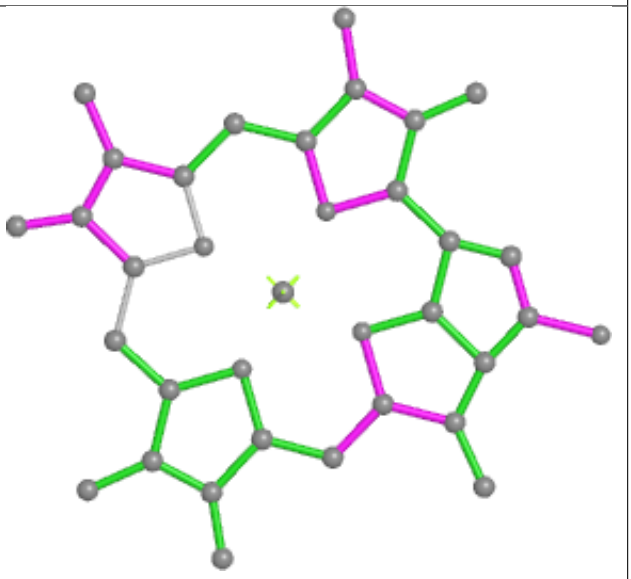
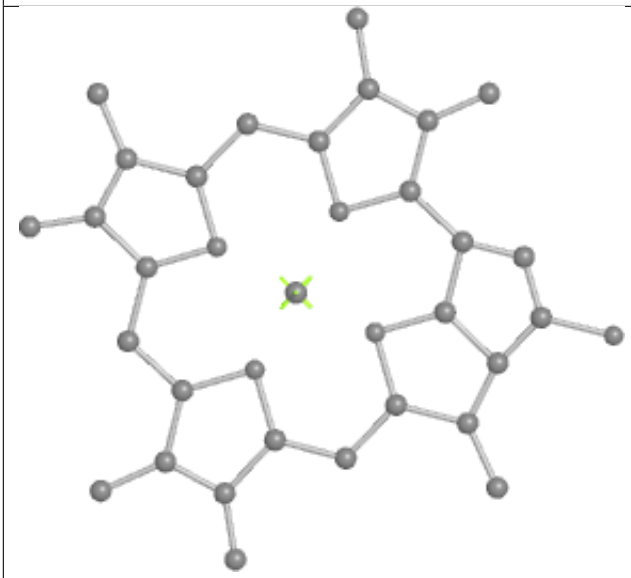


Bond angles



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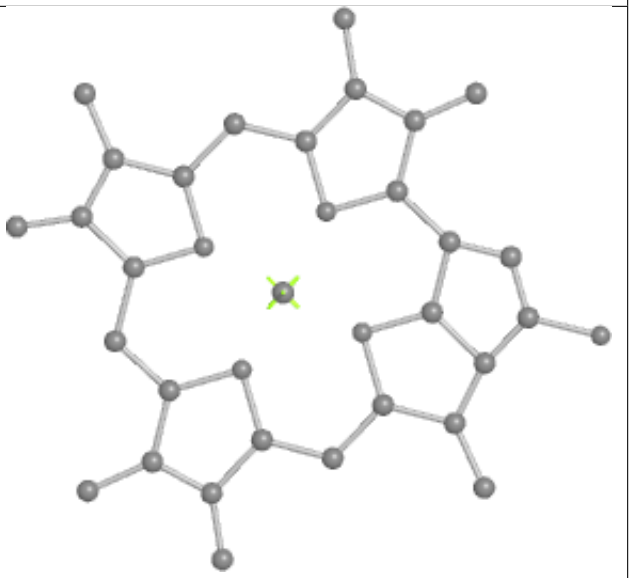
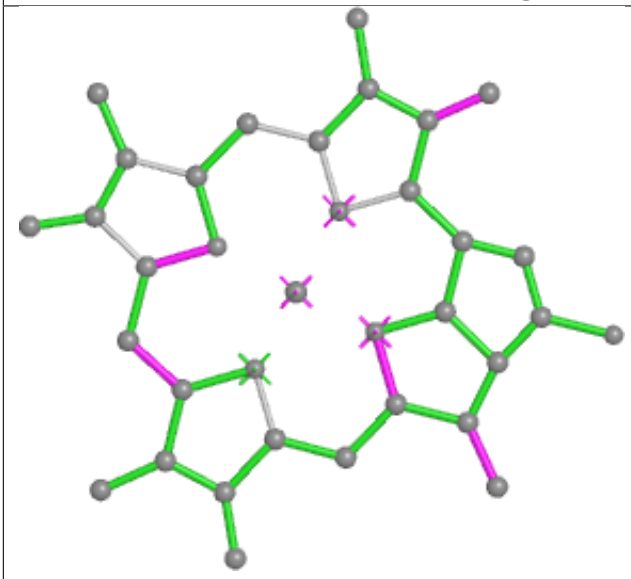


Rings

Ligand CLA L 1109



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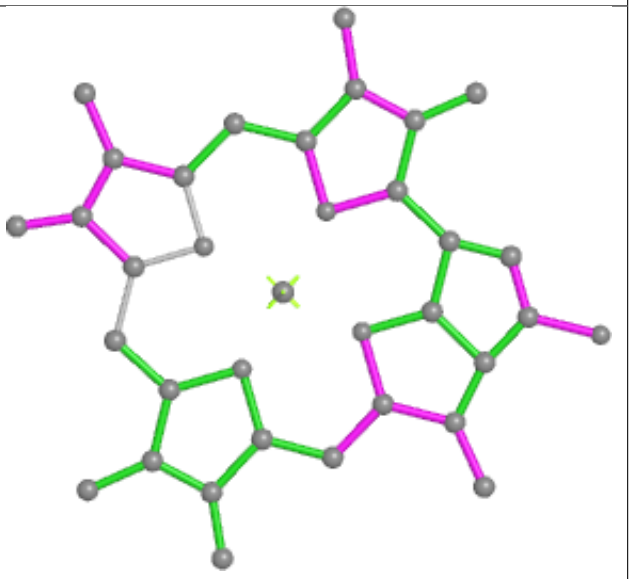
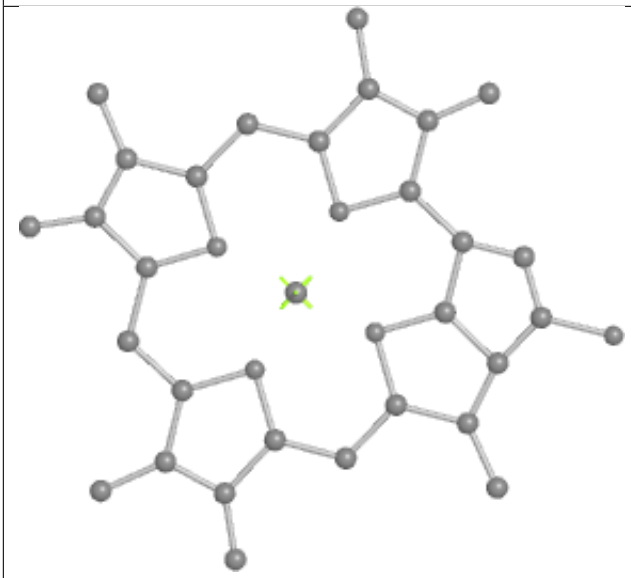


Bond angles



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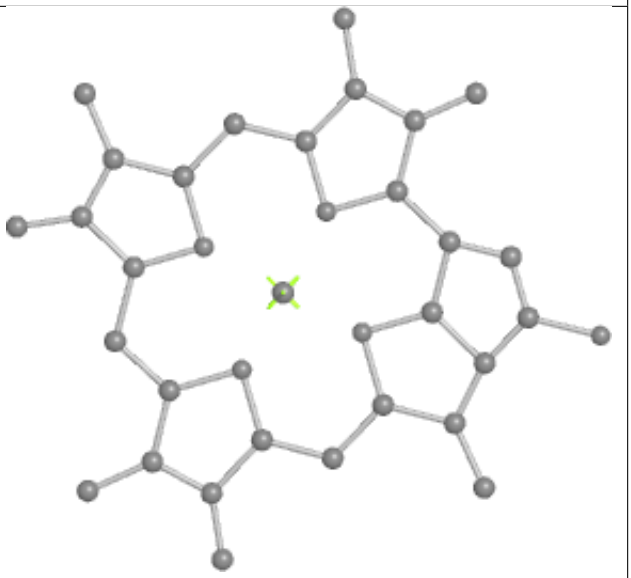
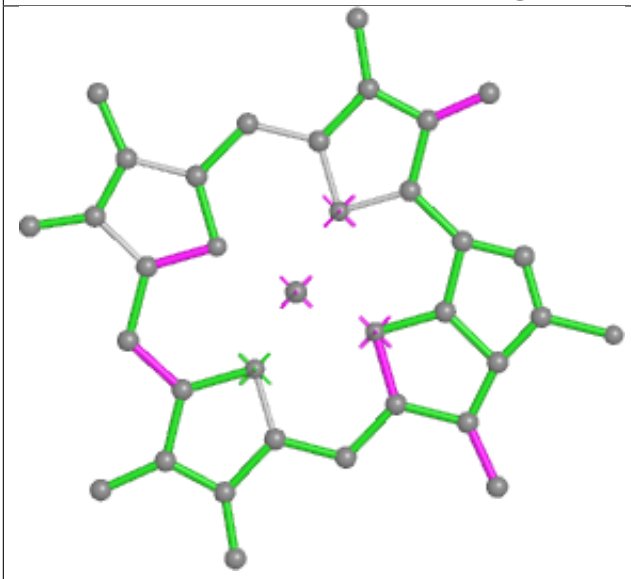


Rings

Ligand CLA M 1079



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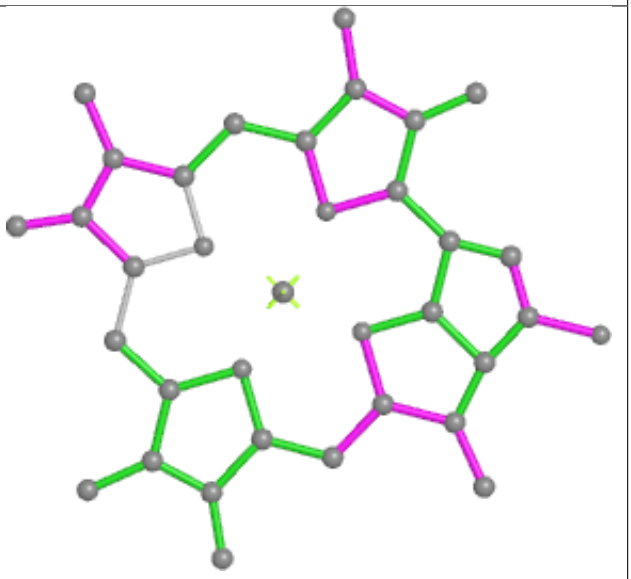
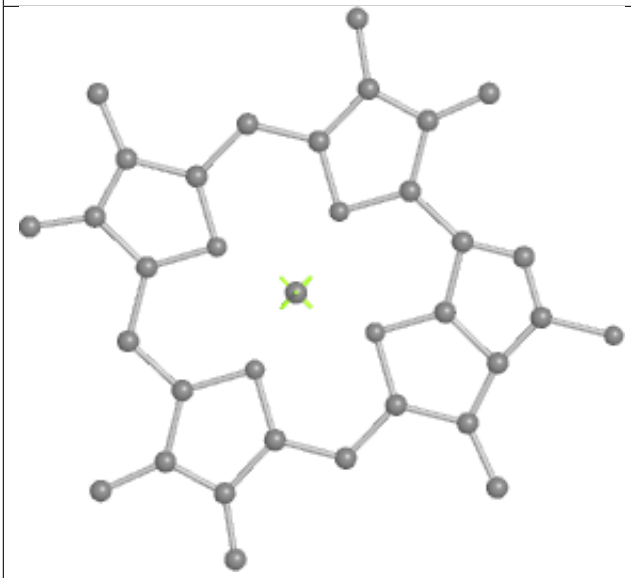
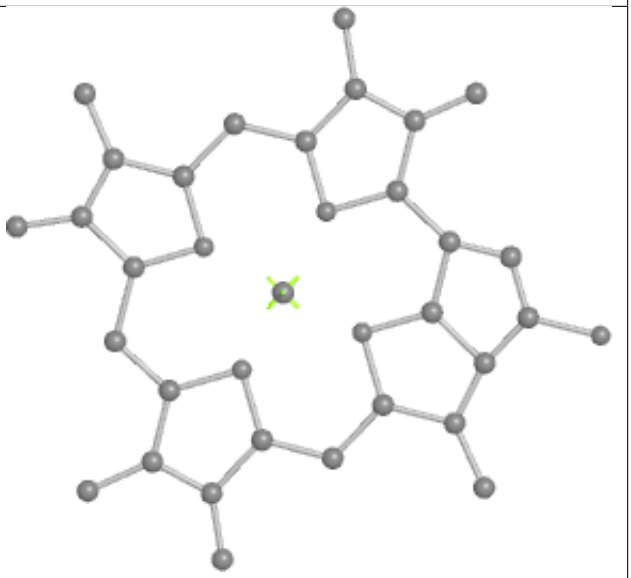


Bond angles

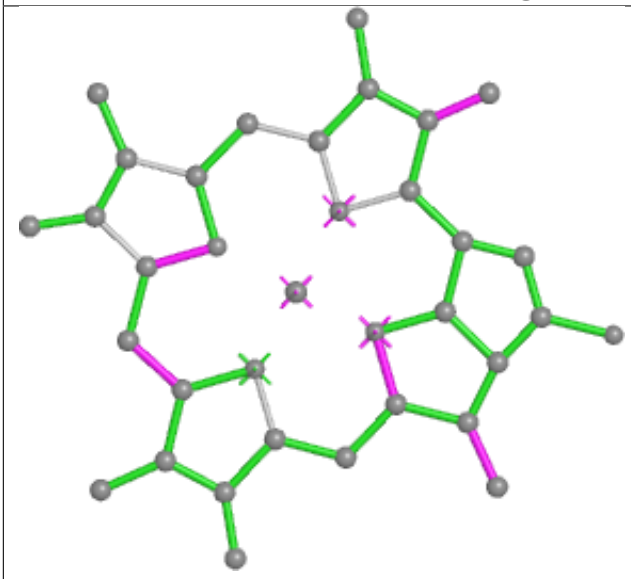


Torsions



Rings

Ligand CLA L 1113



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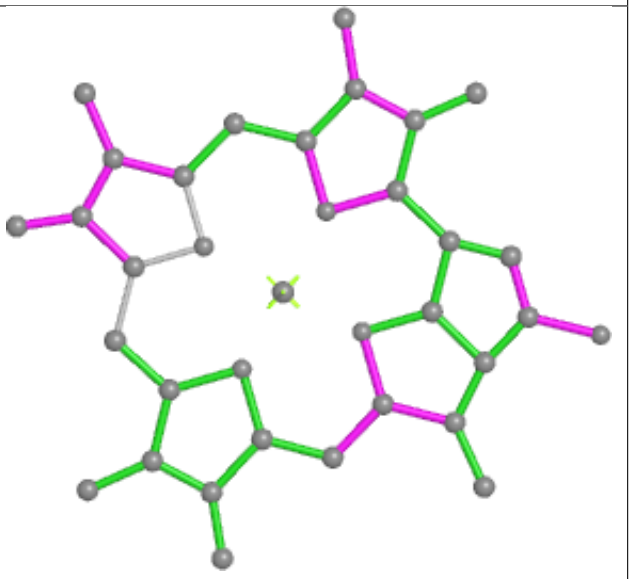
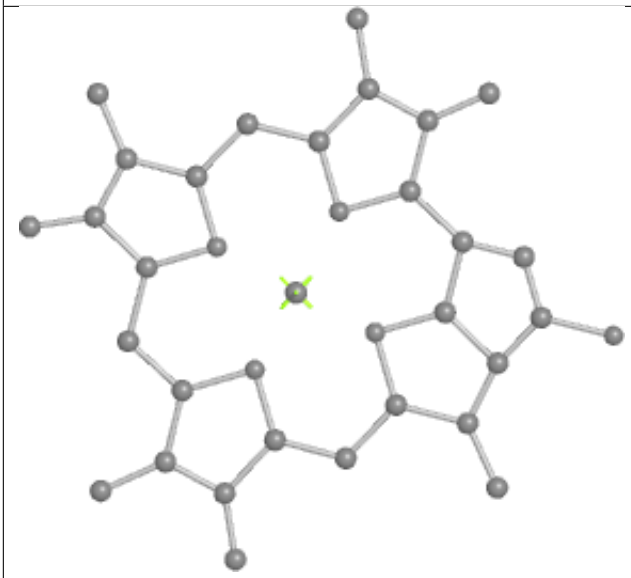
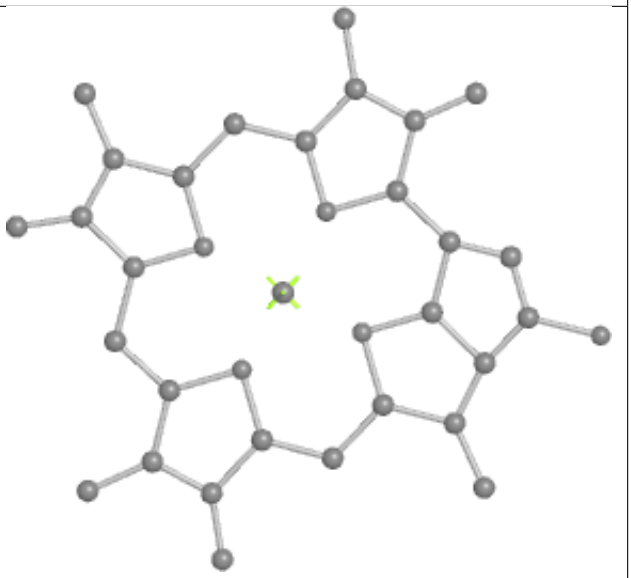


Bond angles

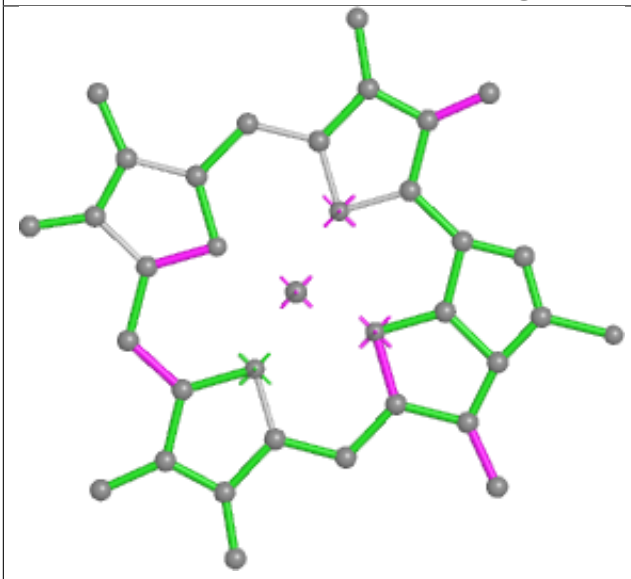


Torsions



Rings

Ligand CLA B 1113



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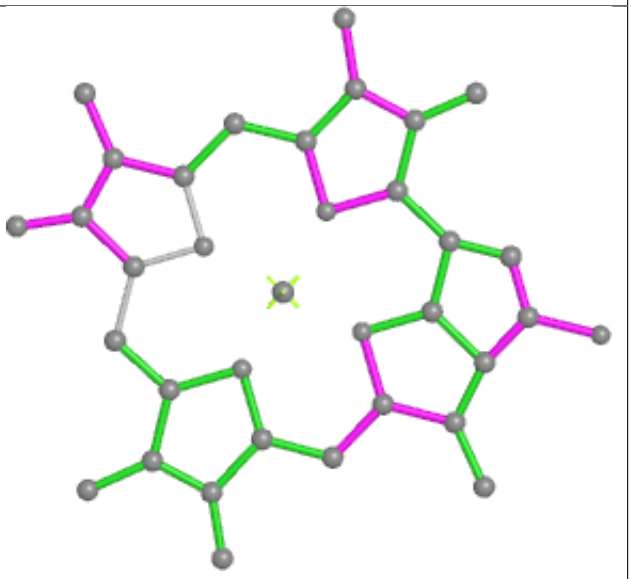
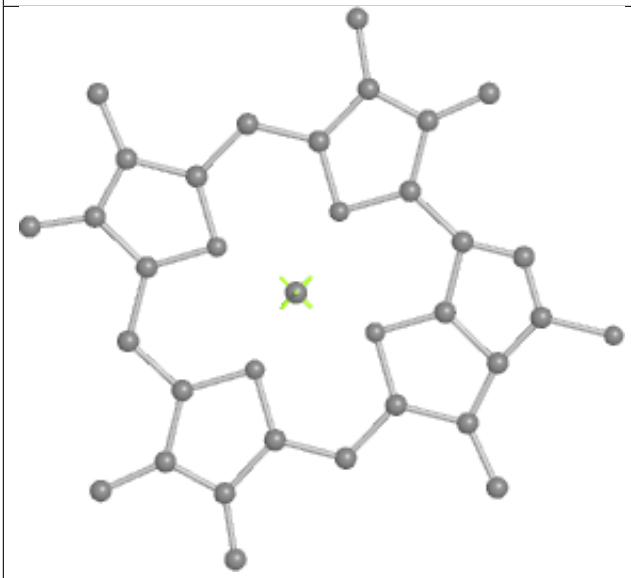
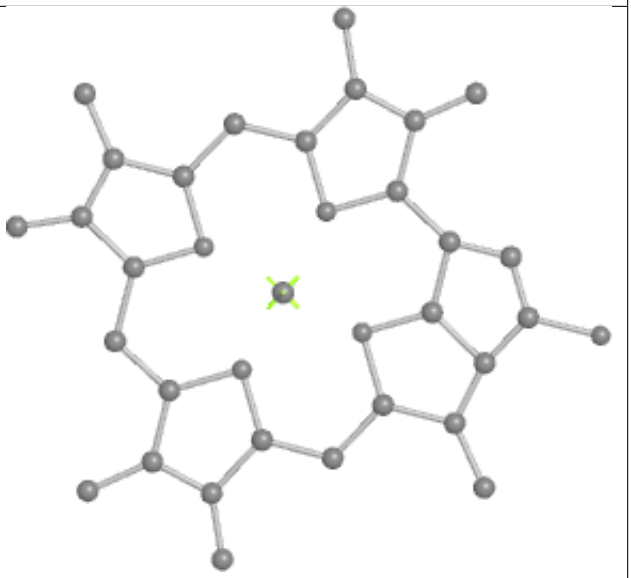


Bond angles

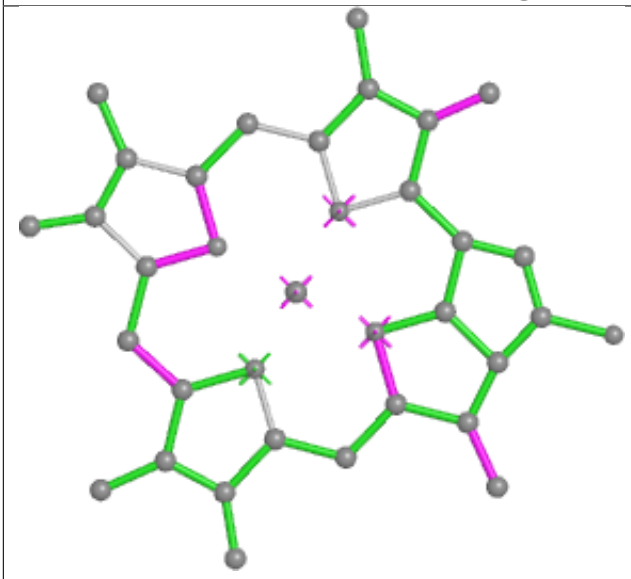


Torsions



Rings

Ligand CLA C 1081



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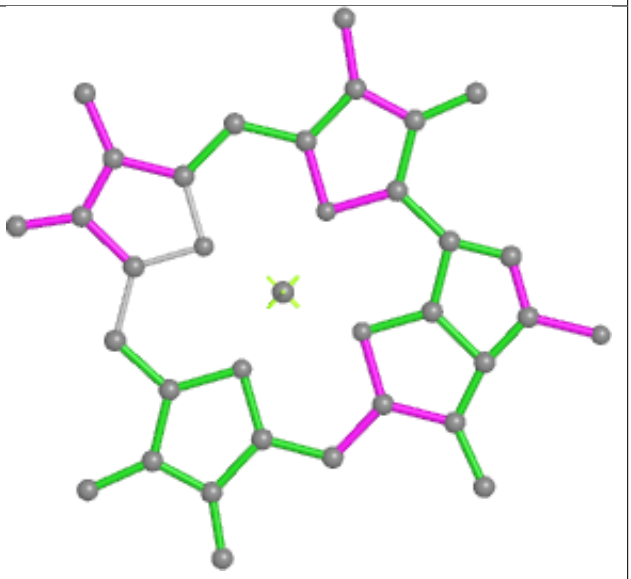
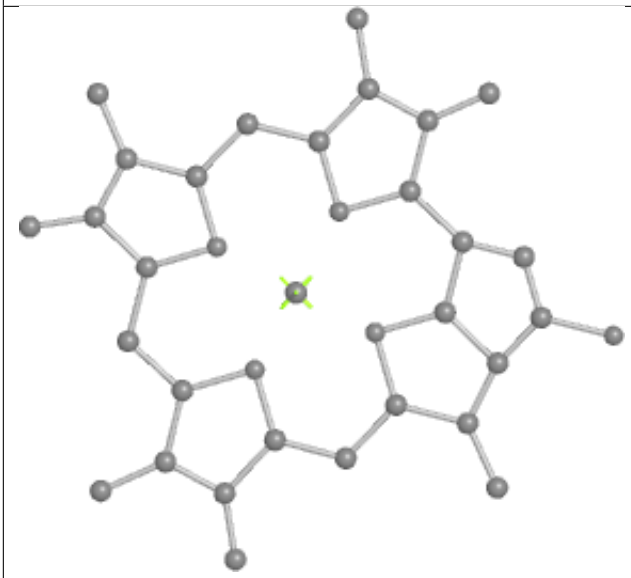
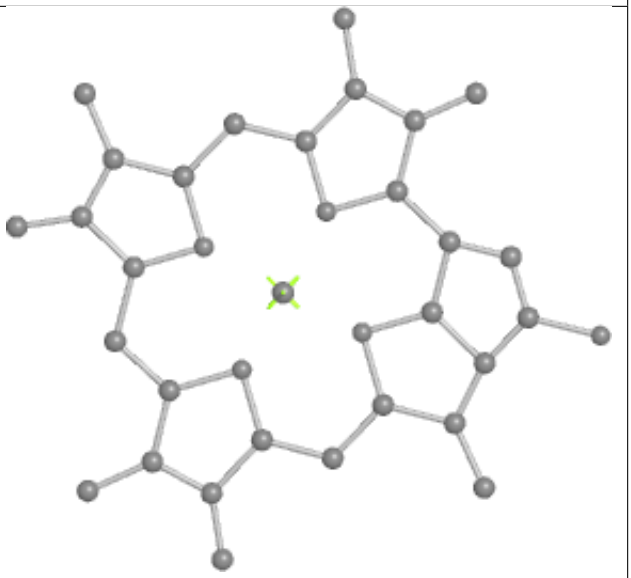


Bond angles

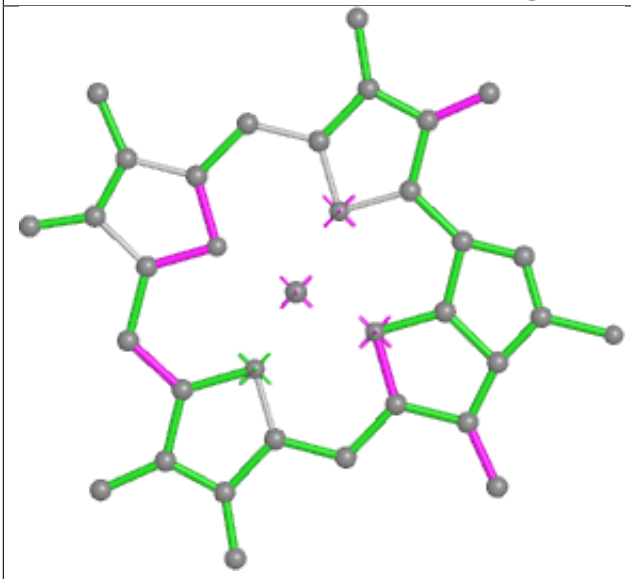


Torsions



Rings

Ligand CLA D 357



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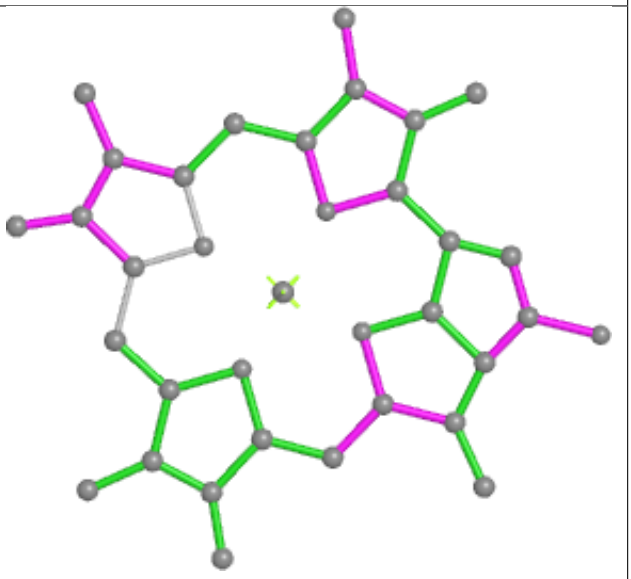
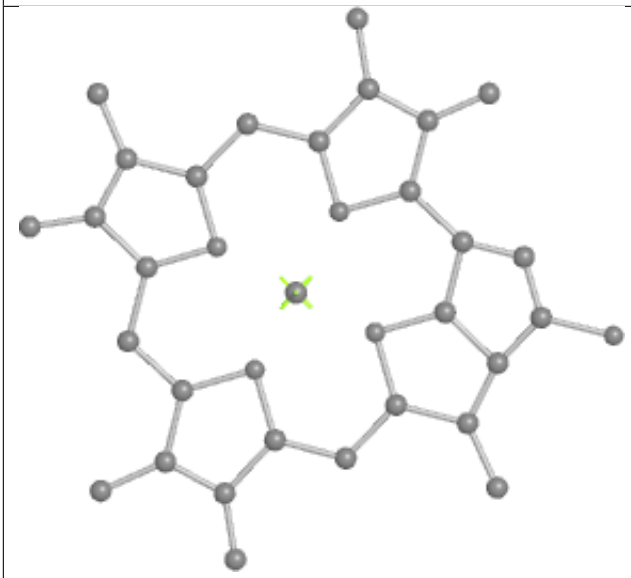
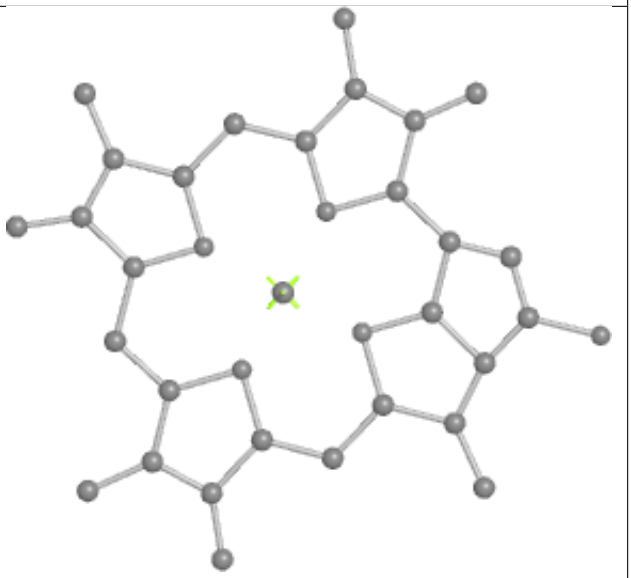


