Full wwPDB X-ray Structure Validation Report ⓘ

Aug 20, 2023 – 07:27 AM EDT

PDB ID	:	2IJ7
Title	:	Structure of Mycobacterium tuberculosis CYP121 in complex with the anti-fungal drug fluconazole
Authors	:	Roujeinikova, A.; Leys, D.
Deposited on	:	2006-09-29
Resolution	:	1.90 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:

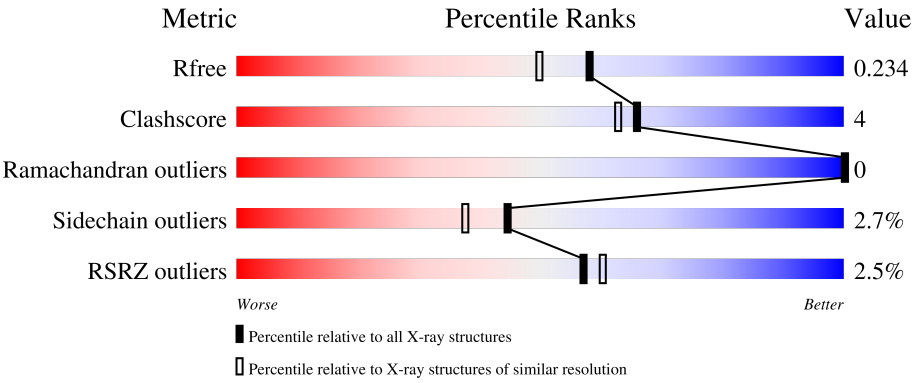
MolProbity	:	4.02b-467
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.35
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.35

1 Overall quality at a glance (i)

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

The reported resolution of this entry is 1.90 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	6207 (1.90-1.90)
Clashscore	141614	6847 (1.90-1.90)
Ramachandran outliers	138981	6760 (1.90-1.90)
Sidechain outliers	138945	6760 (1.90-1.90)
RSRZ outliers	127900	6082 (1.90-1.90)

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	396	3% 92% 6%
1	B	396	2% 91% 6%
1	C	396	% 89% 9%
1	D	396	2% 90% 8%
1	E	396	3% 88% 10%

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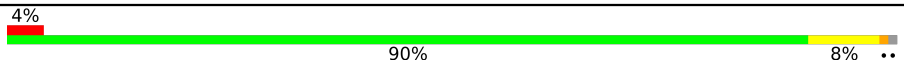
Mol	Chain	Length	Quality of chain
1	F	396	

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
3	TPF	A	2472[A]	-	-	X	-
3	TPF	D	2473[A]	-	-	X	-
3	TPF	F	2474[A]	-	-	X	-

2 Entry composition (i)

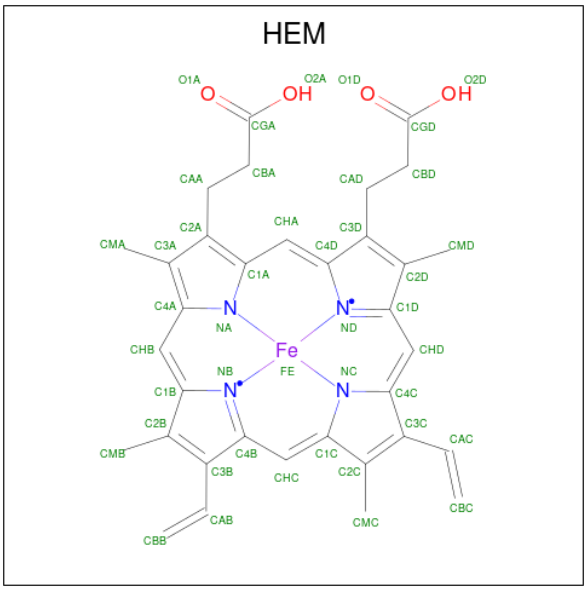
There are 4 unique types of molecules in this entry. The entry contains 20488 atoms, of which 0 are hydrogens and 0 are deuteriums.

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 Cytochrome P450 121.

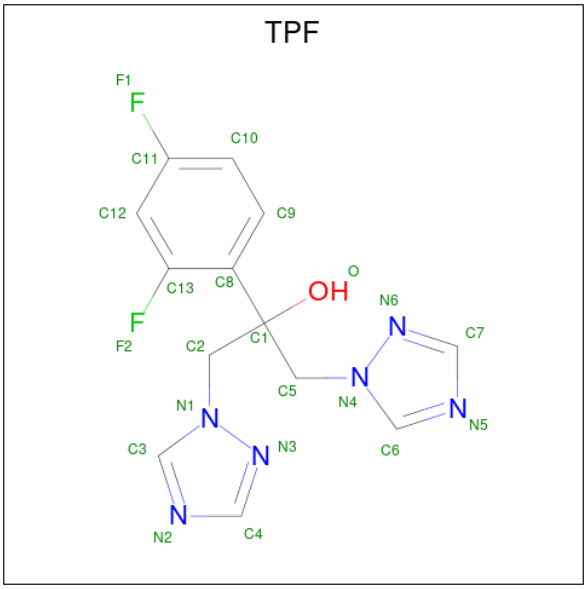
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	391	Total	C	N	O	S	0	0	0
			3012	1914	537	551	10			
1	B	391	Total	C	N	O	S	0	0	0
			3012	1914	537	551	10			
1	C	391	Total	C	N	O	S	0	0	0
			3012	1914	537	551	10			
1	D	391	Total	C	N	O	S	0	0	0
			3012	1914	537	551	10			
1	E	391	Total	C	N	O	S	0	0	0
			3012	1914	537	551	10			
1	F	391	Total	C	N	O	S	0	0	0
			3012	1914	537	551	10			

- 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		

- Molecule 3 is 2-(2,4-DIFLUOROPHENYL)-1,3-DI(1H-1,2,4-TRIAZOL-1-YL)PROPAN-2-OL (three-letter code: TPF) (formula: $C_{13}H_{12}F_2N_6O$).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
3	A	1	Total	C	F	N	O	0	1
			44	26	4	12	2		
3	B	1	Total	C	F	N	O	0	0
			22	13	2	6	1		
3	C	1	Total	C	F	N	O	0	0
			22	13	2	6	1		
3	D	1	Total	C	F	N	O	0	1
			44	26	4	12	2		
3	F	1	Total	C	F	N	O	0	1
			44	26	4	12	2		

- Molecule 4 is water.

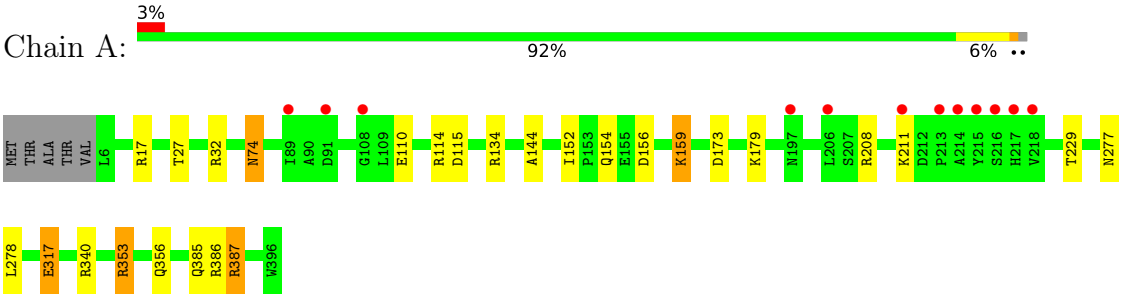
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
4	A	320	Total O 320 320	0	3
4	B	364	Total O 364 364	0	0
4	C	346	Total O 346 346	0	0
4	D	275	Total O 275 275	0	1
4	E	387	Total O 387 387	0	0
4	F	290	Total O 290 290	0	1

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.

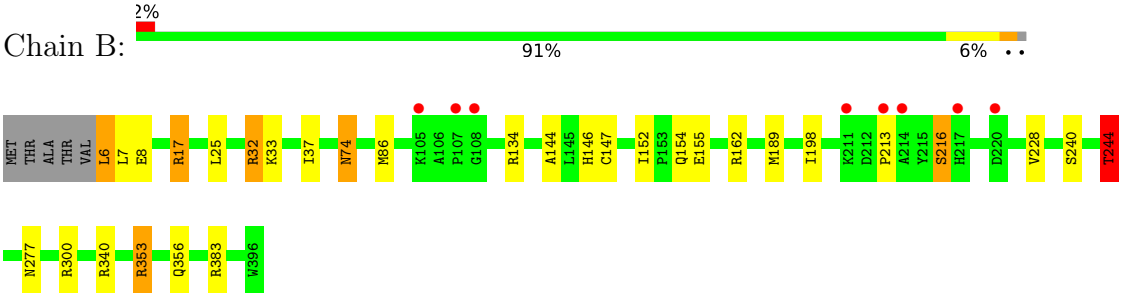
• Molecule 1: Cytochrome P450 121

Chain A:



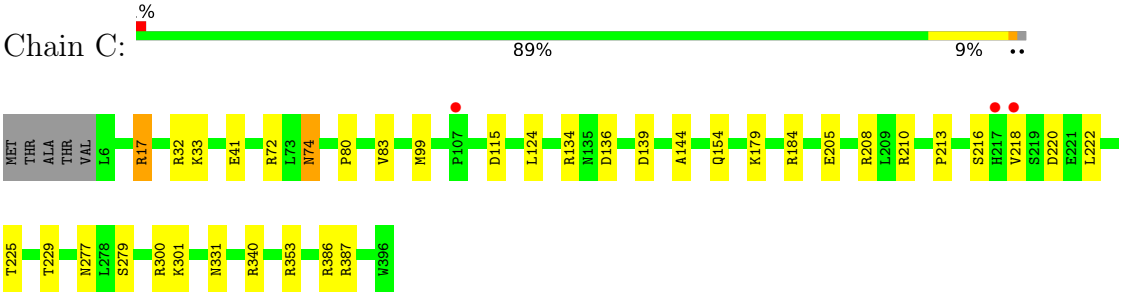
• Molecule 1: Cytochrome P450 121

Chain B:



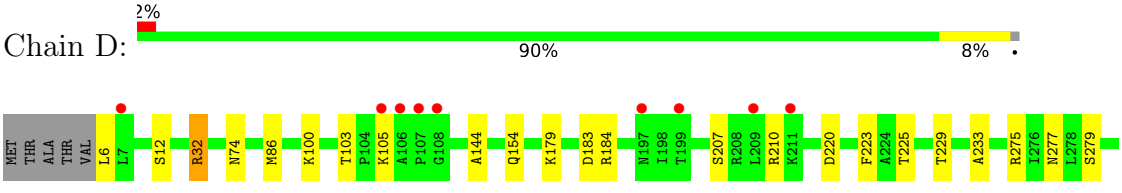
• Molecule 1: Cytochrome P450 121

Chain C:

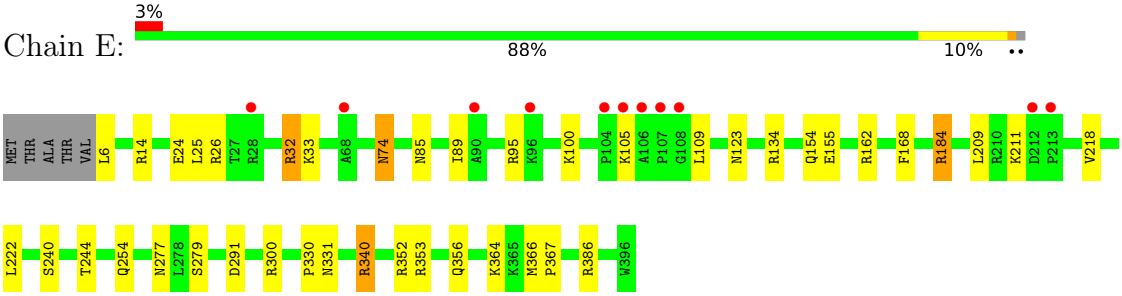


• Molecule 1: Cytochrome P450 121

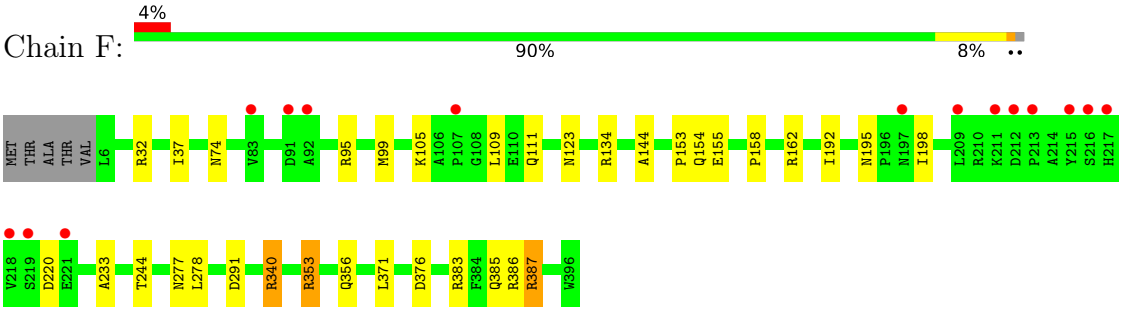
Chain D:



• Molecule 1: Cytochrome P450 121



• Molecule 1: Cytochrome P450 121



4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α, β, γ	60.80Å 129.90Å 323.39Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	20.00 – 1.90 19.97 – 1.90	Depositor EDS
% Data completeness (in resolution range)	89.9 (20.00-1.90) 86.7 (19.97-1.90)	Depositor EDS
R_{merge}	0.09	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	1.75 (at 1.90Å)	Xtriage
Refinement program	REFMAC 5.2.0005	Depositor
R, R_{free}	0.167 , 0.226 0.176 , 0.234	Depositor DCC
R_{free} test set	8786 reflections (5.01%)	wwPDB-VP
Wilson B-factor (Å^2)	23.5	Xtriage
Anisotropy	0.090	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.34 , 54.0	EDS
L-test for twinning[2]	$< \|L\| > = 0.49$, $< L^2 > = 0.32$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o,F_c correlation	0.96	EDS
Total number of atoms	20488	wwPDB-VP
Average B, all atoms (Å^2)	30.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.40% 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: HEM, TPF

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	0.78	1/3075 (0.0%)	0.83	7/4181 (0.2%)
1	B	0.80	2/3075 (0.1%)	0.80	5/4181 (0.1%)
1	C	0.80	0/3075	0.81	9/4181 (0.2%)
1	D	0.77	0/3075	0.80	5/4181 (0.1%)
1	E	0.83	2/3075 (0.1%)	0.84	8/4181 (0.2%)
1	F	0.78	0/3075	0.83	7/4181 (0.2%)
All	All	0.79	5/18450 (0.0%)	0.82	41/25086 (0.2%)

All (5) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	244	THR	CB-CG2	-6.43	1.31	1.52
1	B	8	GLU	CB-CG	5.32	1.62	1.52
1	E	364	LYS	CB-CG	-5.23	1.38	1.52
1	E	24	GLU	CG-CD	5.17	1.59	1.51
1	A	317	GLU	CB-CG	5.12	1.61	1.52

All (41) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	F	340	ARG	NE-CZ-NH2	-13.28	113.66	120.30
1	F	340	ARG	NE-CZ-NH1	12.08	126.34	120.30
1	A	134	ARG	NE-CZ-NH2	9.48	125.04	120.30
1	E	134	ARG	NE-CZ-NH1	-9.21	115.70	120.30
1	A	387	ARG	NE-CZ-NH2	-8.62	115.99	120.30
1	C	387	ARG	NE-CZ-NH2	-8.52	116.04	120.30
1	A	134	ARG	NE-CZ-NH1	-8.14	116.23	120.30
1	C	387	ARG	NE-CZ-NH1	7.89	124.25	120.30
1	E	134	ARG	NE-CZ-NH2	7.58	124.09	120.30
1	B	134	ARG	NE-CZ-NH1	-7.53	116.54	120.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	D	383	ARG	NE-CZ-NH2	7.40	124.00	120.30
1	A	387	ARG	NE-CZ-NH1	7.39	123.99	120.30
1	E	291	ASP	CB-CG-OD1	6.83	124.45	118.30
1	F	353	ARG	NE-CZ-NH1	6.75	123.67	120.30
1	F	387	ARG	NE-CZ-NH2	-6.67	116.96	120.30
1	F	134	ARG	NE-CZ-NH1	-6.31	117.14	120.30
1	B	134	ARG	NE-CZ-NH2	6.30	123.45	120.30
1	D	32	ARG	NE-CZ-NH2	-6.17	117.22	120.30
1	D	184	ARG	NE-CZ-NH1	-6.14	117.23	120.30
1	A	115	ASP	CB-CG-OD1	6.09	123.78	118.30
1	E	352	ARG	NE-CZ-NH1	6.00	123.30	120.30
1	D	387	ARG	NE-CZ-NH1	5.94	123.27	120.30
1	C	184	ARG	NE-CZ-NH1	-5.94	117.33	120.30
1	C	134	ARG	NE-CZ-NH2	5.92	123.26	120.30
1	E	14	ARG	NE-CZ-NH1	5.90	123.25	120.30
1	E	300	ARG	NE-CZ-NH2	-5.68	117.46	120.30
1	C	134	ARG	NE-CZ-NH1	-5.66	117.47	120.30
1	D	370	ASP	CB-CG-OD1	5.64	123.38	118.30
1	B	162	ARG	NE-CZ-NH1	5.61	123.11	120.30
1	B	300	ARG	NE-CZ-NH1	5.61	123.11	120.30
1	A	353	ARG	NE-CZ-NH2	5.56	123.08	120.30
1	F	291	ASP	CB-CG-OD1	5.51	123.26	118.30
1	C	115	ASP	CB-CG-OD1	5.47	123.22	118.30
1	C	300	ARG	NE-CZ-NH1	5.30	122.95	120.30
1	E	352	ARG	NE-CZ-NH2	-5.27	117.67	120.30
1	A	340	ARG	NE-CZ-NH1	5.18	122.89	120.30
1	F	376	ASP	CB-CG-OD2	-5.16	113.65	118.30
1	B	300	ARG	NE-CZ-NH2	-5.13	117.73	120.30
1	C	115	ASP	CB-CG-OD2	-5.13	113.69	118.30
1	C	139	ASP	CB-CG-OD2	-5.01	113.79	118.30
1	E	26	ARG	NE-CZ-NH2	5.01	122.80	120.30

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts (i)

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	3012	0	3074	14	0
1	B	3012	0	3074	18	0
1	C	3012	0	3074	16	0
1	D	3012	0	3074	20	0
1	E	3012	0	3074	21	0
1	F	3012	0	3074	24	0
2	A	43	0	30	7	0
2	B	43	0	30	2	0
2	C	43	0	30	0	0
2	D	43	0	30	3	0
2	E	43	0	30	1	0
2	F	43	0	30	4	0
3	A	44	0	24	14	0
3	B	22	0	12	0	0
3	C	22	0	12	0	0
3	D	44	0	24	15	0
3	F	44	0	24	18	0
4	A	320	0	0	5	1
4	B	364	0	0	3	0
4	C	346	0	0	3	1
4	D	275	0	0	9	0
4	E	387	0	0	6	2
4	F	290	0	0	7	2
All	All	20488	0	18720	148	3

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 4.

