



Full wwPDB X-ray Structure Validation Report ⓘ

Aug 4, 2026 – 09:17 PM EDT

PDB ID : 6E1C / pdb_00006e1c
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	:	4-5-2 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	:	9.0.015 (Gargrove)
Density-Fitness	:	1.0.12
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.50

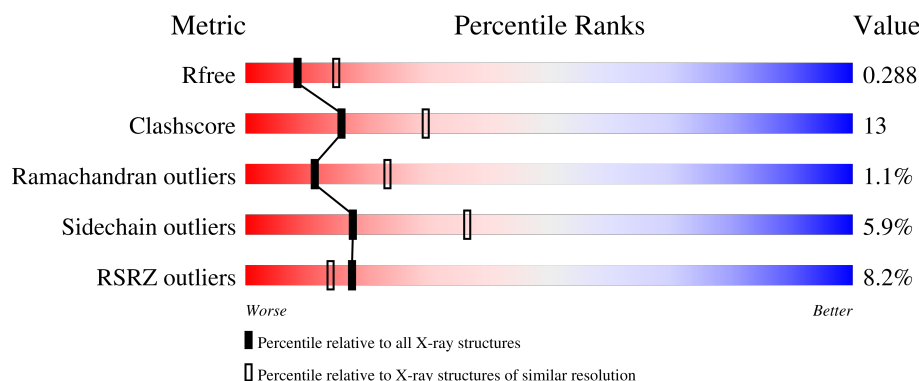
1 Overall quality at a glance

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}	180053	4951 (2.64-2.60)
Clashscore	190562	5303 (2.64-2.60)
Ramachandran outliers	187476	5217 (2.64-2.60)
Sidechain outliers	187428	5217 (2.64-2.60)
RSRZ outliers	180081	4950 (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	3% 71% 17% 10%
1	B	388	11% 59% 18% 5% 17%

The following table lists non-polymeric compounds, carbohydrate monomers and non-standard residues in protein, DNA, RNA chains that are outliers for geometric or electron-density-fit criteria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
2	HEC	A	401	X	-	-	-
2	HEC	A	402	X	-	-	-
2	HEC	B	401	X	-	-	-
2	HEC	B	402	X	-	-	-

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.

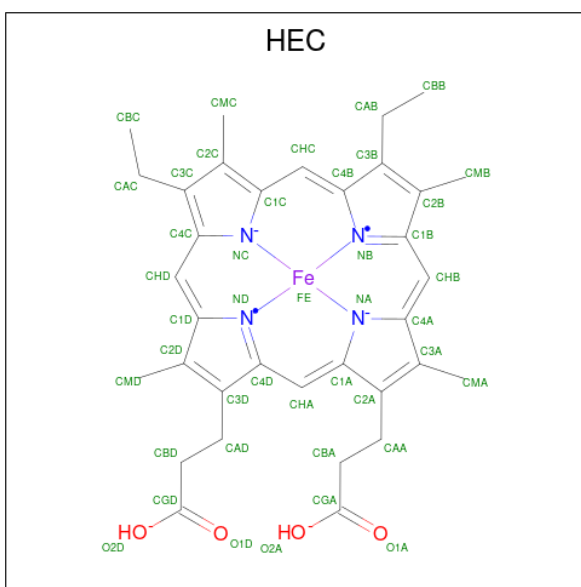
- Molecule 1 is a protein called Di-heme enzyme.

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 (CCD ID: HEC) (formula: $C_{34}H_{36}FeN_4O_4$).



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 (CCD ID: CA) (formula: Ca).