Bond angles

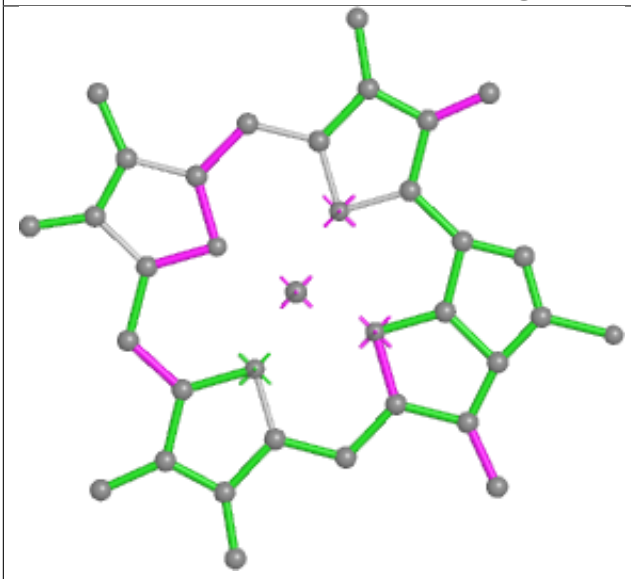


Torsions

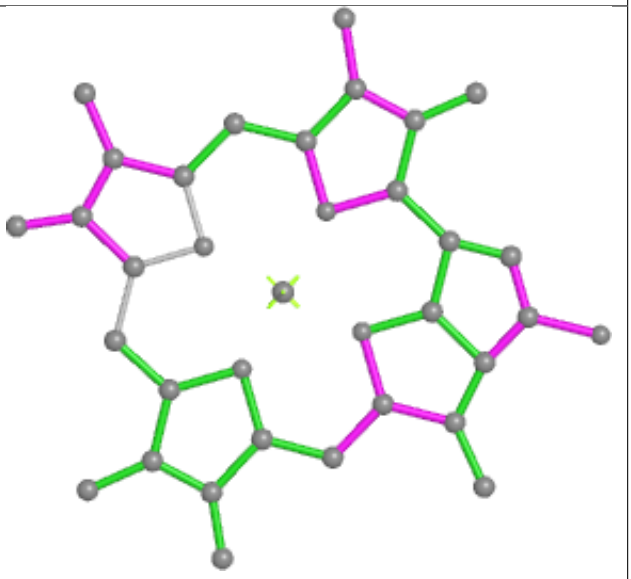


Rings

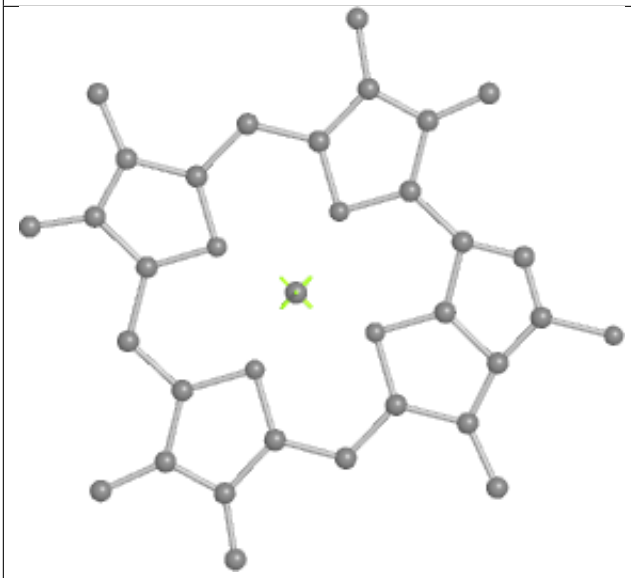
Ligand CLA B 1110



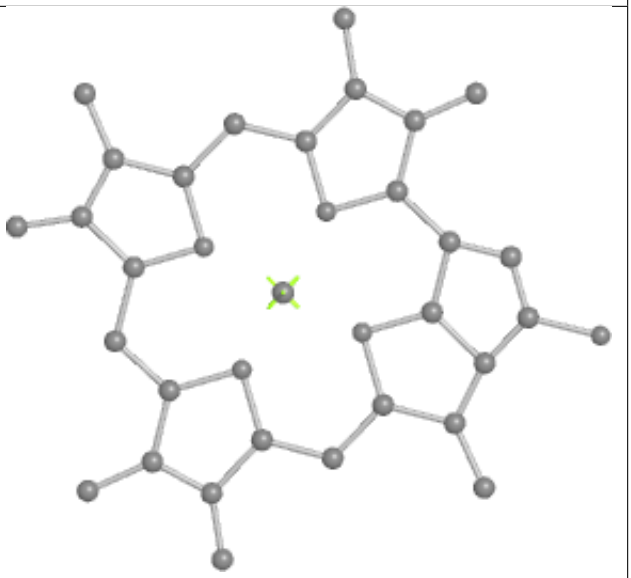
Bond lengths



Bond angles

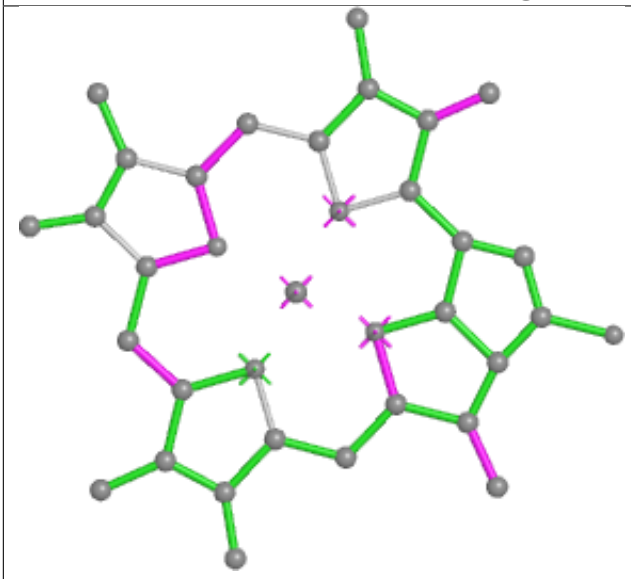


Torsions

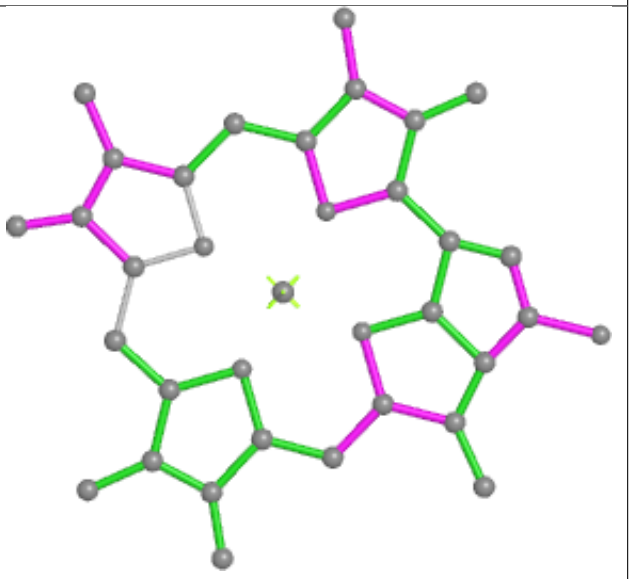


Rings

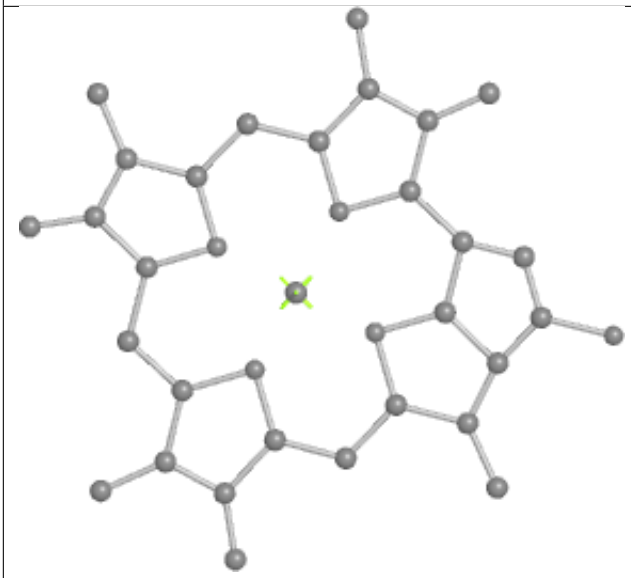
Ligand CLA L 1120



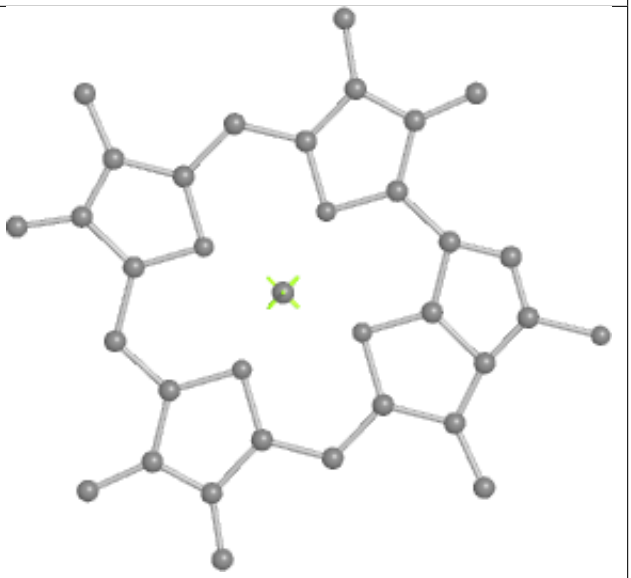
Bond lengths



Bond angles

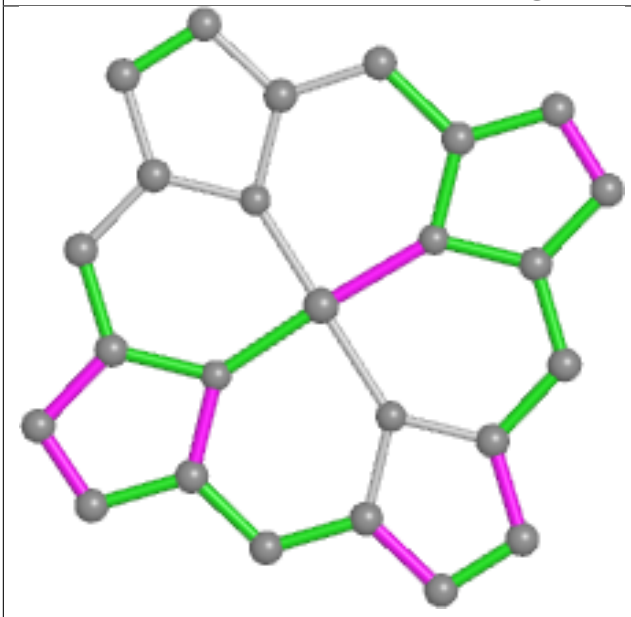


Torsions

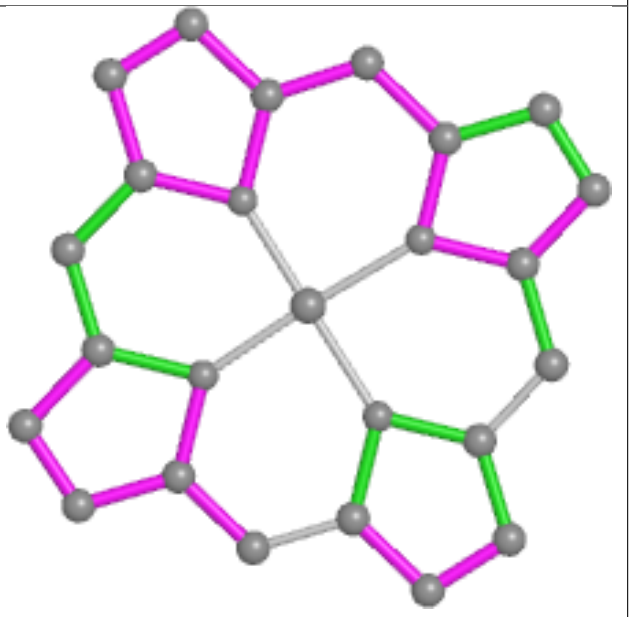


Rings

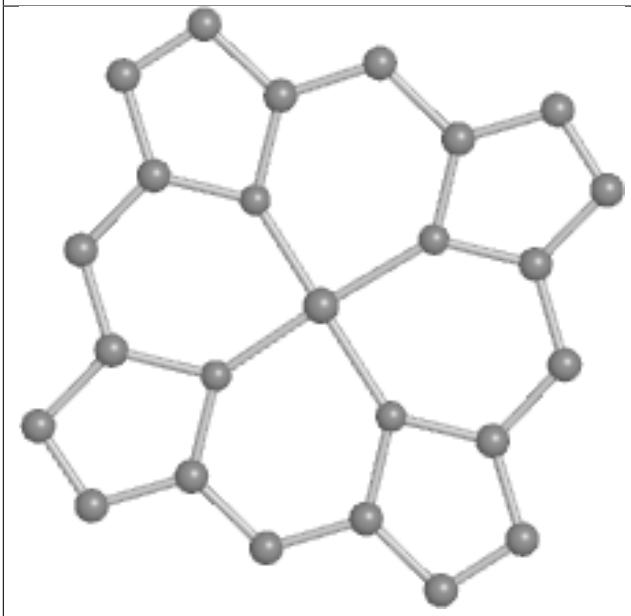
Ligand HEM P 92



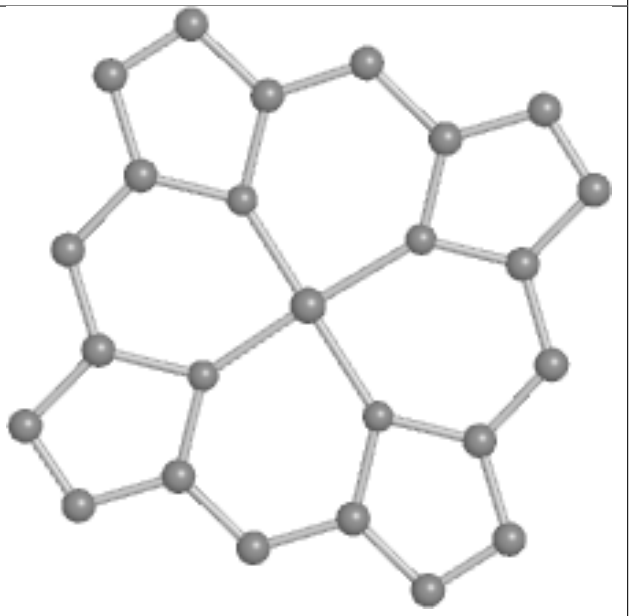
Bond lengths



Bond angles

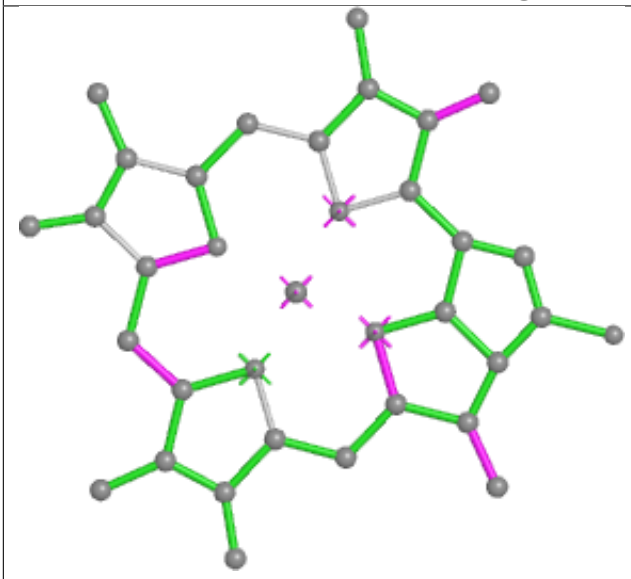


Torsions

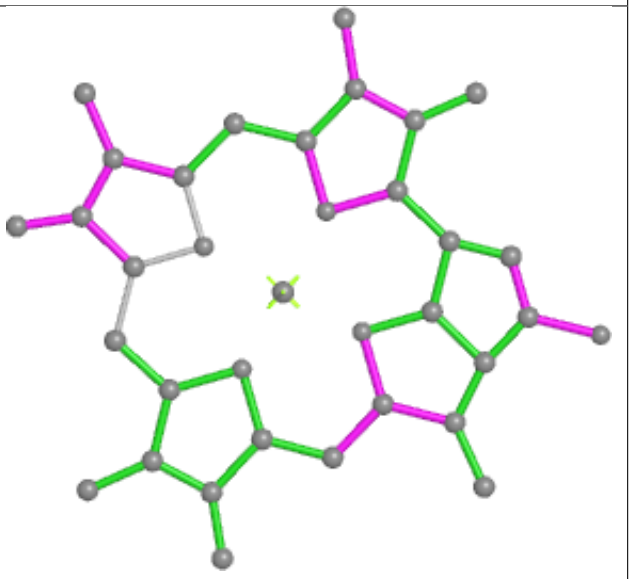


Rings

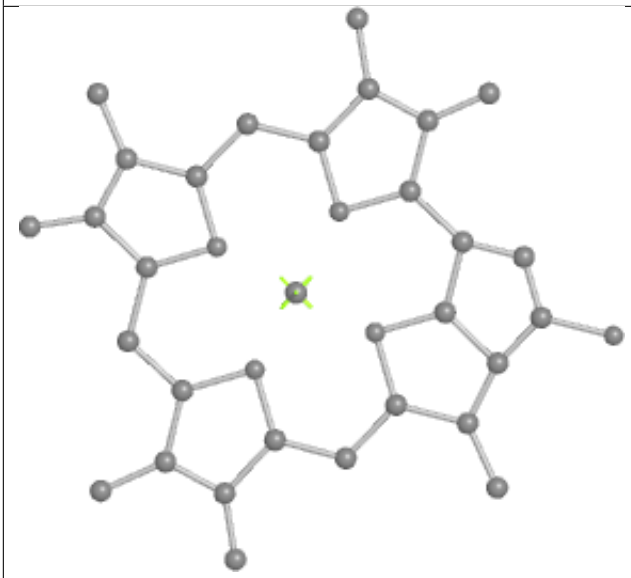
Ligand CLA B 1109



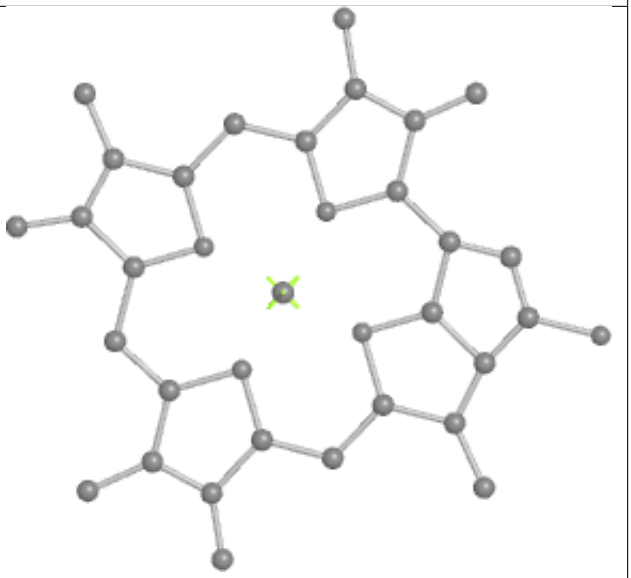
Bond lengths



Bond angles

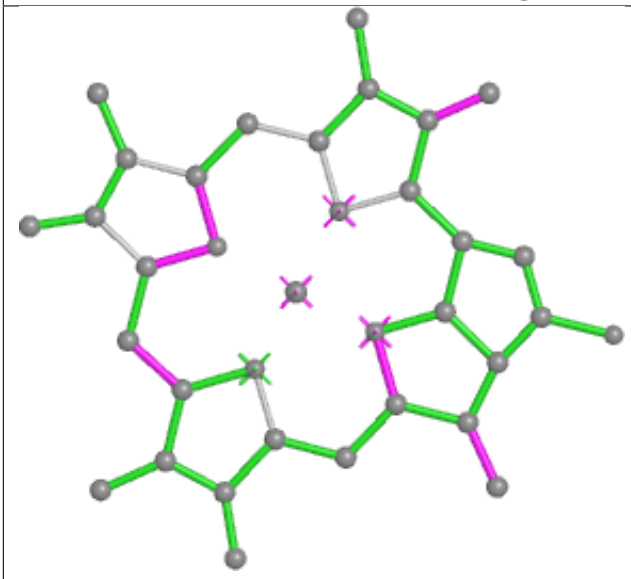


Torsions



Rings

Ligand CLA B 1117



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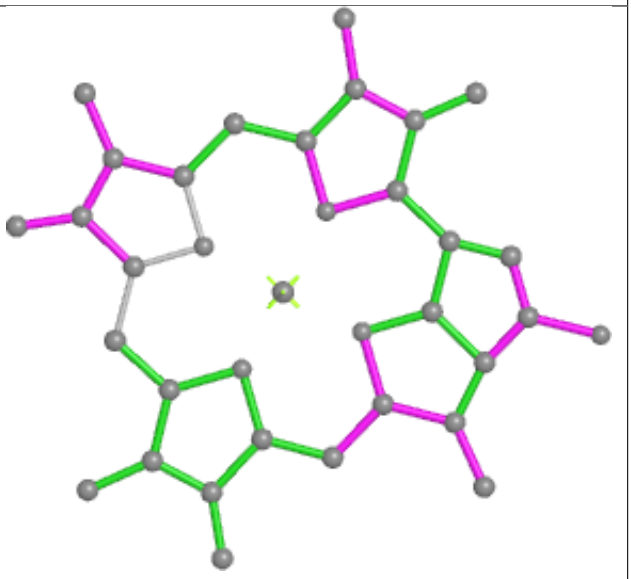
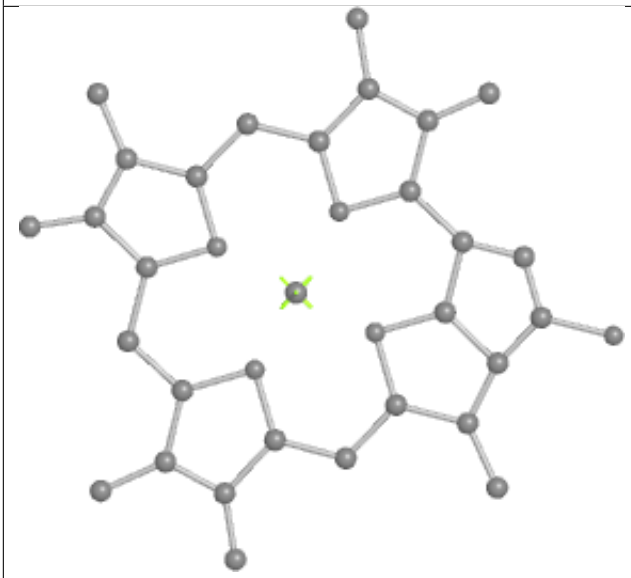
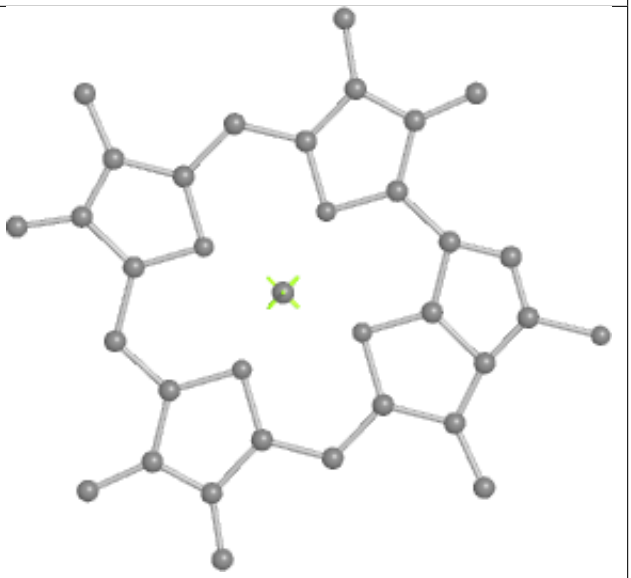


Bond angles

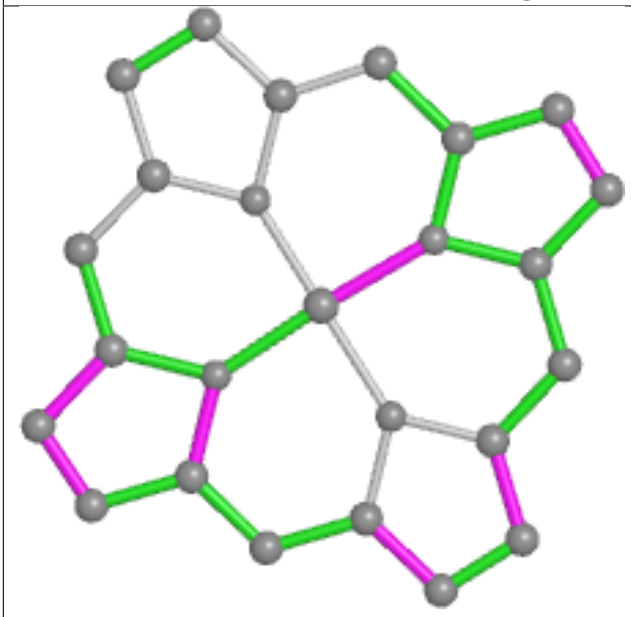


Torsions



Rings

Ligand HEM V 138



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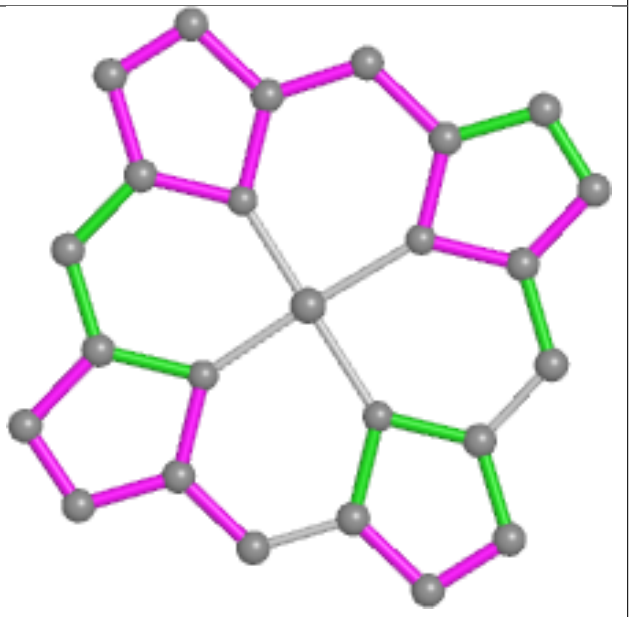
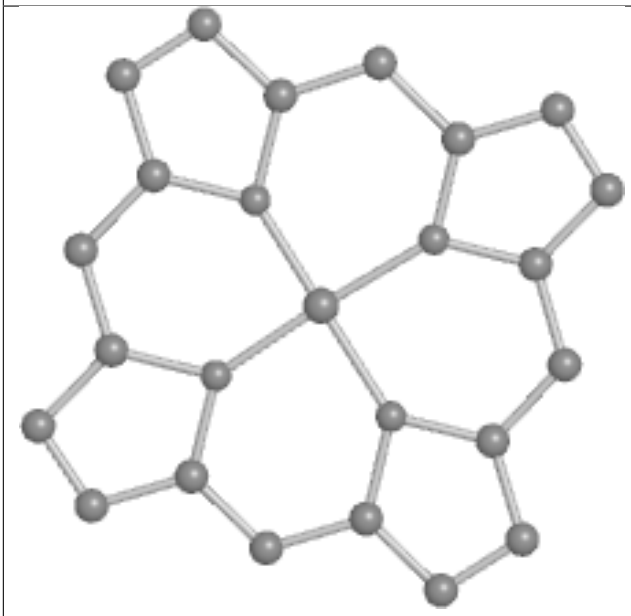
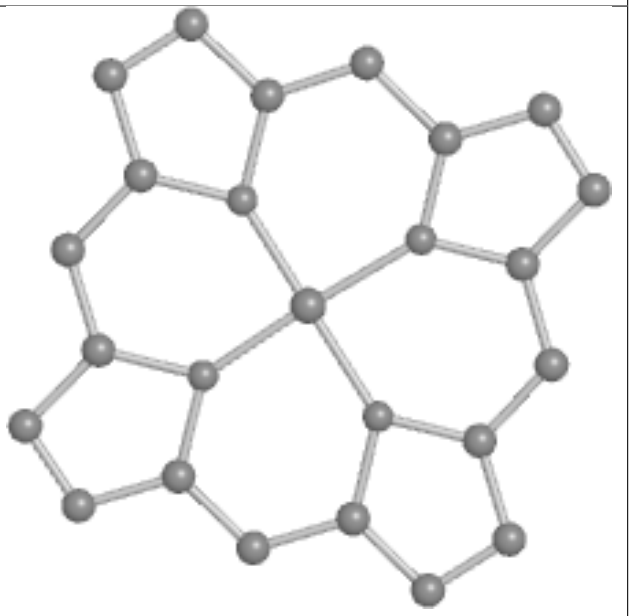


Bond angles

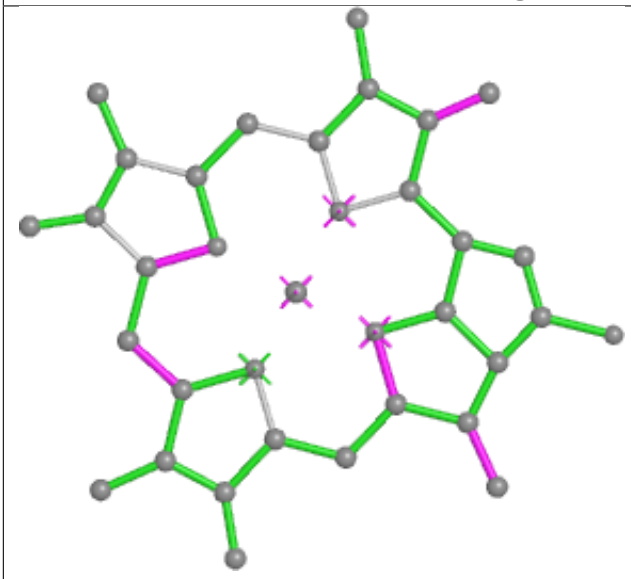


Torsions



Rings

Ligand CLA M 1082



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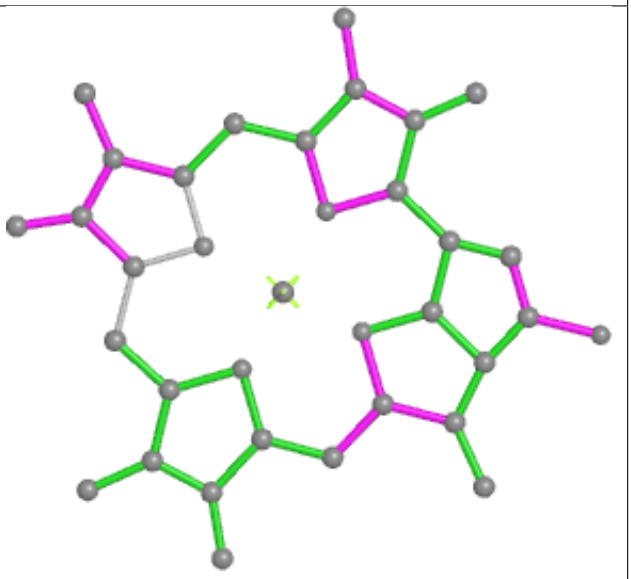
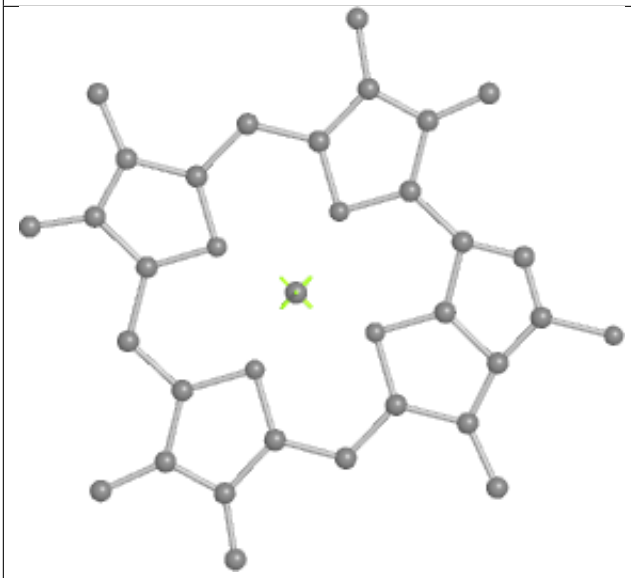
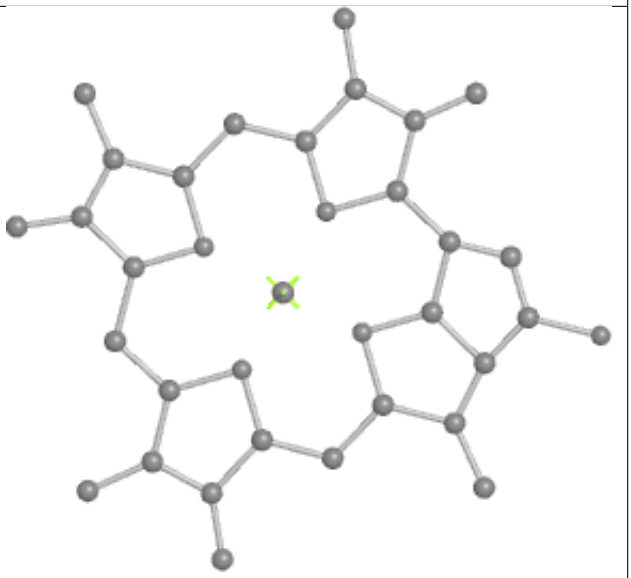


Bond angles

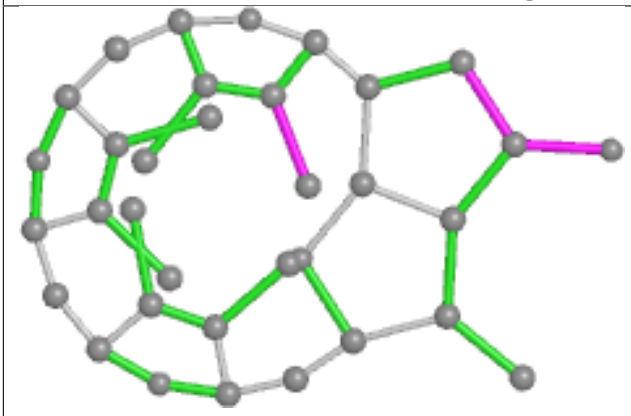


Torsions



Rings

Ligand PHO D 356



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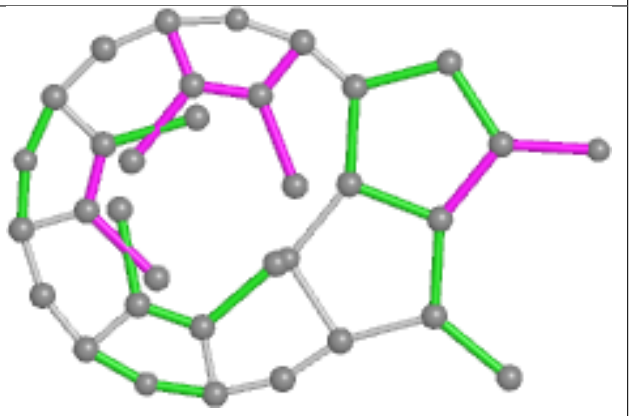
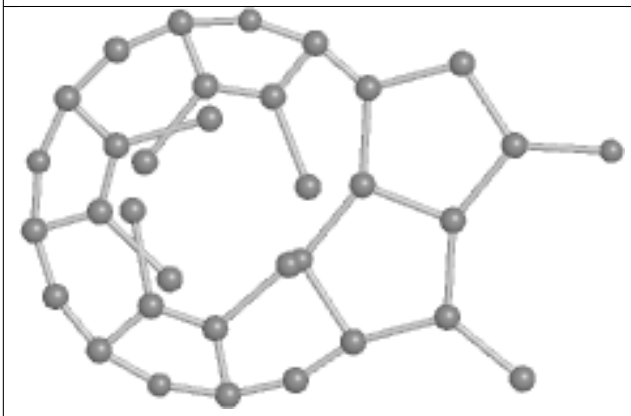


Bond angles



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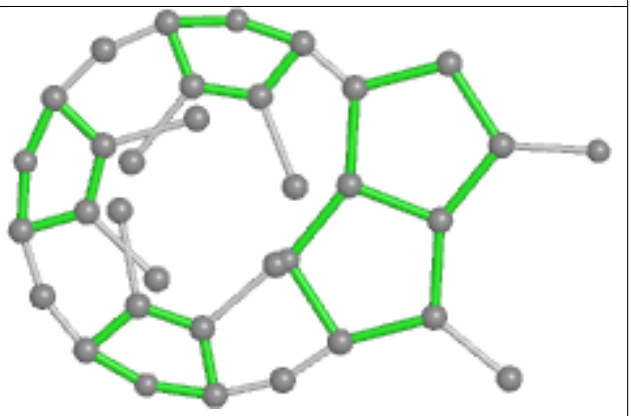
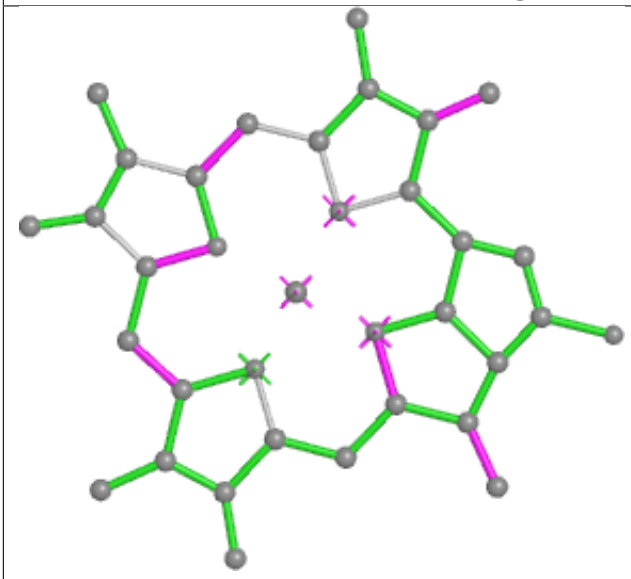


Rings

Ligand CLA M 1087



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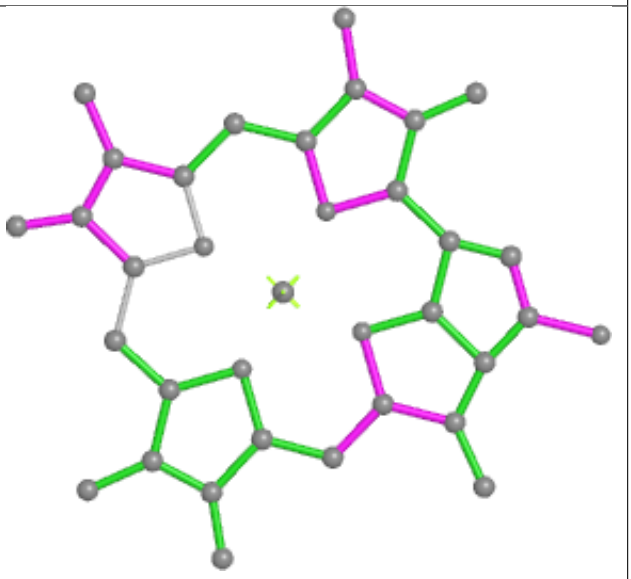
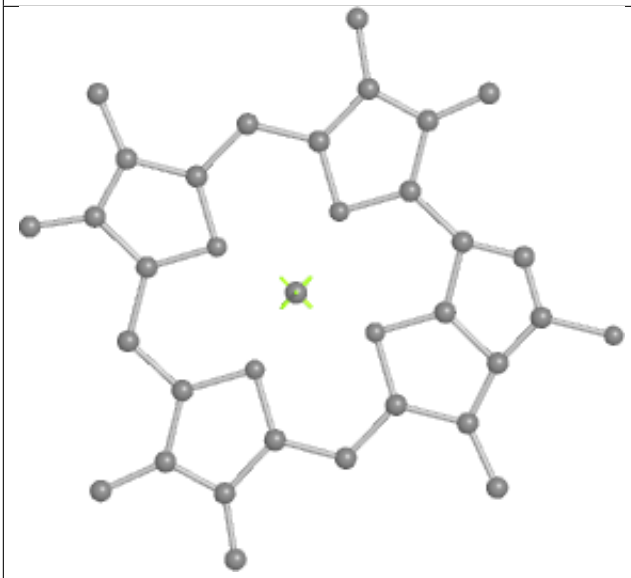


Bond angles



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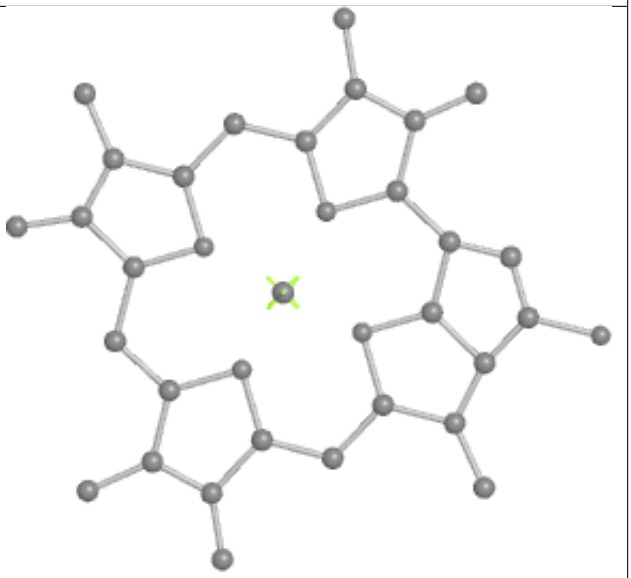
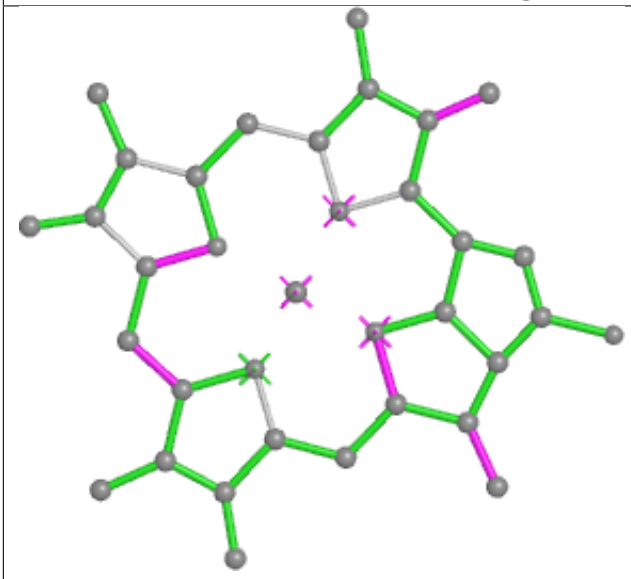


