



Full wwPDB X-ray Structure Validation Report ⓘ

Dec 15, 2024 – 10:31 AM EST

PDB ID : 6E1C
Title : Crystal structure of a MauG-like protein associated with microbial copper homeostasis
Authors : Dassama, L.M.K.; Rosenzweig, A.C.
Deposited on : 2018-07-09
Resolution : 2.62 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	:	2022.3.0, CSD as543be (2022)
Xtriage (Phenix)	:	1.21
EDS	:	3.0
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20231227.v01 (using entries in the PDB archive December 27th 2023)
CCP4	:	9.0.004 (Gargrove)
Density-Fitness	:	1.0.11
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.40

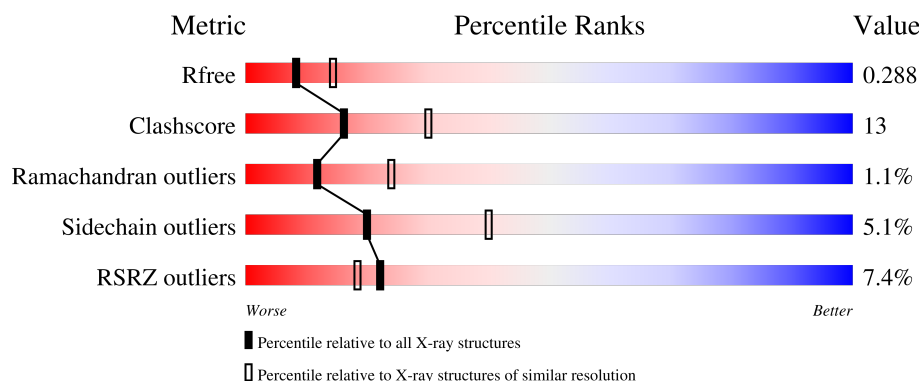
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.62 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}	164625	4623 (2.64-2.60)
Clashscore	180529	5071 (2.64-2.60)
Ramachandran outliers	177936	5006 (2.64-2.60)
Sidechain outliers	177891	5006 (2.64-2.60)
RSRZ outliers	164620	4622 (2.64-2.60)

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	388	
1	B	388	

2 Entry composition

There are 4 unique types of molecules in this entry. The entry contains 5457 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.

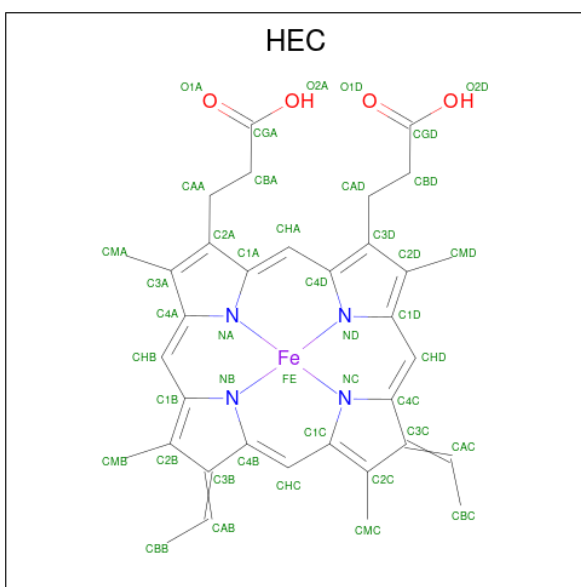
- Molecule 1 is a protein called Di-heme enzyme.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	350	Total	C	N	O	S	0	0	0
			2727	1720	481	516	10			
1	B	323	Total	C	N	O	S	0	0	0
			2504	1576	440	479	9			

There are 16 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	381	TRP	-	expression tag	UNP A0A2D2CY72
A	382	SER	-	expression tag	UNP A0A2D2CY72
A	383	HIS	-	expression tag	UNP A0A2D2CY72
A	384	PRO	-	expression tag	UNP A0A2D2CY72
A	385	GLN	-	expression tag	UNP A0A2D2CY72
A	386	PHE	-	expression tag	UNP A0A2D2CY72
A	387	GLU	-	expression tag	UNP A0A2D2CY72
A	388	LYS	-	expression tag	UNP A0A2D2CY72
B	381	TRP	-	expression tag	UNP A0A2D2CY72
B	382	SER	-	expression tag	UNP A0A2D2CY72
B	383	HIS	-	expression tag	UNP A0A2D2CY72
B	384	PRO	-	expression tag	UNP A0A2D2CY72
B	385	GLN	-	expression tag	UNP A0A2D2CY72
B	386	PHE	-	expression tag	UNP A0A2D2CY72
B	387	GLU	-	expression tag	UNP A0A2D2CY72
B	388	LYS	-	expression tag	UNP A0A2D2CY72

- 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 43	C 34	Fe 1	N 4	O 4	0	0
2	A	1	Total 43	C 34	Fe 1	N 4	O 4	0	0
2	B	1	Total 43	C 34	Fe 1	N 4	O 4	0	0
2	B	1	Total 43	C 34	Fe 1	N 4	O 4	0	0

- Molecule 3 is CALCIUM ION (three-letter code: CA) (formula: Ca).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	1	Total	Ca	0	0
			1	1		
3	B	1	Total	Ca	0	0
			1	1		

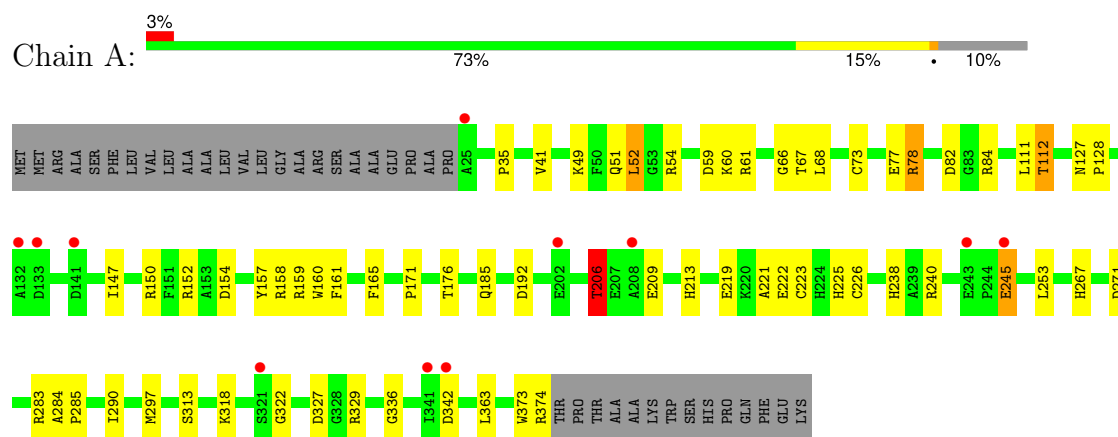
- Molecule 4 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	26	Total	O	0	0
			26	26		
4	B	26	Total	O	0	0
			26	26		