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

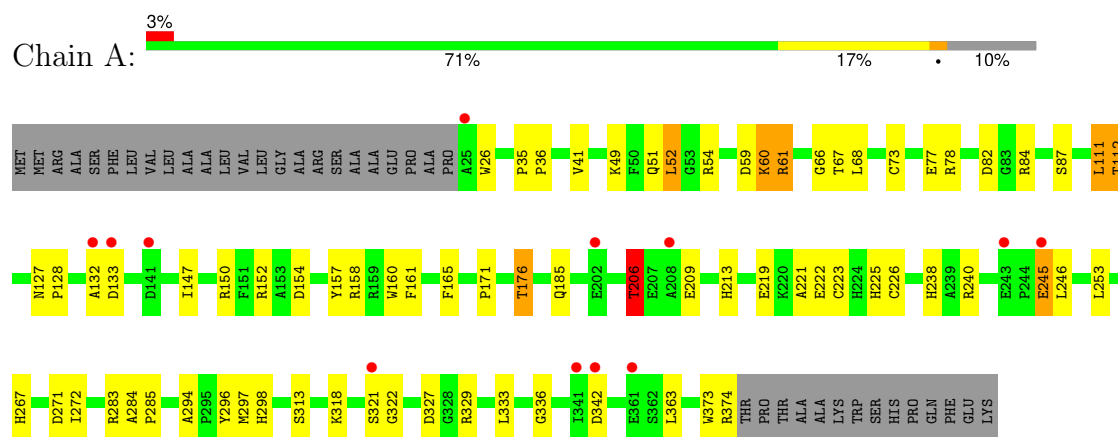
- Molecule 4 is water.

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

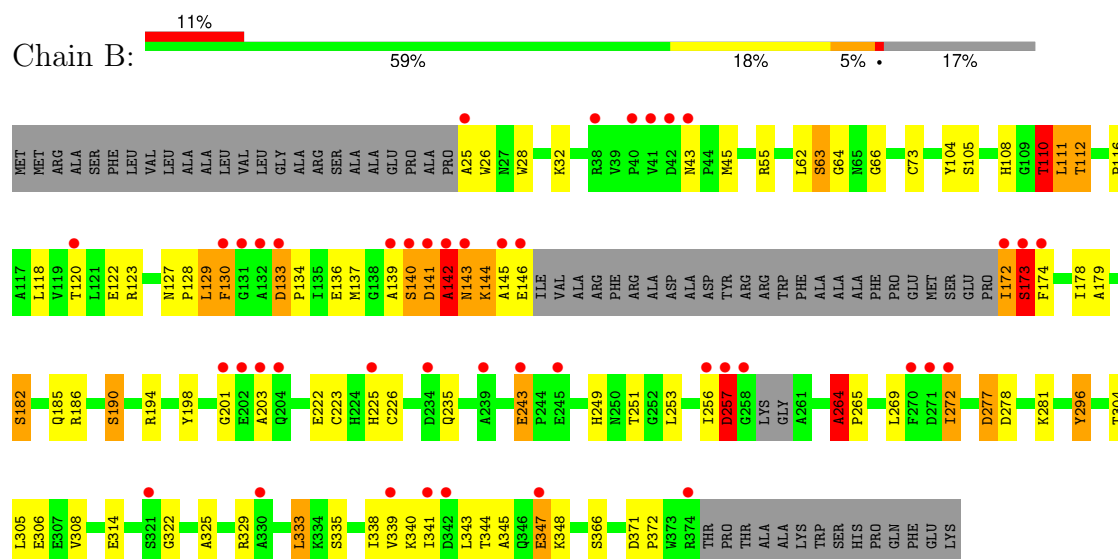
3 Residue-property plots [i](#)

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

• Molecule 1: 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	2000 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 [i](#)

5.1 Standard geometry [i](#)

Bond lengths and bond angles in the following residue types are not validated in this section: CA, 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	1.01	5/2802 (0.2%)	1.29	13/3805 (0.3%)
1	B	0.98	6/2569 (0.2%)	1.54	33/3487 (0.9%)
All	All	0.99	11/5371 (0.2%)	1.42	46/7292 (0.6%)

All (11) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	133	ASP	CA-C	7.23	1.58	1.53
1	A	298	HIS	C-O	-6.87	1.15	1.24
1	B	296	TYR	C-O	-6.47	1.15	1.23
1	A	296	TYR	C-O	-5.65	1.16	1.23
1	B	345	ALA	C-O	-5.64	1.16	1.24
1	A	133	ASP	CA-CB	5.62	1.56	1.52
1	B	142	ALA	CA-C	5.55	1.60	1.52
1	B	110	THR	C-O	-5.53	1.17	1.23
1	A	294	ALA	CA-C	-5.39	1.47	1.53
1	B	141	ASP	C-O	-5.31	1.17	1.24
1	B	130	PHE	N-CA	5.28	1.52	1.46