Rings

Ligand CLA L 1121



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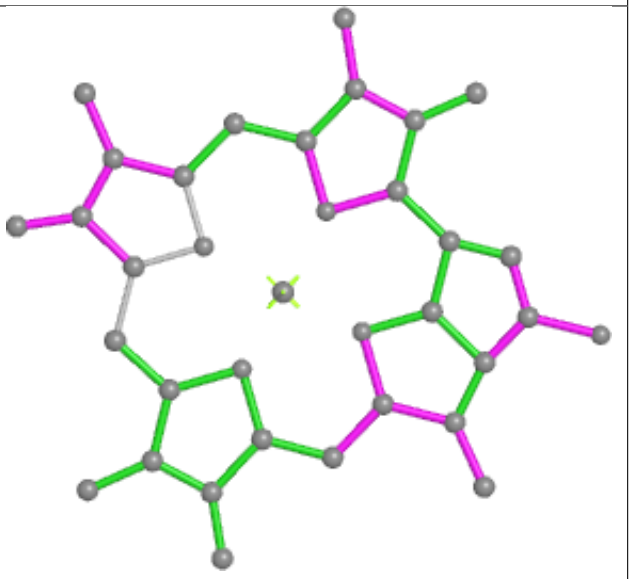
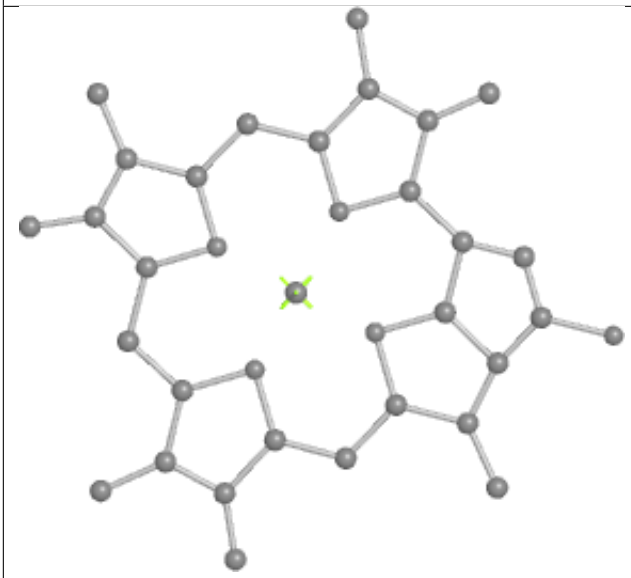
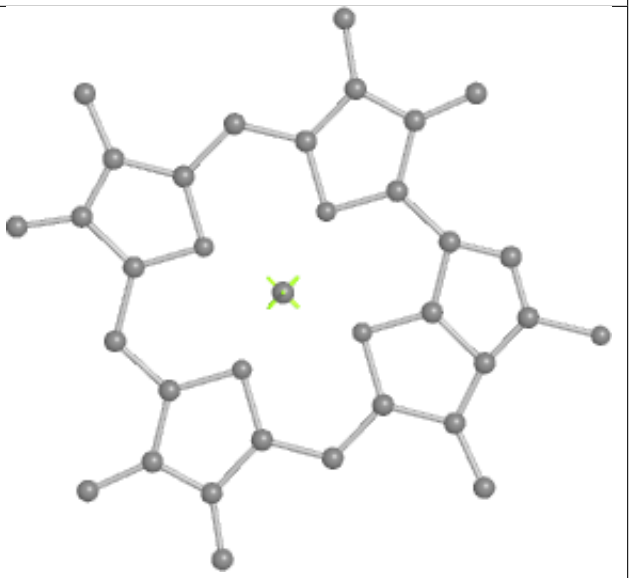


Bond angles

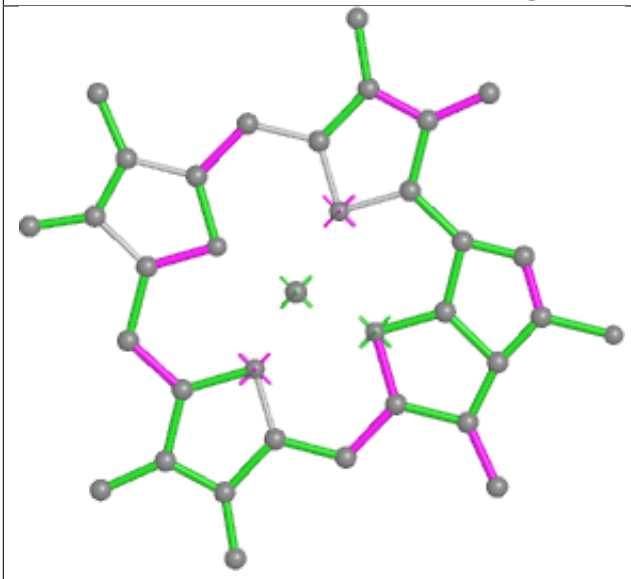


Torsions



Rings

Ligand CLA G 221



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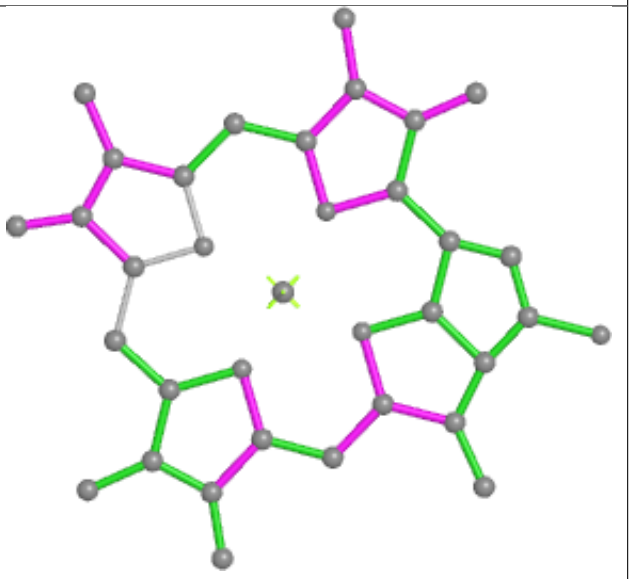
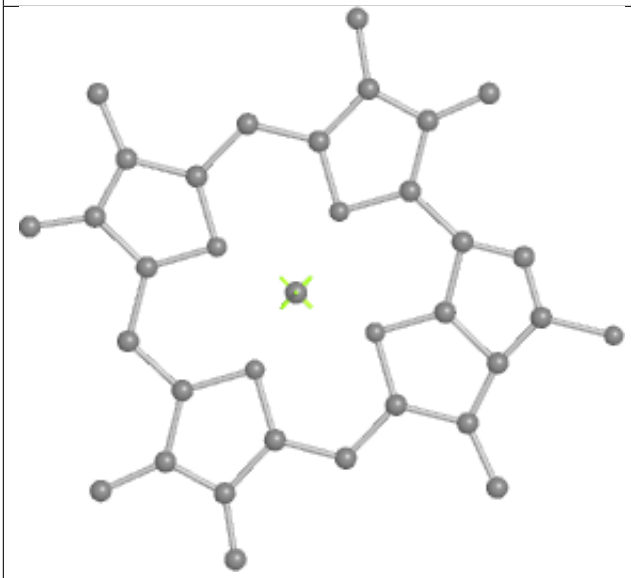
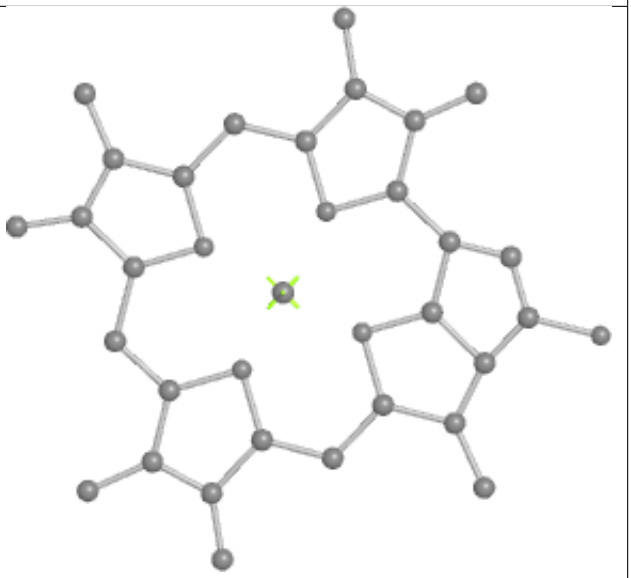


Bond angles

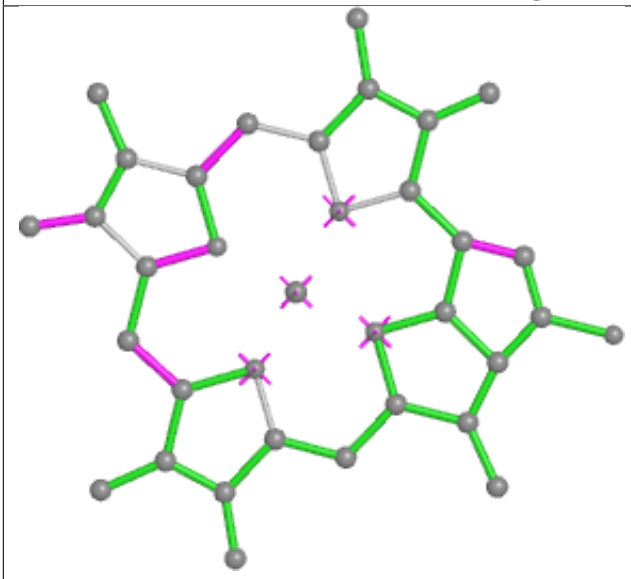


Torsions



Rings

Ligand CLA J 365



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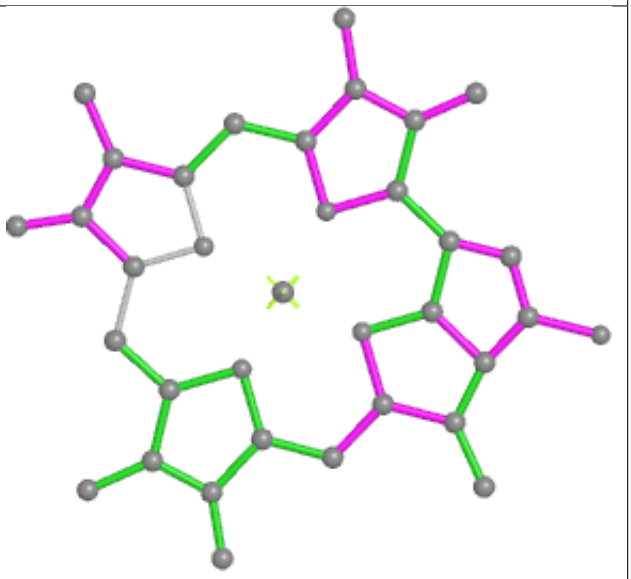
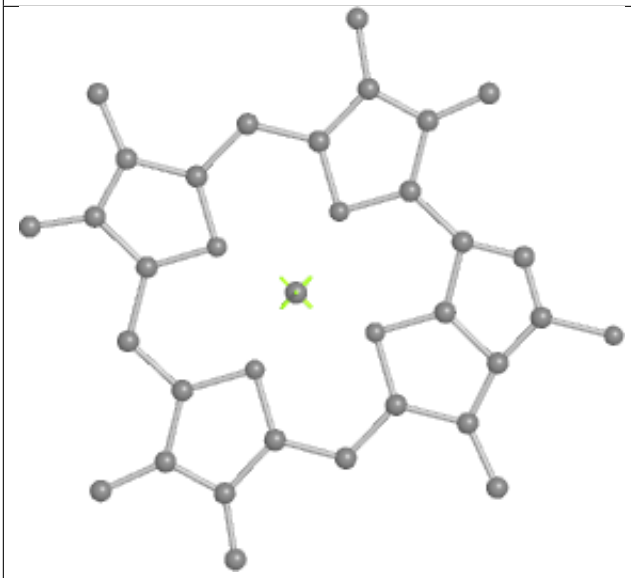
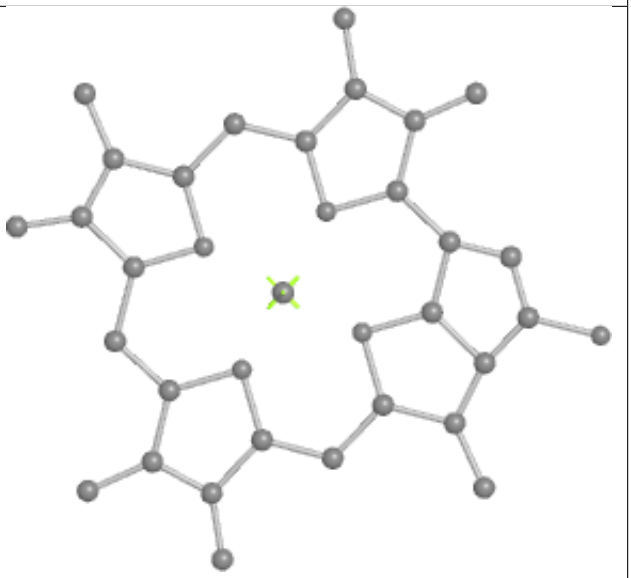


Bond angles

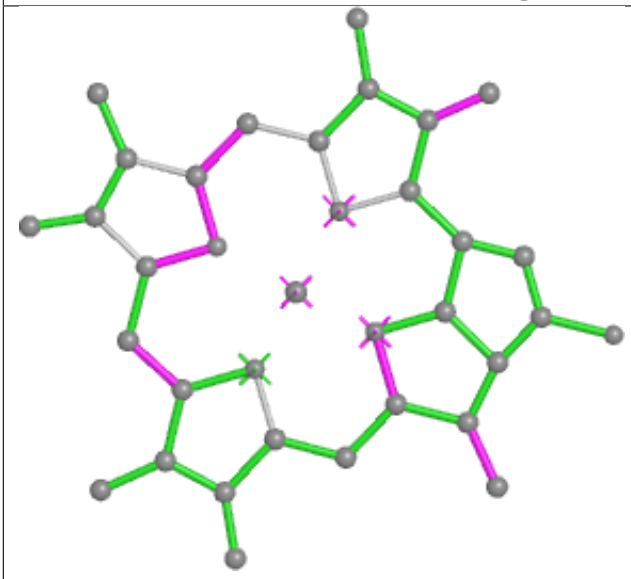


Torsions



Rings

Ligand CLA B 1112



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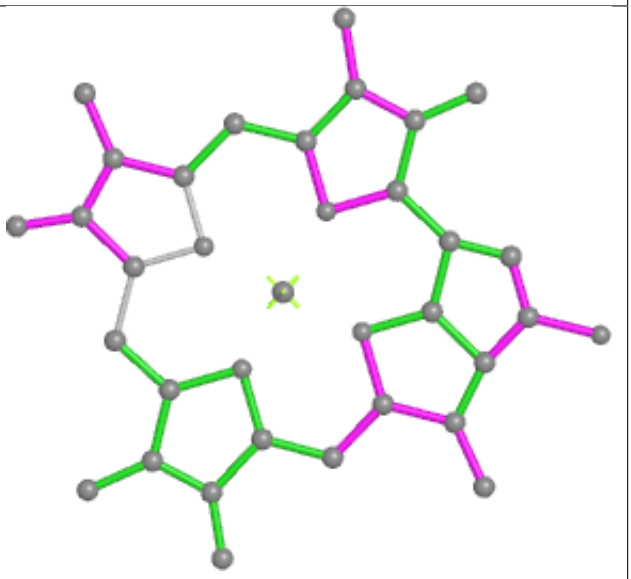
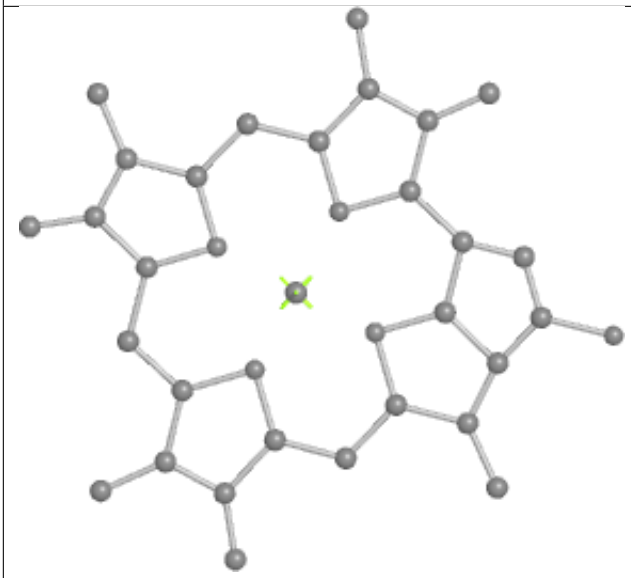


Bond angles



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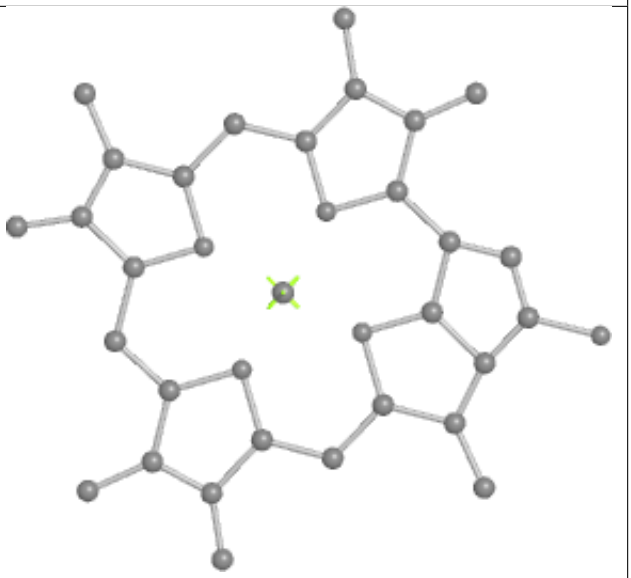
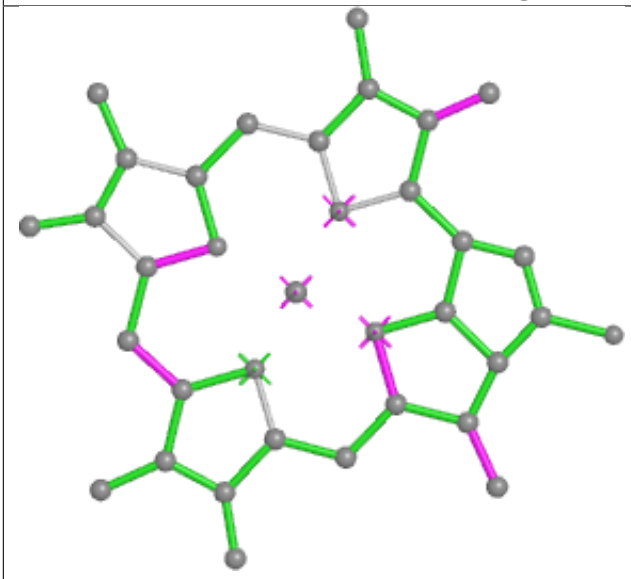


Rings

Ligand CLA B 1107



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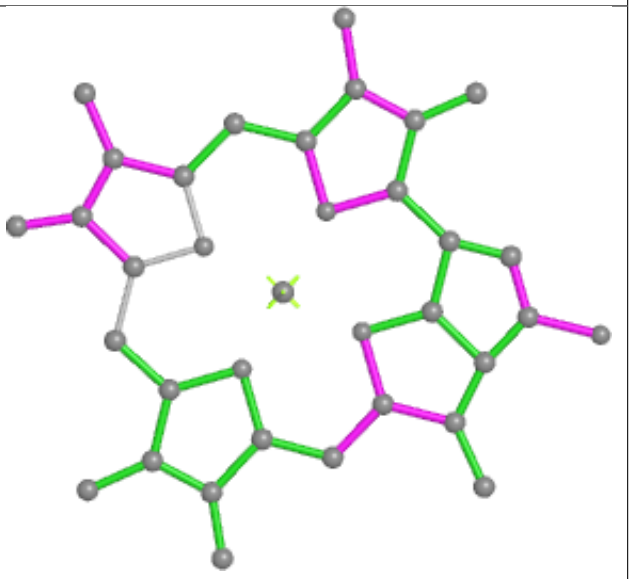
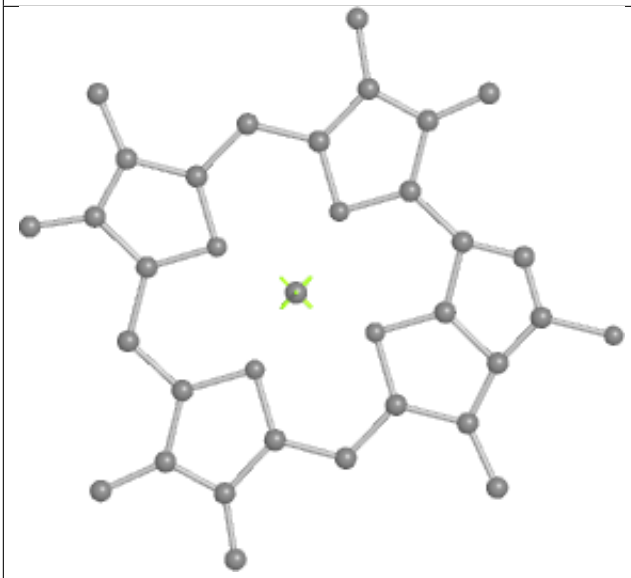
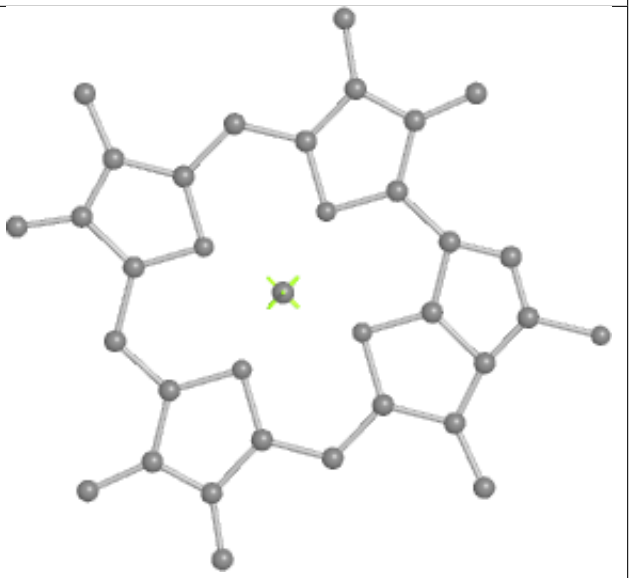


Bond angles

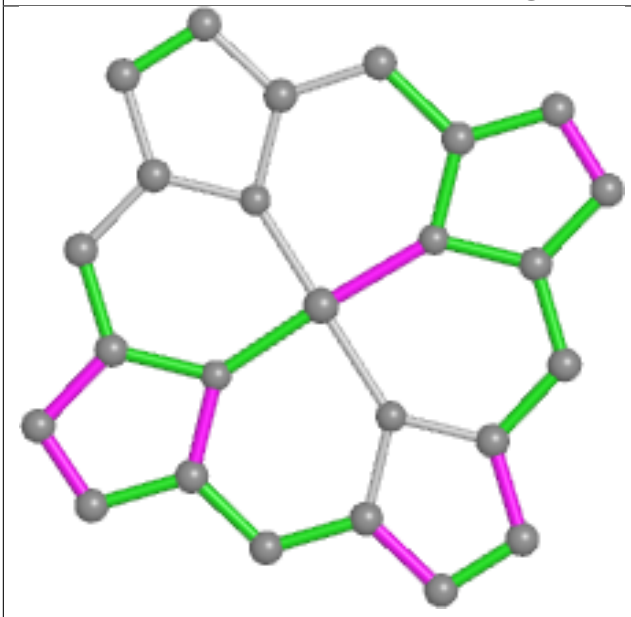


Torsions



Rings

Ligand HEM 0 138



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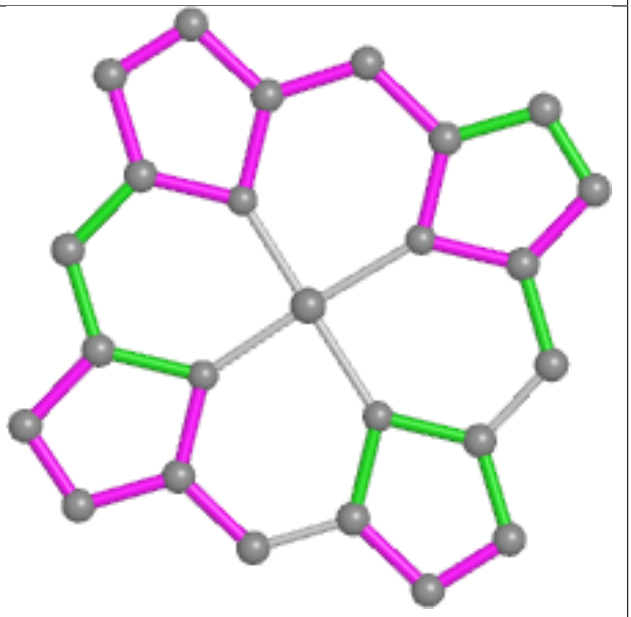

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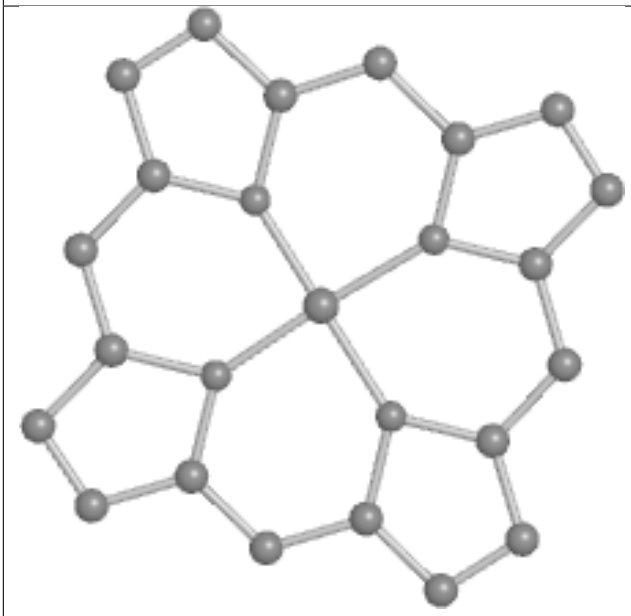
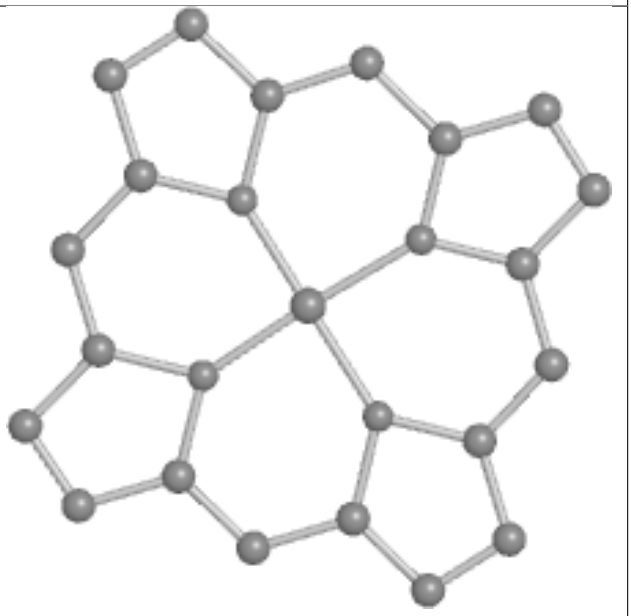
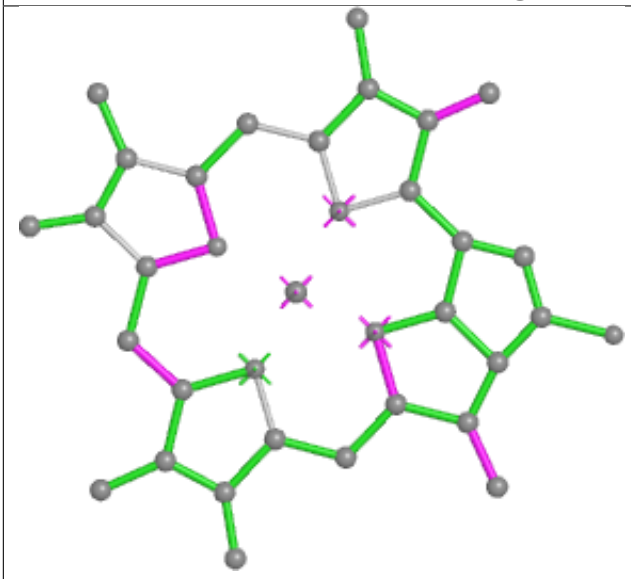


Torsions

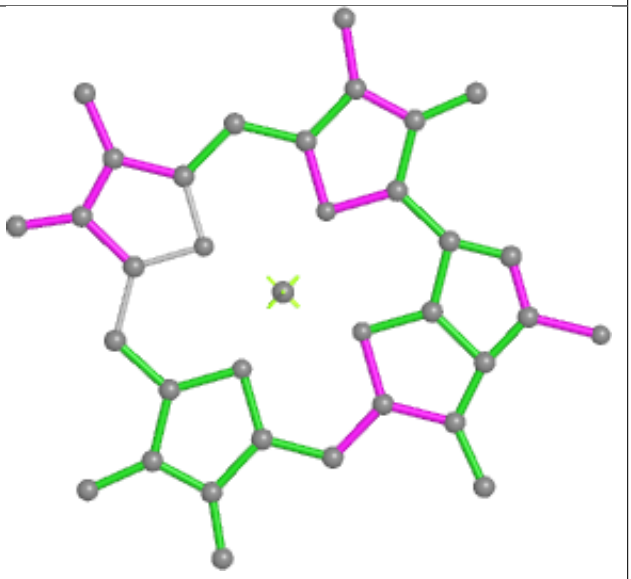


Rings

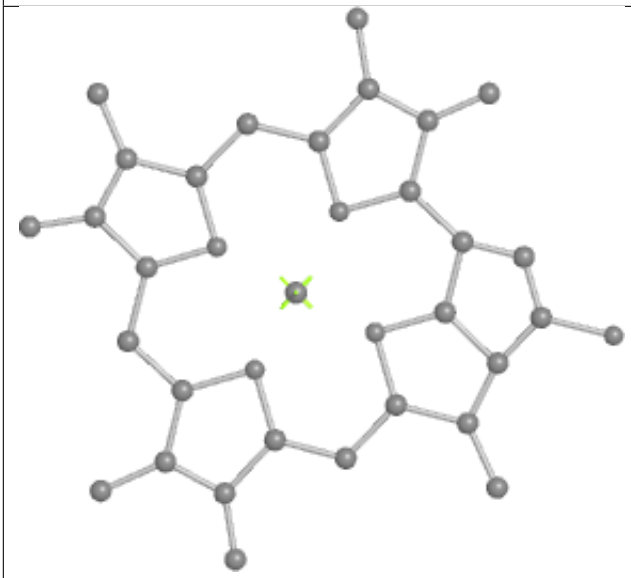
Ligand CLA M 1086



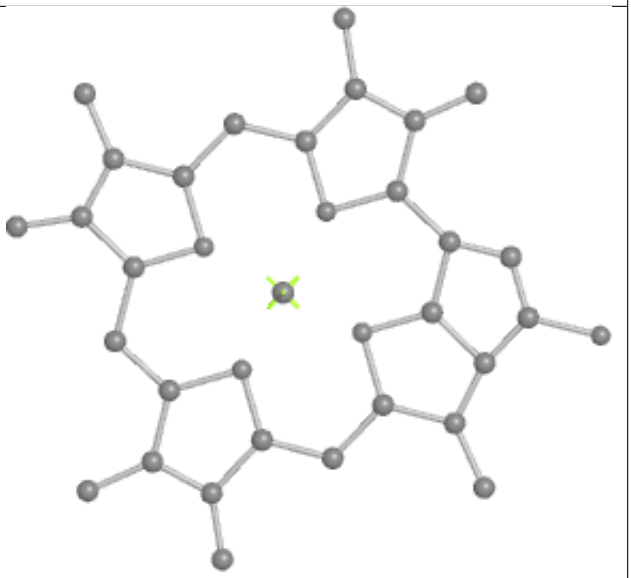
Bond lengths



Bond angles

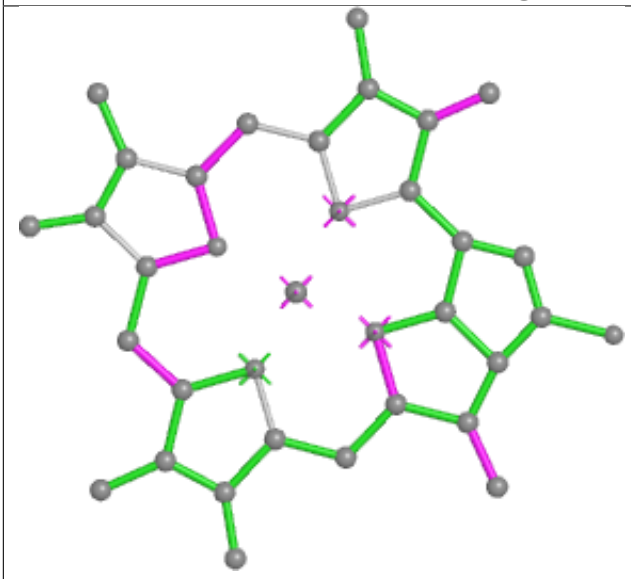


Torsions



Rings

Ligand CLA B 1116



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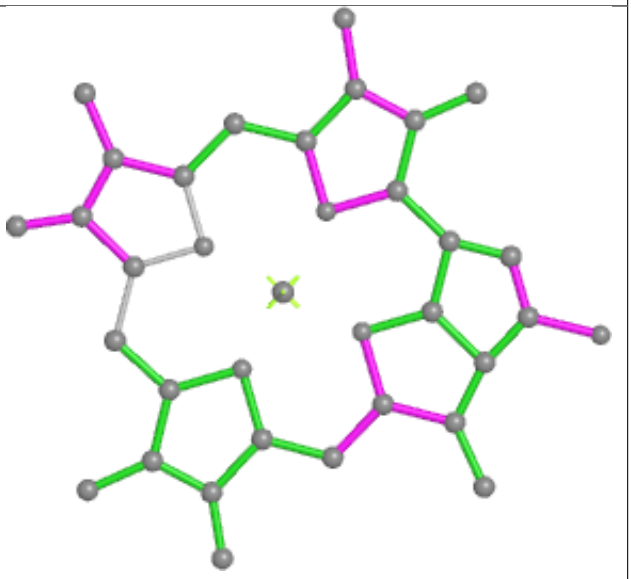
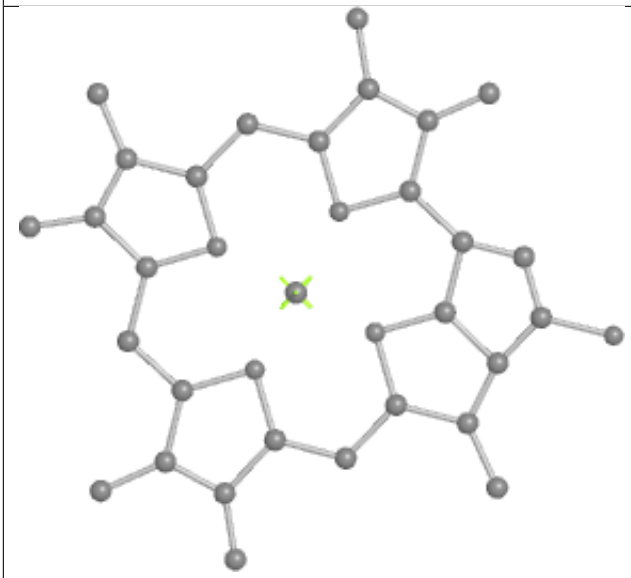
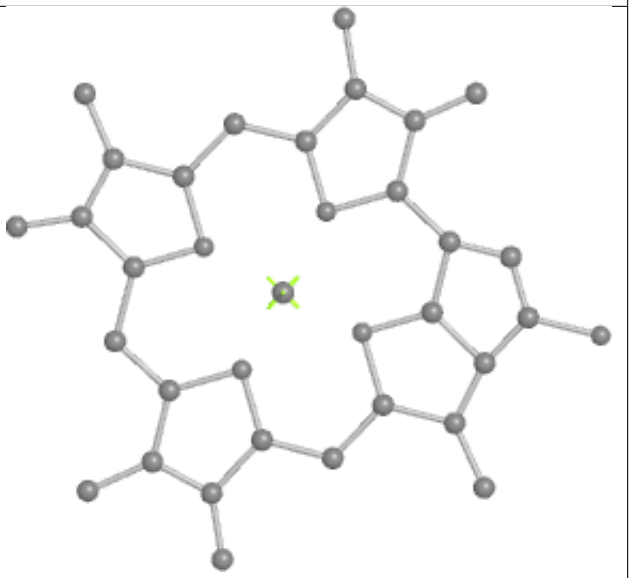


