



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 9, 2026 – 10:11 AM UTC

PDB ID : 4JJ3 / pdb_00004jj3
Title : Crystal structure of MamP soaked with iron(II)
Authors : Siponen, M.; Pignol, D.; Arnoux, P.
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 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 : 4-5-2 with Phenix2.0
Mogul : 2022.3.0, CSD as543be (2022)
Xtriage (Phenix) : 2.0
EDS : 3.0
Buster-report : wwPDB partial adaption of 1.1.7 (2018)
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)
CCP4 : 9.0.010 (Gargrove)
Density-Fitness : 1.0.12
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.49

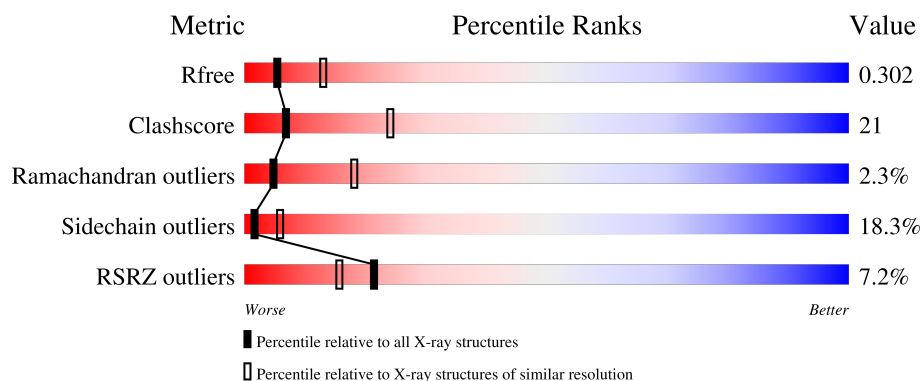
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.80 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}	180053	3866 (2.80-2.80)
Clashscore	190562	4276 (2.80-2.80)
Ramachandran outliers	187476	4196 (2.80-2.80)
Sidechain outliers	187428	4198 (2.80-2.80)
RSRZ outliers	180081	3869 (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 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 $\leq 5\%$. 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	5% 41% 26% 7% 26%
1	B	243	5% 44% 20% 9% 27%

2 Entry composition [i](#)

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 (CCD ID: HEC) (formula: $C_{34}H_{34}FeN_4O_4$).

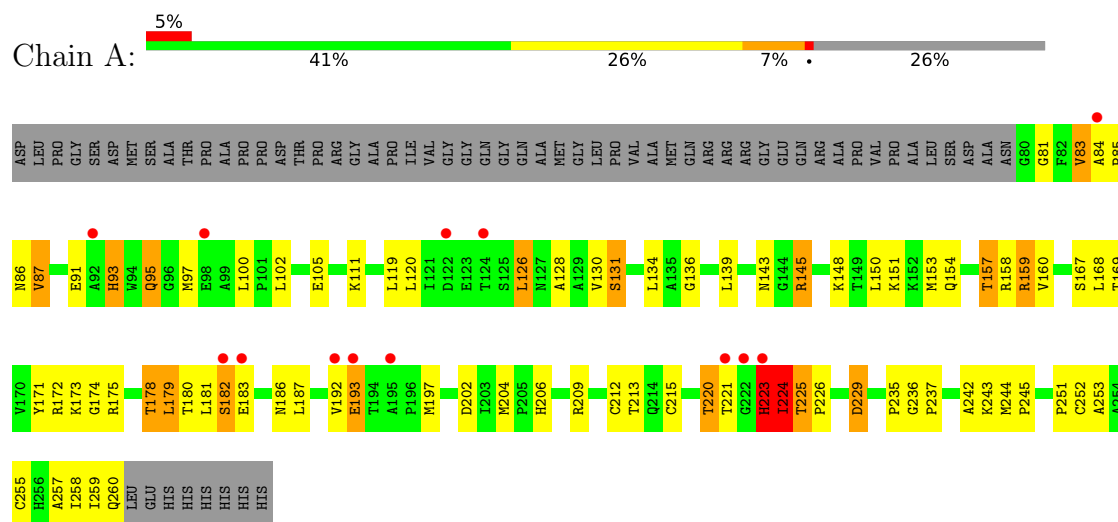


Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
2	A	1	Total	C	Fe	N	O	0	0
			43	34	1	4	4		
2	A	1	Total	C	Fe	N	O	0	0
			43	34	1	4	4		
2	B	1	Total	C	Fe	N	O	0	0
			43	34	1	4	4		
2	B	1	Total	C	Fe	N	O	0	0
			43	34	1	4	4		

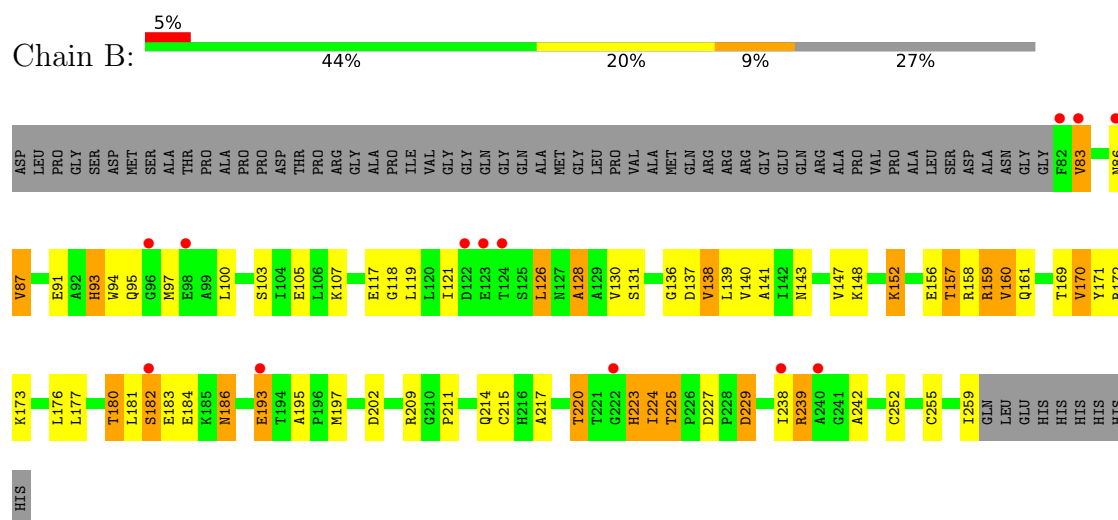
3 Residue-property plots

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: MamP



• Molecule 1: MamP



4 Data and refinement statistics

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 58.87 – 2.80	Depositor EDS
% Data completeness (in resolution range)	97.6 (58.87-2.80) 97.7 (58.87-2.80)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.01 (at 2.81Å)	Xtriage
Refinement program	REFMAC 5.6.0117	Depositor
R, R_{free}	0.264 , 0.298 0.268 , 0.302	Depositor DCC
R_{free} test set	508 reflections (5.34%)	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)	0.32 , 23.9	EDS
L-test for twinning ²	$\langle L \rangle = 0.48$, $\langle L^2 \rangle = 0.32$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.87	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.*

¹Intensities estimated from amplitudes.

