Full wwPDB X-ray Structure Validation Report ⓘ

Jun 18, 2024 – 12:14 PM JST

PDB ID	:	8JS7
Title	:	Dimeric PAS domains of oxygen sensor FixL in complex with imidazole-bound heme
Authors	:	Kamaya, M.; Koteishi, H.; Sawai, H.; Sugimoto, H.; Shiro, Y.
Deposited on	:	2023-06-19
Resolution	:	2.85 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:

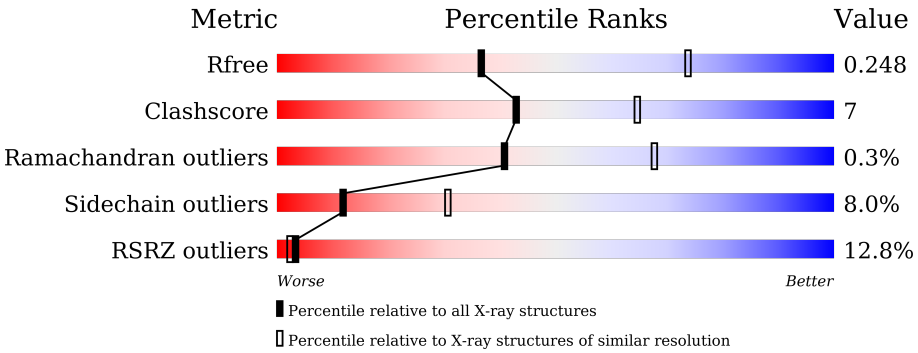
MolProbity	:	4.02b-467
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.37.1
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.37.1

1 Overall quality at a glance

The following experimental techniques were used to determine the structure:
X-RAY DIFFRACTION

The reported resolution of this entry is 2.85 Å.

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



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	130704	3168 (2.90-2.82)
Clashscore	141614	3438 (2.90-2.82)
Ramachandran outliers	138981	3348 (2.90-2.82)
Sidechain outliers	138945	3351 (2.90-2.82)
RSRZ outliers	127900	3103 (2.90-2.82)

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

Mol	Chain	Length	Quality of chain
1	A	273	6% 69% 19% • 8%
1	B	273	15% 74% 19% 7%
1	C	273	7% 73% 17% • 8%
1	D	273	4% 74% 17% • 8%
1	E	273	12% 74% 16% • 8%
1	F	273	10% 68% 21% • 9%

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Mol	Chain	Length	Quality of chain
1	G	273	5% 71% 19% 9%
1	H	273	11% 77% 14% 7%
1	I	273	25% 73% 18% 9%
1	J	273	22% 76% 15% 9%

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
4	IMD	D	303	-	-	X	-

2 Entry composition (i)

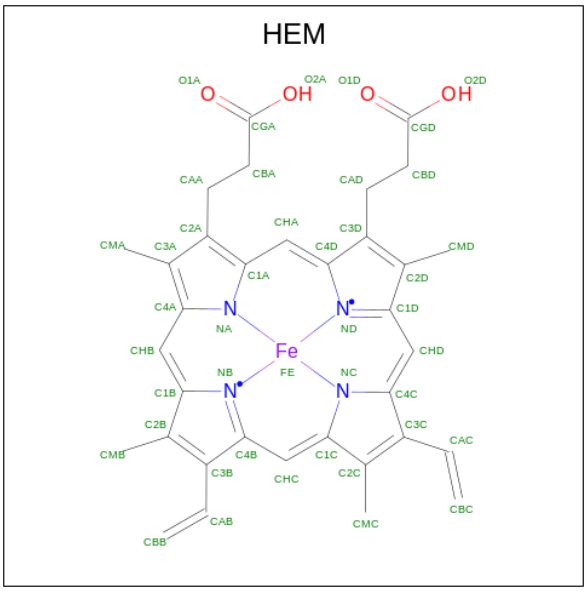
There are 5 unique types of molecules in this entry. The entry contains 20488 atoms, of which 0 are hydrogens and 0 are deuteriums.

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 Sensor protein FixL.

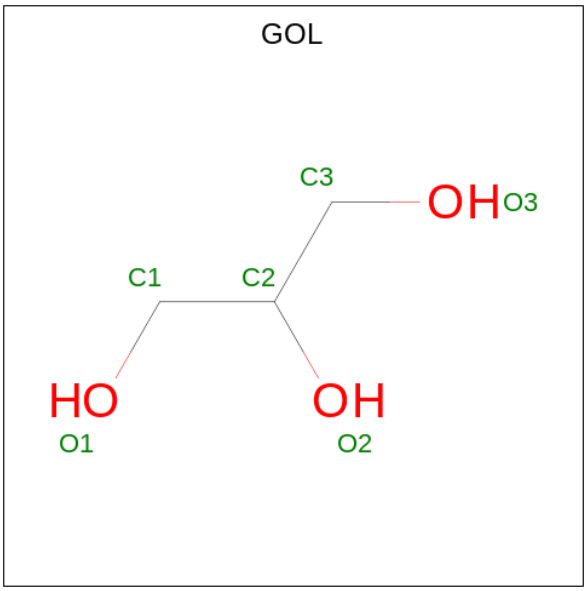
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	250	Total	C	N	O	S	0	3	0
			2000	1247	370	379	4			
1	B	253	Total	C	N	O	S	0	0	0
			1998	1245	365	384	4			
1	C	252	Total	C	N	O	S	0	0	0
			1990	1239	364	383	4			
1	D	251	Total	C	N	O	S	0	1	0
			1988	1239	365	380	4			
1	E	251	Total	C	N	O	S	0	1	0
			1988	1239	365	380	4			
1	F	249	Total	C	N	O	S	0	0	0
			1966	1223	361	378	4			
1	G	249	Total	C	N	O	S	0	0	0
			1966	1223	361	378	4			
1	H	253	Total	C	N	O	S	0	1	0
			2005	1250	367	384	4			
1	I	249	Total	C	N	O	S	0	1	0
			1973	1228	363	378	4			
1	J	249	Total	C	N	O	S	0	1	0
			1973	1228	363	378	4			

- Molecule 2 is PROTOPORPHYRIN IX CONTAINING FE (three-letter code: HEM) (formula: $C_{34}H_{32}FeN_4O_4$).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
2	A	1	Total	C	Fe	N	O	0	0
			43	34	1	4	4		
2	B	1	Total	C	Fe	N	O	0	0
			43	34	1	4	4		
2	C	1	Total	C	Fe	N	O	0	0
			43	34	1	4	4		
2	D	1	Total	C	Fe	N	O	0	0
			43	34	1	4	4		
2	E	1	Total	C	Fe	N	O	0	0
			43	34	1	4	4		
2	F	1	Total	C	Fe	N	O	0	0
			43	34	1	4	4		
2	G	1	Total	C	Fe	N	O	0	0
			43	34	1	4	4		
2	H	1	Total	C	Fe	N	O	0	0
			43	34	1	4	4		
2	I	1	Total	C	Fe	N	O	0	0
			43	34	1	4	4		
2	J	1	Total	C	Fe	N	O	0	0
			43	34	1	4	4		

- Molecule 3 is GLYCEROL (three-letter code: GOL) (formula: $C_3H_8O_3$).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
3	A	1	Total	C	O	0	0
			6	3	3		
3	B	1	Total	C	O	0	0
			6	3	3		
3	B	1	Total	C	O	0	0
			6	3	3		
3	C	1	Total	C	O	0	0
			6	3	3		
3	C	1	Total	C	O	0	0
			6	3	3		
3	D	1	Total	C	O	0	0
			6	3	3		
3	E	1	Total	C	O	0	0
			6	3	3		
3	E	1	Total	C	O	0	0
			6	3	3		
3	F	1	Total	C	O	0	0
			6	3	3		
3	G	1	Total	C	O	0	0
			6	3	3		
3	H	1	Total	C	O	0	0
			6	3	3		
3	H	1	Total	C	O	0	0
			6	3	3		
3	I	1	Total	C	O	0	0
			6	3	3		
3	I	1	Total	C	O	0	0
			6	3	3		

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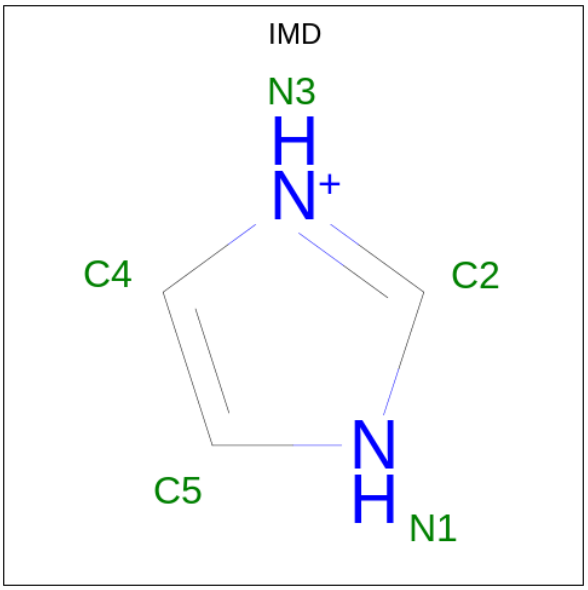
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	J	1	Total C O 6 3 3	0	0

- Molecule 4 is IMIDAZOLE (three-letter code: IMD) (formula: $C_3H_5N_2$) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
4	A	1	Total C N 5 3 2	0	0
4	B	1	Total C N 5 3 2	0	0
4	C	1	Total C N 5 3 2	0	0
4	D	1	Total C N 5 3 2	0	0
4	E	1	Total C N 5 3 2	0	0
4	F	1	Total C N 5 3 2	0	0
4	G	1	Total C N 5 3 2	0	0
4	H	1	Total C N 5 3 2	0	0
4	I	1	Total C N 5 3 2	0	0
4	J	1	Total C N 5 3 2	0	0

- Molecule 5 is water.

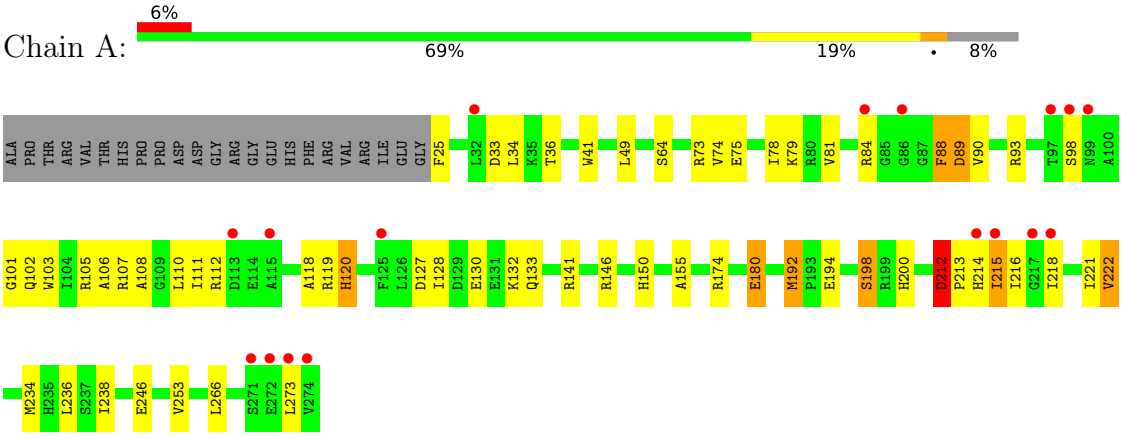
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
5	A	17	Total O 17 17	0	0
5	B	7	Total O 7 7	0	0
5	C	1	Total O 1 1	0	0
5	D	21	Total O 21 21	0	0
5	E	9	Total O 9 9	0	0
5	F	1	Total O 1 1	0	0
5	G	5	Total O 5 5	0	0
5	H	4	Total O 4 4	0	0
5	I	2	Total O 2 2	0	0
5	J	4	Total O 4 4	0	0

3 Residue-property plots (i)

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

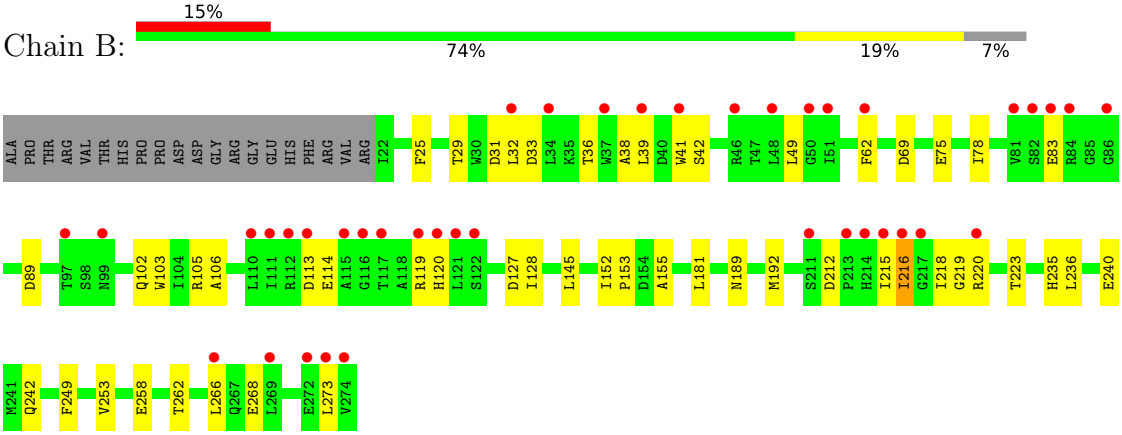
• Molecule 1: Sensor protein FixL

Chain A:



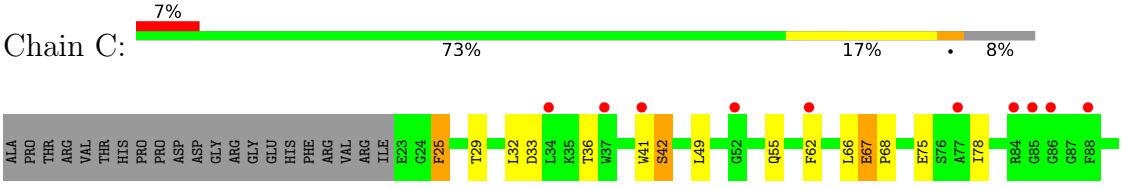
• Molecule 1: Sensor protein FixL

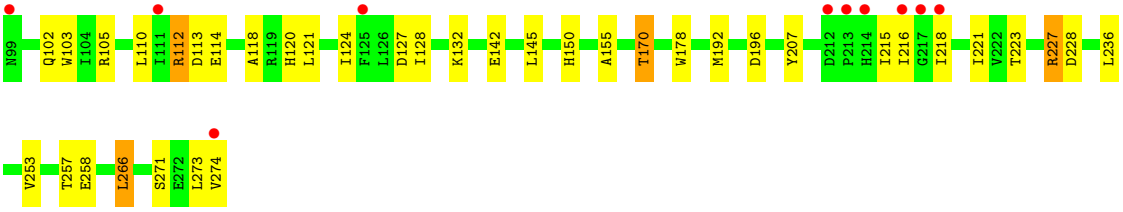
Chain B:



• Molecule 1: Sensor protein FixL

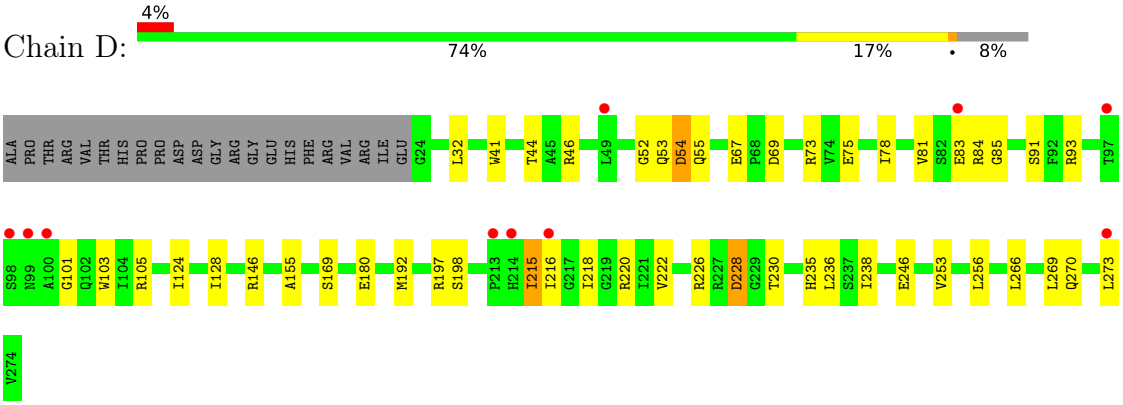
Chain C:





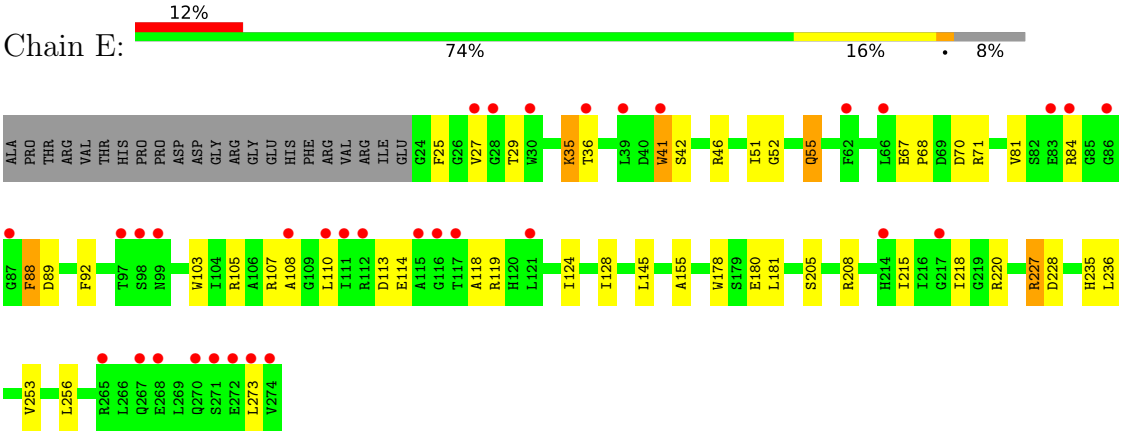
• Molecule 1: Sensor protein FixL

Chain D:



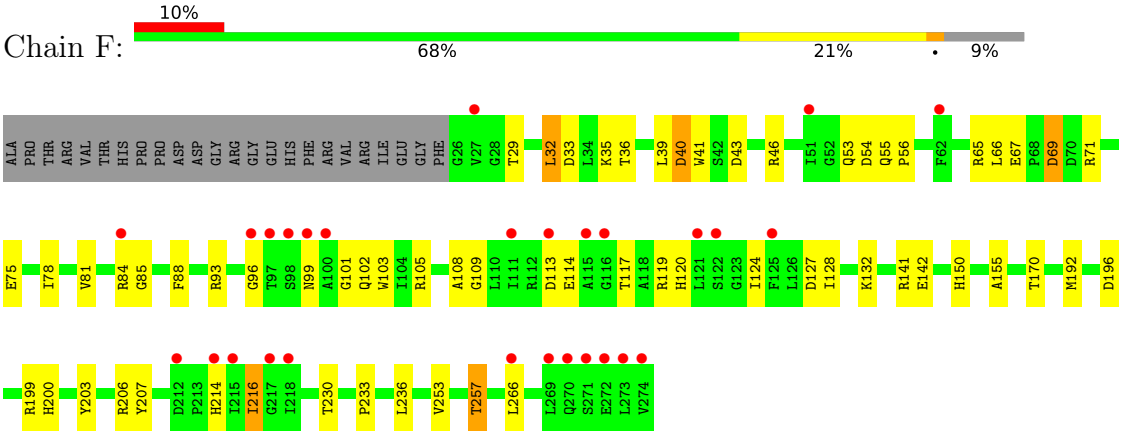
• Molecule 1: Sensor protein FixL

Chain E:



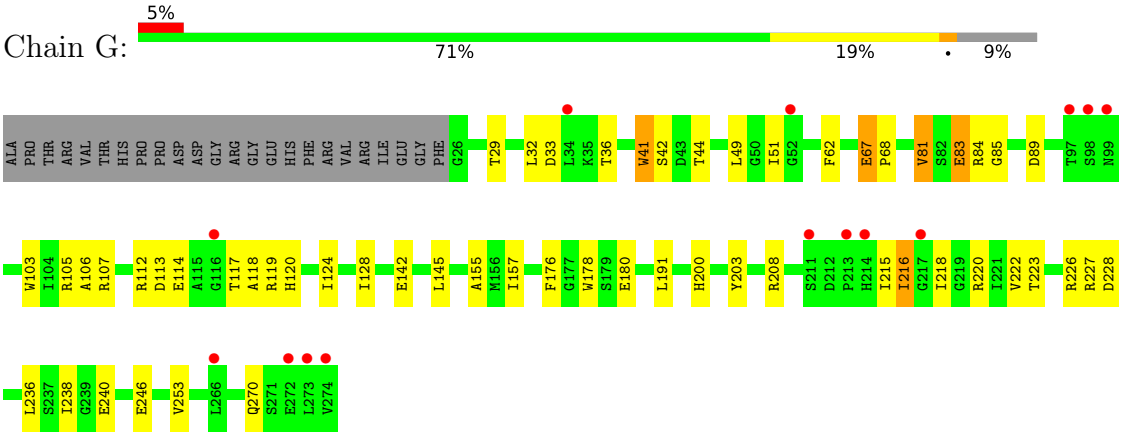
• Molecule 1: Sensor protein FixL

Chain F:



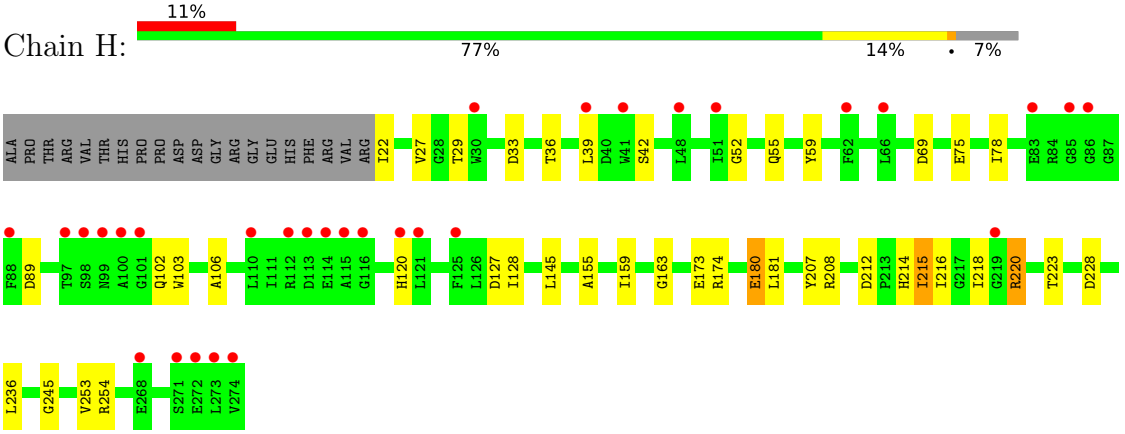
• Molecule 1: Sensor protein FixL

Chain G:



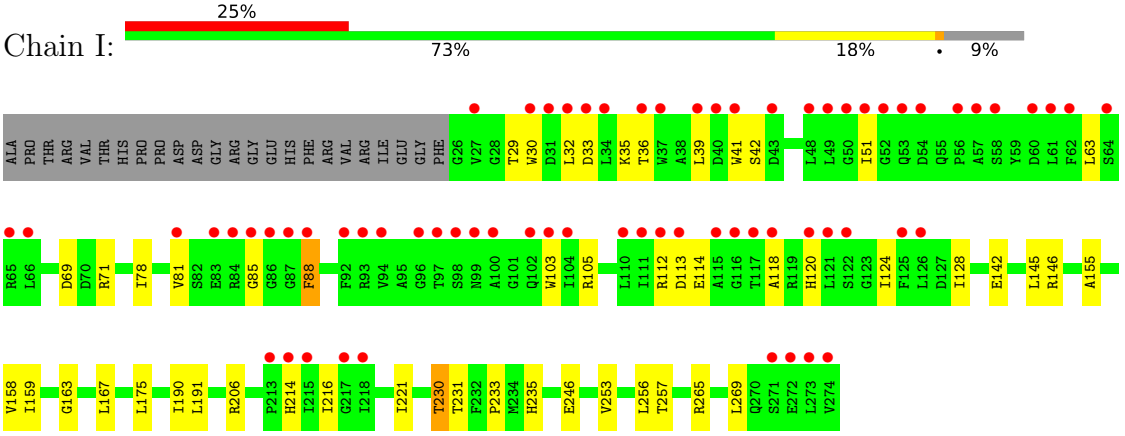
• Molecule 1: Sensor protein FixL

Chain H:



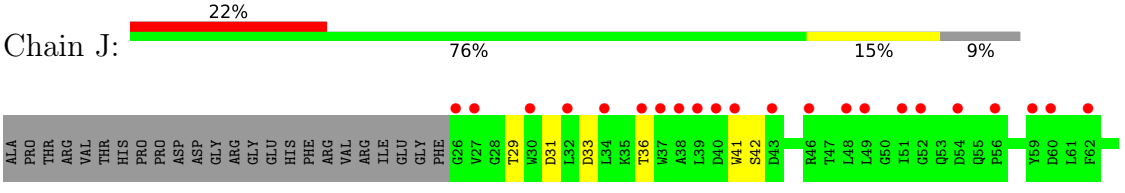
• Molecule 1: Sensor protein FixL

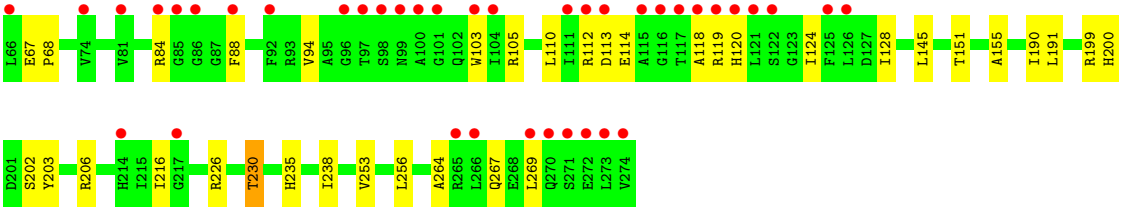
Chain I:



• Molecule 1: Sensor protein FixL

Chain J:




L66
E67
P68
V74
V81
R84
G85
G86
G87
F88
F92
R93
V94
A95
G96
T97
S98
N99
A100
G101
Q102
W103
I104
R105
L110
I111
R112
D113
E114
A115
G116
T117
A118
R119
H120
L121
S122
G123
I124
F125
L126
D127
I128
L145
T151
A155
I190
L191
R199
H200

D201
S202
Y203
R206
H214
I215
I216
G217
R226
T230
H235
I238
V253
L256
A264
R266
L266
Q267
E268
L269
Q270
S271
E272
L273
V274

4 Data and refinement statistics (i)

Property	Value	Source
Space group	C 2 2 21	Depositor
Cell constants a, b, c, α, β, γ	188.85Å 199.31Å 270.01Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	49.83 – 2.85 49.83 – 2.85	Depositor EDS
% Data completeness (in resolution range)	99.7 (49.83-2.85) 92.3 (49.83-2.85)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	1.25 (at 2.86Å)	Xtriage
Refinement program	PHENIX 1.20.1_4487	Depositor
R, R_{free}	0.216 , 0.248 0.217 , 0.248	Depositor DCC
R_{free} test set	5941 reflections (5.04%)	wwPDB-VP
Wilson B-factor (Å^2)	66.3	Xtriage
Anisotropy	0.203	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.30 , 61.9	EDS
L-test for twinning[2]	$< \|L\| > = 0.50$, $< L^2 > = 0.33$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o,F_c correlation	0.94	EDS
Total number of atoms	20488	wwPDB-VP
Average B, all atoms (Å^2)	115.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.47% of the height of the origin peak. No significant pseudotranslation is detected.*

[1] Intensities estimated from amplitudes.

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

5 Model quality

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: IMD, HEM, GOL

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	0.35	0/2049	0.74	0/2769
1	B	0.31	0/2037	0.68	0/2754
1	C	0.32	0/2029	0.67	0/2743
1	D	0.33	0/2031	0.70	0/2746
1	E	0.30	0/2031	0.67	0/2746
1	F	0.31	0/2004	0.67	0/2710
1	G	0.31	0/2004	0.68	0/2710
1	H	0.29	0/2048	0.67	0/2769
1	I	0.29	0/2015	0.66	0/2725
1	J	0.29	0/2015	0.67	0/2725
All	All	0.31	0/20263	0.68	0/27397

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	2000	0	1961	32	0
1	B	1998	0	1948	26	0
1	C	1990	0	1937	26	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	D	1988	0	1938	29	0
1	E	1988	0	1938	24	0
1	F	1966	0	1919	33	0
1	G	1966	0	1919	27	0
1	H	2005	0	1955	20	0
1	I	1973	0	1926	25	0
1	J	1973	0	1926	20	0
2	A	43	0	30	4	0
2	B	43	0	30	2	0
2	C	43	0	30	5	0
2	D	43	0	30	6	0
2	E	43	0	30	4	0
2	F	43	0	30	1	0
2	G	43	0	30	4	0
2	H	43	0	30	1	0
2	I	43	0	30	1	0
2	J	43	0	30	3	0
3	A	6	0	8	1	0
3	B	12	0	16	1	0
3	C	12	0	16	1	0
3	D	6	0	8	0	0
3	E	12	0	16	1	0
3	F	6	0	8	2	0
3	G	6	0	8	0	0
3	H	12	0	16	1	0
3	I	12	0	16	2	0
3	J	6	0	8	0	0
4	A	5	0	4	3	0
4	B	5	0	4	2	0
4	C	5	0	4	0	0
4	D	5	0	4	6	0
4	E	5	0	4	1	0
4	F	5	0	4	0	0
4	G	5	0	4	2	0
4	H	5	0	4	1	0
4	I	5	0	4	0	0
4	J	5	0	4	3	0
5	A	17	0	0	0	0
5	B	7	0	0	0	0
5	C	1	0	0	0	0
5	D	21	0	0	1	0
5	E	9	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
5	F	1	0	0	0	0
5	G	5	0	0	0	0
5	H	4	0	0	0	0
5	I	2	0	0	0	0
5	J	4	0	0	0	0
All	All	20488	0	19827	272	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 7.