Bond angles

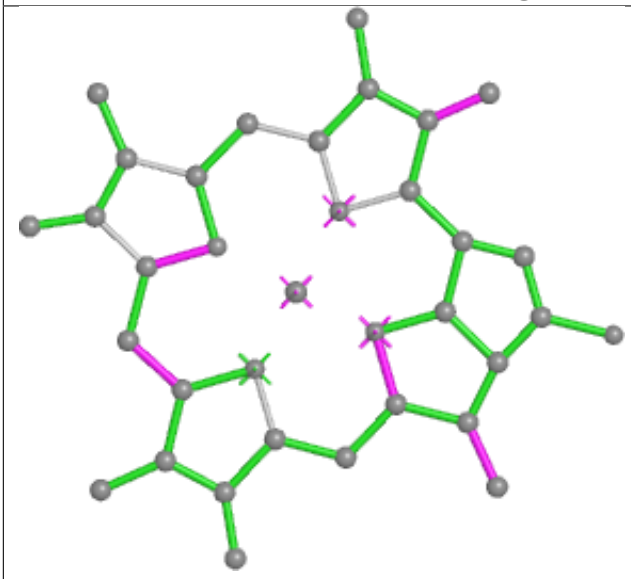


Torsions

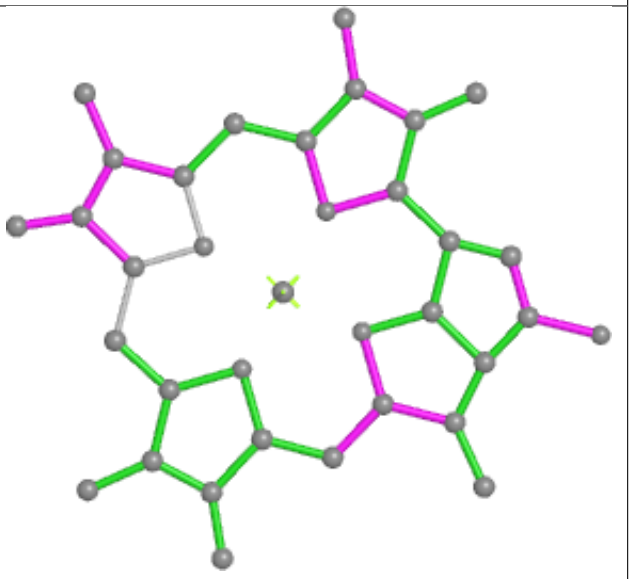


Rings

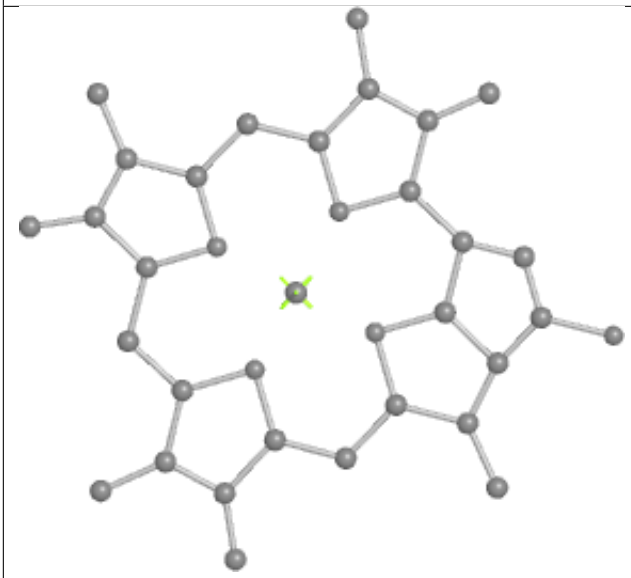
Ligand CLA B 1108



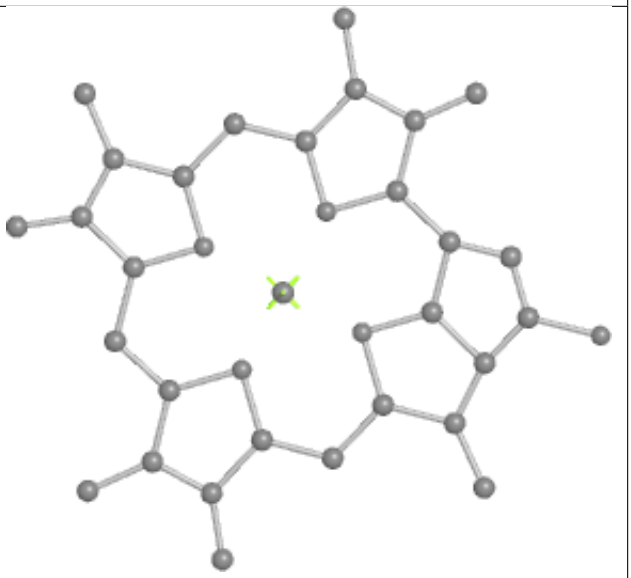
Bond lengths



Bond angles

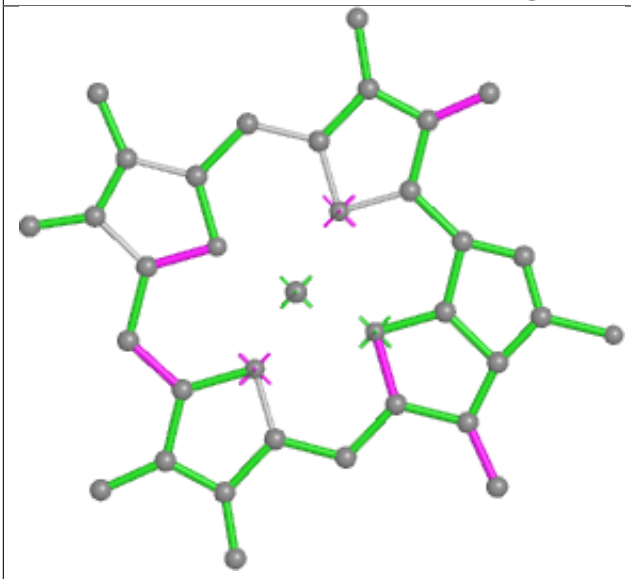


Torsions

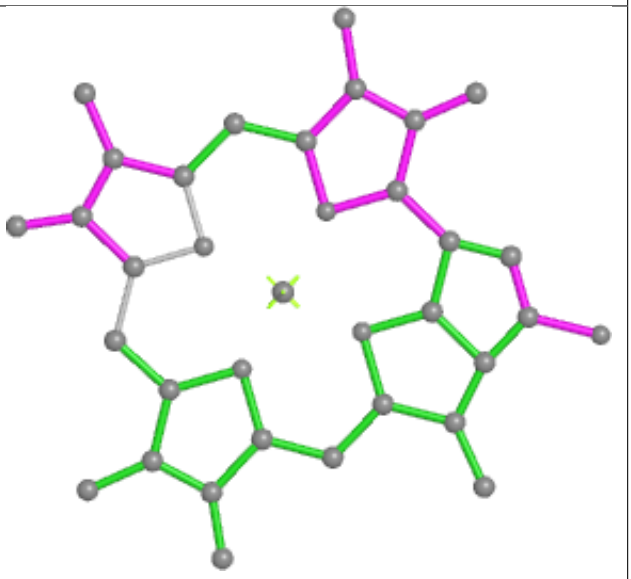


Rings

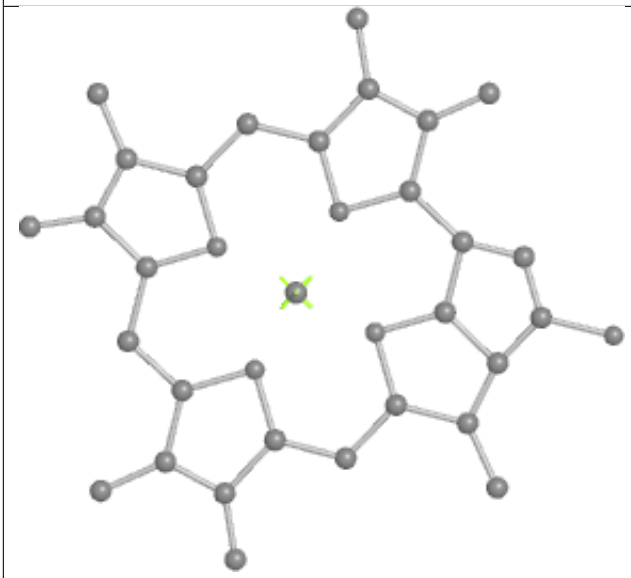
Ligand CLA D 355



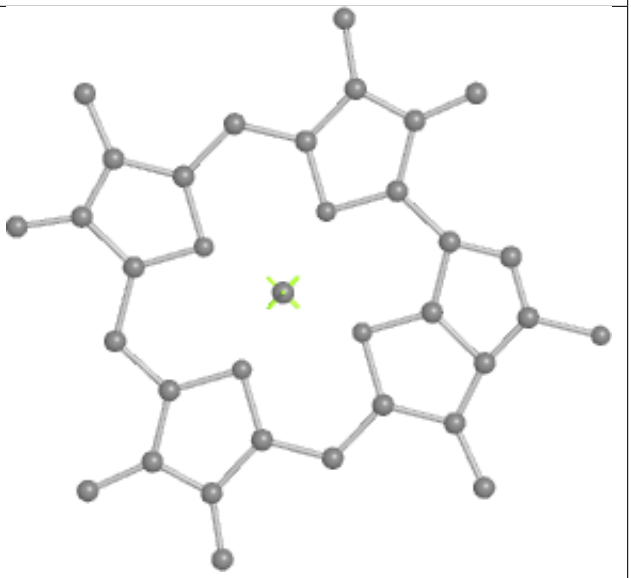
Bond lengths



Bond angles

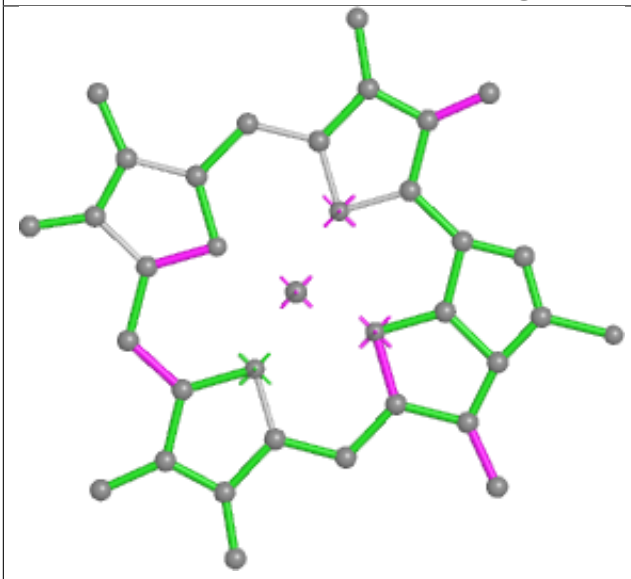


Torsions



Rings

Ligand CLA C 1086



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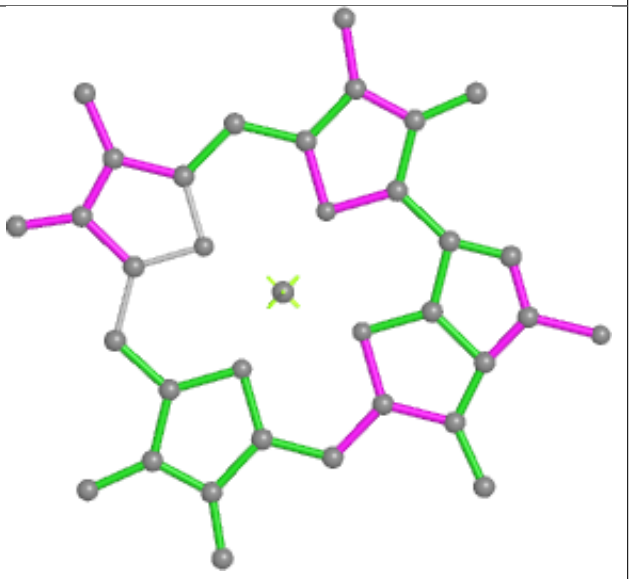
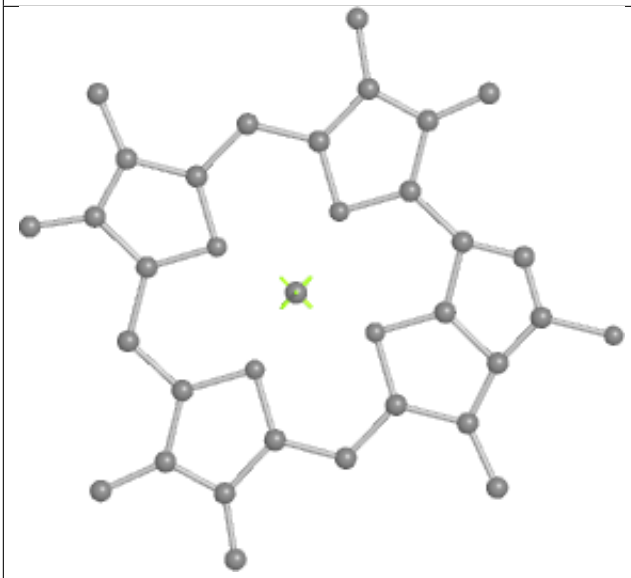
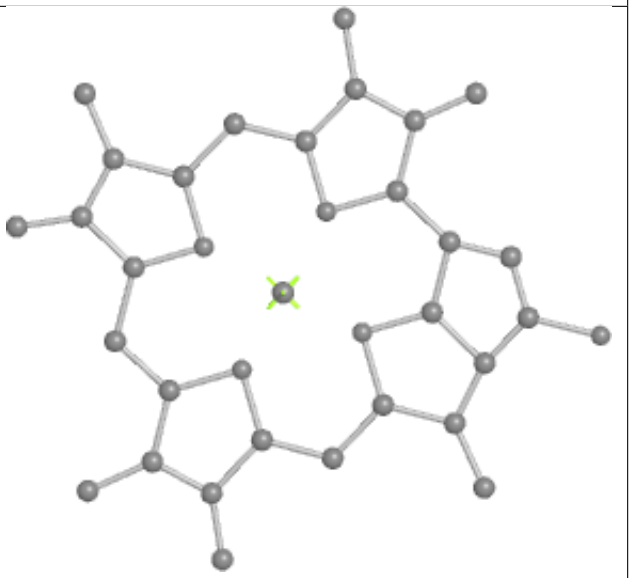