²Theoretical values of $\langle |L| \rangle$, $\langle L^2 \rangle$ for acentric reflections are 0.5, 0.333 respectively for untwinned datasets, and 0.375, 0.2 for perfectly twinned datasets.

5 Model quality [i](#)

5.1 Standard geometry [i](#)

Bond lengths and bond angles in the following residue types are not validated in this section: 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	0.94	0/1397	1.12	6/1892 (0.3%)
1	B	1.00	0/1380	1.10	6/1870 (0.3%)
All	All	0.97	0/2777	1.11	12/3762 (0.3%)

There are no bond length outliers.

All (12) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	236	GLY	CA-C-N	8.51	130.48	119.84
1	A	236	GLY	C-N-CA	8.51	130.48	119.84
1	B	182	SER	N-CA-C	7.24	119.75	108.96
1	A	136	GLY	N-CA-C	-6.03	107.08	114.92
1	A	182	SER	N-CA-C	6.02	119.01	109.50
1	B	136	GLY	N-CA-C	-5.79	106.53	114.64
1	A	212	CYS	N-CA-C	5.70	117.58	111.36
1	B	128	ALA	N-CA-C	-5.44	105.00	111.69
1	B	157	THR	N-CA-C	-5.36	105.88	112.90
1	B	143	ASN	N-CA-C	-5.18	105.60	112.24
1	A	157	THR	N-CA-C	-5.04	105.88	112.23
1	B	118	GLY	N-CA-C	-5.02	103.25	110.38

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	1371	0	1431	59	1
1	B	1354	0	1418	62	1
2	A	86	0	64	13	0
2	B	86	0	64	11	0
All	All	2897	0	2977	121	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 21.

All (121) 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:HG3	1:A:145:ARG:NH1	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:HD22	1:B:186:ASN:N	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:A:225:THR:HA	1:A:226:PRO:C	2.24	0.63
1:A:255:CYS:HG	2:A:502:HEC:CAC	2.12	0.62
1:A:237:PRO:HA	1:A:257:ALA:O	2.00	0.61
1:A:81:GLY:HA2	1:A:197:MET:HE1	1.82	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
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: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:197:MET:HE1	1:B:220:THR:HA	1.87	0.57
1:B:121:ILE:HD11	1:B:139:LEU:HB2	1.86	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:CG	1:A:145:ARG:NH1	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:O	1:A:224:ILE:CG2	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:B:197:MET:HE1	1:B:220:THR:CA	2.37	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
1:A:221:THR:C	1:A:223:HIS:N	2.65	0.54
1:B:91:GLU:HG2	1:B:193:GLU:HB3	1.90	0.54
1:B:137:ASP:CG	1:B:172:ARG:HH11	2.16	0.53
1:B:197:MET:HG2	1:B:217:ALA:O	2.09	0.53
1:A:167:SER:C	1:A:168:LEU:HD23	2.34	0.53
1:A:204:MET:HG2	1:A:206:HIS:O	2.08	0.53
1:B:148:LYS:H	1:B:152:LYS:HZ2	1.55	0.53
1:A:243:LYS:O	1:A:245:PRO:HD3	2.10	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:229:ASP:N	1:A:229:ASP:OD1	2.42	0.52
1:B:223:HIS:O	1:B:224:ILE:C	2.53	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:HG23	1:B:147:VAL:O	2.10	0.50
1:B:224:ILE:O	1:B:224:ILE:CG2	2.58	0.50
1:A:251:PRO:C	1:A:253:ALA:H	2.20	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: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:171:TYR:CD2	1:B:171:TYR:C	2.90	0.49
1:B:197:MET:HG3	1:B:217:ALA:HB3	1.93	0.49
1:A:160:VAL:O	1:A:160:VAL:HG23	2.13	0.49
1:B:160:VAL:O	1:B:160:VAL:HG23	2.12	0.49
1:A:134:LEU:HD12	1:A:172:ARG:CZ	2.44	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:A:221:THR:C	1:A:223:HIS:H	2.21	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:B:197:MET:HE2	1:B:197:MET:HB3	1.62	0.46
1:A:91:GLU:HG2	1:A:193:GLU:HB3	1.98	0.46
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:259:ILE:O	1:B:259:ILE:HG22	2.18	0.44
1:A:159:ARG:CZ	1:A:159:ARG:HB3	2.46	0.44
1:A:259:ILE:O	1:A:260:GLN:HB2	2.17	0.44
1:B:239:ARG:O	1:B:242:ALA:HB2	2.17	0.44
1:A:251:PRO:C	1:A:253:ALA:N	2.76	0.44
1:A:105:GLU:OE1	1:A:209:ARG:NE	2.52	0.43
1:B:259:ILE:O	1:B:259:ILE:CG2	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:93:HIS:ND1	1:B:93:HIS:N	2.68	0.41
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:ND1	1:A:93:HIS:N	2.69	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	11
1	B	176/243 (72%)	158 (90%)	16 (9%)	2 (1%)	11	36
All	All	355/486 (73%)	315 (89%)	32 (9%)	8 (2%)	5	18

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
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%)	118 (80%)	30 (20%)	1	4
1	B	147/195 (75%)	123 (84%)	24 (16%)	2	8
All	All	295/390 (76%)	241 (82%)	54 (18%)	2	6

All (54) 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	126	LEU
1	A	130	VAL
1	A	131	SER
1	A	145	ARG
1	A	148	LYS
1	A	151	LYS
1	A	153	MET
1	A	159	ARG
1	A	169	THR
1	A	173	LYS
1	A	175	ARG

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Mol	Chain	Res	Type
1	A	178	THR
1	A	179	LEU
1	A	182	SER
1	A	183	GLU
1	A	192	VAL
1	A	193	GLU
1	A	202	ASP
1	A	220	THR
1	A	223	HIS
1	A	224	ILE
1	A	225	THR
1	A	229	ASP
1	A	244	MET
1	A	258	ILE
1	B	83	VAL
1	B	86	ASN
1	B	87	VAL
1	B	93	HIS
1	B	100	LEU
1	B	126	LEU
1	B	138	VAL
1	B	140	VAL
1	B	152	LYS
1	B	159	ARG
1	B	160	VAL
1	B	170	VAL
1	B	173	LYS
1	B	176	LEU
1	B	180	THR
1	B	182	SER
1	B	184	GLU
1	B	186	ASN
1	B	193	GLU
1	B	202	ASP
1	B	220	THR
1	B	223	HIS
1	B	225	THR
1	B	239	ARG

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (4) such sidechains are listed below:

Mol	Chain	Res	Type
1	B	86	ASN
1	B	127	ASN
1	B	161	GLN
1	B	186	ASN

5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

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	A	501	1	46,50,50	2.71	23 (50%)	58,82,82	2.16	23 (39%)
2	HEC	B	502	1	46,50,50	2.74	24 (52%)	58,82,82	2.13	23 (39%)
2	HEC	B	501	1	46,50,50	2.77	25 (54%)	58,82,82	2.13	21 (36%)
2	HEC	A	502	1	46,50,50	2.80	25 (54%)	58,82,82	2.26	22 (37%)

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	A	501	1	-	4/14/54/54	-
2	HEC	B	502	1	-	8/14/54/54	-
2	HEC	B	501	1	-	8/14/54/54	-
2	HEC	A	502	1	-	9/14/54/54	-

All (97) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	502	HEC	CHD-C4C	6.21	1.50	1.38
2	A	501	HEC	CHC-C4B	5.89	1.49	1.38
2	A	502	HEC	C2A-C3A	5.64	1.48	1.36
2	B	501	HEC	CHA-C1A	5.61	1.49	1.38
2	B	501	HEC	C2A-C3A	5.37	1.48	1.36
2	A	501	HEC	C2A-C3A	5.34	1.48	1.36
2	B	502	HEC	CHD-C4C	5.30	1.48	1.38
2	A	501	HEC	CHA-C1A	5.24	1.48	1.38
2	B	502	HEC	C2A-C3A	5.19	1.48	1.36
2	A	502	HEC	CHB-C4A	5.16	1.48	1.38
2	B	502	HEC	CHA-C1A	5.15	1.48	1.38
2	B	502	HEC	CAB-C3B	5.11	1.51	1.35
2	B	501	HEC	CHC-C4B	5.04	1.48	1.38
2	B	502	HEC	CHB-C4A	4.85	1.47	1.38
2	A	502	HEC	CAB-C3B	4.81	1.50	1.35
2	B	502	HEC	CHC-C4B	4.79	1.47	1.38
2	A	502	HEC	CHA-C1A	4.78	1.47	1.38
2	A	502	HEC	CHC-C4B	4.71	1.47	1.38
2	B	501	HEC	CHB-C4A	4.65	1.47	1.38
2	B	501	HEC	CAC-C3C	4.61	1.50	1.35
2	A	501	HEC	CHC-C1C	4.52	1.49	1.39
2	B	502	HEC	CAC-C3C	4.45	1.49	1.35
2	A	501	HEC	CAC-C3C	4.35	1.49	1.35
2	A	501	HEC	CHB-C4A	4.31	1.46	1.38
2	A	502	HEC	CAC-C3C	4.27	1.48	1.35
2	A	501	HEC	CHD-C4C	4.21	1.46	1.38
2	B	501	HEC	CHD-C4C	4.10	1.46	1.38
2	B	501	HEC	CHA-C4D	4.04	1.48	1.39
2	A	501	HEC	CHB-C1B	4.01	1.48	1.39
2	B	501	HEC	CHB-C1B	4.01	1.48	1.39
2	A	502	HEC	CHD-C1D	3.87	1.48	1.39
2	A	501	HEC	CAB-C3B	3.87	1.47	1.35
2	B	501	HEC	CAB-C3B	3.85	1.47	1.35
2	B	501	HEC	CHC-C1C	3.76	1.47	1.39

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	502	HEC	C3D-C2D	3.75	1.48	1.38
2	A	502	HEC	CHB-C1B	3.72	1.47	1.39
2	B	502	HEC	CHB-C1B	3.72	1.47	1.39
2	B	502	HEC	CHC-C1C	3.62	1.47	1.39
2	A	502	HEC	CHC-C1C	3.59	1.47	1.39
2	B	502	HEC	CHD-C1D	3.57	1.47	1.39
2	A	502	HEC	CHA-C4D	3.52	1.47	1.39
2	B	501	HEC	C4D-C3D	3.51	1.51	1.44
2	A	501	HEC	CHA-C4D	3.49	1.47	1.39
2	B	502	HEC	CHA-C4D	3.47	1.47	1.39
2	B	501	HEC	C4C-NC	-3.43	1.33	1.39
2	A	501	HEC	C4D-C3D	3.28	1.51	1.44
2	A	501	HEC	C4C-NC	-3.23	1.33	1.39
2	B	501	HEC	CHD-C1D	3.21	1.46	1.39
2	B	502	HEC	C4D-C3D	3.19	1.51	1.44
2	A	502	HEC	C4A-C3A	3.16	1.51	1.45
2	A	502	HEC	C4B-NB	-3.12	1.33	1.39
2	B	501	HEC	C4B-NB	-3.11	1.33	1.39
2	B	501	HEC	C3D-C2D	3.09	1.47	1.38
2	B	502	HEC	C1B-NB	-3.02	1.33	1.39
2	A	501	HEC	CHD-C1D	3.01	1.46	1.39
2	A	501	HEC	C1D-ND	-3.01	1.33	1.39
2	B	501	HEC	C1A-NA	-2.92	1.34	1.39
2	B	501	HEC	C1C-NC	-2.91	1.34	1.39
2	A	502	HEC	C3D-C2D	2.87	1.46	1.38
2	A	501	HEC	C1C-C2C	2.85	1.49	1.43
2	B	501	HEC	C1D-ND	-2.80	1.34	1.39
2	B	502	HEC	C4B-NB	-2.78	1.34	1.39
2	A	501	HEC	C3D-C2D	2.75	1.46	1.38
2	A	502	HEC	C4D-C3D	2.74	1.50	1.44
2	A	501	HEC	C4A-NA	-2.74	1.34	1.39
2	A	502	HEC	C1B-NB	-2.70	1.34	1.39
2	A	502	HEC	C1D-C2D	2.68	1.49	1.43
2	A	501	HEC	C1A-NA	-2.67	1.34	1.39
2	B	502	HEC	C4A-C3A	2.67	1.50	1.45
2	B	501	HEC	C4D-ND	-2.63	1.34	1.39
2	A	502	HEC	C1C-C2C	2.62	1.49	1.43
2	B	502	HEC	C1C-C2C	2.60	1.49	1.43
2	A	502	HEC	CBB-CAB	2.60	1.59	1.49
2	B	502	HEC	C1D-C2D	2.59	1.49	1.43
2	B	501	HEC	C1A-C2A	2.59	1.49	1.45
2	A	502	HEC	C4A-NA	-2.58	1.34	1.39