All (148) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:D:2473[A]:TPF:C7	4:D:2516:HOH:O	1.69	1.39
3:D:2473[A]:TPF:N5	4:D:2652:HOH:O	1.57	1.32
3:F:2474[A]:TPF:C6	4:F:2575:HOH:O	1.81	1.22
3:D:2473[A]:TPF:HC6	4:D:2658:HOH:O	1.41	1.15
3:F:2474[A]:TPF:HC6	4:F:2575:HOH:O	1.43	1.11
3:A:2472[A]:TPF:HC6	4:A:2583:HOH:O	1.61	0.99
3:F:2474[A]:TPF:C6	3:F:2474[A]:TPF:HC21	1.98	0.94
3:D:2473[A]:TPF:C6	4:D:2658:HOH:O	2.03	0.92
1:E:123:ASN:OD1	4:E:552:HOH:O	1.94	0.86
1:D:385:GLN:HE21	3:D:2473[A]:TPF:HC7	1.40	0.84
1:D:385:GLN:NE2	3:D:2473[A]:TPF:HC7	1.96	0.81

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:F:2474[A]:TPF:N6	3:F:2474[A]:TPF:C2	2.46	0.77
1:D:353:ARG:HH11	1:D:356:GLN:HE21	1.34	0.76
3:F:2474[A]:TPF:N6	3:F:2474[A]:TPF:HC22	2.01	0.76
2:A:462:HEM:HAD1	3:A:2472[A]:TPF:H10	1.66	0.76
1:C:144:ALA:HA	1:C:154:GLN:HE22	1.54	0.73
1:B:198:ILE:O	4:B:2725:HOH:O	2.09	0.68
3:D:2473[A]:TPF:F2	3:D:2473[A]:TPF:HC22	1.84	0.66
1:A:152:ILE:O	4:A:2764:HOH:O	2.11	0.66
1:F:386:ARG:HH22	3:F:2474[A]:TPF:C7	2.08	0.66
1:A:353:ARG:HH11	1:A:356:GLN:HE21	1.45	0.63
1:E:353:ARG:HH11	1:E:356:GLN:HE21	1.44	0.63
1:D:6:LEU:N	4:D:2651:HOH:O	2.32	0.62
1:F:158:PRO:O	1:F:162:ARG:HG3	2.00	0.61
1:E:240:SER:O	1:E:244:THR:HG23	2.00	0.61
1:E:184:ARG:CZ	4:E:626:HOH:O	2.49	0.61
3:D:2473[A]:TPF:C6	4:D:2652:HOH:O	2.21	0.60
1:A:208:ARG:O	1:A:211:LYS:HG2	2.01	0.60
1:B:33:LYS:NZ	4:B:2503:HOH:O	2.24	0.59
1:D:210:ARG:HD2	1:D:220:ASP:OD2	2.04	0.58
1:D:233:ALA:HB1	3:D:2473[A]:TPF:N3	2.17	0.58
1:F:353:ARG:HH11	1:F:356:GLN:HE21	1.50	0.58
1:D:353:ARG:HH11	1:D:356:GLN:NE2	1.99	0.58
1:F:233:ALA:HB1	3:F:2474[A]:TPF:N3	2.19	0.58
1:B:353:ARG:HH11	1:B:356:GLN:HE21	1.52	0.57
1:D:225:THR:O	1:D:229:THR:HG23	2.05	0.57
3:D:2473[A]:TPF:C6	3:D:2473[A]:TPF:HC21	2.36	0.56
1:B:37:ILE:HD11	1:B:383:ARG:CZ	2.36	0.56
1:A:386:ARG:HH22	3:A:2472[A]:TPF:HC7	1.70	0.56
1:F:386:ARG:HH22	3:F:2474[A]:TPF:HC7	1.69	0.56
1:B:144:ALA:HA	1:B:154:GLN:HE22	1.70	0.55
1:D:144:ALA:HA	1:D:154:GLN:HE22	1.71	0.55
1:C:205:GLU:HA	1:C:208:ARG:NH1	2.22	0.55
3:A:2472[A]:TPF:N6	3:A:2472[A]:TPF:C2	2.69	0.55
1:C:205:GLU:OE1	1:C:208:ARG:NH1	2.40	0.55
1:C:74:ASN:HD22	1:C:74:ASN:C	2.09	0.54
1:F:195:ASN:HB3	1:F:198:ILE:HG12	1.89	0.54
2:A:462:HEM:CAD	3:A:2472[A]:TPF:H10	2.36	0.54
1:C:33:LYS:HD2	1:C:41:GLU:HB3	1.90	0.54
1:F:144:ALA:HA	1:F:154:GLN:HE22	1.72	0.54
1:F:385:GLN:HE21	3:F:2474[A]:TPF:C7	2.20	0.54
1:C:225:THR:O	1:C:229:THR:HG23	2.07	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:74:ASN:C	1:A:74:ASN:HD22	2.12	0.53
1:A:144:ALA:HA	1:A:154:GLN:HE22	1.73	0.53
2:E:462:HEM:HMC1	2:E:462:HEM:HBC2	1.89	0.53
2:A:462:HEM:NA	3:A:2472[A]:TPF:C3	2.71	0.53
3:D:2473[A]:TPF:HC7	4:D:2516:HOH:O	1.60	0.52
1:F:153:PRO:HB3	1:F:155:GLU:OE1	2.09	0.52
1:F:278:LEU:O	1:F:387:ARG:HD2	2.08	0.52
1:B:6:LEU:N	4:B:2712:HOH:O	2.43	0.52
1:E:25:LEU:HD11	1:E:32:ARG:HG2	1.92	0.52
2:D:462:HEM:CAD	3:D:2473[A]:TPF:HC9	2.40	0.52
1:D:385:GLN:NE2	3:D:2473[A]:TPF:C7	2.70	0.52
1:F:37:ILE:HD11	1:F:383:ARG:NE	2.25	0.51
1:B:25:LEU:HD11	1:B:32:ARG:HD2	1.91	0.51
2:F:462:HEM:C1A	3:F:2474[A]:TPF:HC3	2.46	0.51
1:E:366:MET:N	1:E:367:PRO:HD3	2.27	0.50
1:D:100:LYS:O	1:D:103:THR:HG22	2.12	0.49
1:B:17:ARG:N	1:B:17:ARG:HD2	2.27	0.49
2:F:462:HEM:NA	3:F:2474[A]:TPF:C3	2.75	0.49
1:A:156:ASP:O	1:A:159:LYS:HG3	2.12	0.49
1:C:17:ARG:O	1:C:17:ARG:HD3	2.12	0.48
1:F:244:THR:CB	4:F:2667:HOH:O	2.60	0.48
1:B:240:SER:O	1:B:244:THR:CG2	2.62	0.48
2:A:462:HEM:C1A	3:A:2472[A]:TPF:HC3	2.48	0.48
1:A:278:LEU:O	1:A:387:ARG:HD2	2.14	0.48
1:C:210:ARG:NE	1:C:220:ASP:OD2	2.38	0.48
1:D:210:ARG:HG3	1:D:223:PHE:CE1	2.49	0.48
1:A:229:THR:CG2	3:A:2472[A]:TPF:F1	2.52	0.47
1:F:123:ASN:HB3	4:F:2694:HOH:O	2.15	0.47
2:A:462:HEM:C1A	3:A:2472[A]:TPF:C3	2.97	0.47
2:F:462:HEM:HAD2	3:F:2474[A]:TPF:HC9	1.97	0.47
1:F:385:GLN:NE2	3:F:2474[A]:TPF:C7	2.77	0.47
3:F:2474[A]:TPF:HC21	3:F:2474[A]:TPF:N6	2.19	0.47
1:F:37:ILE:HD11	1:F:383:ARG:CZ	2.45	0.46
1:F:233:ALA:HB1	3:F:2474[A]:TPF:C4	2.46	0.46
1:C:124:LEU:HD21	1:C:136:ASP:HB3	1.98	0.46
1:F:155:GLU:H	1:F:155:GLU:CD	2.19	0.46
1:C:179:LYS:NZ	4:C:2642:HOH:O	2.46	0.46
1:C:279:SER:O	1:C:386:ARG:HA	2.16	0.46
1:E:32:ARG:HD3	1:E:33:LYS:N	2.31	0.46
1:F:244:THR:HB	4:F:2667:HOH:O	2.16	0.46
2:F:462:HEM:HAD1	3:F:2474[A]:TPF:H10	1.98	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:218:VAL:HG13	1:C:222:LEU:HD23	1.97	0.45
1:D:279:SER:CB	4:D:2572:HOH:O	2.65	0.45
1:E:162:ARG:NH2	4:E:657:HOH:O	2.49	0.45
1:A:173:ASP:OD1	4:A:2751:HOH:O	2.21	0.45
1:B:213:PRO:O	1:B:216:SER:OG	2.35	0.45
1:A:385:GLN:HE21	3:A:2472[A]:TPF:C7	2.30	0.44
1:D:275:ARG:O	1:D:313:ASN:HB3	2.18	0.44
1:A:110:GLU:HG2	1:A:114:ARG:NH1	2.32	0.44
1:B:37:ILE:HD11	1:B:383:ARG:NE	2.33	0.44
3:A:2472[A]:TPF:N6	3:A:2472[A]:TPF:HC21	2.31	0.44
3:F:2474[A]:TPF:HC21	3:F:2474[A]:TPF:N5	2.32	0.44
1:F:111:GLN:NE2	4:F:2746:HOH:O	2.49	0.44
2:A:462:HEM:HMC1	2:A:462:HEM:HBC2	1.99	0.44
1:C:301:LYS:NZ	4:C:2710:HOH:O	2.36	0.44
1:D:279:SER:O	1:D:386:ARG:HA	2.18	0.44
1:E:218:VAL:HG13	1:E:222:LEU:HD22	2.00	0.44
1:F:162:ARG:HG2	4:F:2681:HOH:O	2.18	0.44
1:B:86:MET:HG3	2:B:462:HEM:CGD	2.47	0.44
1:B:240:SER:O	1:B:244:THR:HG23	2.16	0.44
1:E:154:GLN:NE2	4:E:818:HOH:O	2.45	0.43
3:A:2472[A]:TPF:C6	4:A:2583:HOH:O	2.40	0.43
3:A:2472[A]:TPF:N6	3:A:2472[A]:TPF:HC22	2.34	0.43
1:B:74:ASN:C	1:B:74:ASN:HD22	2.22	0.43
1:E:74:ASN:C	1:E:74:ASN:HD22	2.22	0.43
2:D:462:HEM:HMD3	3:D:2473[B]:TPF:H10	2.01	0.43
1:F:192:ILE:HG23	1:F:198:ILE:HG13	2.01	0.43
1:D:179:LYS:NZ	1:D:183:ASP:OD2	2.50	0.42
1:E:155:GLU:H	1:E:155:GLU:CD	2.22	0.42
1:C:213:PRO:HA	1:C:216:SER:OG	2.19	0.42
1:D:210:ARG:CD	1:D:220:ASP:OD2	2.67	0.42
1:D:233:ALA:HB1	3:D:2473[A]:TPF:C4	2.49	0.42
1:E:184:ARG:NH2	4:E:626:HOH:O	2.51	0.42
3:F:2474[A]:TPF:HC21	3:F:2474[A]:TPF:C7	2.50	0.42
1:B:155:GLU:CD	1:B:155:GLU:H	2.23	0.42
1:B:189:MET:HG3	1:B:228:VAL:HG23	2.02	0.42
1:E:89:ILE:HB	1:E:95:ARG:HG3	2.01	0.42
1:F:144:ALA:CA	1:F:154:GLN:HE22	2.32	0.42
1:C:99:MET:HE3	4:C:2792:HOH:O	2.20	0.42
1:E:218:VAL:CG1	1:E:222:LEU:HD22	2.49	0.41
1:E:353:ARG:HE	1:E:353:ARG:HA	1.85	0.41
1:F:105:LYS:HA	1:F:105:LYS:HD3	1.86	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:147:CYS:HA	1:B:152:ILE:HB	2.02	0.41
1:A:386:ARG:HH22	3:A:2472[A]:TPF:C7	2.33	0.41
1:D:6:LEU:N	4:D:2722:HOH:O	2.52	0.41
1:F:95:ARG:O	1:F:99:MET:HG2	2.19	0.41
1:A:179:LYS:NZ	4:A:2640:HOH:O	2.54	0.41
1:E:85:ASN:HB3	1:E:168:PHE:CZ	2.56	0.41
1:E:222:LEU:O	1:E:222:LEU:HG	2.20	0.41
1:E:330:PRO:O	1:E:331:ASN:C	2.58	0.41
1:E:340:ARG:HD3	4:E:571:HOH:O	2.20	0.41
2:A:462:HEM:HMB2	2:A:462:HEM:HBB2	2.03	0.40
1:B:146:HIS:NE2	2:B:462:HEM:HBC2	2.36	0.40
1:E:279:SER:O	1:E:386:ARG:HA	2.21	0.40
1:D:86:MET:HG3	2:D:462:HEM:HBD2	2.03	0.40
1:C:80:PRO:O	1:C:83:VAL:HG12	2.21	0.40

All (3) symmetry-related close contacts are listed below. The label for Atom-2 includes the symmetry operator and encoded unit-cell translations to be applied.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:E:695:HOH:O	4:F:2599:HOH:O[2_564]	1.92	0.28
4:A:2699:HOH:O	4:F:2728:HOH:O[4_456]	2.16	0.04
4:C:2601:HOH:O	4:E:730:HOH:O[4_566]	2.19	0.01

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	389/396 (98%)	384 (99%)	5 (1%)	0	100	100
1	B	389/396 (98%)	384 (99%)	5 (1%)	0	100	100
1	C	389/396 (98%)	386 (99%)	3 (1%)	0	100	100
1	D	389/396 (98%)	386 (99%)	3 (1%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	E	389/396 (98%)	385 (99%)	4 (1%)	0	100	100
1	F	389/396 (98%)	382 (98%)	7 (2%)	0	100	100
All	All	2334/2376 (98%)	2307 (99%)	27 (1%)	0	100	100

There are no Ramachandran outliers to report.

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	322/326 (99%)	315 (98%)	7 (2%)	52	47
1	B	322/326 (99%)	312 (97%)	10 (3%)	40	32
1	C	322/326 (99%)	314 (98%)	8 (2%)	47	41
1	D	322/326 (99%)	314 (98%)	8 (2%)	47	41
1	E	322/326 (99%)	310 (96%)	12 (4%)	34	25
1	F	322/326 (99%)	315 (98%)	7 (2%)	52	47
All	All	1932/1956 (99%)	1880 (97%)	52 (3%)	44	38

All (52) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	17	ARG
1	A	27	THR
1	A	32	ARG
1	A	74	ASN
1	A	159	LYS
1	A	277	ASN
1	A	317	GLU
1	B	6	LEU
1	B	7	LEU
1	B	17	ARG
1	B	32	ARG
1	B	74	ASN

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Mol	Chain	Res	Type
1	B	216	SER
1	B	244	THR
1	B	277	ASN
1	B	340	ARG
1	B	353	ARG
1	C	17	ARG
1	C	32	ARG
1	C	72	ARG
1	C	74	ASN
1	C	277	ASN
1	C	331	ASN
1	C	340	ARG
1	C	353	ARG
1	D	12	SER
1	D	32	ARG
1	D	74	ASN
1	D	105	LYS
1	D	207	SER
1	D	277	ASN
1	D	340	ARG
1	D	375	ILE
1	E	6	LEU
1	E	32	ARG
1	E	74	ASN
1	E	100	LYS
1	E	105	LYS
1	E	109	LEU
1	E	184	ARG
1	E	209	LEU
1	E	211	LYS
1	E	254	GLN
1	E	277	ASN
1	E	340	ARG
1	F	32	ARG
1	F	74	ASN
1	F	109	LEU
1	F	220	ASP
1	F	277	ASN
1	F	340	ARG
1	F	371	LEU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (33) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	74	ASN
1	A	111	GLN
1	A	154	GLN
1	A	342	GLN
1	A	356	GLN
1	A	385	GLN
1	B	74	ASN
1	B	154	GLN
1	B	356	GLN
1	B	385	GLN
1	C	74	ASN
1	C	154	GLN
1	C	342	GLN
1	C	356	GLN
1	C	385	GLN
1	D	74	ASN
1	D	154	GLN
1	D	342	GLN
1	D	356	GLN
1	D	385	GLN
1	E	74	ASN
1	E	85	ASN
1	E	154	GLN
1	E	197	ASN
1	E	342	GLN
1	E	356	GLN
1	E	385	GLN
1	F	74	ASN
1	F	154	GLN
1	F	217	HIS
1	F	342	GLN
1	F	356	GLN
1	F	385	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)

14 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	D	462	3,1,4	41,50,50	1.78	5 (12%)	45,82,82	1.61	8 (17%)
2	HEM	E	462	4,1	41,50,50	1.60	5 (12%)	45,82,82	1.49	8 (17%)
2	HEM	C	462	4,1	41,50,50	1.87	8 (19%)	45,82,82	1.53	8 (17%)
3	TPF	F	2474[B]	-	18,24,24	3.61	10 (55%)	24,34,34	4.87	10 (41%)
3	TPF	D	2473[B]	-	18,24,24	3.78	11 (61%)	24,34,34	5.01	11 (45%)
2	HEM	A	462	3,1,4	41,50,50	1.94	10 (24%)	45,82,82	1.68	4 (8%)
3	TPF	B	2470	-	18,24,24	3.74	9 (50%)	24,34,34	4.68	13 (54%)
3	TPF	A	2472[B]	-	18,24,24	3.82	12 (66%)	24,34,34	4.85	10 (41%)
2	HEM	F	462	3,1,4	41,50,50	2.04	8 (19%)	45,82,82	1.71	7 (15%)
3	TPF	D	2473[A]	2	18,24,24	3.33	9 (50%)	24,34,34	4.72	11 (45%)
3	TPF	F	2474[A]	2	18,24,24	3.22	8 (44%)	24,34,34	5.15	12 (50%)
3	TPF	C	2471	-	18,24,24	3.48	10 (55%)	24,34,34	5.00	12 (50%)
3	TPF	A	2472[A]	2	18,24,24	3.44	10 (55%)	24,34,34	4.97	11 (45%)
2	HEM	B	462	4,1	41,50,50	1.86	10 (24%)	45,82,82	2.04	11 (24%)

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	D	462	3,1,4	-	2/12/54/54	-
2	HEM	E	462	4,1	-	2/12/54/54	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	HEM	C	462	4,1	-	1/12/54/54	-
3	TPF	F	2474[B]	-	-	4/16/16/16	0/3/3/3
3	TPF	D	2473[B]	-	-	1/16/16/16	0/3/3/3
2	HEM	A	462	3,1,4	-	0/12/54/54	-
3	TPF	B	2470	-	-	2/16/16/16	0/3/3/3
3	TPF	A	2472[B]	-	-	1/16/16/16	0/3/3/3
2	HEM	F	462	3,1,4	-	0/12/54/54	-
3	TPF	D	2473[A]	2	-	5/16/16/16	0/3/3/3
3	TPF	F	2474[A]	2	-	4/16/16/16	0/3/3/3
3	TPF	C	2471	-	-	1/16/16/16	0/3/3/3
3	TPF	A	2472[A]	2	-	3/16/16/16	0/3/3/3
2	HEM	B	462	4,1	-	0/12/54/54	-

All (125) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	B	2470	TPF	C3-N1	12.09	1.45	1.33
3	D	2473[B]	TPF	C3-N1	11.20	1.44	1.33
3	A	2472[B]	TPF	C3-N1	11.08	1.44	1.33
3	D	2473[A]	TPF	C3-N1	10.58	1.44	1.33
3	C	2471	TPF	C3-N1	10.33	1.43	1.33
3	A	2472[A]	TPF	C3-N1	10.32	1.43	1.33
3	F	2474[B]	TPF	C3-N1	10.32	1.43	1.33
3	F	2474[A]	TPF	C3-N1	9.95	1.43	1.33
2	F	462	HEM	C3D-C2D	7.88	1.53	1.36
2	D	462	HEM	C3D-C2D	7.24	1.52	1.36
2	C	462	HEM	C3D-C2D	7.23	1.52	1.36
2	B	462	HEM	C3D-C2D	7.01	1.51	1.36
2	A	462	HEM	C3D-C2D	6.53	1.50	1.36
2	E	462	HEM	C3D-C2D	6.31	1.50	1.36
3	A	2472[B]	TPF	C6-N5	5.01	1.46	1.34
2	C	462	HEM	C3C-C2C	-5.01	1.33	1.40
3	D	2473[B]	TPF	C6-N5	4.90	1.46	1.34
3	B	2470	TPF	C9-C8	4.85	1.45	1.39
3	F	2474[B]	TPF	C6-N5	4.67	1.45	1.34
3	F	2474[A]	TPF	C6-N5	4.57	1.45	1.34
3	F	2474[B]	TPF	C8-C13	4.48	1.45	1.38
3	C	2471	TPF	C6-N5	4.47	1.45	1.34
3	A	2472[A]	TPF	C6-N5	4.46	1.45	1.34
3	C	2471	TPF	C8-C13	4.37	1.45	1.38
3	D	2473[A]	TPF	C6-N5	4.36	1.44	1.34