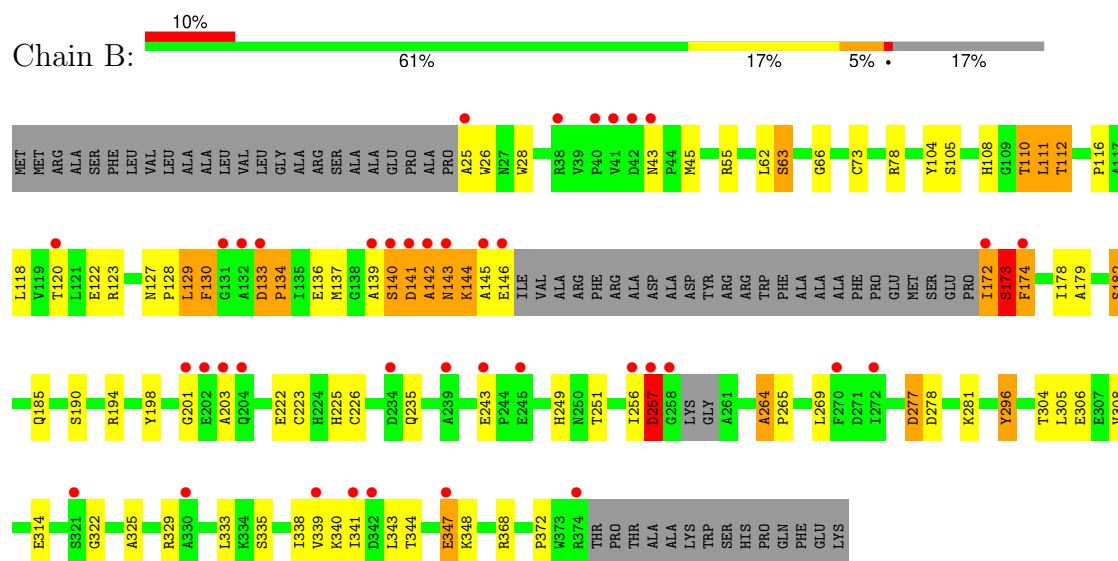
3 Residue-property plots

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: Di-heme enzyme



• Molecule 1: Di-heme enzyme



4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α , β , γ	71.56Å 85.76Å 133.60Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	42.88 – 2.62 42.88 – 2.62	Depositor EDS
% Data completeness (in resolution range)	97.6 (42.88-2.62) 97.6 (42.88-2.62)	Depositor EDS
R_{merge}	0.15	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	4.20 (at 2.61Å)	Xtriage
Refinement program	PHENIX 1.10.1_2155	Depositor
R, R_{free}	0.198 , 0.278 0.228 , 0.288	Depositor DCC
R_{free} test set	22860 reflections (8.05%)	wwPDB-VP
Wilson B-factor (Å ²)	26.1	Xtriage
Anisotropy	0.123	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.33 , 30.8	EDS
L-test for twinning ²	$\langle L \rangle = 0.48$, $\langle L^2 \rangle = 0.31$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.89	EDS
Total number of atoms	5457	wwPDB-VP
Average B, all atoms (Å ²)	27.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.32% of the height of the origin peak. No significant pseudotranslation is detected.*

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

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: HEC, CA

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	0.79	1/2802 (0.0%)	0.94	6/3805 (0.2%)
1	B	0.77	1/2569 (0.0%)	1.13	19/3487 (0.5%)
All	All	0.78	2/5371 (0.0%)	1.04	25/7292 (0.3%)

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	296	TYR	CE1-CZ	-6.33	1.30	1.38
1	A	77	GLU	CD-OE2	-5.14	1.20	1.25

All (25) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	25	ALA	CB-CA-C	20.34	140.61	110.10
1	A	111	LEU	C-N-CA	17.57	165.63	121.70
1	B	140	SER	N-CA-C	13.43	147.27	111.00
1	B	25	ALA	N-CA-C	-12.71	76.68	111.00
1	B	140	SER	CB-CA-C	-9.52	92.02	110.10
1	B	129	LEU	N-CA-C	9.45	136.50	111.00
1	B	340	LYS	N-CA-CB	-9.33	93.80	110.60
1	B	257	ASP	CB-CA-C	-8.52	93.36	110.40
1	A	322	GLY	N-CA-C	7.67	132.29	113.10
1	B	257	ASP	N-CA-C	7.44	131.08	111.00
1	B	173	SER	CB-CA-C	-7.31	96.21	110.10
1	B	339	VAL	N-CA-C	-7.18	91.61	111.00
1	B	78	ARG	NE-CZ-NH2	-7.18	116.71	120.30
1	B	26	TRP	N-CA-CB	6.97	123.15	110.60
1	B	129	LEU	CA-CB-CG	6.72	130.76	115.30
1	B	63	SER	N-CA-C	6.45	128.41	111.00
1	B	130	PHE	N-CA-C	-6.39	93.75	111.00

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	141	ASP	C-N-CA	6.29	137.43	121.70
1	A	112	THR	N-CA-CB	-6.24	98.45	110.30
1	A	111	LEU	N-CA-C	-6.18	94.31	111.00
1	B	174	PHE	N-CA-C	5.61	126.14	111.00
1	B	111	LEU	N-CA-C	-5.53	96.08	111.00
1	B	26	TRP	N-CA-C	-5.40	96.42	111.00
1	A	78	ARG	NE-CZ-NH1	5.21	122.90	120.30
1	A	245	GLU	N-CA-C	5.00	124.50	111.00

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	2727	0	2610	68	1
1	B	2504	0	2395	74	1
2	A	86	0	63	22	0
2	B	86	0	63	16	0
3	A	1	0	0	0	0
3	B	1	0	0	0	0
4	A	26	0	0	2	0
4	B	26	0	0	1	0
All	All	5457	0	5131	136	1

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 13.

All (136) 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:223:CYS:SG	2:A:401:HEC:HBB3	1.46	1.53
1:A:223:CYS:SG	2:A:401:HEC:CBB	2.07	1.42
1:B:223:CYS:SG	2:B:402:HEC:HBB3	1.59	1.40
1:B:223:CYS:SG	2:B:402:HEC:CBB	2.23	1.24

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:318:LYS:HG3	1:A:327:ASP:OD2	1.34	1.23
1:B:110:THR:OG1	1:B:235:GLN:OE1	1.61	1.19
1:A:223:CYS:SG	2:A:401:HEC:CAB	2.31	1.16
1:B:133:ASP:HB3	1:B:134:PRO:HD3	1.35	1.08
1:B:226:CYS:SG	2:B:402:HEC:CAC	2.43	1.06
1:B:223:CYS:SG	2:B:402:HEC:CAB	2.47	1.03
1:A:226:CYS:SG	2:A:401:HEC:CAC	2.51	0.99
1:B:223:CYS:HG	2:B:402:HEC:HBB3	1.28	0.98
1:A:318:LYS:CG	1:A:327:ASP:OD2	2.12	0.96
1:A:223:CYS:HG	2:A:401:HEC:HBB3	1.32	0.94
1:A:73:CYS:SG	2:A:402:HEC:CAC	2.57	0.93
1:A:219:GLU:OE1	1:B:314:GLU:OE1	1.90	0.89
1:A:51:GLN:HE22	1:A:54:ARG:HH11	1.23	0.87
1:B:133:ASP:CB	1:B:134:PRO:HD3	2.05	0.87
1:A:154:ASP:O	1:A:158:ARG:HG3	1.80	0.82
1:A:318:LYS:HG3	1:A:327:ASP:CG	2.00	0.82
1:B:73:CYS:SG	2:B:401:HEC:CAC	2.69	0.81
1:B:185:GLN:HE22	2:B:401:HEC:HHB	1.45	0.81
1:B:226:CYS:SG	2:B:402:HEC:CBC	2.69	0.80
1:B:73:CYS:SG	2:B:401:HEC:HBC3	2.22	0.79
1:A:185:GLN:HE22	2:A:402:HEC:HHB	1.46	0.79
1:B:133:ASP:HB3	1:B:134:PRO:CD	2.13	0.78
1:B:264:ALA:HB1	1:B:265:PRO:HD3	1.64	0.78
1:B:142:ALA:O	1:B:144:LYS:HE3	1.84	0.78
1:B:226:CYS:SG	2:B:402:HEC:HBC3	2.25	0.76
1:A:226:CYS:SG	2:A:401:HEC:CBC	2.74	0.76
1:B:257:ASP:OD1	1:B:257:ASP:N	2.19	0.75
1:A:73:CYS:SG	2:A:402:HEC:HBC3	2.27	0.74
1:A:73:CYS:SG	2:A:402:HEC:CBC	2.77	0.72
1:B:63:SER:O	1:B:137:MET:O	2.07	0.72
1:B:105:SER:HA	1:B:108:HIS:CD2	2.26	0.70
1:B:73:CYS:SG	2:B:401:HEC:CBC	2.80	0.70
1:A:253:LEU:HD11	1:A:297:MET:HE3	1.73	0.70
1:A:206:THR:HG22	1:A:209:GLU:H	1.56	0.69
1:A:226:CYS:SG	2:A:401:HEC:HBC3	2.32	0.68
1:B:140:SER:O	1:B:141:ASP:C	2.32	0.67
1:B:264:ALA:HB1	1:B:265:PRO:CD	2.23	0.67
1:B:269:LEU:HB3	1:B:278:ASP:HB3	1.78	0.66
1:A:253:LEU:HD11	1:A:297:MET:CE	2.26	0.65
1:A:219:GLU:OE1	1:A:222:GLU:OE2	2.14	0.64
1:A:318:LYS:CD	1:A:327:ASP:OD2	2.46	0.64