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	502	HEC	C1C-NC	-2.55	1.34	1.39
2	B	501	HEC	C1B-C2B	2.55	1.49	1.43
2	B	502	HEC	C1A-C2A	2.53	1.49	1.45
2	A	501	HEC	C1D-C2D	2.50	1.49	1.43
2	A	501	HEC	C1B-C2B	2.44	1.48	1.43
2	B	502	HEC	C4C-NC	-2.40	1.35	1.39
2	A	502	HEC	C4C-NC	-2.36	1.35	1.39
2	A	502	HEC	C1D-ND	-2.35	1.35	1.39
2	B	501	HEC	C1D-C2D	2.35	1.48	1.43
2	A	502	HEC	C1B-C2B	2.32	1.48	1.43
2	B	502	HEC	C4A-NA	-2.29	1.35	1.39
2	B	502	HEC	C1B-C2B	2.29	1.48	1.43
2	B	501	HEC	C1C-C2C	2.27	1.48	1.43
2	A	501	HEC	C1A-C2A	2.26	1.49	1.45
2	B	501	HEC	C4A-NA	-2.25	1.35	1.39
2	A	502	HEC	C3B-C2B	2.25	1.48	1.41
2	A	501	HEC	C4D-ND	-2.23	1.35	1.39
2	B	501	HEC	CBC-CAC	2.16	1.57	1.49
2	B	502	HEC	C3B-C2B	2.13	1.48	1.41
2	A	501	HEC	CBD-CGD	2.07	1.55	1.50
2	B	502	HEC	CBD-CGD	2.05	1.55	1.50

All (89) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	A	502	HEC	C2A-C1A-NA	5.70	115.82	110.32
2	A	501	HEC	C3D-C4D-ND	5.56	116.32	110.15
2	A	502	HEC	C3D-C4D-ND	5.43	116.18	110.15
2	B	502	HEC	C3D-C4D-ND	5.35	116.09	110.15
2	A	501	HEC	CBA-CAA-C2A	-4.94	98.88	112.53
2	A	501	HEC	C2D-C1D-ND	4.76	117.77	110.14
2	B	501	HEC	C3D-C4D-ND	4.54	115.18	110.15
2	A	502	HEC	CHB-C4A-NA	-4.49	119.57	124.45
2	B	501	HEC	C2D-C1D-ND	4.35	117.11	110.14
2	B	502	HEC	C2A-C1A-NA	4.25	114.42	110.32
2	B	501	HEC	C1D-C2D-C3D	-4.13	102.09	106.82
2	B	502	HEC	C2C-C1C-NC	4.05	116.63	110.14
2	A	501	HEC	C1D-C2D-C3D	-4.00	102.24	106.82
2	B	501	HEC	C4A-C3A-C2A	-3.90	101.19	106.97
2	A	502	HEC	CBC-CAC-C3C	-3.85	119.73	127.43
2	B	502	HEC	C2D-C1D-ND	3.82	116.27	110.14
2	B	501	HEC	CBA-CAA-C2A	-3.78	102.07	112.53

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	A	502	HEC	CAD-C3D-C4D	3.62	132.00	124.94
2	A	502	HEC	C2C-C1C-NC	3.56	115.85	110.14
2	A	502	HEC	C2D-C1D-ND	3.54	115.81	110.14
2	B	502	HEC	C4D-C3D-C2D	-3.52	101.42	106.87
2	A	502	HEC	CMD-C2D-C1D	3.45	130.67	125.42
2	B	501	HEC	CBB-CAB-C3B	-3.44	120.57	127.43
2	A	502	HEC	C1A-C2A-C3A	-3.43	102.59	107.11
2	B	501	HEC	C2B-C1B-NB	3.41	115.60	110.14
2	A	502	HEC	C4D-C3D-C2D	-3.35	101.68	106.87
2	A	501	HEC	C4A-C3A-C2A	-3.30	102.08	106.97
2	B	501	HEC	CMA-C3A-C4A	3.25	130.46	124.73
2	B	502	HEC	CAD-C3D-C4D	3.24	131.26	124.94
2	B	502	HEC	CBA-CAA-C2A	-3.22	103.63	112.53
2	A	501	HEC	C2A-C1A-NA	3.22	113.43	110.32
2	A	501	HEC	C4D-C3D-C2D	-3.20	101.91	106.87
2	B	502	HEC	C2B-C1B-NB	3.19	115.25	110.14
2	A	501	HEC	C2B-C1B-NB	3.14	115.18	110.14
2	B	501	HEC	C3A-C4A-NA	3.14	115.44	109.64
2	B	501	HEC	C2C-C1C-NC	3.13	115.16	110.14
2	B	502	HEC	C3A-C4A-NA	3.05	115.27	109.64
2	B	502	HEC	C4A-C3A-C2A	-3.03	102.48	106.97
2	B	501	HEC	C2A-C1A-NA	2.96	113.18	110.32
2	B	502	HEC	CHB-C4A-NA	-2.96	121.23	124.45
2	A	502	HEC	CHA-C1A-C2A	-2.91	120.28	124.86
2	A	501	HEC	C3A-C4A-NA	2.88	114.96	109.64
2	A	502	HEC	C4A-C3A-C2A	-2.87	102.71	106.97
2	B	501	HEC	C4D-C3D-C2D	-2.87	102.43	106.87
2	A	502	HEC	C3A-C4A-NA	2.82	114.85	109.64
2	B	502	HEC	CMA-C3A-C4A	2.79	129.65	124.73
2	B	501	HEC	O2D-CGD-CBD	2.79	122.82	114.00
2	B	502	HEC	C1A-C2A-C3A	-2.78	103.44	107.11
2	A	502	HEC	CMA-C3A-C4A	2.77	129.61	124.73
2	B	502	HEC	C1D-C2D-C3D	-2.76	103.65	106.82
2	A	501	HEC	CBD-CAD-C3D	-2.71	105.05	112.53
2	B	501	HEC	CHA-C4D-ND	-2.68	119.00	123.86
2	A	501	HEC	O2D-CGD-O1D	-2.63	116.56	123.33
2	A	501	HEC	C1A-C2A-C3A	-2.62	103.66	107.11
2	A	502	HEC	C1D-C2D-C3D	-2.57	103.87	106.82
2	B	501	HEC	O2D-CGD-O1D	-2.57	116.73	123.33
2	A	502	HEC	O1A-CGA-CBA	-2.54	115.05	123.09
2	B	501	HEC	CAD-CBD-CGD	2.53	120.37	113.67
2	A	501	HEC	C4D-ND-C1D	-2.51	101.72	105.82