All (46) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	140	SER	N-CA-C	26.38	147.27	111.92
1	A	111	LEU	CA-C-N	23.09	165.63	121.54
1	A	111	LEU	C-N-CA	23.09	165.63	121.54
1	B	129	LEU	N-CA-C	20.80	136.50	111.33
1	B	25	ALA	CB-CA-C	20.07	140.61	110.50
1	B	63	SER	N-CA-C	15.99	128.41	111.14
1	B	140	SER	CB-CA-C	-14.42	92.02	111.63
1	B	257	ASP	N-CA-C	13.74	131.08	114.04

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	174	PHE	N-CA-C	12.55	126.14	111.71
1	B	25	ALA	N-CA-C	-12.26	76.68	111.00
1	A	111	LEU	N-CA-C	-10.21	94.31	110.14
1	B	340	LYS	N-CA-CB	-9.82	93.80	110.80
1	A	322	GLY	N-CA-C	9.78	132.29	112.34
1	B	111	LEU	N-CA-C	-9.07	96.08	110.14
1	B	130	PHE	N-CA-C	-8.88	93.75	108.76
1	B	257	ASP	CB-CA-C	-8.87	93.36	109.15
1	B	339	VAL	N-CA-C	-8.53	91.61	109.34
1	B	141	ASP	CA-C-N	8.32	137.43	121.54
1	B	141	ASP	C-N-CA	8.32	137.43	121.54
1	B	26	TRP	N-CA-CB	8.13	123.15	110.71
1	B	190	SER	CA-C-N	-7.19	112.17	123.24
1	B	190	SER	C-N-CA	-7.19	112.17	123.24
1	B	173	SER	CB-CA-C	-7.14	96.21	110.42
1	A	112	THR	N-CA-CB	-7.13	98.45	110.49
1	A	245	GLU	N-CA-C	6.43	124.50	110.80
1	B	26	TRP	N-CA-C	-6.43	96.42	107.61
1	A	132	ALA	N-CA-C	-6.34	99.98	109.94
1	B	272	ILE	CB-CA-C	6.30	117.35	111.30
1	B	264	ALA	CA-C-N	-6.25	113.81	120.94
1	B	264	ALA	C-N-CA	-6.25	113.81	120.94
1	A	296	TYR	N-CA-C	6.19	119.62	109.72
1	B	190	SER	N-CA-C	-6.08	99.49	108.79
1	A	246	LEU	N-CA-C	5.79	122.60	109.81
1	B	243	GLU	CB-CA-C	5.61	115.88	111.00
1	A	112	THR	CB-CA-C	5.40	121.17	110.42
1	B	296	TYR	CA-C-N	5.27	131.61	121.54
1	B	296	TYR	C-N-CA	5.27	131.61	121.54
1	B	142	ALA	N-CA-C	-5.25	99.63	110.80
1	A	36	PRO	O-C-N	5.12	123.67	121.31
1	B	64	GLY	N-CA-C	-5.11	101.07	113.18
1	B	253	LEU	N-CA-C	-5.09	106.91	113.23
1	A	26	TRP	N-CA-C	5.08	117.06	109.59
1	A	321	SER	N-CA-C	5.04	117.82	109.85
1	B	366	SER	N-CA-C	5.04	116.04	109.64
1	B	371	ASP	CA-C-N	-5.02	115.17	121.00
1	B	371	ASP	C-N-CA	-5.02	115.17	121.00

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	69	1
1	B	2504	0	2395	77	1
2	A	86	0	63	21	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	140	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 (140) 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
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:A:318:LYS:CG	1:A:327:ASP:OD2	2.12	0.96
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:B:223:CYS:HG	2:B:402:HEC:HBB3	1.33	0.88
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:318:LYS:HG3	1:A:327:ASP:CG	2.00	0.87
1:A:154:ASP:O	1:A:158:ARG:HG3	1.80	0.82