All (272) 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)
1:F:155:ALA:HB3	1:F:253:VAL:HB	1.72	0.71
1:C:112:ARG:HE	1:C:118:ALA:HB2	1.56	0.70
1:G:67:GLU:HG3	1:G:68:PRO:HD2	1.74	0.69
1:J:155:ALA:HB3	1:J:253:VAL:HB	1.74	0.69
1:B:102:GLN:NE2	1:B:127:ASP:OD1	2.25	0.69
1:J:112:ARG:HE	1:J:118:ALA:HB2	1.58	0.69
1:G:33:ASP:HB3	1:G:120:HIS:HB3	1.76	0.68
1:H:155:ALA:HB3	1:H:253:VAL:HB	1.75	0.68
1:A:155:ALA:HB3	1:A:253:VAL:HB	1.76	0.67
1:A:192:MET:HE1	1:A:200:HIS:HB2	1.76	0.67
1:E:155:ALA:HB3	1:E:253:VAL:HB	1.78	0.66
1:F:43:ASP:HA	1:F:46:ARG:HD2	1.77	0.66
1:I:81:VAL:HA	1:I:85:GLY:HA3	1.78	0.65
1:A:218:ILE:HG12	1:E:218:ILE:HG12	1.79	0.65
1:C:103:TRP:HB3	1:C:128:ILE:HG13	1.79	0.64
1:D:155:ALA:HB3	1:D:253:VAL:HB	1.77	0.64
1:E:29:THR:HG22	1:E:42:SER:HB2	1.78	0.64
1:I:221:ILE:HG22	1:I:235:HIS:HB2	1.78	0.64
2:G:601:HEM:HHC	2:G:601:HEM:HBB2	1.80	0.64
1:E:180:GLU:HG3	1:E:181:LEU:HD12	1.80	0.64
2:J:302:HEM:HHC	2:J:302:HEM:HBB2	1.80	0.62
1:G:215:ILE:HA	1:G:218:ILE:HG13	1.80	0.62
1:C:29:THR:H	1:C:42:SER:HB3	1.62	0.62
1:A:212:ASP:HB3	1:A:213:PRO:HD3	1.82	0.62
1:H:215:ILE:HD11	1:H:220:ARG:HB3	1.82	0.62
1:A:103:TRP:HB3	1:A:128:ILE:HG13	1.80	0.62
1:C:145:LEU:HB2	3:C:602:GOL:H11	1.82	0.62
1:C:155:ALA:HB3	1:C:253:VAL:HB	1.82	0.62

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:180:GLU:OE2	1:I:146:ARG:NH1	2.33	0.62
1:D:228:ASP:N	1:D:228:ASP:OD1	2.29	0.61
1:H:29:THR:H	1:H:42:SER:HB3	1.65	0.61
1:I:269:LEU:HD23	1:J:269:LEU:HD12	1.81	0.61
2:F:302:HEM:HBB2	2:F:302:HEM:HHC	1.82	0.61
1:J:105:ARG:HB2	1:J:128:ILE:HD13	1.83	0.60
1:E:103:TRP:HB3	1:E:128:ILE:HG13	1.83	0.60
1:E:35:LYS:HD3	1:E:119:ARG:HG2	1.82	0.60
1:H:52:GLY:HA2	1:H:55:GLN:HG2	1.85	0.59
1:B:113:ASP:OD2	1:B:119:ARG:NH2	2.36	0.58
1:G:145:LEU:HB2	3:H:302:GOL:H2	1.84	0.58
1:A:33:ASP:HA	1:A:120:HIS:HA	1.84	0.58
2:H:303:HEM:HHC	2:H:303:HEM:HBB2	1.84	0.58
1:I:159:ILE:HD12	1:I:163:GLY:HA2	1.85	0.58
1:J:67:GLU:HG3	1:J:68:PRO:HD2	1.86	0.58
1:F:141:ARG:HH12	3:F:301:GOL:H11	1.68	0.58
2:B:303:HEM:HBB2	2:B:303:HEM:HHC	1.86	0.57
1:B:103:TRP:HB3	1:B:128:ILE:HG13	1.86	0.57
1:D:52:GLY:HA2	1:D:55:GLN:HB2	1.87	0.57
1:D:46:ARG:NH2	1:D:55:GLN:O	2.36	0.57
1:J:238:ILE:HD11	4:J:303:IMD:H2	1.85	0.57
1:D:103:TRP:HB3	1:D:128:ILE:HG13	1.86	0.57
2:D:302:HEM:ND	4:D:303:IMD:C2	2.67	0.57
1:B:155:ALA:HB3	1:B:253:VAL:HB	1.87	0.57
1:H:33:ASP:HB3	1:H:120:HIS:HB3	1.86	0.57
1:J:264:ALA:O	1:J:267:GLN:NE2	2.36	0.57
1:E:215:ILE:HB	2:E:601:HEM:HBA1	1.87	0.56
1:A:102:GLN:NE2	1:A:127:ASP:OD1	2.38	0.56
1:I:233:PRO:HD2	1:I:257:THR:HG22	1.86	0.56
1:E:52:GLY:H	1:E:55:GLN:HE21	1.53	0.56
1:G:29:THR:HG22	1:G:124:ILE:HG22	1.87	0.56
1:I:155:ALA:HB3	1:I:253:VAL:HB	1.88	0.56
2:A:601:HEM:ND	4:A:603:IMD:C2	2.68	0.56
1:F:69:ASP:OD1	1:F:69:ASP:N	2.30	0.56
1:B:33:ASP:HA	1:B:120:HIS:HA	1.87	0.56
1:J:190:ILE:HG13	1:J:191:LEU:HD12	1.88	0.56
1:E:89:ASP:HB2	1:E:107:ARG:HG2	1.88	0.56
1:I:29:THR:HG22	1:I:124:ILE:HG22	1.88	0.55
1:G:113:ASP:OD1	1:G:114:GLU:N	2.39	0.55
1:I:206:ARG:NH2	2:I:601:HEM:O1A	2.38	0.55
1:F:102:GLN:NE2	1:F:127:ASP:OD1	2.37	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:192:MET:HE3	1:F:196:ASP:HB3	1.88	0.55
1:C:192:MET:HE3	1:C:196:ASP:HB3	1.89	0.55
1:D:93:ARG:HH11	1:D:101:GLY:H	1.53	0.55
1:D:73:ARG:NH2	1:D:91:SER:O	2.38	0.55
1:E:178:TRP:CE2	1:E:227:ARG:HB2	2.42	0.55
1:B:113:ASP:OD1	1:B:114:GLU:N	2.39	0.54
1:E:110:LEU:HD11	1:E:118:ALA:HB1	1.89	0.54
1:A:236:LEU:HD21	1:A:238:ILE:HD11	1.90	0.54
1:G:155:ALA:HB3	1:G:253:VAL:HB	1.90	0.54
1:H:102:GLN:NE2	1:H:127:ASP:OD1	2.37	0.54
2:E:601:HEM:HHC	2:E:601:HEM:HBB2	1.88	0.54
1:F:29:THR:HG22	1:F:124:ILE:HG22	1.89	0.54
1:E:113:ASP:OD1	1:E:114:GLU:N	2.41	0.53
1:I:113:ASP:OD1	1:I:114:GLU:N	2.40	0.53
1:F:233:PRO:HD2	1:F:257:THR:HG23	1.91	0.53
1:F:40:ASP:OD1	1:F:40:ASP:N	2.41	0.53
1:B:215:ILE:HA	1:B:218:ILE:HD12	1.91	0.52
1:J:103:TRP:HB3	1:J:128:ILE:HG13	1.90	0.52
1:B:105:ARG:HB2	1:B:128:ILE:HD13	1.91	0.52
1:B:32:LEU:HD13	1:B:39:LEU:HD12	1.90	0.52
1:B:218:ILE:HG12	1:C:218:ILE:HG12	1.89	0.52
1:H:207:TYR:HE1	1:H:216:ILE:HG12	1.74	0.52
1:B:29:THR:H	1:B:42:SER:HB3	1.75	0.52
1:G:29:THR:H	1:G:42:SER:HB3	1.75	0.52
1:F:35:LYS:HE2	1:F:119:ARG:HG3	1.91	0.51
1:A:74:VAL:HG22	1:A:90:VAL:HG21	1.91	0.51
1:I:69:ASP:OD1	1:I:69:ASP:N	2.41	0.51
1:H:69:ASP:N	1:H:69:ASP:OD1	2.43	0.51
1:F:192:MET:HE2	1:F:200:HIS:HB2	1.93	0.51
1:J:113:ASP:OD2	1:J:119:ARG:NH2	2.44	0.51
1:I:29:THR:H	1:I:42:SER:HB3	1.76	0.51
1:J:235:HIS:HB2	1:J:256:LEU:HD11	1.93	0.50
1:C:150:HIS:HA	1:C:170:THR:HG23	1.94	0.50
1:F:113:ASP:OD1	1:F:114:GLU:N	2.44	0.50
1:D:93:ARG:HE	1:D:101:GLY:HA3	1.77	0.49
1:I:63:LEU:HD22	1:I:71:ARG:HB2	1.93	0.49
1:I:190:ILE:HG13	1:I:191:LEU:HD12	1.93	0.49
1:J:113:ASP:OD1	1:J:114:GLU:N	2.45	0.49
1:H:236:LEU:HD21	4:H:304:IMD:C5	2.42	0.49
1:D:105:ARG:HB2	1:D:128:ILE:HD13	1.95	0.49
1:E:235:HIS:HB2	1:E:256:LEU:HD11	1.94	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:240:GLU:OE1	1:B:242:GLN:NE2	2.45	0.49
1:A:194:GLU:OE1	1:A:198:SER:OG	2.28	0.48
1:H:215:ILE:HD11	1:H:220:ARG:HD2	1.95	0.48
1:D:236:LEU:HD23	4:D:303:IMD:C5	2.42	0.48
1:I:105:ARG:HB2	1:I:128:ILE:HD13	1.95	0.48
1:A:112:ARG:HG2	1:A:118:ALA:HA	1.96	0.48
1:C:49:LEU:HD21	1:C:62:PHE:HD1	1.78	0.48
1:J:226:ARG:HH11	1:J:230:THR:HB	1.78	0.48
1:C:113:ASP:OD1	1:C:114:GLU:N	2.43	0.48
1:A:81:VAL:HG22	1:A:110:LEU:HD23	1.95	0.48
2:D:302:HEM:NB	4:D:303:IMD:C4	2.76	0.48
1:A:105:ARG:HB2	1:A:128:ILE:HD13	1.96	0.48
1:C:215:ILE:HG13	2:C:601:HEM:HAA2	1.96	0.48
1:D:192:MET:HE2	1:D:197:ARG:HA	1.96	0.48
1:I:103:TRP:HB3	1:I:128:ILE:HG13	1.96	0.48
1:J:200:HIS:HA	1:J:203:TYR:CD2	2.49	0.48
2:J:302:HEM:NB	4:J:303:IMD:C4	2.77	0.48
1:A:212:ASP:HB3	1:A:213:PRO:CD	2.43	0.47
1:D:226:ARG:NH2	5:D:401:HOH:O	2.46	0.47
2:D:302:HEM:HHC	2:D:302:HEM:HBB2	1.94	0.47
1:G:220:ARG:NH2	2:G:601:HEM:O1A	2.47	0.47
1:F:103:TRP:HB3	1:F:128:ILE:HG13	1.96	0.47
1:I:112:ARG:HE	1:I:118:ALA:HB2	1.80	0.47
2:A:601:HEM:ND	4:A:603:IMD:H2	2.28	0.47
1:B:145:LEU:HB2	3:B:302:GOL:H32	1.97	0.47
1:D:236:LEU:HD13	1:D:253:VAL:HG22	1.96	0.47
1:D:266:LEU:O	1:D:270:GLN:HB2	2.14	0.47
1:G:216:ILE:HG22	1:G:238:ILE:HB	1.96	0.47
1:A:89:ASP:HB2	1:A:107:ARG:HG2	1.97	0.47
2:G:601:HEM:C4A	4:G:603:IMD:H4	2.50	0.47
1:D:218:ILE:HG12	1:H:218:ILE:HG12	1.96	0.46
2:D:302:HEM:ND	4:D:303:IMD:H2	2.30	0.46
1:A:146[B]:ARG:NH2	1:D:180:GLU:OE2	2.49	0.46
1:C:33:ASP:HA	1:C:120:HIS:HA	1.97	0.46
1:D:236:LEU:HD21	1:D:238:ILE:HD11	1.98	0.46
1:A:222:VAL:HG12	1:A:234:MET:HG3	1.98	0.46
1:G:49:LEU:HD21	1:G:62:PHE:HD1	1.80	0.46
1:G:105:ARG:HB2	1:G:128:ILE:HD13	1.97	0.46
1:A:75:GLU:O	1:A:78:ILE:HG13	2.15	0.46
1:A:33:ASP:N	1:A:33:ASP:OD1	2.46	0.46
1:C:110:LEU:HD22	1:C:118:ALA:HB1	1.98	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:145:LEU:HB2	3:E:602:GOL:H2	1.97	0.46
1:I:145:LEU:HD13	3:I:602:GOL:H11	1.98	0.46
1:J:33:ASP:HA	1:J:120:HIS:HA	1.97	0.46
1:A:88:PHE:HD2	1:A:108:ALA:HB3	1.79	0.46
1:C:178:TRP:CE2	1:C:227:ARG:HB2	2.51	0.46
1:H:103:TRP:HB3	1:H:128:ILE:HG13	1.98	0.46
1:H:207:TYR:CE1	1:H:216:ILE:HG12	2.49	0.46
1:F:54:ASP:N	1:F:54:ASP:OD1	2.49	0.46
1:G:81:VAL:HA	1:G:85:GLY:HA3	1.98	0.46
1:A:34:LEU:N	1:A:119:ARG:O	2.45	0.45
1:B:49:LEU:HD21	1:B:62:PHE:HD1	1.81	0.45
1:C:102:GLN:NE2	1:C:127:ASP:OD1	2.49	0.45
1:E:41:TRP:NE1	1:E:46:ARG:HG2	2.31	0.45
1:F:81:VAL:HA	1:F:85:GLY:HA3	1.98	0.45
1:C:227:ARG:HG2	1:H:245:GLY:HA2	1.98	0.45
1:I:158:VAL:HB	1:I:167:LEU:HB2	1.99	0.45
2:J:302:HEM:C1B	4:J:303:IMD:H4	2.51	0.45
2:D:302:HEM:C1B	4:D:303:IMD:H4	2.51	0.45
1:E:215:ILE:N	2:E:601:HEM:O2D	2.32	0.45
1:F:88:PHE:HB3	1:F:108:ALA:HB3	1.98	0.45
1:F:200:HIS:HA	1:F:203:TYR:CD2	2.52	0.45
1:G:89:ASP:HB2	1:G:107:ARG:HG2	1.97	0.45
1:D:235:HIS:HB2	1:D:256:LEU:HD11	1.99	0.45
1:E:52:GLY:HA2	1:E:55:GLN:HG2	1.98	0.45
1:E:68:PRO:HA	1:E:71:ARG:HG2	1.99	0.45
1:F:75:GLU:O	1:F:78:ILE:HG13	2.17	0.45
1:E:105:ARG:HB2	1:E:128:ILE:HD13	1.98	0.45
1:C:132:LYS:HD2	1:C:132:LYS:HA	1.83	0.44
1:F:32:LEU:HB3	1:F:39:LEU:HD13	1.98	0.44
1:E:51:ILE:HG13	1:E:55:GLN:NE2	2.32	0.44
1:F:105:ARG:HB2	1:F:128:ILE:HD13	1.99	0.44
1:G:89:ASP:HA	1:G:106:ALA:O	2.18	0.44
1:I:30:TRP:HH2	1:I:88:PHE:HE2	1.66	0.44
1:J:29:THR:H	1:J:42:SER:HB3	1.83	0.44
1:F:55:GLN:HG3	1:F:56:PRO:HD2	1.99	0.44
1:H:39:LEU:HD12	1:H:59:TYR:HA	1.98	0.44
1:F:199:ARG:NH1	1:F:203:TYR:OH	2.50	0.44
1:A:192:MET:HE2	1:A:192:MET:HB2	1.83	0.44
1:A:266:LEU:HD12	1:B:266:LEU:HD23	2.00	0.43
1:C:150:HIS:ND1	1:C:170:THR:HG21	2.33	0.43
1:G:176:PHE:CD1	1:G:191:LEU:HG	2.53	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:J:199:ARG:O	1:J:202:SER:OG	2.27	0.43
1:A:180:GLU:OE2	1:D:146:ARG:NH1	2.51	0.43
1:B:75:GLU:O	1:B:78:ILE:HG13	2.18	0.43
1:F:66:LEU:HB2	1:F:71:ARG:HB3	1.99	0.43
1:G:200:HIS:HA	1:G:203:TYR:CD2	2.52	0.43
1:G:215:ILE:HB	2:G:601:HEM:O2D	2.18	0.43
1:F:35:LYS:H	1:F:35:LYS:HG2	1.68	0.43
1:F:46:ARG:HD3	1:F:53:GLN:O	2.18	0.43
1:F:207:TYR:CE1	1:F:216:ILE:HG12	2.53	0.43
1:B:152:ILE:HA	1:B:153:PRO:HD3	1.92	0.43
2:C:601:HEM:HHC	2:C:601:HEM:HBB2	1.99	0.43
1:I:33:ASP:HA	1:I:120:HIS:HA	2.00	0.43
1:I:51:ILE:HD12	1:I:51:ILE:HA	1.91	0.43
1:H:159:ILE:HD12	1:H:163:GLY:HA2	2.00	0.43
1:A:103:TRP:CG	1:A:132:LYS:HG3	2.53	0.43
1:E:25:PHE:HB2	1:F:109:GLY:HA3	2.01	0.43
1:H:33:ASP:OD1	1:H:33:ASP:N	2.51	0.43
1:H:75:GLU:O	1:H:78:ILE:HG12	2.19	0.43
1:G:51:ILE:HD12	1:G:51:ILE:HA	1.82	0.43
1:A:215:ILE:HG13	2:A:601:HEM:O2D	2.18	0.42
1:B:216:ILE:H	1:B:216:ILE:HG13	1.61	0.42
1:G:113:ASP:HB3	1:G:119:ARG:HG3	2.01	0.42
2:B:303:HEM:C1B	4:B:304:IMD:H4	2.54	0.42
1:G:83:GLU:H	1:G:83:GLU:HG2	1.67	0.42
1:J:110:LEU:HD23	1:J:110:LEU:H	1.85	0.42
1:G:112:ARG:HA	1:G:118:ALA:HA	2.02	0.42
1:H:173:GLU:OE2	1:H:180:GLU:N	2.48	0.42
1:B:219:GLY:HA3	1:B:235:HIS:NE2	2.34	0.42
1:C:216:ILE:H	1:C:216:ILE:HG13	1.65	0.42
2:C:601:HEM:HMC2	2:C:601:HEM:HBC2	2.02	0.42
1:A:236:LEU:HD23	4:A:603:IMD:C5	2.49	0.42
1:D:215:ILE:HG12	1:D:220:ARG:HD2	2.01	0.42
1:G:103:TRP:HB3	1:G:128:ILE:HG13	2.02	0.42
1:I:265:ARG:HA	1:I:265:ARG:HD3	1.81	0.42
1:B:240:GLU:HG3	1:B:249:PHE:CE2	2.55	0.42
1:A:112:ARG:HE	1:A:118:ALA:HB2	1.85	0.42
1:D:53:GLN:HG2	1:D:54:ASP:OD1	2.20	0.42
1:E:88:PHE:HD2	1:E:108:ALA:HB3	1.85	0.42
1:A:89:ASP:HA	1:A:106:ALA:O	2.20	0.41
1:B:258:GLU:O	1:B:262:THR:HG23	2.20	0.41
1:D:192:MET:HE2	1:D:192:MET:HB2	1.82	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:215:ILE:HD12	1:D:215:ILE:HA	1.81	0.41
1:D:216:ILE:H	1:D:216:ILE:HG13	1.56	0.41
2:D:302:HEM:C1D	4:D:303:IMD:H2	2.55	0.41
1:G:41:TRP:HZ3	1:G:62:PHE:HB2	1.85	0.41
1:C:207:TYR:HB2	2:C:601:HEM:HBD2	2.02	0.41
1:C:266:LEU:HD12	1:D:266:LEU:HD23	2.01	0.41
1:D:269:LEU:O	1:D:273:LEU:HB2	2.20	0.41
1:E:236:LEU:HD21	4:E:604:IMD:C5	2.50	0.41
1:F:65:ARG:HH12	1:F:96:GLY:HA2	1.85	0.41
1:F:150:HIS:HA	1:F:170:THR:HG23	2.02	0.41
1:C:75:GLU:O	1:C:78:ILE:HG13	2.20	0.41
1:C:105:ARG:HB2	1:C:128:ILE:HD13	2.01	0.41
1:F:103:TRP:CD2	1:F:132:LYS:HD3	2.55	0.41
3:I:602:GOL:H32	1:J:145:LEU:HD13	2.02	0.41
1:G:178:TRP:CE2	1:G:227:ARG:HB2	2.54	0.41
1:H:89:ASP:HA	1:H:106:ALA:O	2.21	0.41
2:C:601:HEM:HBD1	2:C:601:HEM:HHA	2.01	0.41
1:D:75:GLU:O	1:D:78:ILE:HG13	2.20	0.41
1:A:141:ARG:NH2	3:A:602:GOL:O1	2.39	0.41
1:B:236:LEU:HD23	4:B:304:IMD:C5	2.50	0.41
1:A:174:ARG:HH22	1:C:216:ILE:HD13	1.84	0.41
1:B:89:ASP:HA	1:B:106:ALA:O	2.20	0.41
1:D:84:ARG:HG3	1:D:85:GLY:H	1.86	0.41
1:F:33:ASP:HA	1:F:120:HIS:HA	2.03	0.41
1:G:216:ILE:H	1:G:216:ILE:HG13	1.60	0.41
2:A:601:HEM:HBB2	2:A:601:HEM:HHC	2.02	0.41
1:B:189:ASN:HA	1:B:192:MET:HE3	2.02	0.41
1:B:218:ILE:HD13	1:C:218:ILE:HG23	2.02	0.41
1:C:67:GLU:HG3	1:C:68:PRO:HD2	2.02	0.40
1:G:236:LEU:HD21	4:G:603:IMD:C5	2.51	0.40
1:I:32:LEU:HB3	1:I:39:LEU:HG	2.03	0.40
1:D:192:MET:CE	1:D:197:ARG:HA	2.51	0.40
1:I:230:THR:OG1	1:I:231:THR:N	2.55	0.40
1:J:29:THR:HG22	1:J:124:ILE:HG22	2.03	0.40
1:A:93:ARG:HH11	1:A:101:GLY:N	2.19	0.40
2:E:601:HEM:HMC1	2:E:601:HEM:HBC2	2.03	0.40
1:F:93:ARG:CZ	1:F:101:GLY:HA3	2.52	0.40
1:F:141:ARG:NH2	3:F:301:GOL:O2	2.37	0.40
1:B:33:ASP:OD1	1:B:38:ALA:N	2.48	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	251/273 (92%)	245 (98%)	3 (1%)	3 (1%)	13	35
1	B	251/273 (92%)	245 (98%)	6 (2%)	0	100	100
1	C	250/273 (92%)	246 (98%)	3 (1%)	1 (0%)	34	62
1	D	250/273 (92%)	248 (99%)	2 (1%)	0	100	100
1	E	250/273 (92%)	246 (98%)	3 (1%)	1 (0%)	34	62
1	F	247/273 (90%)	243 (98%)	3 (1%)	1 (0%)	34	62
1	G	247/273 (90%)	242 (98%)	4 (2%)	1 (0%)	34	62
1	H	252/273 (92%)	246 (98%)	6 (2%)	0	100	100
1	I	248/273 (91%)	245 (99%)	3 (1%)	0	100	100
1	J	248/273 (91%)	244 (98%)	3 (1%)	1 (0%)	34	62
All	All	2494/2730 (91%)	2450 (98%)	36 (1%)	8 (0%)	41	68

All (8) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	98	SER
1	A	212	ASP
1	A	84	ARG
1	C	25	PHE
1	G	84	ARG
1	E	84	ARG
1	F	84	ARG
1	J	84	ARG

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	212/228 (93%)	186 (88%)	26 (12%)	4 12
1	B	211/228 (92%)	198 (94%)	13 (6%)	18 43
1	C	210/228 (92%)	186 (89%)	24 (11%)	5 15
1	D	210/228 (92%)	194 (92%)	16 (8%)	13 33
1	E	210/228 (92%)	193 (92%)	17 (8%)	11 30
1	F	208/228 (91%)	192 (92%)	16 (8%)	13 32
1	G	208/228 (91%)	188 (90%)	20 (10%)	8 22
1	H	212/228 (93%)	197 (93%)	15 (7%)	14 36
1	I	209/228 (92%)	197 (94%)	12 (6%)	20 47
1	J	209/228 (92%)	200 (96%)	9 (4%)	29 59
All	All	2099/2280 (92%)	1931 (92%)	168 (8%)	12 31

All (168) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	25	PHE
1	A	36	THR
1	A	41	TRP
1	A	49	LEU
1	A	64	SER
1	A	73	ARG
1	A	79	LYS
1	A	88	PHE
1	A	89	ASP
1	A	111	ILE
1	A	120	HIS
1	A	130	GLU
1	A	133	GLN
1	A	150[A]	HIS
1	A	150[B]	HIS
1	A	180	GLU
1	A	192	MET
1	A	198	SER
1	A	212	ASP
1	A	214	HIS
1	A	215	ILE
1	A	216	ILE

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Mol	Chain	Res	Type
1	A	221	ILE
1	A	222	VAL
1	A	246	GLU
1	A	273	LEU
1	B	25	PHE
1	B	31	ASP
1	B	36	THR
1	B	41	TRP
1	B	69	ASP
1	B	83	GLU
1	B	181	LEU
1	B	212	ASP
1	B	216	ILE
1	B	220	ARG
1	B	223	THR
1	B	268	GLU
1	B	273	LEU
1	C	25	PHE
1	C	32	LEU
1	C	36	THR
1	C	41	TRP
1	C	42	SER
1	C	55	GLN
1	C	66	LEU
1	C	67	GLU
1	C	112	ARG
1	C	121	LEU
1	C	124	ILE
1	C	142	GLU
1	C	170	THR
1	C	221	ILE
1	C	223	THR
1	C	227	ARG
1	C	228	ASP
1	C	236	LEU
1	C	257	THR
1	C	258	GLU
1	C	266	LEU
1	C	271	SER
1	C	273	LEU
1	C	274	VAL
1	D	32	LEU

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Mol	Chain	Res	Type
1	D	41	TRP
1	D	44	THR
1	D	54	ASP
1	D	67	GLU
1	D	69	ASP
1	D	81	VAL
1	D	83	GLU
1	D	124	ILE
1	D	169	SER
1	D	198	SER
1	D	215	ILE
1	D	222	VAL
1	D	228	ASP
1	D	230	THR
1	D	246	GLU
1	E	27	VAL
1	E	35	LYS
1	E	36	THR
1	E	41	TRP
1	E	55	GLN
1	E	67	GLU
1	E	70	ASP
1	E	81	VAL
1	E	88	PHE
1	E	92	PHE
1	E	124	ILE
1	E	205	SER
1	E	208	ARG
1	E	220	ARG
1	E	227	ARG
1	E	228	ASP
1	E	273	LEU
1	F	32	LEU
1	F	36	THR
1	F	40	ASP
1	F	41	TRP
1	F	67	GLU
1	F	69	ASP
1	F	99	ASN
1	F	117	THR
1	F	142	GLU
1	F	206	ARG

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Mol	Chain	Res	Type
1	F	214	HIS
1	F	216	ILE
1	F	230	THR
1	F	236	LEU
1	F	257	THR
1	F	266	LEU
1	G	32	LEU
1	G	36	THR
1	G	41	TRP
1	G	44	THR
1	G	67	GLU
1	G	81	VAL
1	G	83	GLU
1	G	117	THR
1	G	142	GLU
1	G	157	ILE
1	G	180	GLU
1	G	208	ARG
1	G	216	ILE
1	G	222	VAL
1	G	223	THR
1	G	226	ARG
1	G	228	ASP
1	G	240	GLU
1	G	246	GLU
1	G	270	GLN
1	H	22	ILE
1	H	27	VAL
1	H	36	THR
1	H	145	LEU
1	H	174	ARG
1	H	180	GLU
1	H	181	LEU
1	H	208	ARG
1	H	212	ASP
1	H	214	HIS
1	H	215	ILE
1	H	220	ARG
1	H	223	THR
1	H	228	ASP
1	H	254	ARG
1	I	35	LYS

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Mol	Chain	Res	Type
1	I	36	THR
1	I	41	TRP
1	I	78	ILE
1	I	88	PHE
1	I	142	GLU
1	I	175	LEU
1	I	214	HIS
1	I	216	ILE
1	I	230	THR
1	I	246	GLU
1	I	256	LEU
1	J	31	ASP
1	J	36	THR
1	J	41	TRP
1	J	88	PHE
1	J	94	VAL
1	J	151	THR
1	J	206	ARG
1	J	216	ILE
1	J	230	THR

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (5) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	102	GLN
1	C	102	GLN
1	E	55	GLN
1	E	102	GLN
1	G	261	GLN

5.3.3 RNA (i)

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates (i)

There are no monosaccharides in this entry.