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	A	502	HEC	C2B-C1B-NB	2.50	114.16	110.14
2	A	502	HEC	CBA-CAA-C2A	-2.50	105.63	112.53
2	A	502	HEC	O2A-CGA-CBA	2.48	121.83	114.00
2	A	501	HEC	O2D-CGD-CBD	2.46	121.77	114.00
2	A	501	HEC	CMA-C3A-C4A	2.40	128.96	124.73
2	B	502	HEC	CAD-CBD-CGD	2.40	120.03	113.67
2	A	502	HEC	CMC-C2C-C1C	2.38	129.04	125.42
2	B	502	HEC	O1A-CGA-CBA	-2.35	115.64	123.09
2	A	501	HEC	CHA-C4D-ND	-2.33	119.64	123.86
2	A	501	HEC	CHD-C4C-C3C	-2.33	121.29	125.21
2	A	501	HEC	CHD-C1D-ND	-2.32	119.65	123.86
2	A	501	HEC	CMC-C2C-C1C	2.30	128.92	125.42
2	B	501	HEC	CAD-C3D-C4D	2.28	129.39	124.94
2	A	501	HEC	CBB-CAB-C3B	-2.28	122.88	127.43
2	B	501	HEC	CHB-C4A-NA	-2.26	121.99	124.45
2	B	501	HEC	CMD-C2D-C3D	2.24	130.37	125.62
2	A	502	HEC	O2D-CGD-CBD	2.22	121.01	114.00
2	B	502	HEC	CMB-C2B-C3B	2.22	131.77	126.55
2	A	501	HEC	CAD-C3D-C4D	2.20	129.23	124.94
2	B	502	HEC	CMC-C2C-C1C	2.18	128.74	125.42
2	B	502	HEC	CHD-C1D-C2D	-2.14	121.21	127.43
2	B	501	HEC	CMB-C2B-C3B	2.14	131.57	126.55
2	B	502	HEC	CHA-C1A-C2A	-2.09	121.56	124.86
2	B	502	HEC	CBC-CAC-C3C	-2.08	123.27	127.43
2	B	502	HEC	O2A-CGA-CBA	2.08	120.56	114.00
2	A	502	HEC	C4D-ND-C1D	-2.06	102.46	105.82
2	B	501	HEC	CMB-C2B-C1B	2.06	128.55	125.42
2	B	502	HEC	O2D-CGD-O1D	-2.03	118.10	123.33
2	A	501	HEC	C2C-C1C-NC	2.03	113.40	110.14
2	A	501	HEC	CBC-CAC-C3C	-2.01	123.42	127.43

There are no chirality outliers.

All (29) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	A	501	HEC	C2C-C3C-CAC-CBC
2	A	501	HEC	C4C-C3C-CAC-CBC
2	A	502	HEC	C2B-C3B-CAB-CBB
2	A	502	HEC	C4B-C3B-CAB-CBB
2	A	502	HEC	C2C-C3C-CAC-CBC
2	A	502	HEC	C4C-C3C-CAC-CBC
2	B	501	HEC	C2B-C3B-CAB-CBB

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Mol	Chain	Res	Type	Atoms
2	B	501	HEC	C4B-C3B-CAB-CBB
2	B	501	HEC	C2C-C3C-CAC-CBC
2	B	501	HEC	C4C-C3C-CAC-CBC
2	B	502	HEC	C2B-C3B-CAB-CBB
2	B	502	HEC	C4B-C3B-CAB-CBB
2	B	502	HEC	C2C-C3C-CAC-CBC
2	B	502	HEC	C4C-C3C-CAC-CBC
2	A	502	HEC	C2A-CAA-CBA-CGA
2	A	501	HEC	CAD-CBD-CGD-O1D
2	A	502	HEC	CAD-CBD-CGD-O1D
2	B	501	HEC	CAD-CBD-CGD-O1D
2	B	501	HEC	CAA-CBA-CGA-O1A
2	A	502	HEC	CAD-CBD-CGD-O2D
2	B	501	HEC	CAA-CBA-CGA-O2A
2	A	501	HEC	CAD-CBD-CGD-O2D
2	B	501	HEC	CAD-CBD-CGD-O2D
2	B	502	HEC	CAD-CBD-CGD-O2D
2	B	502	HEC	CAD-CBD-CGD-O1D
2	A	502	HEC	CAA-CBA-CGA-O1A
2	B	502	HEC	C2A-CAA-CBA-CGA
2	B	502	HEC	CAA-CBA-CGA-O1A
2	A	502	HEC	CAA-CBA-CGA-O2A

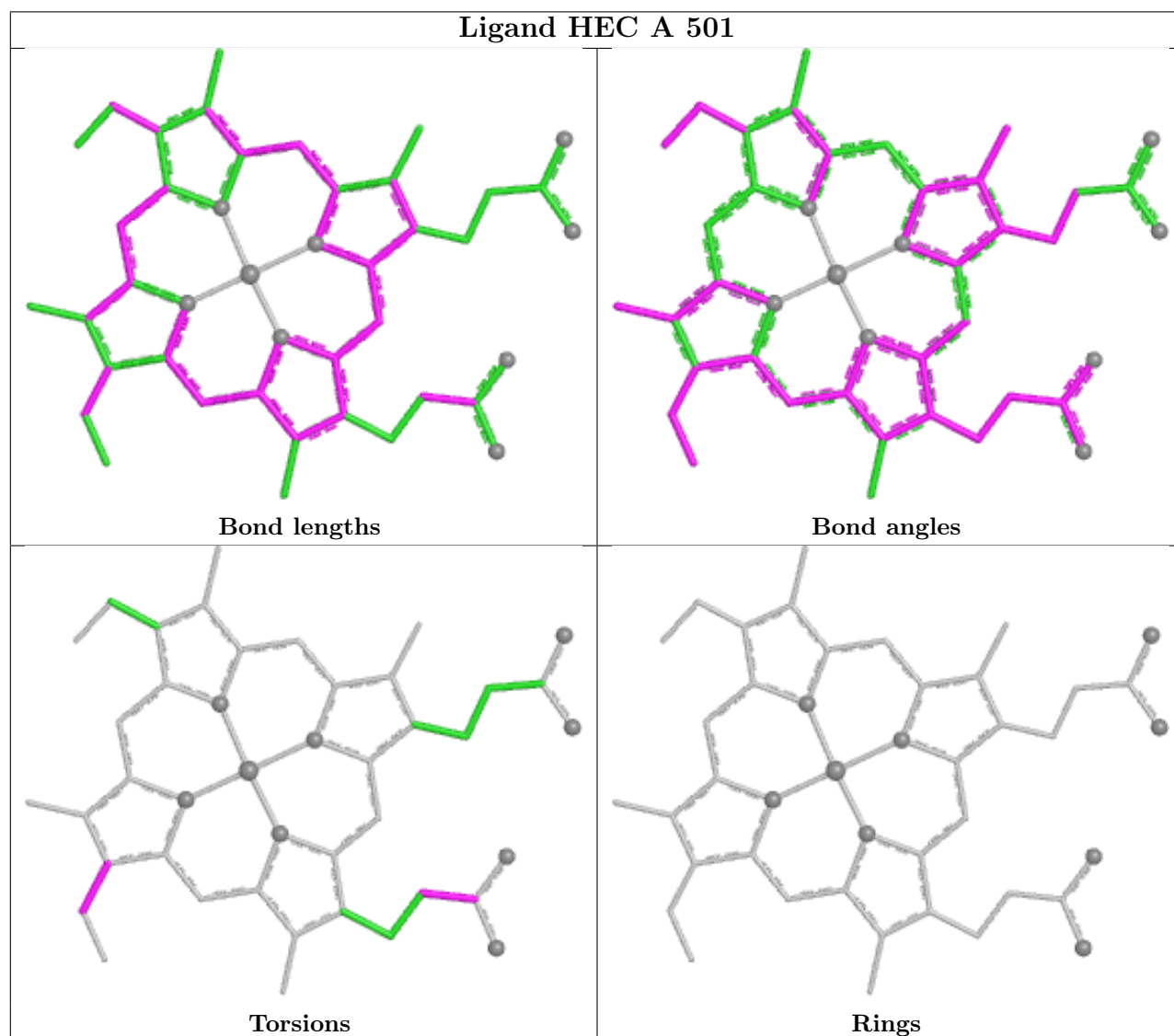
There are no ring outliers.