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	C	2471	TPF	C9-C8	4.33	1.45	1.39
2	F	462	HEM	C3C-C2C	-4.32	1.34	1.40
3	D	2473[B]	TPF	C12-C13	4.23	1.44	1.37
2	F	462	HEM	C3C-CAC	4.21	1.56	1.47
2	A	462	HEM	C3C-C2C	-4.16	1.34	1.40
3	A	2472[B]	TPF	C8-C13	4.09	1.44	1.38
3	A	2472[B]	TPF	N3-N1	4.02	1.41	1.35
3	C	2471	TPF	N3-N1	3.99	1.41	1.35
2	B	462	HEM	C3C-C2C	-3.99	1.34	1.40
3	A	2472[A]	TPF	N3-N1	3.98	1.41	1.35
3	D	2473[B]	TPF	N6-N4	3.97	1.41	1.35
3	D	2473[B]	TPF	N3-N1	3.89	1.41	1.35
3	A	2472[B]	TPF	C12-C13	3.79	1.44	1.37
3	A	2472[A]	TPF	C12-C13	3.77	1.44	1.37
2	A	462	HEM	C3C-CAC	3.76	1.55	1.47
3	F	2474[B]	TPF	C12-C13	3.68	1.43	1.37
3	B	2470	TPF	C10-C11	3.68	1.44	1.37
3	F	2474[B]	TPF	C12-C11	3.67	1.43	1.37
2	D	462	HEM	C3C-C2C	-3.65	1.35	1.40
3	F	2474[B]	TPF	N6-N4	3.64	1.40	1.35
3	A	2472[A]	TPF	N6-N4	3.62	1.40	1.35
3	F	2474[B]	TPF	N3-N1	3.60	1.40	1.35
3	B	2470	TPF	C6-N5	3.59	1.42	1.34
3	B	2470	TPF	N3-N1	3.58	1.40	1.35
3	F	2474[B]	TPF	C9-C8	3.56	1.44	1.39
3	A	2472[A]	TPF	C12-C11	3.51	1.43	1.37
3	A	2472[B]	TPF	C12-C11	3.48	1.43	1.37
3	D	2473[B]	TPF	C9-C8	3.47	1.44	1.39
3	F	2474[A]	TPF	N6-N4	3.47	1.40	1.35
3	F	2474[A]	TPF	C8-C13	3.45	1.44	1.38
3	A	2472[A]	TPF	C8-C13	3.40	1.43	1.38
3	A	2472[B]	TPF	C9-C8	3.40	1.43	1.39
3	D	2473[B]	TPF	C12-C11	3.38	1.43	1.37
2	E	462	HEM	C3C-CAC	3.37	1.54	1.47
3	D	2473[A]	TPF	N3-N1	3.32	1.40	1.35
3	D	2473[A]	TPF	C12-C13	3.31	1.43	1.37
3	B	2470	TPF	C12-C13	3.28	1.43	1.37
3	C	2471	TPF	C10-C11	3.26	1.43	1.37
3	F	2474[A]	TPF	N3-N1	3.18	1.40	1.35
3	D	2473[A]	TPF	C12-C11	3.16	1.43	1.37
3	D	2473[B]	TPF	C10-C11	3.16	1.43	1.37
3	A	2472[B]	TPF	N6-N4	3.16	1.39	1.35

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	F	2474[B]	TPF	C10-C11	3.12	1.43	1.37
2	C	462	HEM	C3C-CAC	3.07	1.54	1.47
3	D	2473[A]	TPF	C8-C13	3.05	1.43	1.38
3	B	2470	TPF	N6-N4	3.03	1.39	1.35
3	D	2473[B]	TPF	C8-C13	3.02	1.43	1.38
2	B	462	HEM	C3C-CAC	3.01	1.54	1.47
3	A	2472[B]	TPF	C10-C11	2.96	1.42	1.37
2	E	462	HEM	C3C-C2C	-2.94	1.36	1.40
3	A	2472[B]	TPF	C6-N4	2.93	1.36	1.33
3	F	2474[A]	TPF	C12-C11	2.89	1.42	1.37
3	F	2474[A]	TPF	C12-C13	2.84	1.42	1.37
3	B	2470	TPF	C8-C13	2.81	1.43	1.38
2	C	462	HEM	CAA-C2A	2.81	1.56	1.52
3	A	2472[B]	TPF	C10-C9	2.79	1.43	1.38
2	B	462	HEM	CAB-C3B	2.78	1.55	1.47
2	C	462	HEM	CMD-C2D	2.74	1.56	1.50
2	F	462	HEM	CAB-C3B	2.73	1.54	1.47
3	C	2471	TPF	C12-C13	2.69	1.42	1.37
3	A	2472[A]	TPF	C10-C11	2.68	1.42	1.37
3	D	2473[A]	TPF	N6-N4	2.66	1.39	1.35
2	D	462	HEM	CAB-C3B	2.63	1.54	1.47
2	A	462	HEM	C4A-NA	2.61	1.41	1.36
2	A	462	HEM	CAA-C2A	2.55	1.55	1.52
2	F	462	HEM	C1B-NB	-2.53	1.35	1.40
3	F	2474[B]	TPF	C10-C9	2.52	1.43	1.38
2	A	462	HEM	CMD-C2D	2.52	1.56	1.50
2	B	462	HEM	FE-ND	2.50	2.09	1.96
3	C	2471	TPF	C12-C11	2.46	1.41	1.37
2	F	462	HEM	CMB-C2B	2.46	1.56	1.50
3	D	2473[A]	TPF	C10-C11	2.45	1.41	1.37
3	B	2470	TPF	C12-C11	2.45	1.41	1.37
2	F	462	HEM	CMC-C2C	2.45	1.57	1.51
3	D	2473[A]	TPF	C9-C8	2.44	1.42	1.39
2	C	462	HEM	CAB-C3B	2.44	1.54	1.47
2	B	462	HEM	C4A-NA	2.43	1.41	1.36
3	D	2473[B]	TPF	C6-N4	2.43	1.36	1.33
3	A	2472[B]	TPF	F1-C11	2.43	1.42	1.36
2	D	462	HEM	CMB-C2B	2.34	1.55	1.50
2	F	462	HEM	CAA-C2A	2.34	1.55	1.52
3	D	2473[B]	TPF	C10-C9	2.33	1.43	1.38
2	B	462	HEM	CAA-C2A	2.32	1.55	1.52
2	B	462	HEM	FE-NB	2.31	2.08	1.96

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	C	2471	TPF	C10-C9	2.30	1.42	1.38
2	B	462	HEM	CMB-C2B	2.29	1.55	1.50
2	D	462	HEM	FE-NB	2.29	2.08	1.96
2	A	462	HEM	CMA-C3A	2.26	1.56	1.51
2	A	462	HEM	FE-ND	2.25	2.08	1.96
2	A	462	HEM	CMB-C2B	2.24	1.55	1.50
3	F	2474[A]	TPF	C10-C11	2.21	1.41	1.37
2	A	462	HEM	CAB-C3B	2.20	1.53	1.47
3	A	2472[A]	TPF	C9-C8	2.16	1.42	1.39
2	E	462	HEM	CMB-C2B	2.15	1.55	1.50
2	E	462	HEM	CAB-C3B	2.15	1.53	1.47
2	C	462	HEM	C2C-C1C	2.14	1.47	1.42
3	A	2472[A]	TPF	C10-C9	2.06	1.42	1.38
2	C	462	HEM	C4A-CHB	-2.06	1.35	1.41
2	B	462	HEM	C2C-C1C	2.04	1.47	1.42
3	C	2471	TPF	N6-N4	2.01	1.38	1.35

All (136) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
3	C	2471	TPF	C3-N2-C4	14.40	118.56	102.34
3	F	2474[A]	TPF	C3-N2-C4	13.85	117.95	102.34
3	F	2474[B]	TPF	C3-N2-C4	13.68	117.75	102.34
3	D	2473[B]	TPF	C3-N2-C4	13.48	117.53	102.34
3	A	2472[A]	TPF	C3-N2-C4	12.99	116.97	102.34
3	D	2473[A]	TPF	C3-N2-C4	12.78	116.74	102.34
3	A	2472[B]	TPF	C3-N2-C4	12.61	116.54	102.34
3	F	2474[A]	TPF	N5-C6-N4	-11.70	98.10	112.24
3	B	2470	TPF	C3-N2-C4	11.65	115.47	102.34
3	C	2471	TPF	N2-C3-N1	-11.20	98.70	112.24
3	F	2474[A]	TPF	C6-N5-C7	11.11	114.86	102.34
3	A	2472[A]	TPF	C6-N5-C7	11.01	114.74	102.34
3	D	2473[B]	TPF	N5-C6-N4	-10.92	99.04	112.24
3	D	2473[B]	TPF	N2-C3-N1	-10.91	99.05	112.24
3	A	2472[A]	TPF	N5-C6-N4	-10.80	99.19	112.24
3	D	2473[A]	TPF	N5-C6-N4	-10.62	99.40	112.24
3	F	2474[A]	TPF	N2-C3-N1	-10.39	99.68	112.24
3	A	2472[A]	TPF	N2-C3-N1	-10.25	99.85	112.24
3	F	2474[B]	TPF	N2-C3-N1	-10.22	99.88	112.24
3	D	2473[B]	TPF	C6-N5-C7	10.14	113.77	102.34
3	A	2472[B]	TPF	C6-N5-C7	10.08	113.70	102.34
3	A	2472[B]	TPF	N5-C6-N4	-9.86	100.33	112.24

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
3	F	2474[B]	TPF	N5-C6-N4	-9.66	100.56	112.24
3	D	2473[A]	TPF	N2-C3-N1	-9.64	100.58	112.24
3	A	2472[B]	TPF	N2-C3-N1	-9.52	100.73	112.24
3	F	2474[B]	TPF	C6-N5-C7	9.46	112.99	102.34
3	B	2470	TPF	N5-C6-N4	-9.38	100.90	112.24
3	D	2473[A]	TPF	C6-N5-C7	9.37	112.89	102.34
3	B	2470	TPF	C6-N5-C7	9.28	112.80	102.34
3	C	2471	TPF	N5-C6-N4	-8.89	101.49	112.24
3	B	2470	TPF	N2-C3-N1	-8.65	101.78	112.24
2	B	462	HEM	C4D-ND-C1D	7.94	113.28	105.07
3	C	2471	TPF	C6-N5-C7	7.62	110.93	102.34
2	D	462	HEM	C4D-ND-C1D	6.29	111.58	105.07
3	A	2472[B]	TPF	C13-C12-C11	5.81	122.72	116.62
2	A	462	HEM	C4D-ND-C1D	5.79	111.05	105.07
3	B	2470	TPF	C13-C12-C11	5.39	122.28	116.62
3	C	2471	TPF	F2-C13-C8	5.26	125.31	118.98
3	A	2472[B]	TPF	C10-C11-C12	-5.10	116.67	123.29
3	F	2474[B]	TPF	C12-C13-C8	-5.08	118.49	124.00
2	F	462	HEM	C4D-ND-C1D	5.07	110.31	105.07
3	C	2471	TPF	C12-C13-C8	-4.65	118.95	124.00
3	B	2470	TPF	C12-C13-C8	-4.54	119.07	124.00
2	F	462	HEM	C4C-CHD-C1D	4.54	128.55	122.56
2	A	462	HEM	C4C-CHD-C1D	4.53	128.54	122.56
3	F	2474[B]	TPF	C13-C12-C11	4.51	121.36	116.62
3	C	2471	TPF	C1-C8-C13	-4.50	119.14	122.84
2	A	462	HEM	CMC-C2C-C3C	4.31	132.73	124.68
3	D	2473[A]	TPF	C1-C8-C13	-4.21	119.37	122.84
3	D	2473[B]	TPF	C12-C13-C8	-4.18	119.47	124.00
3	B	2470	TPF	C10-C11-C12	-4.17	117.88	123.29
3	B	2470	TPF	C1-C8-C13	-4.16	119.41	122.84
2	F	462	HEM	CMC-C2C-C3C	4.15	132.44	124.68
2	B	462	HEM	C1B-NB-C4B	4.14	109.35	105.07
2	C	462	HEM	C4D-ND-C1D	4.07	109.28	105.07
3	B	2470	TPF	F2-C13-C8	4.05	123.85	118.98
3	A	2472[B]	TPF	C12-C13-C8	-3.95	119.71	124.00
3	A	2472[A]	TPF	C12-C13-C8	-3.80	119.88	124.00
3	C	2471	TPF	C13-C12-C11	3.78	120.59	116.62
3	D	2473[A]	TPF	C12-C13-C8	-3.74	119.95	124.00
2	F	462	HEM	C2C-C3C-C4C	3.67	109.46	106.90
2	B	462	HEM	C4C-CHD-C1D	3.66	127.39	122.56
3	F	2474[B]	TPF	F2-C13-C8	3.65	123.37	118.98
2	C	462	HEM	CMC-C2C-C3C	3.64	131.49	124.68

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
3	A	2472[B]	TPF	C9-C10-C11	3.63	122.11	118.36
2	E	462	HEM	C4D-ND-C1D	3.59	108.78	105.07
2	D	462	HEM	CMC-C2C-C3C	3.58	131.38	124.68
3	D	2473[A]	TPF	C9-C8-C13	3.55	120.52	116.10
3	A	2472[A]	TPF	C9-C8-C1	-3.43	116.72	120.95
3	B	2470	TPF	C9-C10-C11	3.36	121.83	118.36
3	D	2473[B]	TPF	C13-C12-C11	3.35	120.14	116.62
3	C	2471	TPF	C9-C8-C13	3.26	120.15	116.10
3	D	2473[B]	TPF	C1-C8-C13	-3.25	120.16	122.84
3	F	2474[A]	TPF	C12-C13-C8	-3.25	120.48	124.00
2	B	462	HEM	C3D-C4D-ND	-3.24	106.56	110.17
3	A	2472[A]	TPF	C13-C12-C11	3.23	120.01	116.62
3	D	2473[B]	TPF	C9-C8-C13	3.22	120.11	116.10
3	C	2471	TPF	F1-C11-C10	3.22	124.01	118.54
2	E	462	HEM	C3B-C2B-C1B	3.19	108.86	106.49
2	B	462	HEM	C4B-CHC-C1C	3.19	126.77	122.56
3	A	2472[A]	TPF	C10-C11-C12	-3.19	119.15	123.29
3	F	2474[A]	TPF	C10-C11-C12	-3.17	119.18	123.29
3	F	2474[A]	TPF	F1-C11-C12	3.13	122.72	118.25
3	A	2472[A]	TPF	F1-C11-C12	3.10	122.69	118.25
3	B	2470	TPF	C9-C8-C13	3.09	119.94	116.10
3	F	2474[A]	TPF	C9-C10-C11	3.07	121.54	118.36
3	F	2474[B]	TPF	C9-C8-C13	3.02	119.86	116.10
2	F	462	HEM	CHD-C1D-ND	3.02	127.71	124.43
3	F	2474[A]	TPF	C13-C12-C11	3.02	119.79	116.62
2	B	462	HEM	CHC-C4B-NB	2.99	127.68	124.43
2	C	462	HEM	C4C-CHD-C1D	2.97	126.48	122.56
2	B	462	HEM	CHA-C4D-ND	2.95	128.03	124.38
3	A	2472[B]	TPF	F1-C11-C12	2.92	122.42	118.25
2	E	462	HEM	CMC-C2C-C3C	2.88	130.07	124.68
3	A	2472[A]	TPF	C9-C8-C13	2.83	119.62	116.10
2	B	462	HEM	CMC-C2C-C3C	2.80	129.91	124.68
3	B	2470	TPF	F1-C11-C10	2.77	123.24	118.54
3	F	2474[B]	TPF	C10-C11-C12	-2.74	119.73	123.29
3	A	2472[A]	TPF	C9-C10-C11	2.68	121.13	118.36
2	A	462	HEM	C2C-C3C-C4C	2.66	108.76	106.90
2	E	462	HEM	CHD-C1D-ND	2.66	127.32	124.43
2	B	462	HEM	CBD-CAD-C3D	-2.62	105.34	112.63
3	C	2471	TPF	F1-C11-C12	-2.59	114.55	118.25
3	D	2473[B]	TPF	C10-C11-C12	-2.58	119.94	123.29
2	C	462	HEM	C4A-C3A-C2A	2.54	108.76	107.00
3	C	2471	TPF	C2-C1-C8	-2.52	104.59	110.87

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	B	462	HEM	CMD-C2D-C1D	2.50	128.85	125.04
2	E	462	HEM	C4C-CHD-C1D	2.50	125.86	122.56
3	D	2473[A]	TPF	C6-N4-N6	2.49	112.78	109.01
3	F	2474[B]	TPF	C9-C8-C1	-2.48	117.89	120.95
3	F	2474[A]	TPF	C9-C8-C13	2.46	119.16	116.10
3	D	2473[A]	TPF	C9-C10-C11	2.44	120.88	118.36
2	E	462	HEM	CAD-C3D-C4D	2.42	128.88	124.66
2	D	462	HEM	C4B-CHC-C1C	2.36	125.67	122.56
2	B	462	HEM	CHD-C1D-ND	2.33	126.96	124.43
2	C	462	HEM	CHC-C4B-C3B	2.33	128.14	124.57
2	E	462	HEM	C1B-NB-C4B	2.32	107.47	105.07
2	D	462	HEM	C2C-C3C-C4C	2.32	108.52	106.90
2	C	462	HEM	CAD-C3D-C4D	2.30	128.68	124.66
2	F	462	HEM	C1B-NB-C4B	2.30	107.45	105.07
3	D	2473[A]	TPF	C13-C12-C11	2.26	119.00	116.62
2	C	462	HEM	CBD-CAD-C3D	-2.23	106.43	112.63
2	D	462	HEM	C4A-C3A-C2A	2.23	108.55	107.00
3	F	2474[A]	TPF	C6-N4-N6	2.18	112.32	109.01
3	D	2473[B]	TPF	C6-N4-N6	2.16	112.28	109.01
3	D	2473[A]	TPF	C10-C11-C12	-2.15	120.50	123.29
2	F	462	HEM	C4B-CHC-C1C	2.15	125.39	122.56
2	C	462	HEM	CHD-C1D-ND	2.08	126.69	124.43
2	E	462	HEM	C4B-CHC-C1C	2.06	125.28	122.56
3	F	2474[A]	TPF	F2-C13-C8	2.05	121.45	118.98
2	D	462	HEM	CHA-C4D-ND	2.03	126.89	124.38
2	D	462	HEM	C4C-CHD-C1D	2.03	125.24	122.56
3	D	2473[B]	TPF	C2-C1-C8	-2.02	105.83	110.87
3	B	2470	TPF	C2-C1-C8	-2.02	105.83	110.87
2	D	462	HEM	C3D-C4D-ND	-2.01	107.92	110.17
3	A	2472[B]	TPF	C2-C1-C8	-2.00	105.88	110.87

There are no chirality outliers.

All (26) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	A	2472[B]	TPF	C1-C5-N4-C6
3	B	2470	TPF	C1-C5-N4-C6
3	C	2471	TPF	C1-C5-N4-C6
3	D	2473[A]	TPF	C2-C1-C5-N4
3	D	2473[A]	TPF	C8-C1-C5-N4
3	D	2473[A]	TPF	C1-C2-N1-C3
3	D	2473[A]	TPF	C1-C5-N4-C6

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Mol	Chain	Res	Type	Atoms
3	D	2473[B]	TPF	C1-C5-N4-C6
3	F	2474[A]	TPF	C2-C1-C5-N4
3	F	2474[A]	TPF	C8-C1-C5-N4
3	F	2474[A]	TPF	C1-C2-N1-C3
3	F	2474[B]	TPF	C1-C5-N4-C6
3	D	2473[A]	TPF	O-C1-C5-N4
3	F	2474[A]	TPF	O-C1-C5-N4
3	A	2472[A]	TPF	C2-C1-C5-N4
3	F	2474[B]	TPF	C8-C1-C2-N1
3	F	2474[B]	TPF	C5-C1-C2-N1
3	A	2472[A]	TPF	O-C1-C5-N4
3	A	2472[A]	TPF	C8-C1-C5-N4
2	D	462	HEM	CAD-CBD-CGD-O2D
2	E	462	HEM	CAD-CBD-CGD-O2D
3	F	2474[B]	TPF	O-C1-C2-N1
2	D	462	HEM	CAD-CBD-CGD-O1D
3	B	2470	TPF	C5-C1-C2-N1
2	C	462	HEM	CAD-CBD-CGD-O2D
2	E	462	HEM	CAD-CBD-CGD-O1D

There are no ring outliers.