5.6 Ligand geometry (i)

35 ligands are modelled in this entry.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\| > 2$	Counts	RMSZ	$\#\|Z\| > 2$
2	HEM	I	601	1,4	41,50,50	1.41	4 (9%)	45,82,82	1.46	8 (17%)
3	GOL	E	603	-	5,5,5	0.91	0	5,5,5	1.04	0
4	IMD	D	303	2	3,5,5	0.49	0	4,5,5	0.58	0
3	GOL	F	301	-	5,5,5	0.89	0	5,5,5	1.16	0
3	GOL	C	602	-	5,5,5	1.14	0	5,5,5	0.84	0
2	HEM	E	601	1,4	41,50,50	1.46	6 (14%)	45,82,82	1.56	10 (22%)
4	IMD	A	603	2	3,5,5	0.49	0	4,5,5	0.66	0
4	IMD	E	604	2	3,5,5	0.47	0	4,5,5	0.53	0
3	GOL	H	302	-	5,5,5	0.79	0	5,5,5	0.97	0
4	IMD	F	303	2	3,5,5	0.42	0	4,5,5	0.53	0
3	GOL	J	301	-	5,5,5	1.10	0	5,5,5	0.87	0
4	IMD	B	304	2	3,5,5	0.48	0	4,5,5	0.30	0
3	GOL	C	603	-	5,5,5	0.90	0	5,5,5	1.15	0
2	HEM	G	601	1,4	41,50,50	1.50	4 (9%)	45,82,82	1.72	13 (28%)
4	IMD	H	304	2	3,5,5	0.48	0	4,5,5	0.66	0
2	HEM	H	303	1,4	41,50,50	1.44	5 (12%)	45,82,82	1.62	11 (24%)
3	GOL	H	301	-	5,5,5	0.92	0	5,5,5	1.04	0
3	GOL	D	301	-	5,5,5	0.88	0	5,5,5	1.13	1 (20%)
3	GOL	A	602	-	5,5,5	1.10	0	5,5,5	0.93	0
4	IMD	C	604	2	3,5,5	0.40	0	4,5,5	0.67	0
2	HEM	J	302	1,4	41,50,50	1.49	6 (14%)	45,82,82	1.61	12 (26%)
4	IMD	I	604	2	3,5,5	0.44	0	4,5,5	0.53	0
2	HEM	F	302	1,4	41,50,50	1.48	6 (14%)	45,82,82	1.60	8 (17%)
3	GOL	I	602	-	5,5,5	0.94	0	5,5,5	0.95	0
4	IMD	G	603	2	3,5,5	0.41	0	4,5,5	0.72	0
3	GOL	E	602	-	5,5,5	0.95	0	5,5,5	1.03	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
2	HEM	A	601	1,4	41,50,50	1.50	6 (14%)	45,82,82	1.51	9 (20%)
2	HEM	C	601	1,4	41,50,50	1.51	5 (12%)	45,82,82	1.95	16 (35%)
2	HEM	D	302	1,4	41,50,50	1.47	6 (14%)	45,82,82	1.64	12 (26%)
2	HEM	B	303	1,4	41,50,50	1.50	5 (12%)	45,82,82	1.55	8 (17%)
3	GOL	B	302	-	5,5,5	1.03	0	5,5,5	0.88	0
3	GOL	G	602	-	5,5,5	0.87	0	5,5,5	1.22	1 (20%)
3	GOL	B	301	-	5,5,5	0.69	0	5,5,5	1.22	1 (20%)
3	GOL	I	603	-	5,5,5	0.79	0	5,5,5	1.18	0
4	IMD	J	303	2	3,5,5	0.44	0	4,5,5	0.43	0

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
2	HEM	I	601	1,4	-	2/12/54/54	-
3	GOL	E	603	-	-	2/4/4/4	-
4	IMD	D	303	2	-	-	0/1/1/1
3	GOL	F	301	-	-	3/4/4/4	-
3	GOL	C	602	-	-	0/4/4/4	-
2	HEM	E	601	1,4	-	4/12/54/54	-
4	IMD	A	603	2	-	-	0/1/1/1
4	IMD	E	604	2	-	-	0/1/1/1
3	GOL	H	302	-	-	0/4/4/4	-
4	IMD	F	303	2	-	-	0/1/1/1
3	GOL	J	301	-	-	1/4/4/4	-
4	IMD	B	304	2	-	-	0/1/1/1
3	GOL	C	603	-	-	0/4/4/4	-
2	HEM	G	601	1,4	-	5/12/54/54	-
4	IMD	H	304	2	-	-	0/1/1/1
2	HEM	H	303	1,4	-	4/12/54/54	-
3	GOL	H	301	-	-	4/4/4/4	-
3	GOL	D	301	-	-	2/4/4/4	-
3	GOL	A	602	-	-	2/4/4/4	-
4	IMD	C	604	2	-	-	0/1/1/1
2	HEM	J	302	1,4	-	3/12/54/54	-
4	IMD	I	604	2	-	-	0/1/1/1
2	HEM	F	302	1,4	-	4/12/54/54	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
3	GOL	I	602	-	-	2/4/4/4	-
4	IMD	G	603	2	-	-	0/1/1/1
3	GOL	E	602	-	-	0/4/4/4	-
2	HEM	A	601	1,4	-	3/12/54/54	-
2	HEM	C	601	1,4	-	8/12/54/54	-
2	HEM	D	302	1,4	-	3/12/54/54	-
2	HEM	B	303	1,4	-	3/12/54/54	-
3	GOL	B	302	-	-	0/4/4/4	-
3	GOL	G	602	-	-	2/4/4/4	-
3	GOL	B	301	-	-	2/4/4/4	-
3	GOL	I	603	-	-	2/4/4/4	-
4	IMD	J	303	2	-	-	0/1/1/1

All (53) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	G	601	HEM	C3C-CAC	3.88	1.55	1.47
2	A	601	HEM	C3C-CAC	3.85	1.55	1.47
2	B	303	HEM	C3C-CAC	3.80	1.55	1.47
2	C	601	HEM	C3C-CAC	3.79	1.55	1.47
2	C	601	HEM	C3C-C2C	-3.77	1.35	1.40
2	H	303	HEM	C3C-CAC	3.76	1.55	1.47
2	D	302	HEM	C3C-CAC	3.75	1.55	1.47
2	J	302	HEM	C3C-CAC	3.75	1.55	1.47
2	I	601	HEM	C3C-CAC	3.73	1.55	1.47
2	D	302	HEM	C3C-C2C	-3.69	1.35	1.40
2	A	601	HEM	C3C-C2C	-3.65	1.35	1.40
2	E	601	HEM	C3C-CAC	3.62	1.55	1.47
2	J	302	HEM	C3C-C2C	-3.62	1.35	1.40
2	F	302	HEM	C3C-CAC	3.59	1.55	1.47
2	G	601	HEM	C3C-C2C	-3.58	1.35	1.40
2	F	302	HEM	C3C-C2C	-3.57	1.35	1.40
2	I	601	HEM	C3C-C2C	-3.53	1.35	1.40
2	E	601	HEM	C3C-C2C	-3.50	1.35	1.40
2	H	303	HEM	C3C-C2C	-3.50	1.35	1.40
2	B	303	HEM	C3C-C2C	-3.25	1.35	1.40
2	E	601	HEM	CAB-C3B	3.21	1.56	1.47
2	B	303	HEM	CAB-C3B	3.00	1.55	1.47
2	J	302	HEM	CAB-C3B	2.97	1.55	1.47
2	G	601	HEM	CAB-C3B	2.92	1.55	1.47

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	C	601	HEM	CAB-C3B	2.89	1.55	1.47
2	I	601	HEM	CAB-C3B	2.86	1.55	1.47
2	H	303	HEM	CAB-C3B	2.85	1.55	1.47
2	A	601	HEM	CAB-C3B	2.85	1.55	1.47
2	F	302	HEM	CAB-C3B	2.81	1.55	1.47
2	D	302	HEM	CAB-C3B	2.80	1.55	1.47
2	B	303	HEM	CAA-C2A	2.56	1.55	1.52
2	E	601	HEM	FE-NB	2.56	2.09	1.96
2	J	302	HEM	CAA-C2A	2.52	1.55	1.52
2	D	302	HEM	FE-NB	2.47	2.09	1.96
2	F	302	HEM	CAA-C2A	2.45	1.55	1.52
2	G	601	HEM	CAA-C2A	2.45	1.55	1.52
2	A	601	HEM	CMD-C2D	2.41	1.55	1.50
2	J	302	HEM	FE-ND	2.39	2.08	1.96
2	H	303	HEM	CAA-C2A	2.34	1.55	1.52
2	D	302	HEM	CAA-C2A	2.31	1.55	1.52
2	C	601	HEM	CAA-C2A	2.27	1.55	1.52
2	E	601	HEM	CAA-C2A	2.27	1.55	1.52
2	F	302	HEM	FE-ND	2.23	2.07	1.96
2	A	601	HEM	FE-NB	2.22	2.07	1.96
2	A	601	HEM	CAA-C2A	2.19	1.55	1.52
2	D	302	HEM	CMD-C2D	2.19	1.55	1.50
2	F	302	HEM	CMD-C2D	2.15	1.55	1.50
2	H	303	HEM	CMD-C2D	2.15	1.55	1.50
2	B	303	HEM	FE-NB	2.12	2.07	1.96
2	E	601	HEM	CMD-C2D	2.08	1.55	1.50
2	I	601	HEM	CAA-C2A	2.08	1.55	1.52
2	C	601	HEM	CMD-C2D	2.03	1.55	1.50
2	J	302	HEM	CMD-C2D	2.00	1.55	1.50

All (110) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	J	302	HEM	C1B-NB-C4B	3.92	109.12	105.07
2	C	601	HEM	CMA-C3A-C4A	-3.83	122.58	128.46
2	H	303	HEM	C3B-C2B-C1B	3.74	109.26	106.49
2	F	302	HEM	C4B-CHC-C1C	3.68	127.41	122.56
2	E	601	HEM	C3B-C2B-C1B	3.61	109.16	106.49
2	D	302	HEM	C4C-CHD-C1D	3.58	127.29	122.56
2	G	601	HEM	C1B-NB-C4B	3.49	108.67	105.07
2	I	601	HEM	C4D-ND-C1D	3.48	108.66	105.07
2	A	601	HEM	C4B-CHC-C1C	3.45	127.11	122.56

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	C	601	HEM	C1B-NB-C4B	3.42	108.60	105.07
2	D	302	HEM	C3B-C2B-C1B	3.39	109.00	106.49
2	J	302	HEM	C3B-C2B-C1B	3.38	108.99	106.49
2	H	303	HEM	C1B-NB-C4B	3.37	108.55	105.07
2	B	303	HEM	C1B-NB-C4B	3.35	108.53	105.07
2	C	601	HEM	C3B-C2B-C1B	3.34	108.96	106.49
2	H	303	HEM	C4D-ND-C1D	3.26	108.44	105.07
2	C	601	HEM	C4D-ND-C1D	3.21	108.39	105.07
2	C	601	HEM	CAD-C3D-C4D	3.20	130.26	124.66
2	G	601	HEM	C3B-C2B-C1B	3.19	108.85	106.49
2	E	601	HEM	C1B-NB-C4B	3.15	108.32	105.07
2	C	601	HEM	CAD-C3D-C2D	-3.14	122.03	127.88
2	E	601	HEM	CMC-C2C-C3C	3.12	130.52	124.68
2	F	302	HEM	C1B-NB-C4B	3.11	108.28	105.07
2	H	303	HEM	C4B-CHC-C1C	3.11	126.66	122.56
2	B	303	HEM	C4C-CHD-C1D	3.01	126.53	122.56
2	B	303	HEM	C4D-ND-C1D	2.95	108.12	105.07
2	F	302	HEM	C4D-ND-C1D	2.95	108.12	105.07
2	F	302	HEM	CMA-C3A-C4A	-2.95	123.93	128.46
2	A	601	HEM	C4D-ND-C1D	2.93	108.10	105.07
2	E	601	HEM	C4D-ND-C1D	2.92	108.09	105.07
2	B	303	HEM	C3B-C2B-C1B	2.92	108.65	106.49
2	C	601	HEM	C4B-CHC-C1C	2.91	126.40	122.56
2	G	601	HEM	CAD-CBD-CGD	-2.91	107.34	113.60
2	B	303	HEM	CMA-C3A-C4A	-2.89	124.02	128.46
2	J	302	HEM	CMA-C3A-C4A	-2.88	124.04	128.46
2	D	302	HEM	CBD-CAD-C3D	-2.87	104.65	112.63
2	G	601	HEM	C4D-ND-C1D	2.86	108.03	105.07
2	A	601	HEM	C1B-NB-C4B	2.86	108.02	105.07
2	H	303	HEM	CMC-C2C-C3C	2.85	130.01	124.68
2	A	601	HEM	CMC-C2C-C3C	2.82	129.95	124.68
2	A	601	HEM	CMA-C3A-C4A	-2.81	124.15	128.46
2	C	601	HEM	C4C-CHD-C1D	2.80	126.25	122.56
2	J	302	HEM	C4B-CHC-C1C	2.78	126.22	122.56
2	F	302	HEM	C3B-C2B-C1B	2.77	108.54	106.49
2	D	302	HEM	C4D-ND-C1D	2.75	107.92	105.07
2	C	601	HEM	CBA-CAA-C2A	2.74	117.30	112.62
2	I	601	HEM	C1B-NB-C4B	2.70	107.86	105.07
2	F	302	HEM	CMC-C2C-C3C	2.69	129.70	124.68
2	I	601	HEM	CMC-C2C-C3C	2.68	129.69	124.68
2	D	302	HEM	CMA-C3A-C4A	-2.68	124.35	128.46
2	A	601	HEM	C3B-C2B-C1B	2.67	108.47	106.49

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	D	302	HEM	CMC-C2C-C3C	2.66	129.66	124.68
2	D	302	HEM	C1B-NB-C4B	2.62	107.78	105.07
2	G	601	HEM	CHD-C1D-ND	2.59	127.24	124.43
2	G	601	HEM	C4B-CHC-C1C	2.59	125.97	122.56
2	J	302	HEM	CHC-C4B-C3B	2.58	128.51	124.57
2	C	601	HEM	CMA-C3A-C2A	2.57	129.79	124.94
2	G	601	HEM	CMC-C2C-C3C	2.56	129.47	124.68
2	B	303	HEM	C4B-CHC-C1C	2.56	125.94	122.56
2	G	601	HEM	C3D-C4D-ND	-2.55	107.33	110.17
2	B	303	HEM	CMC-C2C-C3C	2.55	129.44	124.68
2	I	601	HEM	CMB-C2B-C1B	-2.54	121.17	125.04
2	G	601	HEM	CMA-C3A-C4A	-2.53	124.58	128.46
2	G	601	HEM	C4C-CHD-C1D	2.52	125.89	122.56
2	C	601	HEM	CMC-C2C-C3C	2.49	129.34	124.68
2	C	601	HEM	CAA-CBA-CGA	-2.48	106.80	113.76
2	E	601	HEM	C4C-CHD-C1D	2.47	125.82	122.56
2	I	601	HEM	C4C-CHD-C1D	2.47	125.82	122.56
2	F	302	HEM	CAA-CBA-CGA	-2.46	106.87	113.76
2	J	302	HEM	CBA-CAA-C2A	2.44	116.78	112.62
2	I	601	HEM	C3D-C4D-ND	-2.43	107.46	110.17
2	J	302	HEM	C4C-CHD-C1D	2.41	125.73	122.56
2	C	601	HEM	C2B-C1B-NB	-2.39	107.00	109.84
2	H	303	HEM	CHB-C1B-NB	2.36	127.29	124.38
2	B	303	HEM	CHC-C4B-C3B	2.35	128.16	124.57
2	C	601	HEM	C3D-C4D-ND	-2.33	107.57	110.17
2	J	302	HEM	C2B-C1B-NB	-2.32	107.09	109.84
2	G	601	HEM	CAD-C3D-C2D	-2.32	123.56	127.88
2	C	601	HEM	O2D-CGD-CBD	2.31	121.46	114.03
2	A	601	HEM	C4C-CHD-C1D	2.29	125.58	122.56
2	J	302	HEM	CMC-C2C-C3C	2.29	128.96	124.68
2	D	302	HEM	C3D-C4D-ND	-2.29	107.62	110.17
2	A	601	HEM	C3D-C4D-ND	-2.27	107.64	110.17
2	D	302	HEM	CHC-C4B-C3B	2.27	128.04	124.57
2	D	302	HEM	CHB-C1B-NB	2.27	127.18	124.38
2	J	302	HEM	CAA-CBA-CGA	-2.26	107.42	113.76
2	F	302	HEM	C3D-C4D-ND	-2.24	107.67	110.17
2	H	303	HEM	CHC-C4B-C3B	2.24	128.00	124.57
2	H	303	HEM	C3D-C4D-ND	-2.24	107.68	110.17
2	E	601	HEM	CHC-C4B-C3B	2.22	127.97	124.57
2	G	601	HEM	CHC-C4B-C3B	2.21	127.94	124.57
2	E	601	HEM	CHB-C1B-NB	2.17	127.06	124.38
2	E	601	HEM	CMA-C3A-C4A	-2.16	125.14	128.46

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
3	B	301	GOL	C3-C2-C1	-2.16	103.30	111.70
2	H	303	HEM	C2B-C1B-NB	-2.15	107.29	109.84
2	E	601	HEM	CBD-CAD-C3D	-2.14	106.69	112.63
3	D	301	GOL	C3-C2-C1	-2.12	103.46	111.70
2	C	601	HEM	CHD-C1D-ND	2.11	126.72	124.43
2	I	601	HEM	CAA-CBA-CGA	-2.10	107.87	113.76
2	G	601	HEM	C2B-C1B-NB	-2.09	107.36	109.84
3	G	602	GOL	C3-C2-C1	-2.09	103.57	111.70
2	J	302	HEM	C4D-ND-C1D	2.08	107.22	105.07
2	H	303	HEM	CAA-CBA-CGA	-2.07	107.94	113.76
2	J	302	HEM	CHB-C1B-NB	2.07	126.94	124.38
2	D	302	HEM	O1D-CGD-CBD	-2.04	116.52	123.08
2	I	601	HEM	C3B-C2B-C1B	2.03	107.99	106.49
2	A	601	HEM	CHC-C4B-C3B	2.02	127.67	124.57
2	H	303	HEM	C4C-CHD-C1D	2.02	125.23	122.56
2	D	302	HEM	CAB-C3B-C2B	-2.02	121.94	128.60
2	E	601	HEM	C3D-C4D-ND	-2.02	107.92	110.17

There are no chirality outliers.

All (61) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	C	601	HEM	C1A-C2A-CAA-CBA
2	C	601	HEM	C3A-C2A-CAA-CBA
3	D	301	GOL	O1-C1-C2-C3
3	E	603	GOL	O1-C1-C2-C3
3	H	301	GOL	O1-C1-C2-C3
3	I	603	GOL	C1-C2-C3-O3
2	C	601	HEM	C4D-C3D-CAD-CBD
2	D	302	HEM	C3D-CAD-CBD-CGD
2	E	601	HEM	C3D-CAD-CBD-CGD
3	I	603	GOL	O2-C2-C3-O3
2	C	601	HEM	C2D-C3D-CAD-CBD
3	A	602	GOL	O1-C1-C2-C3
3	B	301	GOL	C1-C2-C3-O3
3	F	301	GOL	O1-C1-C2-C3
3	F	301	GOL	C1-C2-C3-O3
3	G	602	GOL	O1-C1-C2-C3
3	H	301	GOL	C1-C2-C3-O3
3	D	301	GOL	O1-C1-C2-O2
3	E	603	GOL	O1-C1-C2-O2
3	G	602	GOL	O1-C1-C2-O2

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Mol	Chain	Res	Type	Atoms
3	H	301	GOL	O1-C1-C2-O2
2	H	303	HEM	C3D-CAD-CBD-CGD
2	J	302	HEM	C4B-C3B-CAB-CBB
3	A	602	GOL	O1-C1-C2-O2
3	I	602	GOL	O2-C2-C3-O3
2	B	303	HEM	C4B-C3B-CAB-CBB
2	D	302	HEM	C4B-C3B-CAB-CBB
2	E	601	HEM	C4B-C3B-CAB-CBB
2	G	601	HEM	C4B-C3B-CAB-CBB
2	H	303	HEM	C4B-C3B-CAB-CBB
3	B	301	GOL	O2-C2-C3-O3
3	F	301	GOL	O2-C2-C3-O3
3	I	602	GOL	C1-C2-C3-O3
3	J	301	GOL	O2-C2-C3-O3
2	F	302	HEM	C3D-CAD-CBD-CGD
2	F	302	HEM	CAA-CBA-CGA-O1A
2	G	601	HEM	CAD-CBD-CGD-O1D
2	J	302	HEM	CAD-CBD-CGD-O1D
2	G	601	HEM	CAD-CBD-CGD-O2D
2	G	601	HEM	CAA-CBA-CGA-O2A
2	J	302	HEM	CAD-CBD-CGD-O2D
2	A	601	HEM	CAD-CBD-CGD-O2D
2	C	601	HEM	CAD-CBD-CGD-O1D
2	C	601	HEM	CAA-CBA-CGA-O1A
2	H	303	HEM	CAD-CBD-CGD-O1D
2	B	303	HEM	CAD-CBD-CGD-O2D
2	A	601	HEM	CAD-CBD-CGD-O1D
2	F	302	HEM	CAA-CBA-CGA-O2A
2	F	302	HEM	C4B-C3B-CAB-CBB
2	B	303	HEM	CAD-CBD-CGD-O1D
2	I	601	HEM	CAD-CBD-CGD-O2D
2	C	601	HEM	CAA-CBA-CGA-O2A
2	C	601	HEM	CAD-CBD-CGD-O2D
2	H	303	HEM	CAD-CBD-CGD-O2D
3	H	301	GOL	O2-C2-C3-O3
2	G	601	HEM	CAA-CBA-CGA-O1A
2	I	601	HEM	CAD-CBD-CGD-O1D
2	A	601	HEM	CAA-CBA-CGA-O1A
2	E	601	HEM	CAA-CBA-CGA-O1A
2	E	601	HEM	CAA-CBA-CGA-O2A
2	D	302	HEM	CAD-CBD-CGD-O2D

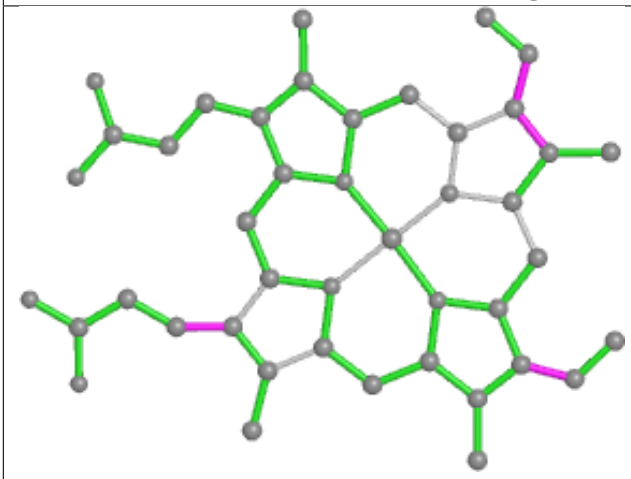
There are no ring outliers.

24 monomers are involved in 47 short contacts:

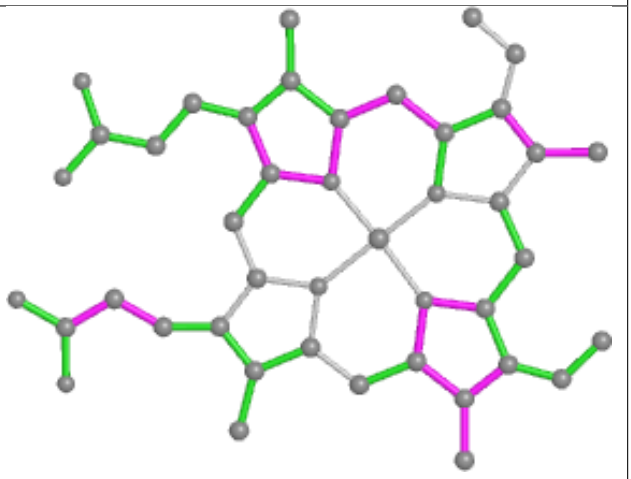
Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	I	601	HEM	1	0
4	D	303	IMD	6	0
3	F	301	GOL	2	0
3	C	602	GOL	1	0
2	E	601	HEM	4	0
4	A	603	IMD	3	0
4	E	604	IMD	1	0
3	H	302	GOL	1	0
4	B	304	IMD	2	0
2	G	601	HEM	4	0
4	H	304	IMD	1	0
2	H	303	HEM	1	0
3	A	602	GOL	1	0
2	J	302	HEM	3	0
2	F	302	HEM	1	0
3	I	602	GOL	2	0
4	G	603	IMD	2	0
3	E	602	GOL	1	0
2	A	601	HEM	4	0
2	C	601	HEM	5	0
2	D	302	HEM	6	0
2	B	303	HEM	2	0
3	B	302	GOL	1	0
4	J	303	IMD	3	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.