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:343:LEU:HD22	1:B:347:GLU:OE2	1.98	0.63
1:A:336:GLY:HA3	1:B:343:LEU:O	1.98	0.63
1:B:198:TYR:HA	1:B:203:ALA:HA	1.80	0.62
1:B:143:ASN:C	1:B:145:ALA:H	2.03	0.61
1:A:221:ALA:HB1	2:A:401:HEC:HBB1	1.82	0.61
1:B:130:PHE:CD1	1:B:139:ALA:HB3	2.36	0.61
1:B:278:ASP:HA	1:B:281:LYS:HE2	1.82	0.61
1:A:297:MET:CE	2:A:401:HEC:HBD1	2.31	0.60
1:B:62:LEU:O	1:B:62:LEU:HG	2.03	0.59
1:B:111:LEU:O	1:B:112:THR:HG22	2.03	0.59
1:B:226:CYS:SG	2:B:402:HEC:C3C	2.91	0.58
1:B:43:ASN:OD1	1:B:179:ALA:HB1	2.03	0.58
1:A:171:PRO:O	1:A:176:THR:HG21	2.04	0.57
1:B:55:ARG:HG2	1:B:372:PRO:HG2	1.85	0.57
1:B:256:ILE:HD12	1:B:256:ILE:N	2.20	0.56
1:A:35:PRO:HG2	1:A:238:HIS:CD2	2.41	0.55
1:B:249:HIS:O	1:B:281:LYS:HA	2.07	0.55
1:A:127:ASN:HB2	1:A:128:PRO:HD3	1.87	0.55
1:A:35:PRO:HG2	1:A:238:HIS:CG	2.41	0.55
1:B:28:TRP:CH2	1:B:45:MET:HE2	2.41	0.55
1:A:225:HIS:NE2	1:B:314:GLU:OE1	2.39	0.55
1:B:104:TYR:OH	1:B:190:SER:O	2.21	0.55
1:A:222:GLU:OE1	1:B:314:GLU:OE1	2.25	0.55
1:A:185:GLN:NE2	2:A:402:HEC:HBB	2.21	0.54
1:B:264:ALA:CB	1:B:265:PRO:CD	2.86	0.54
1:B:28:TRP:HH2	1:B:45:MET:CE	2.21	0.54
1:B:277:ASP:HA	1:B:333:LEU:HD21	1.90	0.53
1:A:223:CYS:SG	2:A:401:HEC:C3B	2.95	0.53
1:A:297:MET:HE1	2:A:401:HEC:HBD1	1.89	0.53
1:B:63:SER:HB3	1:B:66:GLY:H	1.73	0.53
1:A:206:THR:HB	1:A:209:GLU:CD	2.29	0.52
1:B:256:ILE:N	1:B:256:ILE:CD1	2.72	0.52
1:B:133:ASP:CB	1:B:134:PRO:CD	2.78	0.51
1:A:73:CYS:SG	2:A:402:HEC:C3C	2.98	0.51
1:B:178:ILE:O	1:B:182:SER:OG	2.21	0.50
1:A:51:GLN:HE22	1:A:54:ARG:NH1	2.02	0.50
1:A:222:GLU:OE2	1:A:225:HIS:NE2	2.45	0.50
1:B:127:ASN:HB2	1:B:128:PRO:CD	2.42	0.49
1:B:28:TRP:CH2	1:B:45:MET:CE	2.95	0.49
1:B:118:LEU:HA	1:B:123:ARG:HH21	1.77	0.49
1:A:152:ARG:O	1:A:158:ARG:HD3	2.14	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:322:GLY:H	1:B:325:ALA:HB2	1.79	0.48
1:A:112:THR:HB	2:A:402:HEC:O2D	2.14	0.47
1:A:318:LYS:HD2	1:A:327:ASP:OD2	2.13	0.47
1:A:222:GLU:OE2	1:A:225:HIS:CD2	2.69	0.46
1:B:172:ILE:O	1:B:173:SER:HB3	2.15	0.46
1:B:343:LEU:HB3	1:B:348:LYS:HG3	1.97	0.46
1:A:206:THR:HG23	4:A:513:HOH:O	2.15	0.46
1:B:251:THR:HA	1:B:338:ILE:HD13	1.98	0.46
1:A:219:GLU:OE2	1:B:329:ARG:NH2	2.50	0.45
1:A:290:ILE:HG12	2:A:401:HEC:HMA3	1.98	0.45
1:A:267:HIS:HD2	1:A:271:ASP:OD1	2.00	0.45
1:A:147:ILE:O	1:A:150:ARG:HB2	2.17	0.45
1:A:59:ASP:OD1	1:A:61:ARG:HB3	2.17	0.45
1:B:144:LYS:HA	1:B:144:LYS:HD3	1.84	0.44
1:A:336:GLY:CA	1:B:343:LEU:O	2.65	0.44
1:A:219:GLU:OE1	1:A:222:GLU:CD	2.56	0.44
1:A:225:HIS:CE1	1:B:314:GLU:OE2	2.71	0.44
1:B:296:TYR:CZ	1:B:305:LEU:HD13	2.53	0.44
1:A:67:THR:O	1:A:68:LEU:HD23	2.18	0.43
1:B:143:ASN:C	1:B:145:ALA:N	2.71	0.43
1:A:112:THR:O	1:A:283:ARG:CZ	2.66	0.43
1:B:140:SER:C	1:B:142:ALA:N	2.67	0.43
1:A:213:HIS:HE1	4:A:504:HOH:O	2.02	0.43
1:B:343:LEU:HD22	1:B:347:GLU:CD	2.38	0.43
1:B:128:PRO:HA	1:B:136:GLU:OE1	2.18	0.43
1:A:157:TYR:CD1	1:A:161:PHE:HE1	2.37	0.43
1:B:73:CYS:SG	2:B:401:HEC:C3C	3.07	0.42
1:A:297:MET:HE1	2:A:401:HEC:CHA	2.49	0.42
1:B:222:GLU:HG3	1:B:225:HIS:HD2	1.85	0.42
1:B:223:CYS:SG	2:B:402:HEC:C3B	3.08	0.42
2:B:401:HEC:CBB	2:B:401:HEC:HMB1	2.50	0.42
1:A:284:ALA:HA	1:A:285:PRO:HD3	1.92	0.42
1:A:78:ARG:NH1	1:A:78:ARG:HG2	2.34	0.41
1:A:165:PHE:CE1	1:A:176:THR:HG22	2.56	0.41
1:A:226:CYS:SG	2:A:401:HEC:C3C	3.09	0.41
1:A:297:MET:HE3	2:A:401:HEC:HBD1	2.00	0.41
1:B:304:THR:HB	1:B:306:GLU:OE1	2.20	0.41
1:A:52:LEU:HG	1:A:160:TRP:HB3	2.03	0.41
1:A:238:HIS:CE1	1:A:240:ARG:HB2	2.55	0.41
1:B:111:LEU:HD23	1:B:111:LEU:HA	1.88	0.41
1:A:60:LYS:O	1:A:66:GLY:HA2	2.19	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:219:GLU:OE1	1:A:222:GLU:OE1	2.39	0.40
1:B:28:TRP:HD1	4:B:522:HOH:O	2.04	0.40
1:B:304:THR:O	1:B:308:VAL:HG23	2.21	0.40
1:A:82:ASP:HB3	1:A:84:ARG:H	1.87	0.40
1:A:267:HIS:CD2	1:A:271:ASP:OD1	2.74	0.40
1:A:373:TRP:O	1:A:374:ARG:HB2	2.21	0.40
1:B:296:TYR:HB3	2:B:402:HEC:HAA1	2.02	0.40
1:B:116:PRO:HG2	1:B:269:LEU:HD21	2.04	0.40
1:B:120:THR:HG22	1:B:122:GLU:OE2	2.22	0.40