Bond angles

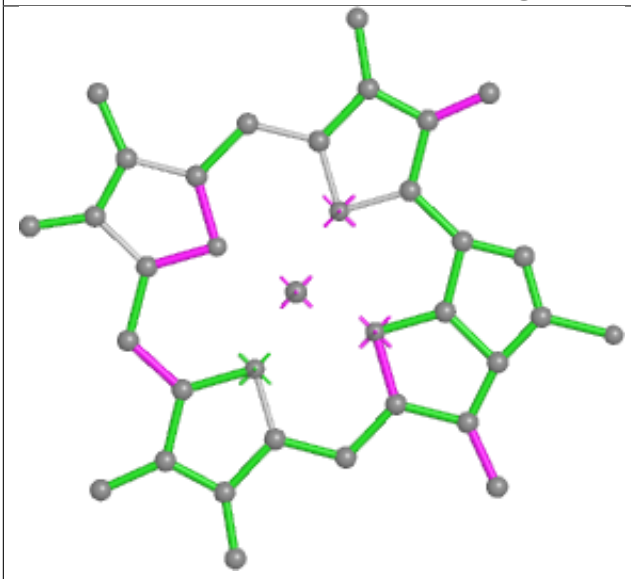


Torsions

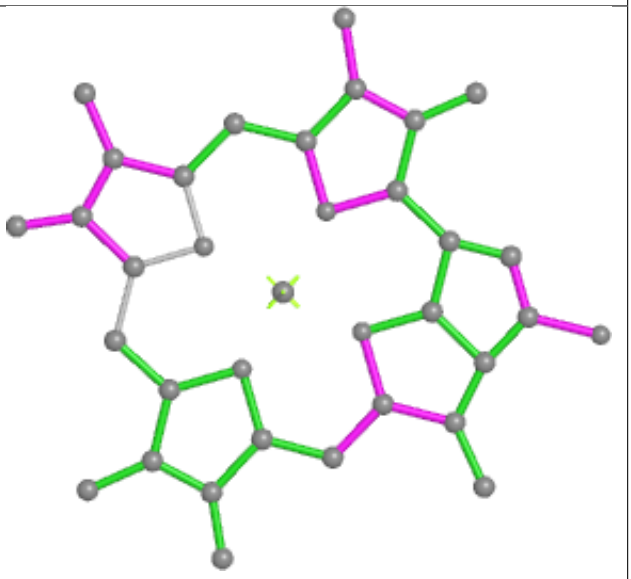


Rings

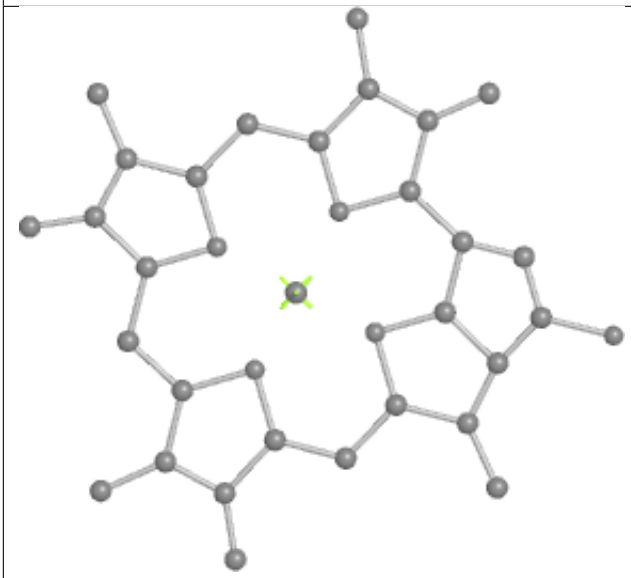
Ligand CLA B 1115



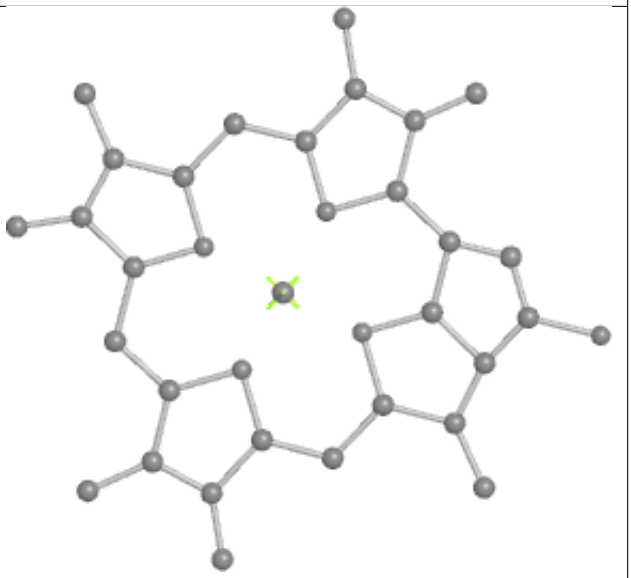
Bond lengths



Bond angles

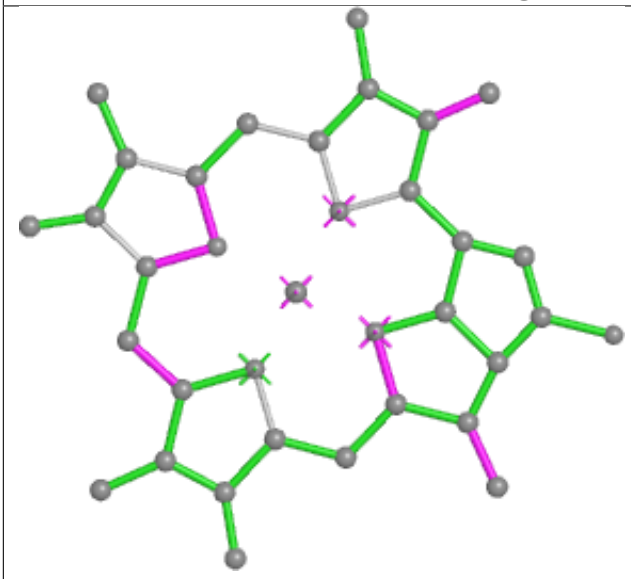


Torsions

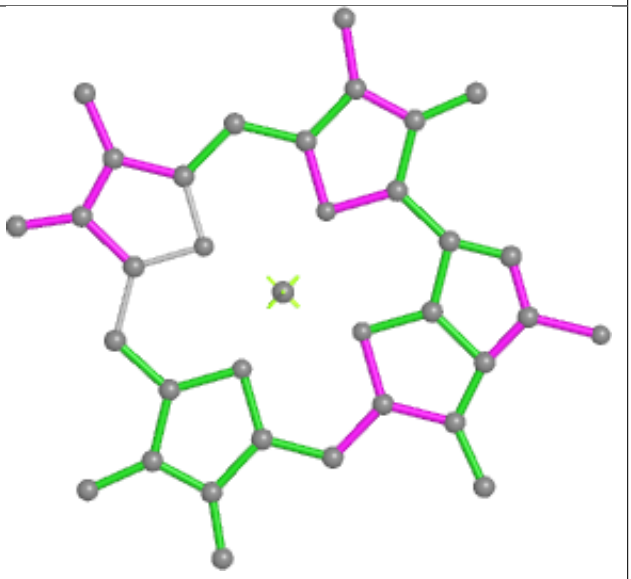


Rings

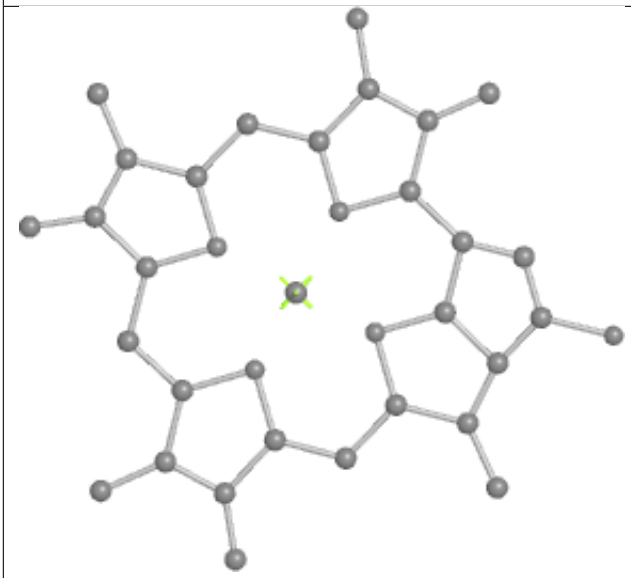
Ligand CLA C 1084



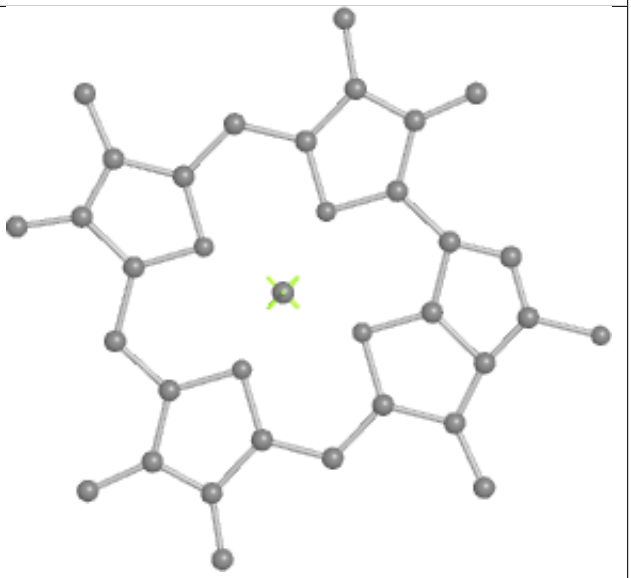
Bond lengths



Bond angles

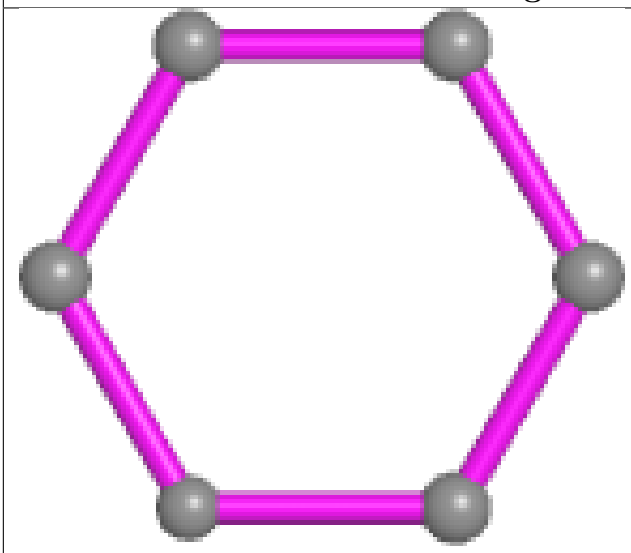


Torsions

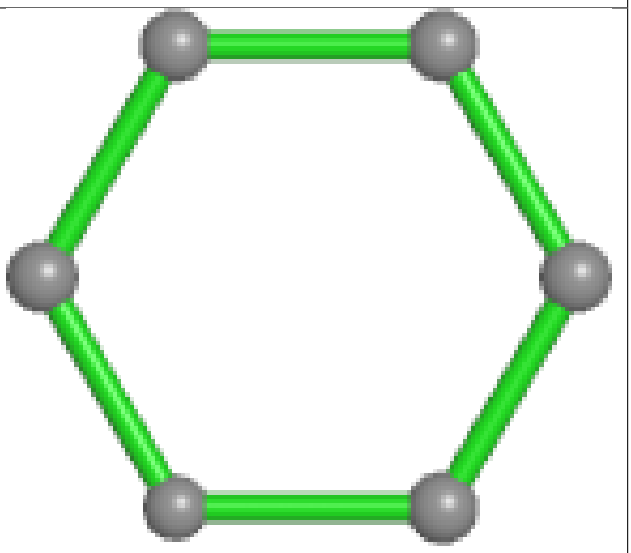


Rings

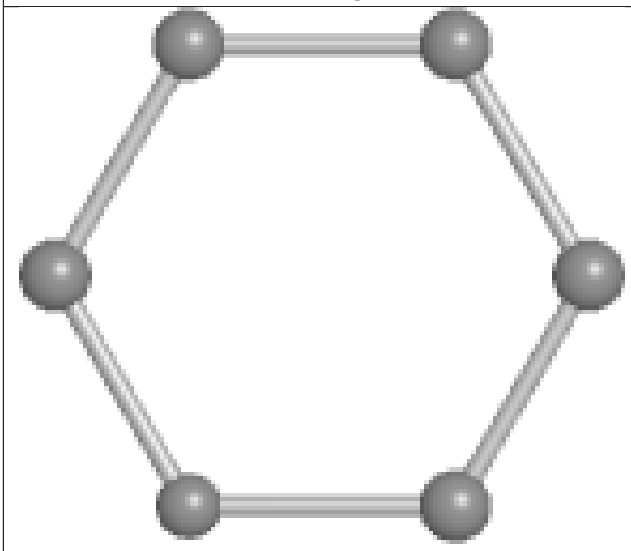
Ligand PLA N 359



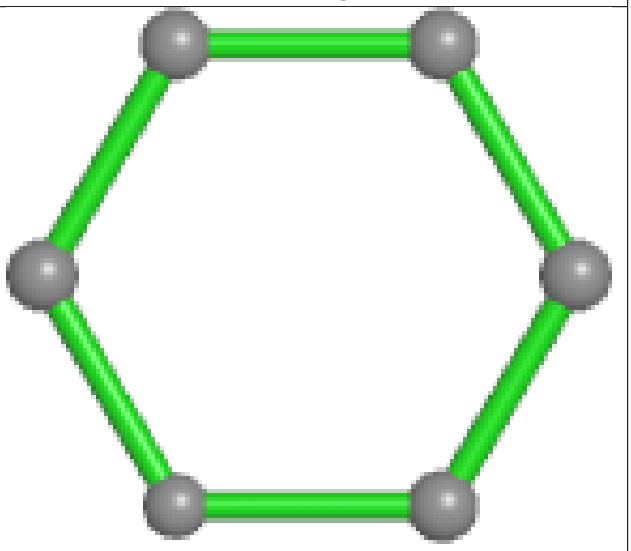
Bond lengths



Bond angles

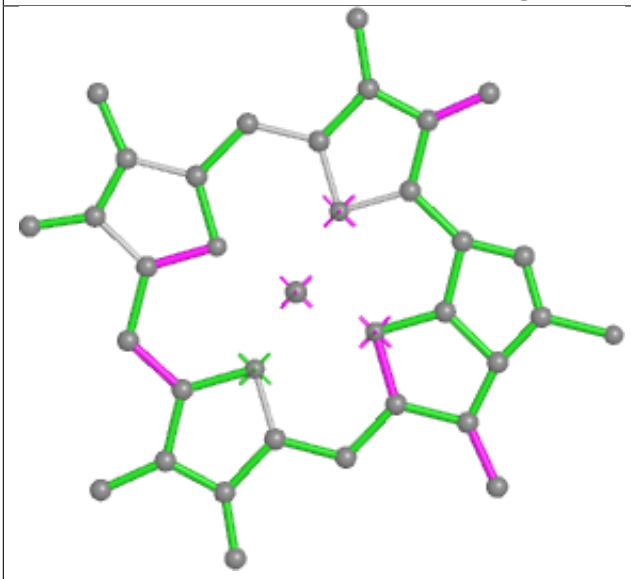


Torsions

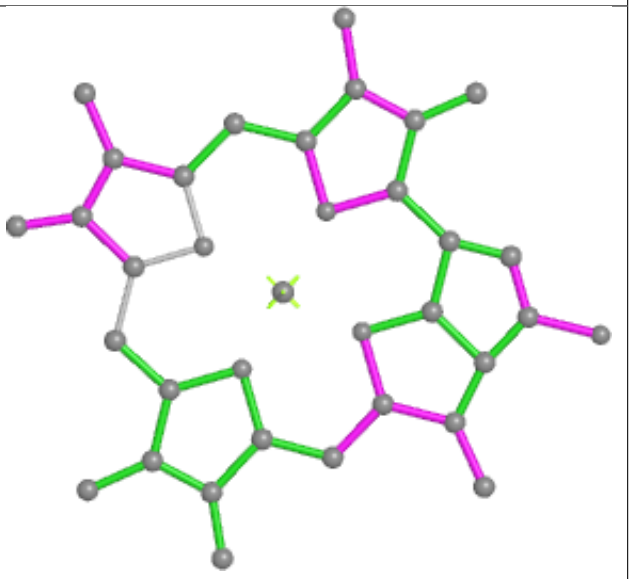


Rings

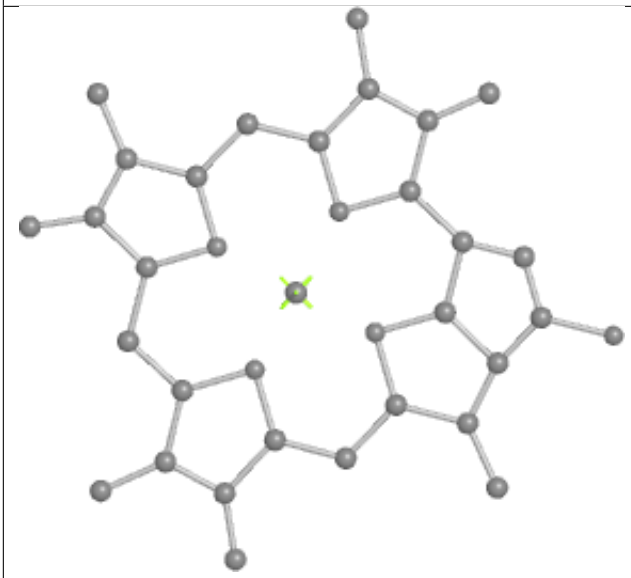
Ligand CLA C 1079



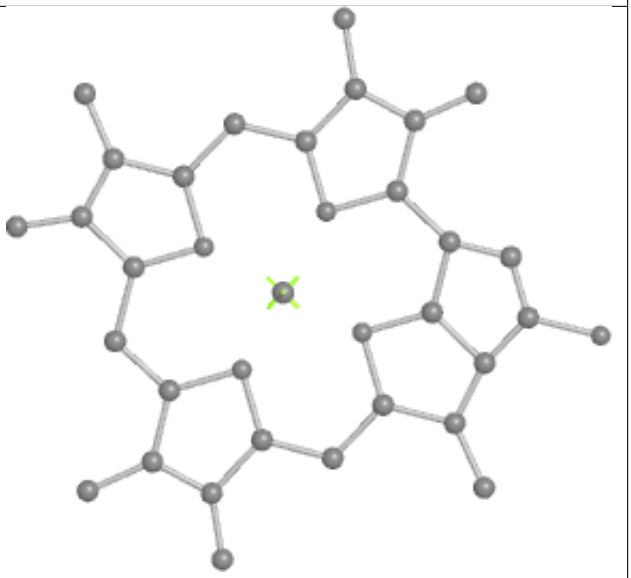
Bond lengths



Bond angles

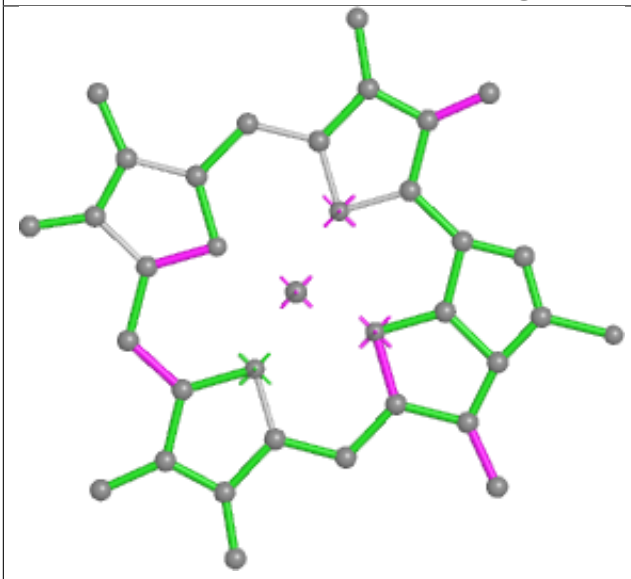


Torsions

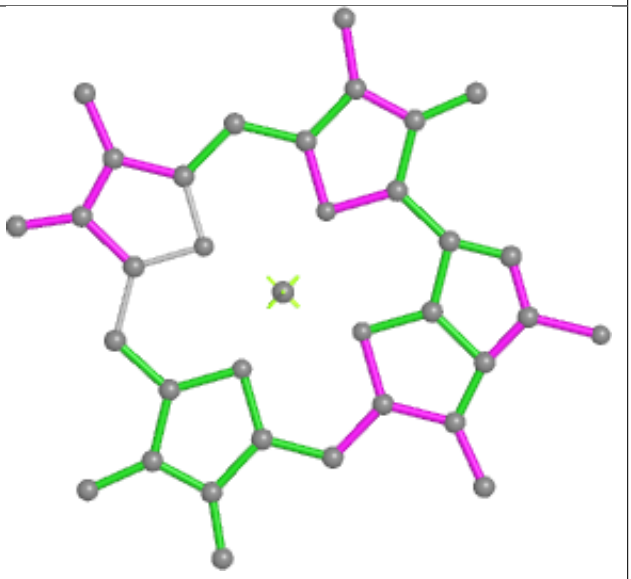


Rings

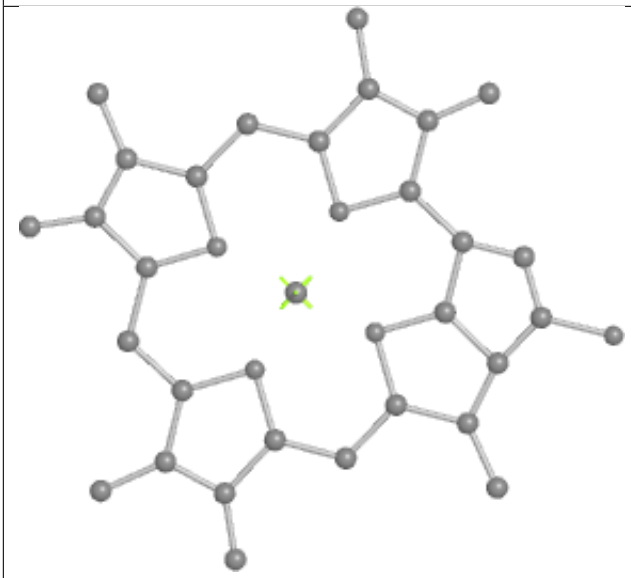
Ligand CLA B 1114



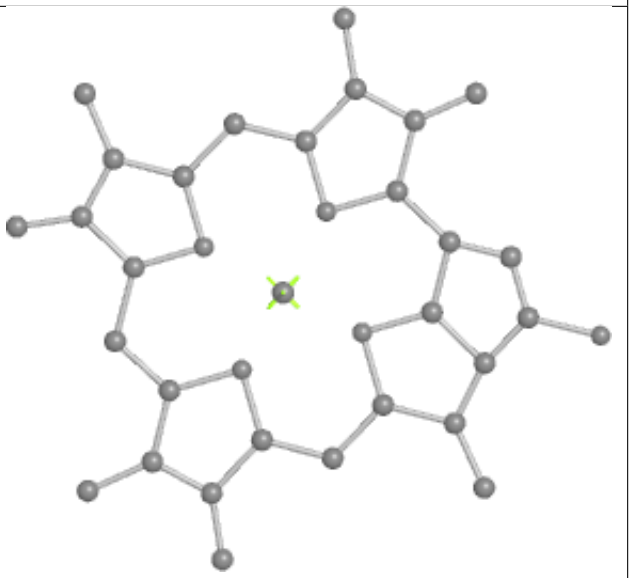
Bond lengths



Bond angles

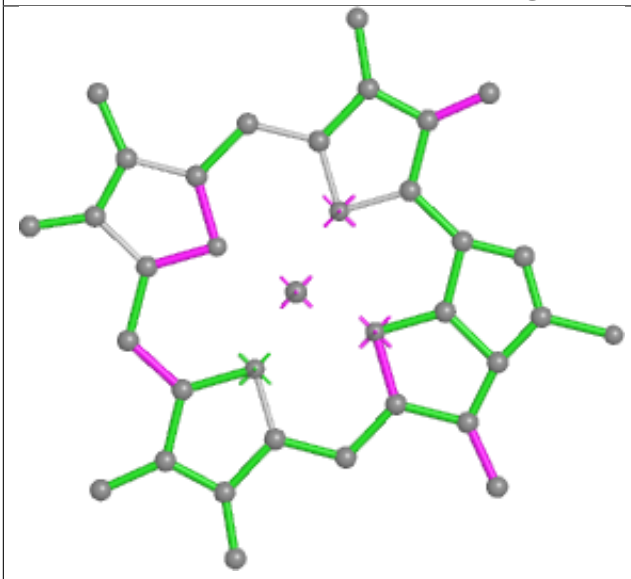


Torsions

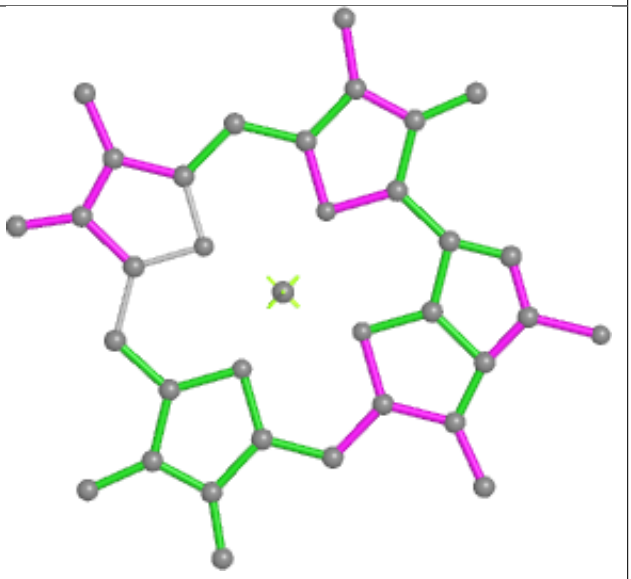


Rings

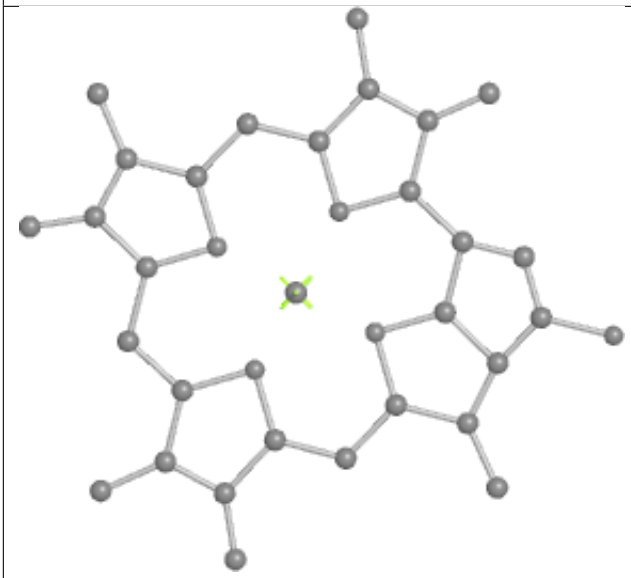
Ligand CLA A 369



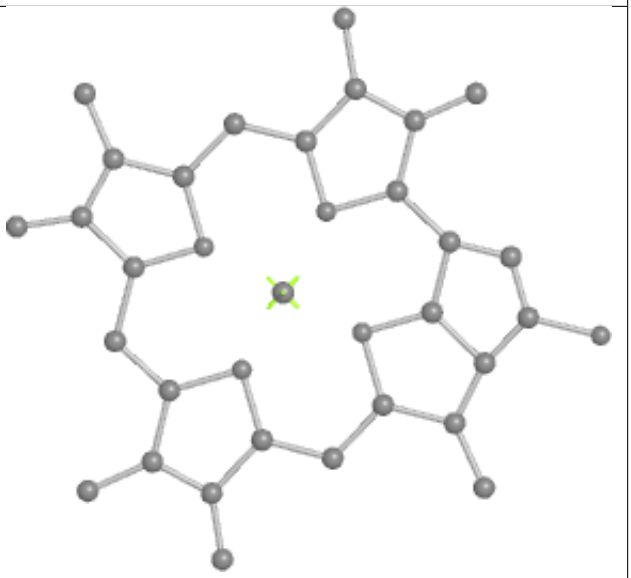
Bond lengths



Bond angles

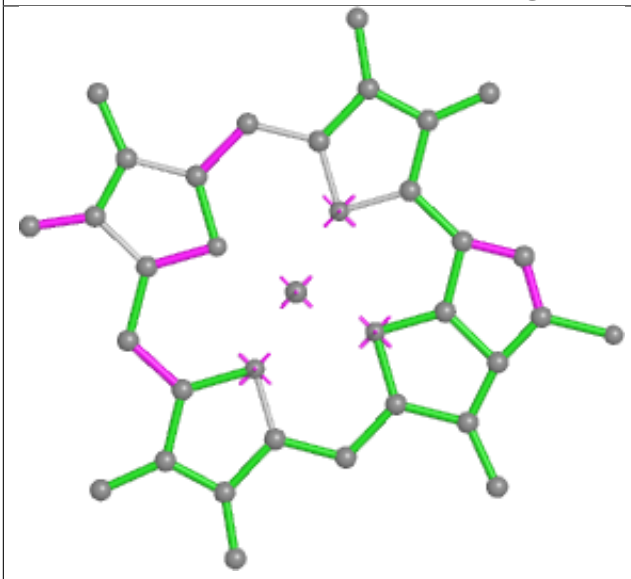


Torsions

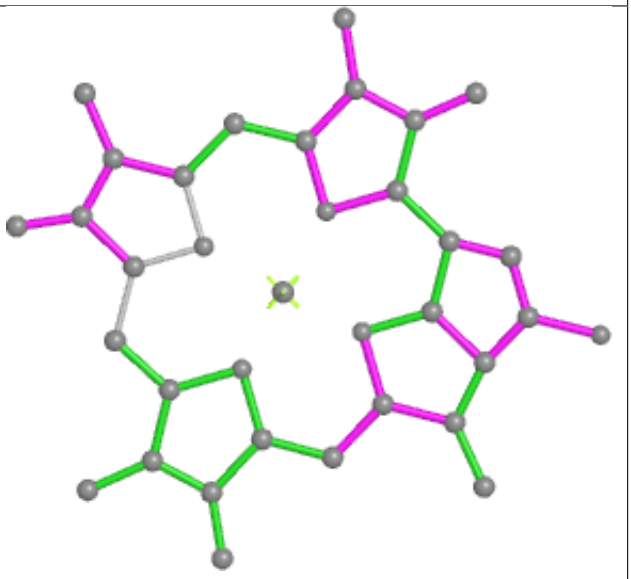


Rings

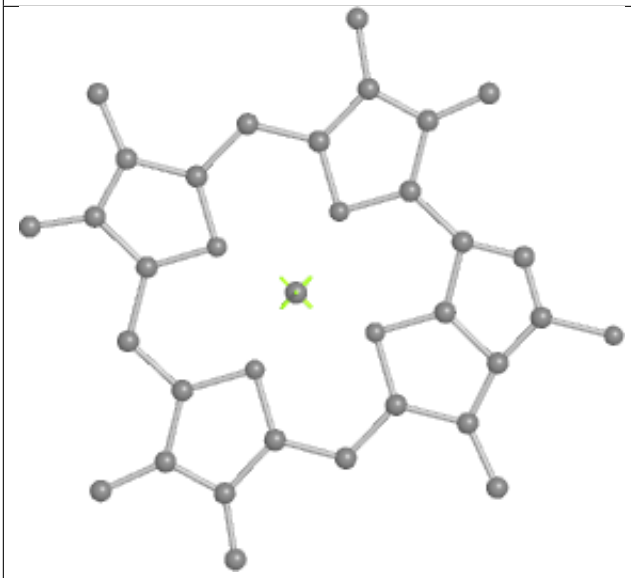
Ligand CLA A 365



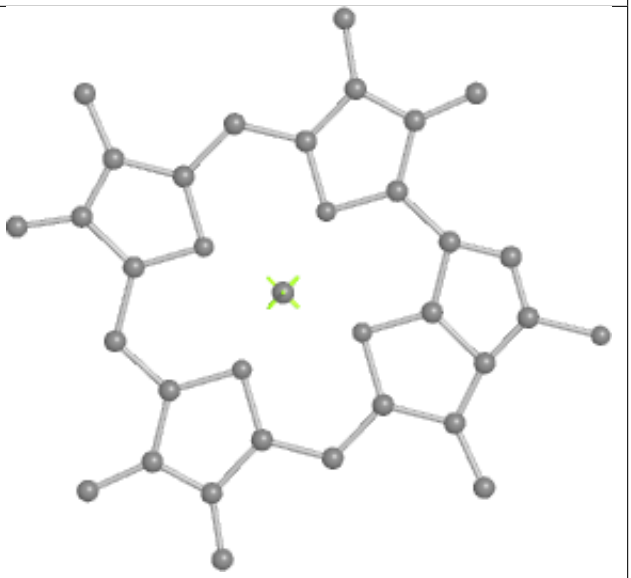
Bond lengths



Bond angles

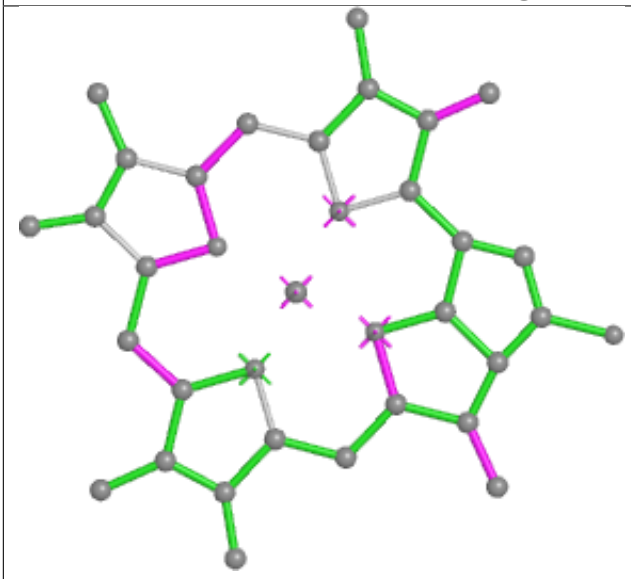


Torsions



Rings

Ligand CLA B 1119



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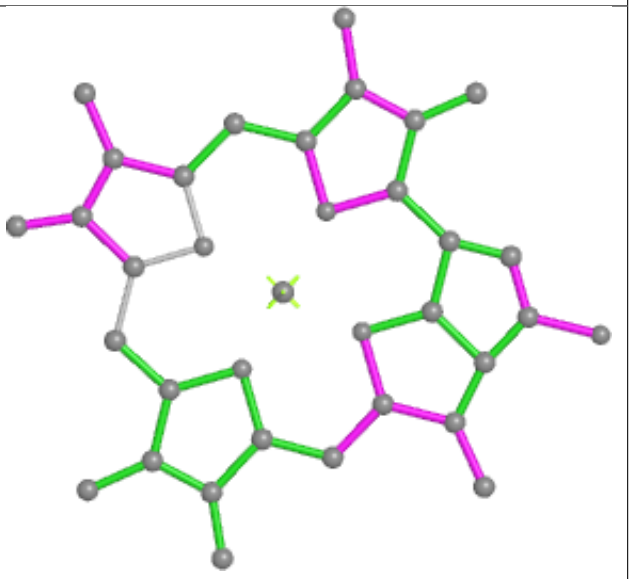
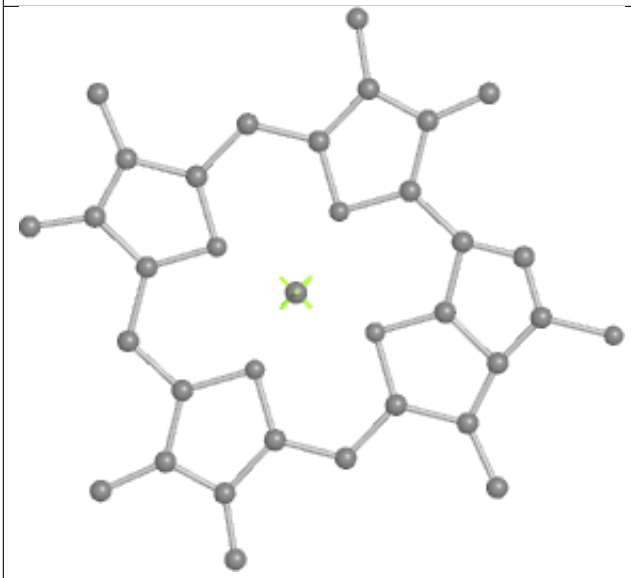
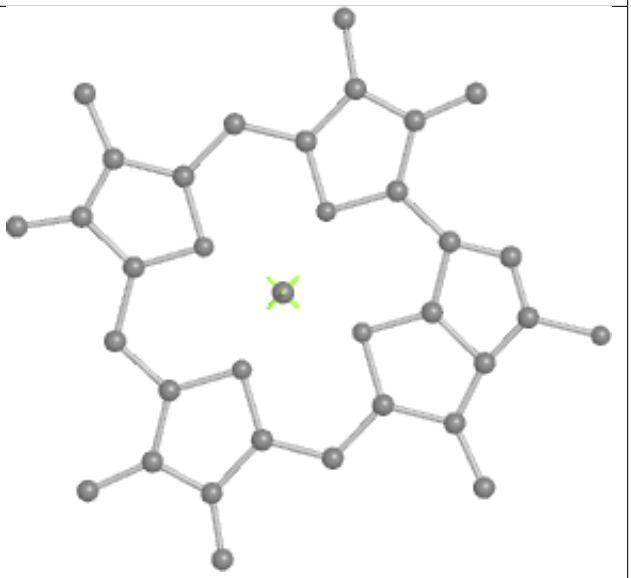


Bond angles

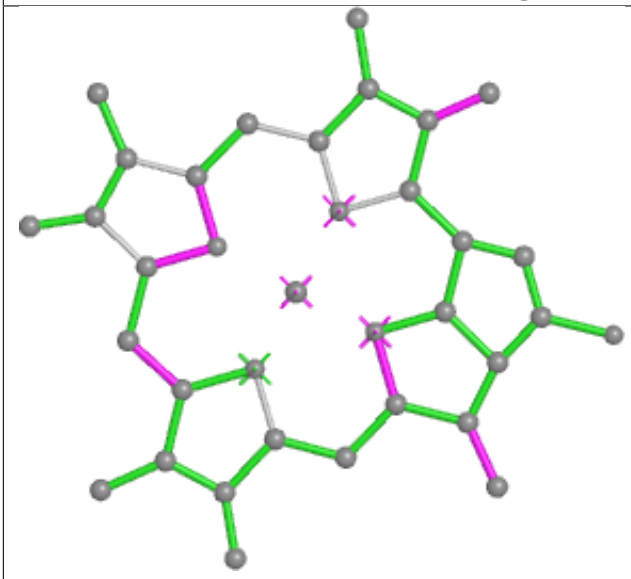


Torsions

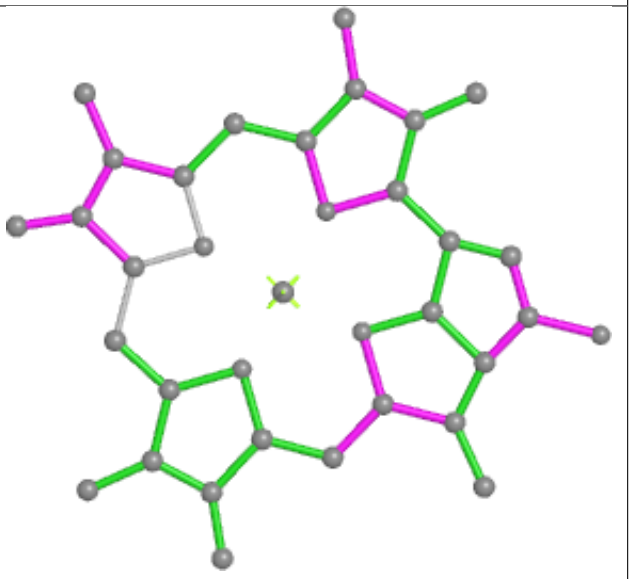


Rings

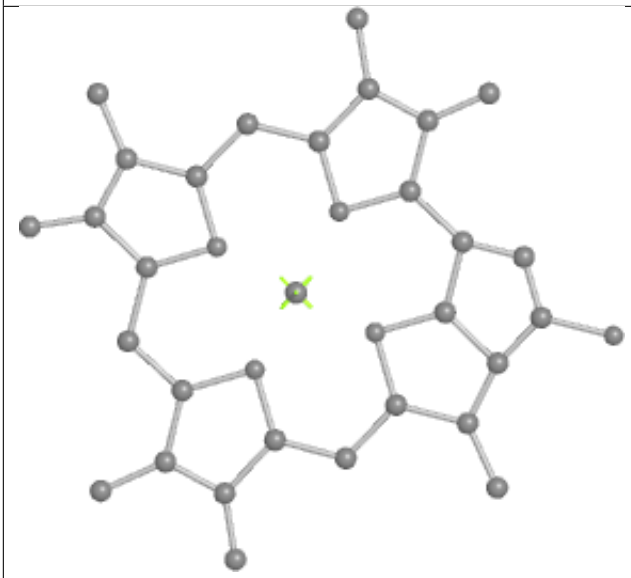
Ligand CLA C 1089



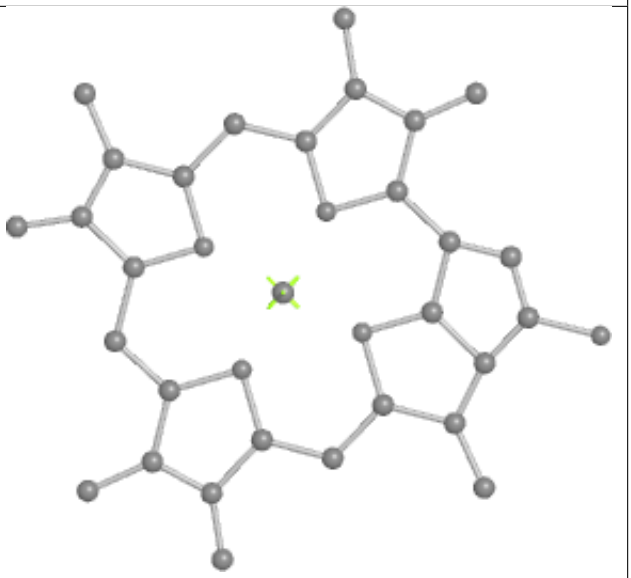
Bond lengths



Bond angles

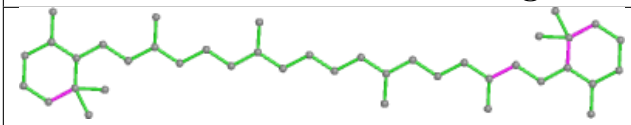


Torsions



Rings

Ligand BCR D 359



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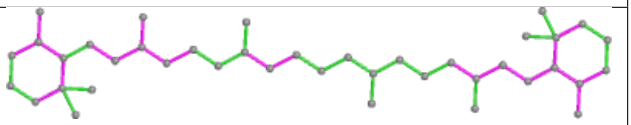
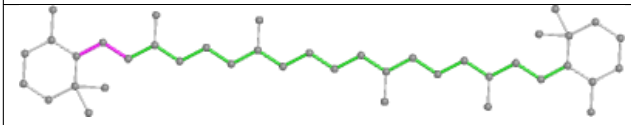
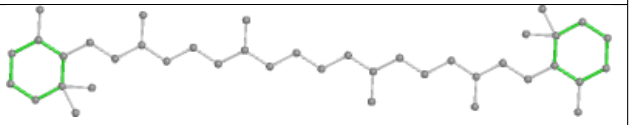


Bond angles

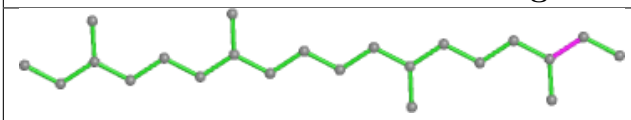


Torsions

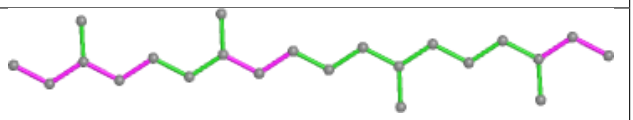


Rings

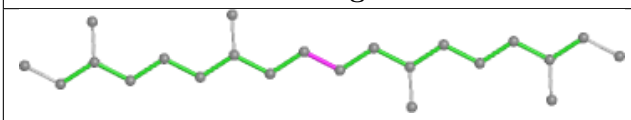
Ligand BCR K 47



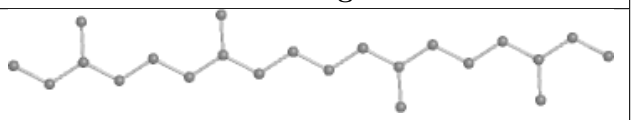
Bond lengths



Bond angles

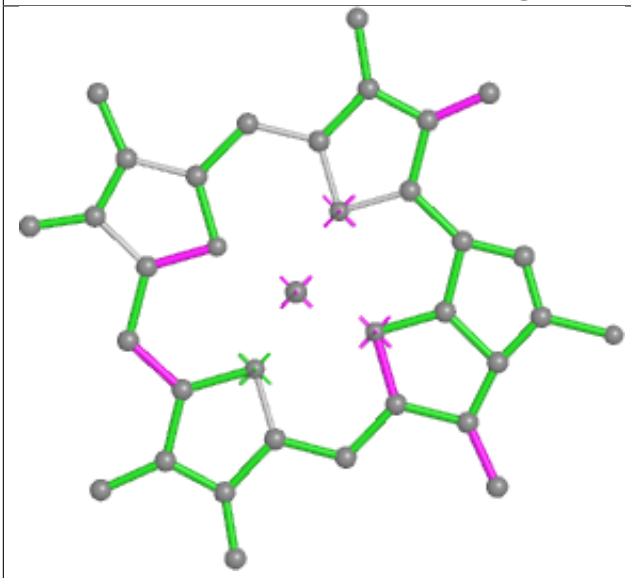


Torsions

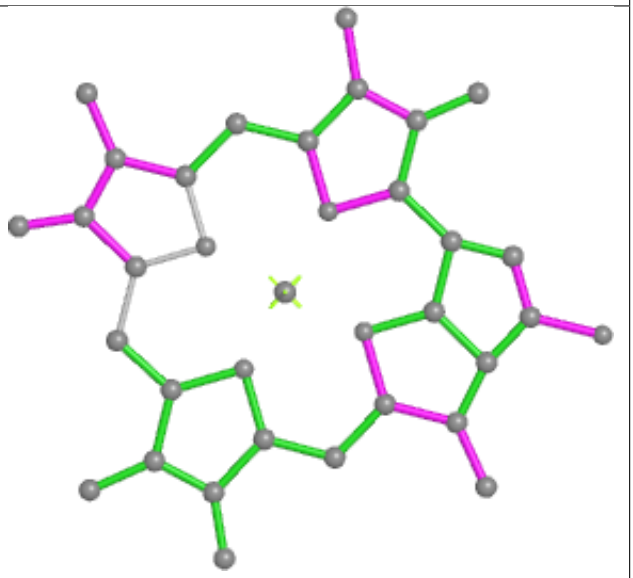


Rings

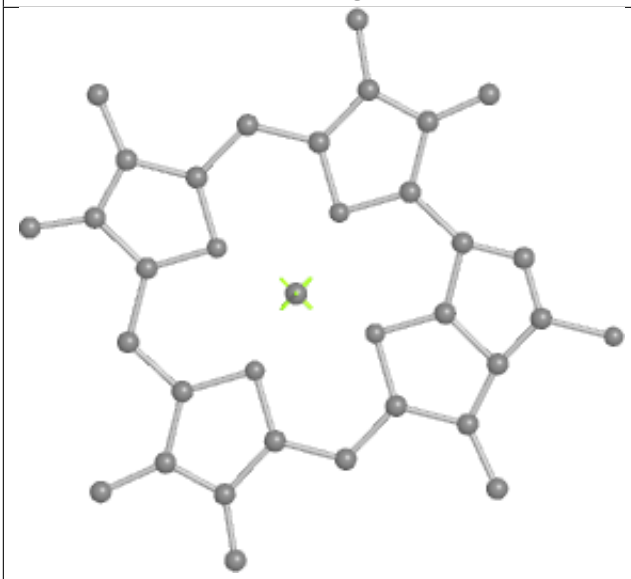
Ligand CLA C 1085



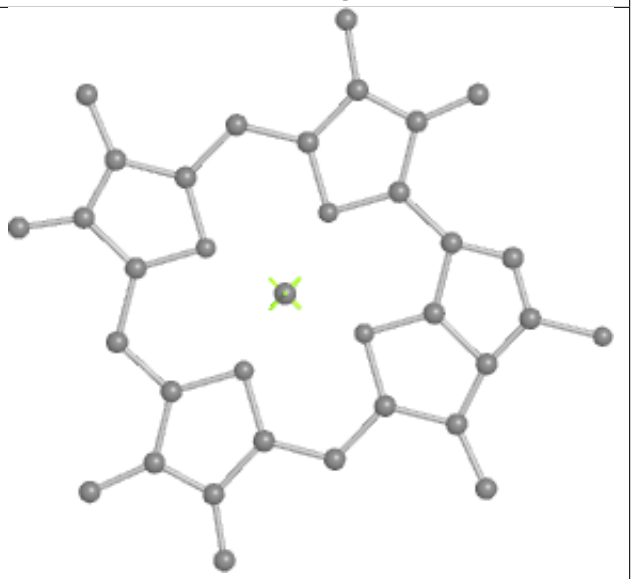
Bond lengths



Bond angles

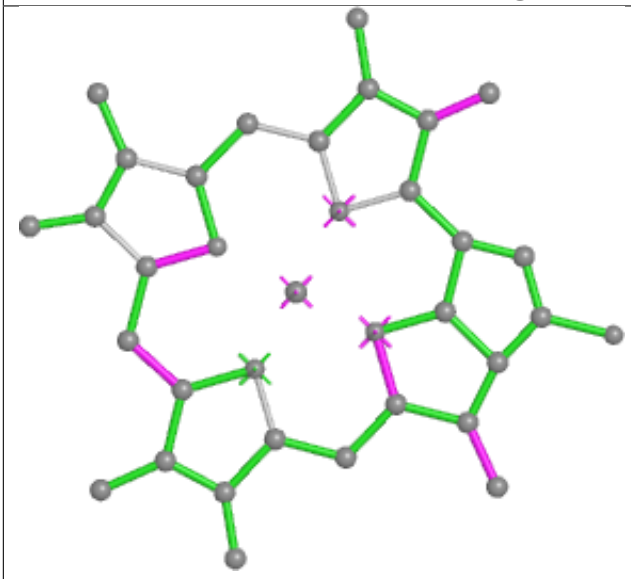


Torsions



Rings

Ligand CLA M 1085



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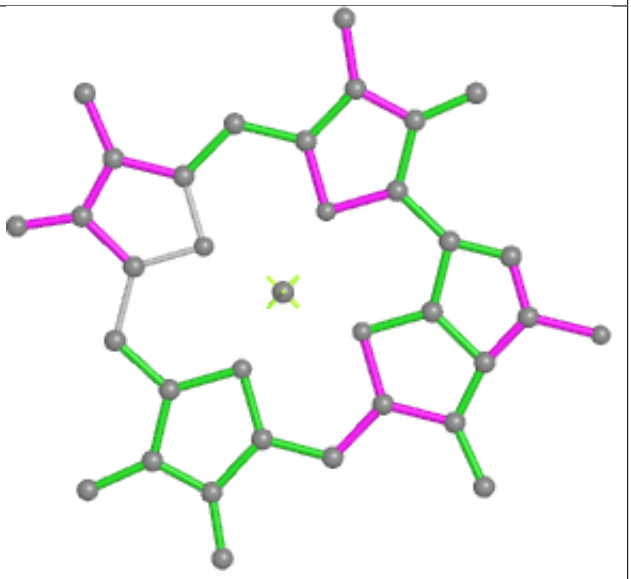
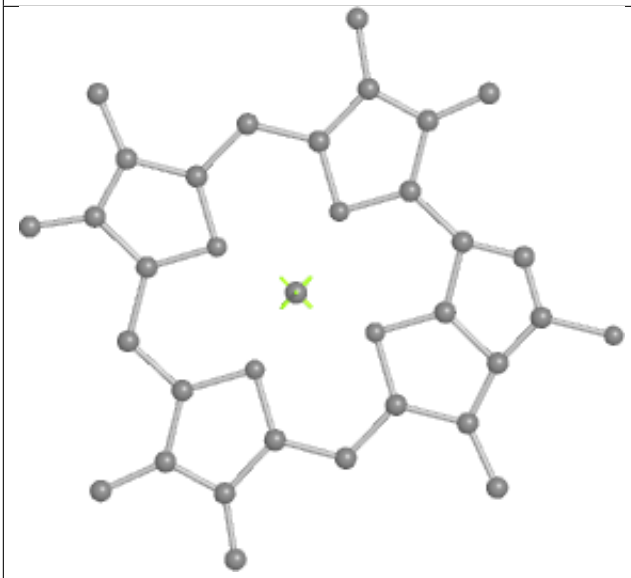


Bond angles



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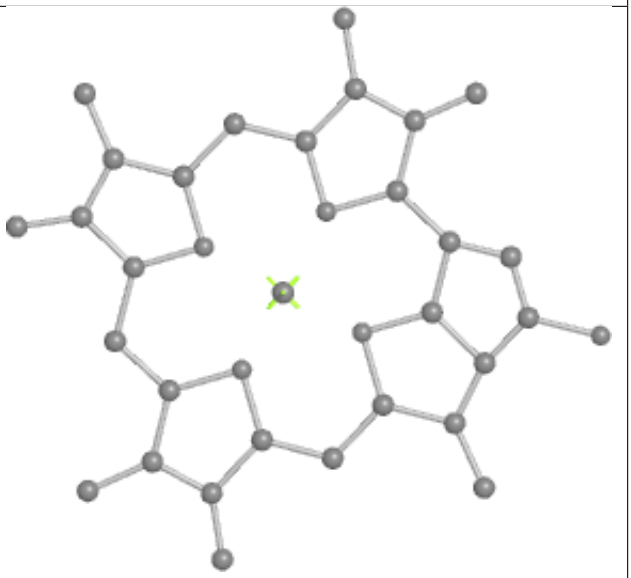
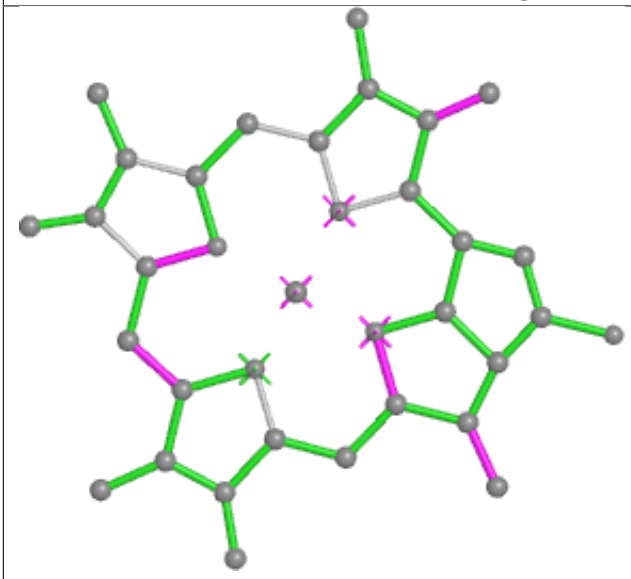


Rings

Ligand CLA C 1087



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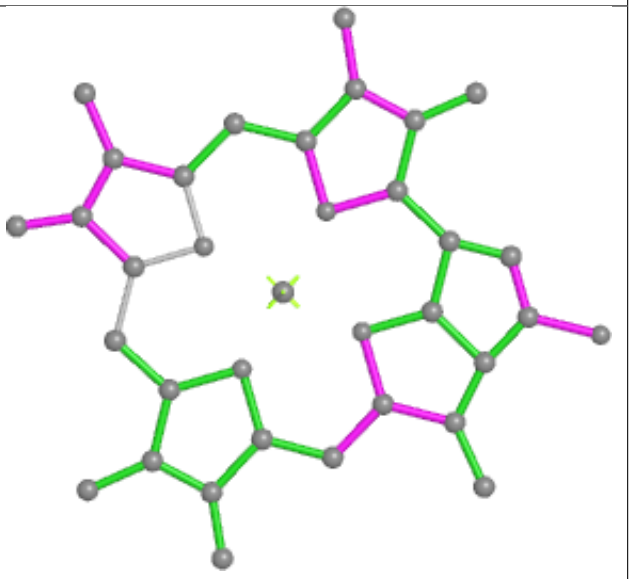
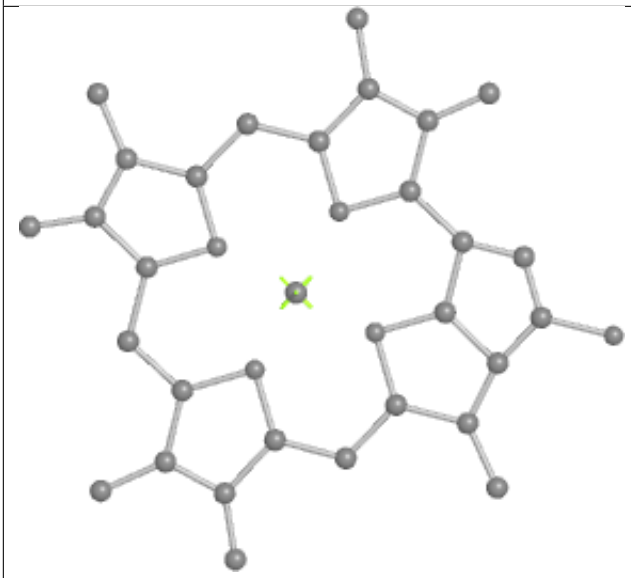
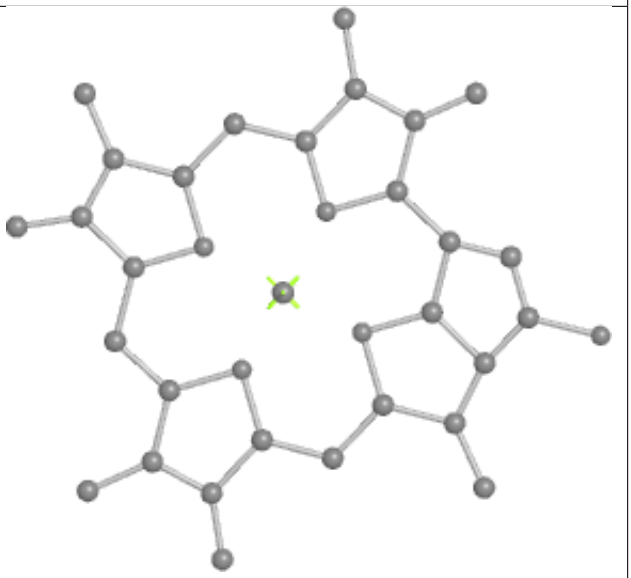