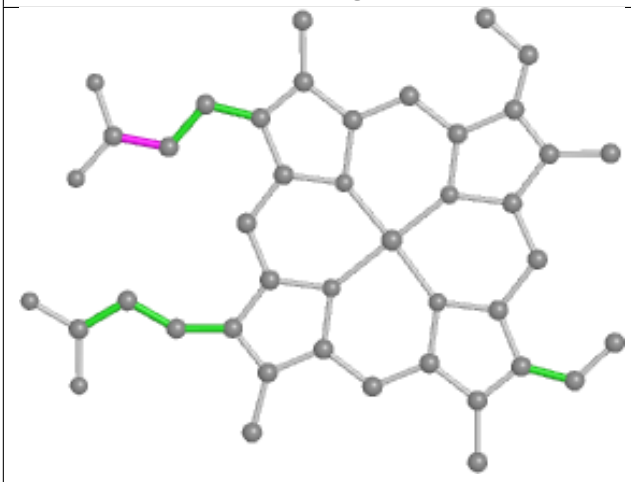
Ligand HEM I 601



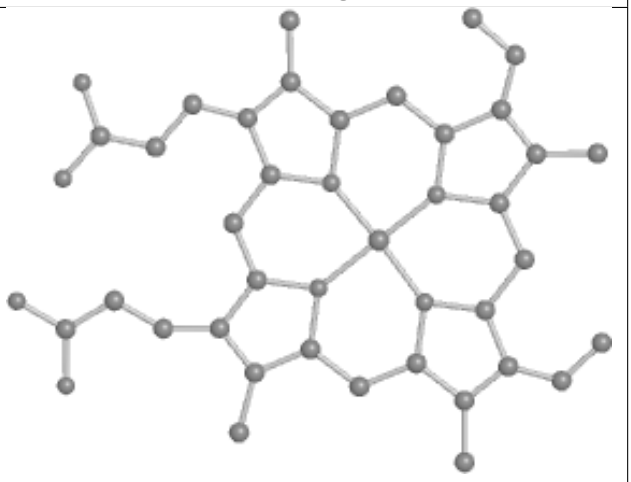
Bond lengths



Bond angles

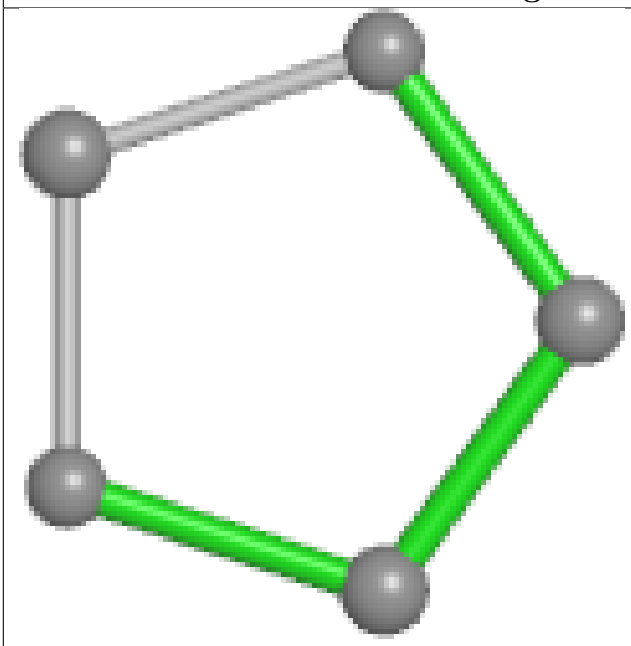


Torsions

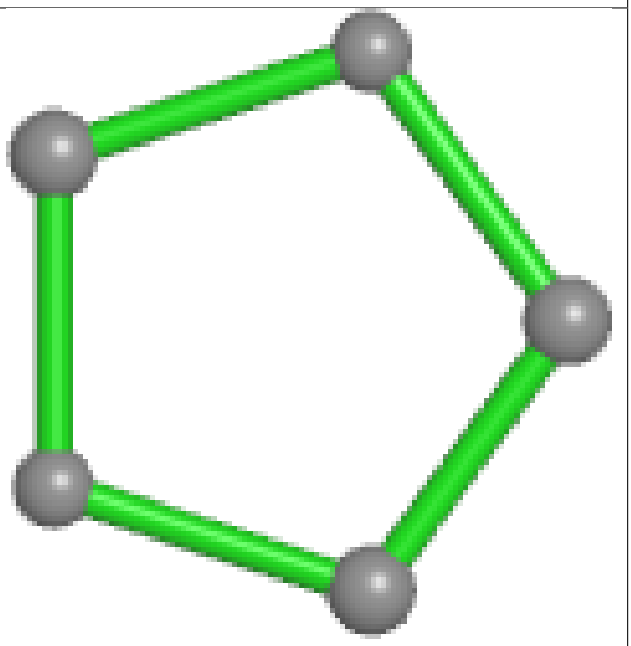


Rings

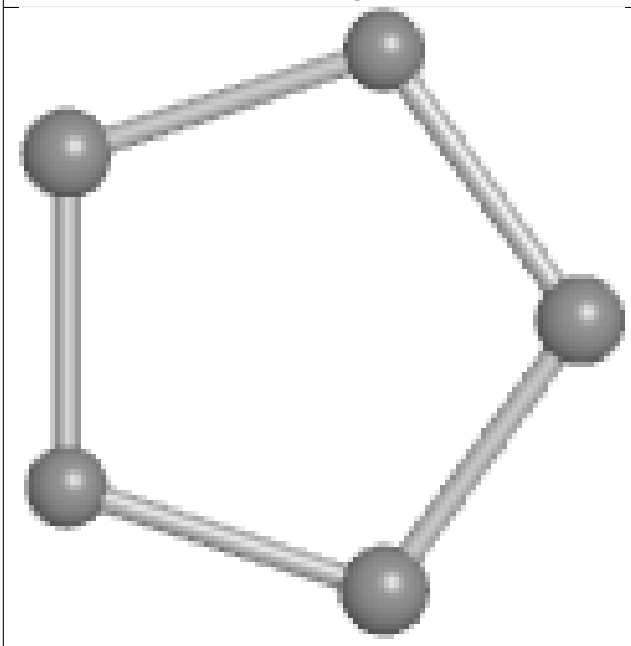
Ligand IMD D 303



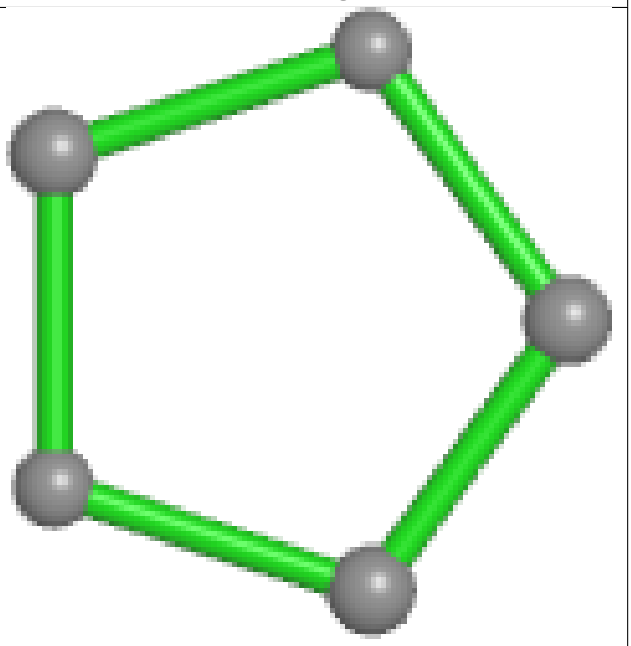
Bond lengths



Bond angles

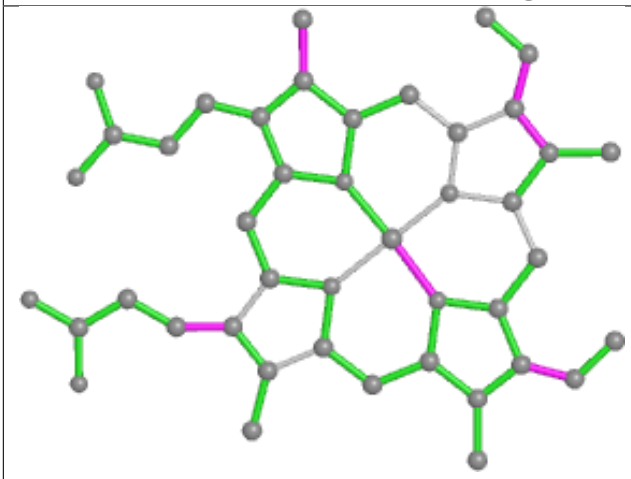


Torsions

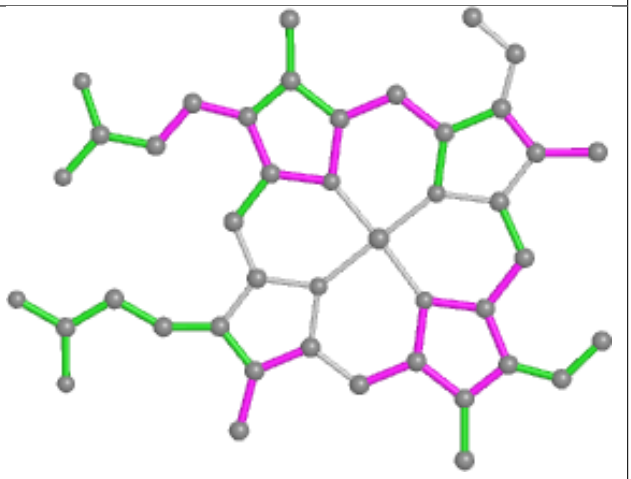


Rings

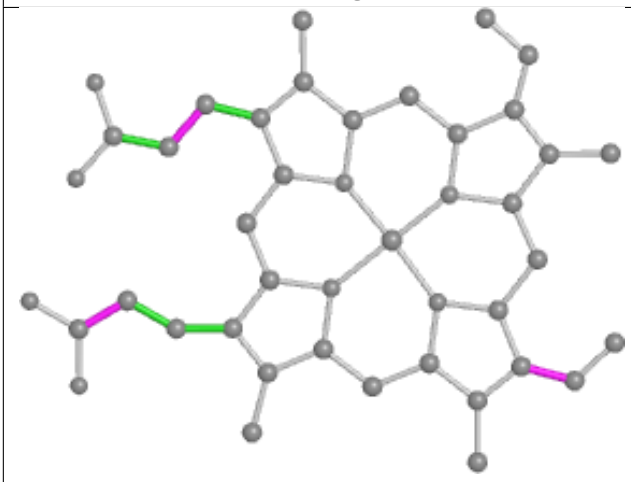
Ligand HEM E 601



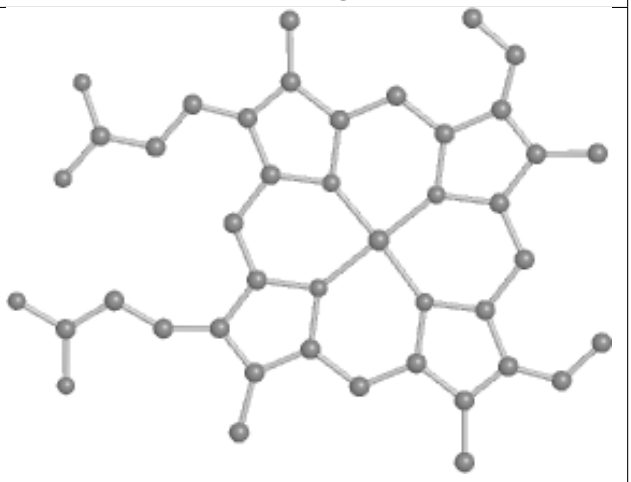
Bond lengths



Bond angles

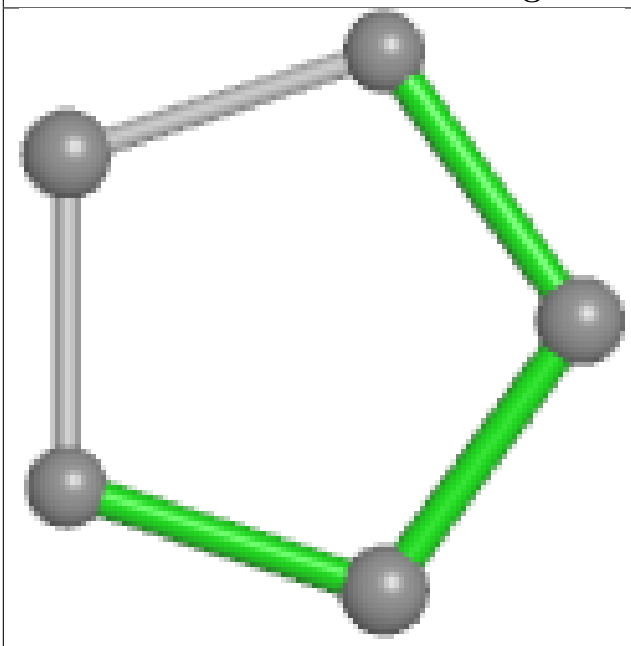


Torsions

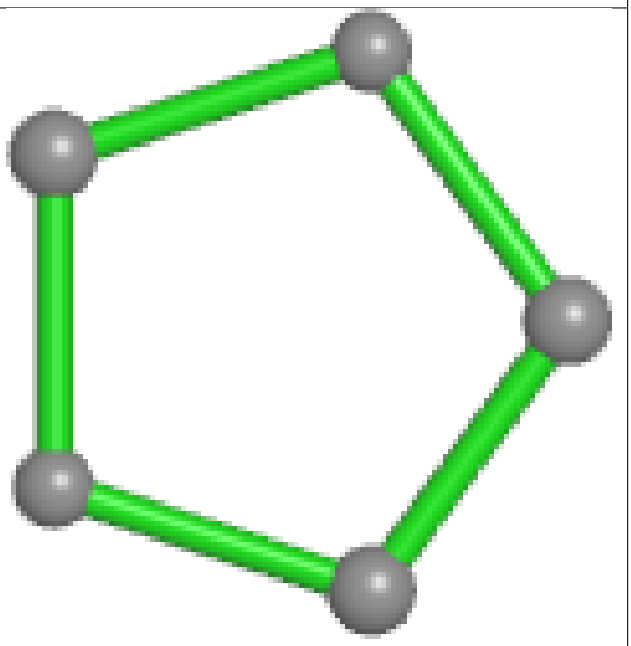


Rings

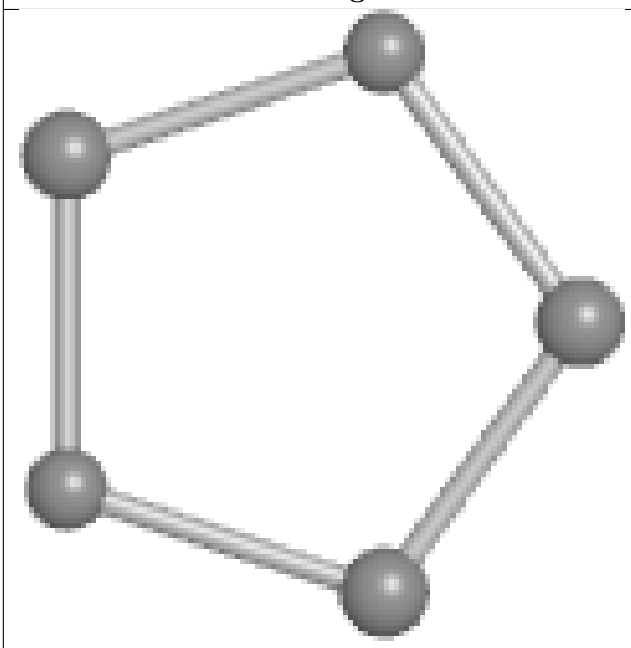
Ligand IMD A 603



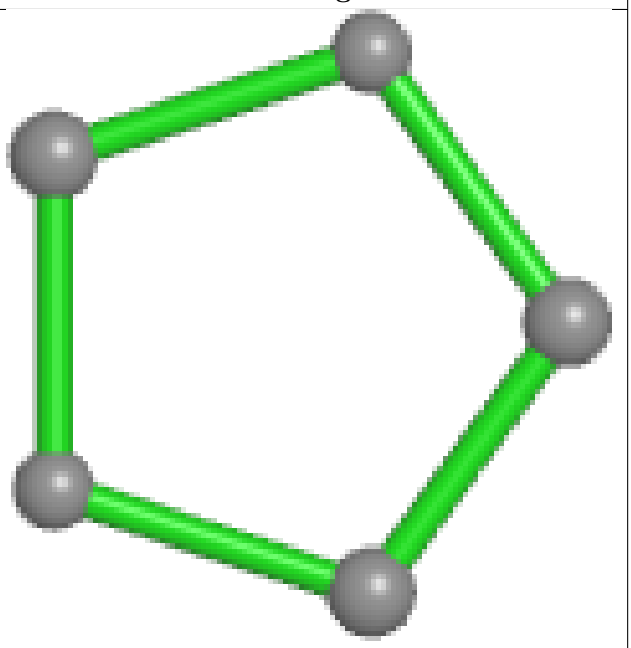
Bond lengths



Bond angles

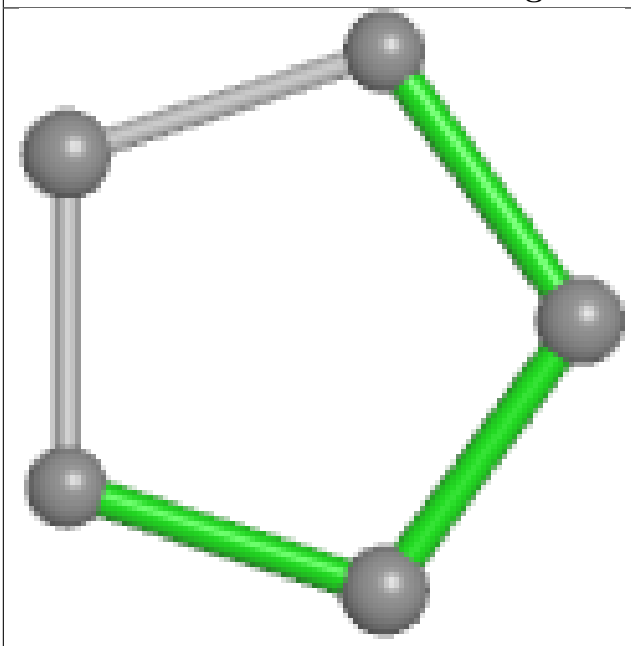


Torsions

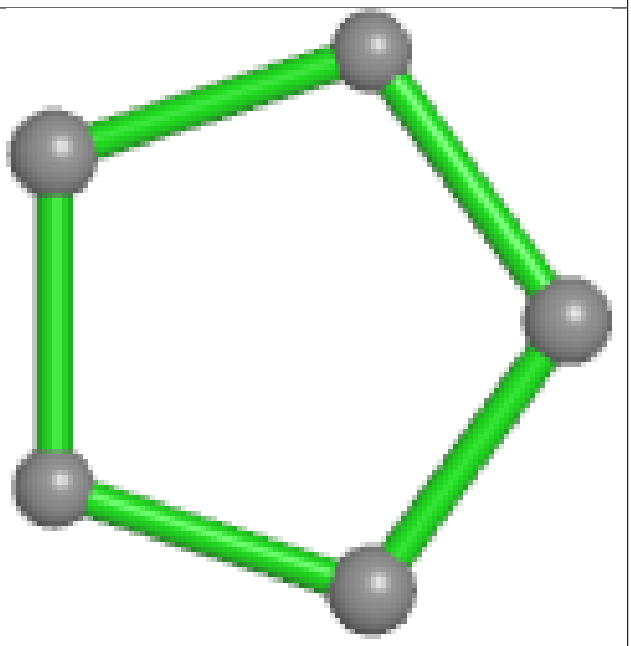


Rings

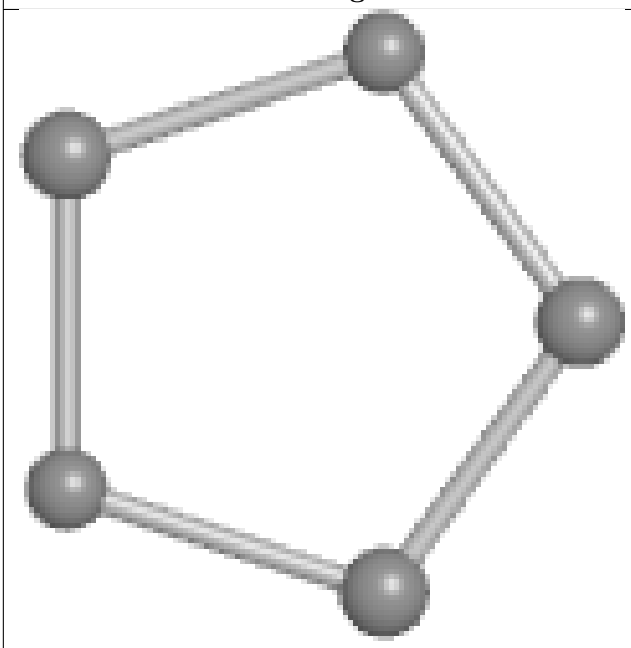
Ligand IMD E 604



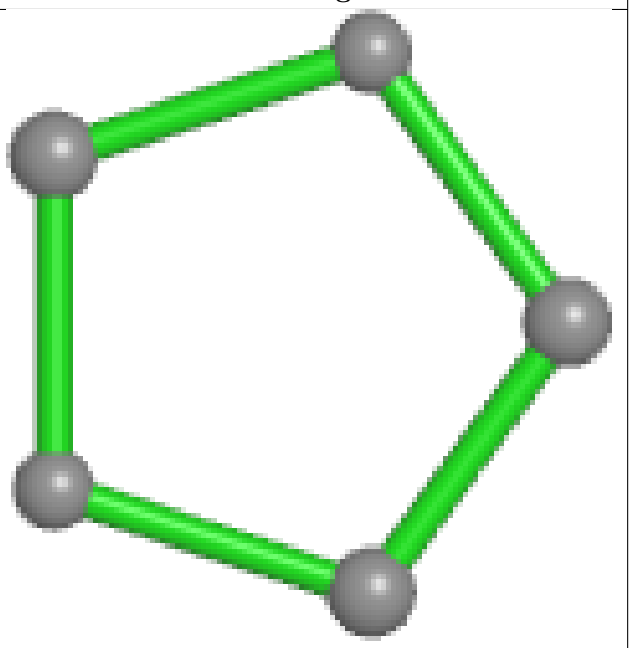
Bond lengths



Bond angles

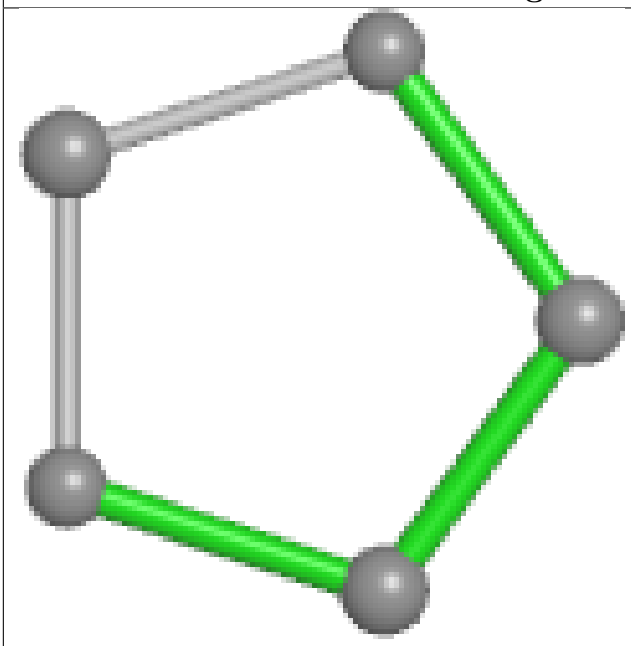


Torsions

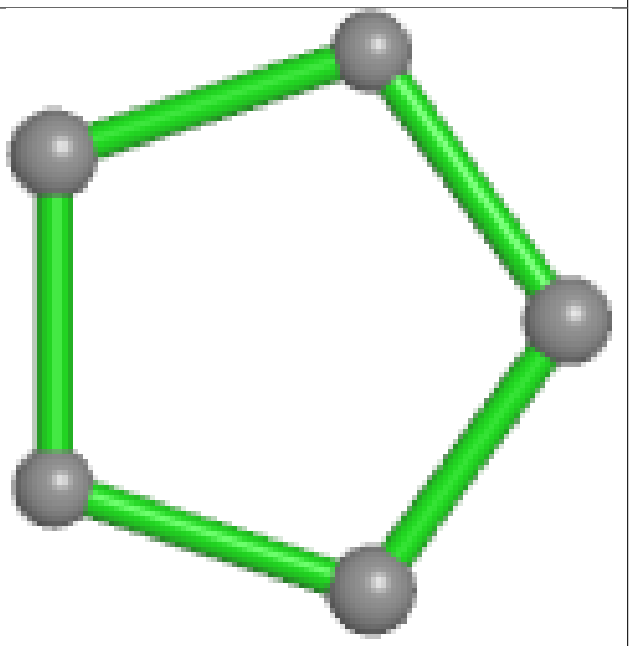


Rings

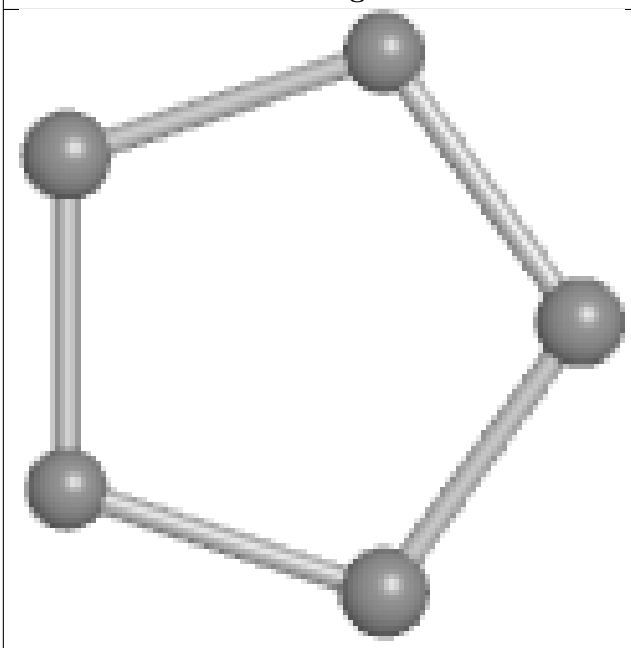
Ligand IMD F 303



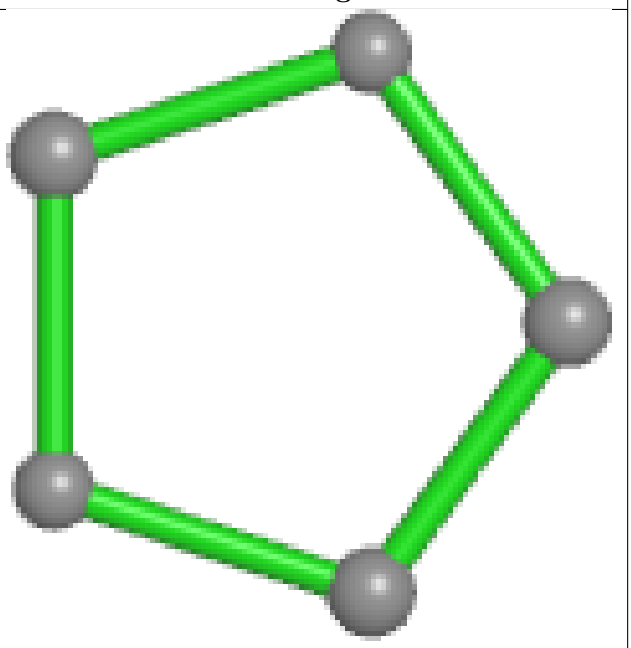
Bond lengths



Bond angles

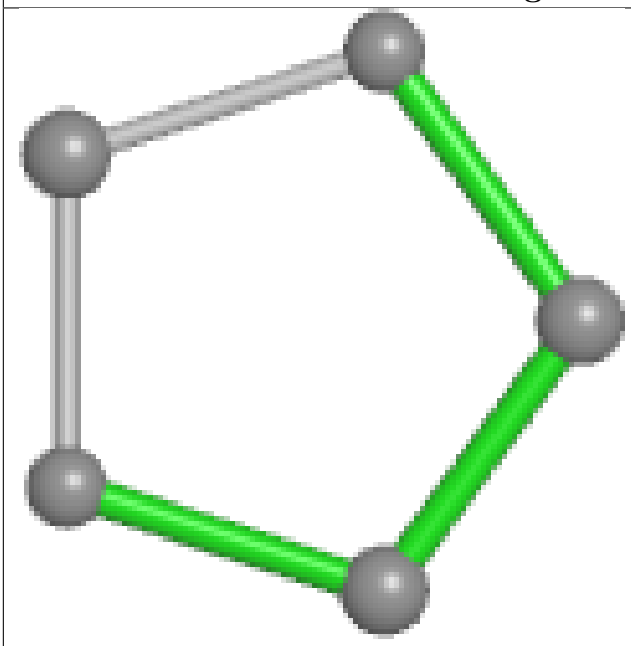


Torsions

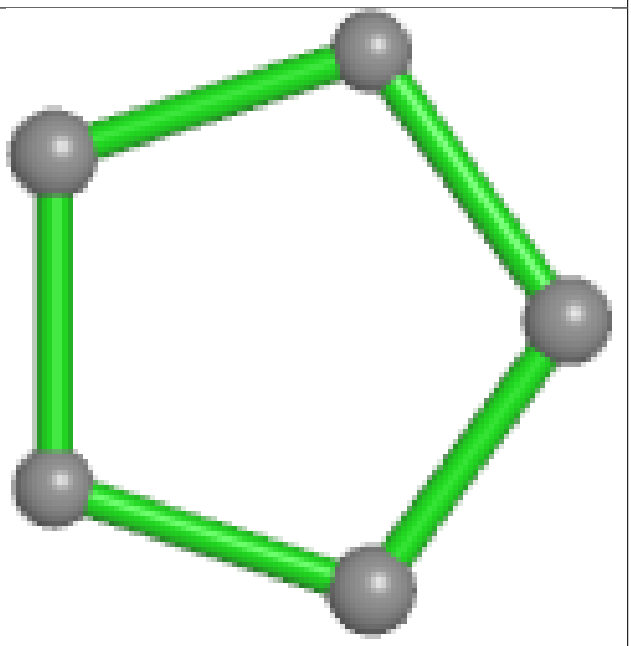


Rings

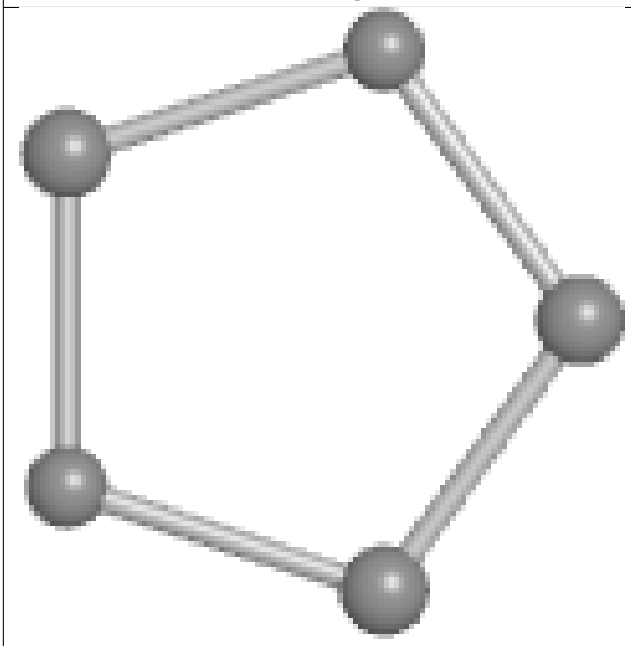
Ligand IMD B 304



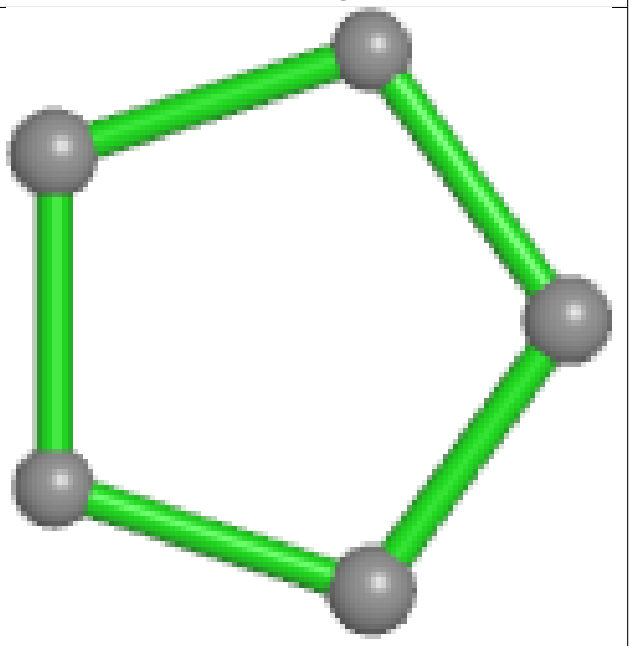
Bond lengths



Bond angles

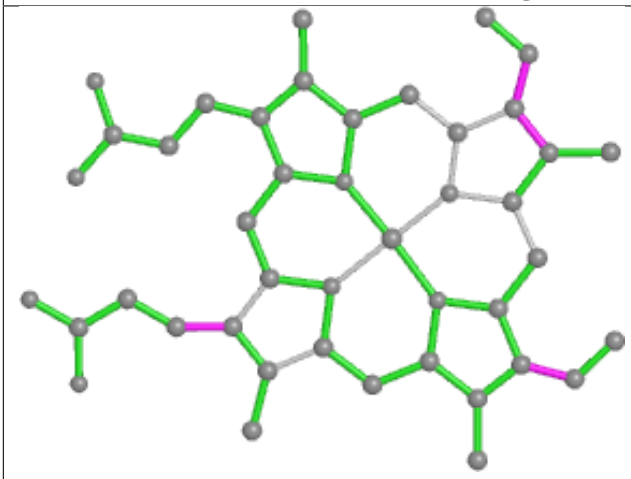


Torsions



Rings

Ligand HEM G 601



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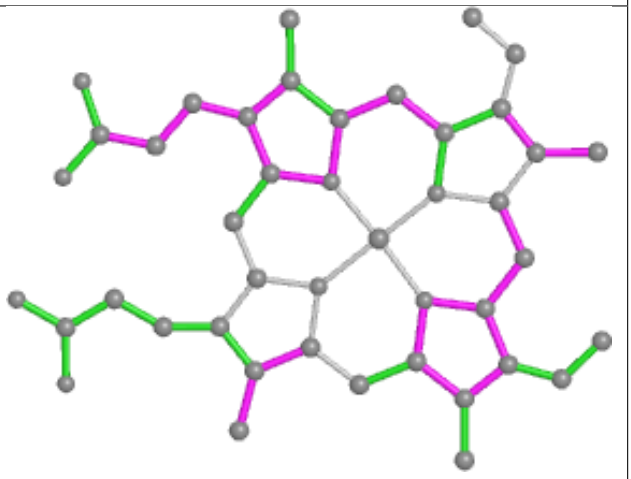
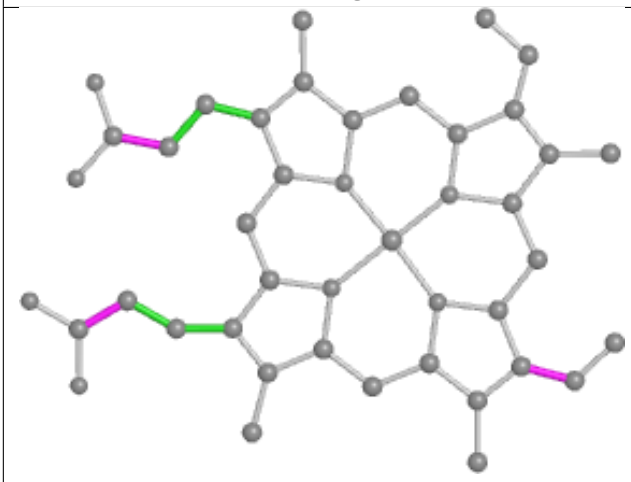


Bond angles



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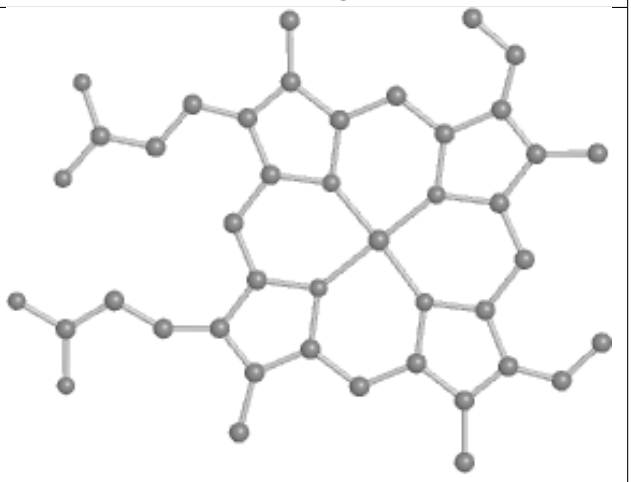
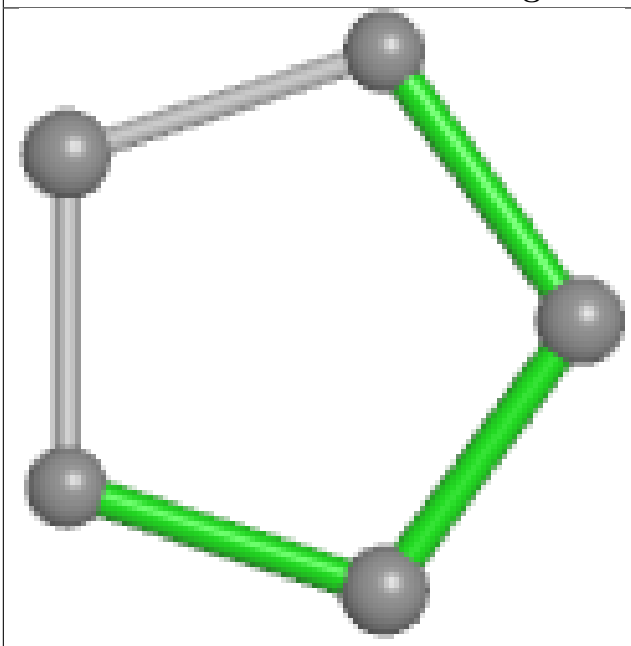
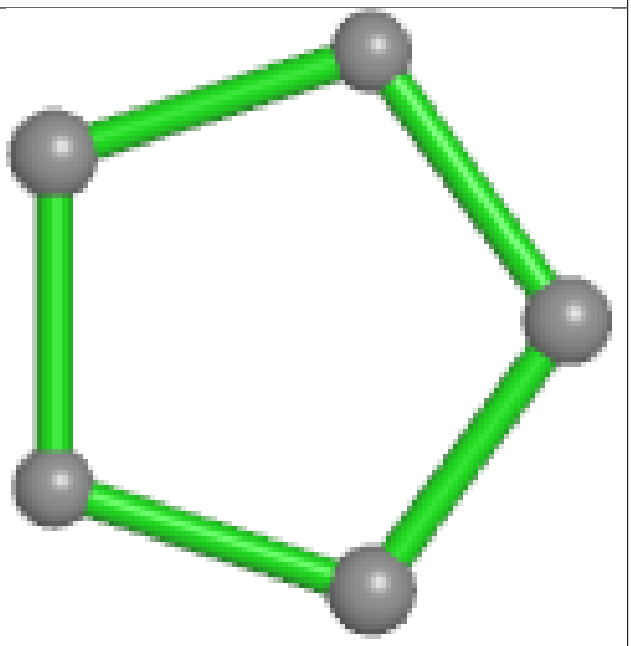