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:253:LEU:HD11	1:A:297:MET:HE2	1.67	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:140:SER:O	1:B:141:ASP:C	2.32	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: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:A:297:MET:HE3	2:A:401:HEC:HBD1	1.75	0.68
1:A:223:CYS:HG	2:A:401:HEC:HBB3	1.54	0.67
1:B:264:ALA:HB1	1:B:265:PRO:CD	2.23	0.67
1:B:143:ASN:C	1:B:145:ALA:H	2.03	0.66
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
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:28:TRP:CH2	1:B:45:MET:HE3	2.34	0.63
1:B:198:TYR:HA	1:B:203:ALA:HA	1.80	0.62
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	0.59
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:62:LEU:O	1:B:62:LEU:HG	2.03	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:206:THR:HB	1:A:209:GLU:CD	2.29	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:A:225:HIS:NE2	1:B:314:GLU:OE1	2.39	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:HHB	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:B:63:SER:HB3	1:B:66:GLY:H	1.73	0.53
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:A:297:MET:HE3	2:A:401:HEC:CBD	2.41	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:45:MET:HE1	1:B:186:ARG:HD2	1.93	0.49
1:B:118:LEU:HA	1:B:123:ARG:HH21	1.77	0.49
1:A:77:GLU:H	1:A:77:GLU:CD	2.15	0.49
1:A:219:GLU:OE1	1:A:222:GLU:CD	2.56	0.49
1:B:104:TYR:OH	1:B:190:SER:O	2.21	0.49
1:B:343:LEU:HD22	1:B:347:GLU:CD	2.38	0.48
1:B:143:ASN:C	1:B:145:ALA:N	2.71	0.48
1:B:140:SER:C	1:B:142:ALA:N	2.67	0.48
1:A:152:ARG:O	1:A:158:ARG:HD3	2.14	0.48
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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:219:GLU:OE2	1:B:329:ARG:NH2	2.50	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: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:A:112:THR:O	1:A:283:ARG:CZ	2.66	0.43
1:B:28:TRP:HH2	1:B:45:MET:HE3	1.77	0.43
1:A:213:HIS:HE1	4:A:504:HOH:O	2.02	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: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:82:ASP:OD2	1:A:87:SER:OG	2.36	0.42
1:A:284:ALA:HA	1:A:285:PRO:HD3	1.92	0.42
1:B:110:THR:OG1	1:B:235:GLN:CD	2.52	0.42
1:A:78:ARG:NH1	1:A:78:ARG:HG2	2.34	0.41
1:A:297:MET:HE3	2:A:401:HEC:CGD	2.49	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: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
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%)	21	39
1	B	317/388 (82%)	275 (87%)	37 (12%)	5 (2%)	7	15
All	All	665/776 (86%)	591 (89%)	67 (10%)	7 (1%)	11	23

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
1	B	142	ALA
1	A	206	THR
1	B	201	GLY

5.3.2 Protein sidechains [i](#)

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	282/310 (91%)	268 (95%)	14 (5%)	22	44

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	B	262/310 (84%)	244 (93%)	18 (7%)	14	30
All	All	544/620 (88%)	512 (94%)	32 (6%)	18	36

All (32) 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	60	LYS
1	A	61	ARG
1	A	111	LEU
1	A	176	THR
1	A	206	THR
1	A	245	GLU
1	A	272	ILE
1	A	313	SER
1	A	329	ARG
1	A	333	LEU
1	A	342	ASP
1	B	32	LYS
1	B	110	THR
1	B	112	THR
1	B	129	LEU
1	B	143	ASN
1	B	144	LYS
1	B	146	GLU
1	B	172	ILE
1	B	182	SER
1	B	194	ARG
1	B	257	ASP
1	B	272	ILE
1	B	277	ASP
1	B	333	LEU
1	B	335	SER
1	B	341	ILE
1	B	344	THR
1	B	347	GLU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (12) 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	267	HIS
1	B	143	ASN
1	B	185	GLN
1	B	224	HIS
1	B	238	HIS
1	B	249	HIS
1	B	267	HIS
1	B	346	GLN

5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

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	402	1	50,50,50	2.94	27 (54%)	68,82,82	2.64	30 (44%)
2	HEC	B	401	1	50,50,50	2.72	28 (56%)	68,82,82	2.83	38 (55%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
2	HEC	A	402	1	50,50,50	2.83	27 (54%)	68,82,82	2.80	32 (47%)
2	HEC	A	401	1	50,50,50	2.89	26 (52%)	68,82,82	2.54	33 (48%)

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	402	1	1/1/3/7	8/14/54/54	-
2	HEC	B	401	1	1/1/3/7	8/14/54/54	-
2	HEC	A	402	1	1/1/3/7	6/14/54/54	-
2	HEC	A	401	1	1/1/3/7	6/14/54/54	-