All (1) 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:A:158:ARG:NH2	1:B:243:GLU:OE2[2_564]	2.16	0.04

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	348/388 (90%)	316 (91%)	30 (9%)	2 (1%)	22	40
1	B	317/388 (82%)	275 (87%)	37 (12%)	5 (2%)	8	15
All	All	665/776 (86%)	591 (89%)	67 (10%)	7 (1%)	12	24

All (7) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	B	133	ASP
1	B	264	ALA
1	B	173	SER
1	A	363	LEU

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Mol	Chain	Res	Type
1	B	142	ALA
1	A	206	THR
1	B	201	GLY

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	282/310 (91%)	272 (96%)	10 (4%)	31	55
1	B	262/310 (84%)	244 (93%)	18 (7%)	13	26
All	All	544/620 (88%)	516 (95%)	28 (5%)	20	40

All (28) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	41	VAL
1	A	49	LYS
1	A	52	LEU
1	A	159	ARG
1	A	192	ASP
1	A	206	THR
1	A	245	GLU
1	A	313	SER
1	A	329	ARG
1	A	342	ASP
1	B	110	THR
1	B	112	THR
1	B	129	LEU
1	B	134	PRO
1	B	143	ASN
1	B	144	LYS
1	B	146	GLU
1	B	172	ILE
1	B	174	PHE
1	B	182	SER

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Mol	Chain	Res	Type
1	B	194	ARG
1	B	257	ASP
1	B	277	ASP
1	B	335	SER
1	B	341	ILE
1	B	344	THR
1	B	347	GLU
1	B	368	ARG

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (10) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	51	GLN
1	A	185	GLN
1	A	210	GLN
1	A	213	HIS
1	A	235	GLN
1	A	267	HIS
1	B	143	ASN
1	B	185	GLN
1	B	249	HIS
1	B	346	GLN

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 ⓘ

There are no oligosaccharides in this entry.

5.6 Ligand geometry ⓘ

Of 6 ligands modelled in this entry, 2 are monoatomic - leaving 4 for Mogul analysis.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\# Z > 2$	Counts	RMSZ	$\# Z > 2$
2	HEC	B	401	1	32,50,50	2.03	7 (21%)	30,82,82	2.87	12 (40%)
2	HEC	A	401	1	32,50,50	2.38	11 (34%)	30,82,82	2.93	11 (36%)
2	HEC	B	402	1	32,50,50	2.46	10 (31%)	30,82,82	2.81	10 (33%)
2	HEC	A	402	1	32,50,50	2.08	10 (31%)	30,82,82	2.84	12 (40%)

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	401	1	-	4/10/54/54	-
2	HEC	A	401	1	-	2/10/54/54	-
2	HEC	B	402	1	-	4/10/54/54	-
2	HEC	A	402	1	-	2/10/54/54	-

All (38) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	402	HEC	C3C-C2C	7.91	1.49	1.40
2	A	401	HEC	C2B-C3B	7.56	1.49	1.40
2	B	402	HEC	C2B-C3B	7.18	1.48	1.40
2	A	401	HEC	C3C-C2C	6.13	1.47	1.40
2	A	402	HEC	C3C-C2C	5.94	1.47	1.40
2	B	401	HEC	C3C-C2C	5.67	1.47	1.40
2	B	401	HEC	C2B-C3B	5.19	1.46	1.40
2	A	402	HEC	C2B-C3B	4.77	1.46	1.40
2	A	401	HEC	C2A-C3A	3.72	1.48	1.37
2	A	402	HEC	C2A-C3A	3.61	1.48	1.37
2	B	401	HEC	C2A-C1A	3.58	1.50	1.42
2	B	401	HEC	C2A-C3A	3.37	1.47	1.37
2	A	401	HEC	C2A-C1A	3.35	1.50	1.42
2	B	402	HEC	C2A-C3A	3.34	1.47	1.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	402	HEC	C2A-C1A	3.27	1.49	1.42
2	A	402	HEC	C2A-C1A	3.13	1.49	1.42
2	B	402	HEC	C1C-CHC	3.12	1.49	1.41
2	A	402	HEC	C3D-C2D	3.10	1.46	1.37
2	B	402	HEC	C3D-C2D	2.88	1.46	1.37
2	A	401	HEC	C3D-C2D	2.86	1.46	1.37
2	A	401	HEC	C3C-C4C	2.84	1.48	1.43
2	A	402	HEC	C4D-CHA	2.81	1.48	1.41
2	B	401	HEC	C3D-C2D	2.77	1.45	1.37
2	A	401	HEC	C1C-CHC	2.65	1.48	1.41
2	A	402	HEC	C3A-C4A	2.60	1.48	1.42
2	B	402	HEC	C3A-C4A	2.57	1.48	1.42
2	B	402	HEC	C1B-CHB	2.53	1.48	1.41
2	B	401	HEC	C4D-CHA	2.52	1.48	1.41
2	B	401	HEC	C3A-C4A	2.49	1.48	1.42
2	A	402	HEC	C1C-NC	-2.41	1.31	1.36
2	B	402	HEC	C4D-CHA	2.39	1.47	1.41
2	A	401	HEC	C4D-CHA	2.37	1.47	1.41
2	B	402	HEC	C1D-CHD	2.36	1.47	1.41
2	A	401	HEC	C3A-C4A	2.29	1.47	1.42
2	A	401	HEC	C1D-CHD	2.19	1.47	1.41
2	A	402	HEC	C1D-CHD	2.11	1.46	1.41
2	A	401	HEC	C1B-CHB	2.03	1.46	1.41
2	A	402	HEC	C1B-CHB	2.02	1.46	1.41

All (45) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	401	HEC	C1D-C2D-C3D	-7.62	101.70	107.00
2	A	401	HEC	C1D-C2D-C3D	-7.23	101.97	107.00
2	B	402	HEC	C1D-C2D-C3D	-6.96	102.16	107.00
2	A	402	HEC	C1D-C2D-C3D	-6.92	102.18	107.00
2	B	401	HEC	CBA-CAA-C2A	-6.83	101.29	112.55
2	A	401	HEC	CBA-CAA-C2A	-6.37	102.05	112.55
2	B	402	HEC	CMC-C2C-C3C	6.35	133.28	125.82
2	A	402	HEC	CBD-CAD-C3D	-6.35	101.87	112.54
2	B	402	HEC	CMB-C2B-C3B	6.31	133.24	125.82
2	B	401	HEC	CBD-CAD-C3D	-6.19	102.12	112.54
2	B	402	HEC	CBD-CAD-C3D	-6.13	102.23	112.54
2	A	401	HEC	CBD-CAD-C3D	-6.10	102.29	112.54
2	A	401	HEC	CMC-C2C-C3C	5.87	132.72	125.82
2	A	402	HEC	CBA-CAA-C2A	-5.72	103.12	112.55