Bond angles

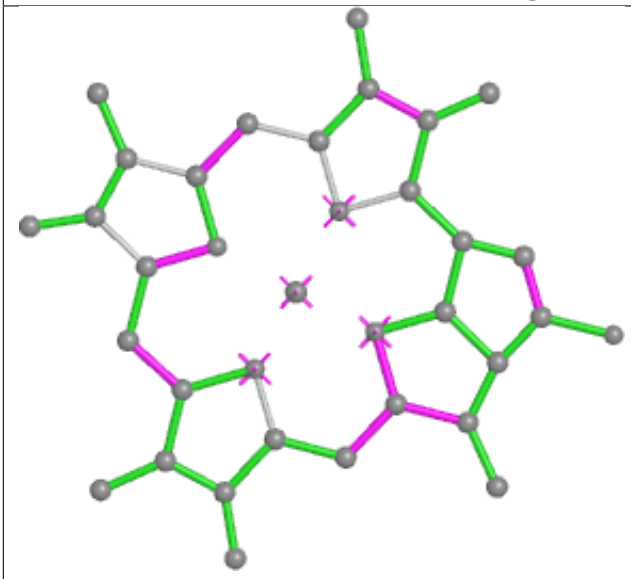


Torsions

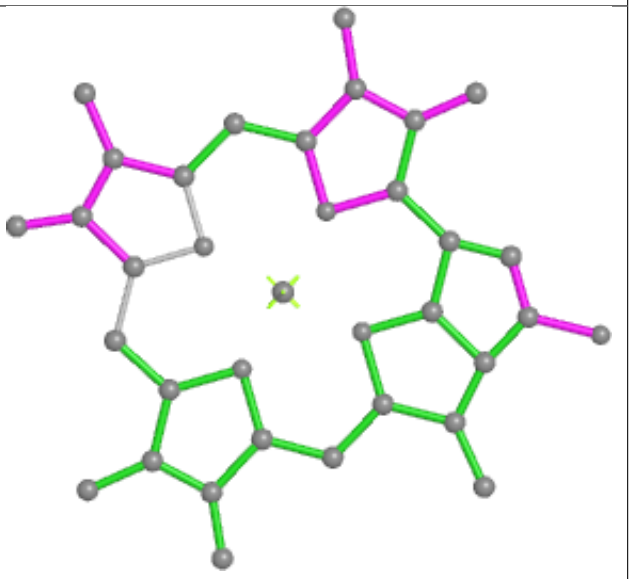


Rings

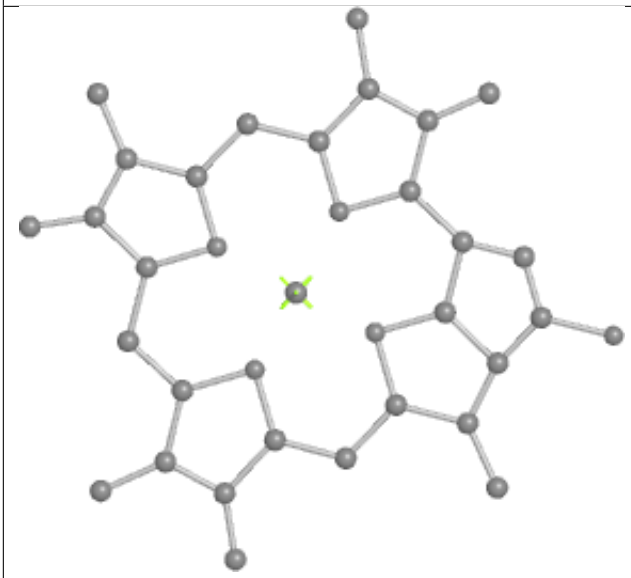
Ligand CLA A 366



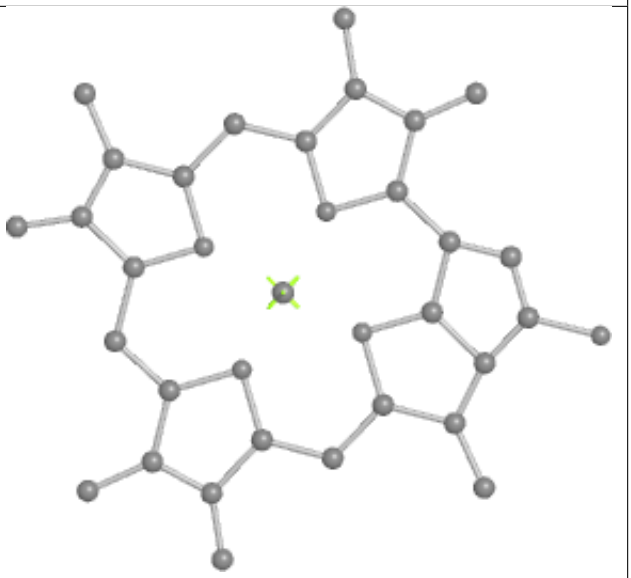
Bond lengths



Bond angles

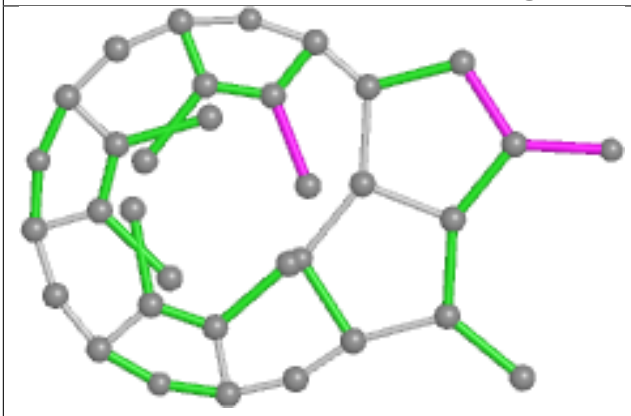


Torsions

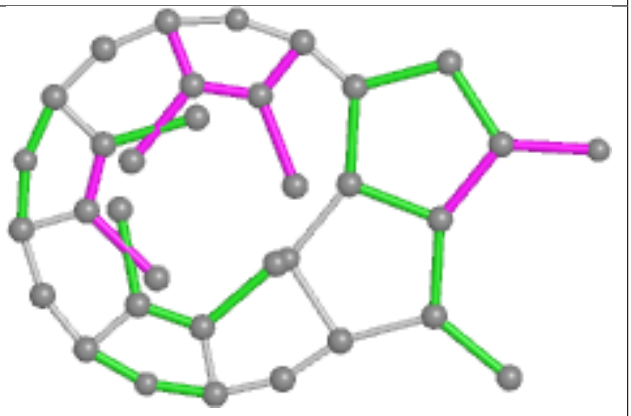


Rings

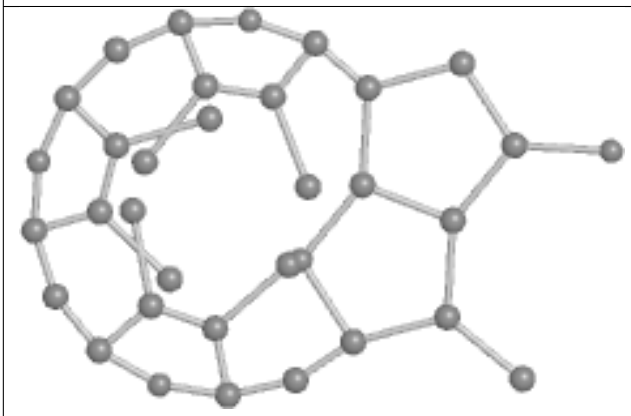
Ligand PHO N 357



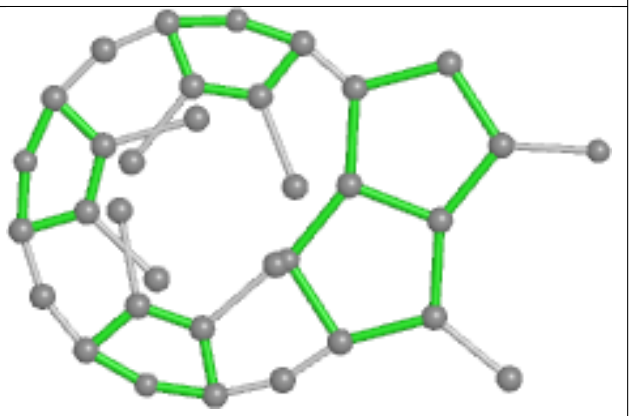
Bond lengths



Bond angles

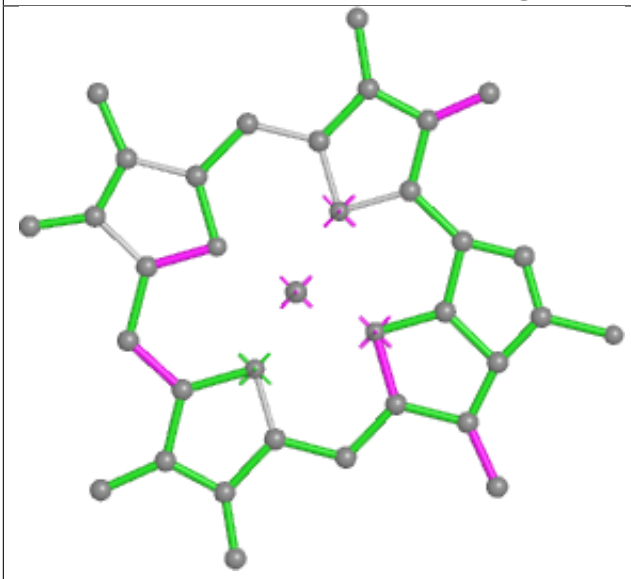


Torsions

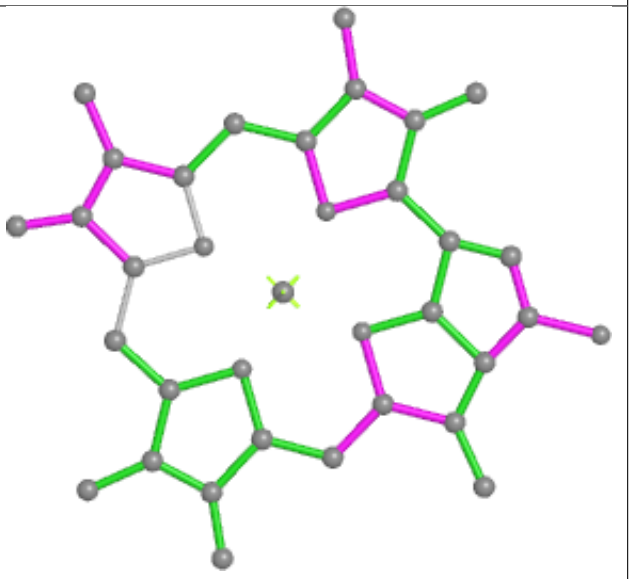


Rings

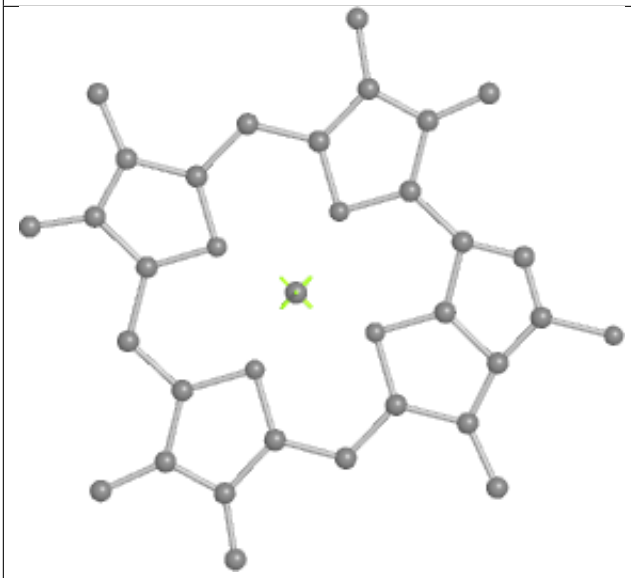
Ligand CLA B 1120



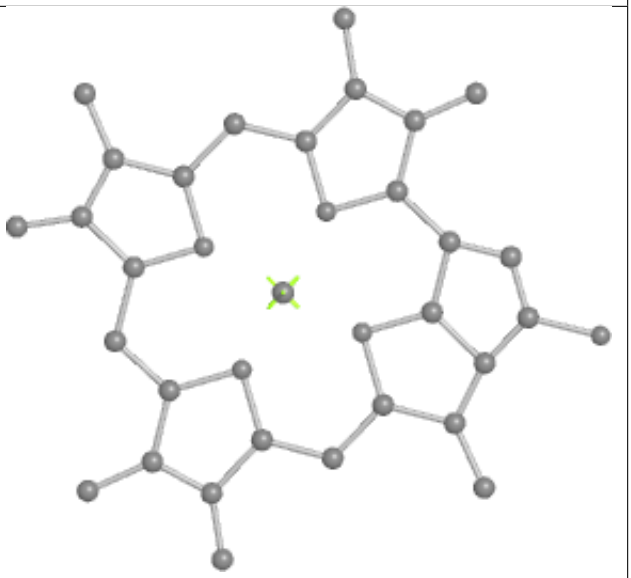
Bond lengths



Bond angles

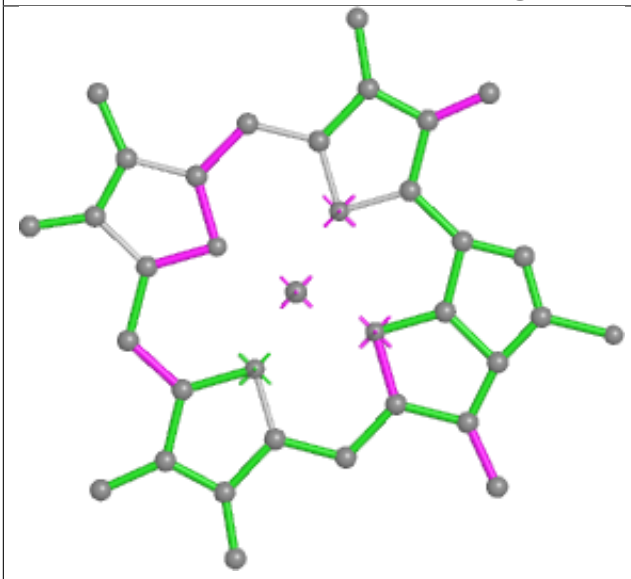


Torsions



Rings

Ligand CLA M 1088



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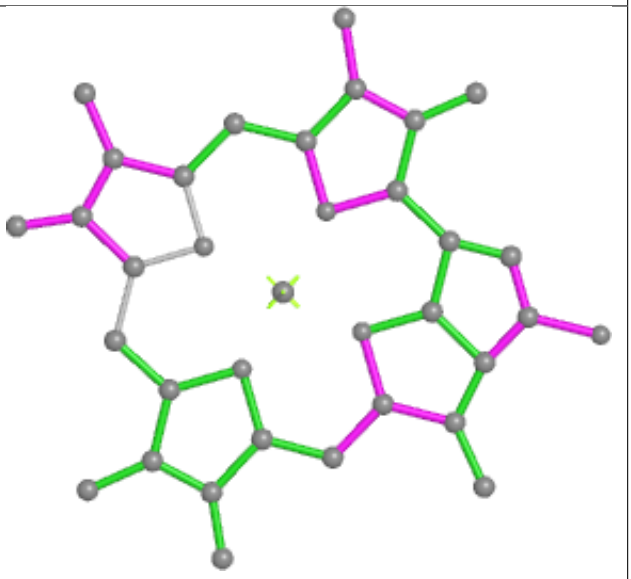
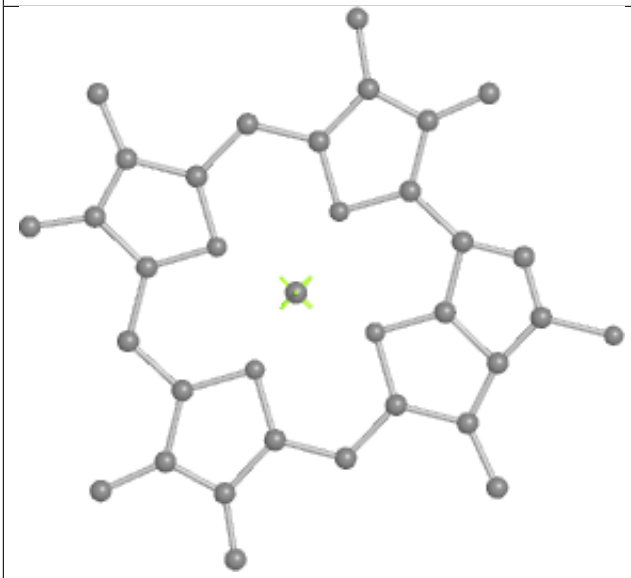
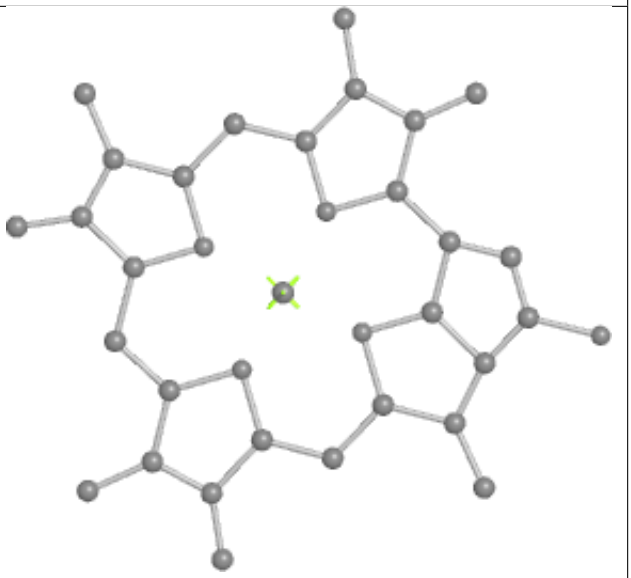


Bond angles

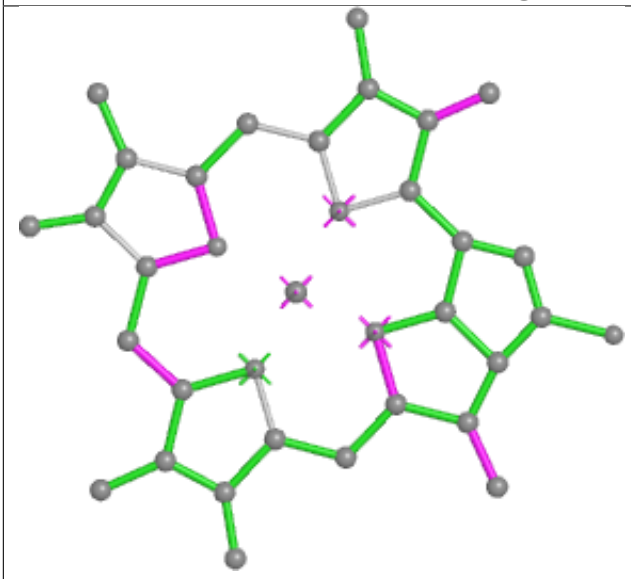


Torsions



Rings

Ligand CLA C 1078



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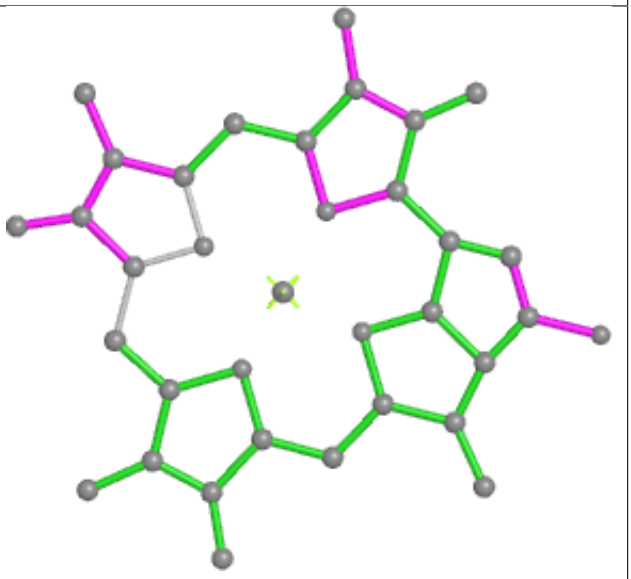
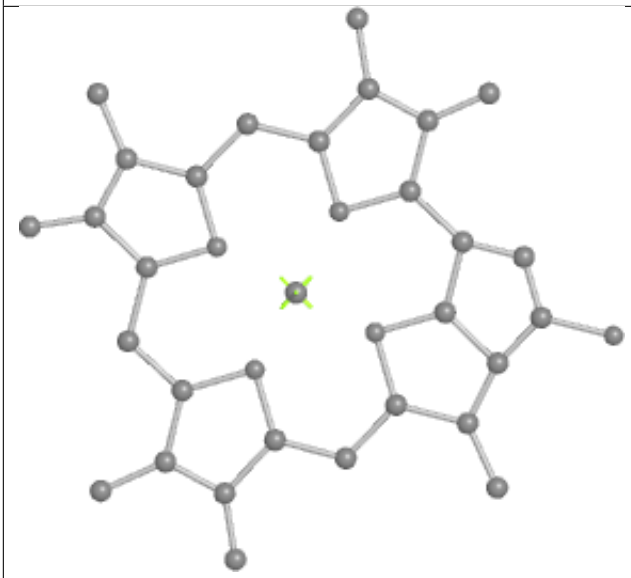
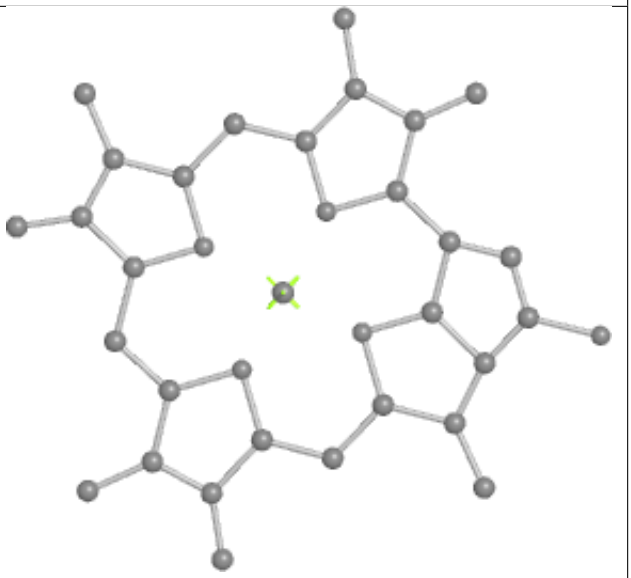


Bond angles

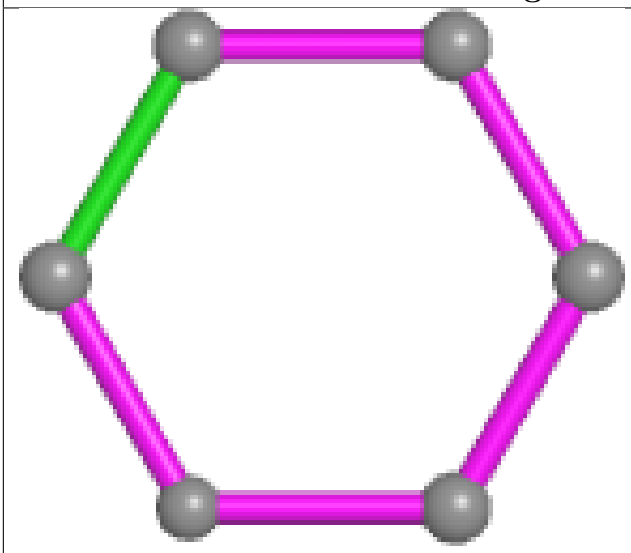


Torsions



Rings

Ligand PLA D 358



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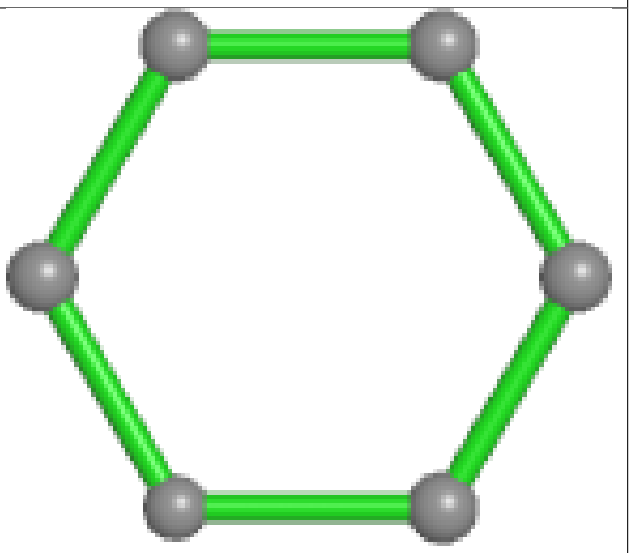
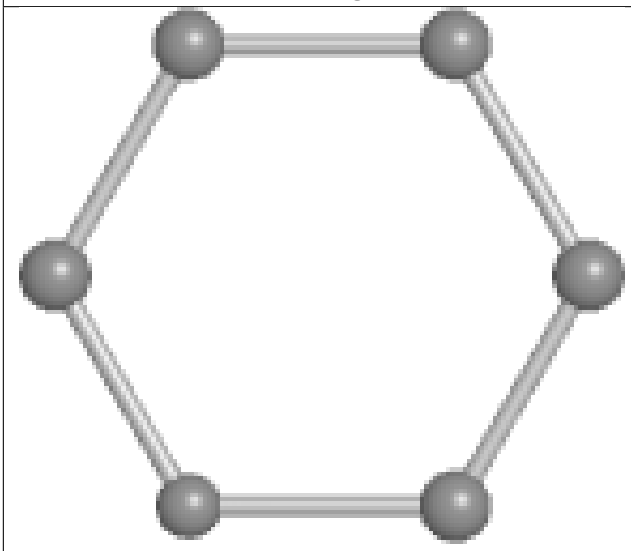
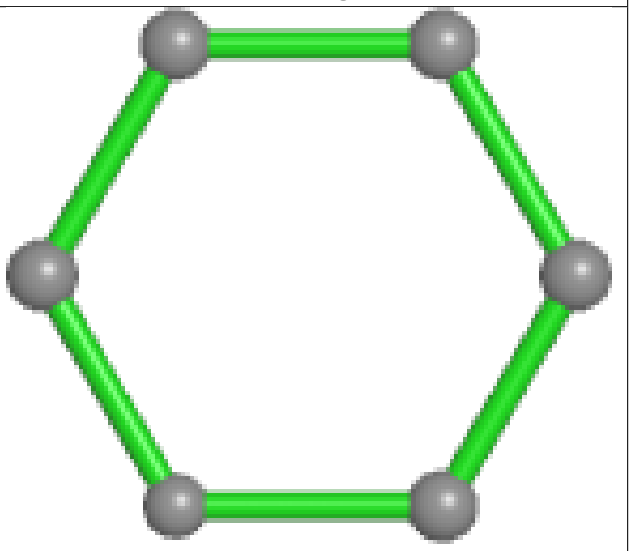


Bond angles

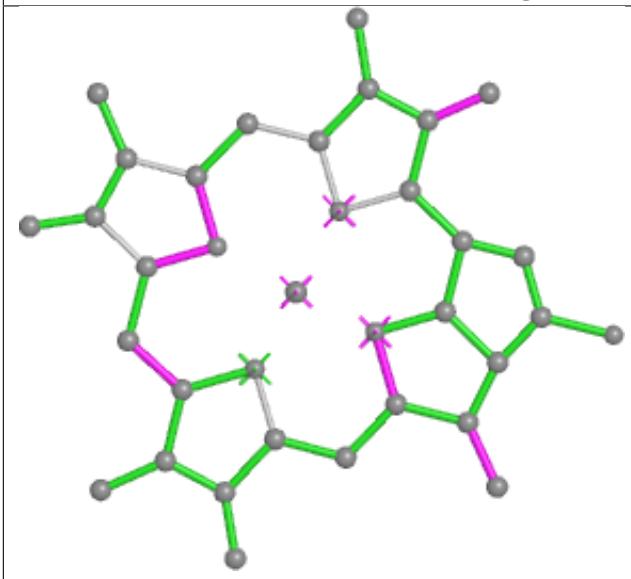


Torsions

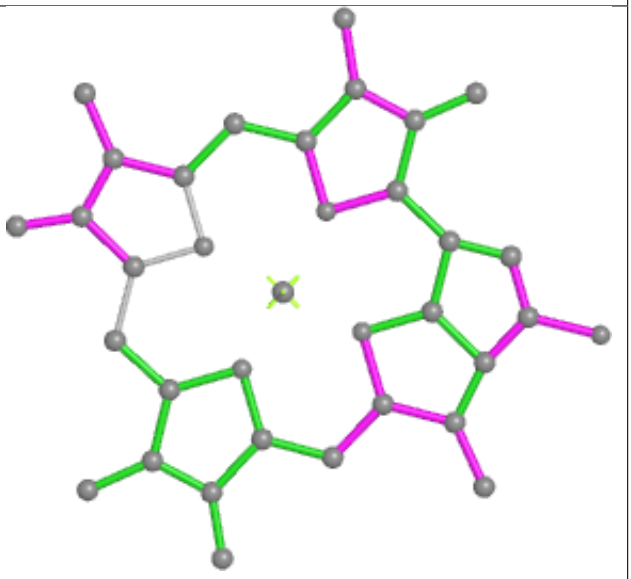


Rings

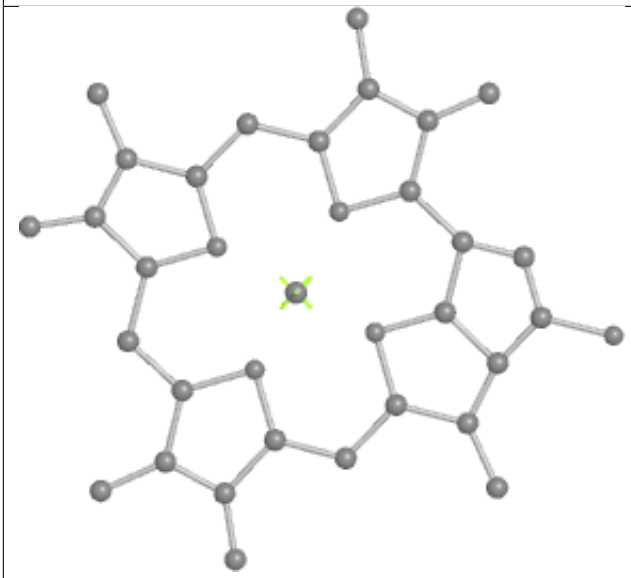
Ligand CLA L 1112



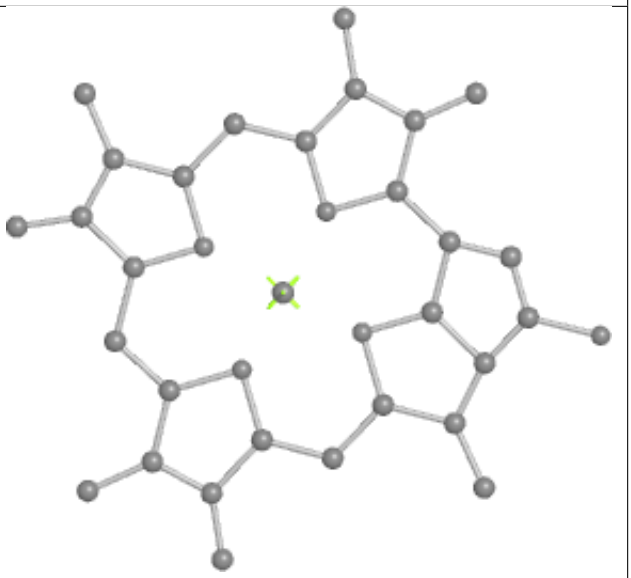
Bond lengths



Bond angles

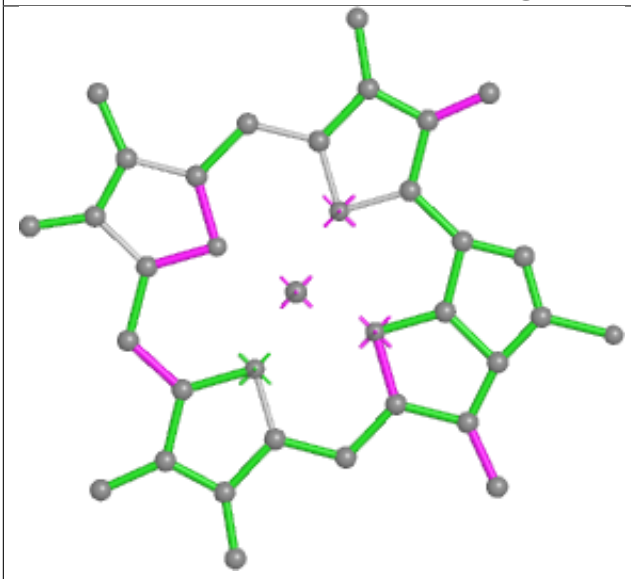


Torsions



Rings

Ligand CLA L 1107



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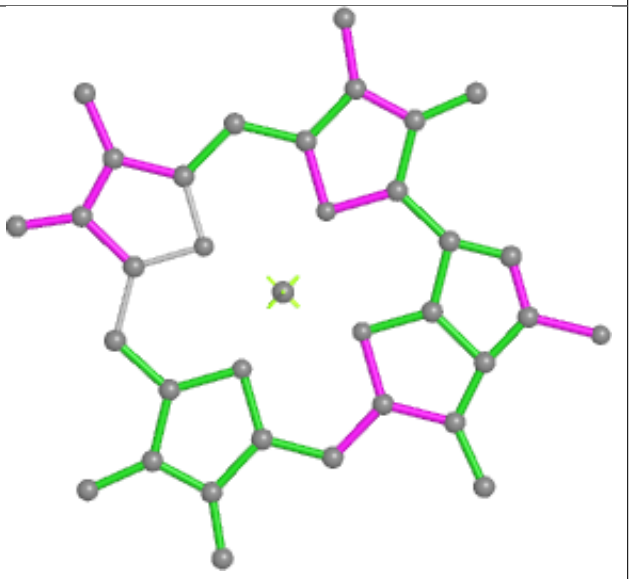
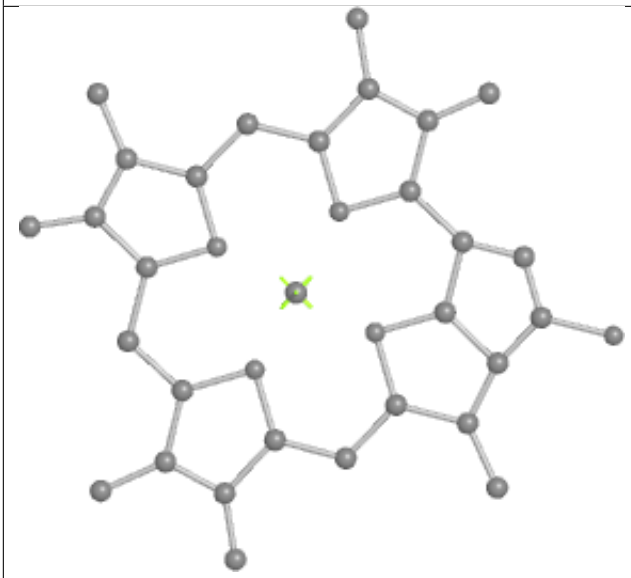
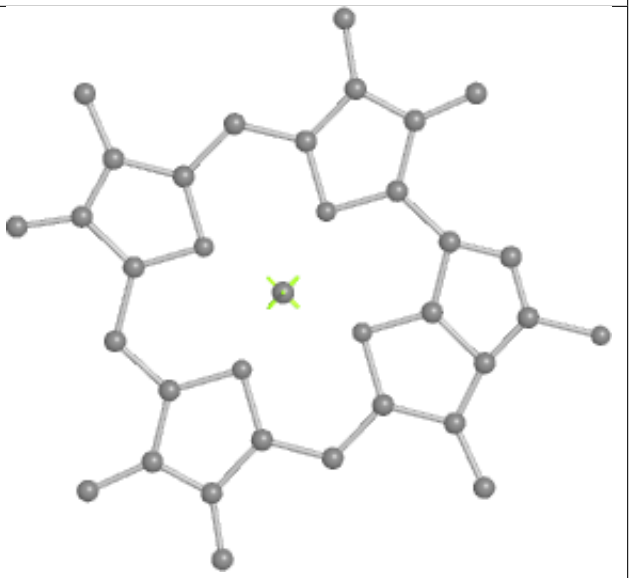


