Full wwPDB X-ray Structure Validation Report ⓘ

May 21, 2020 – 08:51 am BST

PDB ID	:	4JJ3
Title	:	Crystal structure of MamP soaked with iron(II)
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Deposited on	:	2013-03-07
Resolution	:	2.80 Å(reported)

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

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

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

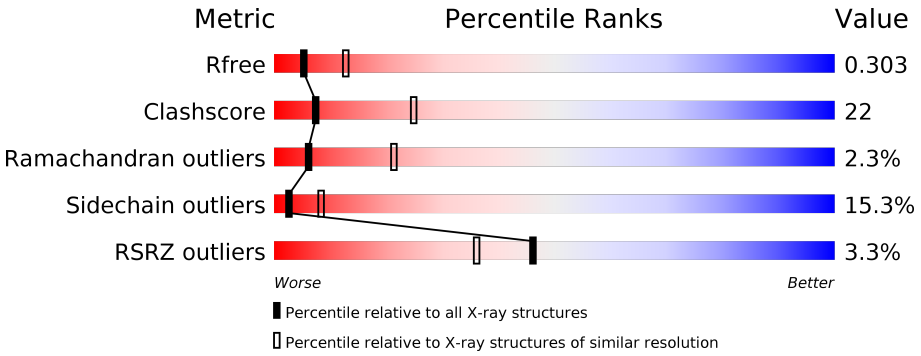
MolProbity	:	4.02b-467
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.11
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber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

1 Overall quality at a glance (i)

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

The reported resolution of this entry is 2.80 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	3140 (2.80-2.80)
Clashscore	141614	3569 (2.80-2.80)
Ramachandran outliers	138981	3498 (2.80-2.80)
Sidechain outliers	138945	3500 (2.80-2.80)
RSRZ outliers	127900	3078 (2.80-2.80)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments on the lower bar indicate the fraction of residues that contain outliers for >=3, 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions <=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	243	3% 42% 27% 26%
1	B	243	2% 46% 20% 7% 27%

2 Entry composition

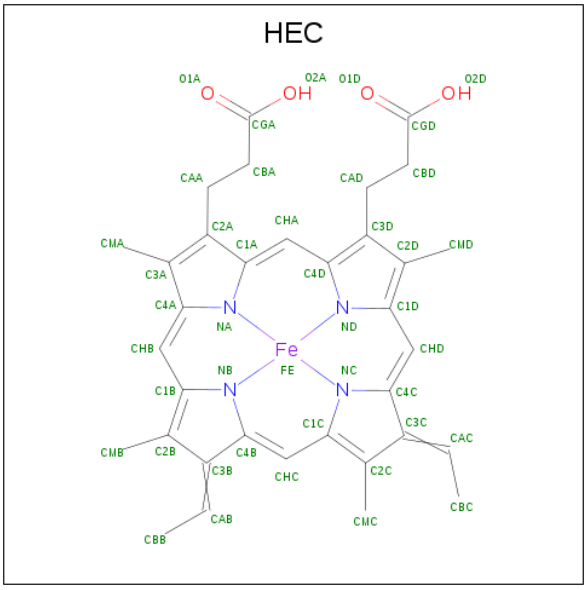
There are 2 unique types of molecules in this entry. The entry contains 2897 atoms, of which 0 are hydrogens and 0 are deuteriums.

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 MamP.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	181	Total	C	N	O	S	0	0	0
			1371	864	252	245	10			
1	B	178	Total	C	N	O	S	0	0	0
			1354	855	248	241	10			

- Molecule 2 is HEME C (three-letter code: HEC) (formula: $C_{34}H_{34}FeN_4O_4$).



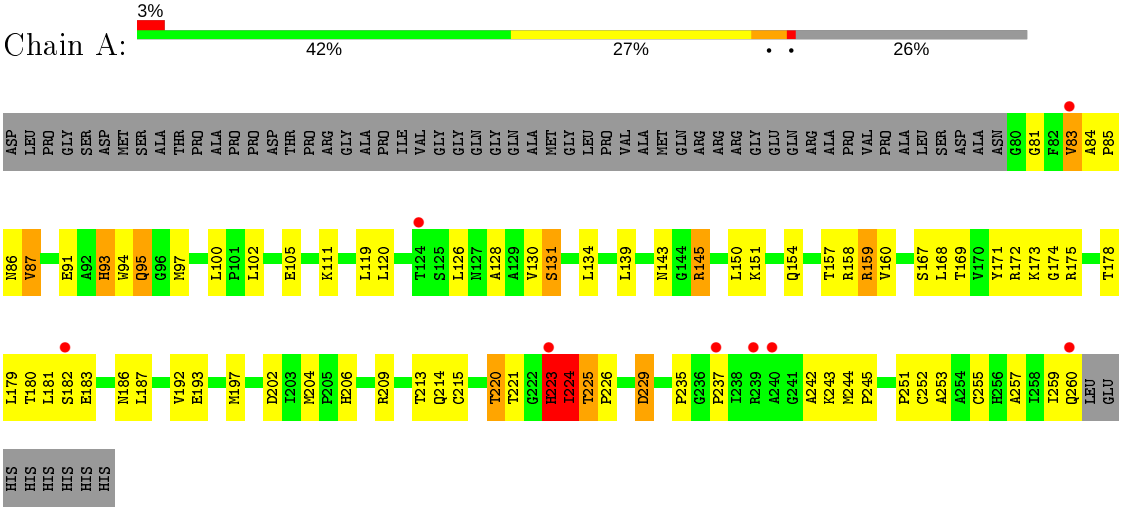
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
2	A	1	Total	C	Fe	N	O	0	0
			43	34	1	4	4		
2	A	1	Total	C	Fe	N	O	0	0
			43	34	1	4	4		
2	B	1	Total	C	Fe	N	O	0	0
			43	34	1	4	4		
2	B	1	Total	C	Fe	N	O	0	0
			43	34	1	4	4		

3 Residue-property plots (i)

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

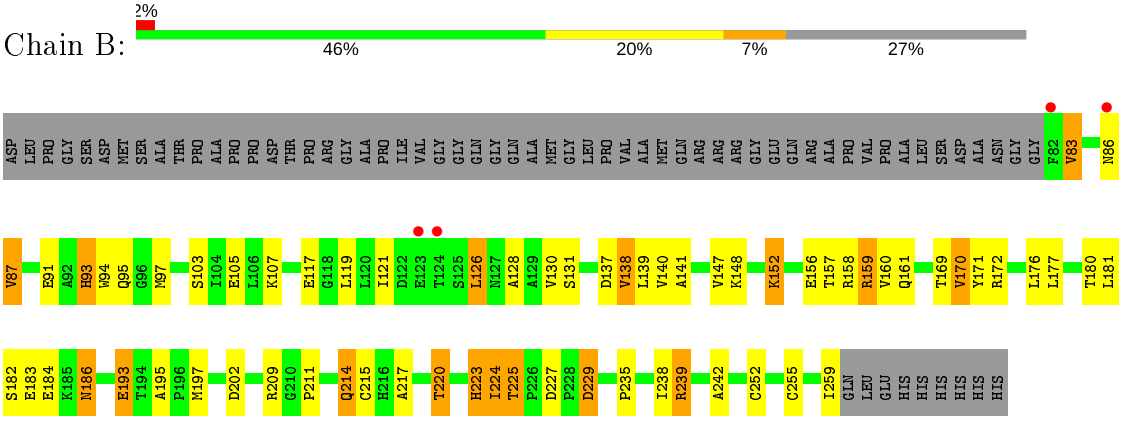
- Molecule 1: MamP

Chain A:



- Molecule 1: MamP

Chain B:



4 Data and refinement statistics (i)

Property	Value	Source
Space group	C 1 2 1	Depositor
Cell constants a, b, c, α, β, γ	81.11Å 96.08Å 54.45Å 90.00° 113.31° 90.00°	Depositor
Resolution (Å)	58.87 – 2.80 34.64 – 2.80	Depositor EDS
% Data completeness (in resolution range)	97.6 (58.87-2.80) 97.8 (34.64-2.80)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	2.01 (at 2.81Å)	Xtriage
Refinement program	REFMAC 5.6.0117	Depositor
R, R_{free}	0.264 , 0.298 0.268 , 0.303	Depositor DCC
R_{free} test set	494 reflections (5.31%)	wwPDB-VP
Wilson B-factor (Å^2)	52.0	Xtriage
Anisotropy	0.055	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.33 , 29.8	EDS
L-test for twinning[2]	$< \|L\| > = 0.48$, $< L^2 > = 0.32$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o,F_c correlation	0.86	EDS
Total number of atoms	2897	wwPDB-VP
Average B, all atoms (Å^2)	48.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The analyses of the Patterson function reveals a significant off-origin peak that is 24.35 % of the origin peak, indicating pseudo-translational symmetry. The chance of finding a peak of this or larger height randomly in a structure without pseudo-translational symmetry is equal to 3.9002e-03. The detected translational NCS is most likely also responsible for the elevated intensity ratio.*

[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: HEC

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	0.71	1/1397 (0.1%)	0.82	0/1892
1	B	0.70	0/1380	0.80	0/1870
All	All	0.71	1/2777 (0.0%)	0.81	0/3762

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	94	TRP	CD2-CE2	5.98	1.48	1.41

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	1371	0	1431	58	1
1	B	1354	0	1418	67	1
2	A	86	0	64	16	0
2	B	86	0	64	14	0
All	All	2897	0	2977	127	2

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 22.

All (127) 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:A:215:CYS:SG	2:A:501:HEC:CAC	2.22	1.27
1:A:145:ARG:HH11	1:A:145:ARG:HG3	1.02	1.09
1:B:137:ASP:OD2	1:B:172:ARG:NH1	1.89	1.05
1:A:145:ARG:HH11	1:A:145:ARG:CG	1.70	1.03
1:B:252:CYS:SG	2:B:502:HEC:CBB	2.48	1.02
1:B:255:CYS:SG	2:B:502:HEC:HAC	2.01	0.98
1:A:145:ARG:NH1	1:A:145:ARG:HG3	1.73	0.96
1:A:131:SER:HB2	1:A:180:THR:O	1.71	0.89
1:A:197:MET:SD	1:A:221:THR:O	2.34	0.86
1:B:215:CYS:SG	2:B:501:HEC:CBC	2.63	0.86
1:A:255:CYS:SG	2:A:502:HEC:C3C	2.64	0.86
1:B:215:CYS:SG	2:B:501:HEC:HAC	2.11	0.85
1:B:252:CYS:SG	2:B:502:HEC:C3B	2.62	0.85
1:A:255:CYS:SG	2:A:502:HEC:HAC	2.18	0.83
1:B:156:GLU:OE2	1:B:159:ARG:NH1	2.11	0.82
1:B:252:CYS:SG	2:B:502:HEC:HBB3	2.17	0.82
1:A:220:THR:O	1:A:223:HIS:HB3	1.80	0.80
1:A:255:CYS:SG	2:A:502:HEC:CBC	2.70	0.79
1:B:215:CYS:SG	2:B:501:HEC:C3C	2.72	0.78
1:B:255:CYS:SG	2:B:502:HEC:C3C	2.71	0.77
1:A:215:CYS:SG	2:A:501:HEC:HAC	2.26	0.76
1:B:186:ASN:N	1:B:186:ASN:HD22	1.86	0.73
1:B:224:ILE:O	1:B:224:ILE:HG23	1.90	0.72
1:B:83:VAL:HG12	1:B:87:VAL:HG21	1.71	0.71
1:A:215:CYS:SG	2:A:501:HEC:CBC	2.79	0.69
1:B:255:CYS:SG	2:B:502:HEC:CBC	2.80	0.69
1:B:238:ILE:HD12	1:B:242:ALA:HB3	1.75	0.69
1:B:252:CYS:SG	2:B:502:HEC:HAB	2.31	0.69
1:A:215:CYS:SG	2:A:501:HEC:C3C	2.80	0.69
1:B:220:THR:O	1:B:223:HIS:HB3	1.92	0.68
1:A:209:ARG:NH2	2:A:501:HEC:O1D	2.23	0.65
1:A:224:ILE:HG23	1:A:224:ILE:O	1.96	0.65
1:B:223:HIS:HB2	1:B:225:THR:OG1	1.96	0.65
1:B:235:PRO:HG3	2:B:502:HEC:HMD3	1.80	0.63
1:A:255:CYS:HG	2:A:502:HEC:CAC	2.12	0.62
1:B:197:MET:HE1	1:B:220:THR:HA	1.81	0.62
1:A:237:PRO:HA	1:A:257:ALA:O	2.00	0.61
1:B:103:SER:O	1:B:107:LYS:HG3	2.02	0.60
1:A:167:SER:O	1:A:168:LEU:HD23	2.01	0.59
1:A:171:TYR:CE1	1:A:174:GLY:HA2	2.36	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:95:GLN:HB2	1:B:181:LEU:HD21	1.85	0.59
1:A:119:LEU:O	1:A:139:LEU:N	2.32	0.58
1:B:197:MET:HE1	1:B:220:THR:CA	2.33	0.58
1:B:131:SER:HB2	1:B:180:THR:O	2.03	0.58
1:B:126:LEU:O	1:B:130:VAL:HG23	2.03	0.58
1:B:157:THR:O	1:B:161:GLN:HB3	2.04	0.57
1:B:121:ILE:HD11	1:B:139:LEU:HB2	1.86	0.57
1:A:225:THR:HA	1:A:226:PRO:C	2.24	0.57
1:B:159:ARG:CZ	1:B:159:ARG:HB3	2.35	0.56
1:A:119:LEU:HD13	1:A:150:LEU:HD23	1.88	0.56
1:A:245:PRO:HG3	2:A:502:HEC:C2A	2.35	0.56
1:A:145:ARG:NH1	1:A:145:ARG:CG	2.40	0.55
1:B:215:CYS:SG	2:B:501:HEC:HBC3	2.46	0.55
1:B:131:SER:HB3	1:B:181:LEU:HD12	1.88	0.55
1:A:251:PRO:O	1:A:253:ALA:N	2.39	0.55
1:A:224:ILE:CG2	1:A:224:ILE:O	2.55	0.55
1:A:95:GLN:HG3	1:A:187:LEU:HD22	1.88	0.54
1:B:211:PRO:O	1:B:214:GLN:HB2	2.06	0.54
1:A:85:PRO:O	1:A:86:ASN:OD1	2.25	0.54
1:A:128:ALA:HA	1:A:181:LEU:HD11	1.88	0.54
2:A:502:HEC:HMC1	2:A:502:HEC:HBC3	1.88	0.54
1:B:91:GLU:HG2	1:B:193:GLU:HB3	1.90	0.54
1:A:235:PRO:HG3	2:A:502:HEC:HMD3	1.91	0.53
1:B:197:MET:HG2	1:B:217:ALA:O	2.09	0.53
1:B:148:LYS:H	1:B:152:LYS:HZ2	1.57	0.53
1:A:204:MET:HG2	1:A:206:HIS:O	2.08	0.53
1:A:243:LYS:O	1:A:245:PRO:HD3	2.10	0.52
1:A:229:ASP:OD1	1:A:229:ASP:N	2.42	0.52
1:B:94:TRP:O	1:B:97:MET:HG2	2.11	0.51
1:B:95:GLN:NE2	1:B:183:GLU:OE1	2.44	0.51
1:B:186:ASN:HD22	1:B:186:ASN:H	1.55	0.51
1:B:147:VAL:O	1:B:147:VAL:HG23	2.10	0.50
1:B:224:ILE:CG2	1:B:224:ILE:O	2.58	0.50
1:B:105:GLU:OE1	1:B:209:ARG:NE	2.45	0.50
1:B:220:THR:O	1:B:223:HIS:CB	2.60	0.49
1:A:255:CYS:SG	2:A:502:HEC:HBC3	2.50	0.49
1:A:221:THR:C	1:A:223:HIS:N	2.65	0.49
1:B:220:THR:O	1:B:223:HIS:CG	2.66	0.49
1:A:102:LEU:HD13	1:A:120:LEU:HB2	1.95	0.49
1:B:197:MET:HG3	1:B:217:ALA:HB3	1.93	0.49
1:A:160:VAL:HG23	1:A:160:VAL:O	2.13	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:160:VAL:HG23	1:B:160:VAL:O	2.12	0.49
1:B:137:ASP:CG	1:B:172:ARG:HH11	2.16	0.48
1:A:134:LEU:HD12	1:A:172:ARG:CZ	2.44	0.48
1:A:167:SER:C	1:A:168:LEU:HD23	2.34	0.48
1:B:117:GLU:HB3	1:B:148:LYS:HG2	1.94	0.48
1:A:128:ALA:HA	1:A:181:LEU:CD1	2.44	0.47
1:A:178:THR:O	1:A:179:LEU:HD23	2.14	0.47
1:B:255:CYS:HG	2:B:502:HEC:HAC	1.72	0.47
1:B:223:HIS:O	1:B:224:ILE:C	2.53	0.47
1:A:84:ALA:HB2	1:A:213:THR:HB	1.96	0.46
1:B:172:ARG:NH2	1:B:177:LEU:HD13	2.30	0.46
1:B:239:ARG:HA	1:B:259:ILE:HB	1.95	0.46
1:B:128:ALA:HA	1:B:181:LEU:HD11	1.96	0.46
1:A:91:GLU:HG2	1:A:193:GLU:HB3	1.98	0.46
1:A:251:PRO:C	1:A:253:ALA:H	2.20	0.45
1:A:81:GLY:HA2	1:A:197:MET:CE	2.46	0.45
1:B:195:ALA:HB3	1:B:215:CYS:O	2.17	0.45
1:A:143:ASN:ND2	1:A:160:VAL:HG11	2.32	0.44
1:B:186:ASN:N	1:B:186:ASN:ND2	2.59	0.44
1:B:259:ILE:HG22	1:B:259:ILE:O	2.18	0.44
1:B:215:CYS:HG	2:B:501:HEC:CAC	2.22	0.44
1:A:159:ARG:HB3	1:A:159:ARG:CZ	2.46	0.44
1:A:259:ILE:O	1:A:260:GLN:HB2	2.17	0.44
1:B:171:TYR:CD2	1:B:171:TYR:C	2.90	0.44
1:B:239:ARG:O	1:B:242:ALA:HB2	2.17	0.44
2:A:501:HEC:CBB	2:A:501:HEC:HMB1	2.48	0.44
1:A:105:GLU:OE1	1:A:209:ARG:NE	2.52	0.43
1:B:259:ILE:CG2	1:B:259:ILE:O	2.66	0.43
1:A:154:GLN:O	1:A:157:THR:N	2.47	0.42
1:B:227:ASP:OD1	1:B:229:ASP:HB2	2.19	0.42
1:A:223:HIS:CG	1:A:224:ILE:H	2.37	0.42
1:A:221:THR:C	1:A:223:HIS:H	2.21	0.42
1:A:223:HIS:O	1:A:224:ILE:HB	2.20	0.42
1:B:91:GLU:O	1:B:193:GLU:N	2.52	0.42
1:A:215:CYS:SG	2:A:501:HEC:HBC3	2.59	0.42
1:B:138:VAL:O	1:B:170:VAL:HG12	2.19	0.42
1:B:128:ALA:HA	1:B:181:LEU:CD1	2.50	0.42
1:A:97:MET:O	1:A:97:MET:CG	2.68	0.42
1:B:119:LEU:O	1:B:138:VAL:HA	2.20	0.41
1:B:197:MET:HB3	1:B:197:MET:HE2	1.95	0.41
1:B:93:HIS:N	1:B:93:HIS:ND1	2.68	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:235:PRO:HB3	2:A:502:HEC:C1D	2.50	0.41
1:A:83:VAL:HG23	1:A:87:VAL:CG2	2.51	0.40
1:B:141:ALA:HB3	1:B:169:THR:HB	2.03	0.40
1:A:93:HIS:N	1:A:93:HIS:ND1	2.69	0.40
1:B:197:MET:HE1	1:B:220:THR:N	2.37	0.40