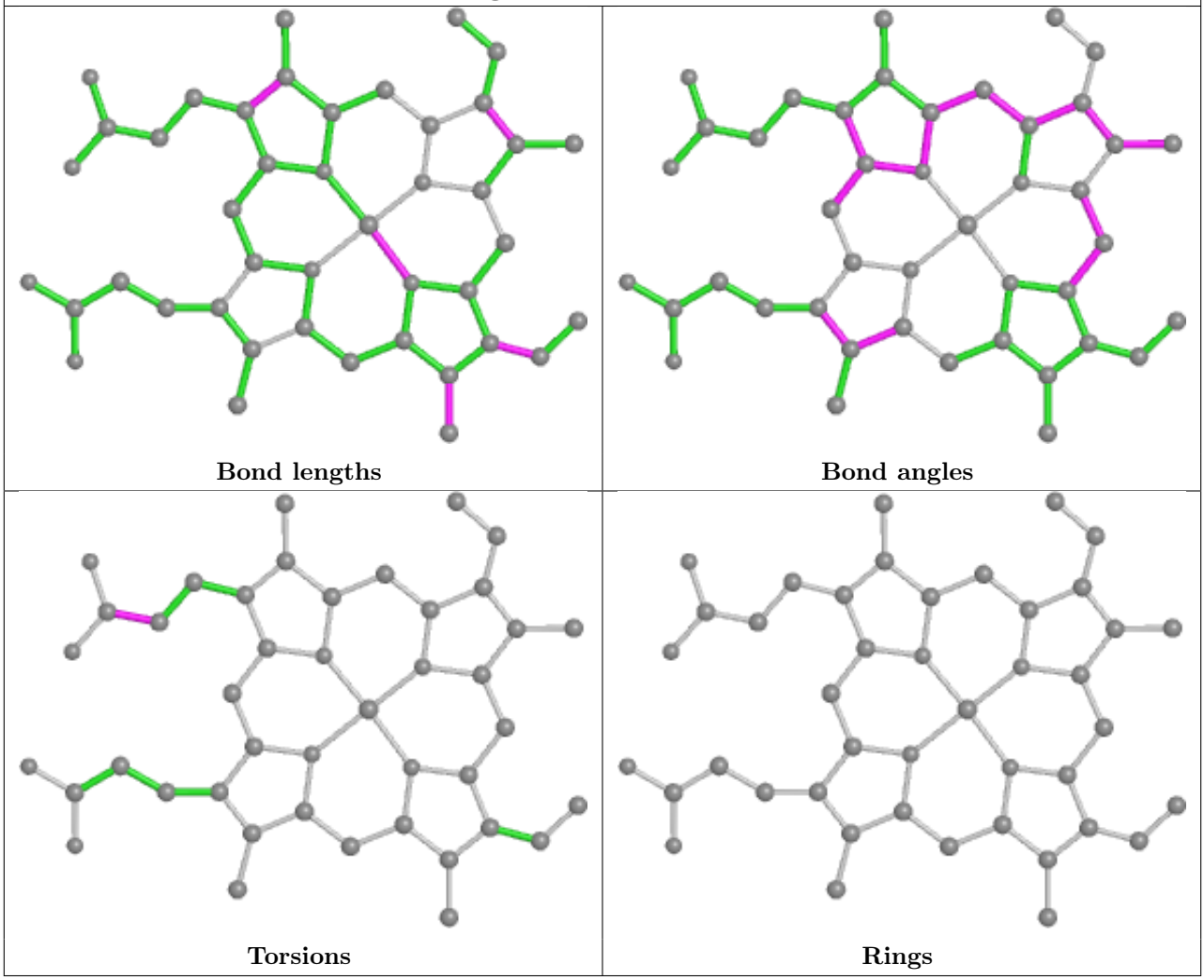
9 monomers are involved in 53 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	D	462	HEM	3	0
2	E	462	HEM	1	0
3	D	2473[B]	TPF	1	0
2	A	462	HEM	7	0
2	F	462	HEM	4	0
3	D	2473[A]	TPF	14	0
3	F	2474[A]	TPF	18	0
3	A	2472[A]	TPF	14	0
2	B	462	HEM	2	0

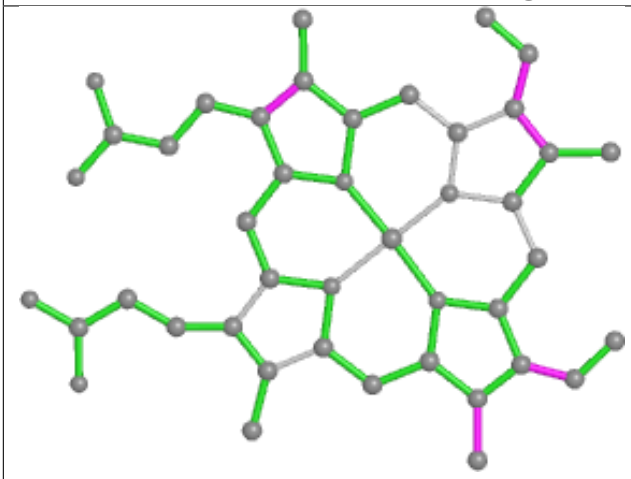
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. 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.

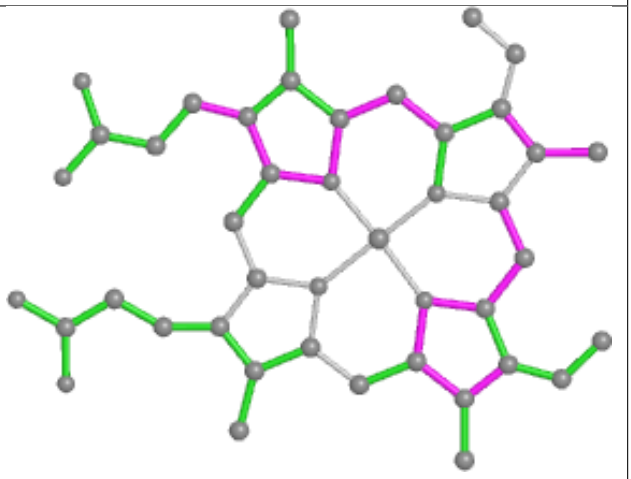
Ligand HEM D 462



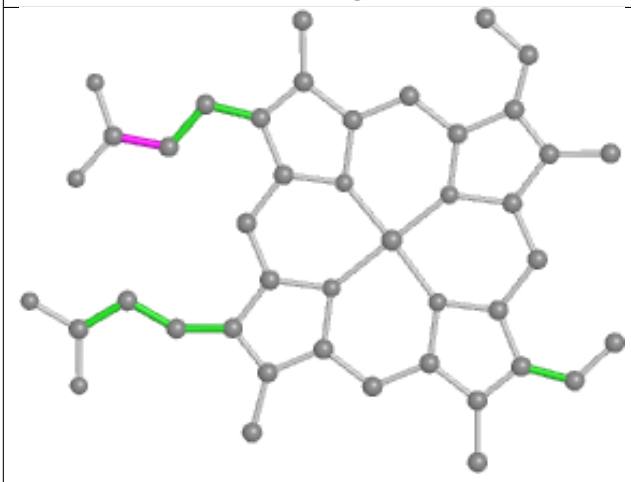
Ligand HEM E 462



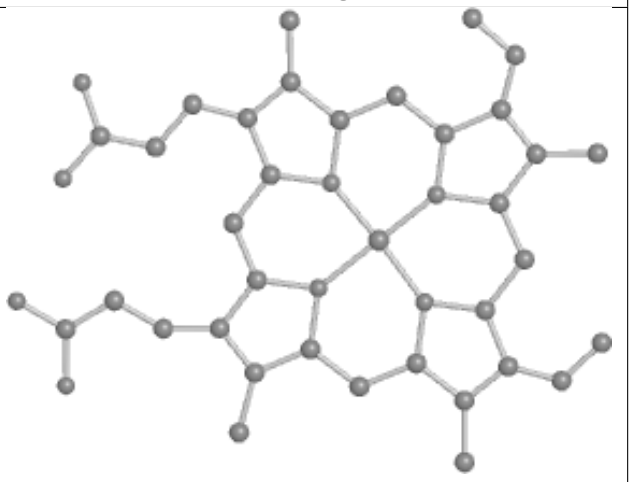
Bond lengths



Bond angles

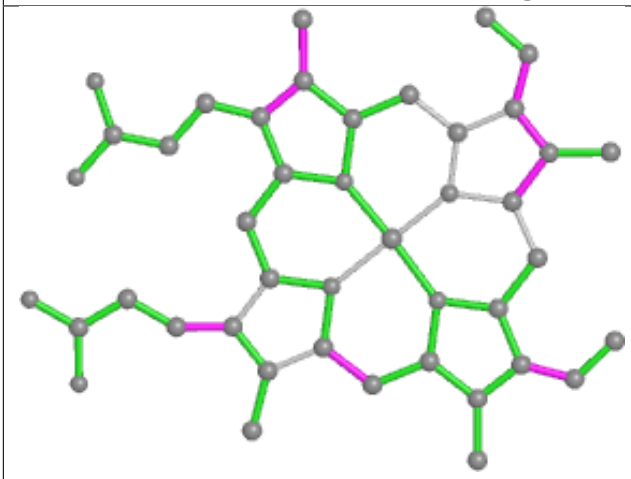


Torsions

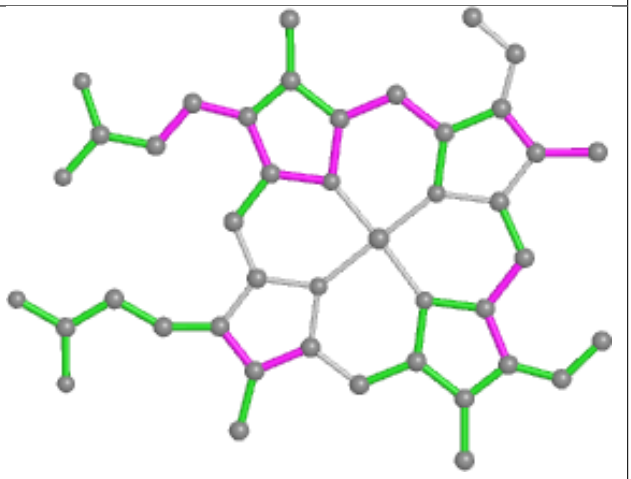


Rings

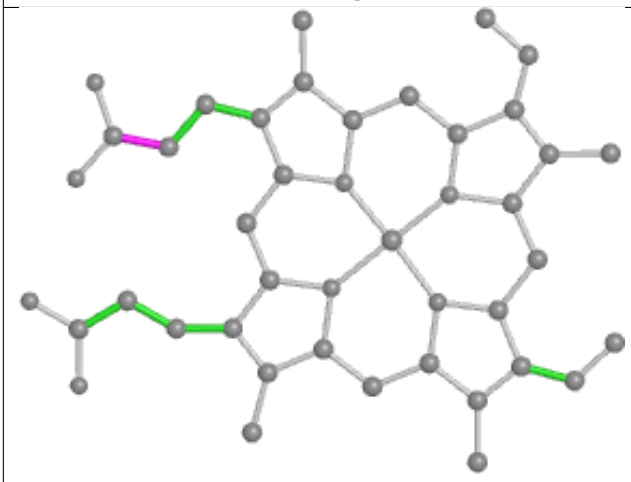
Ligand HEM C 462



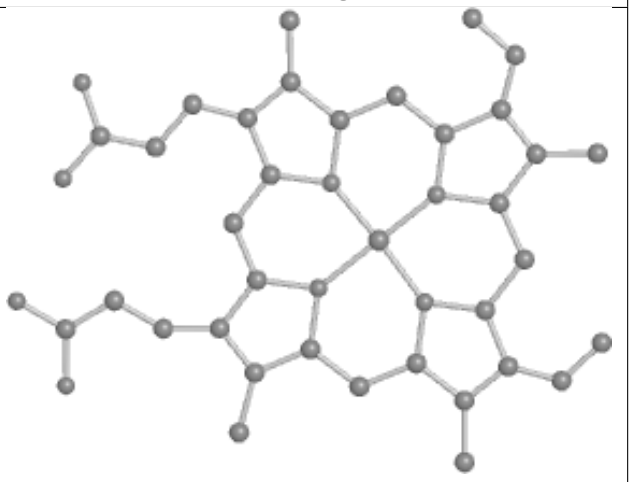
Bond lengths



Bond angles

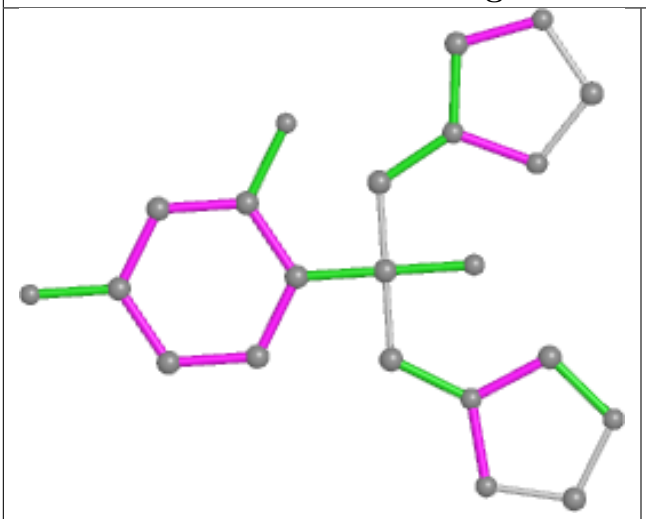


Torsions

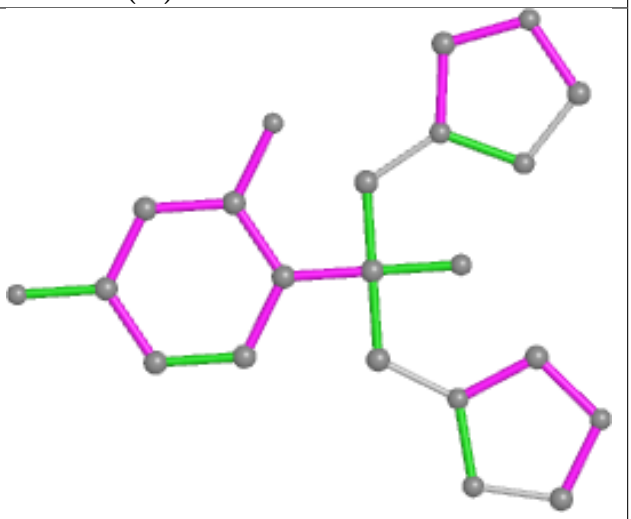


Rings

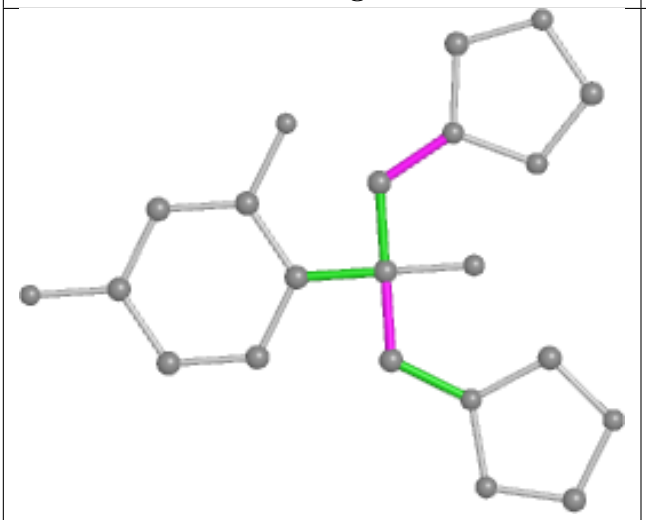
Ligand TPF F 2474 (B)



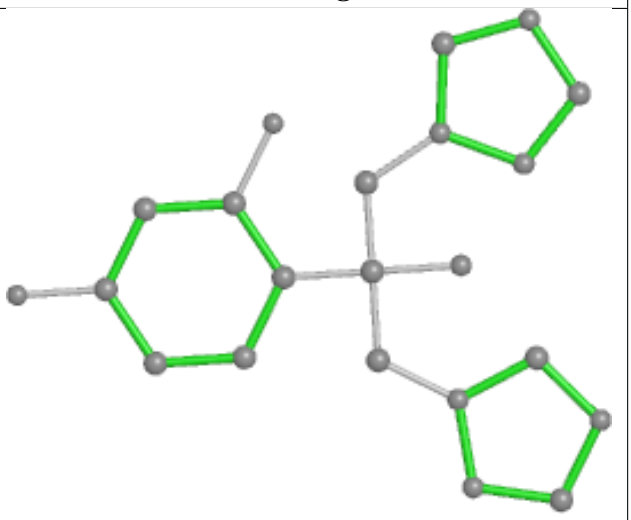
Bond lengths



Bond angles

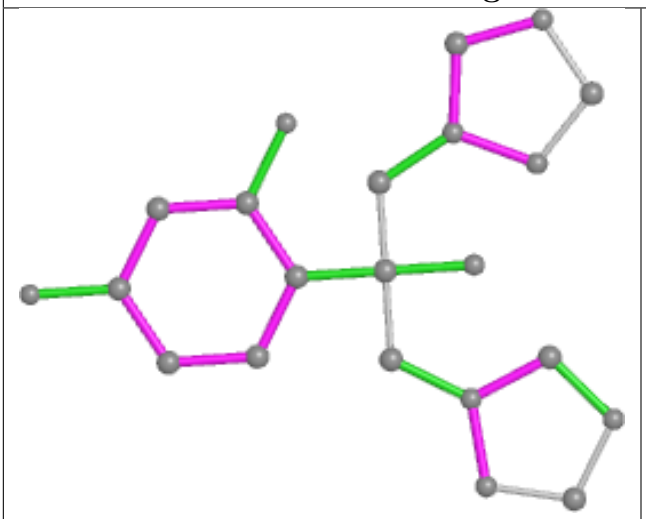


Torsions

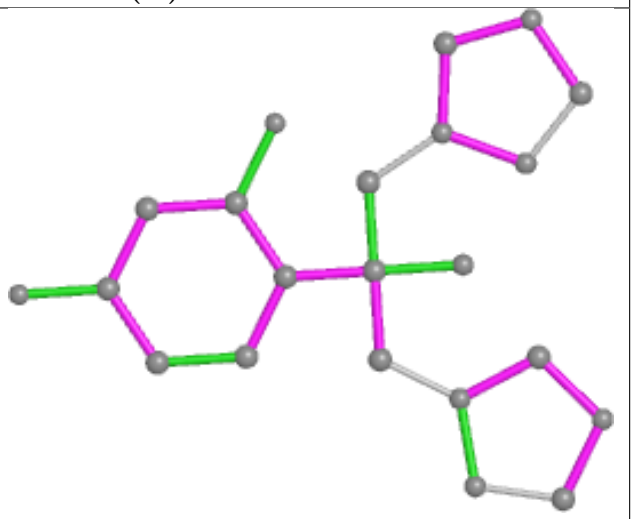


Rings

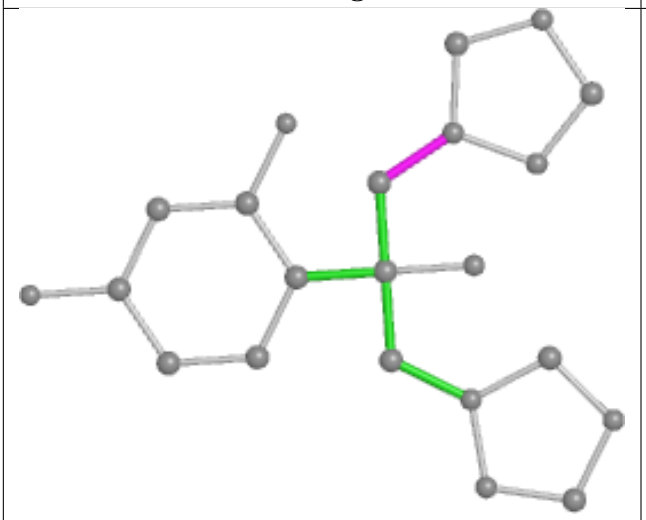
Ligand TPF D 2473 (B)