Bond angles

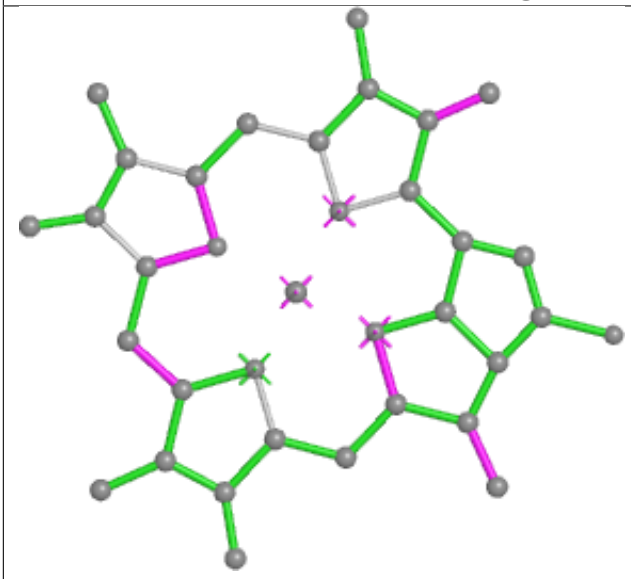


Torsions



Rings

Ligand CLA L 1116



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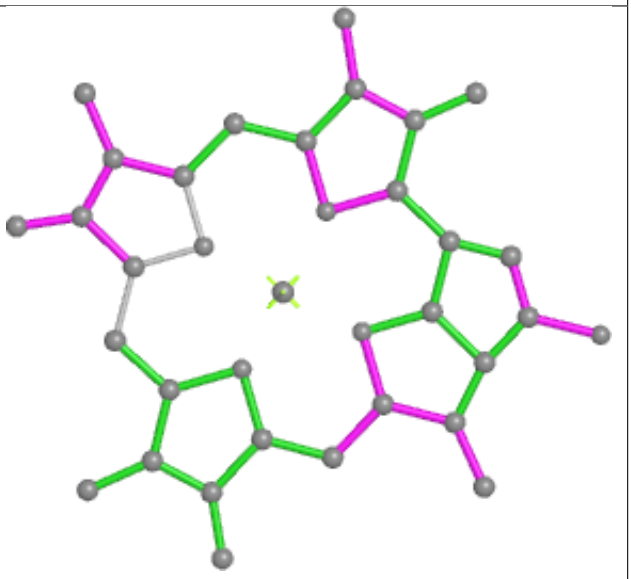
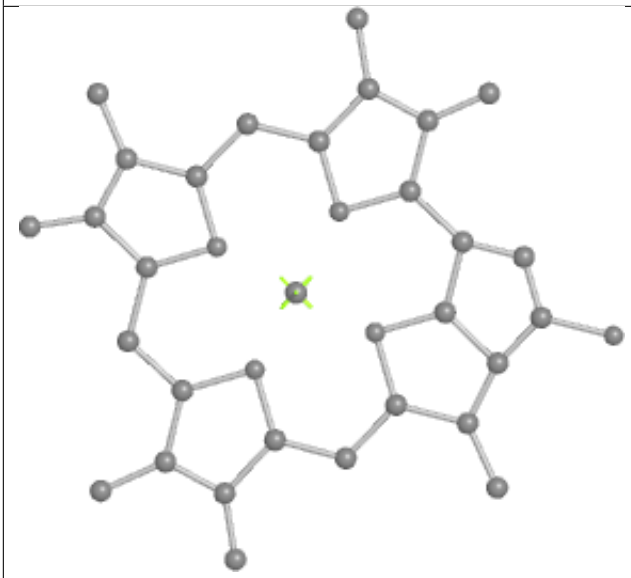
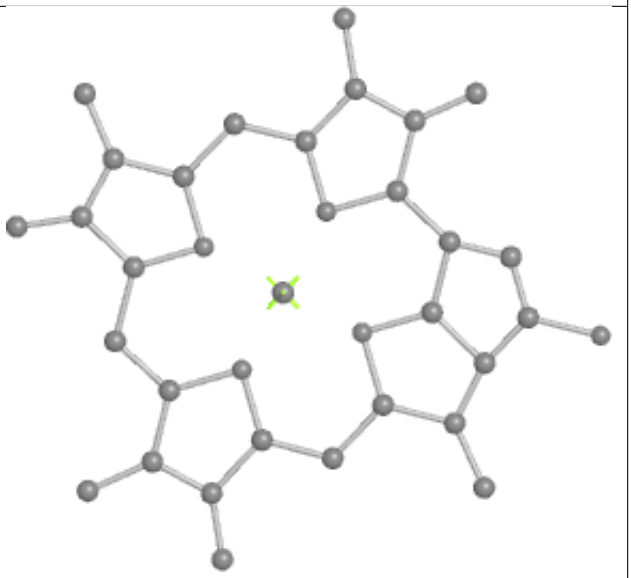


Bond angles

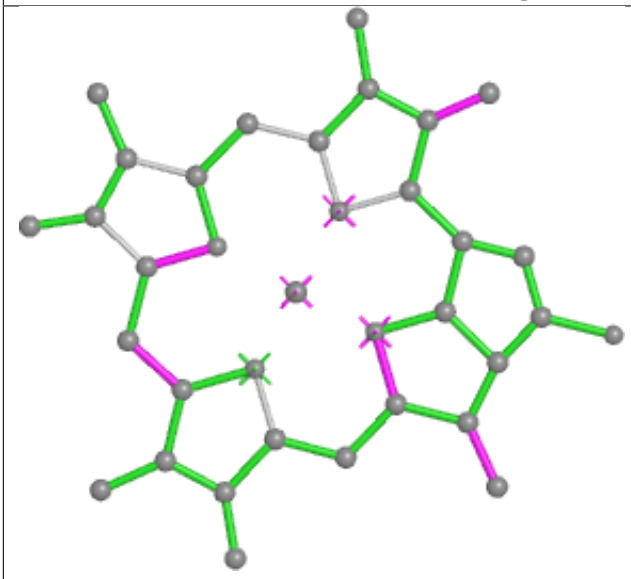


Torsions

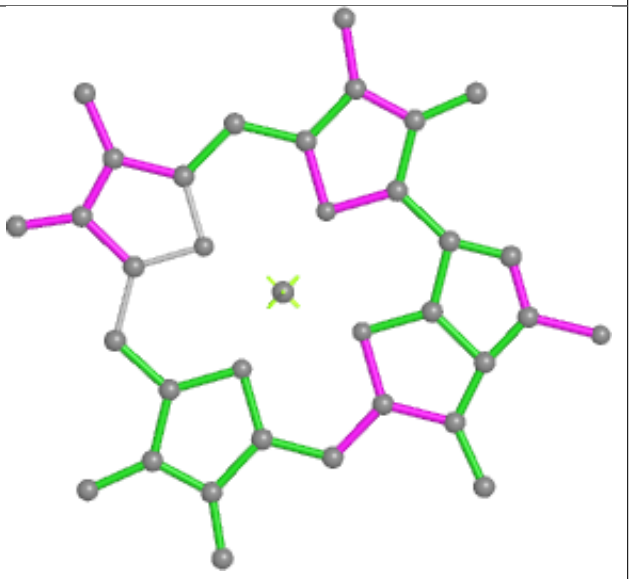


Rings

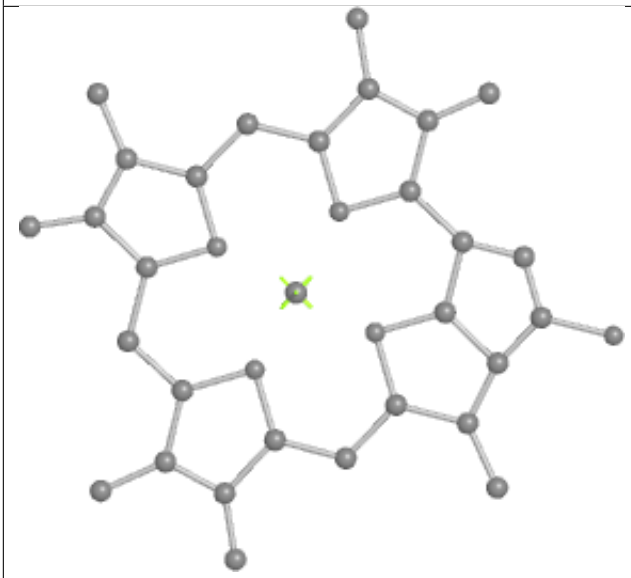
Ligand CLA B 1122



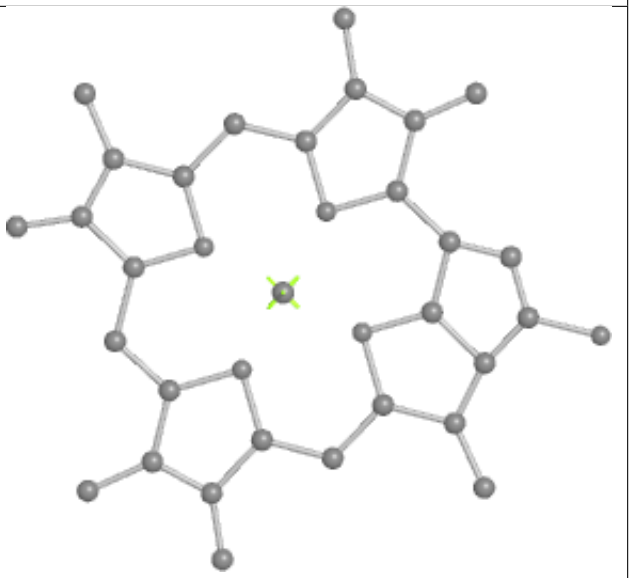
Bond lengths



Bond angles

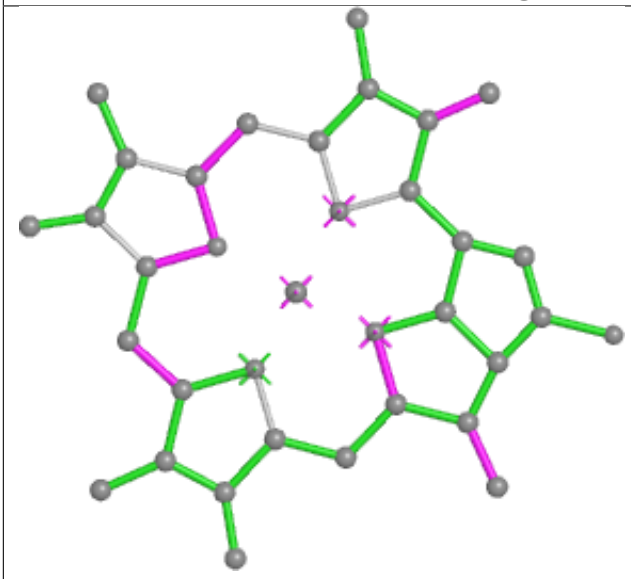


Torsions



Rings

Ligand CLA C 1088



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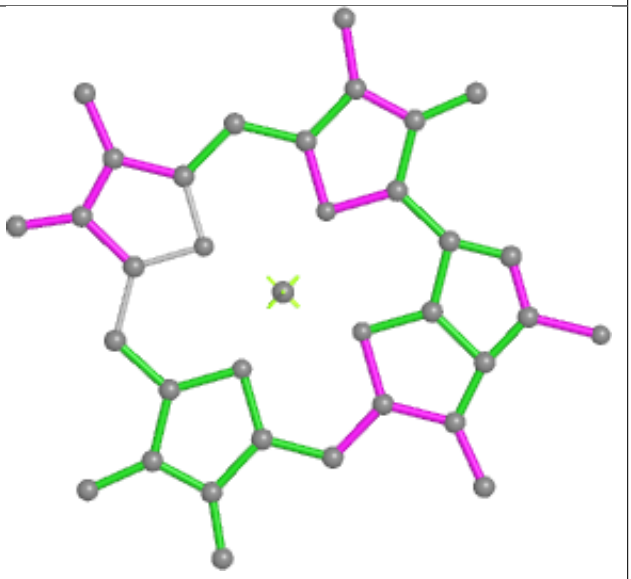
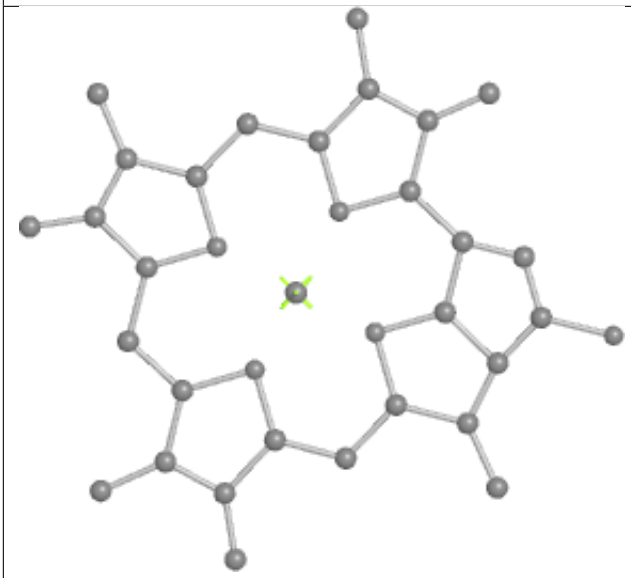
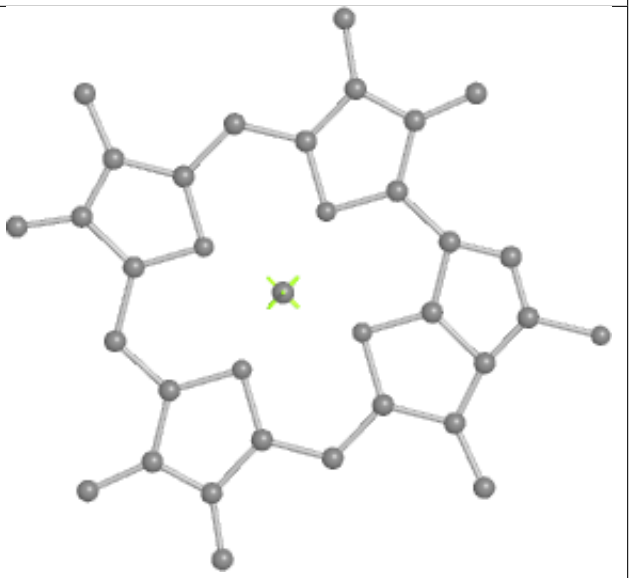


Bond angles

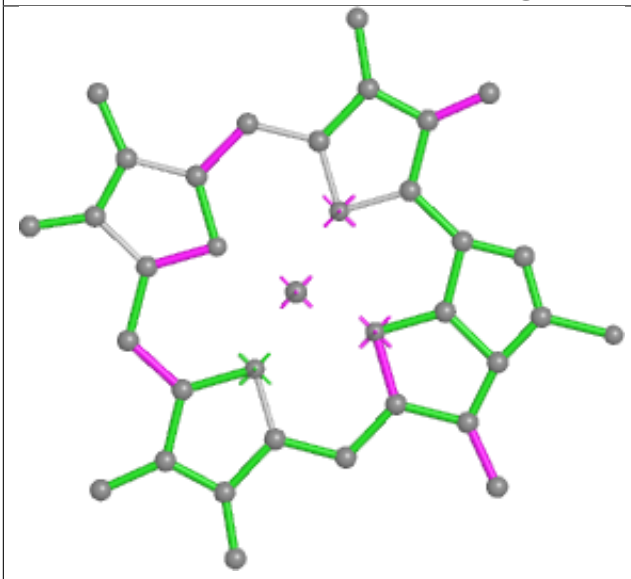


Torsions

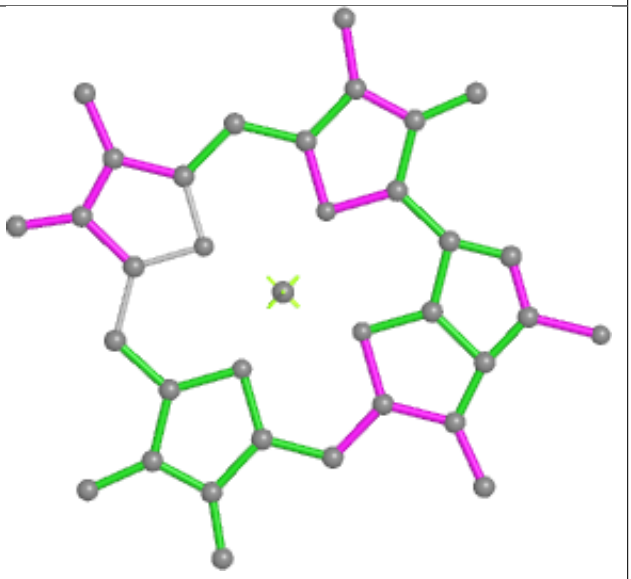


Rings

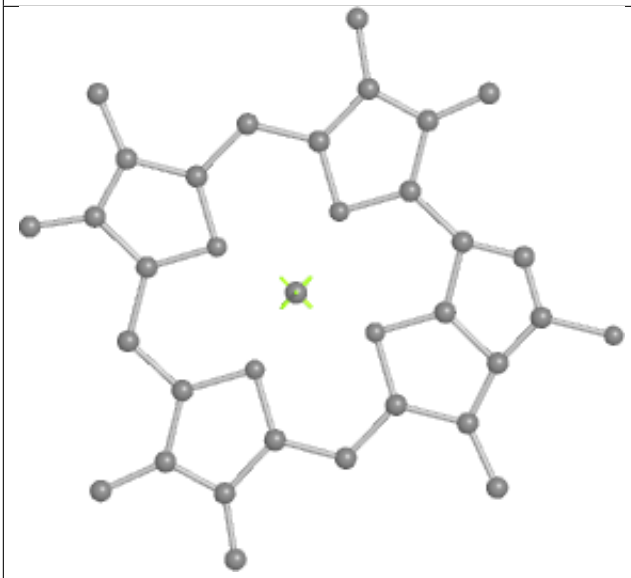
Ligand CLA L 1119



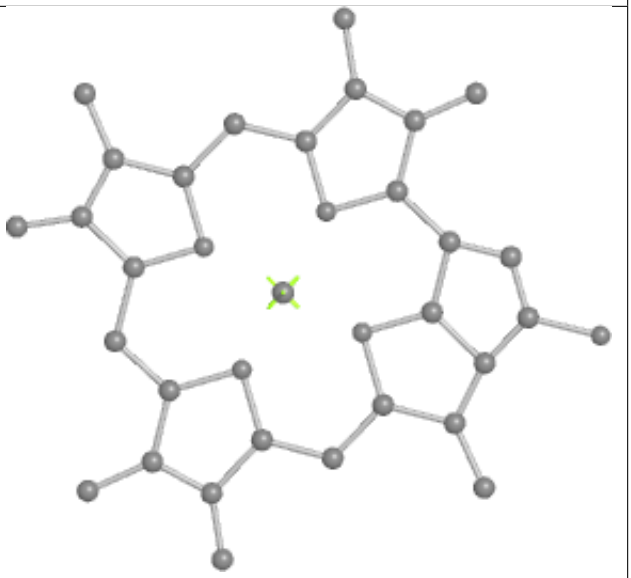
Bond lengths



Bond angles

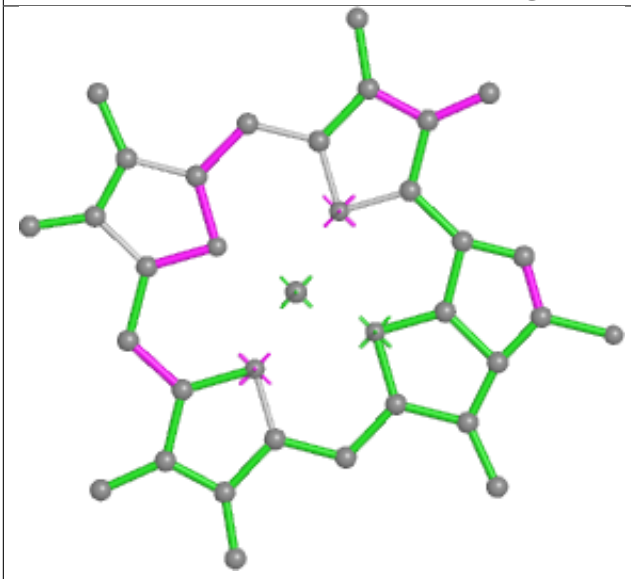


Torsions



Rings

Ligand CLA N 354



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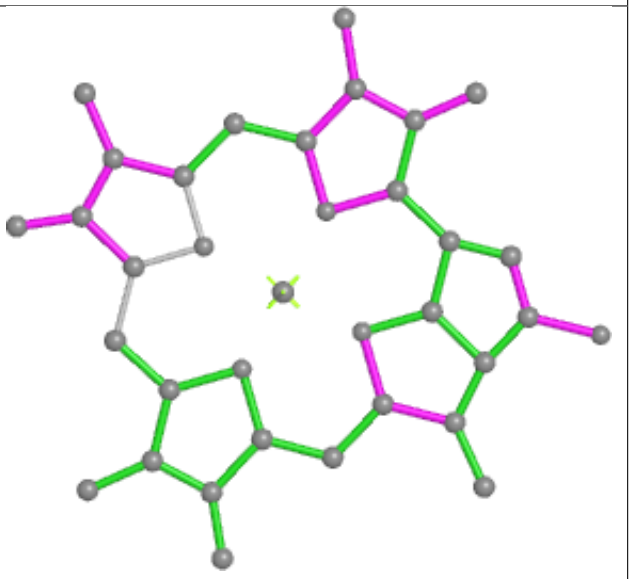
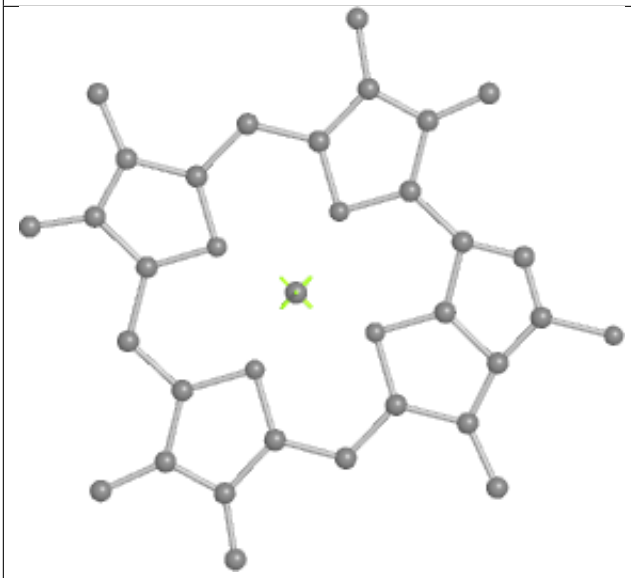
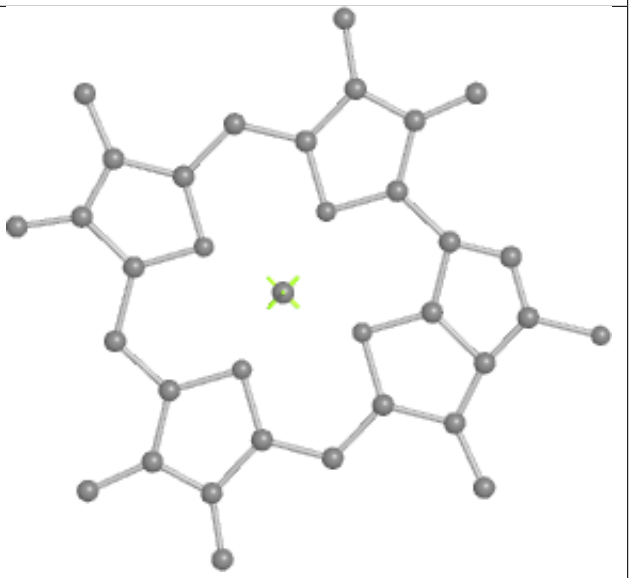


Bond angles

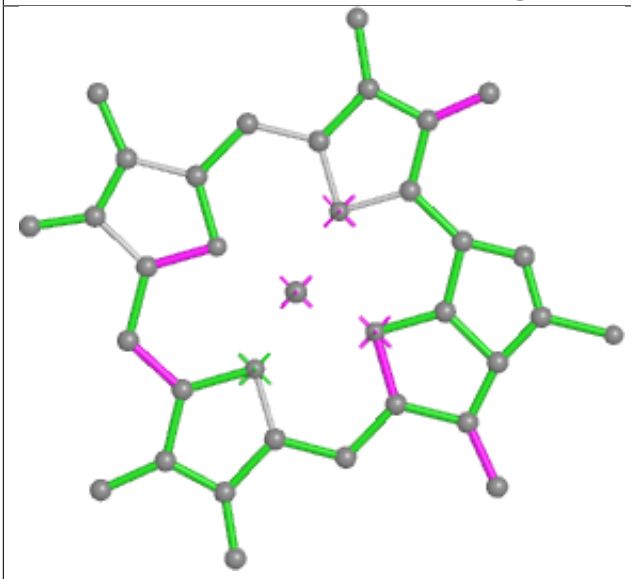


Torsions



Rings

Ligand CLA M 1081



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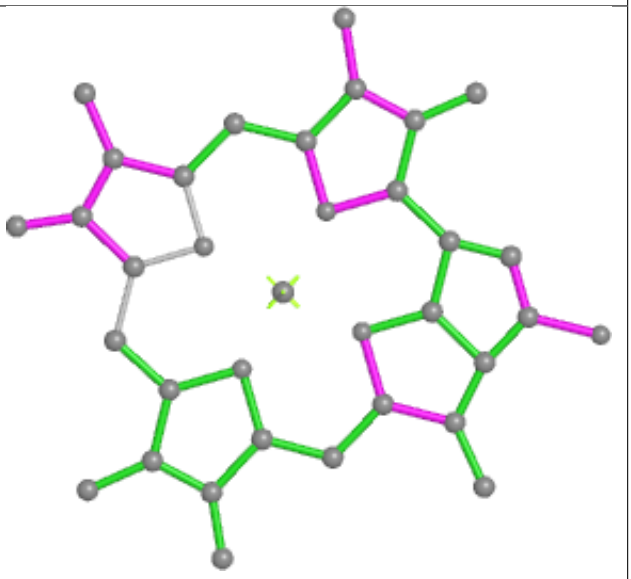
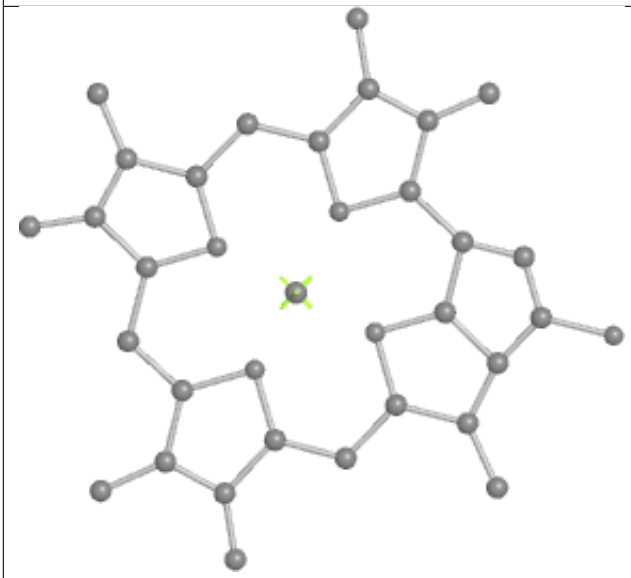
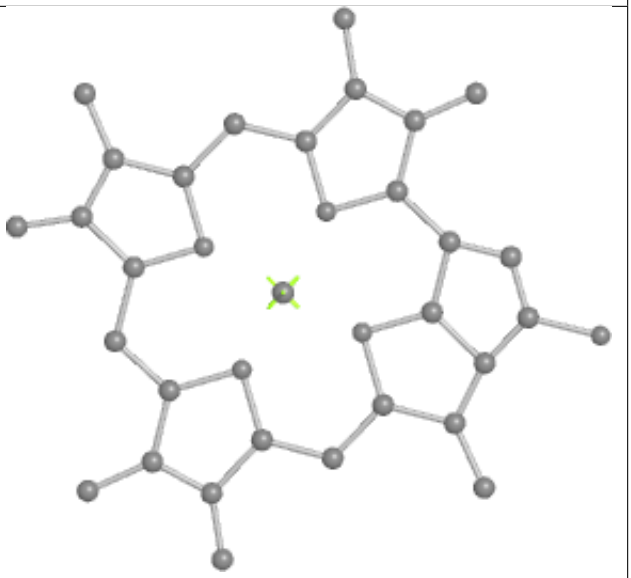


Bond angles

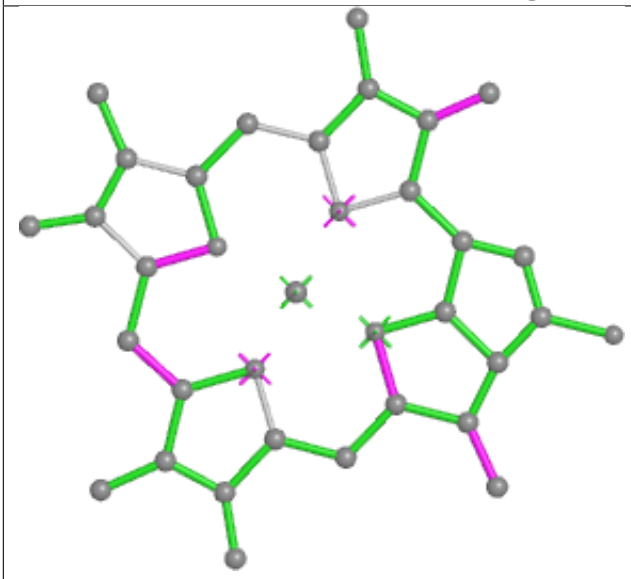


Torsions



Rings

Ligand CLA N 356



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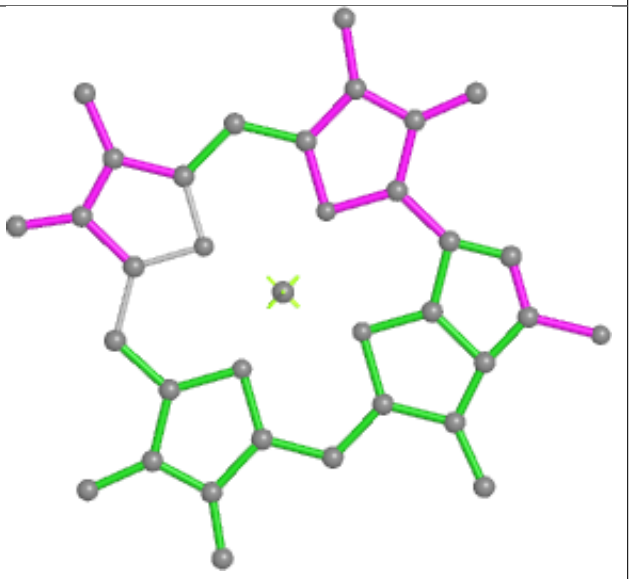
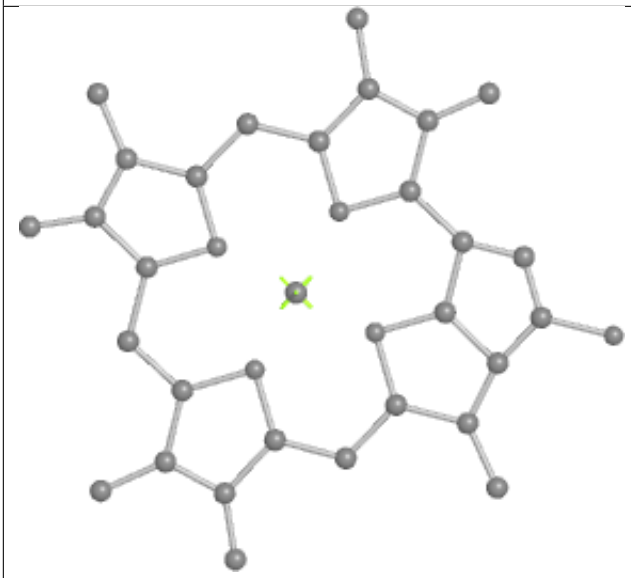
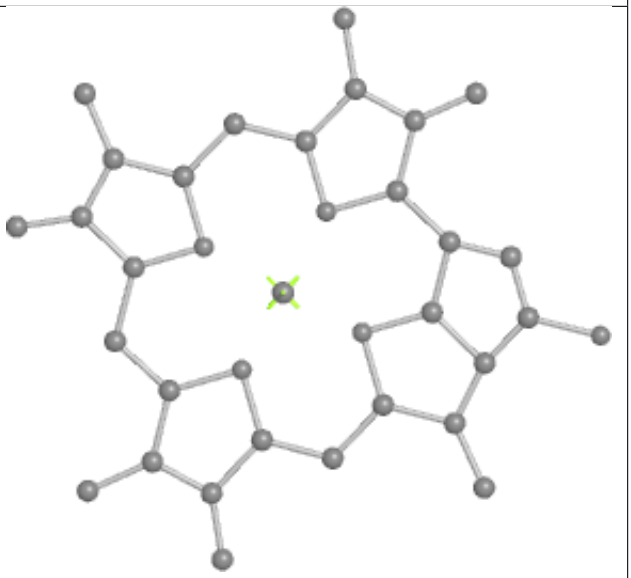


Bond angles

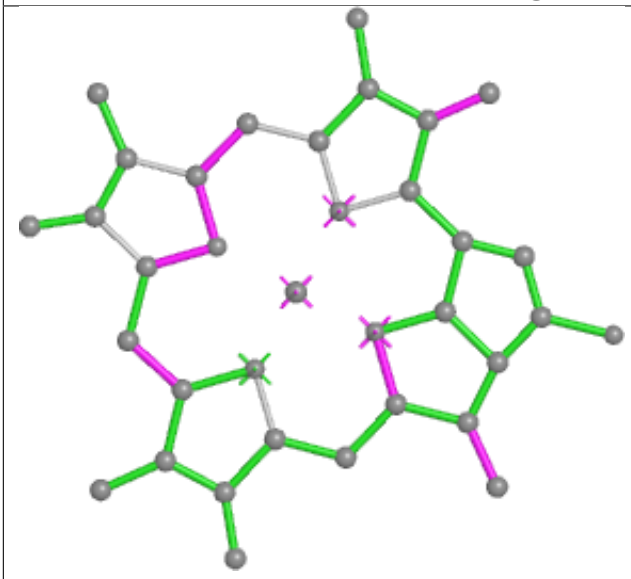


Torsions

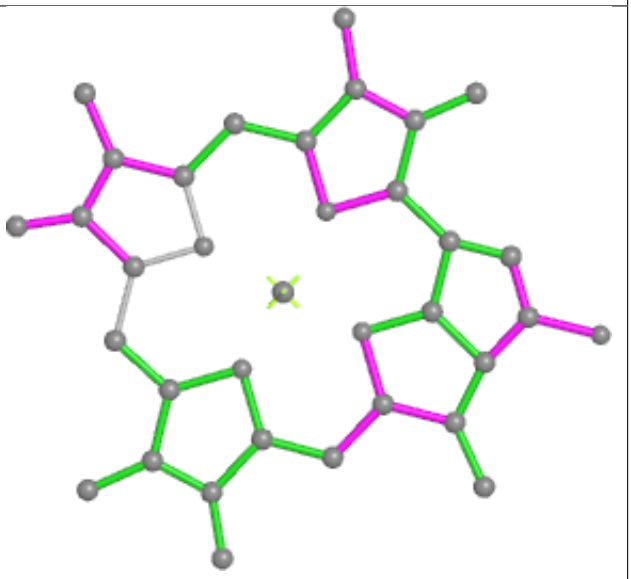


Rings

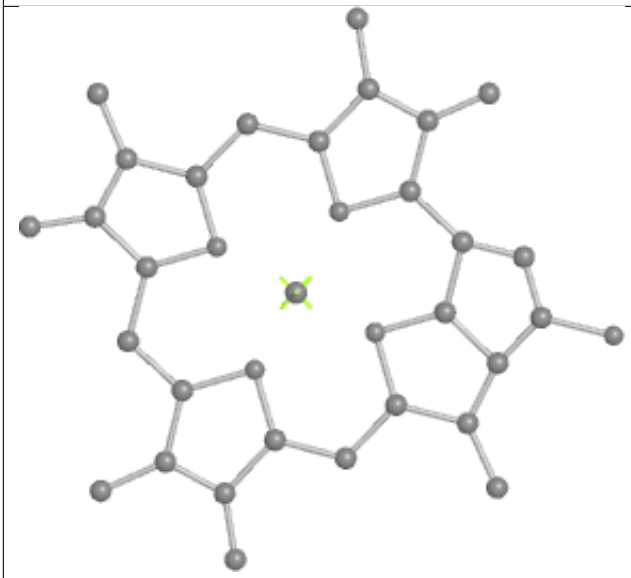
Ligand CLA W 64



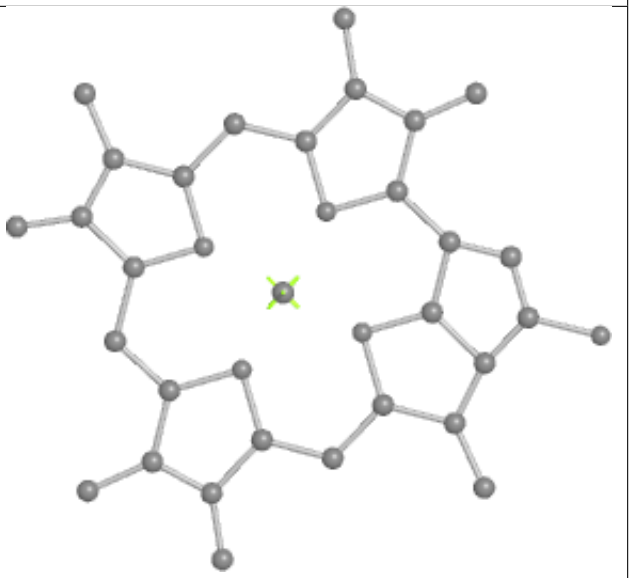
Bond lengths



Bond angles

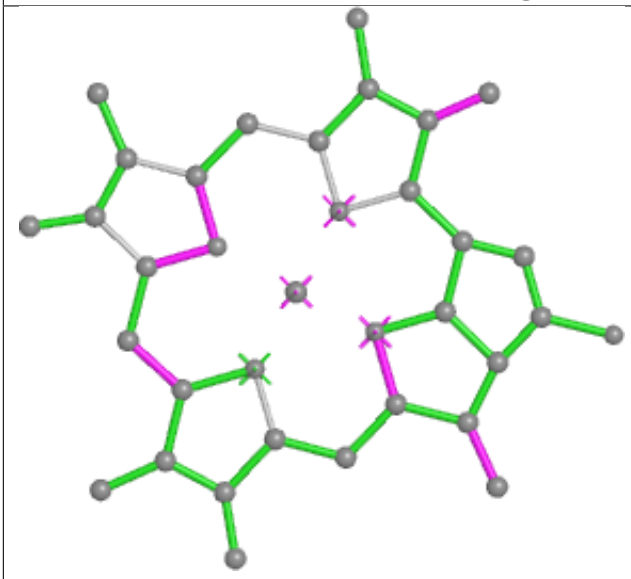


Torsions

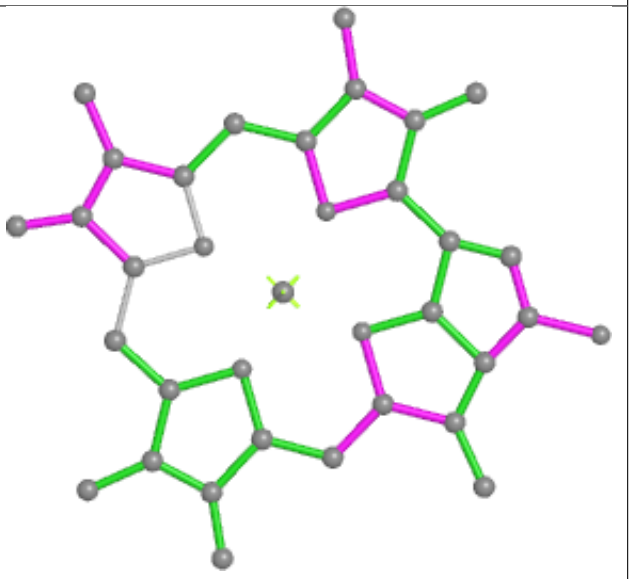


Rings

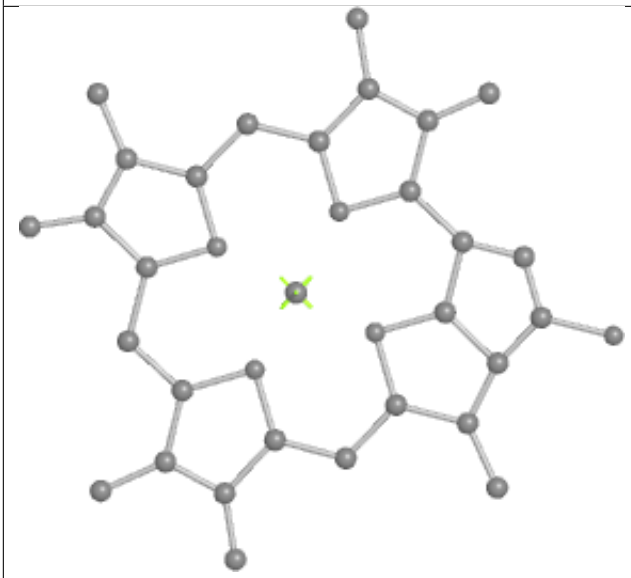
Ligand CLA L 1115



Bond lengths



Bond angles



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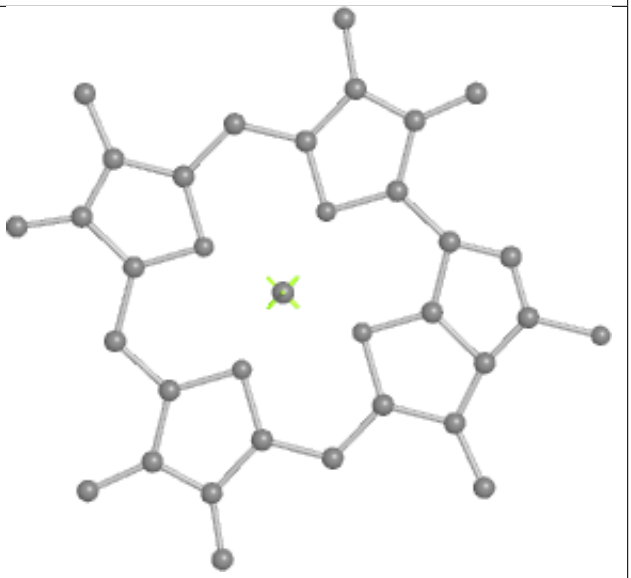
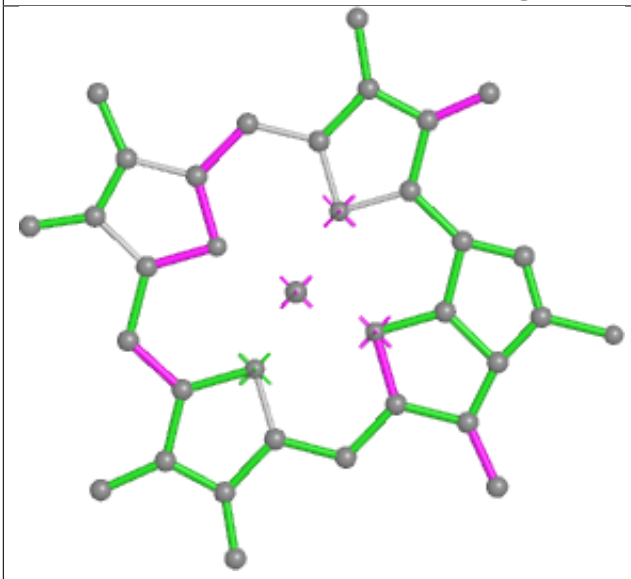
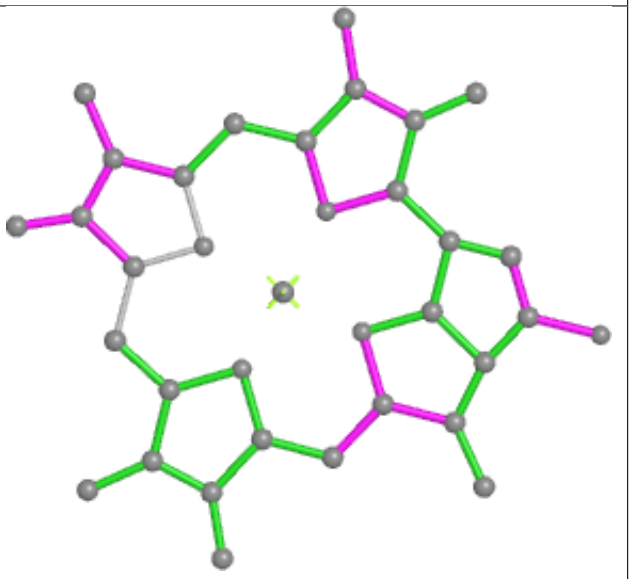