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	A	402	HEC	CMC-C2C-C3C	5.62	132.43	125.82
2	A	401	HEC	CMB-C2B-C3B	5.17	131.90	125.82
2	B	402	HEC	CBA-CAA-C2A	-4.49	105.15	112.55
2	B	401	HEC	CMC-C2C-C3C	4.47	131.08	125.82
2	A	402	HEC	CMB-C2B-C3B	4.04	130.58	125.82
2	B	401	HEC	CMB-C2B-C3B	3.86	130.36	125.82
2	A	401	HEC	CBB-CAB-C3B	-3.77	118.68	127.49
2	A	401	HEC	CMA-C3A-C2A	3.48	131.50	124.94
2	B	401	HEC	CBB-CAB-C3B	-3.23	119.93	127.49
2	A	402	HEC	CMD-C2D-C3D	2.82	130.26	124.94
2	A	402	HEC	CBB-CAB-C3B	-2.76	121.04	127.49
2	B	402	HEC	CBB-CAB-C3B	-2.69	121.19	127.49
2	A	402	HEC	CMA-C3A-C2A	2.64	129.91	124.94
2	B	401	HEC	O1A-CGA-CBA	-2.61	114.82	123.09
2	B	401	HEC	CMD-C2D-C3D	2.59	129.83	124.94
2	A	402	HEC	O2D-CGD-CBD	2.57	122.11	114.00
2	B	401	HEC	C3C-C4C-NC	2.55	115.77	110.94
2	B	402	HEC	O1A-CGA-CBA	-2.52	115.09	123.09
2	A	402	HEC	CBC-CAC-C3C	-2.40	121.88	127.49
2	A	402	HEC	C3B-C4B-NB	2.37	115.41	110.94
2	B	402	HEC	O2A-CGA-CBA	2.29	121.23	114.00
2	B	401	HEC	CMA-C3A-C2A	2.26	129.21	124.94
2	B	401	HEC	O2A-CGA-CBA	2.26	121.15	114.00
2	A	401	HEC	CMD-C2D-C3D	2.26	129.20	124.94
2	B	401	HEC	C4D-CHA-C1A	2.25	130.27	123.67
2	A	401	HEC	CAA-CBA-CGA	2.18	119.70	113.83
2	B	402	HEC	CBC-CAC-C3C	-2.13	122.51	127.49
2	B	402	HEC	CMA-C3A-C2A	2.12	128.94	124.94
2	A	402	HEC	C4D-CHA-C1A	2.08	129.77	123.67
2	A	401	HEC	O2D-CGD-CBD	2.05	120.46	114.00
2	A	401	HEC	O2A-CGA-O1A	-2.04	118.08	123.33

There are no chirality outliers.

All (12) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	A	402	HEC	CAD-CBD-CGD-O1D
2	A	402	HEC	CAD-CBD-CGD-O2D
2	B	402	HEC	CAD-CBD-CGD-O1D
2	B	402	HEC	CAD-CBD-CGD-O2D
2	B	401	HEC	CAD-CBD-CGD-O2D
2	B	401	HEC	CAD-CBD-CGD-O1D

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Mol	Chain	Res	Type	Atoms
2	B	401	HEC	CAA-CBA-CGA-O1A
2	B	402	HEC	CAA-CBA-CGA-O1A
2	A	401	HEC	CAD-CBD-CGD-O1D
2	B	402	HEC	CAA-CBA-CGA-O2A
2	B	401	HEC	CAA-CBA-CGA-O2A
2	A	401	HEC	CAD-CBD-CGD-O2D

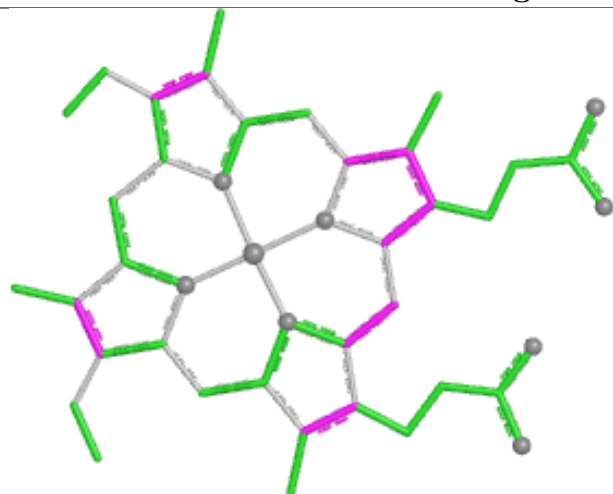
There are no ring outliers.

4 monomers are involved in 38 short contacts:

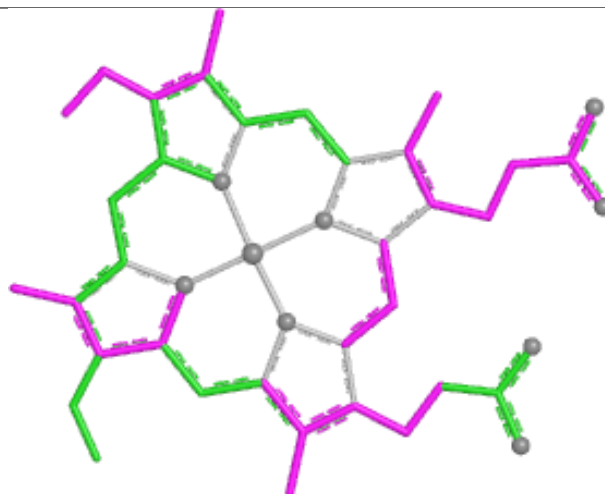
Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	B	401	HEC	6	0
2	A	401	HEC	15	0
2	B	402	HEC	10	0
2	A	402	HEC	7	0

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.