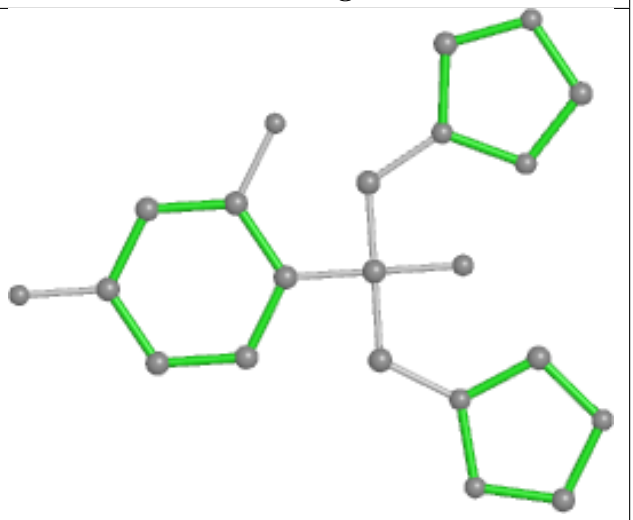
Bond lengths



Bond angles

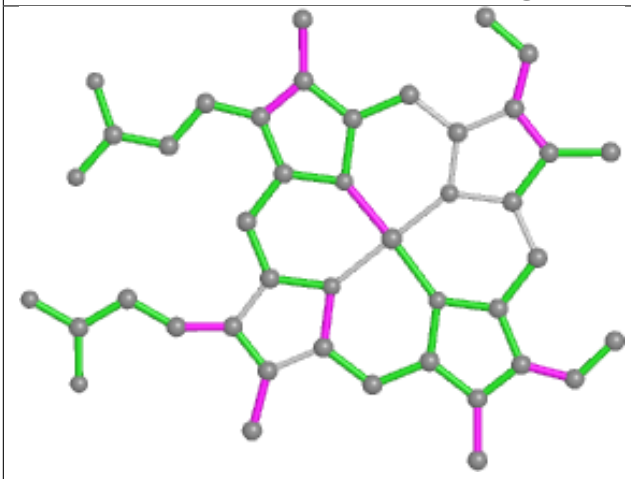


Torsions

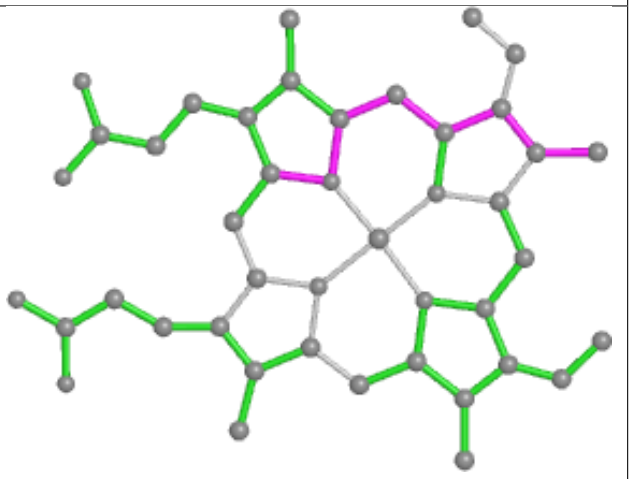


Rings

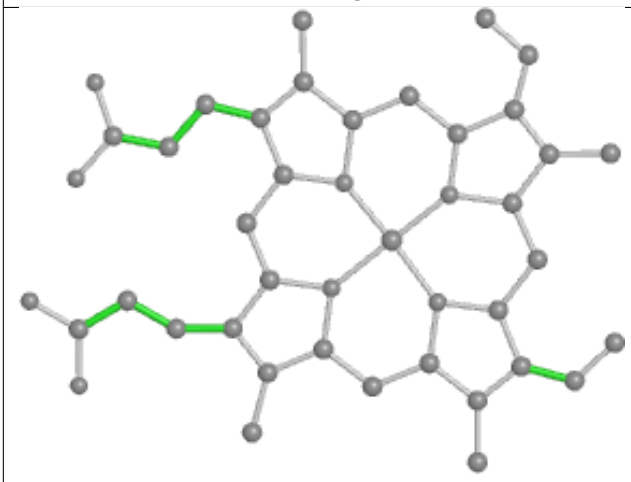
Ligand HEM A 462



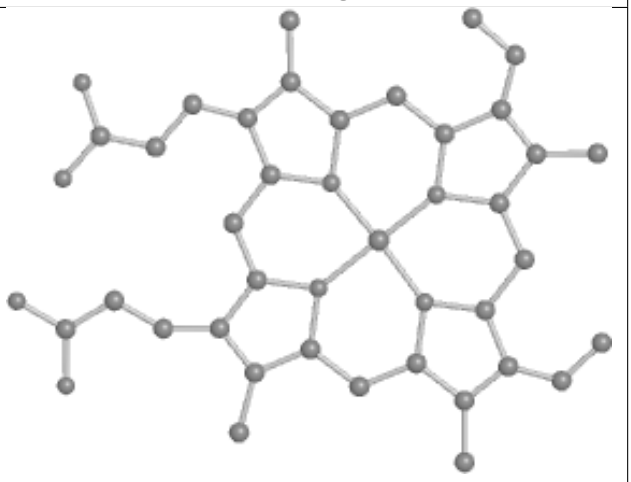
Bond lengths



Bond angles

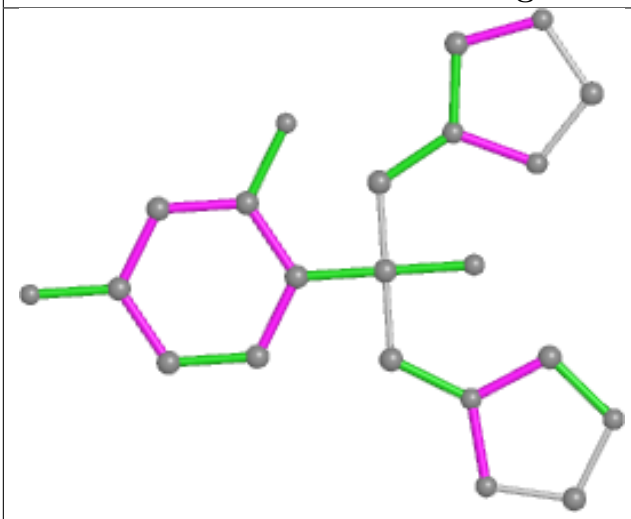


Torsions

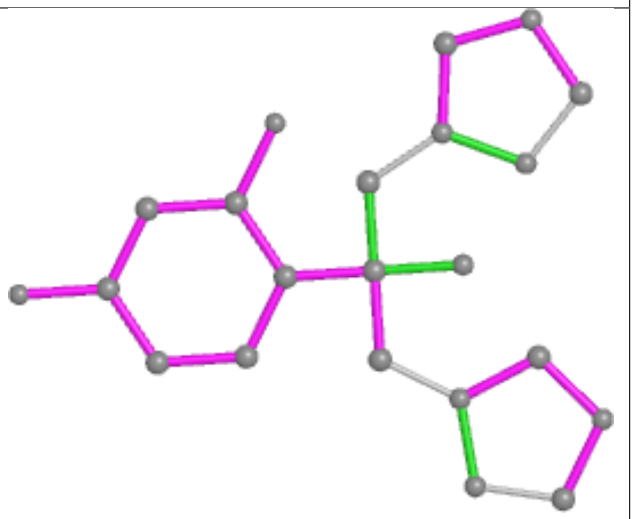


Rings

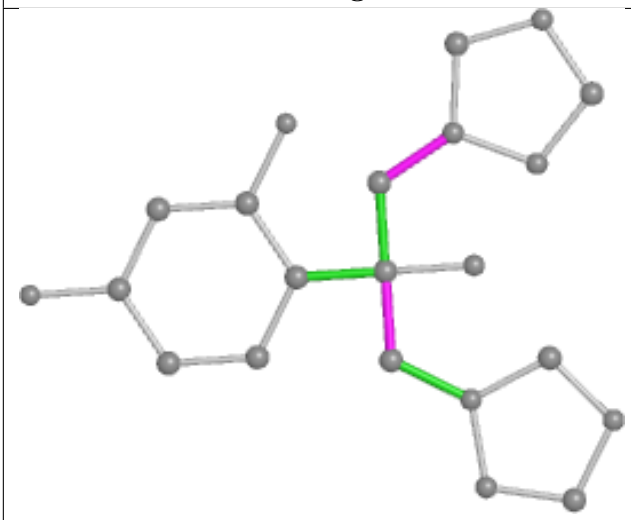
Ligand TPF B 2470



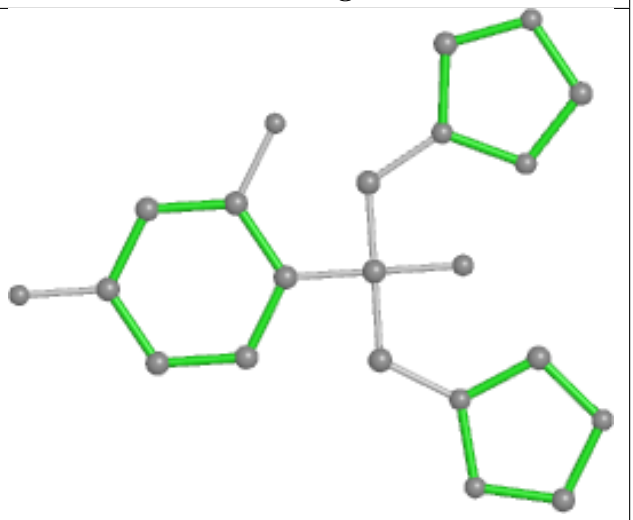
Bond lengths



Bond angles

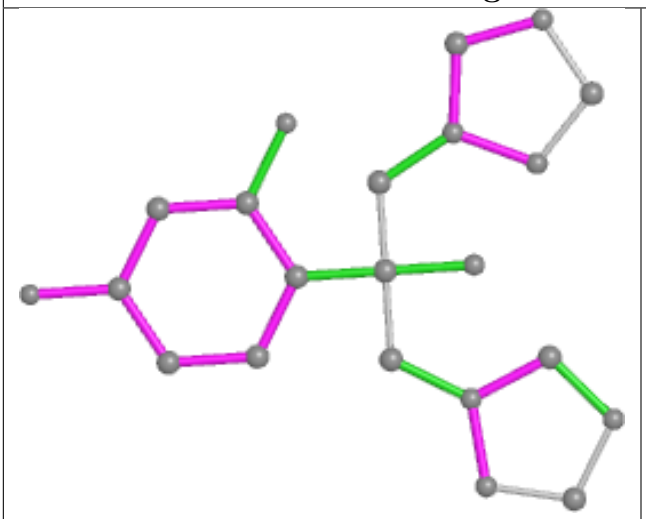


Torsions



Rings

Ligand TPF A 2472 (B)



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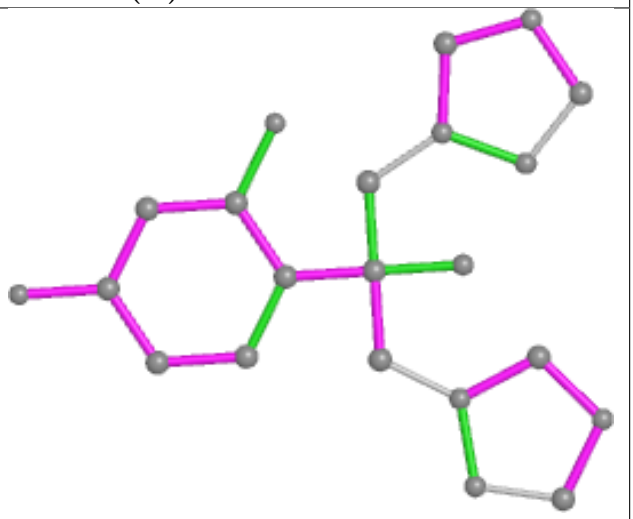
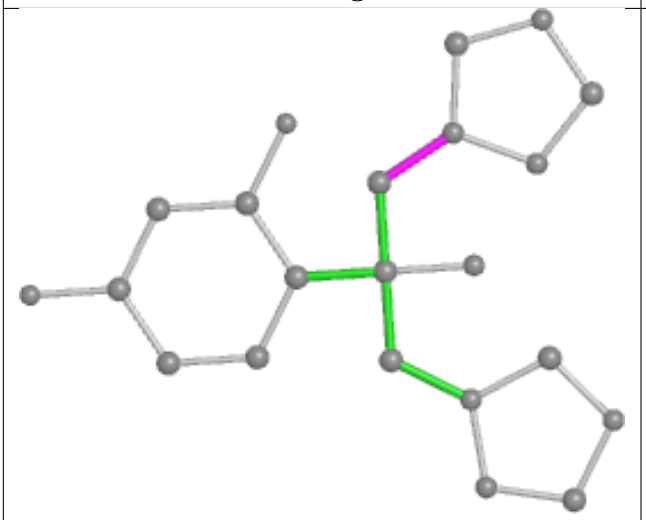
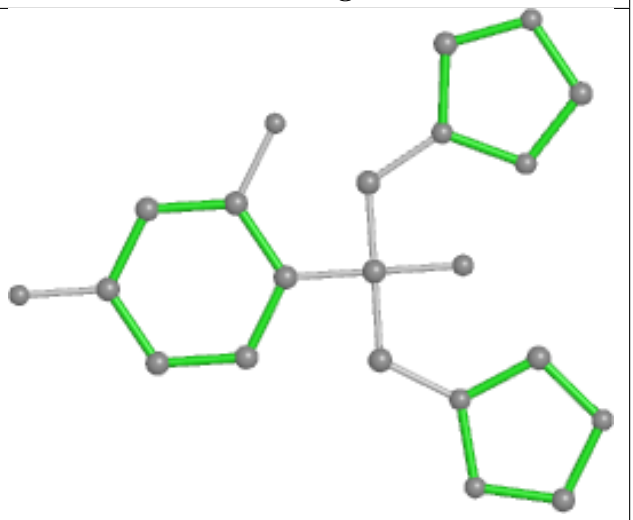


Bond angles

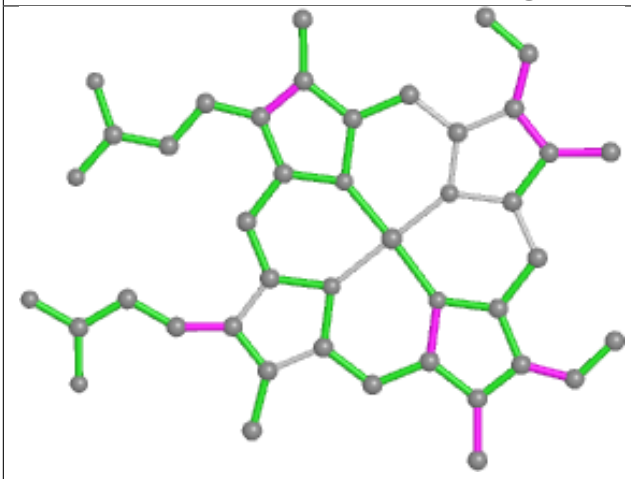


Torsions



Rings

Ligand HEM F 462



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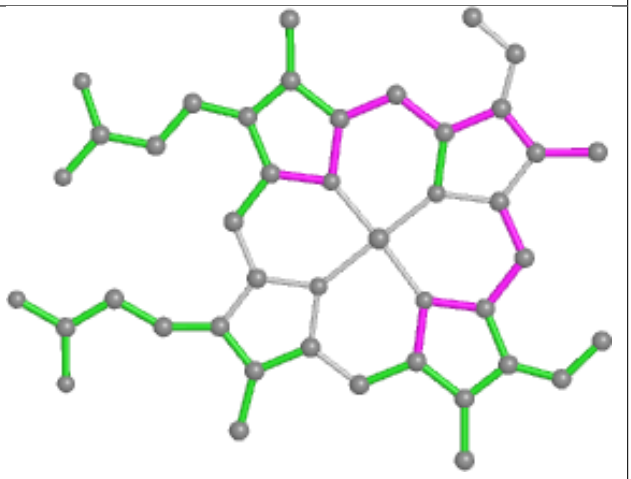
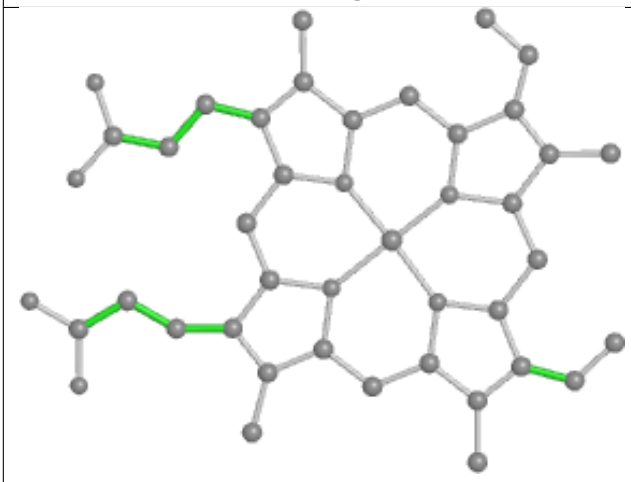
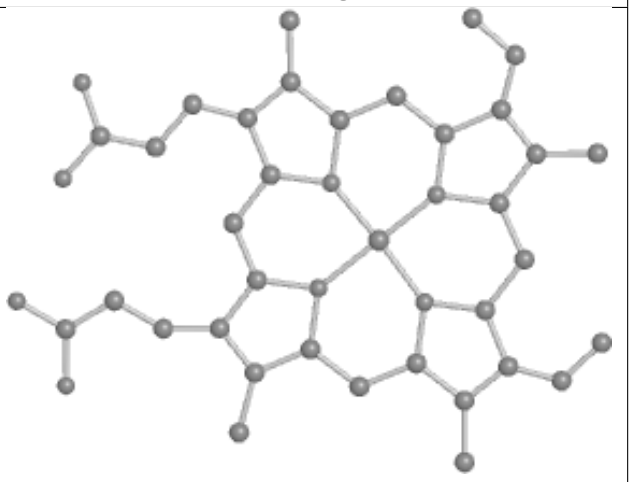


Bond angles

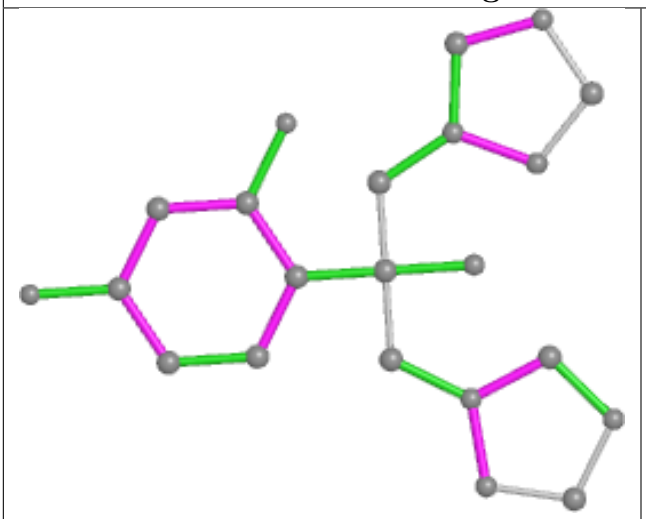


Torsions



Rings

Ligand TPF D 2473 (A)



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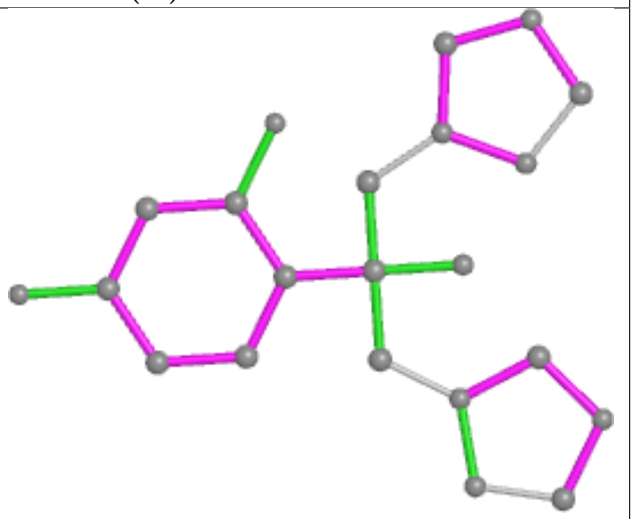
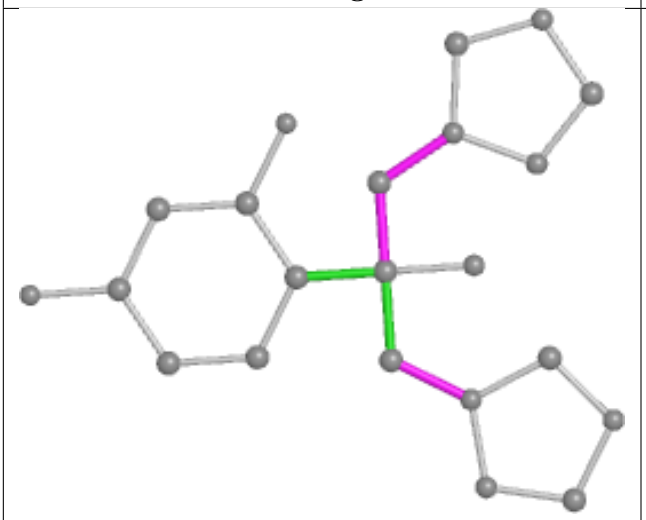
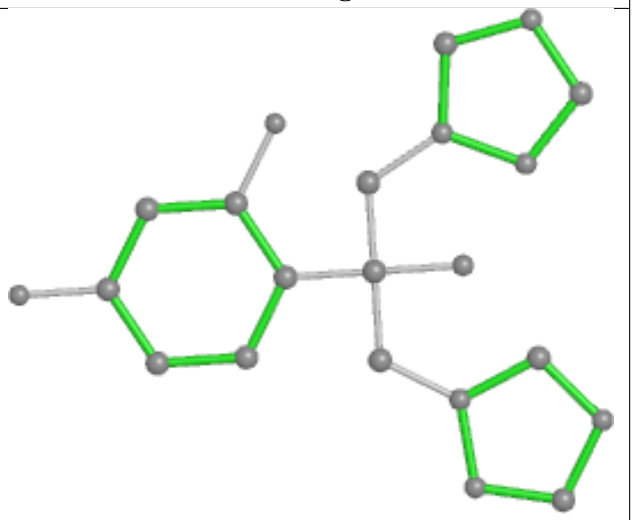