Rings

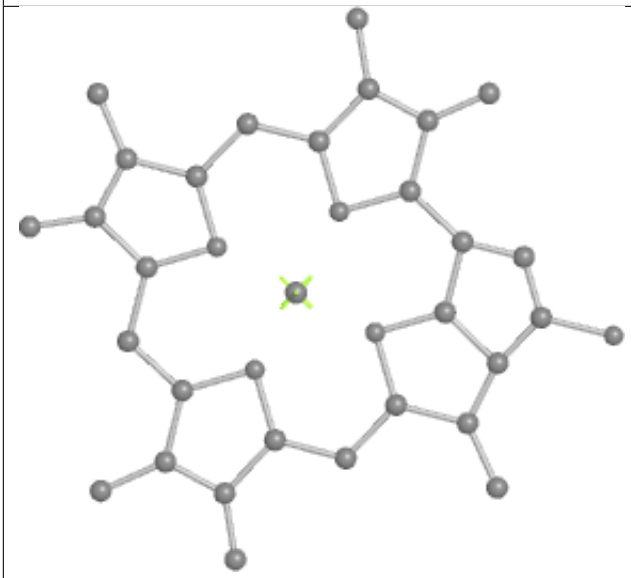
Ligand CLA B 1118



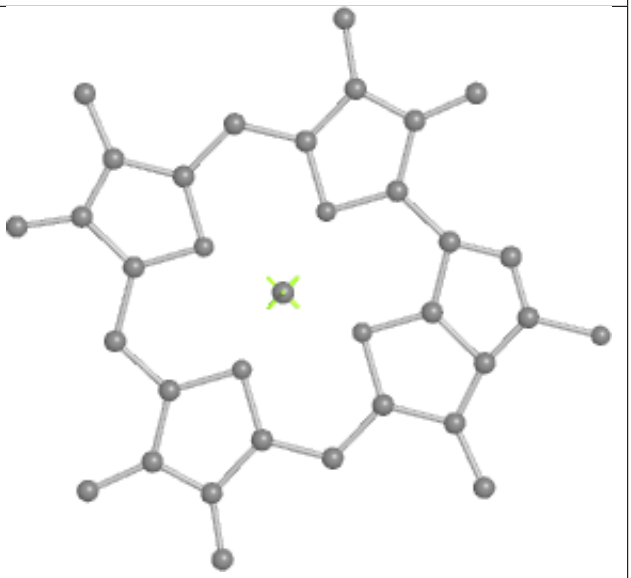
Bond lengths



Bond angles

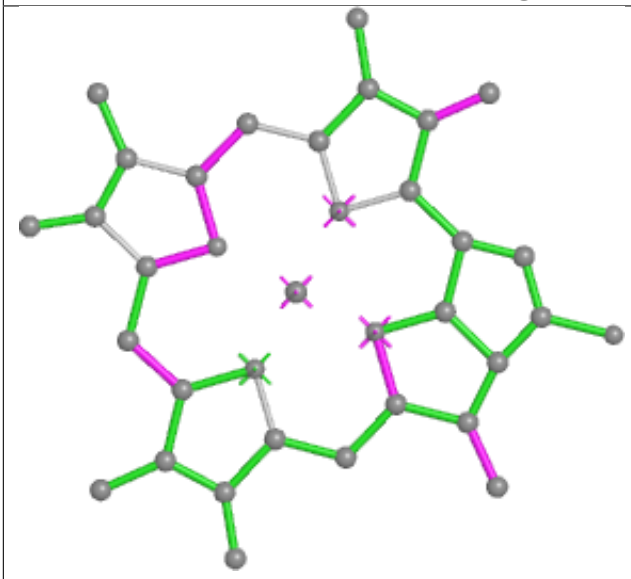


Torsions

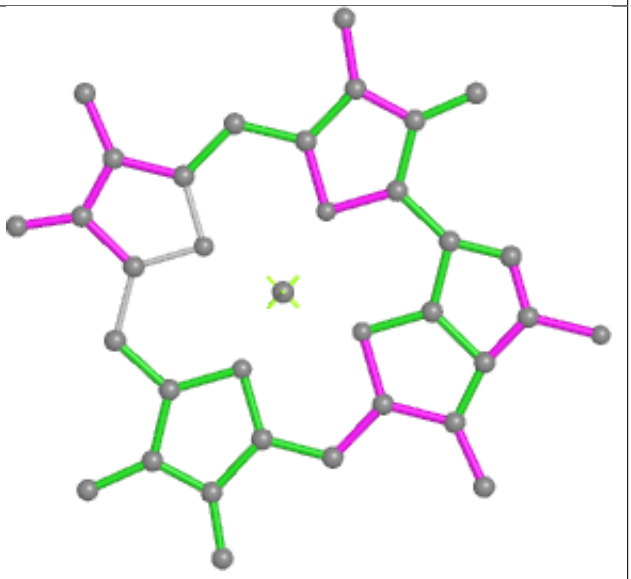


Rings

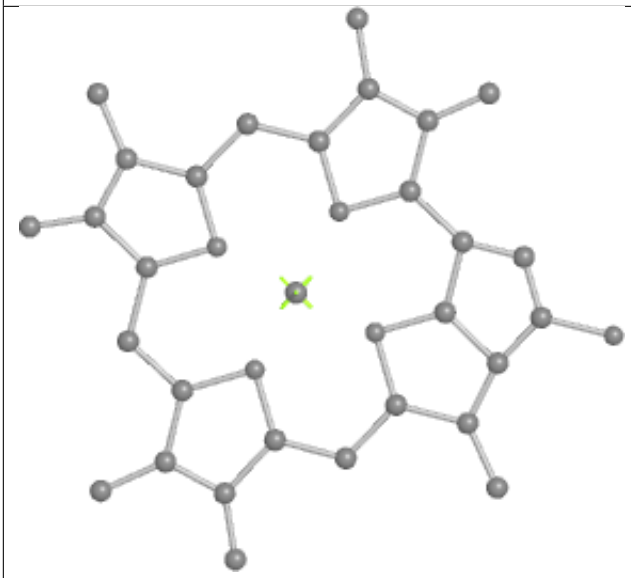
Ligand CLA C 1080



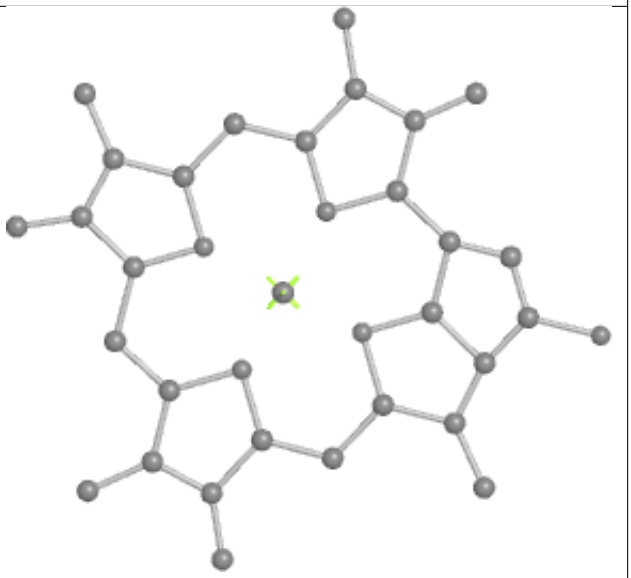
Bond lengths



Bond angles

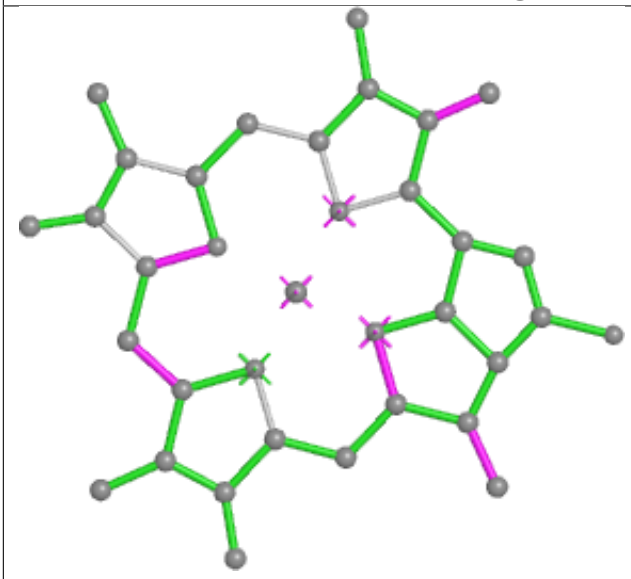


Torsions

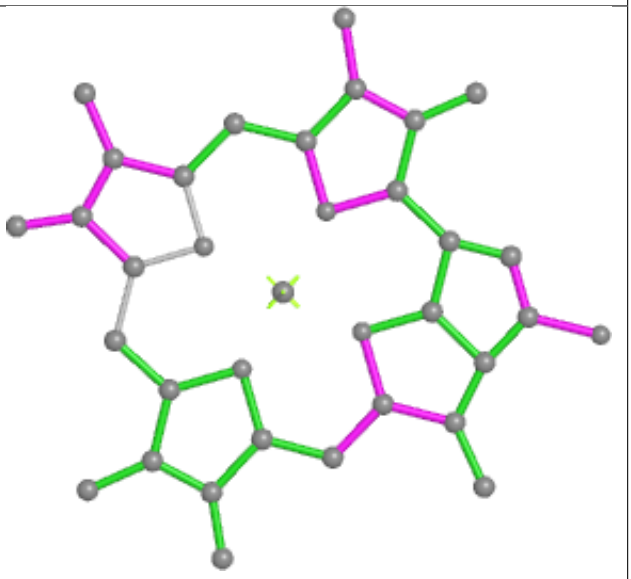


Rings

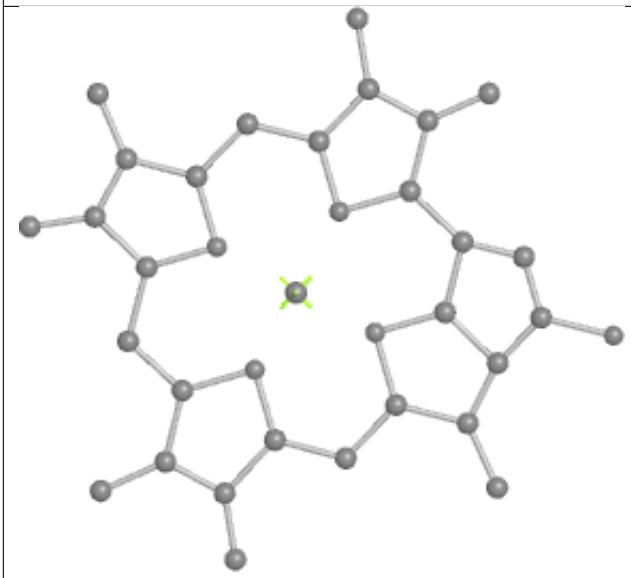
Ligand CLA M 1080



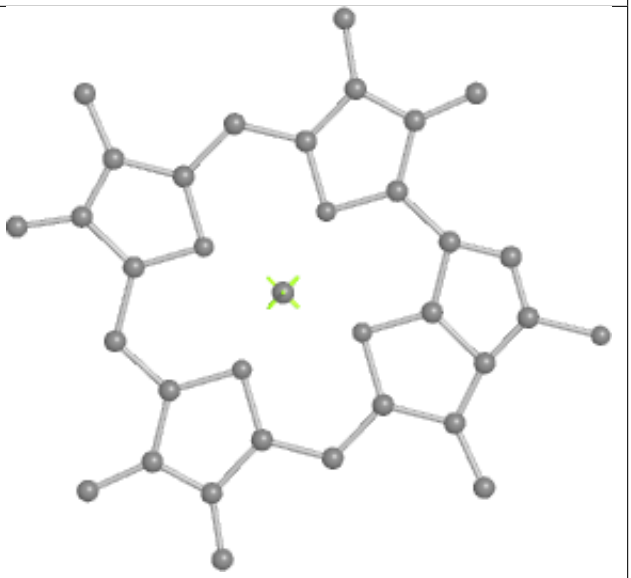
Bond lengths



Bond angles

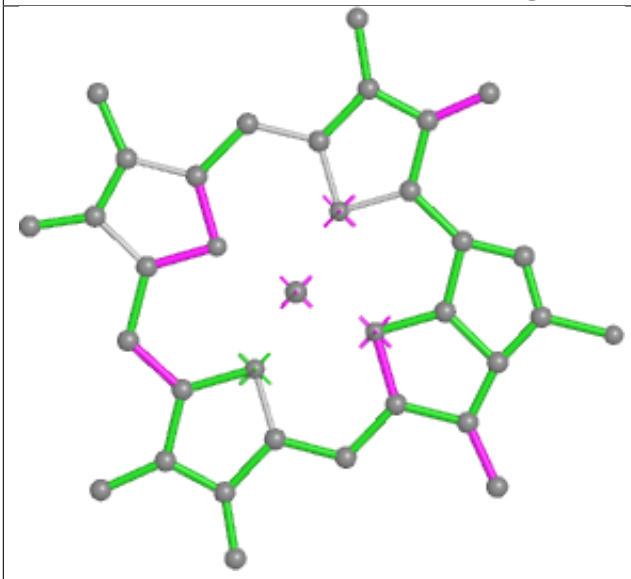


Torsions

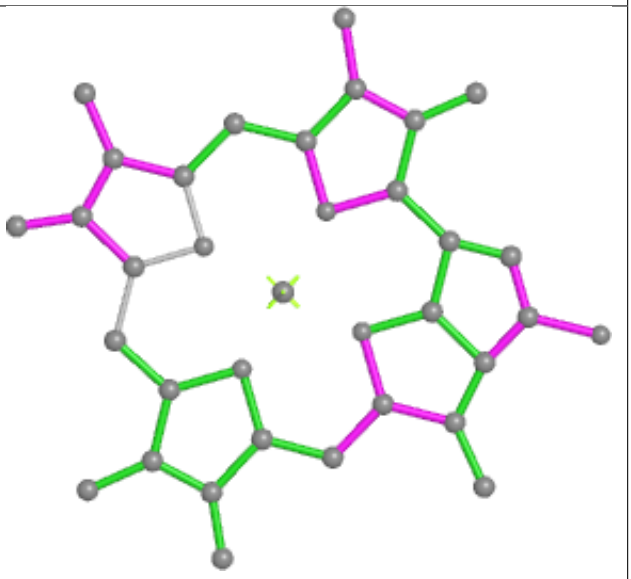


Rings

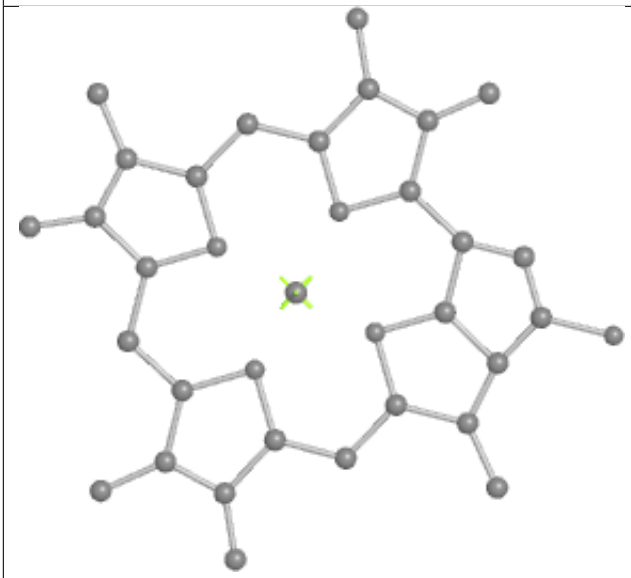
Ligand CLA N 358



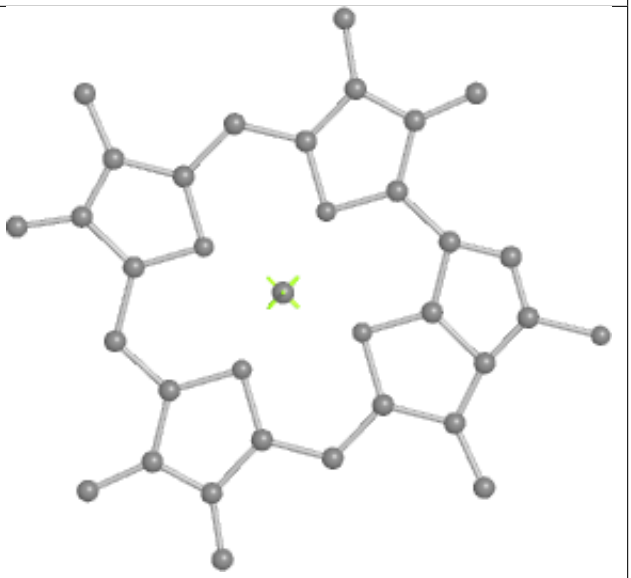
Bond lengths



Bond angles

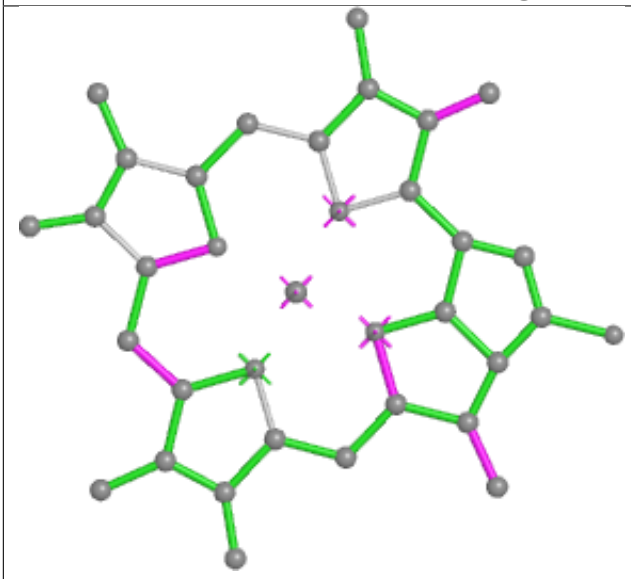


Torsions

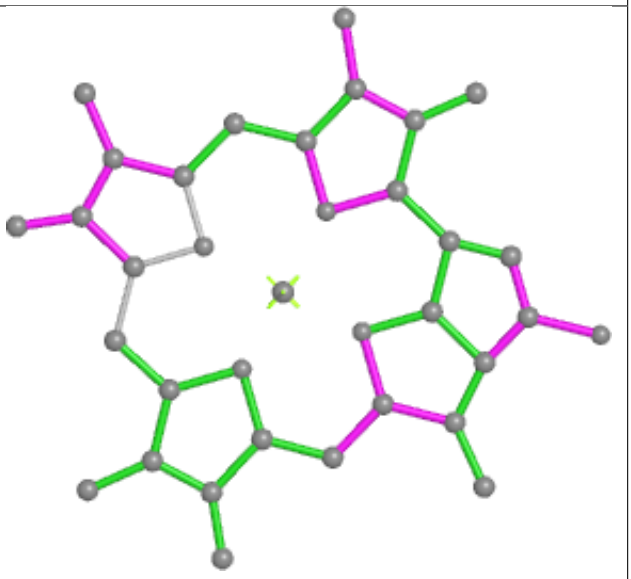


Rings

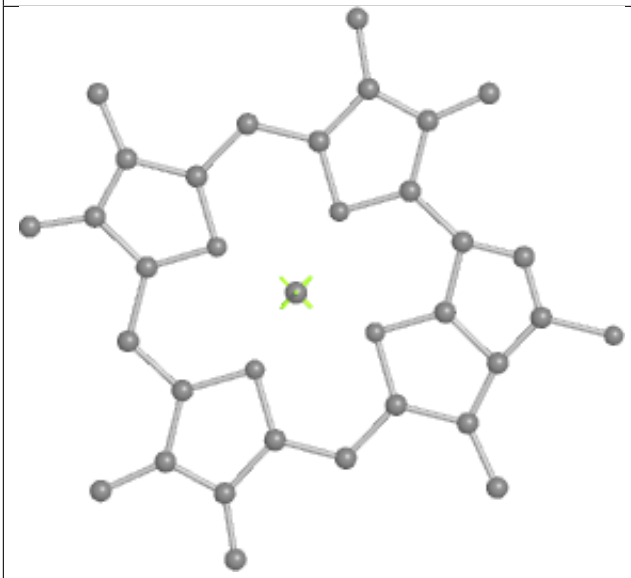
Ligand CLA B 1121



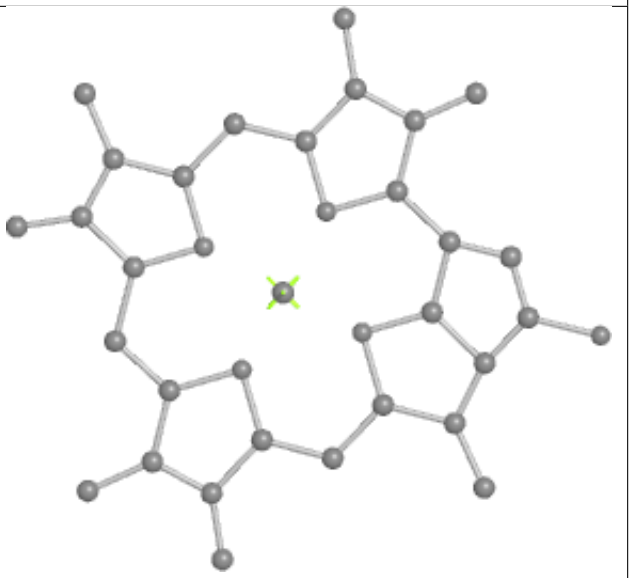
Bond lengths



Bond angles

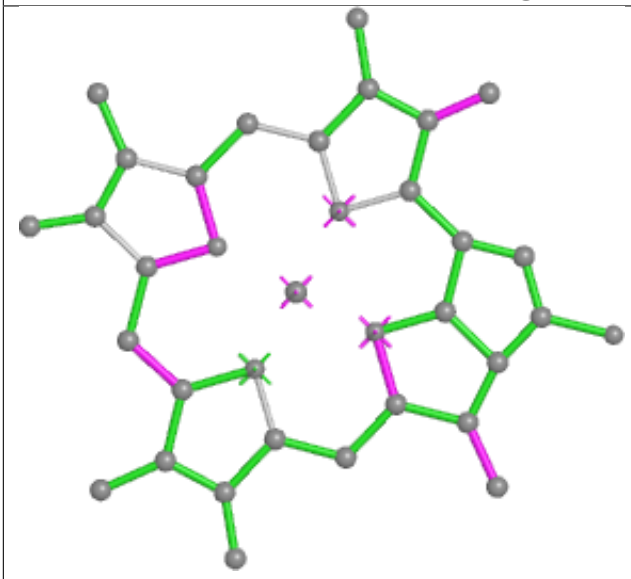


Torsions

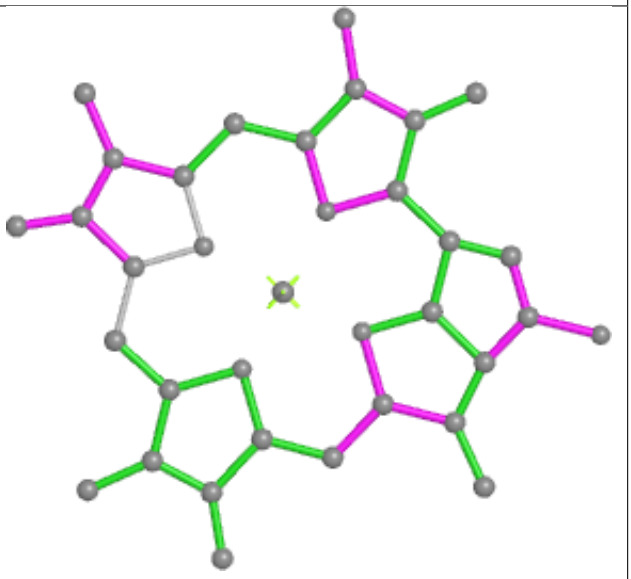


Rings

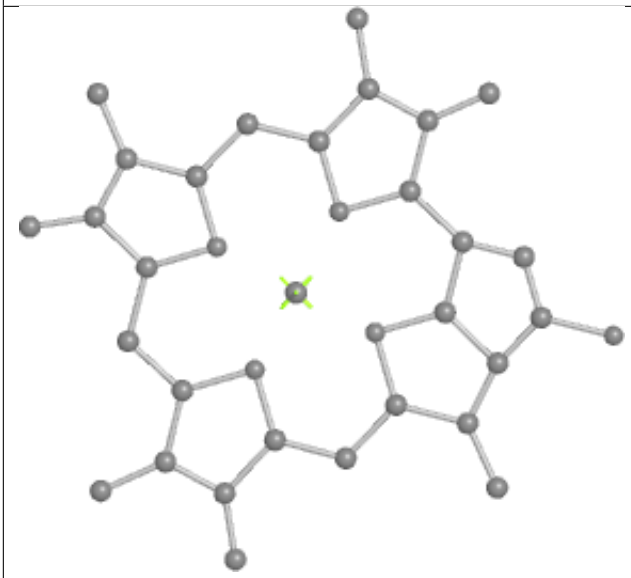
Ligand CLA L 1117



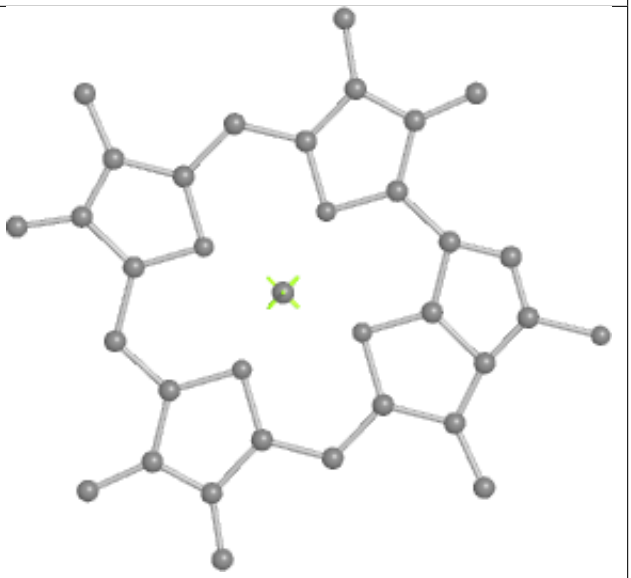
Bond lengths



Bond angles

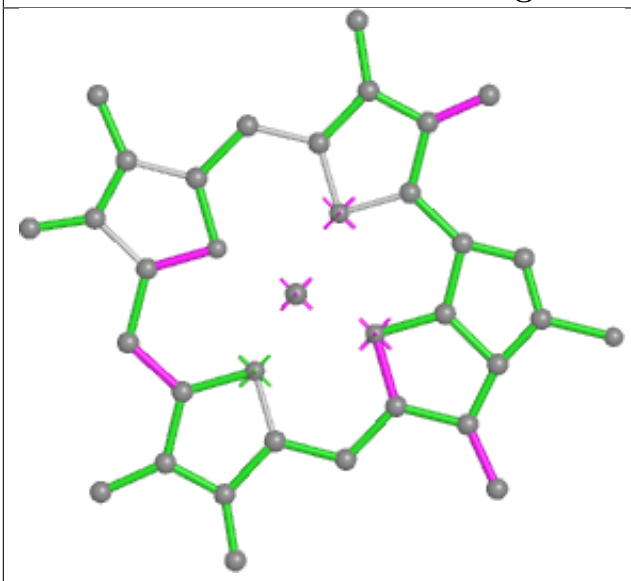


Torsions

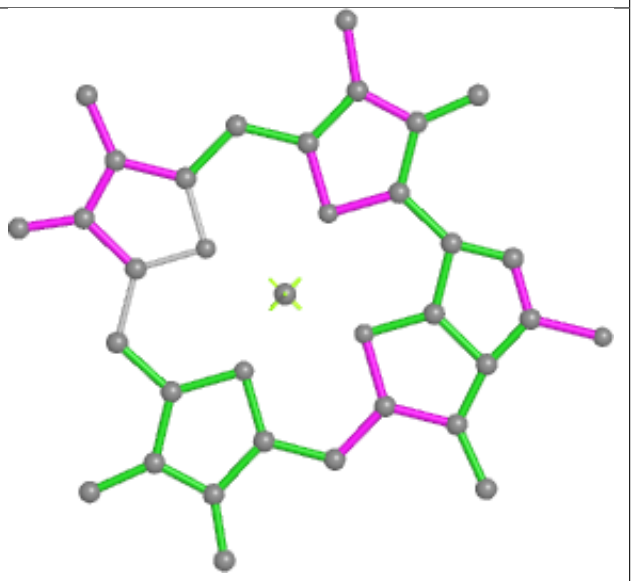


Rings

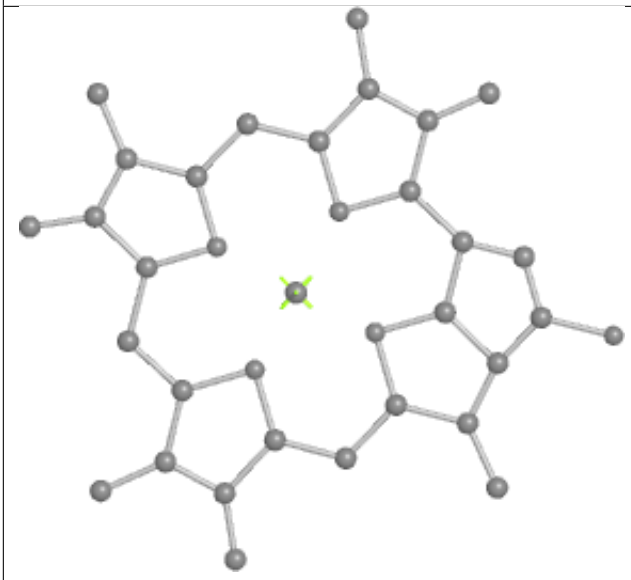
Ligand CLA C 1083



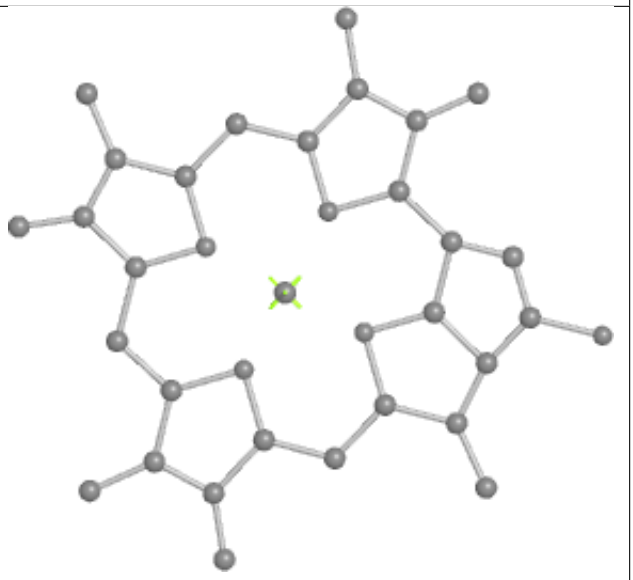
Bond lengths



Bond angles



Torsions



Rings

5.7 Other polymers

There are no such residues in this entry.

5.8 Polymer linkage issues

The following chains have linkage breaks:

Mol	Chain	Number of breaks
11	O	2

Continued on next page...

Continued from previous page...

Mol	Chain	Number of breaks
11	Y	1

All chain breaks are listed below:

Model	Chain	Residue-1	Atom-1	Residue-2	Atom-2	Distance (Å)
1	O	175:UNK	C	176:UNK	N	9.74
1	O	9:UNK	C	10:UNK	N	6.01
1	Y	9:UNK	C	10:UNK	N	5.91

6 Fit of model and data

6.1 Protein, DNA and RNA chains

EDS was not executed - this section is therefore empty.

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

EDS was not executed - this section is therefore empty.

6.3 Carbohydrates

EDS was not executed - this section is therefore empty.

6.4 Ligands

EDS was not executed - this section is therefore empty.

6.5 Other polymers

EDS was not executed - this section is therefore empty.