4 monomers are involved in 24 short contacts:

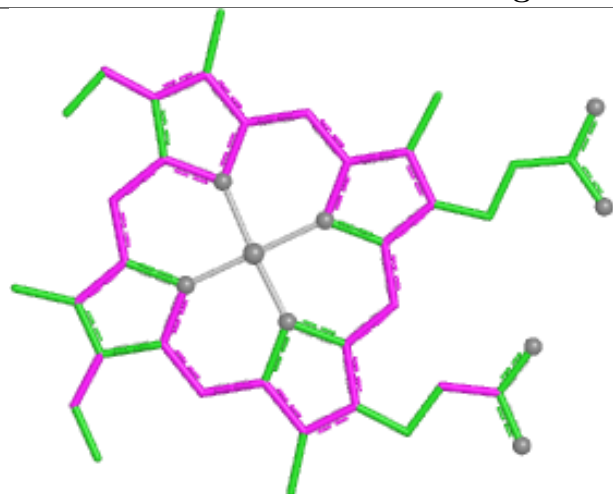
Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	A	501	HEC	6	0
2	B	502	HEC	7	0
2	B	501	HEC	4	0
2	A	502	HEC	7	0

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 than 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.

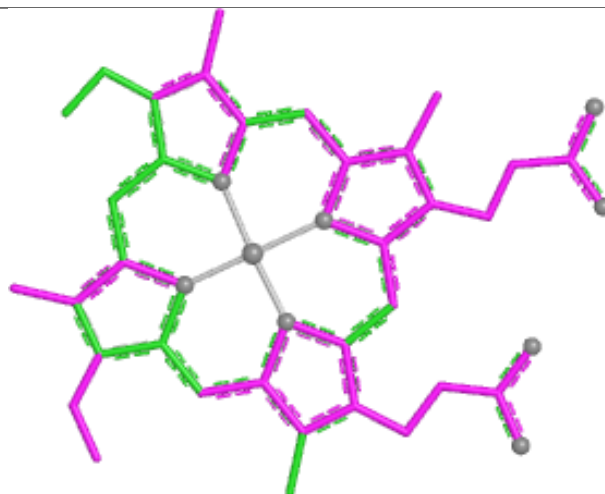
The outliers are highlighted in purple. The color gray indicates Mogul did not find sufficient equivalents in the CSD to analyse the geometry.