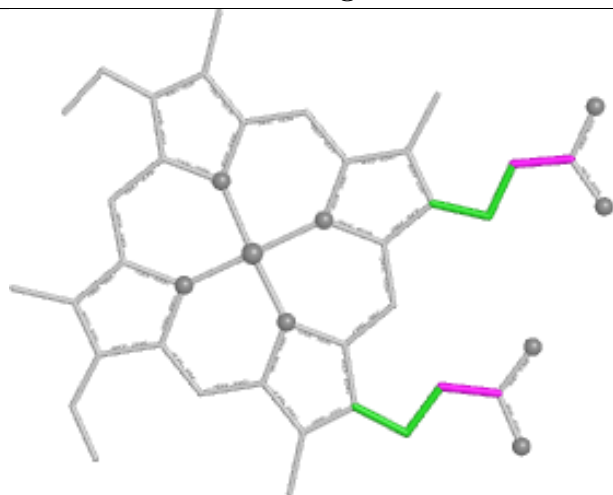
Ligand HEC B 401



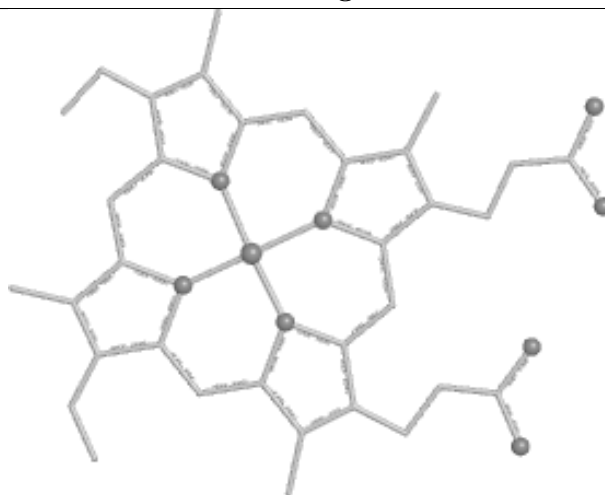
Bond lengths



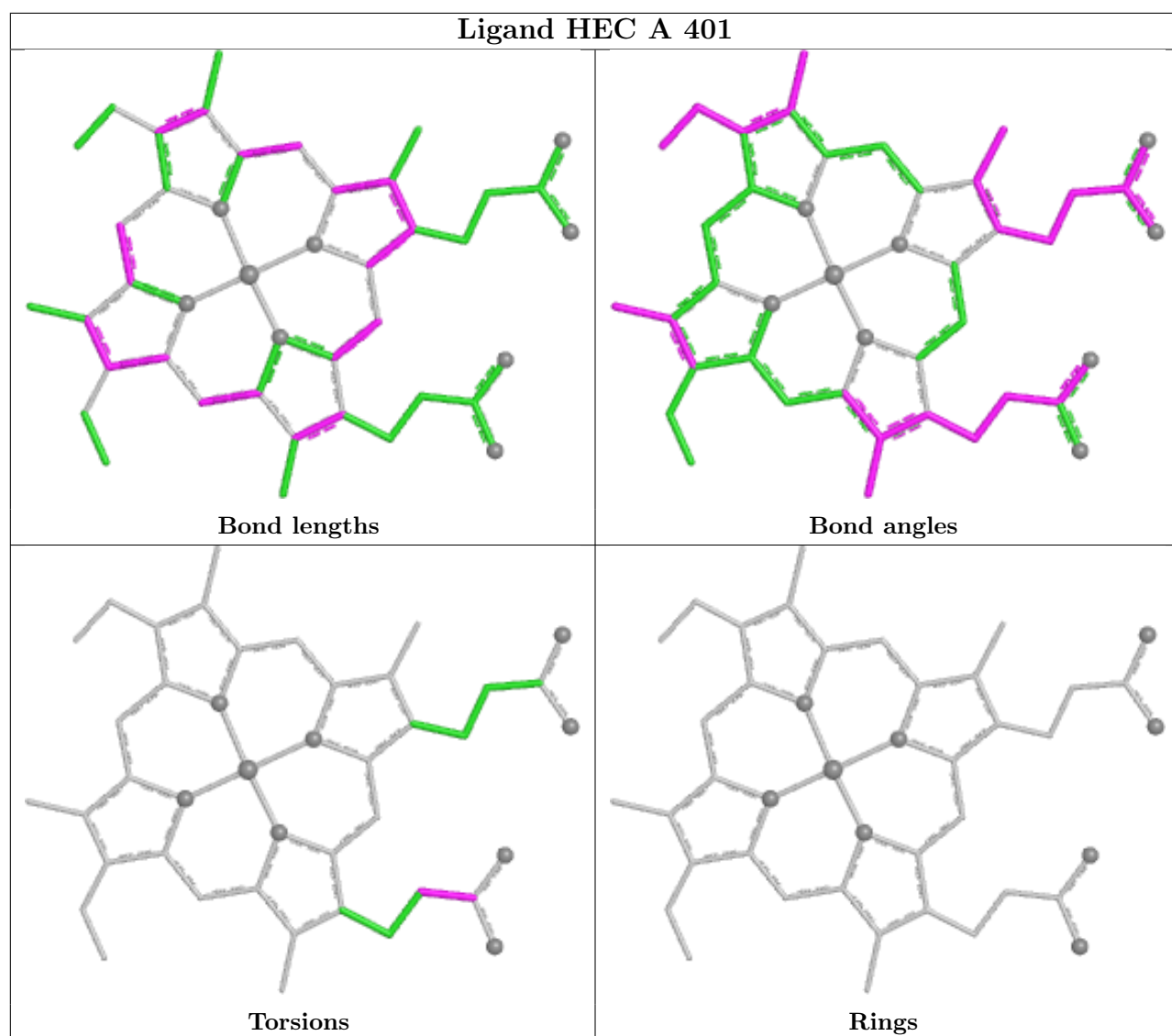
Bond angles



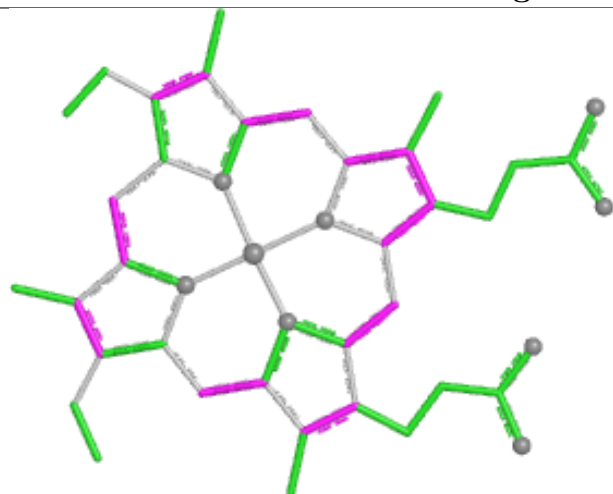
Torsions



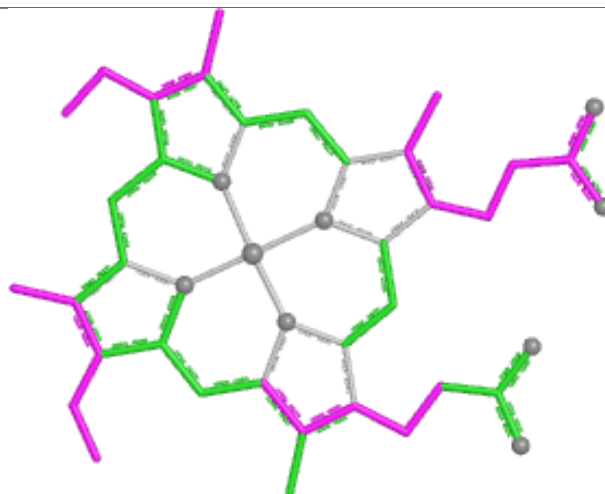
Rings



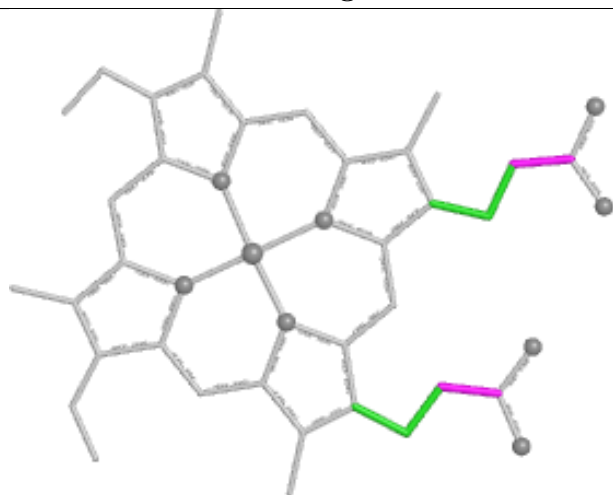
Ligand HEC B 402



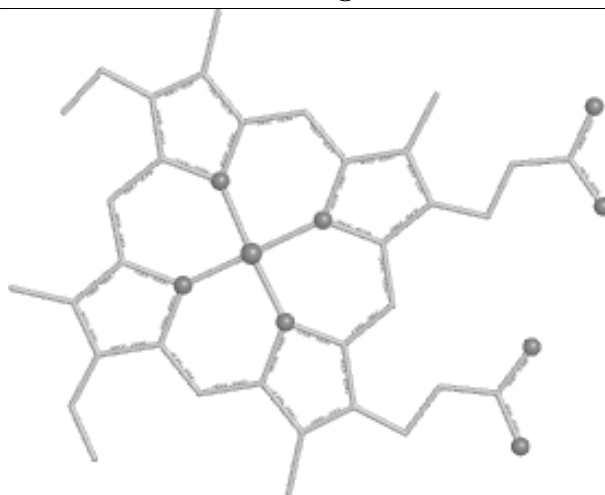
Bond lengths



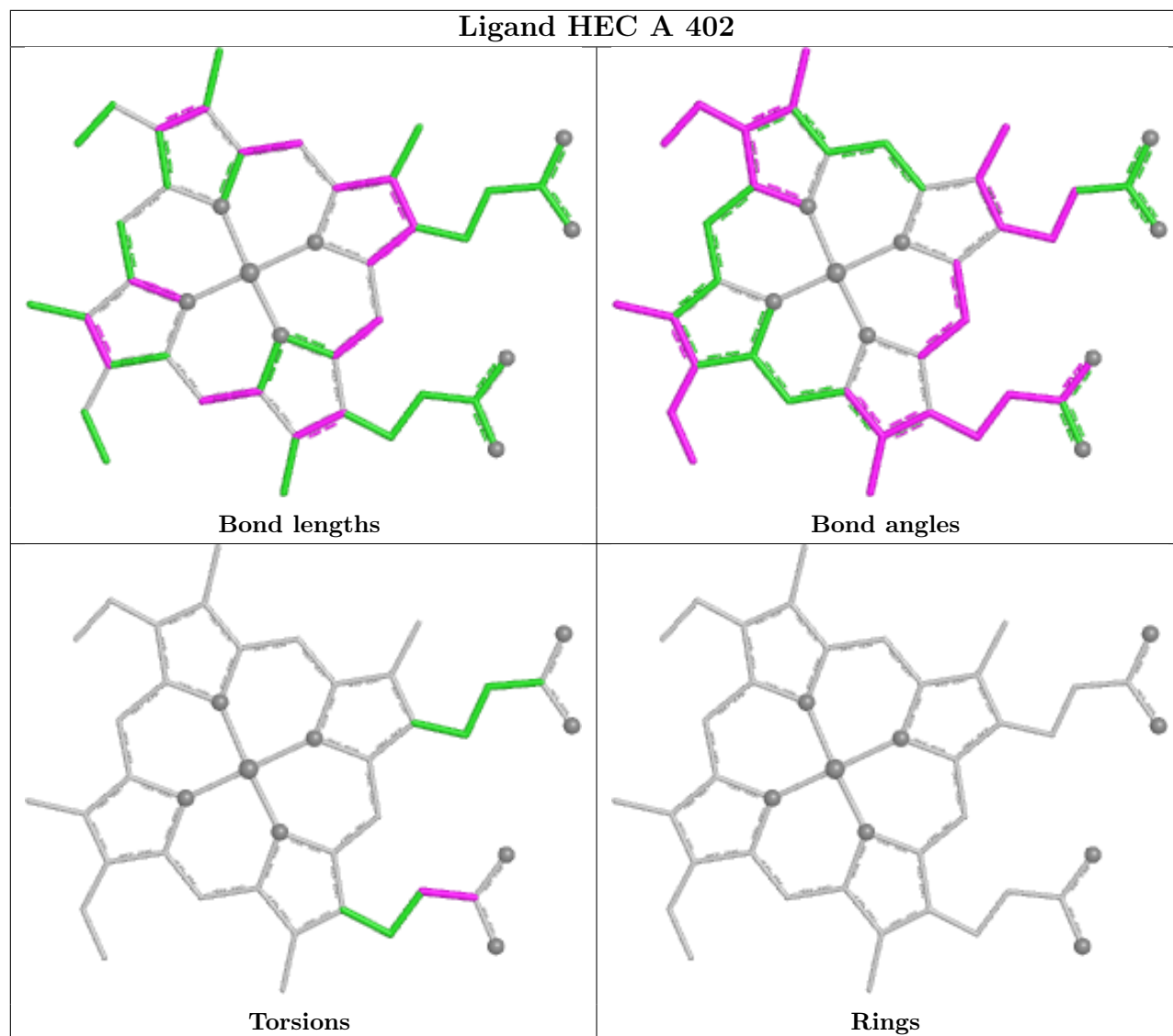
Bond angles



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	350/388 (90%)	0.02	11 (3%) 51 46	5, 22, 47, 66	0
1	B	323/388 (83%)	0.60	39 (12%) 10 8	7, 32, 63, 87	0
All	All	673/776 (86%)	0.30	50 (7%) 22 18	5, 26, 59, 87	0

All (50) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	142	ALA	6.9
1	B	132	ALA	5.8
1	B	172	ILE	5.8
1	B	25	ALA	5.5
1	B	342	ASP	4.5
1	B	141	ASP	4.4
1	B	146	GLU	4.2
1	B	374	ARG	3.9
1	B	140	SER	3.9