Bond angles

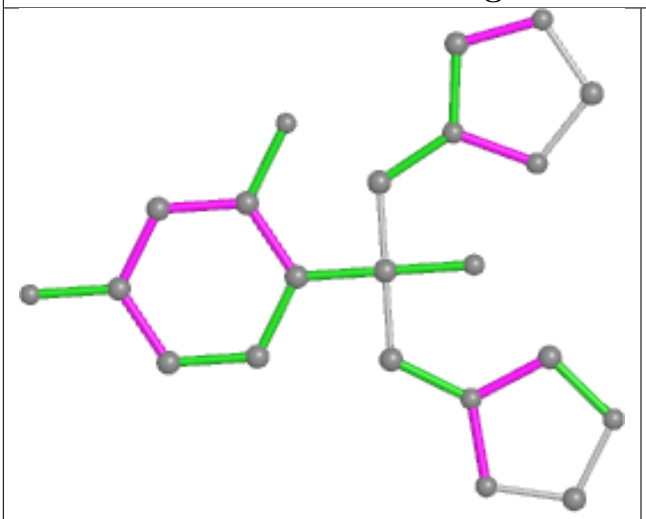


Torsions

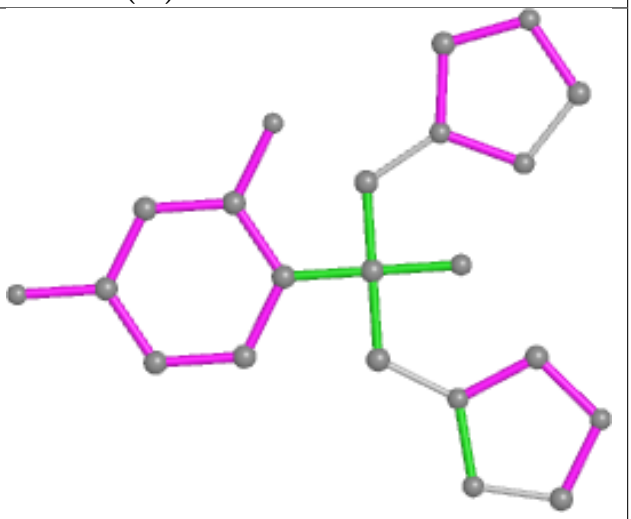


Rings

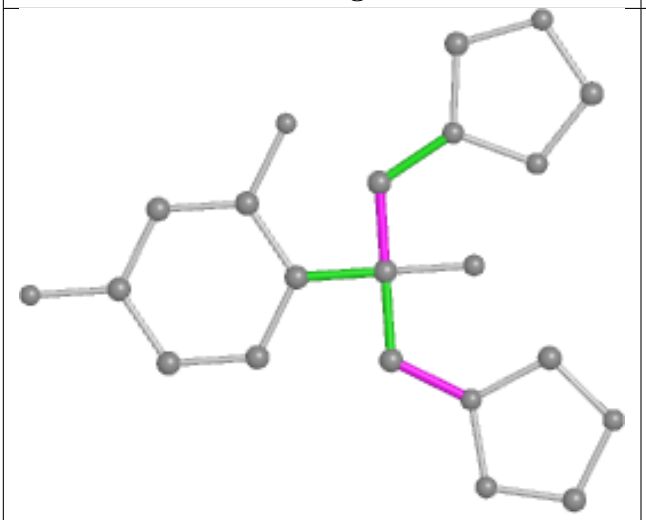
Ligand TPF F 2474 (A)



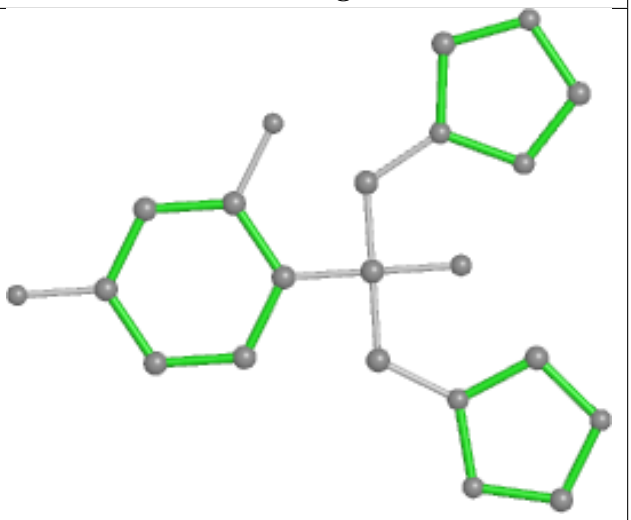
Bond lengths



Bond angles

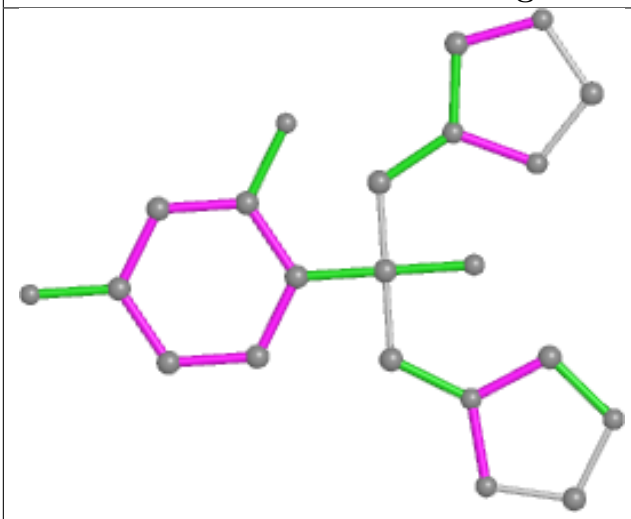


Torsions

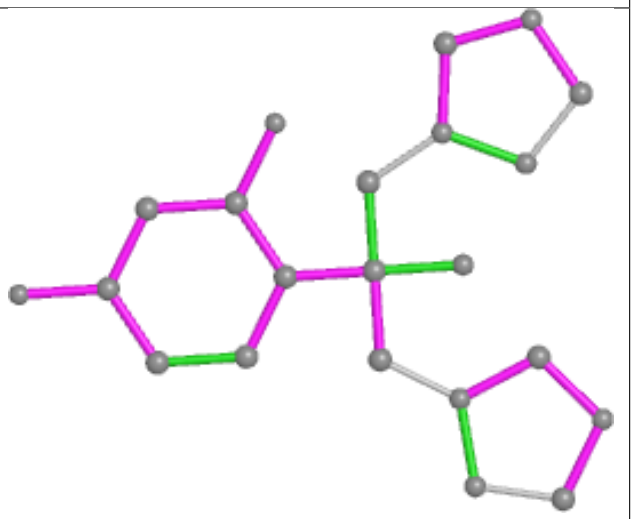


Rings

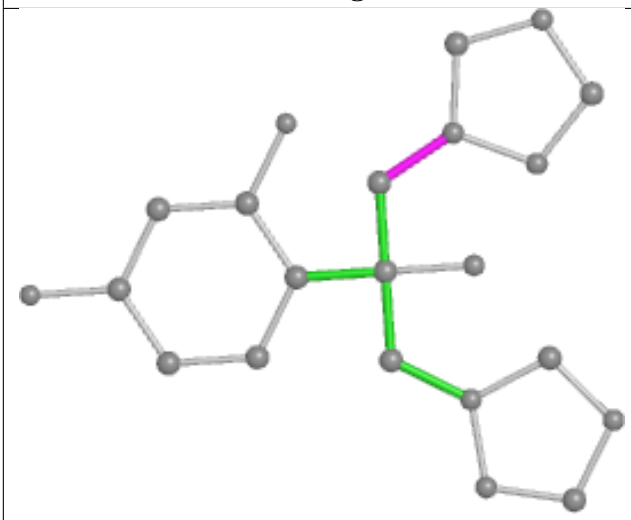
Ligand TPF C 2471



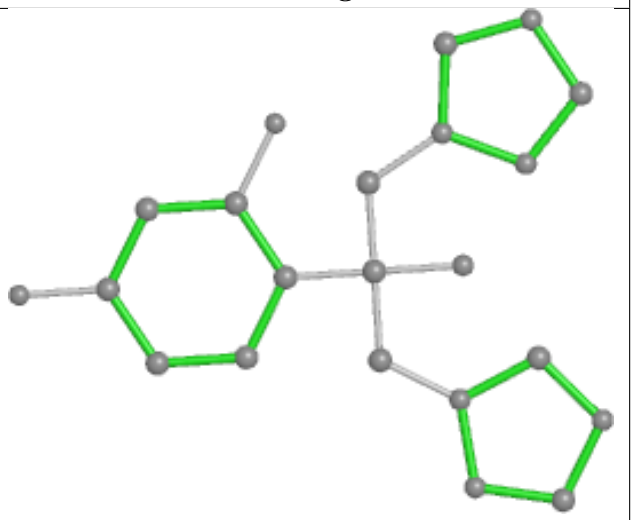
Bond lengths



Bond angles

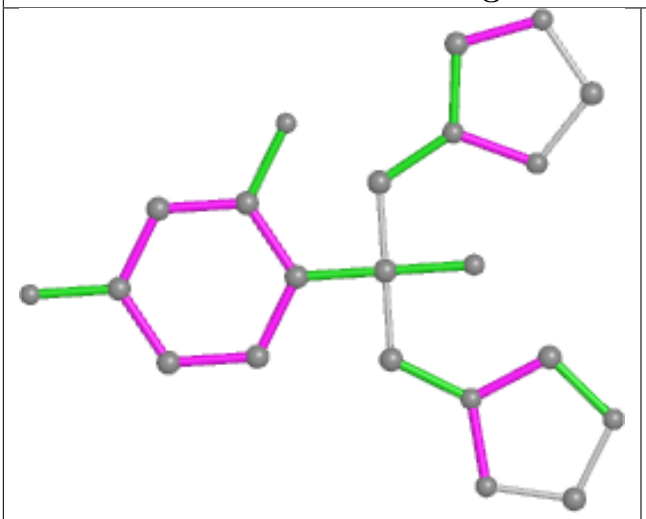


Torsions

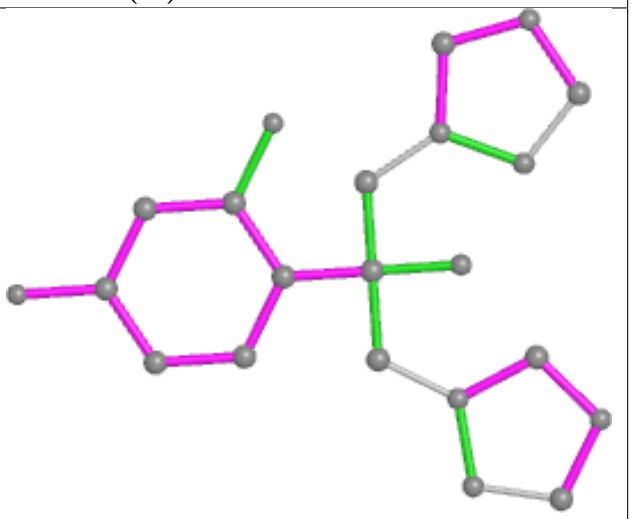


Rings

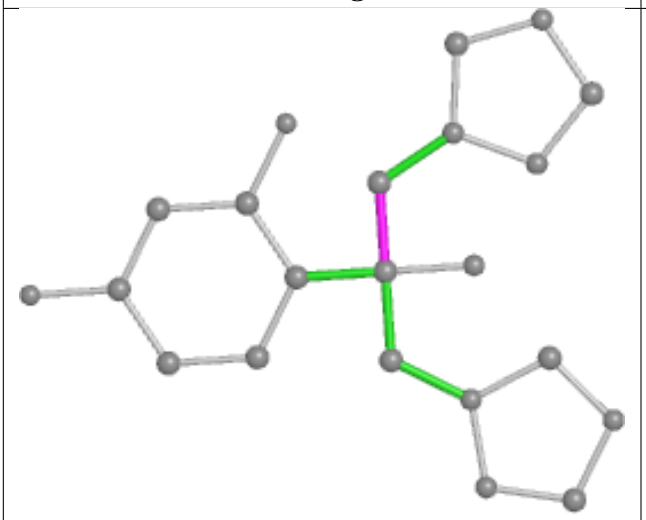
Ligand TPF A 2472 (A)



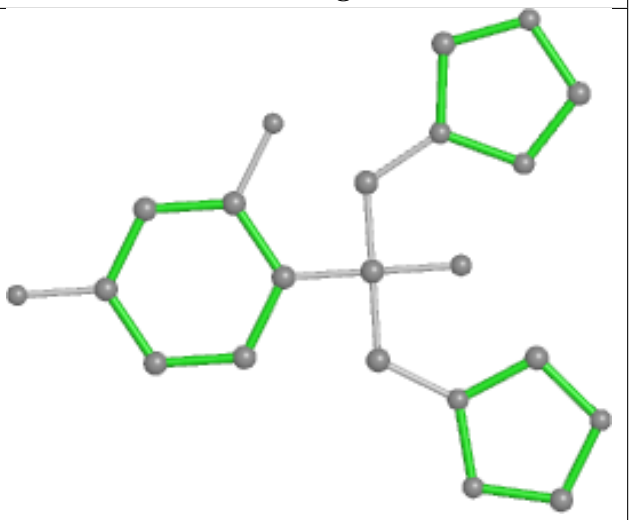
Bond lengths



Bond angles

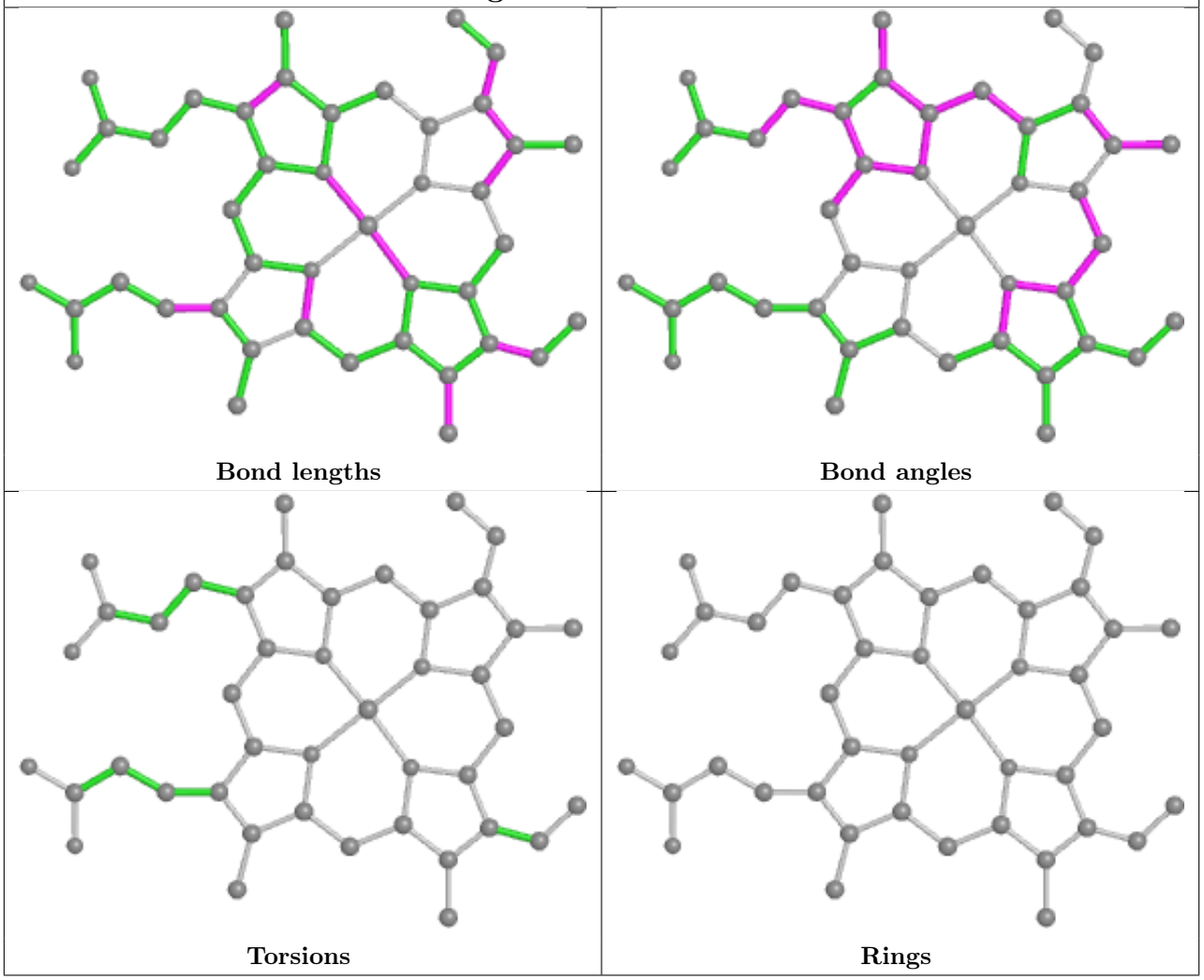


Torsions



Rings

Ligand HEM B 462



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	391/396 (98%)	-0.05	12 (3%)	49	51	17, 29, 53, 65	0
1	B	391/396 (98%)	-0.18	8 (2%)	65	68	18, 27, 46, 62	0
1	C	391/396 (98%)	-0.21	3 (0%)	86	87	18, 28, 41, 54	0
1	D	391/396 (98%)	-0.08	9 (2%)	60	63	19, 30, 50, 59	0
1	E	391/396 (98%)	-0.14	11 (2%)	53	56	16, 26, 47, 58	0
1	F	391/396 (98%)	-0.03	15 (3%)	40	43	17, 29, 54, 70	0
All	All	2346/2376 (98%)	-0.12	58 (2%)	57	60	16, 28, 50, 70	0

All (58) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	E	107	PRO	7.7
1	A	216	SER	5.4
1	F	211	LYS	4.9
1	E	106	ALA	4.9
1	F	107	PRO	4.4
1	A	217	HIS	4.1
1	F	215	TYR	4.1
1	F	216	SER	4.0
1	A	211	LYS	4.0
1	F	217	HIS	3.9
1	C	217	HIS	3.7
1	D	199	THR	3.6
1	E	105	LYS	3.5
1	B	211	LYS	3.5
1	F	213	PRO	3.5
1	E	104	PRO	3.4
1	F	83	VAL	3.4
1	B	214	ALA	3.3
1	F	218	VAL	3.3

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Mol	Chain	Res	Type	RSRZ
1	E	213	PRO	3.2
1	B	105	LYS	3.1
1	B	217	HIS	3.1
1	D	105	LYS	3.1
1	F	219	SER	3.1
1	C	107	PRO	3.1
1	A	218	VAL	3.1
1	F	209	LEU	3.1
1	D	108	GLY	3.0
1	E	108	GLY	3.0
1	F	212	ASP	2.9
1	D	197	ASN	2.8
1	A	197	ASN	2.7
1	A	206	LEU	2.7
1	A	213	PRO	2.7
1	A	214	ALA	2.7
1	D	211	LYS	2.7
1	B	107	PRO	2.7
1	A	91	ASP	2.6
1	D	107	PRO	2.6
1	F	91	ASP	2.6
1	D	7	LEU	2.5
1	F	92	ALA	2.4
1	D	106	ALA	2.3
1	E	212	ASP	2.3
1	B	213	PRO	2.3
1	A	108	GLY	2.2
1	E	96	LYS	2.2
1	A	89	ILE	2.2
1	E	68	ALA	2.2
1	F	197	ASN	2.2
1	C	218	VAL	2.2
1	B	108	GLY	2.1
1	A	215	TYR	2.1
1	B	220	ASP	2.0
1	E	90	ALA	2.0
1	E	28	ARG	2.0
1	F	221	GLU	2.0
1	D	209	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)