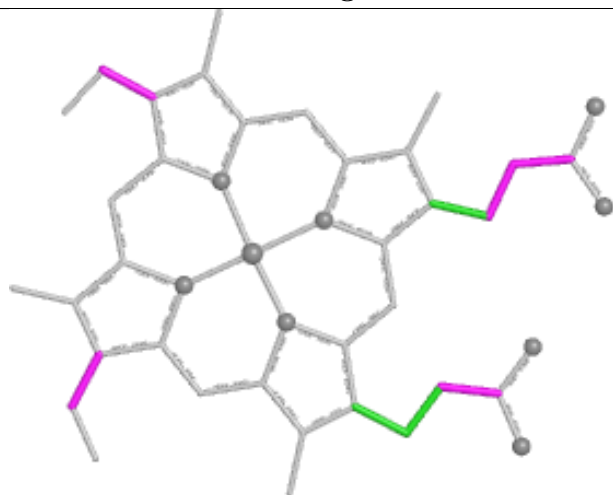
Ligand HEC B 502



Bond lengths



Bond angles

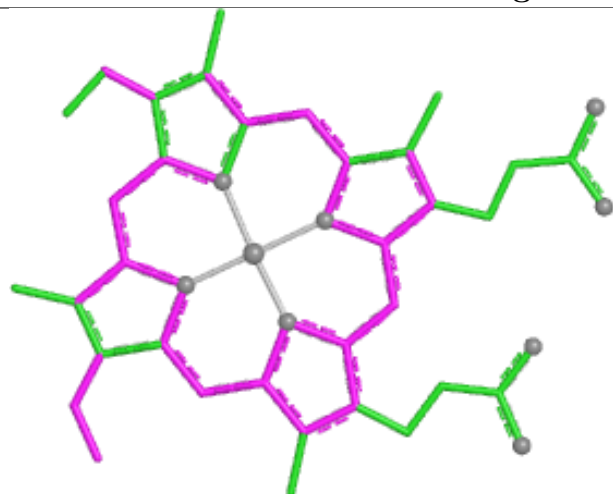


Torsions

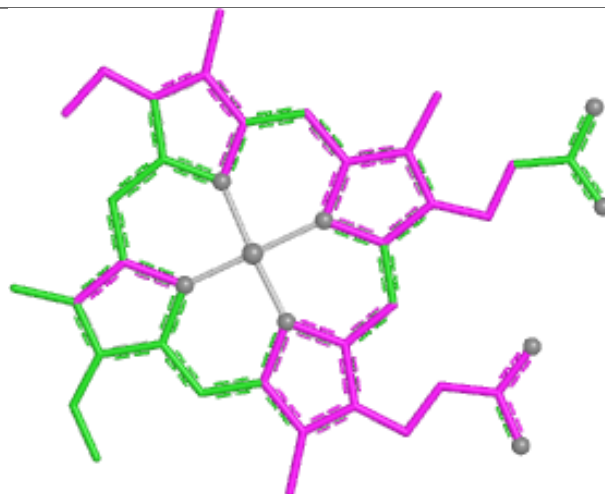


Rings

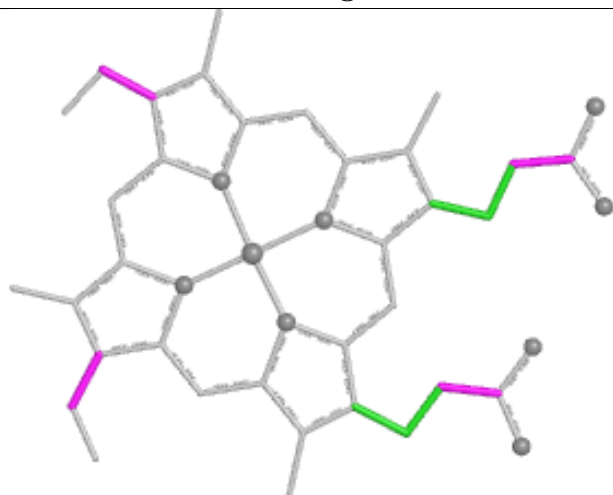
Ligand HEC B 501



Bond lengths



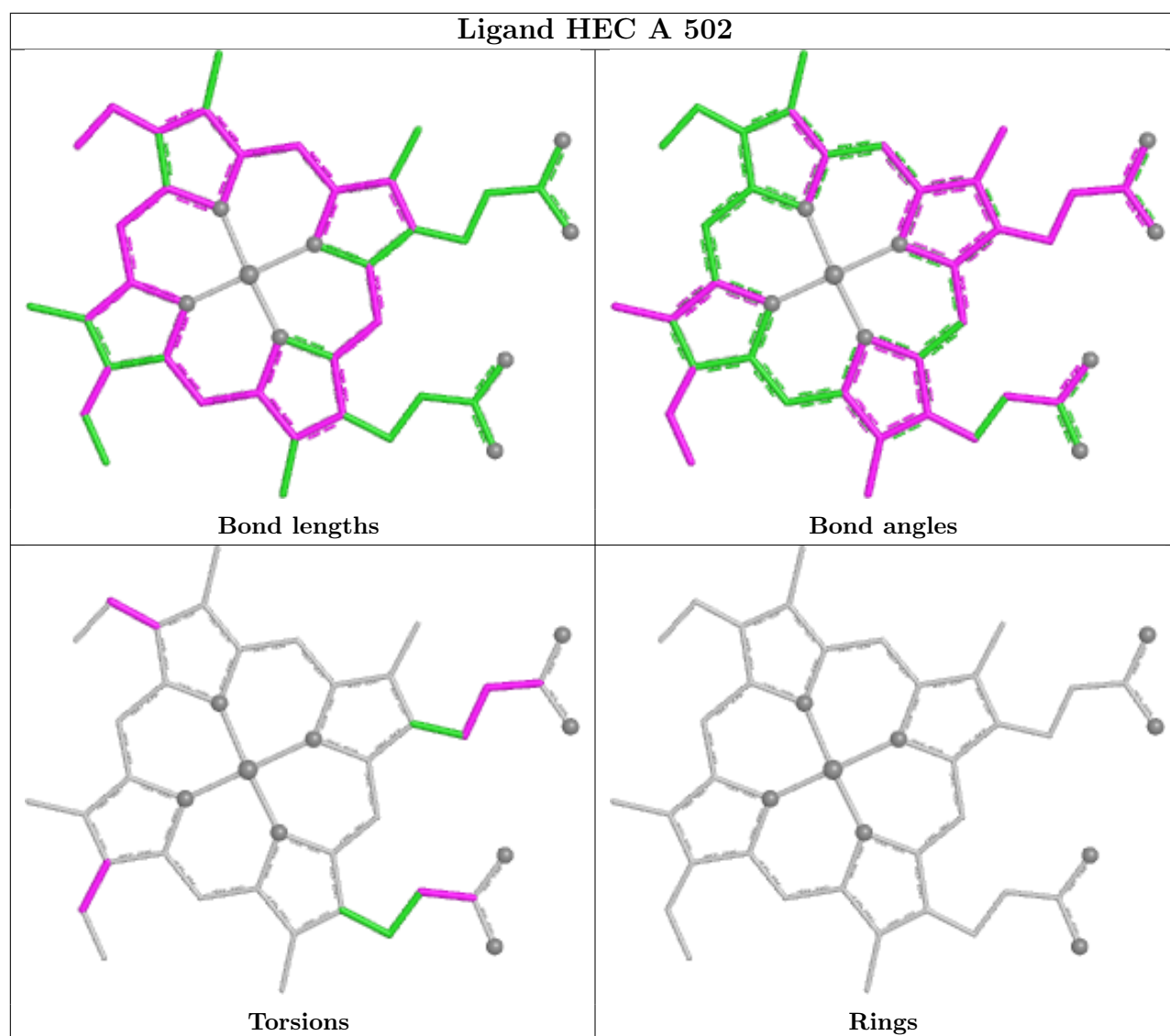
Bond angles



Torsions



Rings



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, 95th percentile and maximum values of the occupancy-weighted average B-factor per residue. The column labelled ‘Q < 0.9’ lists the number of (and percentage) of residues with an average occupancy less than 0.9.

Mol	Chain	Analysed	<RSRZ>	#RSRZ > 2		OWAB(Å ²)	Q < 0.9
1	A	181/243 (74%)	0.86	13 (7%)	21 16	32, 46, 80, 93	0
1	B	178/243 (73%)	0.81	13 (7%)	21 15	32, 44, 76, 89	0
All	All	359/486 (73%)	0.83	26 (7%)	21 16	32, 45, 78, 93	0

All (26) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	182	SER	4.5
1	B	124	THR	4.5
1	A	124	THR	4.1
1	A	122	ASP	4.0
1	B	122	ASP	3.5
1	B	182	SER	3.4
1	B	193	GLU	3.1
1	B	96	GLY	3.0
1	B	123	GLU	2.8
1	B	240	ALA	2.7
1	A	98	GLU	2.7
1	A	223	HIS	2.5
1	A	222	GLY	2.5
1	B	98	GLU	2.4
1	A	84	ALA	2.4
1	A	92	ALA	2.3
1	A	193	GLU	2.2
1	A	192	VAL	2.2
1	B	83	VAL	2.2
1	B	222	GLY	2.2
1	B	238	ILE	2.1
1	B	86	ASN	2.1
1	A	221	THR	2.1
1	A	195	ALA	2.1

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Mol	Chain	Res	Type	RSRZ
1	A	183	GLU	2.0
1	B	82	PHE	2.0

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

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

6.3 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

6.4 Ligands [i](#)

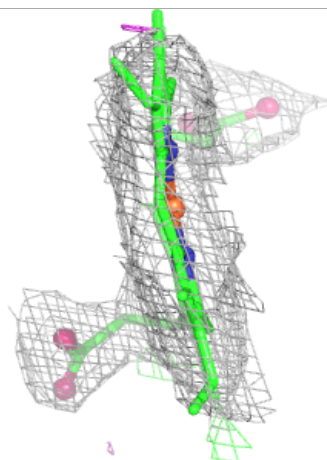
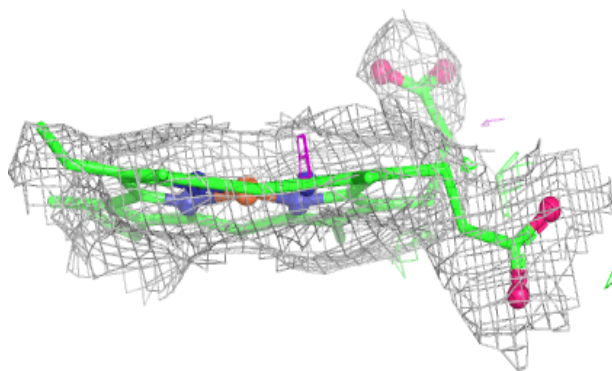
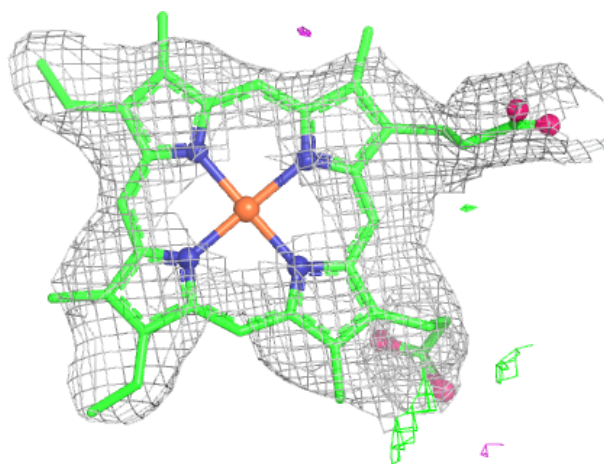
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q < 0.9' lists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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
2	HEC	A	502	43/43	0.91	0.13	35,40,52,63	0
2	HEC	A	501	43/43	0.92	0.12	31,38,47,59	0
2	HEC	B	501	43/43	0.92	0.12	34,39,48,59	0
2	HEC	B	502	43/43	0.92	0.12	31,36,51,62	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.