1	B	203	ALA	3.6
1	B	341	ILE	3.5
1	B	133	ASP	3.5
1	B	41	VAL	3.4
1	A	25	ALA	3.4
1	A	133	ASP	3.3
1	B	139	ALA	3.2
1	B	339	VAL	3.1
1	A	321	SER	3.1
1	B	145	ALA	3.0
1	B	258	GLY	3.0
1	A	202	GLU	2.9
1	B	201	GLY	2.8
1	A	342	ASP	2.8
1	B	321	SER	2.7

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Mol	Chain	Res	Type	RSRZ
1	B	143	ASN	2.6
1	B	131	GLY	2.6
1	B	256	ILE	2.6
1	B	243	GLU	2.6
1	B	42	ASP	2.5
1	A	341	ILE	2.5
1	A	243	GLU	2.5
1	B	347	GLU	2.5
1	B	38	ARG	2.5
1	B	43	ASN	2.5
1	B	239	ALA	2.4
1	B	204	GLN	2.4
1	B	40	PRO	2.4
1	B	234	ASP	2.3
1	B	330	ALA	2.3
1	B	245	GLU	2.3
1	B	257	ASP	2.3
1	B	174	PHE	2.3
1	B	272	ILE	2.3
1	B	120	THR	2.2
1	A	208	ALA	2.1
1	B	202	GLU	2.1
1	A	245	GLU	2.0
1	B	270	PHE	2.0
1	A	141	ASP	2.0
1	A	132	ALA	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](#)

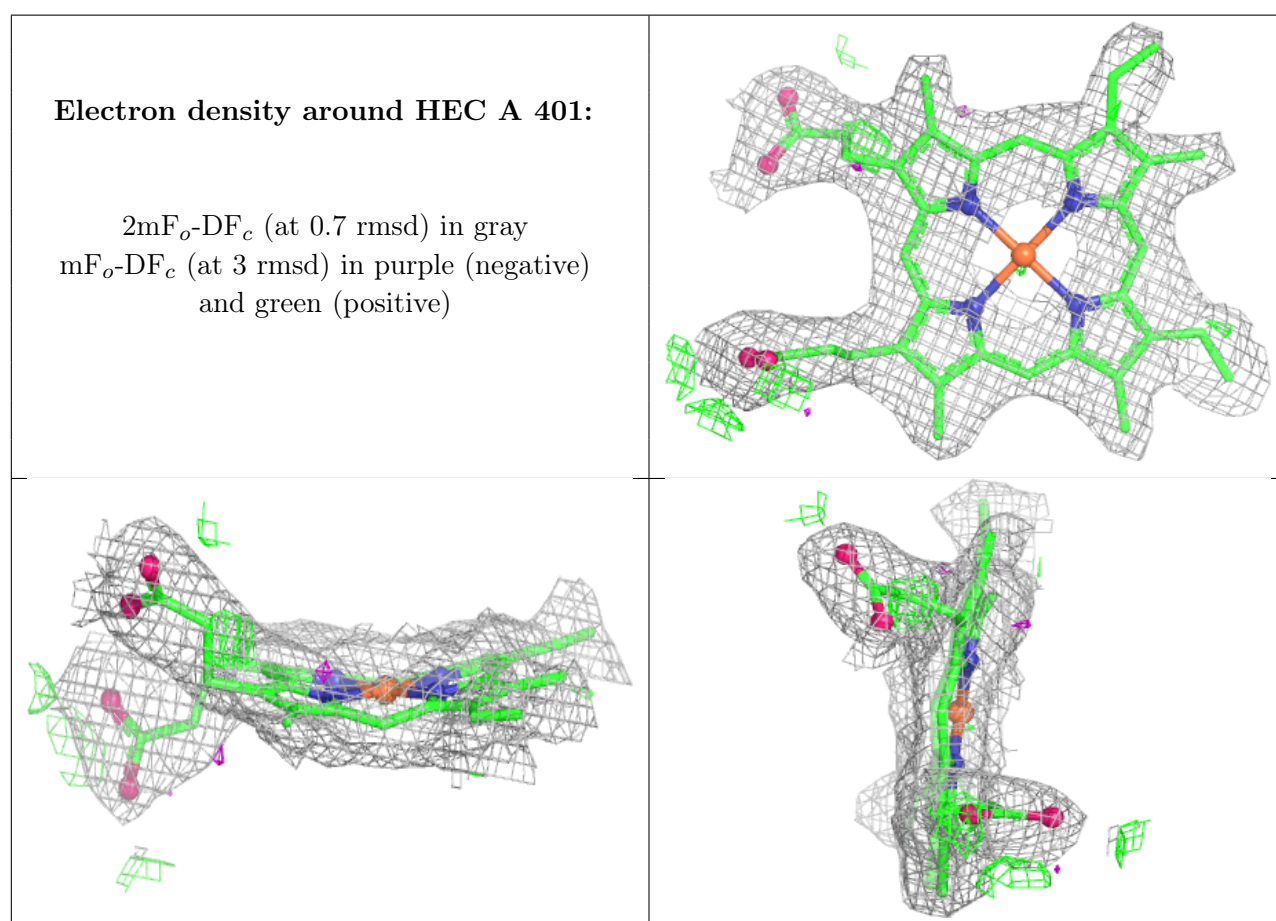
There are no monosaccharides in this entry.