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

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:158:ARG:NH1	1:B:186:ASN:ND2[2_655]	1.73	0.47
1:A:158:ARG:NH1	1:A:186:ASN:OD1[2_655]	1.88	0.32

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	179/243 (74%)	157 (88%)	16 (9%)	6 (3%)	3 13
1	B	176/243 (72%)	158 (90%)	16 (9%)	2 (1%)	14 41
All	All	355/486 (73%)	315 (89%)	32 (9%)	8 (2%)	6 21

All (8) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	223	HIS
1	A	224	ILE
1	A	252	CYS
1	B	229	ASP
1	A	242	ALA
1	A	126	LEU
1	B	224	ILE

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Mol	Chain	Res	Type
1	A	95	GLN

5.3.2 Protein sidechains

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
1	A	148/195 (76%)	124 (84%)	24 (16%)	2 7
1	B	147/195 (75%)	126 (86%)	21 (14%)	3 10
All	All	295/390 (76%)	250 (85%)	45 (15%)	2 8

All (45) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	83	VAL
1	A	87	VAL
1	A	93	HIS
1	A	100	LEU
1	A	111	LYS
1	A	130	VAL
1	A	131	SER
1	A	145	ARG
1	A	151	LYS
1	A	159	ARG
1	A	169	THR
1	A	173	LYS
1	A	175	ARG
1	A	182	SER
1	A	183	GLU
1	A	192	VAL
1	A	202	ASP
1	A	214	GLN
1	A	220	THR
1	A	223	HIS
1	A	224	ILE
1	A	225	THR

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Mol	Chain	Res	Type
1	A	229	ASP
1	A	244	MET
1	B	83	VAL
1	B	86	ASN
1	B	87	VAL
1	B	93	HIS
1	B	126	LEU
1	B	138	VAL
1	B	140	VAL
1	B	152	LYS
1	B	159	ARG
1	B	170	VAL
1	B	176	LEU
1	B	182	SER
1	B	184	GLU
1	B	186	ASN
1	B	193	GLU
1	B	202	ASP
1	B	214	GLN
1	B	220	THR
1	B	223	HIS
1	B	225	THR
1	B	239	ARG

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (2) such sidechains are listed below:

Mol	Chain	Res	Type
1	B	86	ASN
1	B	186	ASN

5.3.3 RNA

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates (i)

There are no carbohydrates in this entry.