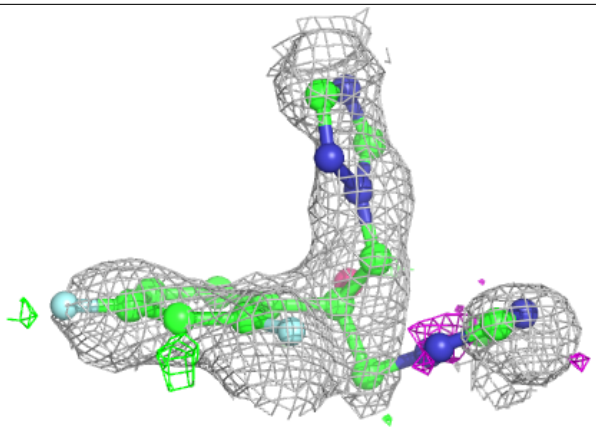
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95^{th} percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9'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

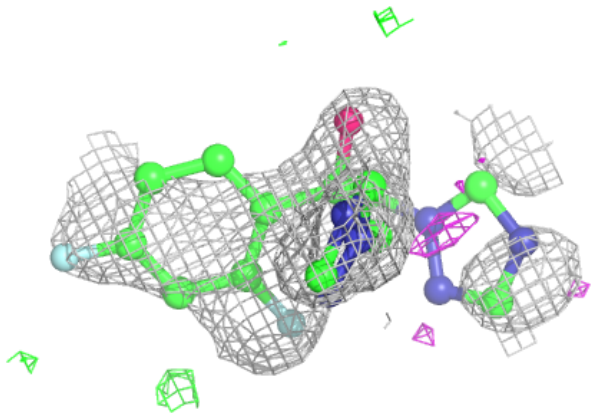
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
3	TPF	F	2474[A]	22/22	0.87	0.22	25,28,29,31	22
3	TPF	F	2474[B]	22/22	0.87	0.22	30,34,36,36	22
3	TPF	D	2473[A]	22/22	0.93	0.18	26,30,31,32	22
3	TPF	D	2473[B]	22/22	0.93	0.18	24,28,30,30	22
3	TPF	A	2472[B]	22/22	0.94	0.14	24,30,33,34	22
3	TPF	C	2471	22/22	0.94	0.10	32,34,36,36	0
3	TPF	A	2472[A]	22/22	0.94	0.14	18,25,28,29	22
3	TPF	B	2470	22/22	0.96	0.08	24,27,28,30	0
2	HEM	E	462	43/43	0.98	0.07	18,21,25,28	0
2	HEM	F	462	43/43	0.98	0.07	17,22,29,34	0
2	HEM	B	462	43/43	0.98	0.08	18,22,26,27	0
2	HEM	C	462	43/43	0.98	0.07	17,20,27,32	0
2	HEM	D	462	43/43	0.98	0.08	21,24,33,37	0
2	HEM	A	462	43/43	0.99	0.07	17,21,28,32	0

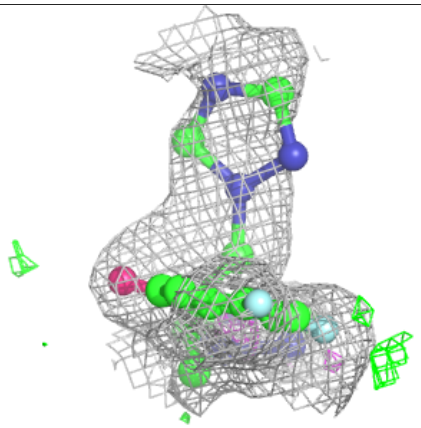
The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation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

Electron density around TPF F 2474 (A):

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

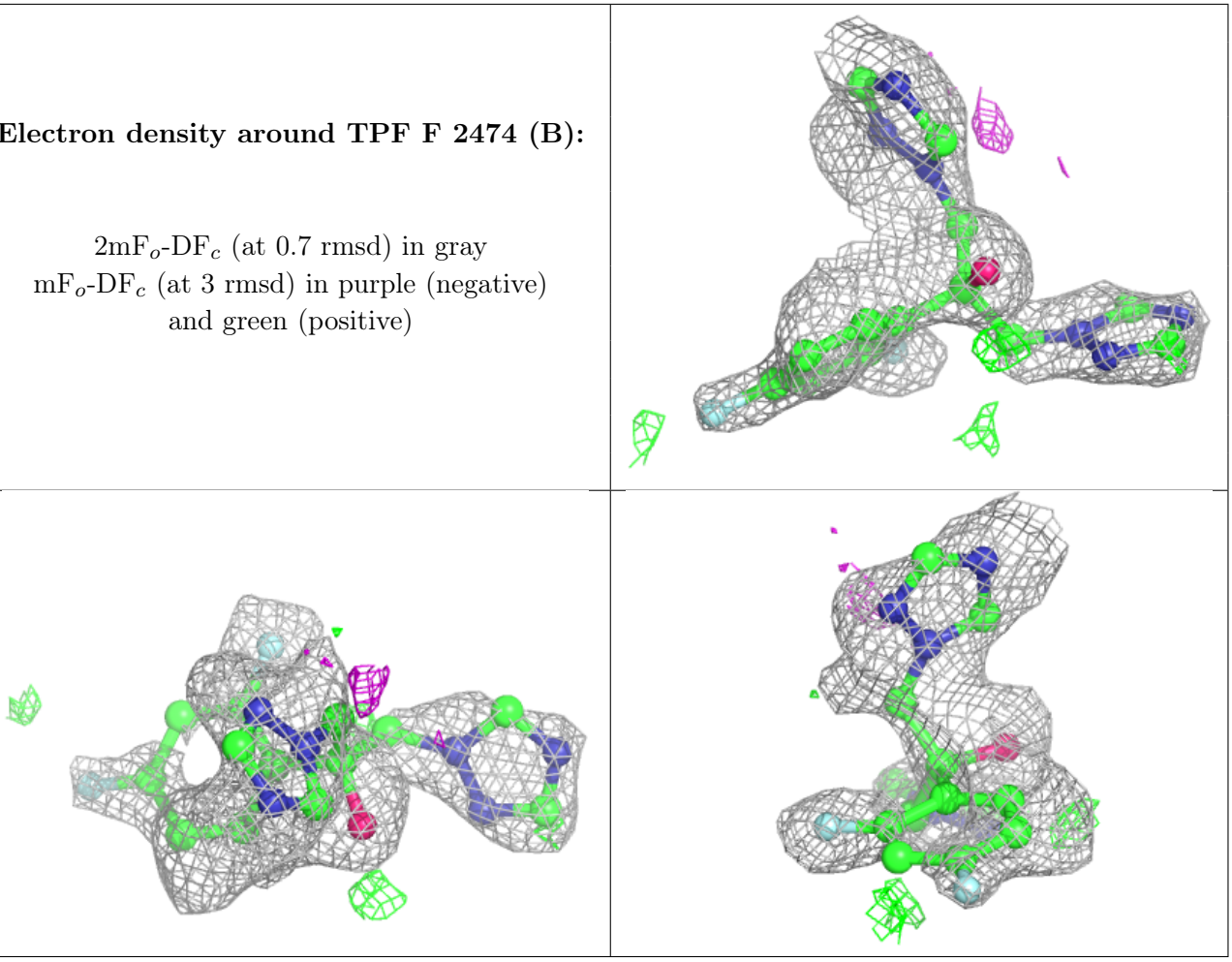






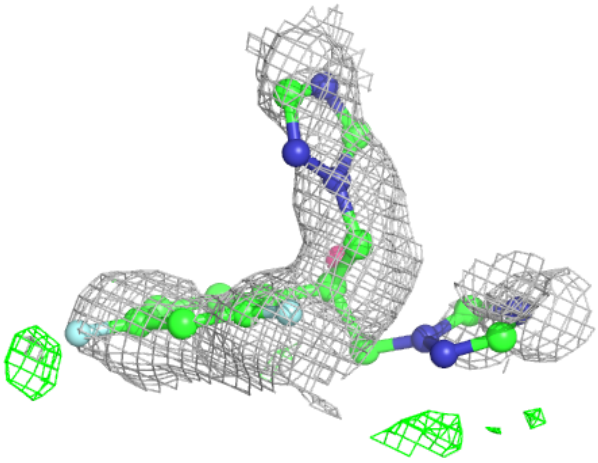
Electron density around TPF F 2474 (B):

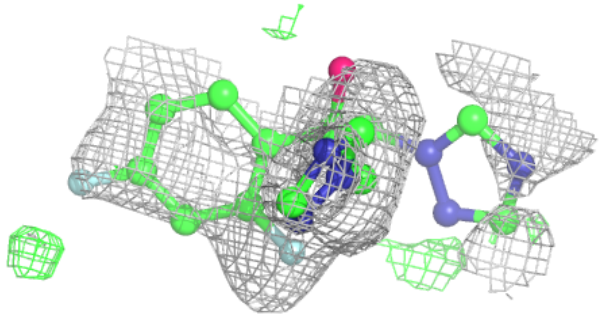
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

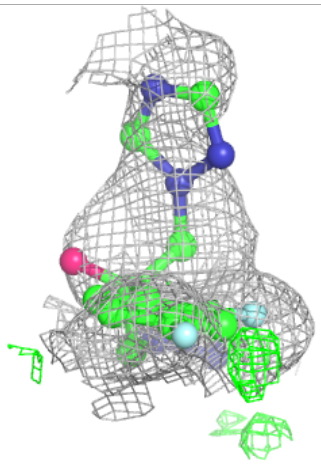


Electron density around TPF D 2473 (A):

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

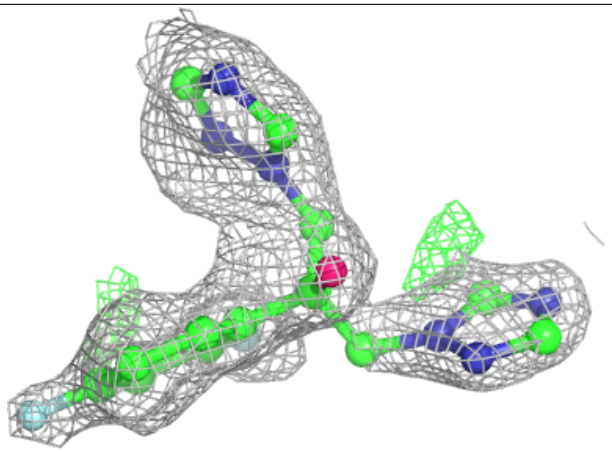


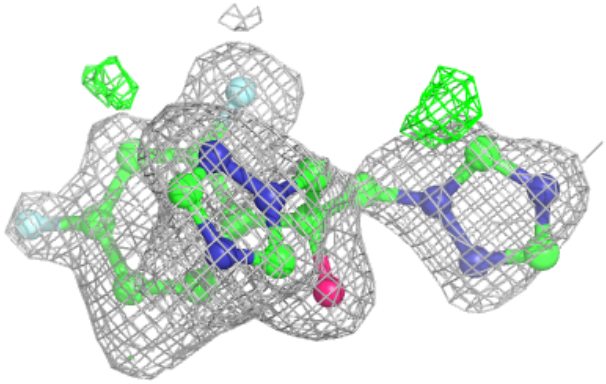


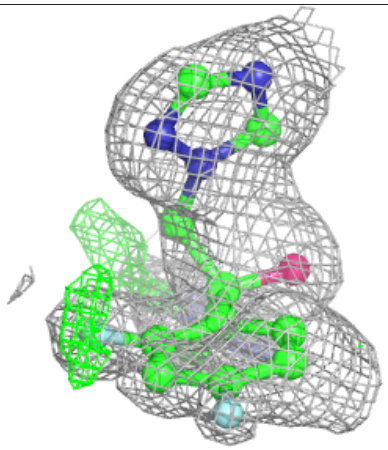


Electron density around TPF D 2473 (B):

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

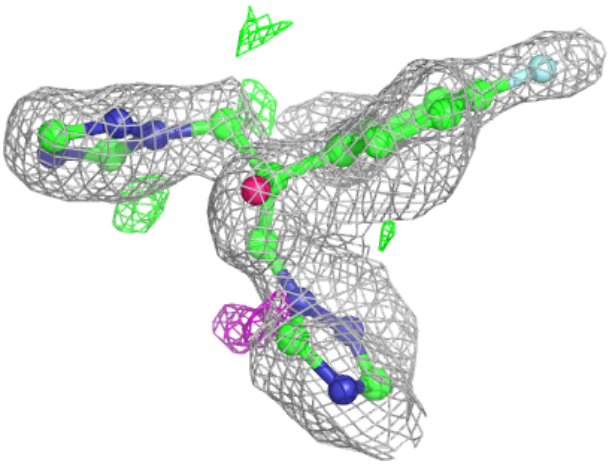


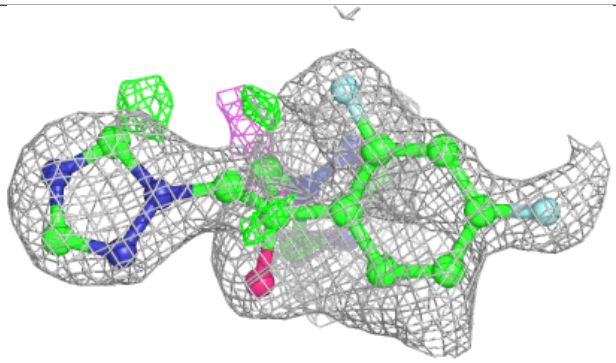


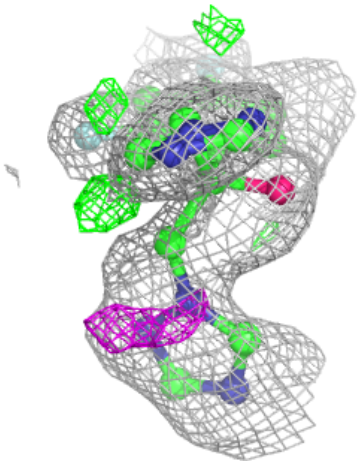


Electron density around TPF A 2472 (B):

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

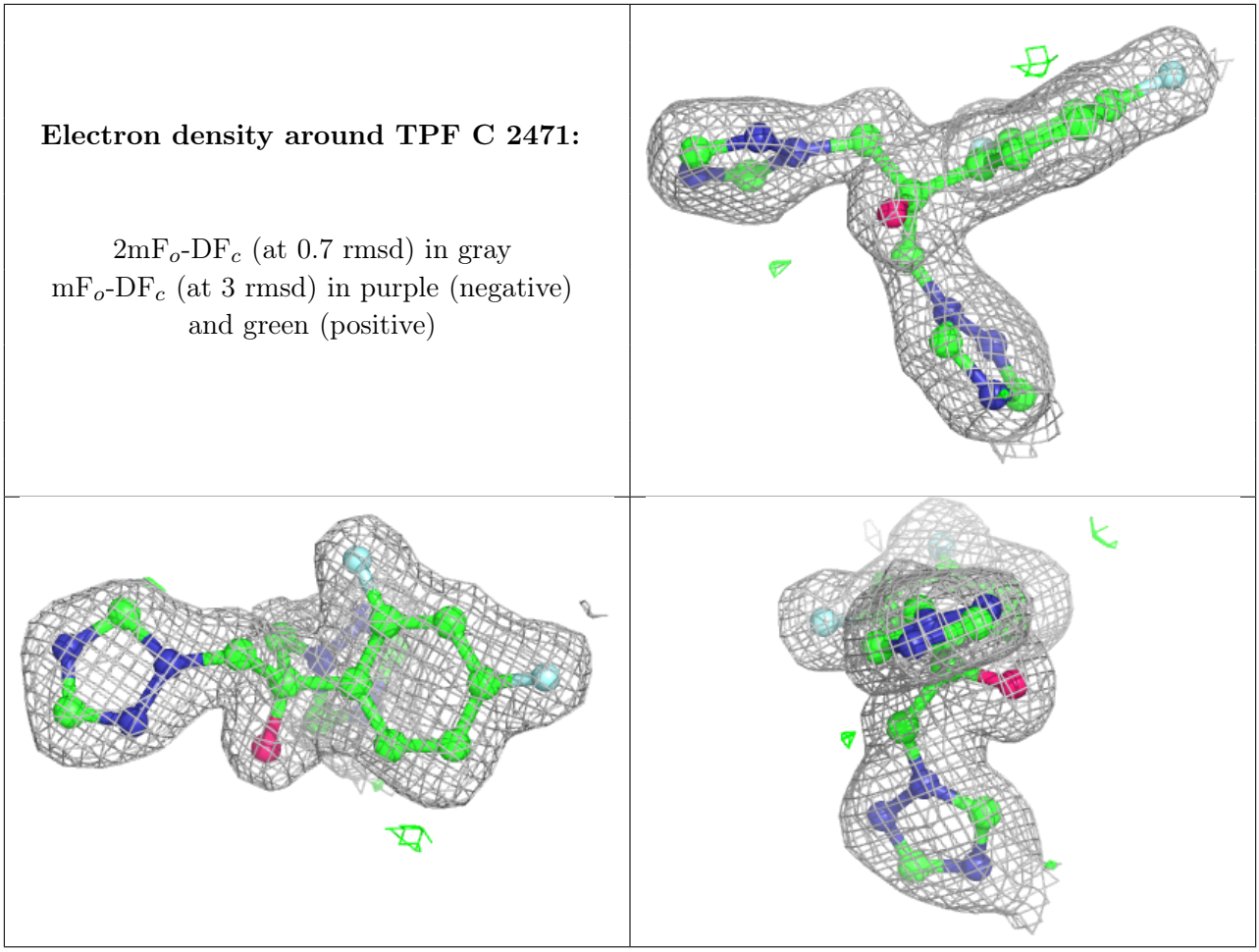






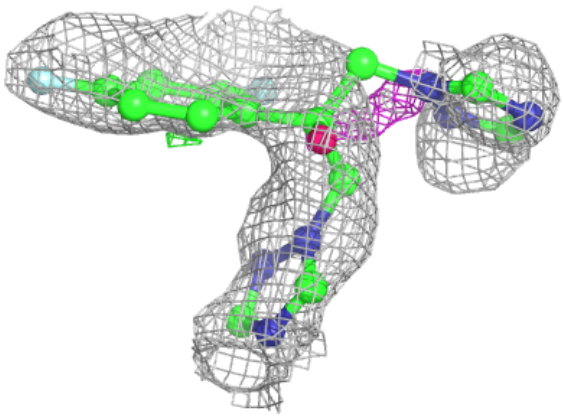
Electron density around TPF C 2471:

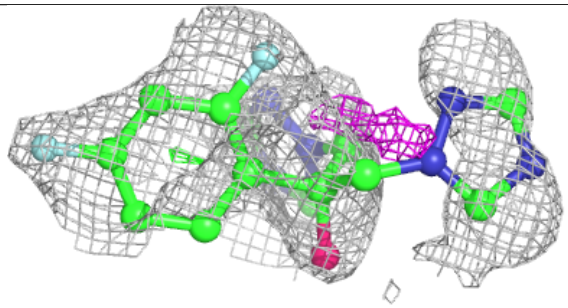
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

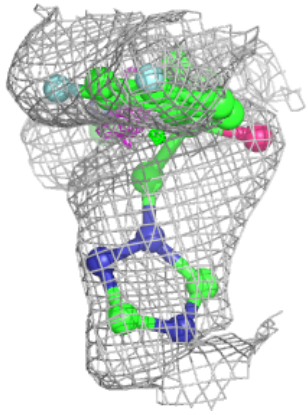


Electron density around TPF A 2472 (A):