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, 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.

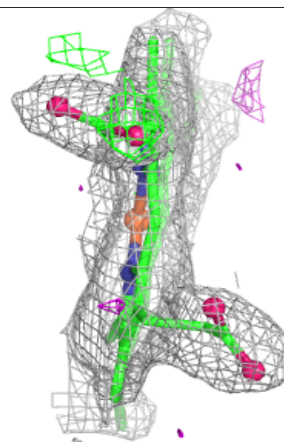
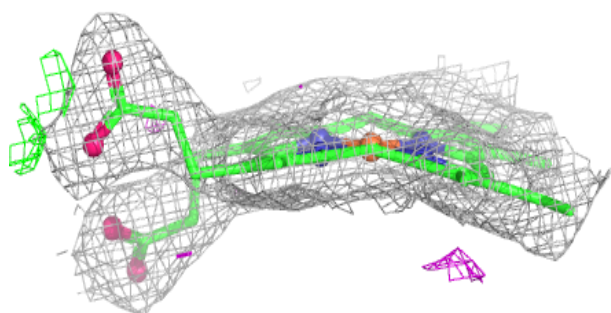
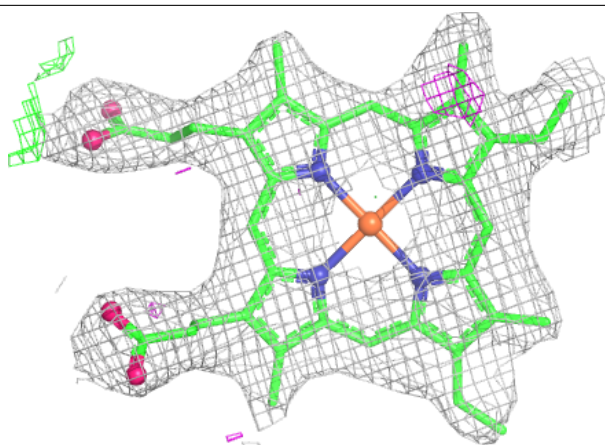
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
3	CA	A	403	1/1	0.80	0.03	5,5,5,5	0
2	HEC	A	401	43/43	0.94	0.10	9,12,15,16	0
2	HEC	B	402	43/43	0.95	0.10	15,18,22,26	0
2	HEC	B	401	43/43	0.95	0.11	14,17,28,33	0
2	HEC	A	402	43/43	0.96	0.09	9,9,17,22	0
3	CA	B	403	1/1	0.97	0.06	11,11,11,11	0

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.



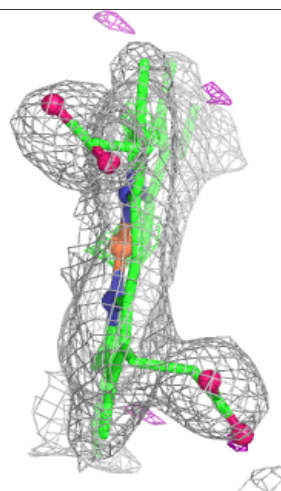
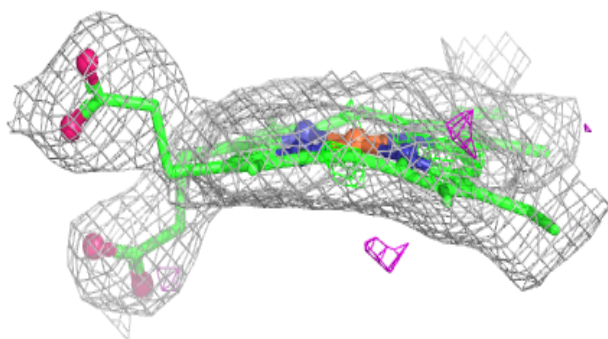
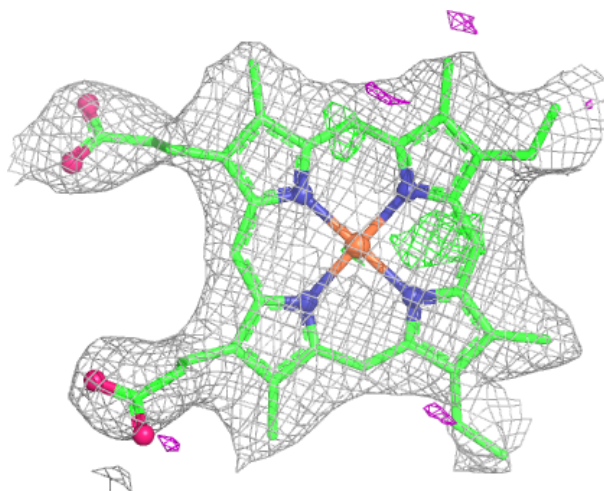
Electron density around HEC B 402:

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



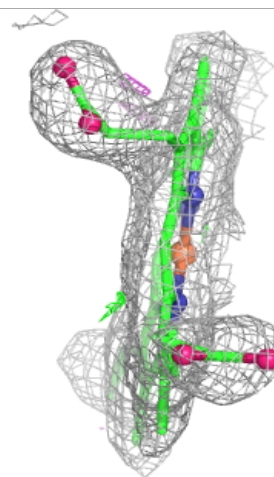
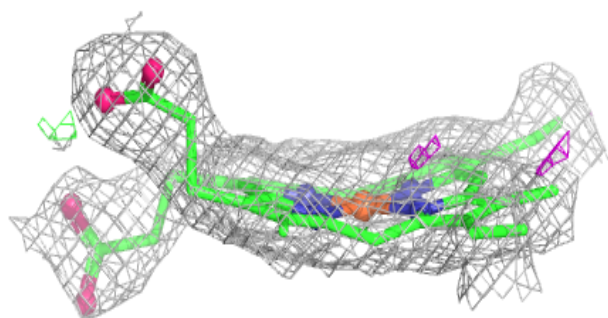
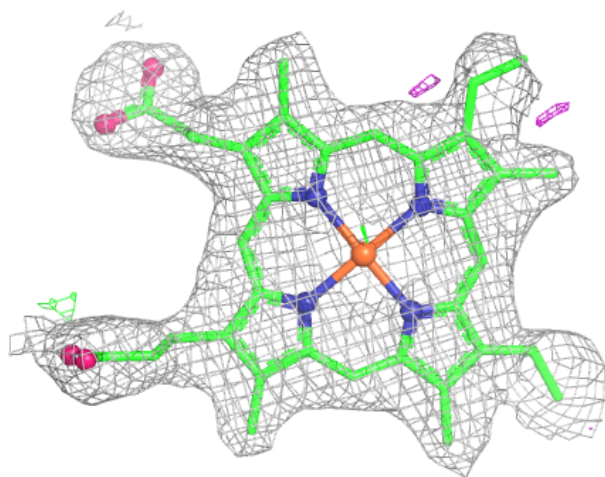
Electron density around HEC B 401:

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



Electron density around HEC A 402:

$2mF_o-DF_c$ (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.