5.6 Ligand geometry (i)

4 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	HEC	B	502	1	26,50,50	2.67	12 (46%)	18,82,82	2.78	7 (38%)
2	HEC	B	501	1	26,50,50	2.45	12 (46%)	18,82,82	3.05	7 (38%)
2	HEC	A	502	1	26,50,50	2.62	13 (50%)	18,82,82	2.31	6 (33%)
2	HEC	A	501	1	26,50,50	2.41	10 (38%)	18,82,82	3.11	8 (44%)

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	HEC	B	502	1	-	0/6/54/54	-
2	HEC	B	501	1	-	0/6/54/54	-
2	HEC	A	502	1	-	0/6/54/54	-
2	HEC	A	501	1	-	0/6/54/54	-

All (47) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	502	HEC	C3B-C2B	7.66	1.48	1.40
2	B	502	HEC	C3B-C2B	7.28	1.48	1.40
2	A	501	HEC	C3C-C2C	6.51	1.47	1.40
2	B	501	HEC	C3B-C2B	6.43	1.47	1.40
2	B	502	HEC	C3C-C2C	6.04	1.47	1.40
2	A	501	HEC	C3B-C2B	5.67	1.46	1.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	501	HEC	C3C-C2C	5.67	1.46	1.40
2	A	502	HEC	C3C-C2C	5.13	1.46	1.40
2	A	502	HEC	C4A-C3A	3.98	1.51	1.42
2	A	502	HEC	C2A-C3A	3.80	1.48	1.37
2	B	502	HEC	C3D-C2D	3.72	1.48	1.37
2	B	501	HEC	C2A-C3A	3.60	1.48	1.37
2	A	501	HEC	C2A-C3A	3.58	1.48	1.37
2	B	502	HEC	C4A-C3A	3.55	1.50	1.42
2	B	502	HEC	C2A-C3A	3.48	1.48	1.37
2	B	501	HEC	C1A-C2A	3.17	1.49	1.42
2	B	501	HEC	C3D-C2D	3.14	1.47	1.37
2	B	502	HEC	C1A-C2A	3.13	1.49	1.42
2	A	501	HEC	C1C-CHC	3.08	1.49	1.41
2	B	502	HEC	C3B-C4B	3.06	1.48	1.43
2	B	502	HEC	C3C-C4C	3.05	1.48	1.43
2	A	502	HEC	C3D-C2D	2.94	1.46	1.37
2	A	501	HEC	C1A-C2A	2.92	1.49	1.42
2	A	502	HEC	C3C-C4C	2.89	1.48	1.43
2	B	501	HEC	C4A-C3A	2.84	1.49	1.42
2	A	501	HEC	C3D-C2D	2.84	1.46	1.37
2	B	501	HEC	C4D-CHA	2.69	1.48	1.41
2	A	501	HEC	C1B-CHB	2.67	1.48	1.41
2	B	501	HEC	C1B-CHB	2.67	1.48	1.41
2	A	501	HEC	C4A-C3A	2.59	1.48	1.42
2	A	502	HEC	C1D-CHD	2.56	1.48	1.41
2	A	502	HEC	CBB-CAB	2.53	1.59	1.49
2	A	501	HEC	C3B-C4B	2.51	1.47	1.43
2	B	501	HEC	C1C-CHC	2.47	1.47	1.41
2	A	502	HEC	C1B-CHB	2.44	1.47	1.41
2	B	502	HEC	C1B-CHB	2.43	1.47	1.41
2	A	502	HEC	C1A-C2A	2.42	1.48	1.42
2	B	502	HEC	C1C-CHC	2.35	1.47	1.41
2	A	502	HEC	C1C-CHC	2.33	1.47	1.41
2	B	502	HEC	C1D-CHD	2.31	1.47	1.41
2	A	502	HEC	C4D-CHA	2.28	1.47	1.41
2	A	501	HEC	C4D-CHA	2.25	1.47	1.41
2	B	501	HEC	C3B-C4B	2.24	1.47	1.43
2	B	502	HEC	C4D-CHA	2.24	1.47	1.41
2	A	502	HEC	C3B-C4B	2.15	1.47	1.43
2	B	501	HEC	CBC-CAC	2.10	1.57	1.49
2	B	501	HEC	C1D-CHD	2.02	1.46	1.41

All (28) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	A	501	HEC	CBA-CAA-C2A	-7.38	98.88	112.48
2	B	501	HEC	C1D-C2D-C3D	-7.05	102.09	107.00
2	A	501	HEC	C1D-C2D-C3D	-6.83	102.24	107.00
2	B	501	HEC	CBA-CAA-C2A	-5.65	102.07	112.48
2	B	502	HEC	CMB-C2B-C3B	5.06	131.77	125.82
2	B	501	HEC	CMB-C2B-C3B	4.89	131.57	125.82
2	B	502	HEC	C1D-C2D-C3D	-4.81	103.65	107.00
2	B	502	HEC	CBA-CAA-C2A	-4.80	103.63	112.48
2	B	501	HEC	CAD-CBD-CGD	4.59	120.37	112.67
2	A	501	HEC	CMB-C2B-C3B	4.56	131.18	125.82
2	A	502	HEC	CMB-C2B-C3B	4.53	131.15	125.82
2	A	502	HEC	C1D-C2D-C3D	-4.49	103.87	107.00
2	B	502	HEC	CAD-CBD-CGD	4.39	120.03	112.67
2	B	502	HEC	CMC-C2C-C3C	4.27	130.84	125.82
2	A	501	HEC	CBD-CAD-C3D	-4.03	105.05	112.49
2	B	501	HEC	CMC-C2C-C3C	3.79	130.28	125.82
2	A	502	HEC	CMC-C2C-C3C	3.75	130.23	125.82
2	A	502	HEC	CBA-CAA-C2A	-3.72	105.63	112.48
2	B	502	HEC	C4B-C3B-C2B	-3.08	103.02	106.35
2	A	502	HEC	CAD-CBD-CGD	3.06	117.80	112.67
2	A	501	HEC	CAD-CBD-CGD	3.04	117.78	112.67
2	A	501	HEC	CMC-C2C-C3C	2.91	129.24	125.82
2	B	501	HEC	CMD-C2D-C3D	2.88	130.37	124.94
2	A	501	HEC	CMD-C2D-C3D	2.42	129.50	124.94
2	B	502	HEC	CMD-C2D-C3D	2.41	129.49	124.94
2	A	501	HEC	CMA-C3A-C2A	2.12	128.95	124.94
2	A	502	HEC	C4B-C3B-C2B	-2.06	104.13	106.35
2	B	501	HEC	C3C-C4C-NC	2.01	114.73	110.94

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

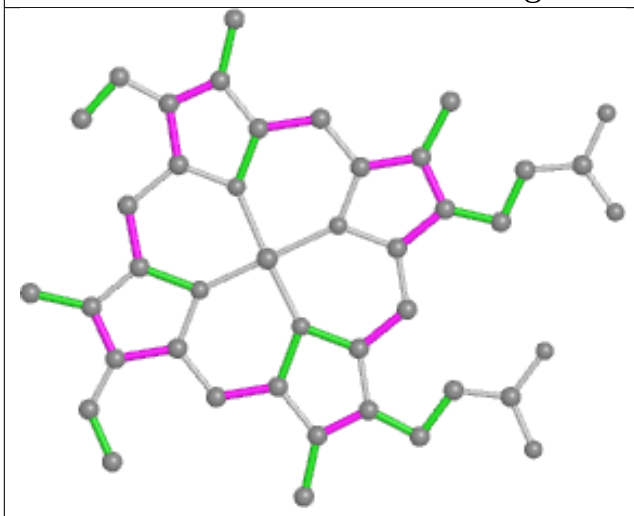
4 monomers are involved in 30 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	B	502	HEC	9	0
2	B	501	HEC	5	0
2	A	502	HEC	9	0
2	A	501	HEC	7	0