Rings

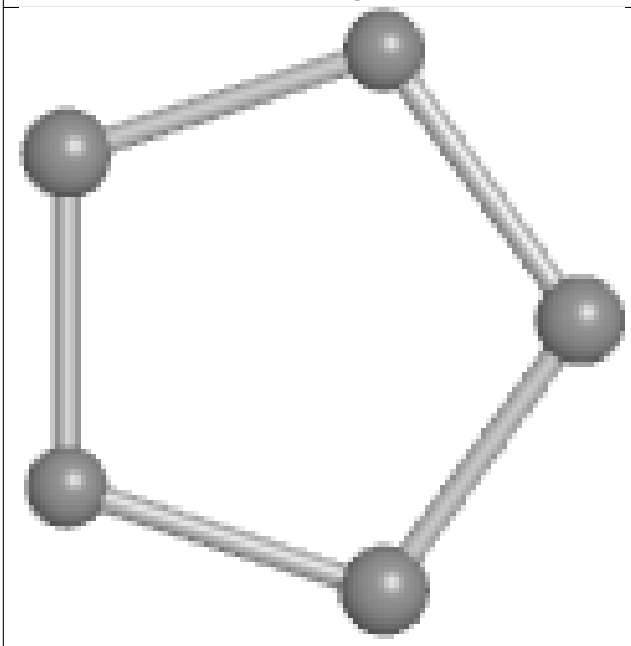
Ligand IMD H 304



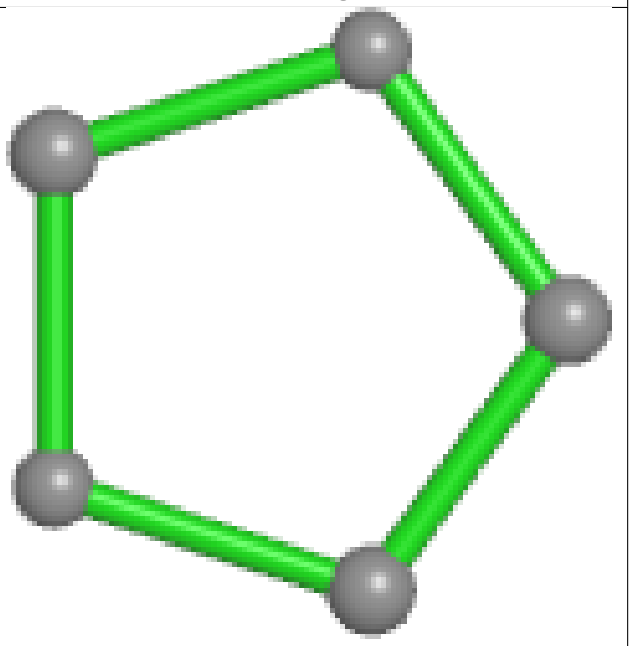
Bond lengths



Bond angles

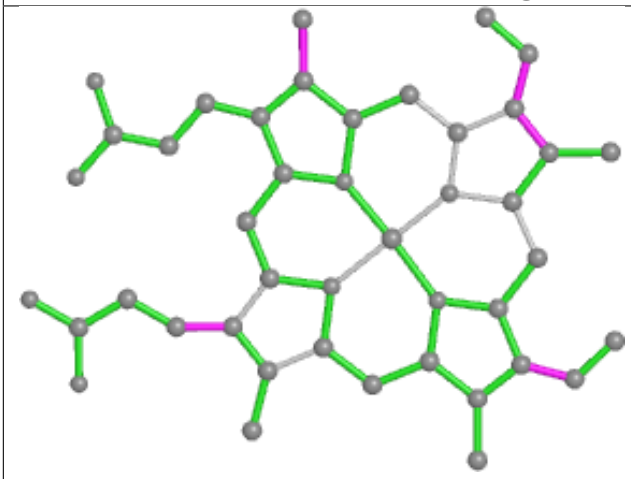


Torsions

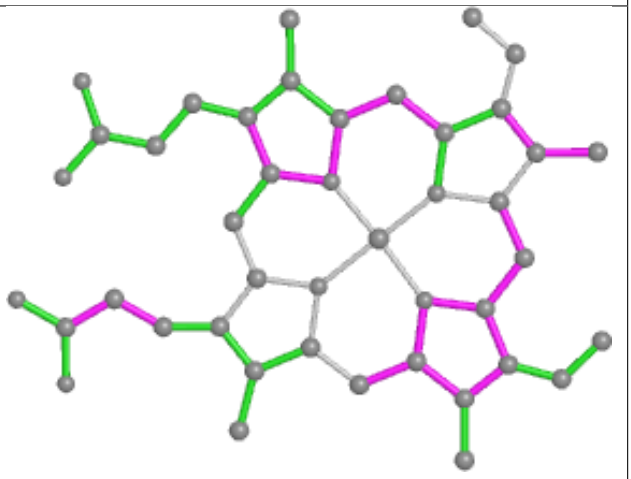


Rings

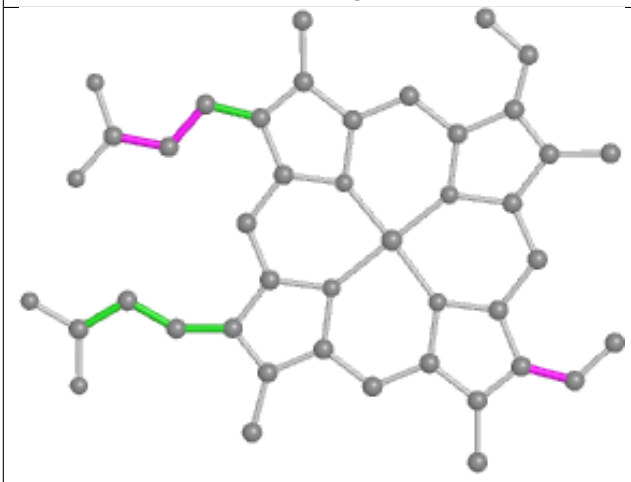
Ligand HEM H 303



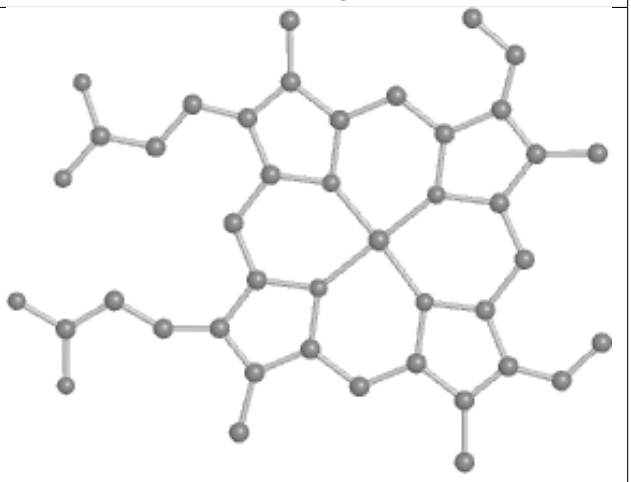
Bond lengths



Bond angles

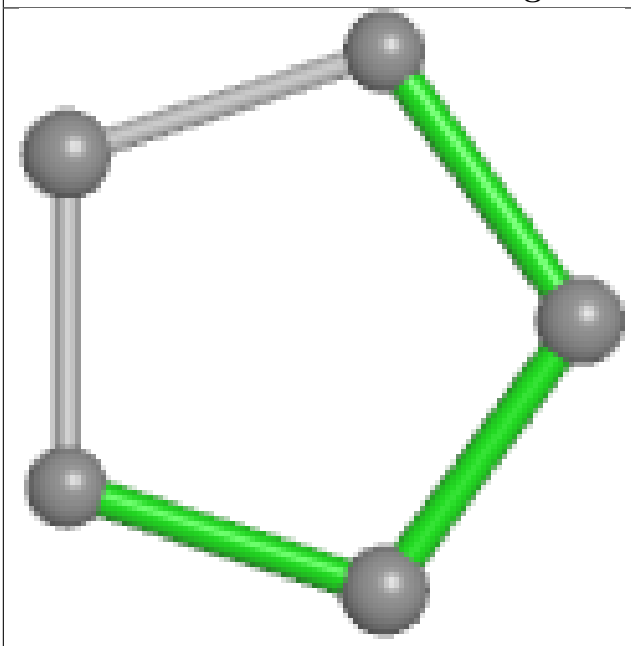


Torsions

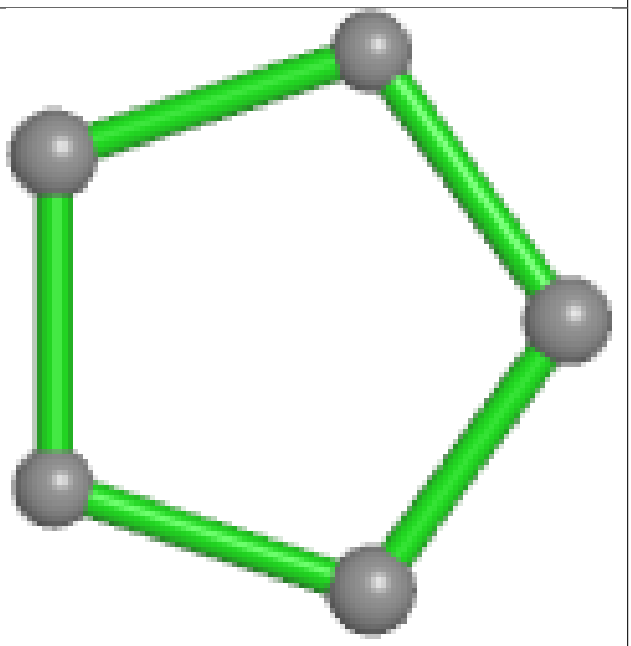


Rings

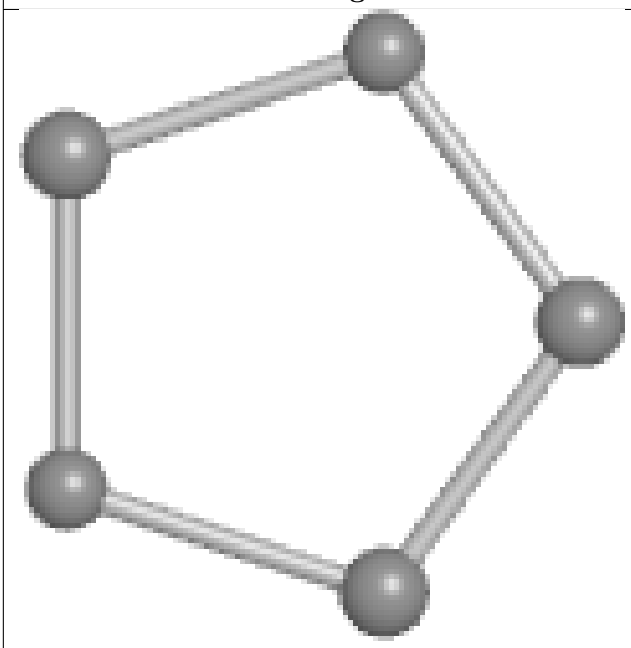
Ligand IMD C 604



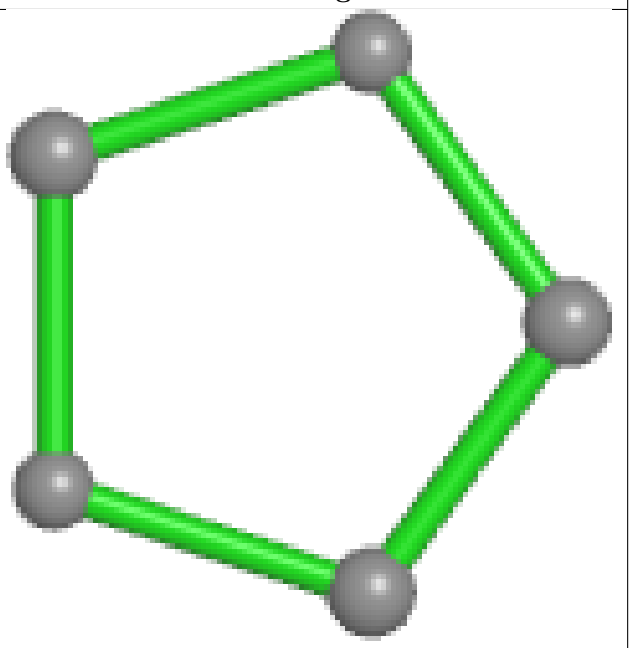
Bond lengths



Bond angles

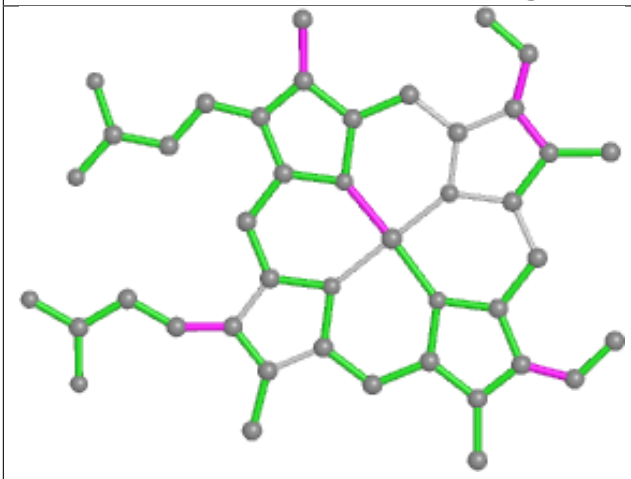


Torsions

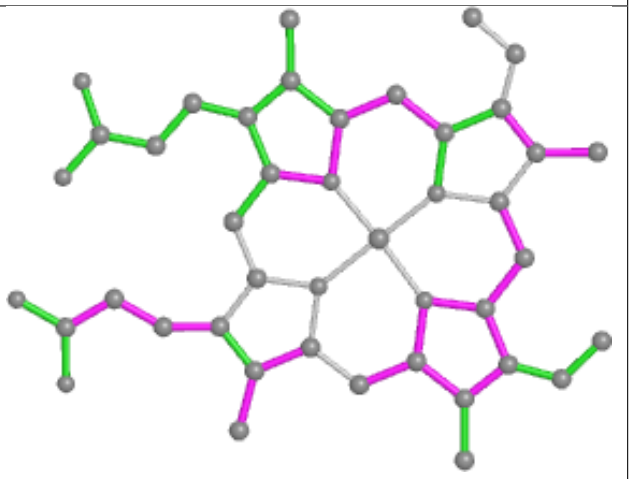


Rings

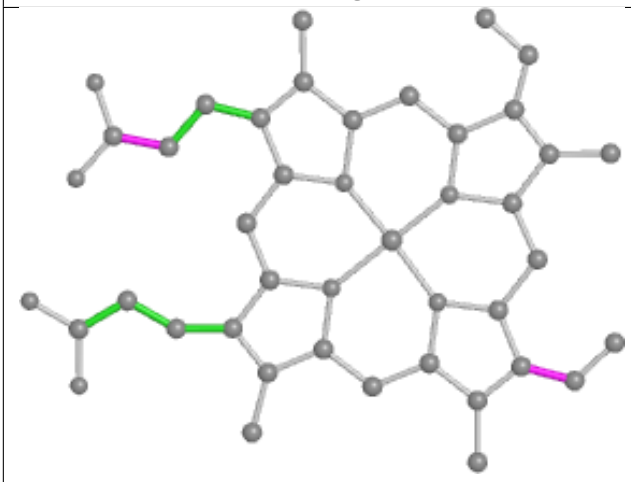
Ligand HEM J 302



Bond lengths



Bond angles



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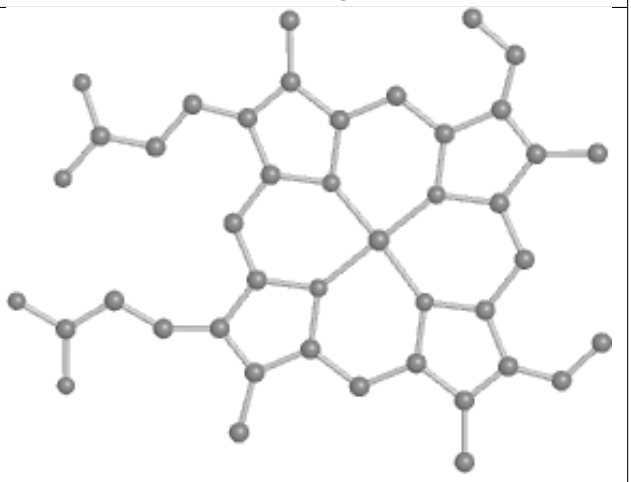
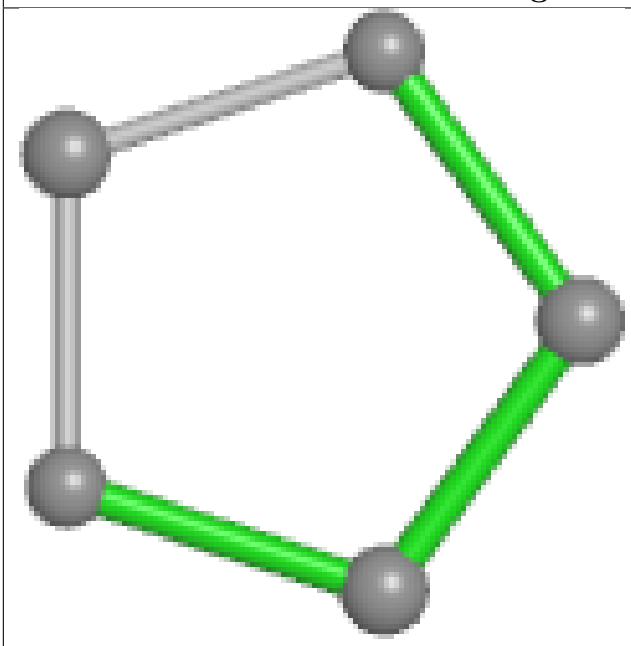
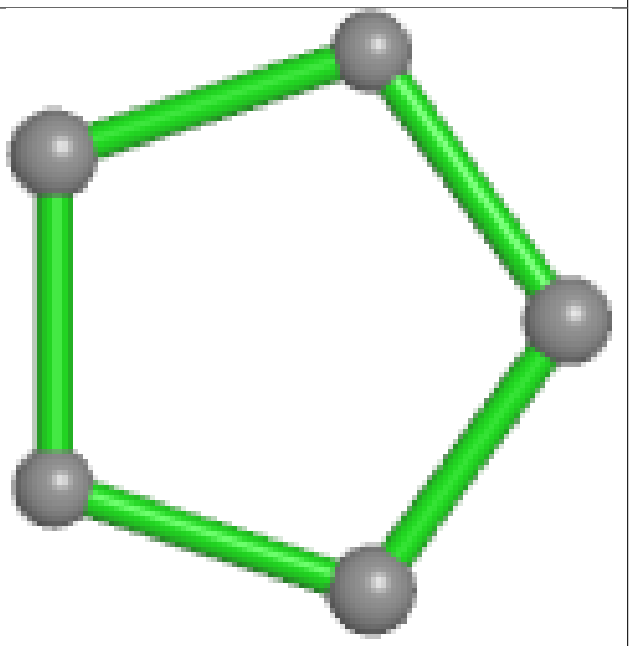