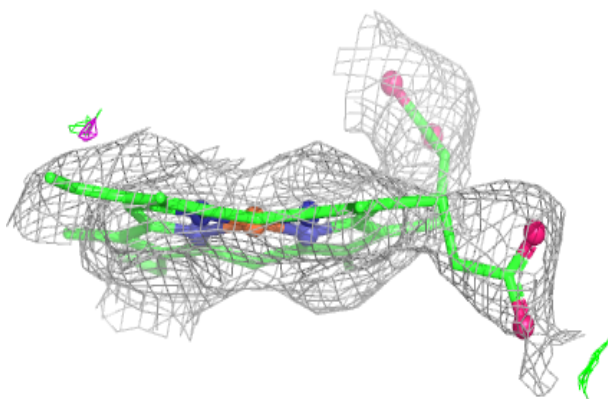
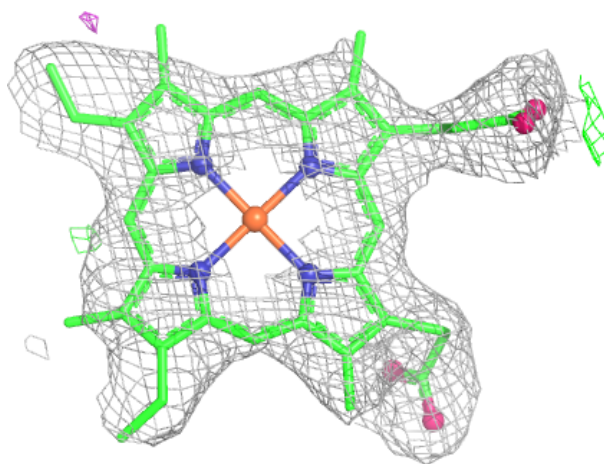
Electron density around HEC A 502:

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



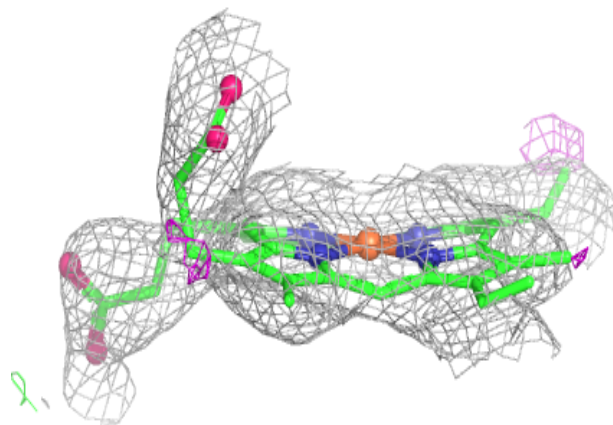
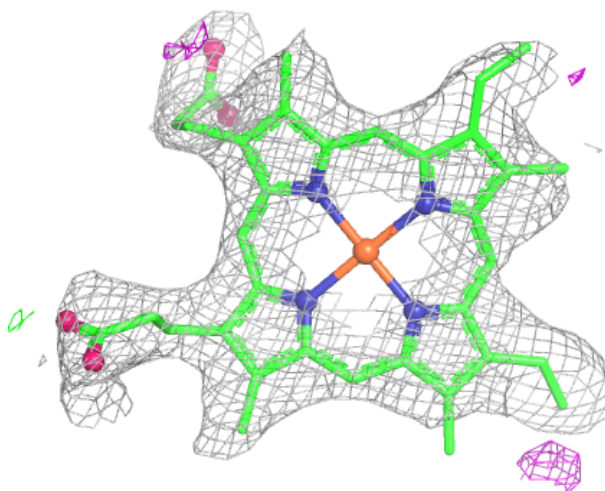
Electron density around HEC A 501:

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



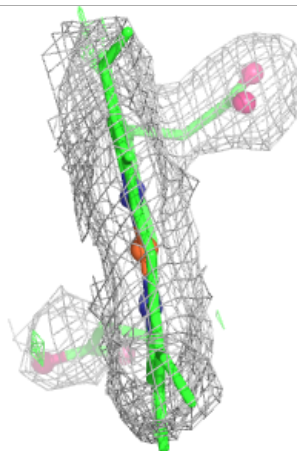
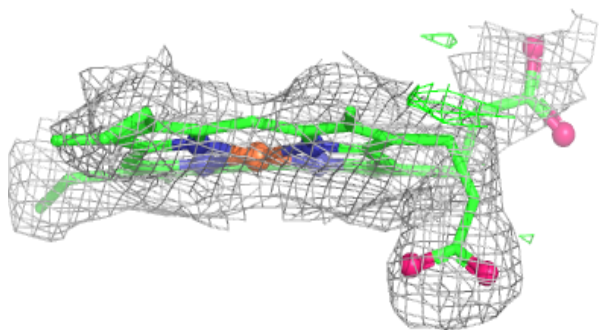
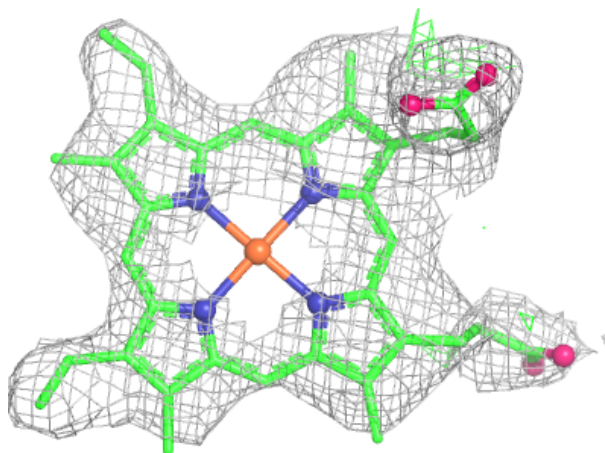
Electron density around HEC B 501:

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



Electron density around HEC 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)



6.5 Other polymers [i](#)

There are no such residues in this entry.