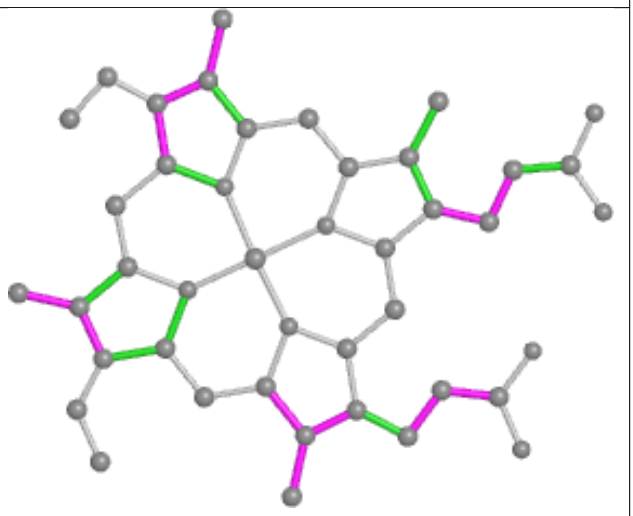
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In

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.

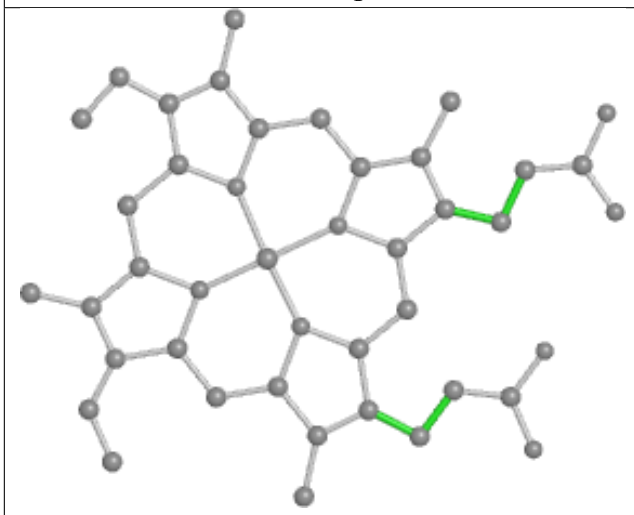
Ligand HEC B 502



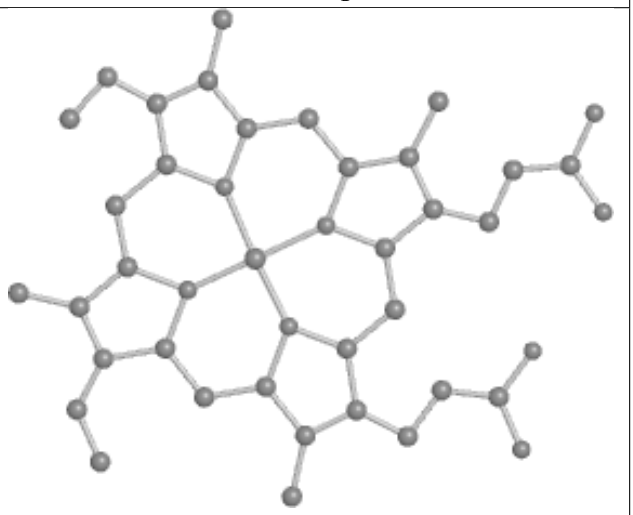
Bond lengths



Bond angles

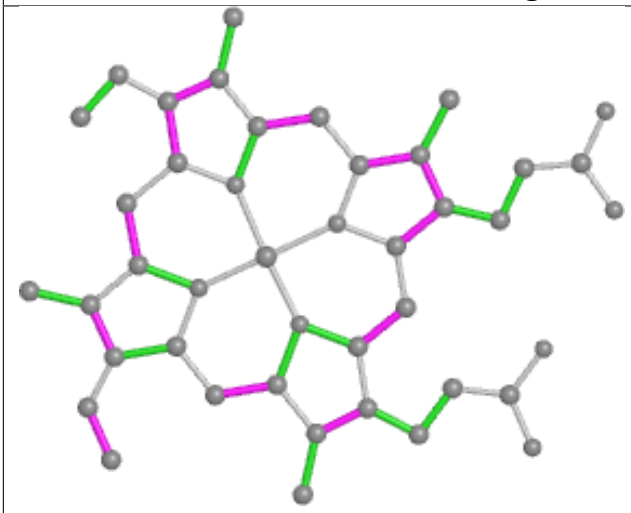


Torsions

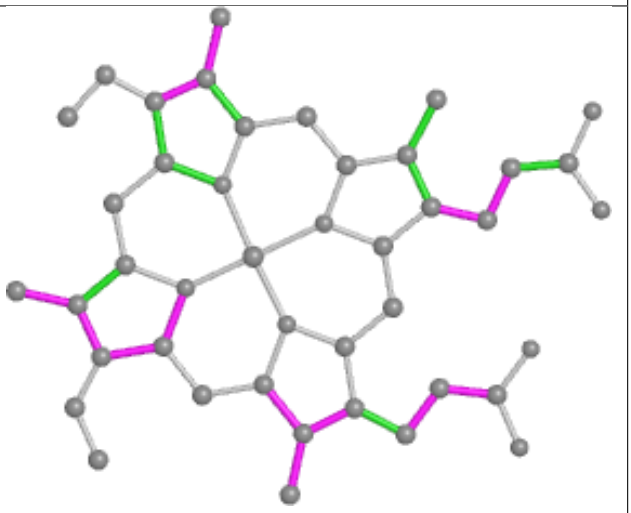


Rings

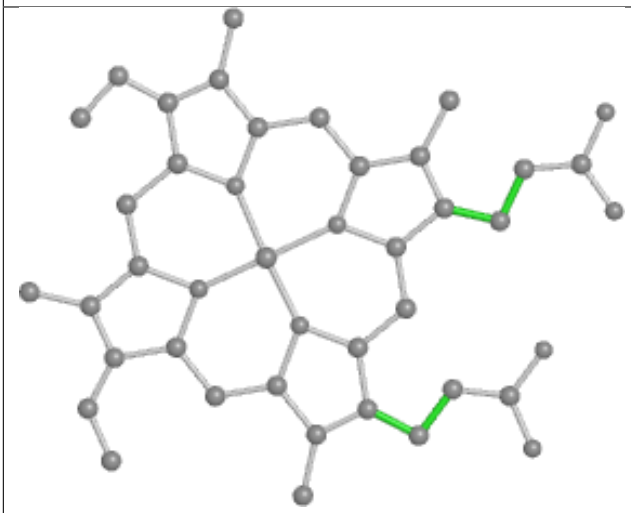
Ligand HEC B 501



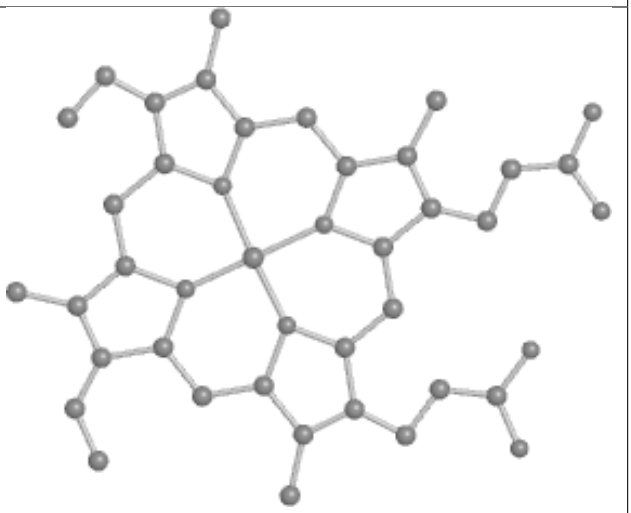
Bond lengths



Bond angles

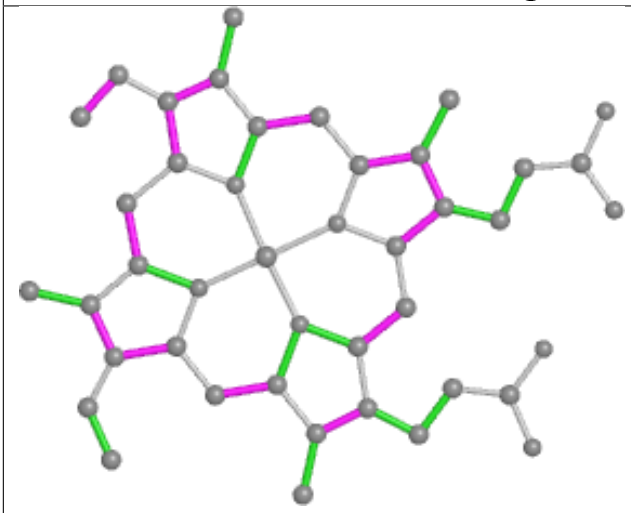


Torsions

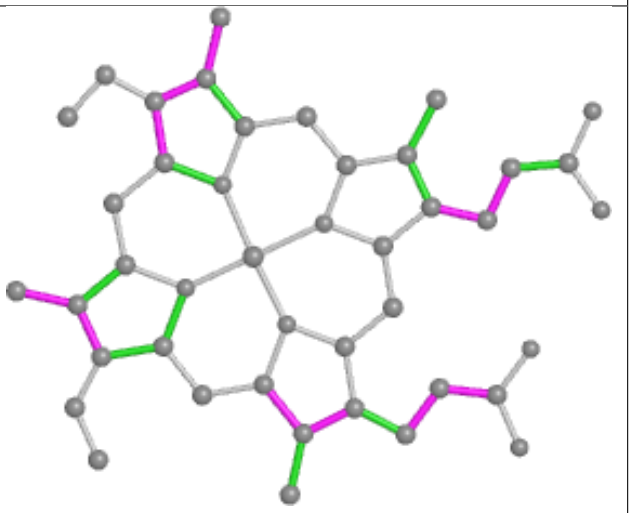


Rings

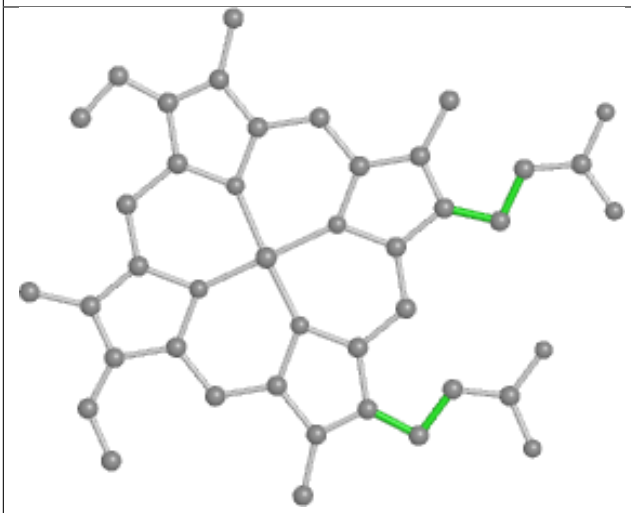
Ligand HEC A 502



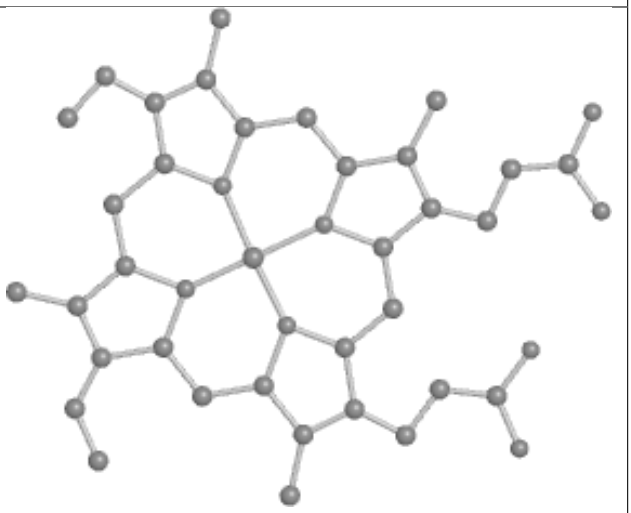