Rings

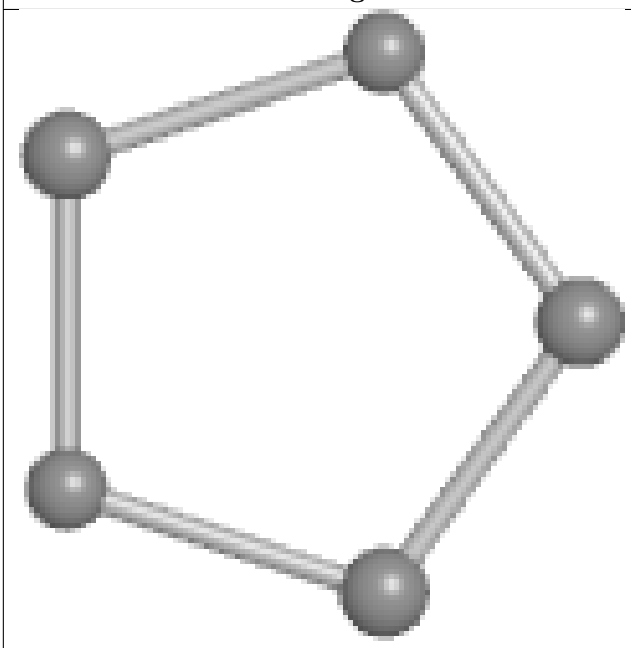
Ligand IMD I 604



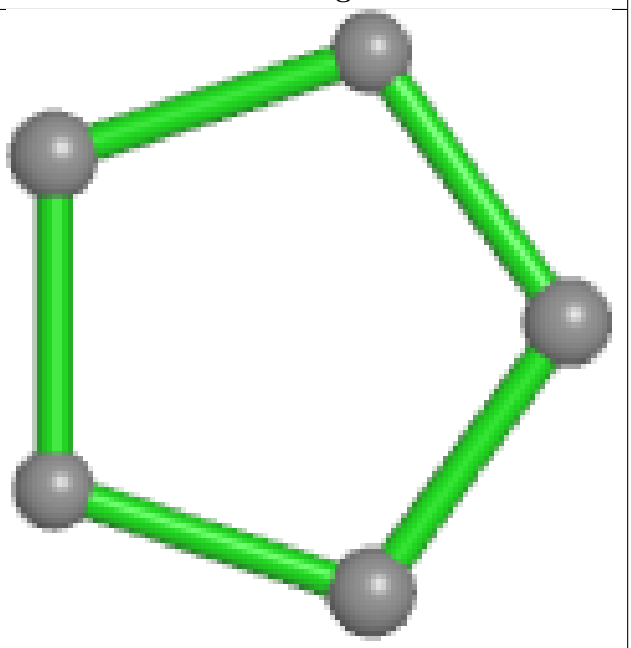
Bond lengths



Bond angles

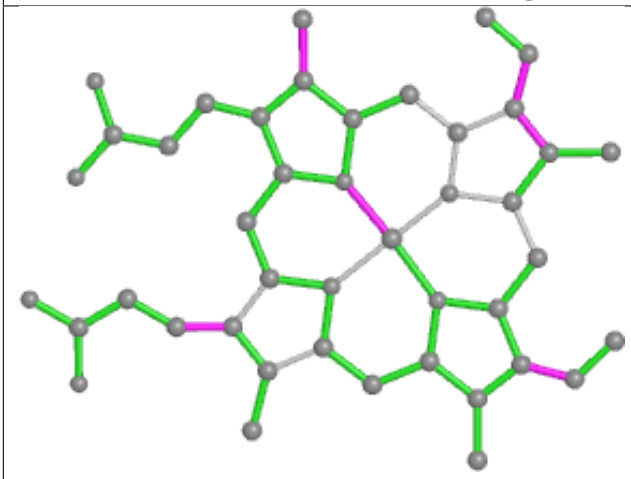


Torsions

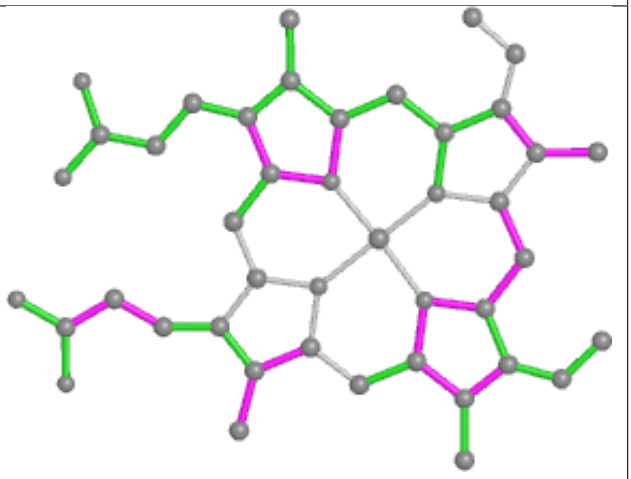


Rings

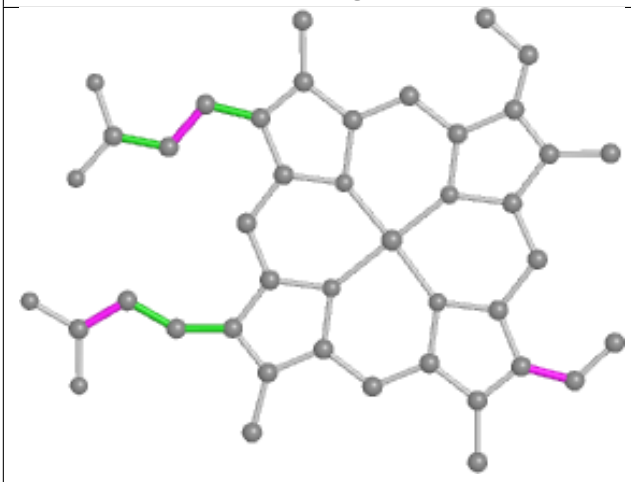
Ligand HEM F 302



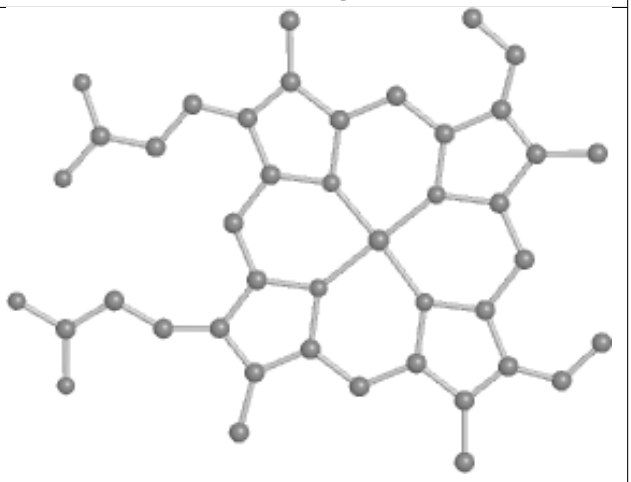
Bond lengths



Bond angles

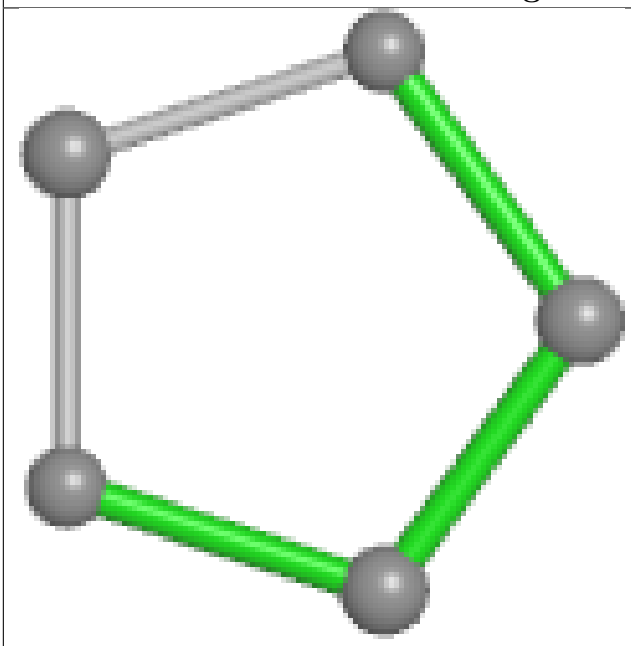


Torsions

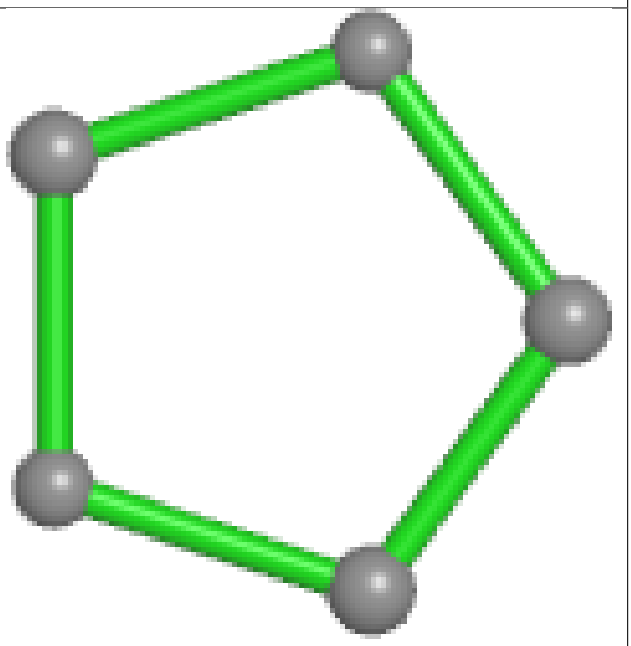


Rings

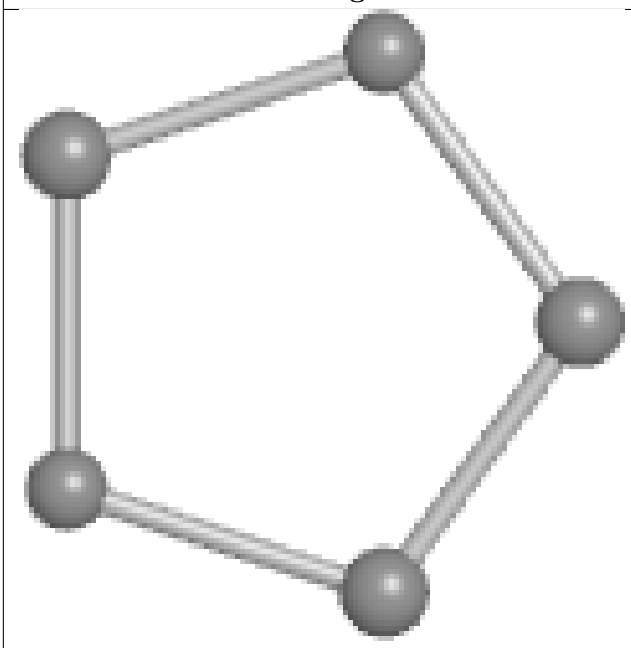
Ligand IMD G 603



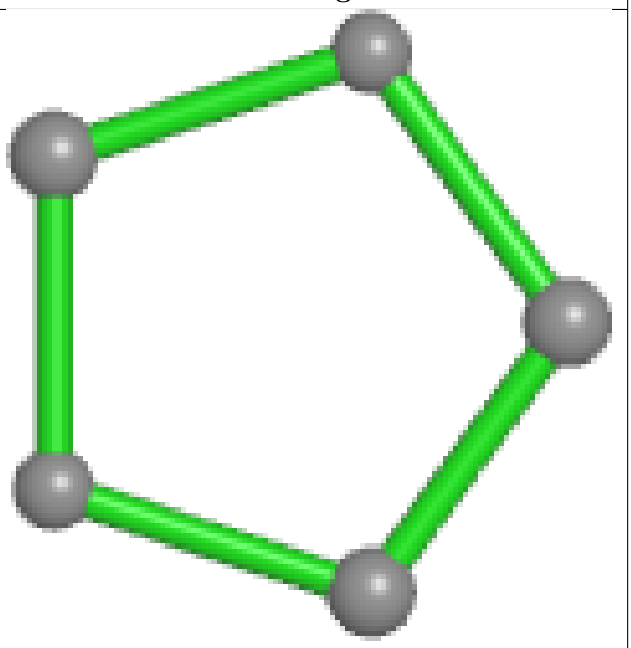
Bond lengths



Bond angles

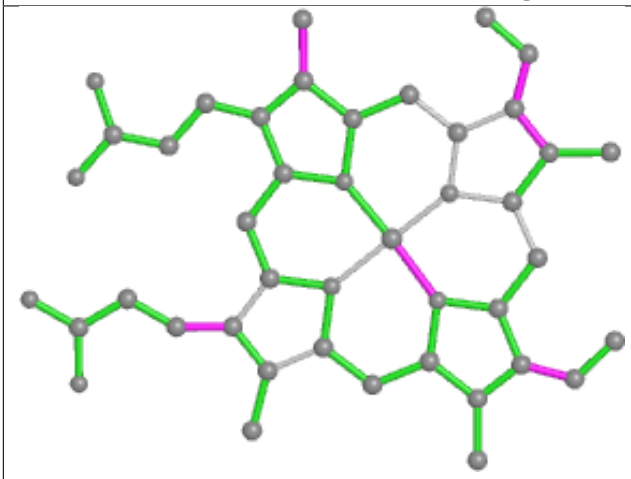


Torsions

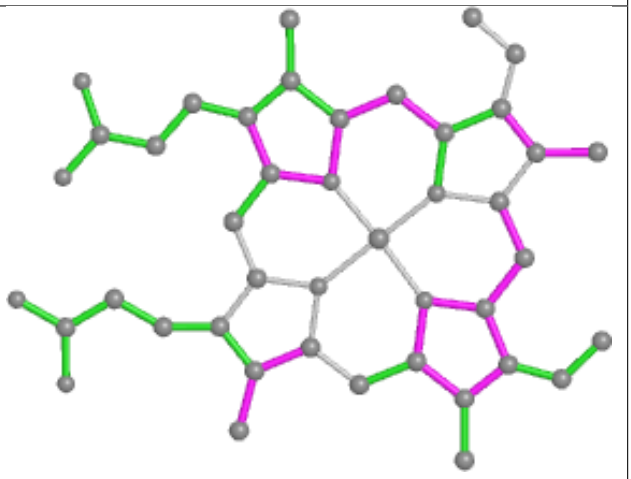


Rings

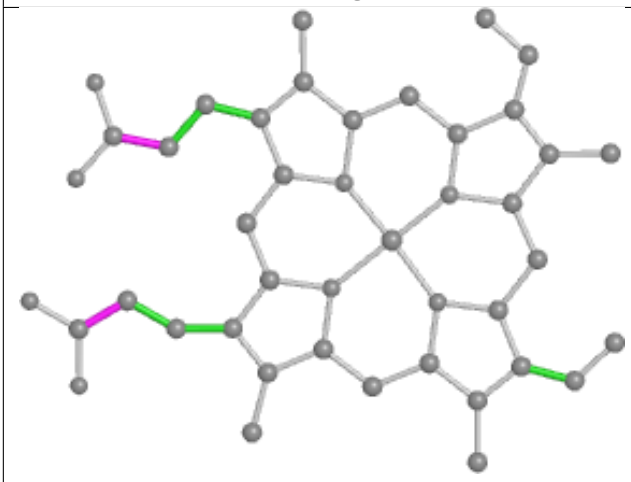
Ligand HEM A 601



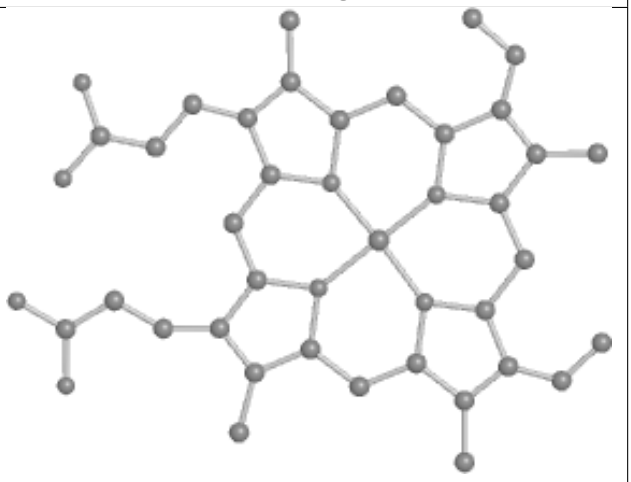
Bond lengths



Bond angles

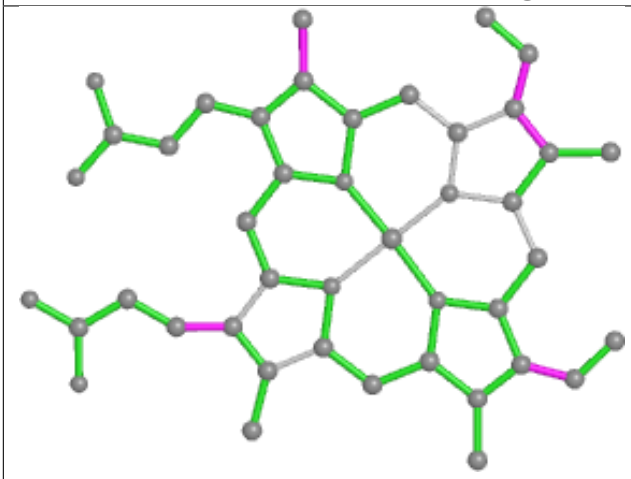


Torsions

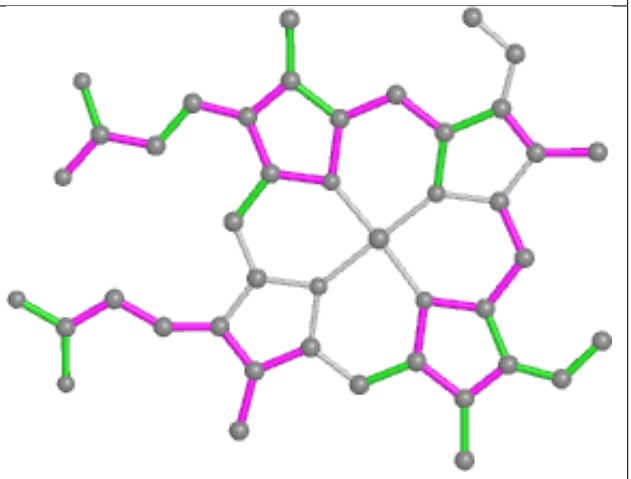


Rings

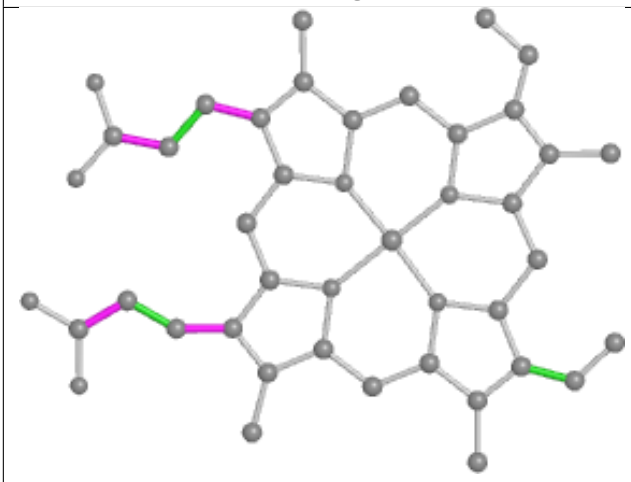
Ligand HEM C 601



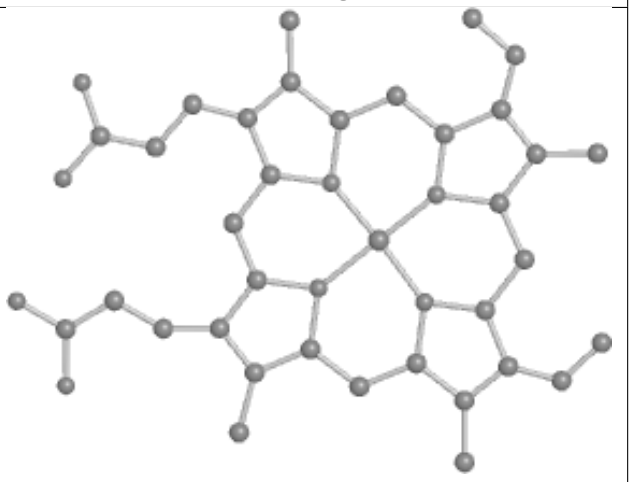
Bond lengths



Bond angles

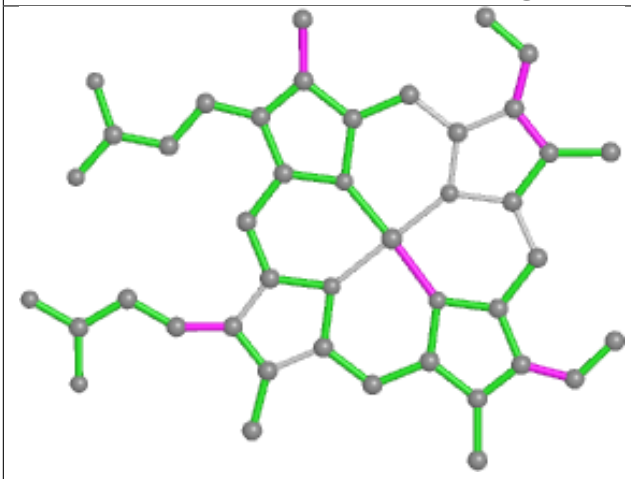


Torsions

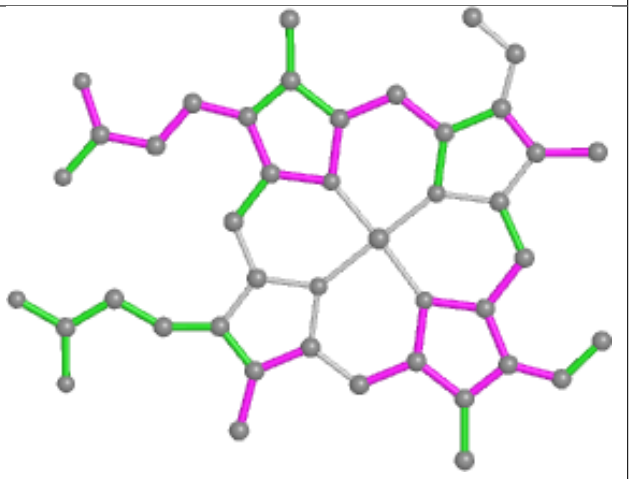


Rings

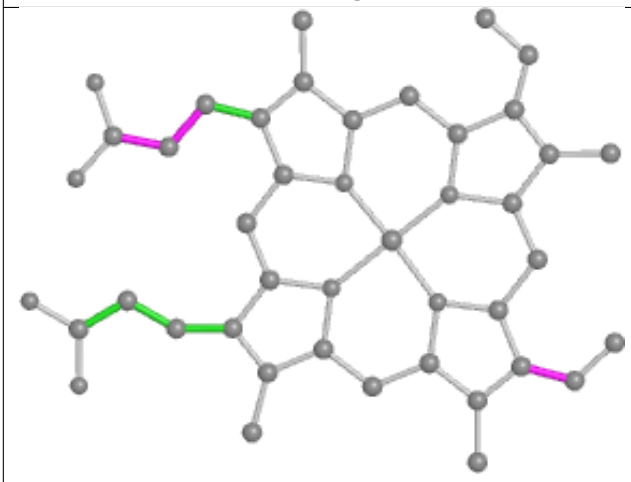
Ligand HEM D 302



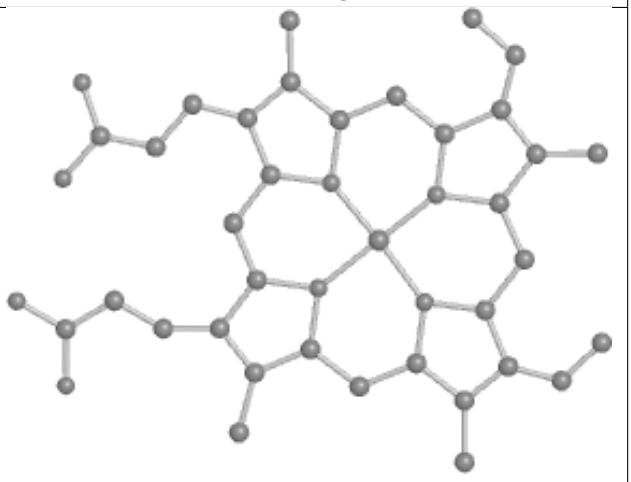
Bond lengths



Bond angles

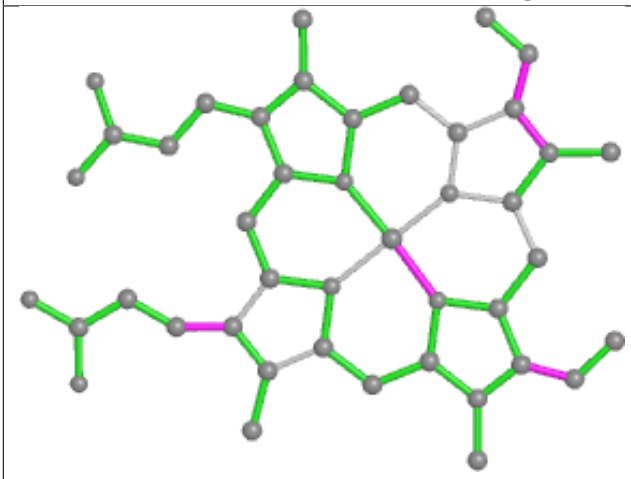


Torsions

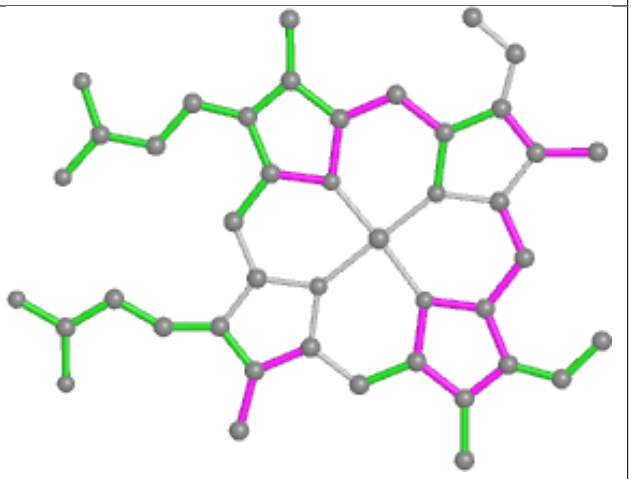


Rings

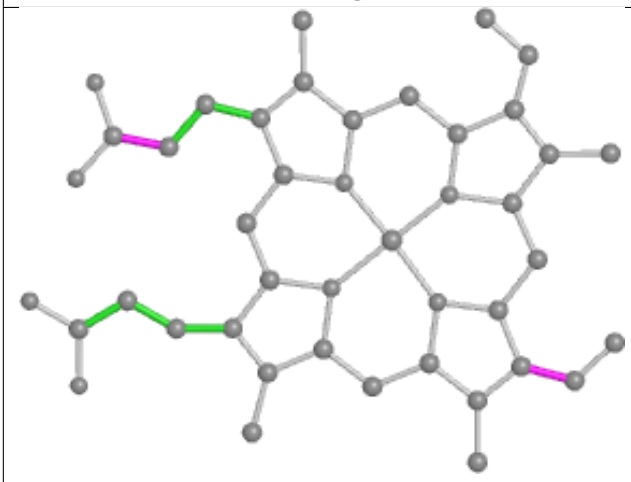
Ligand HEM B 303



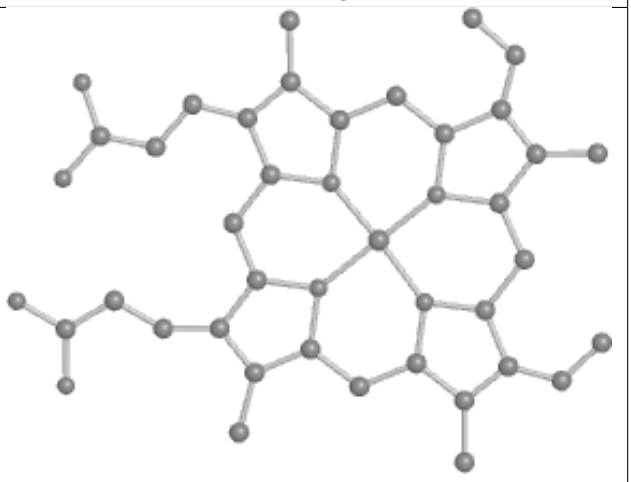
Bond lengths



Bond angles

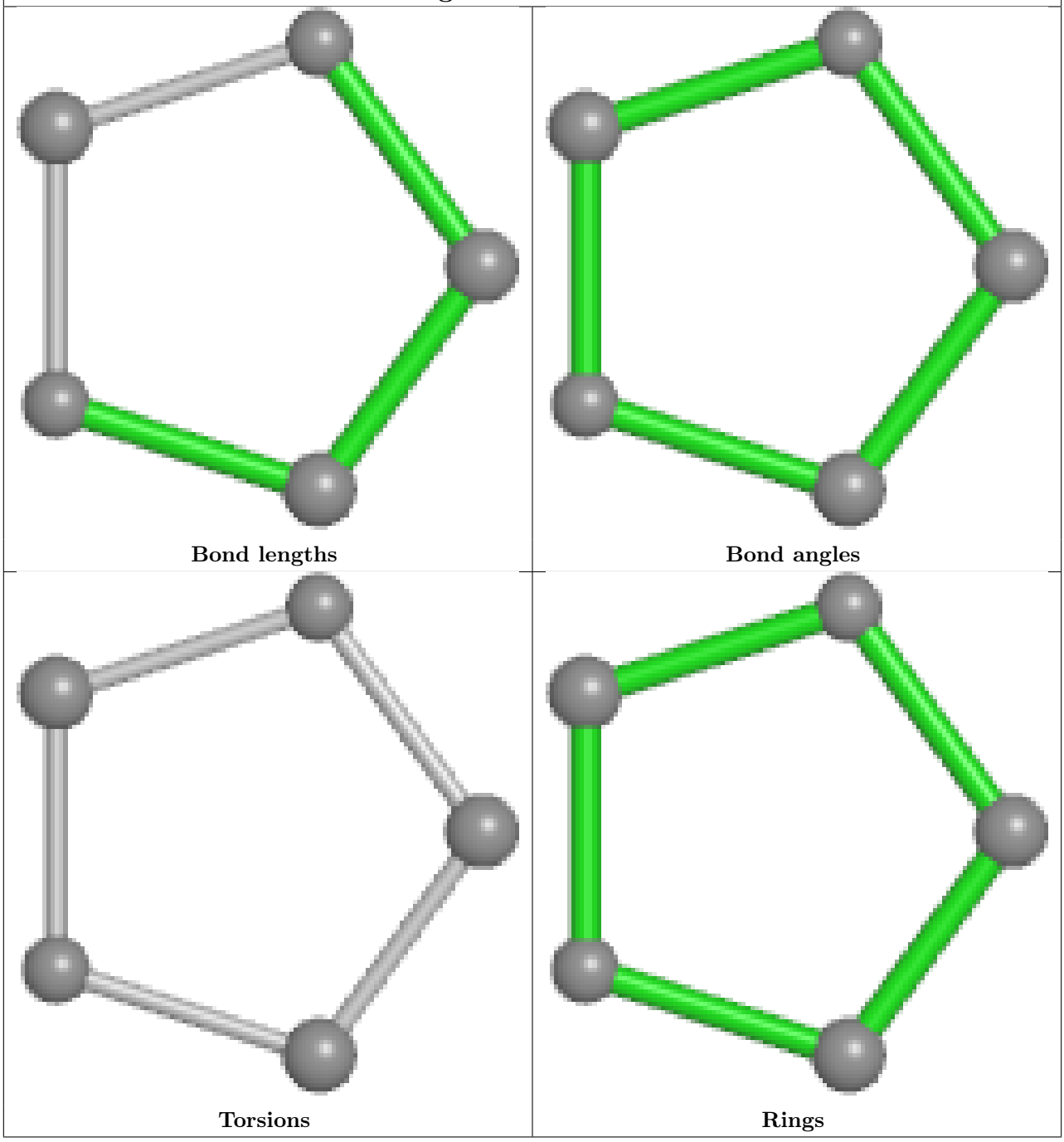


Torsions



Rings

Ligand IMD J 303



5.7 Other polymers (i)

There are no such residues in this entry.

5.8 Polymer linkage issues (i)

There are no chain breaks in this entry.

6 Fit of model and data

6.1 Protein, DNA and RNA chains

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

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å^2)	Q<0.9
1	A	250/273 (91%)	0.41	17 (6%) 17 13	41, 84, 188, 266	0
1	B	253/273 (92%)	0.77	40 (15%) 2 1	46, 101, 217, 265	0
1	C	252/273 (92%)	0.47	20 (7%) 12 9	43, 100, 205, 257	0
1	D	251/273 (91%)	0.29	10 (3%) 38 32	46, 82, 176, 255	0
1	E	251/273 (91%)	0.71	33 (13%) 3 2	51, 109, 217, 264	0
1	F	249/273 (91%)	0.66	28 (11%) 5 3	52, 108, 204, 254	0
1	G	249/273 (91%)	0.43	14 (5%) 24 20	54, 98, 191, 236	0
1	H	253/273 (92%)	0.70	31 (12%) 4 2	54, 112, 221, 269	0
1	I	249/273 (91%)	1.32	68 (27%) 0 0	61, 142, 234, 280	0
1	J	249/273 (91%)	1.21	61 (24%) 0 0	59, 141, 238, 291	0
All	All	2506/2730 (91%)	0.70	322 (12%) 3 2	41, 103, 221, 291	0

All (322) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	H	274	VAL	10.7
1	J	273	LEU	10.2
1	C	213	PRO	9.9
1	I	52	GLY	9.8
1	J	274	VAL	9.6
1	I	48	LEU	8.7
1	E	273	LEU	8.2
1	C	86	GLY	8.1
1	I	274	VAL	8.1
1	A	274	VAL	8.1
1	I	98	SER	8.0
1	I	51	ILE	8.0
1	I	53	GLN	8.0

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Mol	Chain	Res	Type	RSRZ
1	I	30	TRP	7.8
1	I	96	GLY	7.8
1	I	99	ASN	7.6
1	J	52	GLY	7.5
1	F	274	VAL	7.4
1	I	34	LEU	7.2
1	J	51	ILE	7.2
1	I	41	TRP	7.1
1	I	49	LEU	7.1
1	J	41	TRP	7.1
1	H	99	ASN	7.1
1	J	62	PHE	6.8
1	E	271	SER	6.7
1	I	62	PHE	6.7
1	I	121	LEU	6.5
1	J	39	LEU	6.4
1	I	39	LEU	6.2
1	C	214	HIS	6.1
1	J	111	ILE	6.1
1	A	217	GLY	6.1
1	H	51	ILE	6.1
1	E	274	VAL	6.0
1	I	32	LEU	5.9
1	J	121	LEU	5.9
1	F	99	ASN	5.8
1	B	112	ARG	5.8
1	B	213	PRO	5.7
1	G	274	VAL	5.7
1	I	120	HIS	5.7
1	B	274	VAL	5.7
1	I	111	ILE	5.6
1	F	214	HIS	5.5
1	F	116	GLY	5.5
1	J	99	ASN	5.5
1	G	214	HIS	5.4
1	B	81	VAL	5.4
1	I	88	PHE	5.4
1	I	117	THR	5.4
1	J	116	GLY	5.4
1	A	214	HIS	5.4
1	B	214	HIS	5.3
1	J	270	GLN	5.3

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Mol	Chain	Res	Type	RSRZ
1	A	99	ASN	5.2
1	B	116	GLY	5.2
1	I	272	GLU	5.1
1	B	84	ARG	5.1
1	J	40	ASP	5.1
1	B	117	THR	5.1
1	D	99	ASN	5.0
1	J	98	SER	5.0
1	C	84	ARG	5.0
1	J	217	GLY	4.8
1	H	100	ALA	4.7
1	J	117	THR	4.7
1	J	37	TRP	4.7
1	B	34	LEU	4.6
1	F	98	SER	4.6
1	I	271	SER	4.5
1	J	88	PHE	4.5
1	F	273	LEU	4.5
1	E	84	ARG	4.4
1	H	98	SER	4.4
1	B	62	PHE	4.4
1	F	100	ALA	4.4
1	J	32	LEU	4.4
1	J	115	ALA	4.4
1	C	41	TRP	4.3
1	I	97	THR	4.3
1	B	39	LEU	4.3
1	B	99	ASN	4.3
1	J	269	LEU	4.3
1	E	115	ALA	4.2
1	A	218	ILE	4.2
1	B	217	GLY	4.2
1	E	116	GLY	4.2
1	B	51	ILE	4.2
1	B	120	HIS	4.2
1	F	121	LEU	4.2
1	J	97	THR	4.2
1	D	98	SER	4.1
1	I	58	SER	4.1
1	I	126	LEU	4.1
1	D	213	PRO	4.1
1	A	113	ASP	4.0

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Mol	Chain	Res	Type	RSRZ
1	I	50	GLY	4.0
1	B	115	ALA	4.0
1	H	268	GLU	4.0
1	J	38	ALA	3.9
1	J	125	PHE	3.9
1	J	120	HIS	3.9
1	I	86	GLY	3.9
1	I	110	LEU	3.9
1	J	271	SER	3.8
1	C	212	ASP	3.8
1	I	125	PHE	3.8
1	F	271	SER	3.8
1	J	36	THR	3.7
1	J	86	GLY	3.7
1	C	37	TRP	3.7
1	B	50	GLY	3.7
1	I	116	GLY	3.7
1	J	272	GLU	3.7
1	A	273	LEU	3.7
1	G	273	LEU	3.7
1	I	36	THR	3.7
1	I	214	HIS	3.6
1	J	119	ARG	3.6
1	C	274	VAL	3.6
1	J	34	LEU	3.6
1	I	54	ASP	3.6
1	G	98	SER	3.6
1	B	97	THR	3.6
1	J	112	ARG	3.6
1	A	272	GLU	3.6
1	J	84	ARG	3.6
1	H	125	PHE	3.6
1	I	273	LEU	3.6
1	E	66	LEU	3.5
1	G	116	GLY	3.5
1	C	34	LEU	3.5
1	B	48	LEU	3.5
1	E	39	LEU	3.5
1	F	51	ILE	3.5
1	G	213	PRO	3.5
1	C	99	ASN	3.4
1	F	212	ASP	3.4

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Mol	Chain	Res	Type	RSRZ
1	B	216	ILE	3.4
1	G	52	GLY	3.4
1	I	85	GLY	3.4
1	B	273	LEU	3.4
1	H	85	GLY	3.4
1	E	30	TRP	3.4
1	J	118	ALA	3.3
1	E	86	GLY	3.3
1	H	62	PHE	3.3
1	A	97	THR	3.3
1	I	217	GLY	3.3
1	G	97	THR	3.3
1	D	214	HIS	3.3
1	J	113	ASP	3.3
1	J	48	LEU	3.3
1	B	110	LEU	3.2
1	F	111	ILE	3.2
1	I	40	ASP	3.2
1	C	62	PHE	3.2
1	B	121	LEU	3.2
1	I	215	ILE	3.2
1	A	98	SER	3.2
1	H	112	ARG	3.2
1	J	26	GLY	3.2
1	I	213	PRO	3.2
1	J	266	LEU	3.2
1	H	273	LEU	3.1
1	A	215	ILE	3.1
1	E	111	ILE	3.1
1	H	219	GLY	3.1
1	B	37	TRP	3.1
1	I	118	ALA	3.1
1	F	272	GLU	3.1
1	H	113	ASP	3.1
1	J	92	PHE	3.1
1	E	112	ARG	3.1
1	B	211	SER	3.0
1	E	98	SER	3.0
1	E	117	THR	3.0
1	D	100	ALA	3.0
1	H	116	GLY	3.0
1	I	64	SER	3.0

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Mol	Chain	Res	Type	RSRZ
1	D	83	GLU	3.0
1	B	46	ARG	3.0
1	J	54	ASP	3.0
1	E	41	TRP	3.0
1	I	37	TRP	3.0
1	A	84	ARG	3.0
1	E	110	LEU	2.9
1	F	269	LEU	2.9
1	J	126	LEU	2.9
1	A	271	SER	2.9
1	I	84	ARG	2.9
1	G	34	LEU	2.9
1	F	115	ALA	2.9
1	B	122	SER	2.9
1	H	271	SER	2.9
1	B	86	GLY	2.9
1	J	101	GLY	2.9
1	E	27	VAL	2.8
1	F	62	PHE	2.8
1	J	122	SER	2.8
1	H	39	LEU	2.8
1	B	272	GLU	2.8
1	B	41	TRP	2.8
1	F	270	GLN	2.8
1	I	218	ILE	2.8
1	C	88	PHE	2.8
1	F	27	VAL	2.8
1	I	66	LEU	2.8
1	H	66	LEU	2.8
1	E	87	GLY	2.7
1	J	30	TRP	2.7
1	E	272	GLU	2.7
1	J	56	PRO	2.7
1	I	94	VAL	2.7
1	C	77	ALA	2.7
1	E	62	PHE	2.7
1	I	56	PRO	2.7
1	I	100	ALA	2.7
1	H	97	THR	2.7
1	B	111	ILE	2.7
1	E	121	LEU	2.7
1	I	122	SER	2.7

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Mol	Chain	Res	Type	RSRZ
1	J	265	ARG	2.7
1	E	268	GLU	2.7
1	I	115	ALA	2.7
1	B	83	GLU	2.7
1	H	121	LEU	2.6
1	I	102	GLN	2.6
1	J	66	LEU	2.6
1	J	46	ARG	2.6
1	I	57	ALA	2.6
1	H	88	PHE	2.6
1	J	43	ASP	2.6
1	E	270	GLN	2.6
1	J	100	ALA	2.6
1	J	59	TYR	2.6
1	H	120	HIS	2.6
1	C	52	GLY	2.5
1	G	266	LEU	2.5
1	J	81	VAL	2.5
1	J	49	LEU	2.5
1	I	81	VAL	2.5
1	F	96	GLY	2.5
1	C	218	ILE	2.5
1	E	99	ASN	2.5
1	F	266	LEU	2.5
1	I	92	PHE	2.5
1	I	113	ASP	2.5
1	I	93	ARG	2.5
1	A	86	GLY	2.5
1	H	86	GLY	2.5
1	B	269	LEU	2.5
1	C	216	ILE	2.5
1	E	267	GLN	2.4
1	F	217	GLY	2.4
1	H	110	LEU	2.4
1	I	61	LEU	2.4
1	F	125	PHE	2.4
1	G	272	GLU	2.4
1	B	113	ASP	2.4
1	E	97	THR	2.4
1	H	115	ALA	2.4
1	F	215	ILE	2.4
1	J	74	VAL	2.4

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Mol	Chain	Res	Type	RSRZ
1	C	217	GLY	2.4
1	H	83	GLU	2.4
1	J	104	ILE	2.4
1	H	30	TRP	2.4
1	I	65	ARG	2.4
1	A	32	LEU	2.4
1	I	27	VAL	2.4
1	E	28	GLY	2.3
1	D	97	THR	2.3
1	E	265	ARG	2.3
1	E	214	HIS	2.3
1	J	85	GLY	2.3
1	F	84	ARG	2.3
1	I	112	ARG	2.3
1	B	215	ILE	2.3
1	G	99	ASN	2.3
1	I	87	GLY	2.3
1	B	32	LEU	2.3
1	C	111	ILE	2.3
1	F	122	SER	2.3
1	B	266	LEU	2.3
1	I	43	ASP	2.3
1	D	216	ILE	2.3
1	D	273	LEU	2.3
1	I	60	ASP	2.3
1	E	36	THR	2.2
1	J	27	VAL	2.2
1	B	119	ARG	2.2
1	H	41	TRP	2.2
1	I	104	ILE	2.2
1	I	31	ASP	2.2
1	J	96	GLY	2.2
1	E	108	ALA	2.2
1	G	217	GLY	2.2
1	D	49	LEU	2.2
1	F	113	ASP	2.2
1	B	82	SER	2.1
1	H	272	GLU	2.1
1	I	103	TRP	2.1
1	J	214	HIS	2.1
1	C	85	GLY	2.1
1	B	220	ARG	2.1

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Mol	Chain	Res	Type	RSRZ
1	H	114	GLU	2.1
1	E	83	GLU	2.1
1	F	218	ILE	2.1
1	E	217	GLY	2.1
1	J	60	ASP	2.1
1	A	115	ALA	2.1
1	C	125	PHE	2.1
1	G	211	SER	2.1
1	I	33	ASP	2.1
1	J	103	TRP	2.0
1	F	97	THR	2.0
1	H	101	GLY	2.0
1	I	83	GLU	2.0
1	A	125	PHE	2.0
1	H	48	LEU	2.0

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

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

6.3 Carbohydrates (i)

There are no monosaccharides in this entry.