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

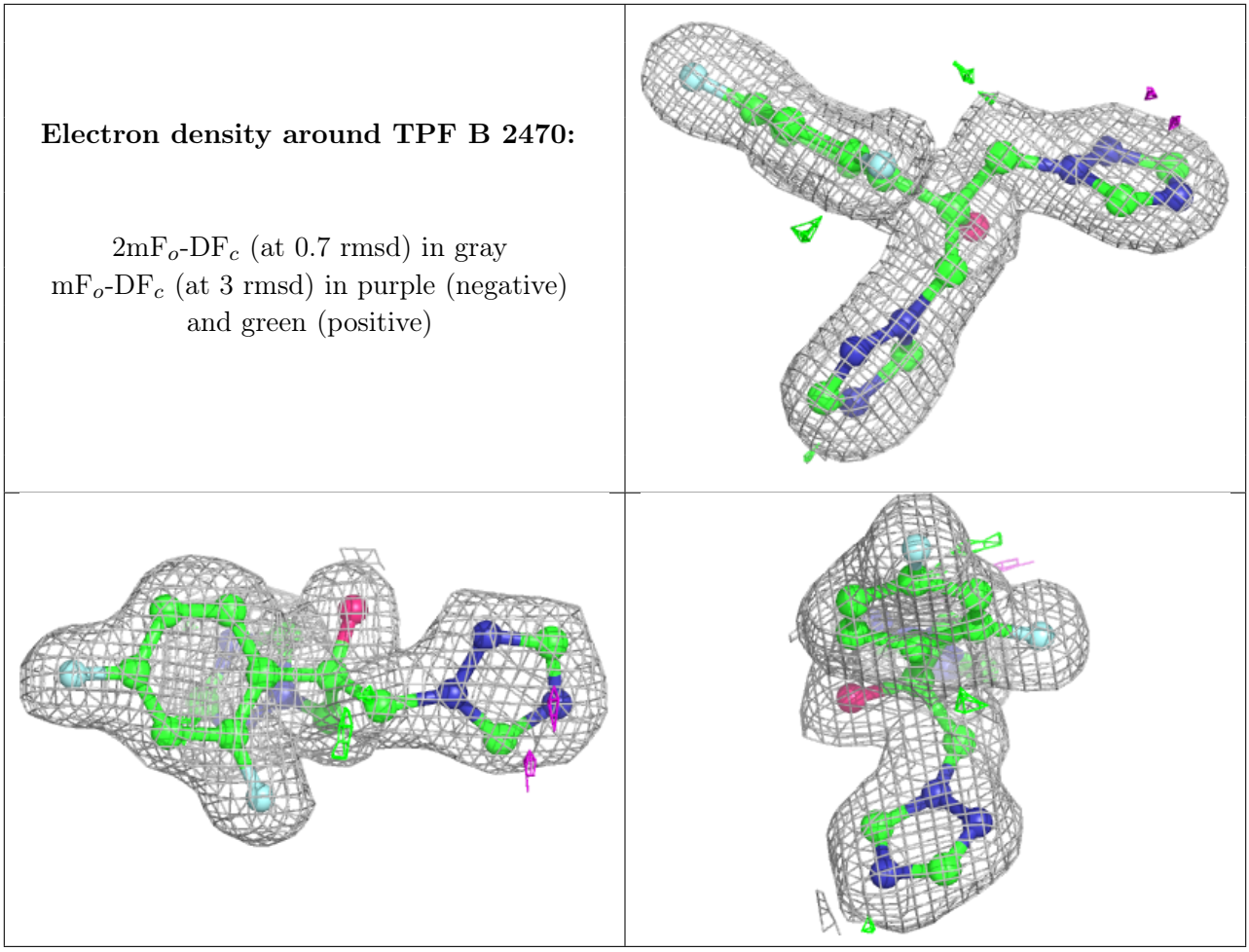






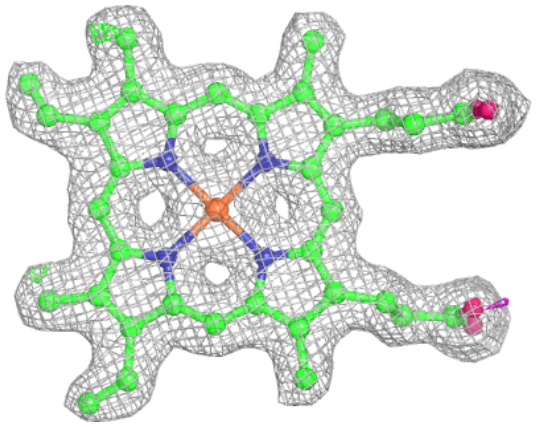
Electron density around TPF B 2470:

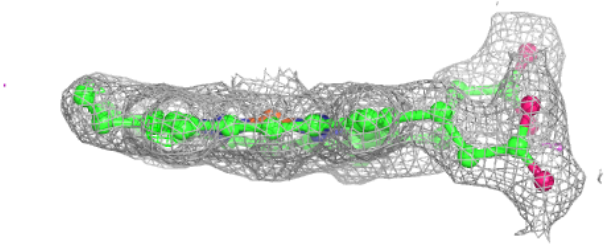
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

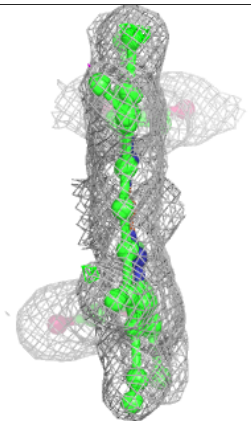


Electron density around HEM E 462:

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

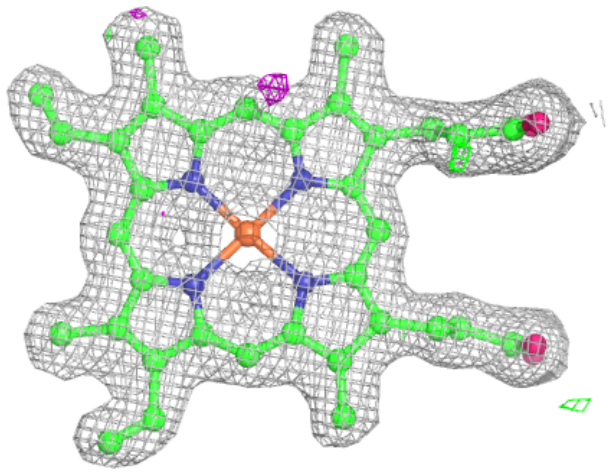


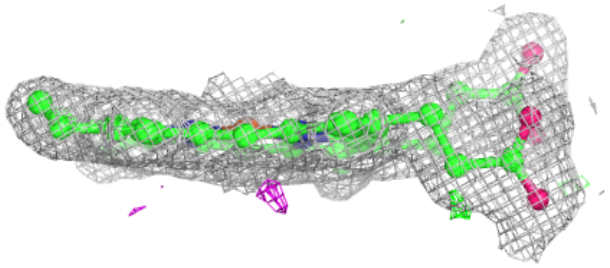


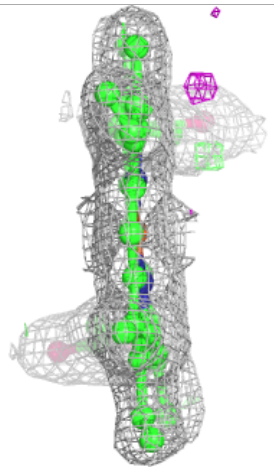


Electron density around HEM F 462:

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

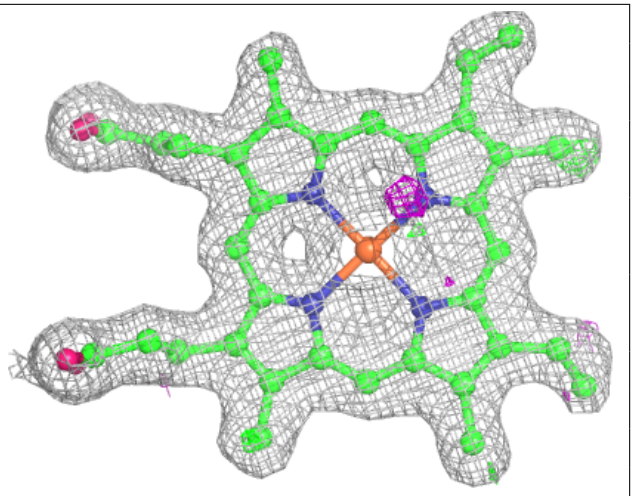


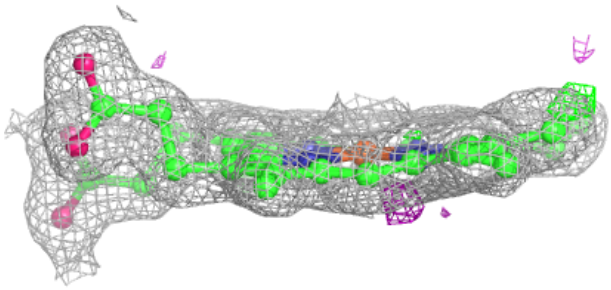


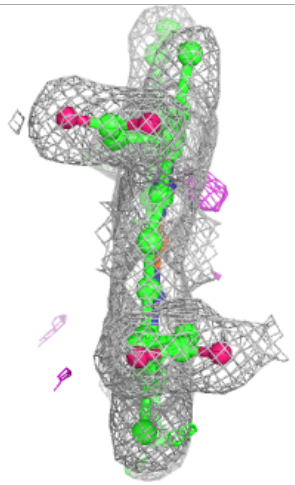


Electron density around HEM B 462:

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

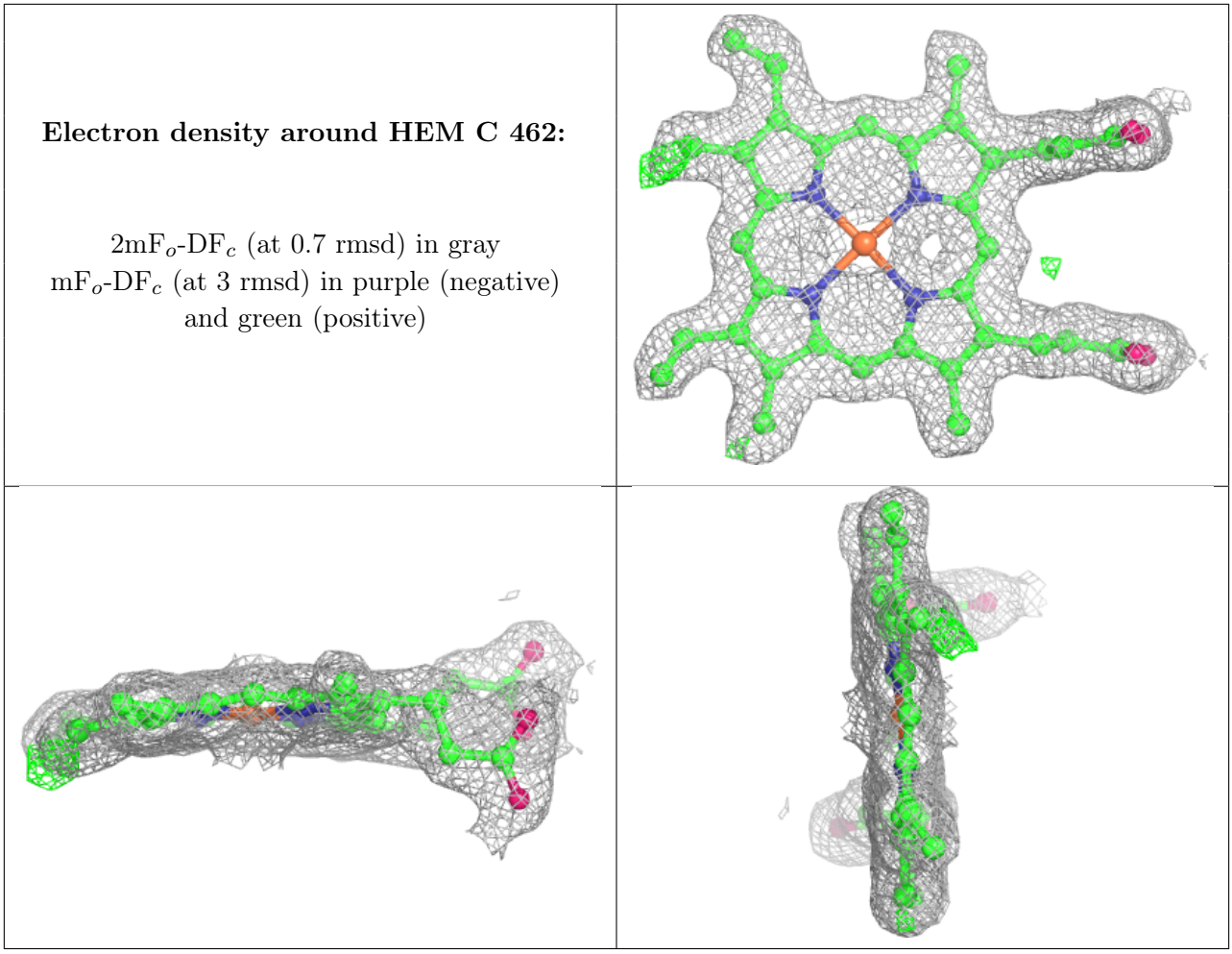






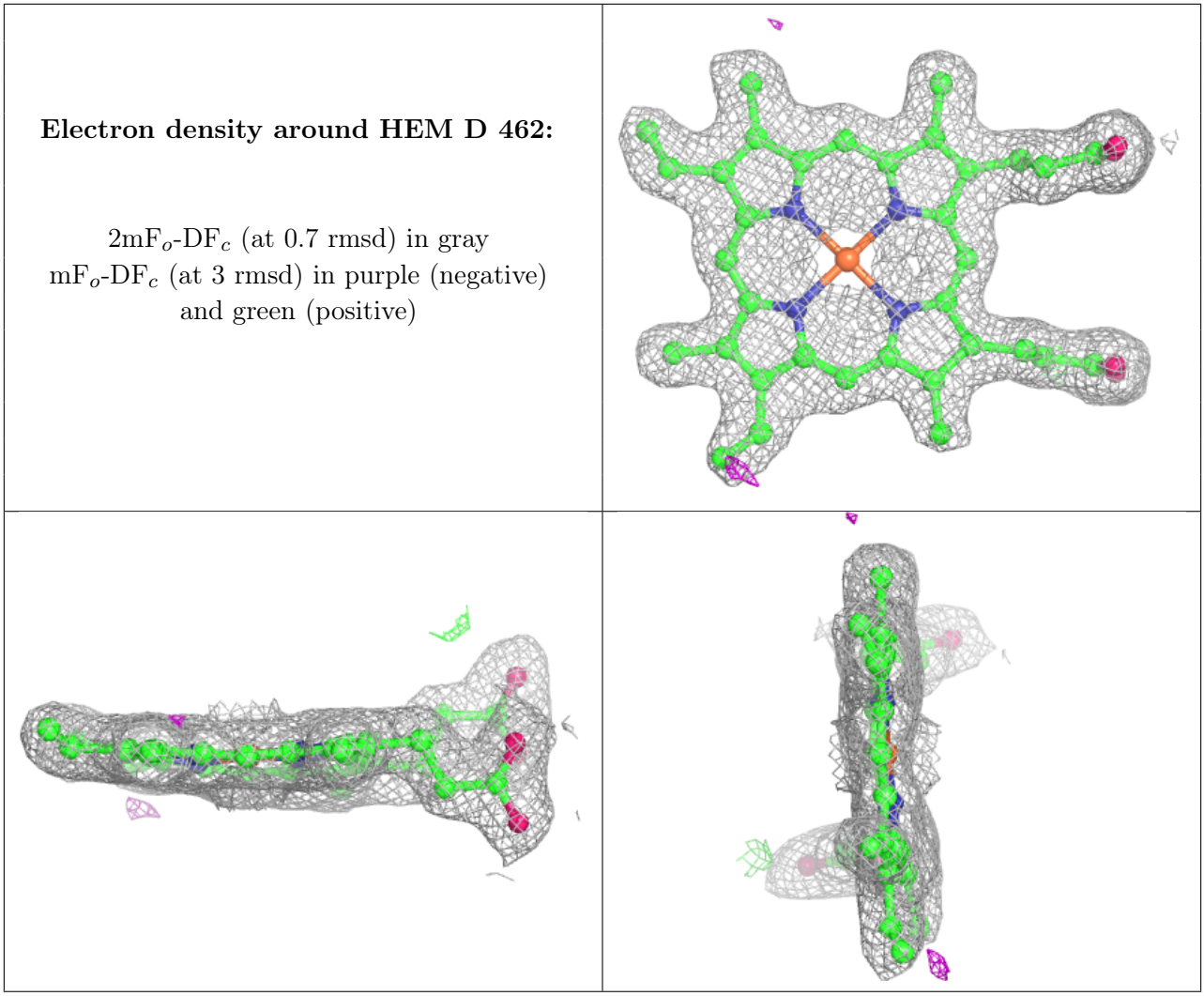
Electron density around HEM C 462:

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



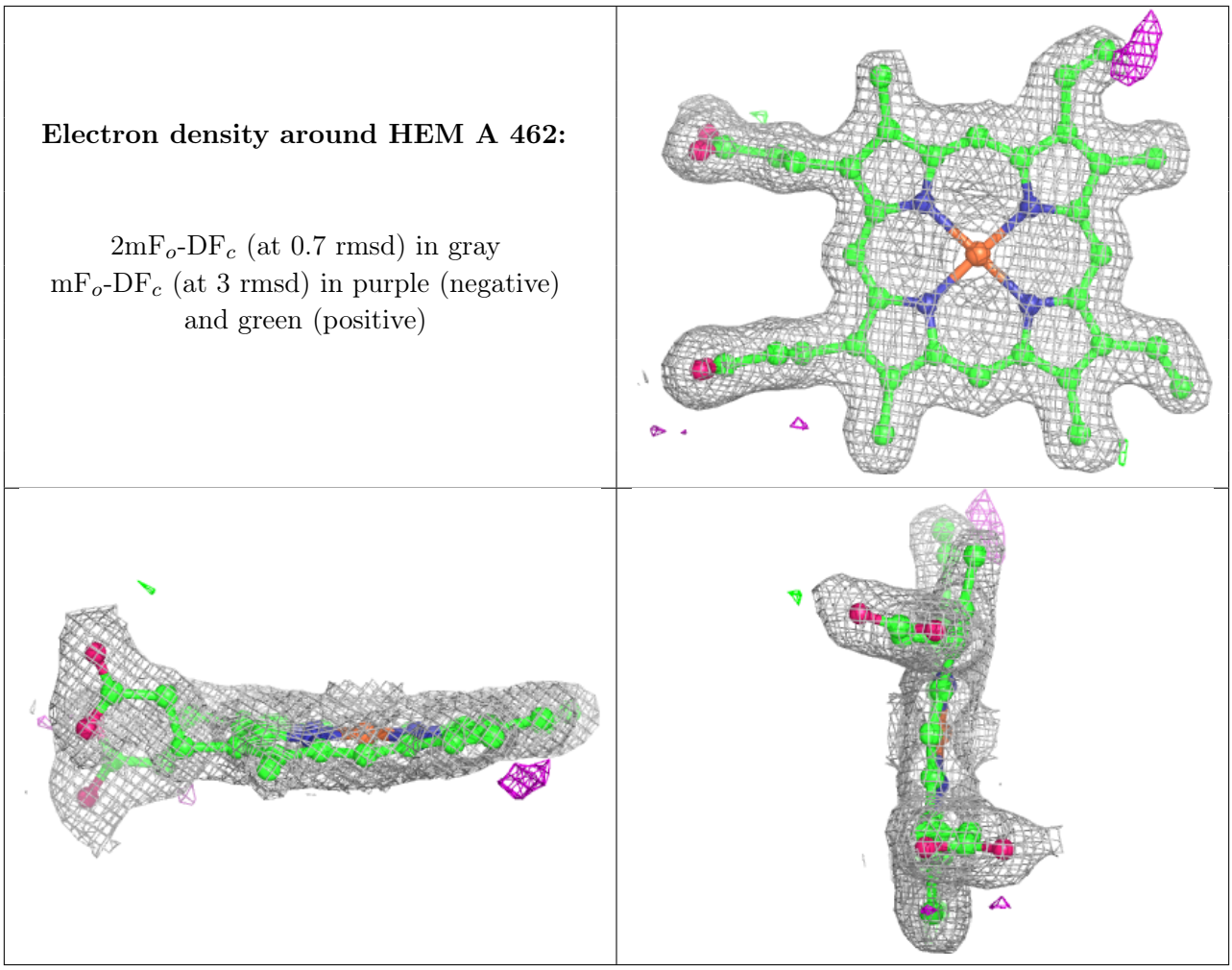
Electron density around HEM D 462:

$2mF_o$-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 462:

$2mF_o$-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.