Bond lengths



Bond angles

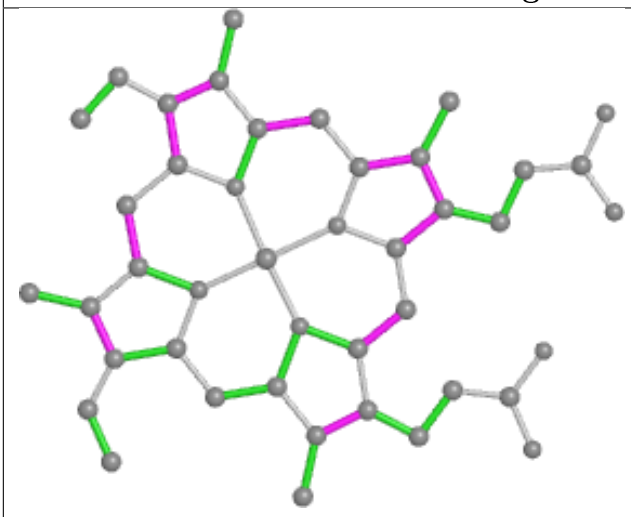


Torsions

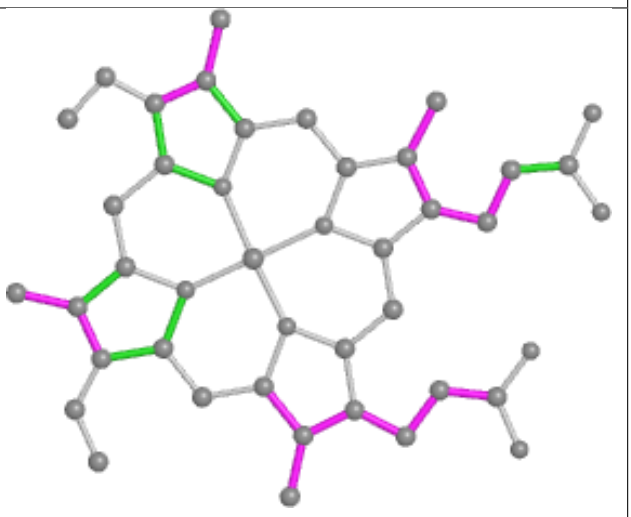


Rings

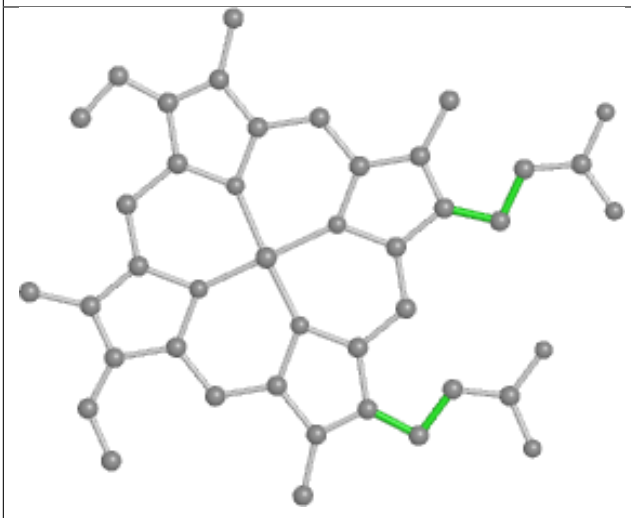
Ligand HEC A 501



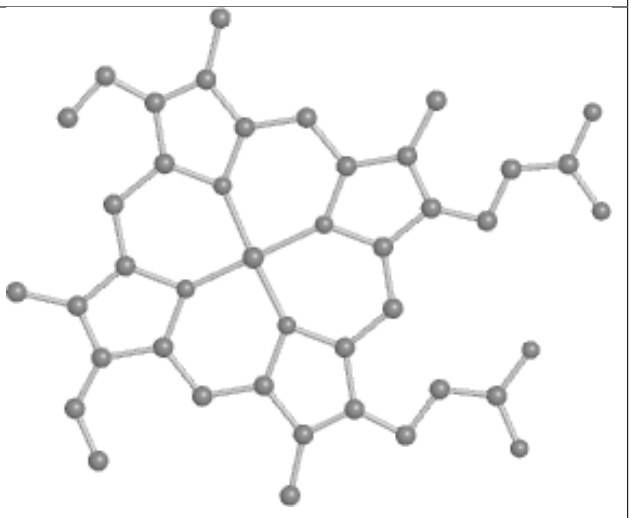
Bond lengths



Bond angles



Torsions



Rings

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	181/243 (74%)	0.39	8 (4%) 34 24	32, 47, 80, 93	0
1	B	178/243 (73%)	0.20	4 (2%) 62 52	32, 44, 76, 89	0
All	All	359/486 (73%)	0.29	12 (3%) 46 36	32, 46, 78, 93	0

All (12) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	124	THR	3.4
1	A	260	GLN	3.4
1	A	223	HIS	2.9
1	A	124	THR	2.9
1	B	82	PHE	2.6
1	A	182	SER	2.5
1	A	240	ALA	2.4
1	B	86	ASN	2.3
1	A	237	PRO	2.2
1	A	83	VAL	2.2
1	A	239	ARG	2.0