6.4 Ligands (i)

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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
3	GOL	G	602	6/6	0.89	0.28	60,83,89,89	0
3	GOL	E	603	6/6	0.90	0.27	65,85,87,89	0
3	GOL	I	603	6/6	0.90	0.25	74,88,90,99	0
3	GOL	C	603	6/6	0.92	0.28	57,71,75,75	0
3	GOL	A	602	6/6	0.92	0.25	62,68,69,73	0
3	GOL	H	301	6/6	0.93	0.22	67,78,78,80	0
3	GOL	J	301	6/6	0.93	0.27	68,72,76,77	0
3	GOL	D	301	6/6	0.94	0.22	60,62,71,74	0

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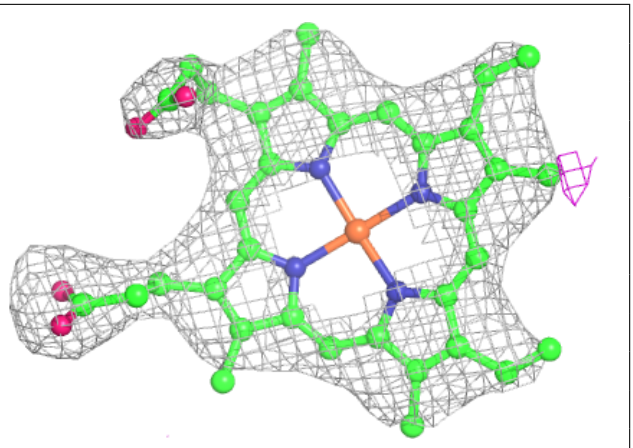
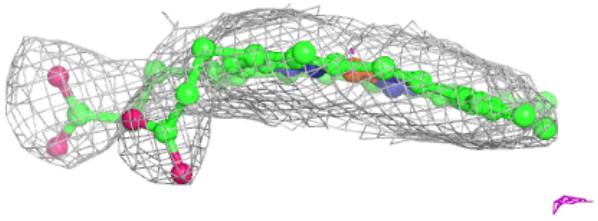
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
3	GOL	B	301	6/6	0.95	0.22	59,68,69,74	0
3	GOL	F	301	6/6	0.95	0.24	65,70,71,74	0
3	GOL	I	602	6/6	0.96	0.33	61,69,76,76	0
2	HEM	B	303	43/43	0.98	0.24	47,69,114,131	0
3	GOL	B	302	6/6	0.98	0.29	59,59,63,64	0
3	GOL	C	602	6/6	0.98	0.38	55,59,61,66	0
2	HEM	C	601	43/43	0.98	0.23	51,64,114,129	0
2	HEM	D	302	43/43	0.98	0.24	54,67,115,135	0
3	GOL	E	602	6/6	0.98	0.39	63,67,67,69	0
2	HEM	E	601	43/43	0.98	0.25	57,73,115,127	0
2	HEM	F	302	43/43	0.98	0.25	58,82,131,145	0
2	HEM	G	601	43/43	0.98	0.23	61,85,128,145	0
2	HEM	H	303	43/43	0.98	0.23	60,81,125,140	0
3	GOL	H	302	6/6	0.98	0.23	61,65,66,69	0
2	HEM	I	601	43/43	0.98	0.25	71,95,137,148	0
2	HEM	J	302	43/43	0.98	0.26	73,91,151,160	0
2	HEM	A	601	43/43	0.98	0.21	49,60,98,115	0
4	IMD	A	603	5/5	0.98	0.26	52,57,60,62	0
4	IMD	D	303	5/5	0.98	0.26	57,60,66,71	0
4	IMD	E	604	5/5	0.98	0.25	67,70,71,73	0
4	IMD	H	304	5/5	0.98	0.27	79,83,85,86	0
4	IMD	I	604	5/5	0.98	0.23	90,90,93,96	0
4	IMD	F	303	5/5	0.99	0.20	79,79,80,84	0
4	IMD	G	603	5/5	0.99	0.21	81,81,82,83	0
4	IMD	B	304	5/5	0.99	0.20	65,66,68,68	0
4	IMD	C	604	5/5	0.99	0.21	66,67,73,73	0
4	IMD	J	303	5/5	0.99	0.21	83,85,87,97	0

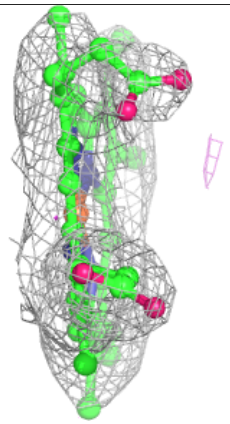
The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation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

Electron density around HEM B 303:

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

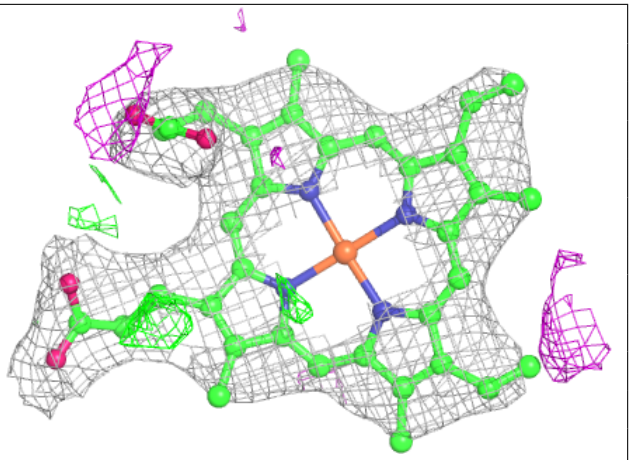


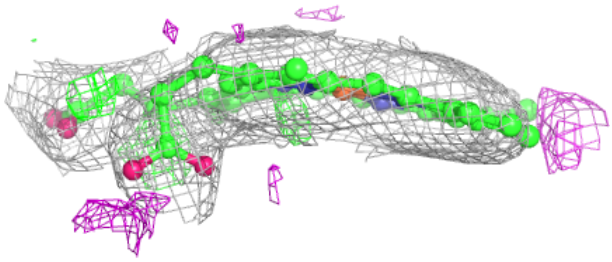


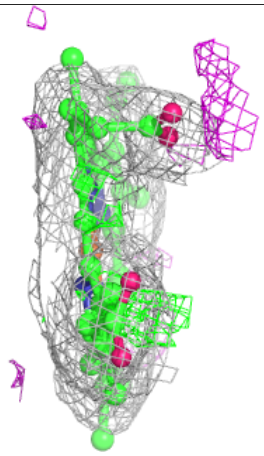


Electron density around HEM C 601:

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

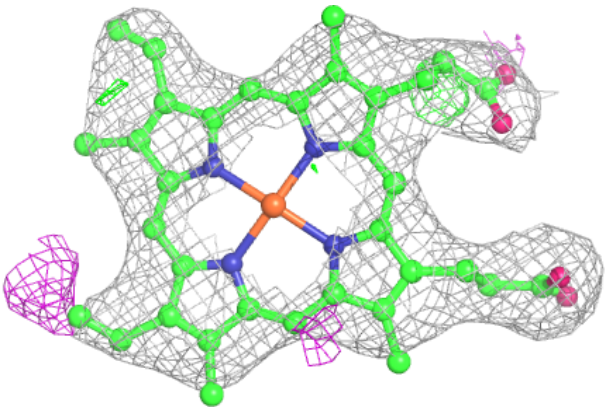


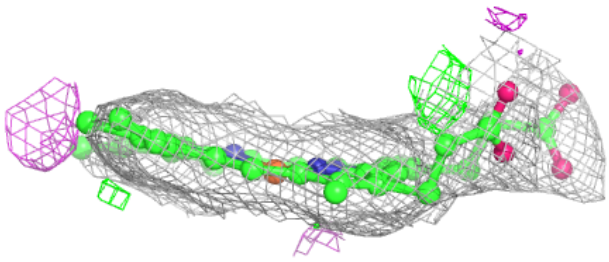


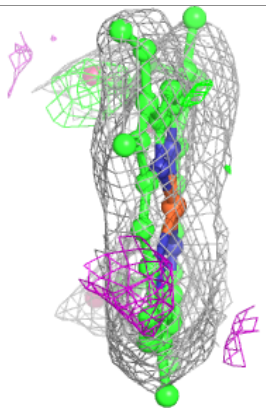


Electron density around HEM D 302:

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

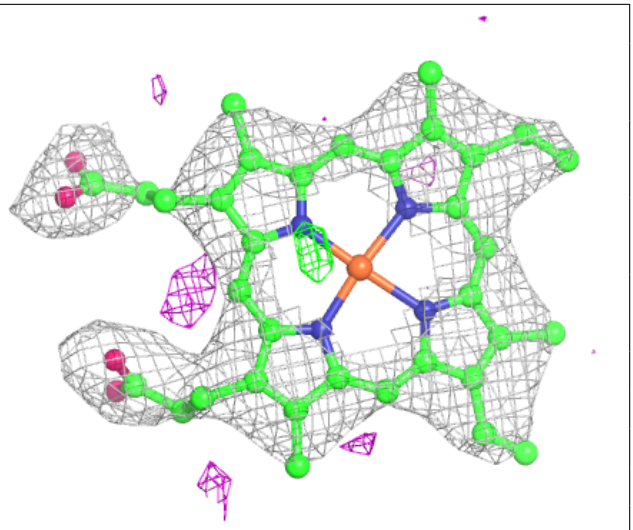


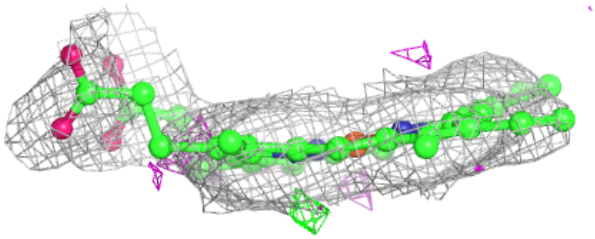


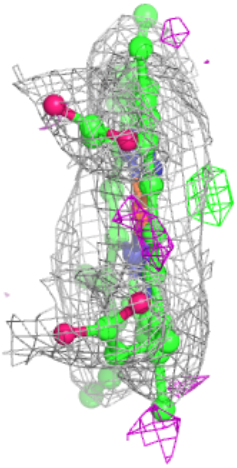


Electron density around HEM E 601:

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

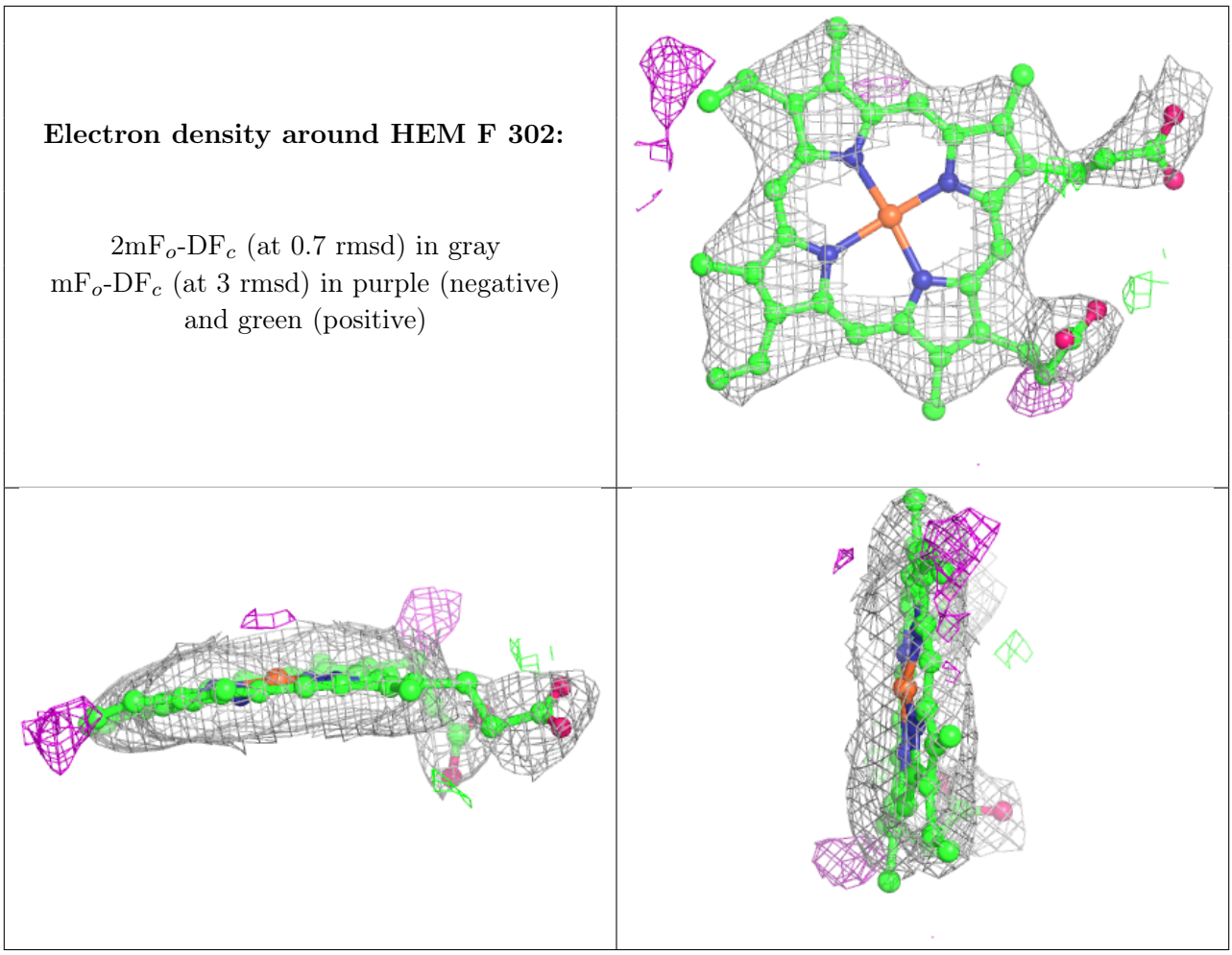






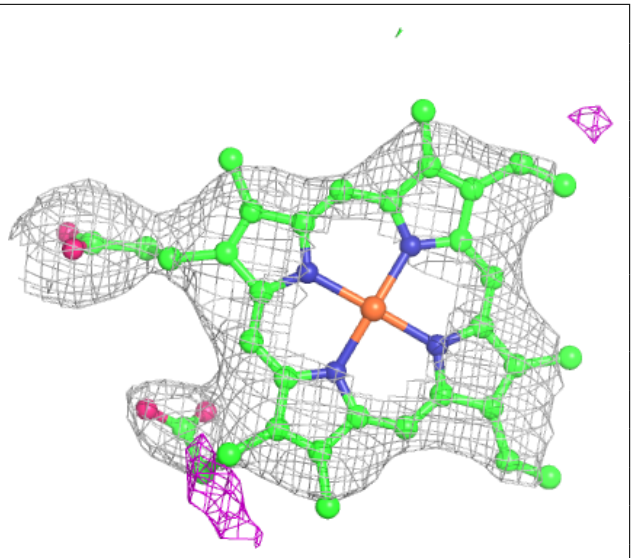
Electron density around HEM F 302:

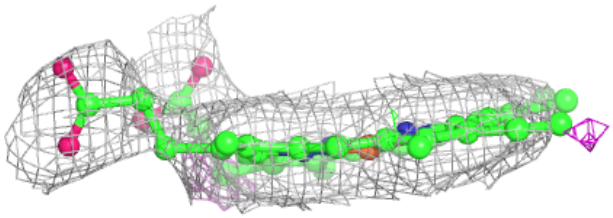
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

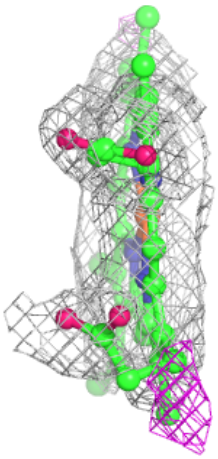


Electron density around HEM G 601:

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

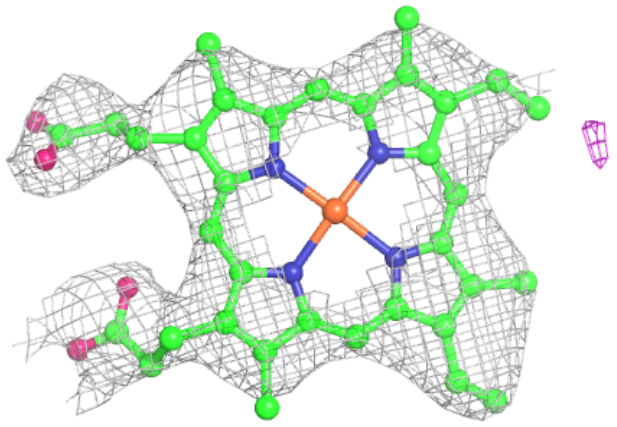


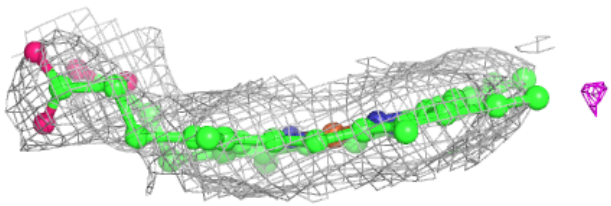


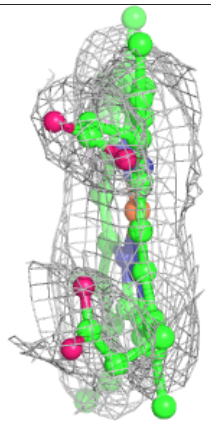


Electron density around HEM H 303:

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

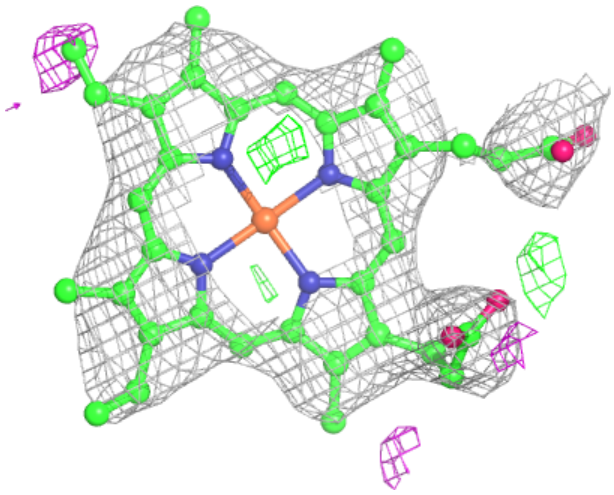


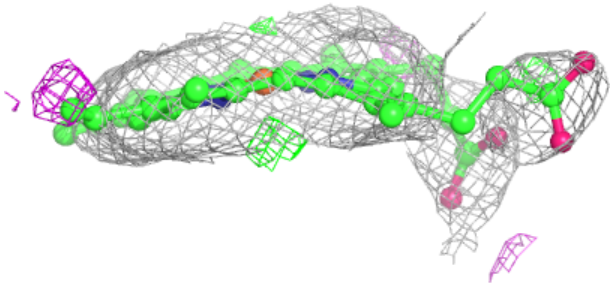


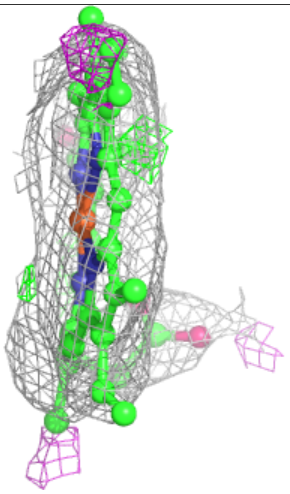


Electron density around HEM I 601:

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

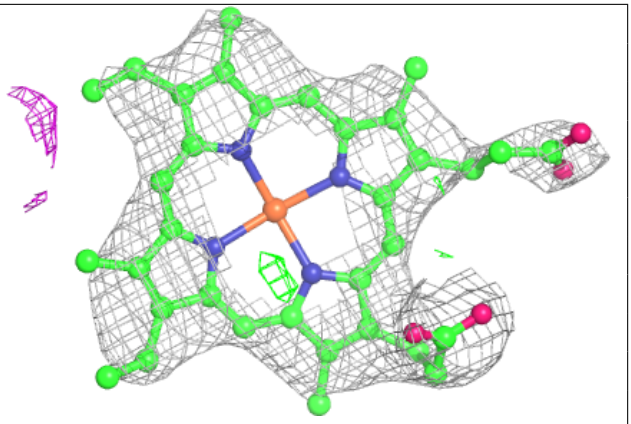


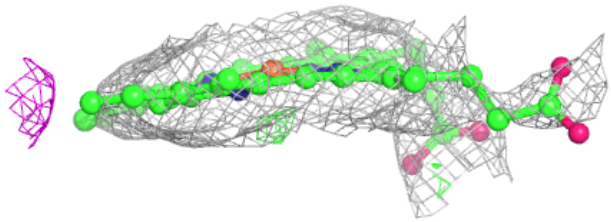


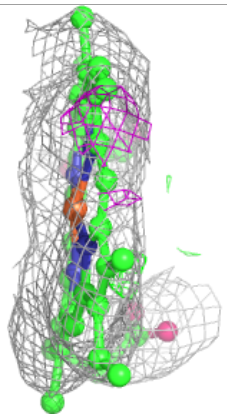


Electron density around HEM J 302:

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

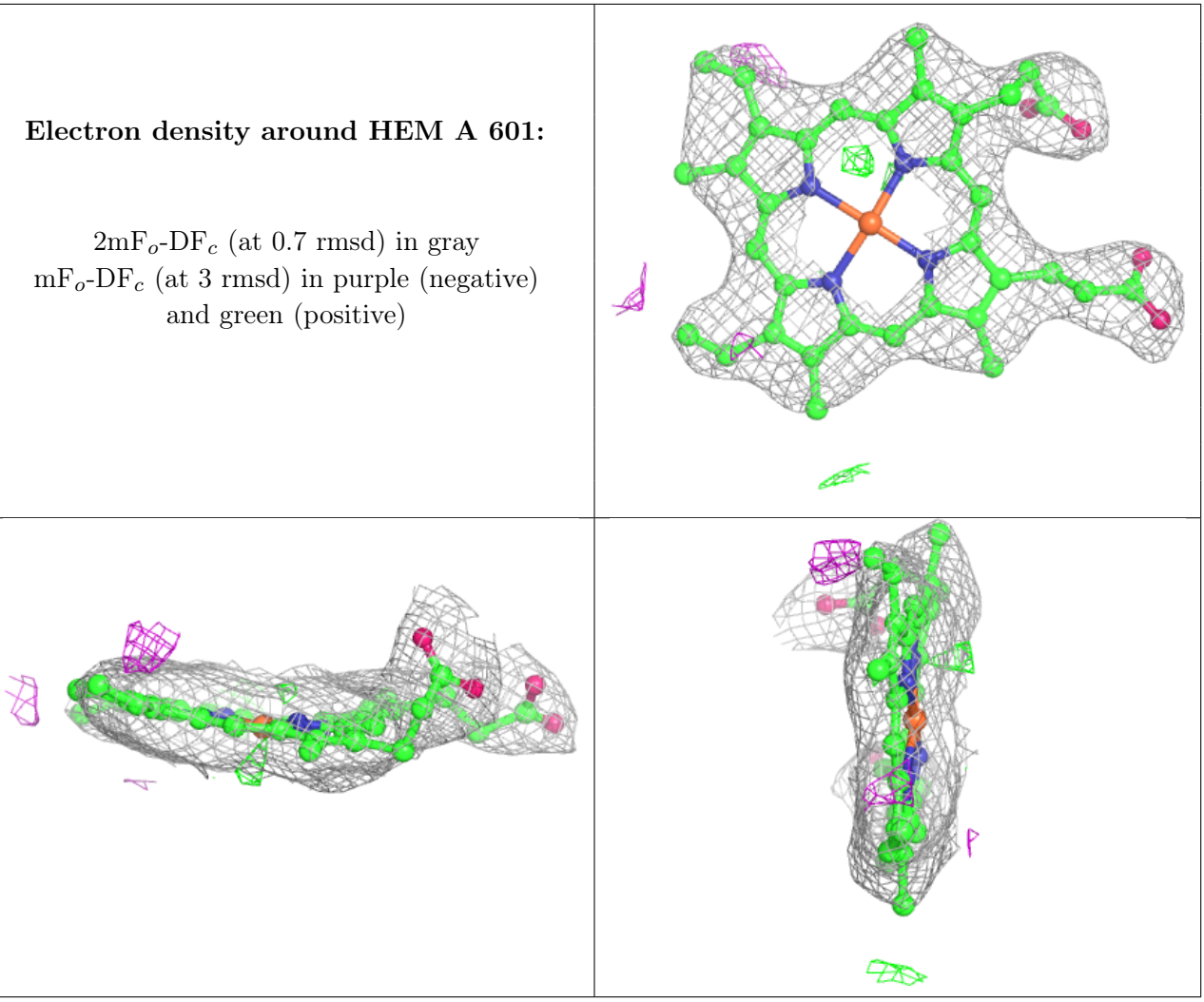






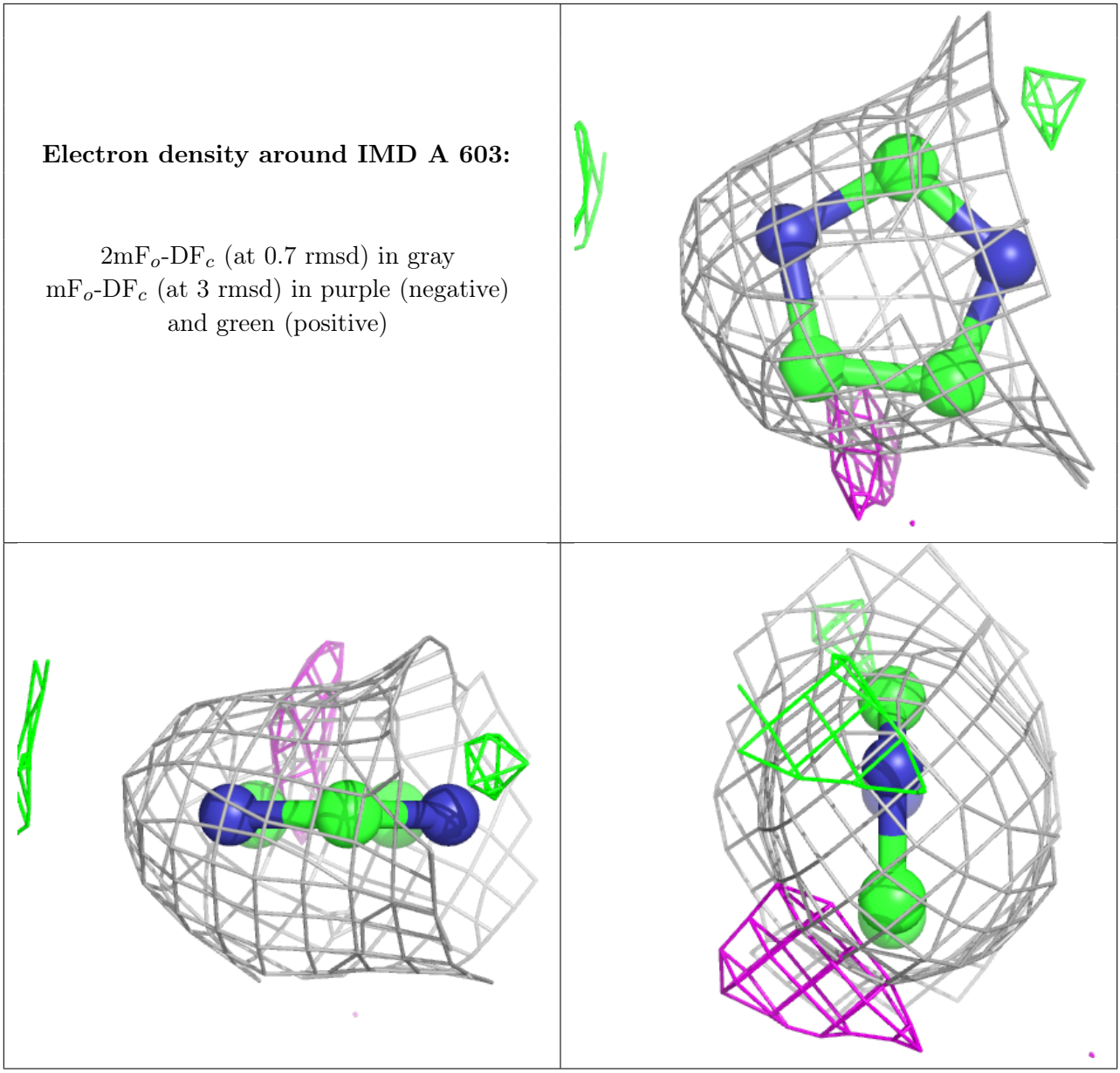
Electron density around HEM A 601:

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



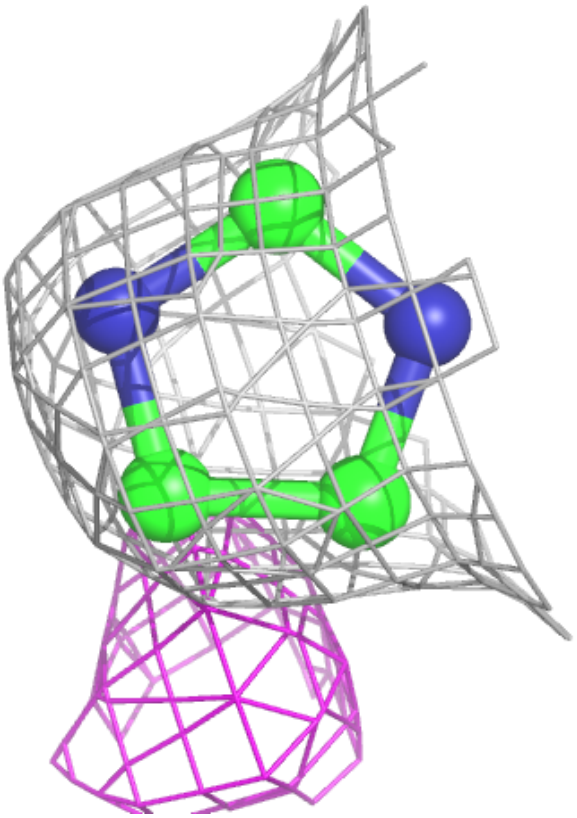
Electron density around IMD A 603:

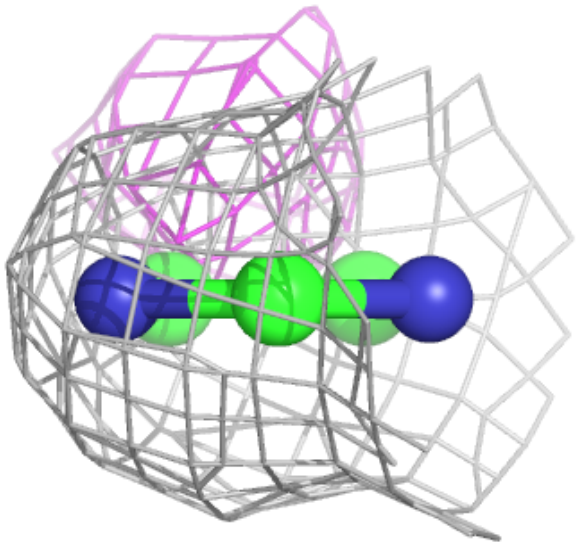
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

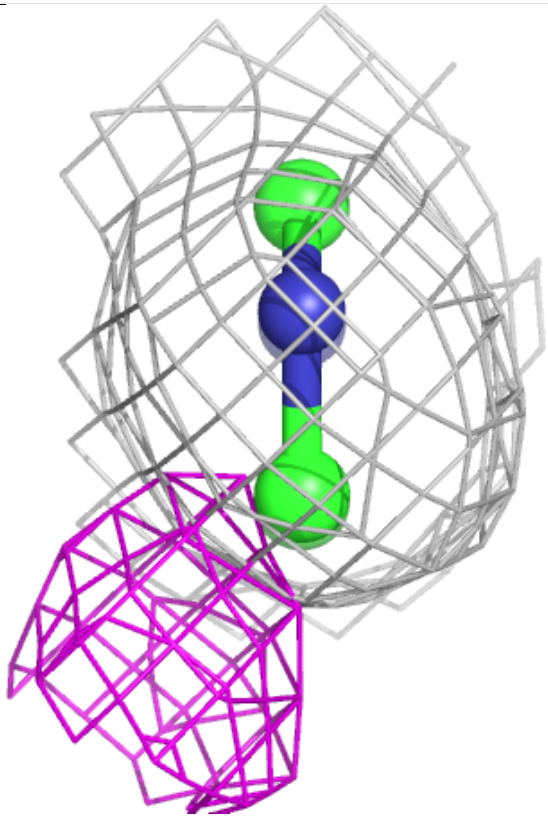


Electron density around IMD D 303:

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

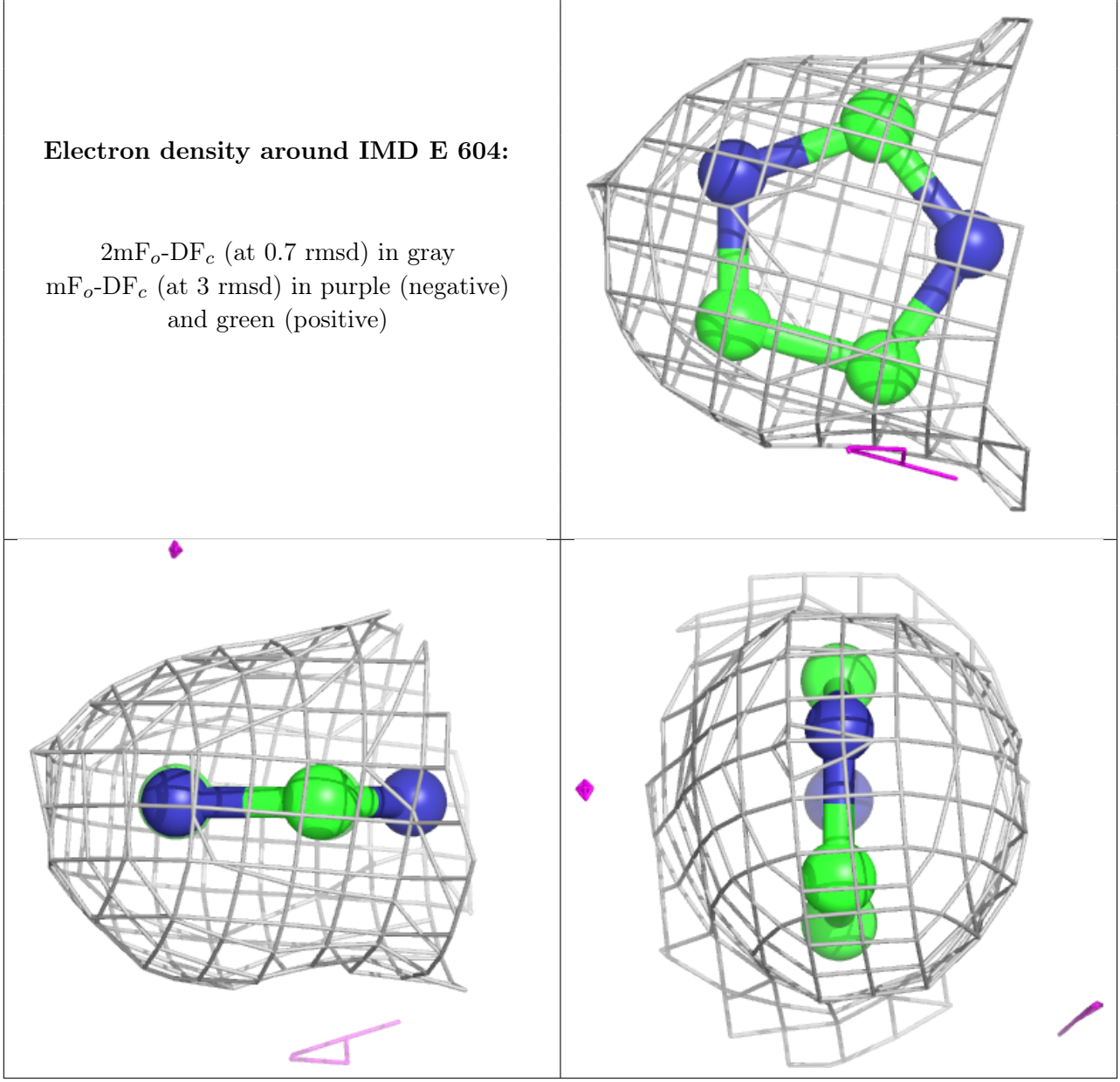






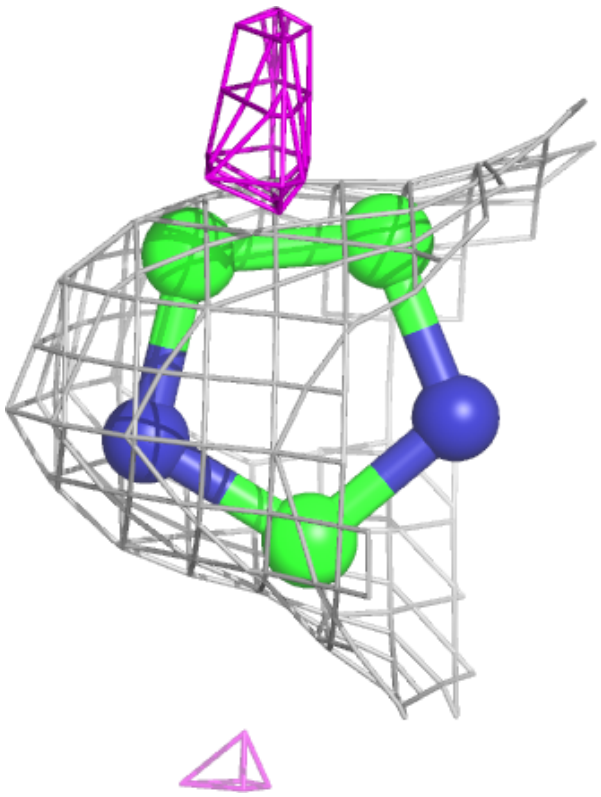
Electron density around IMD E 604:

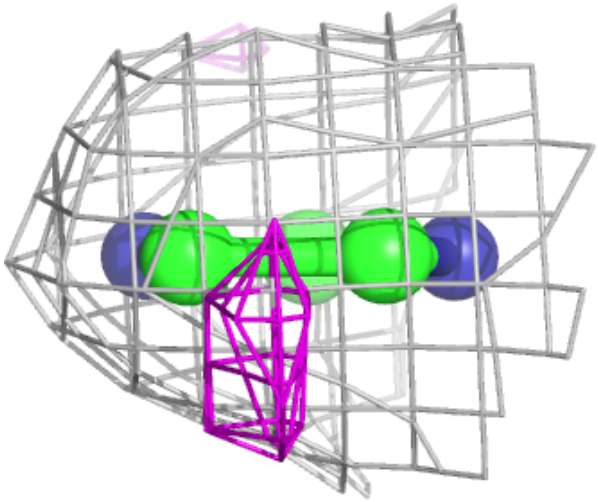
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

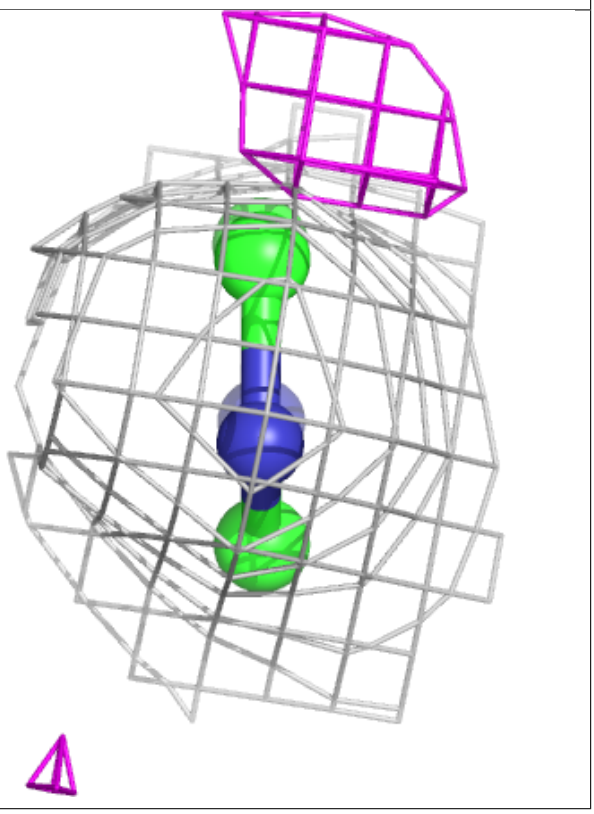


Electron density around IMD H 304:

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

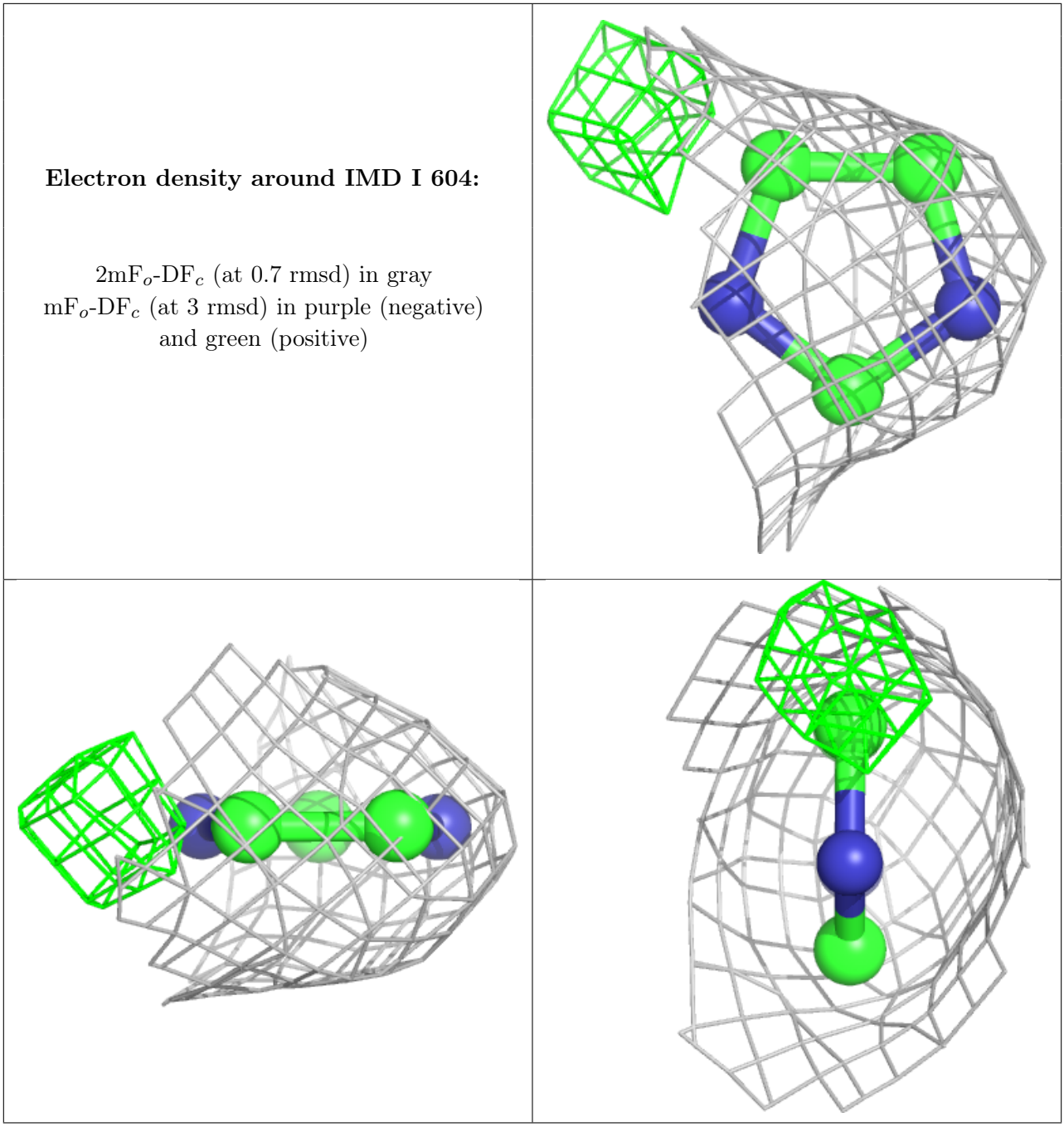






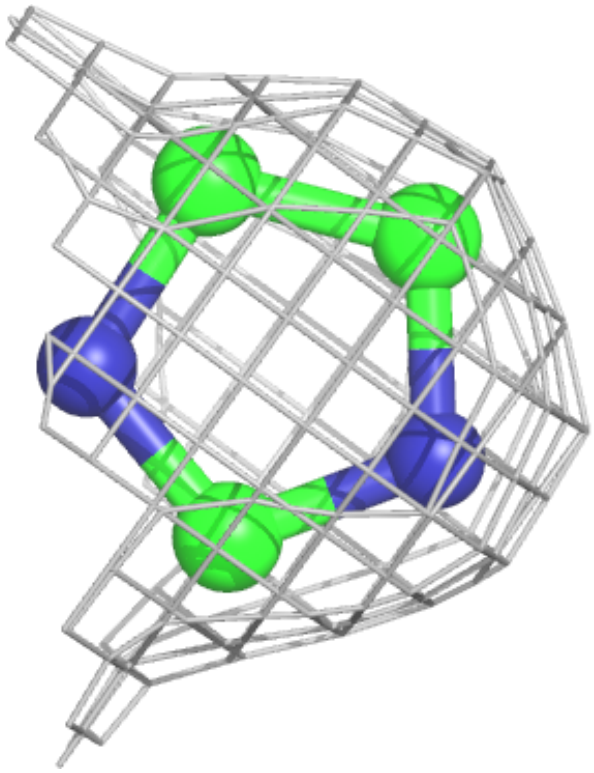
Electron density around IMD I 604:

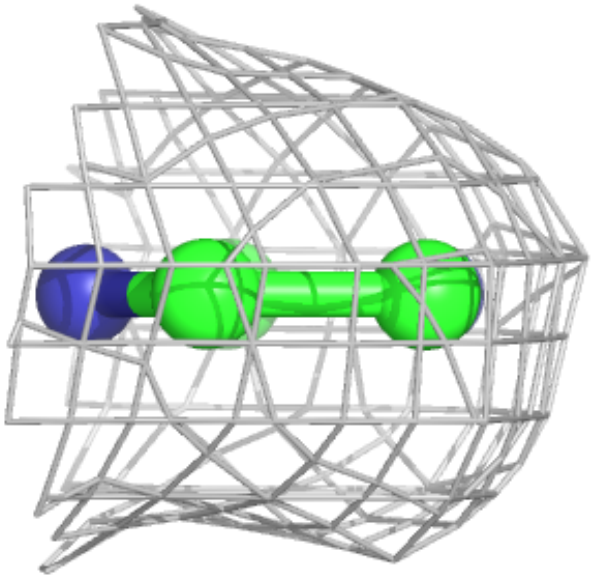
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

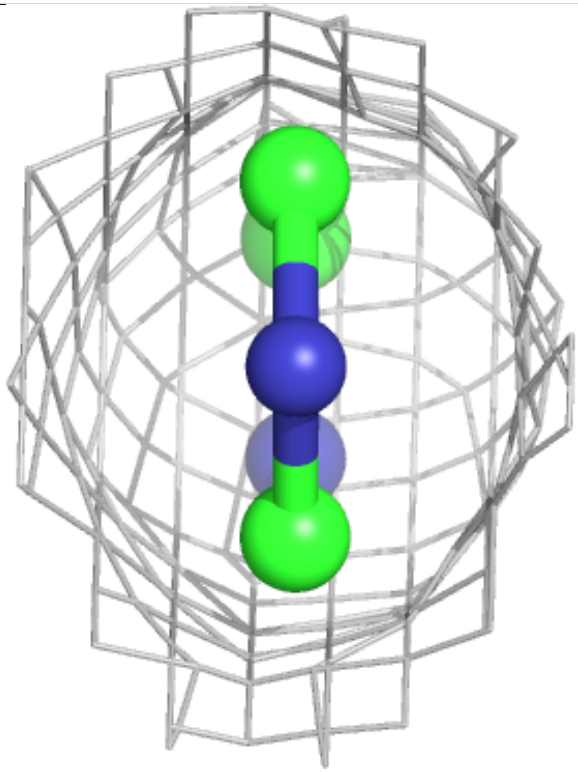


Electron density around IMD F 303:

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

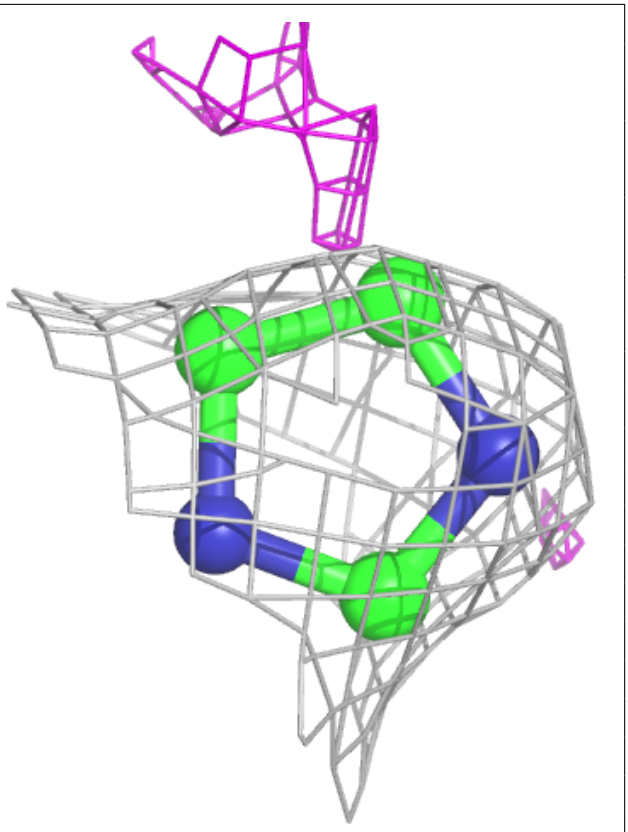


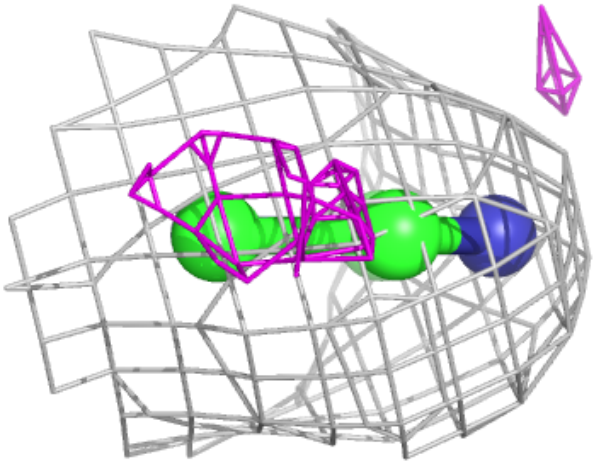


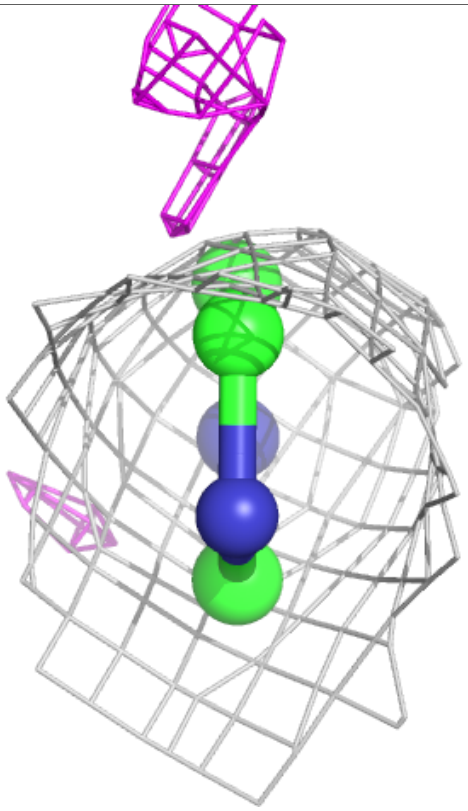


Electron density around IMD G 603:

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

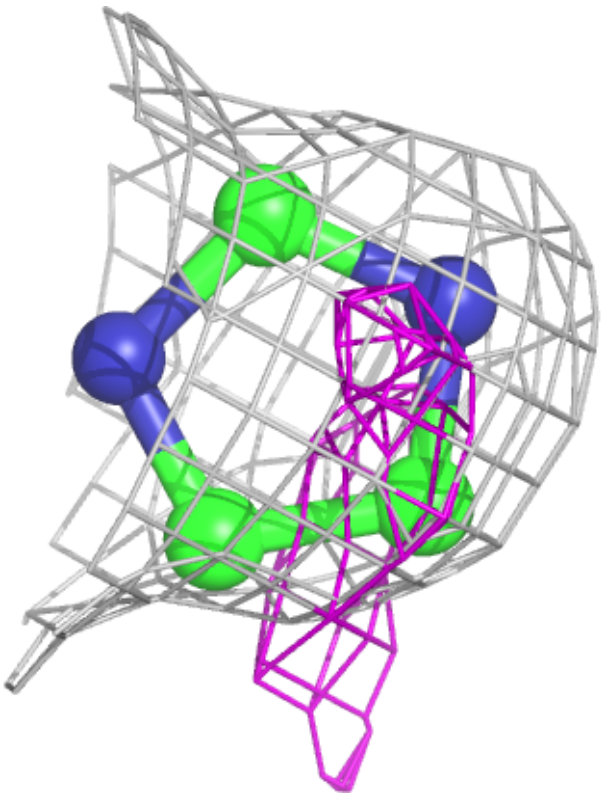


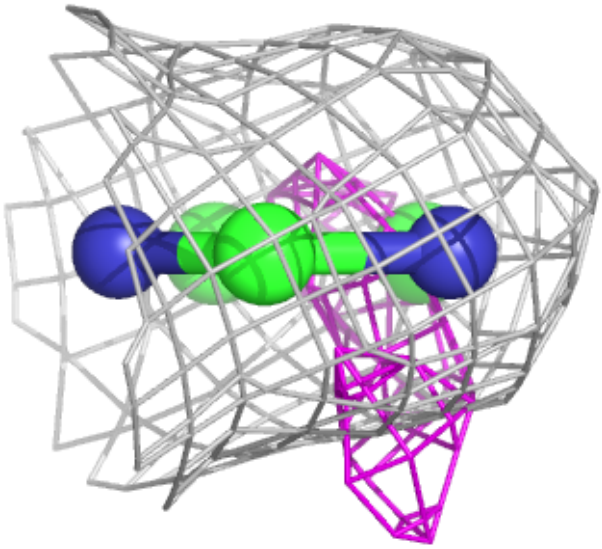


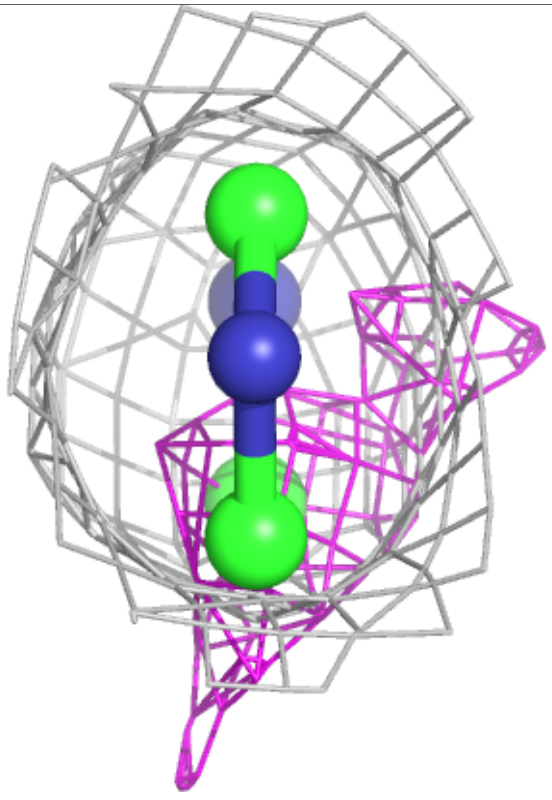


Electron density around IMD B 304:

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

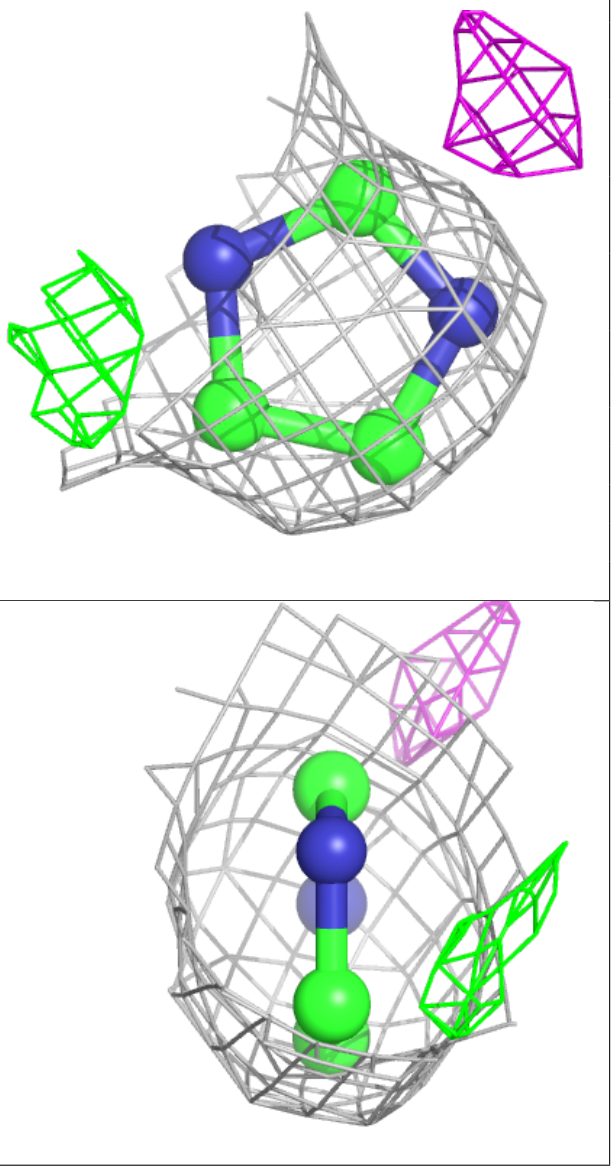


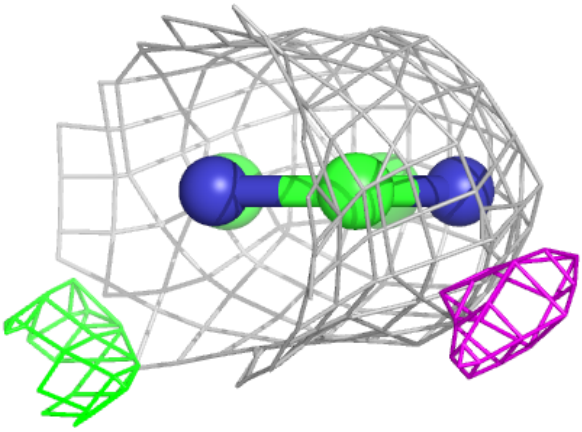




Electron density around IMD C 604:

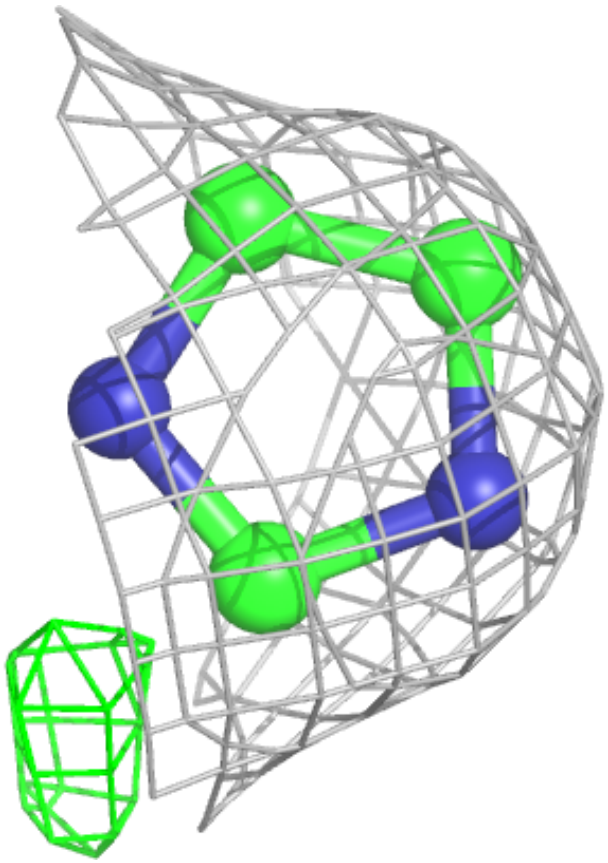
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

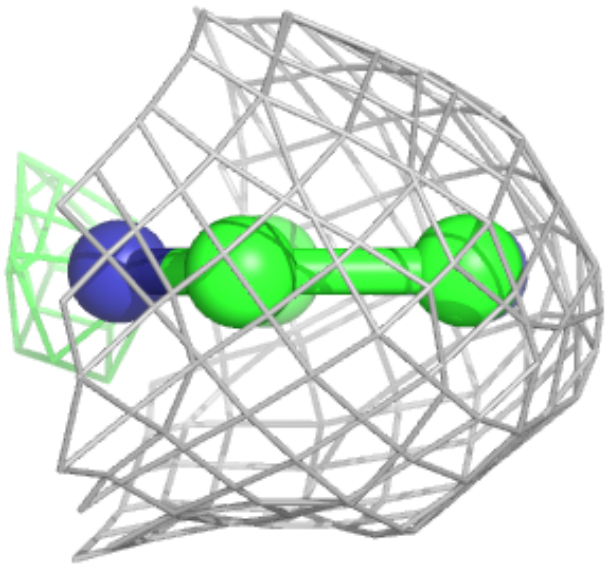


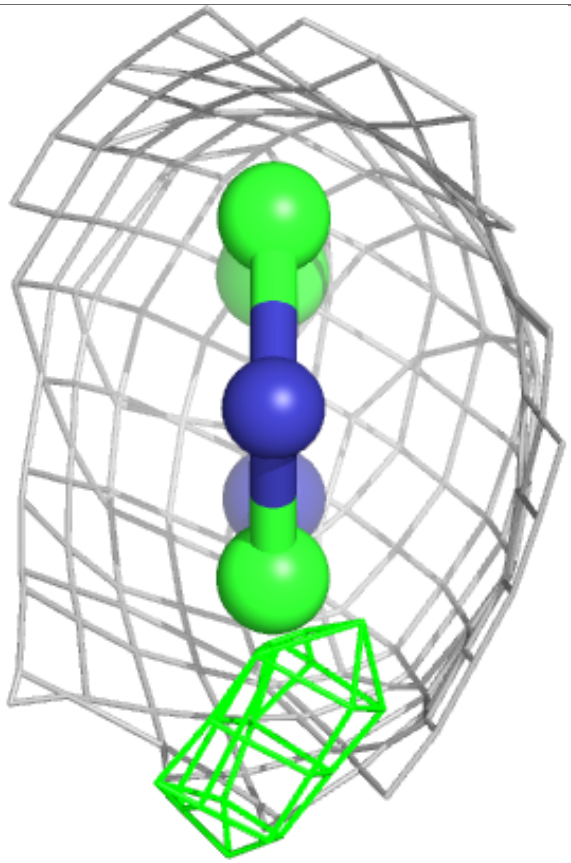


Electron density around IMD J 303:

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







6.5 Other polymers (i)

There are no such residues in this entry.