1	B	123	GLU	2.0

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

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

6.3 Carbohydrates

There are no carbohydrates in this entry.

6.4 Ligands

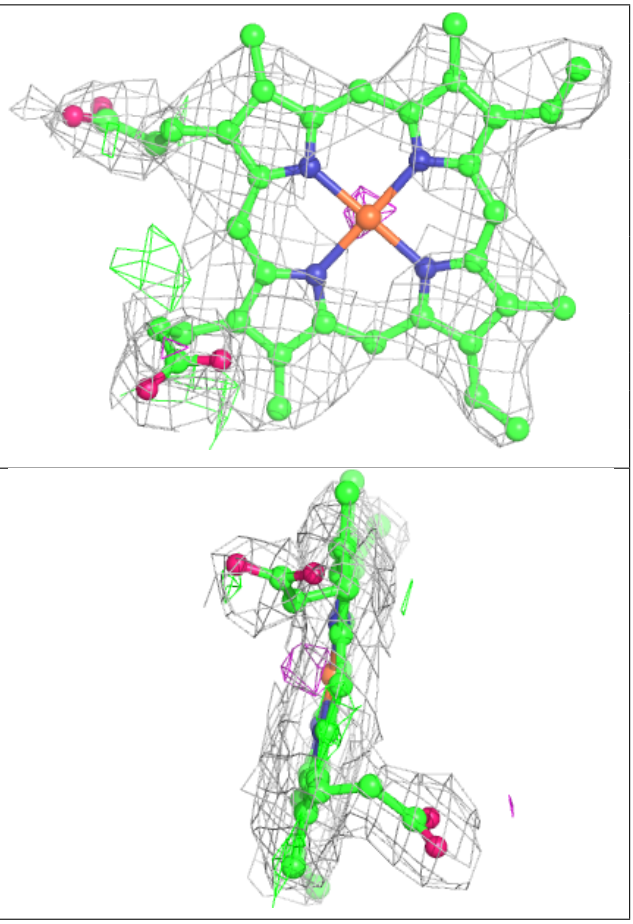
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95^{th} percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' 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
2	HEC	B	502	43/43	0.91	0.21	31,36,51,62	0
2	HEC	B	501	43/43	0.92	0.21	34,39,48,59	0
2	HEC	A	502	43/43	0.92	0.23	35,40,52,63	0
2	HEC	A	501	43/43	0.92	0.21	31,38,47,59	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.

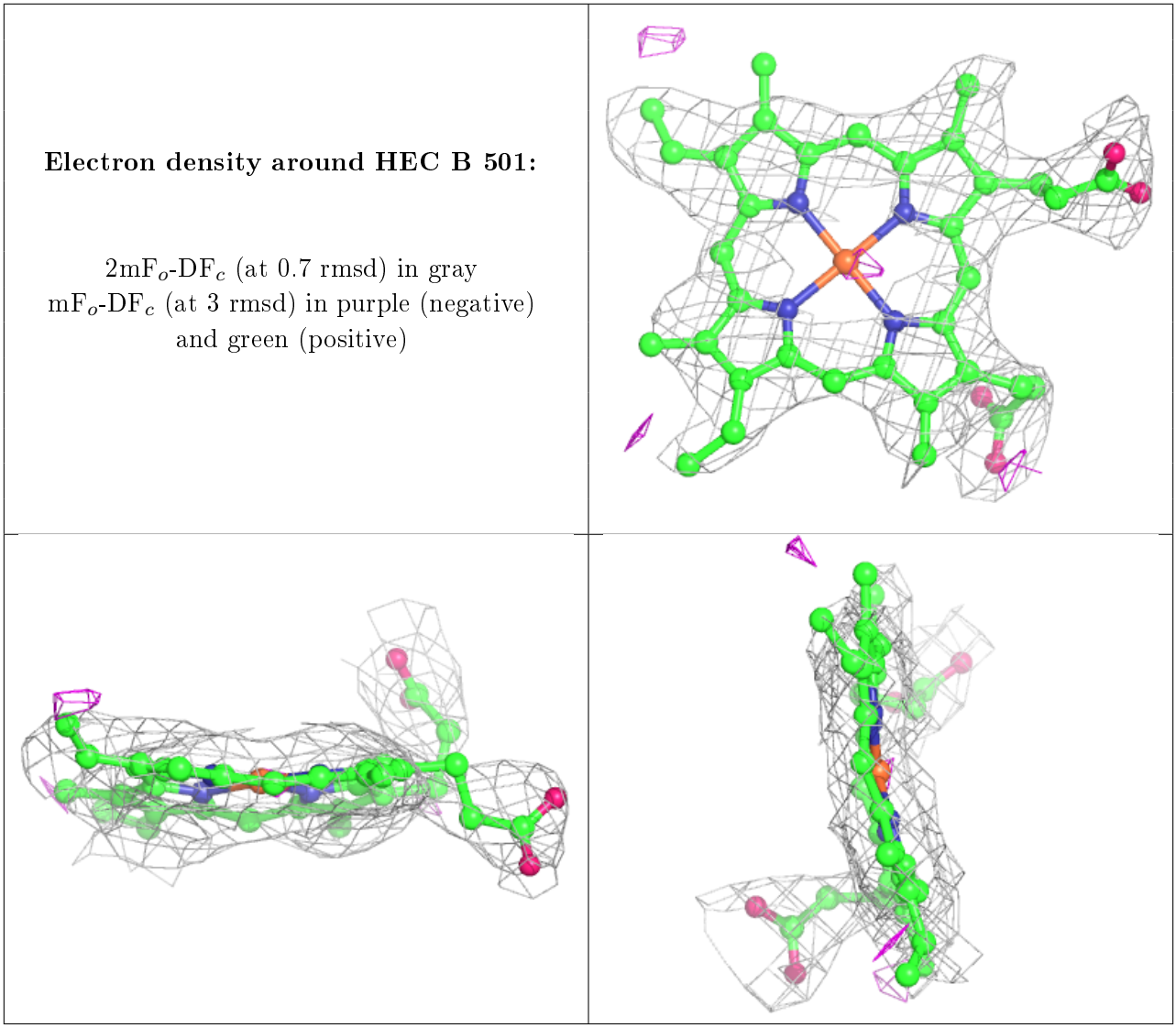
Electron density around HEC B 502:

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



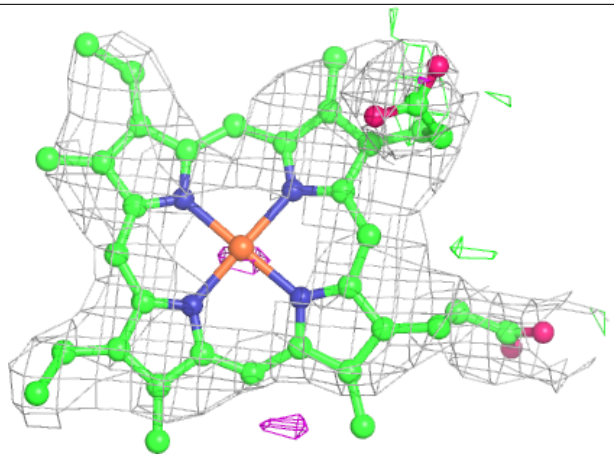
Electron density around HEC B 501:

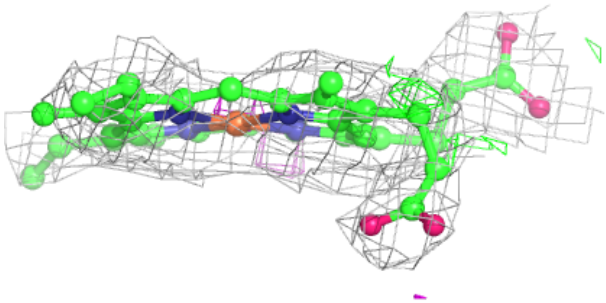
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

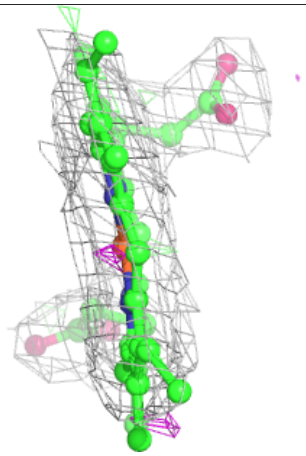


Electron density around HEC A 502:

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

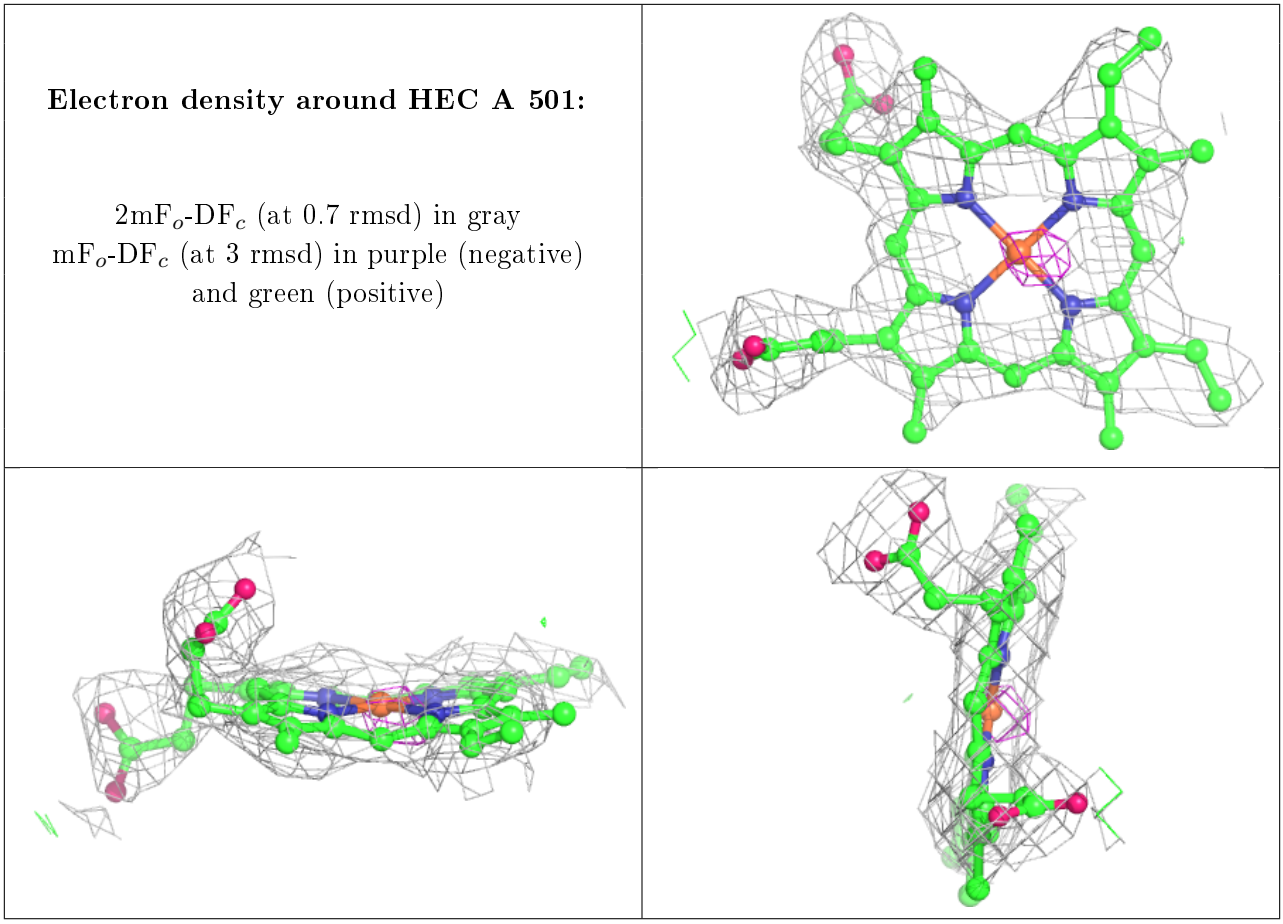






Electron density around HEC A 501:

$2mF_o$-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.