All (108) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	402	HEC	CHA-C1A	5.86	1.49	1.38
2	B	401	HEC	CHA-C1A	5.83	1.49	1.38
2	A	401	HEC	C3B-C2B	5.77	1.49	1.36
2	B	402	HEC	C3B-C2B	5.57	1.48	1.36
2	A	401	HEC	C2A-C3A	5.53	1.48	1.36
2	A	402	HEC	C2A-C3A	5.38	1.48	1.36
2	A	401	HEC	CHA-C1A	5.31	1.48	1.38
2	B	402	HEC	FE-ND	5.21	2.11	1.94
2	B	401	HEC	C2A-C3A	5.05	1.47	1.36
2	B	402	HEC	C2A-C3A	5.01	1.47	1.36
2	A	402	HEC	C4B-NB	-4.97	1.31	1.40
2	B	402	HEC	FE-NC	4.96	2.11	1.95
2	A	401	HEC	FE-ND	4.87	2.09	1.94
2	A	401	HEC	FE-NB	4.86	2.09	1.94
2	A	401	HEC	FE-NC	4.71	2.10	1.95
2	B	402	HEC	CHC-C4B	4.71	1.47	1.38
2	B	401	HEC	FE-ND	4.69	2.09	1.94
2	A	402	HEC	C3D-C2D	4.67	1.46	1.36
2	B	402	HEC	FE-NB	4.60	2.09	1.94
2	B	402	HEC	CHC-C1C	4.57	1.49	1.39
2	B	401	HEC	C3B-C2B	4.54	1.46	1.36
2	B	402	HEC	CHD-C1D	4.53	1.47	1.38
2	A	401	HEC	CHB-C4A	4.47	1.47	1.38
2	B	402	HEC	FE-NA	4.41	2.09	1.95

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	402	HEC	C3D-C2D	4.37	1.46	1.36
2	A	402	HEC	FE-NA	4.34	2.09	1.95
2	A	401	HEC	C3D-C2D	4.34	1.46	1.36
2	A	402	HEC	C1C-NC	-4.34	1.31	1.39
2	A	402	HEC	C3B-C2B	4.32	1.46	1.36
2	A	401	HEC	CHD-C1D	4.29	1.47	1.38
2	A	402	HEC	C1D-ND	-4.27	1.32	1.40
2	B	401	HEC	C4B-NB	-4.26	1.32	1.40
2	A	402	HEC	CHA-C1A	4.24	1.46	1.38
2	B	401	HEC	C4C-NC	-4.22	1.31	1.39
2	B	401	HEC	FE-NA	4.22	2.09	1.95
2	B	401	HEC	C3D-C2D	4.22	1.45	1.36
2	A	402	HEC	CHA-C4D	4.21	1.48	1.39
2	A	402	HEC	FE-NB	4.20	2.07	1.94
2	B	401	HEC	C1D-ND	-4.18	1.33	1.40
2	A	402	HEC	CHD-C1D	4.18	1.46	1.38
2	B	402	HEC	C3C-C2C	4.11	1.49	1.38
2	A	402	HEC	FE-ND	4.07	2.07	1.94
2	B	401	HEC	FE-NC	4.02	2.08	1.95
2	A	401	HEC	CHC-C1C	3.99	1.48	1.39
2	B	402	HEC	C4A-NA	-3.96	1.32	1.39
2	A	401	HEC	C1D-ND	-3.92	1.33	1.40
2	B	402	HEC	CHB-C1B	3.88	1.48	1.39
2	A	401	HEC	FE-NA	3.87	2.07	1.95
2	B	401	HEC	CHA-C4D	3.87	1.48	1.39
2	A	402	HEC	C4C-NC	-3.85	1.32	1.39
2	B	402	HEC	CHB-C4A	3.84	1.45	1.38
2	A	402	HEC	FE-NC	3.72	2.07	1.95
2	A	401	HEC	CHC-C4B	3.71	1.45	1.38
2	B	402	HEC	CHA-C4D	3.70	1.47	1.39
2	A	401	HEC	CHA-C4D	3.68	1.47	1.39
2	A	401	HEC	C4C-NC	-3.60	1.32	1.39
2	B	401	HEC	FE-NB	3.59	2.05	1.94
2	A	402	HEC	C4A-NA	-3.48	1.33	1.39
2	A	402	HEC	CHB-C4A	3.46	1.45	1.38
2	B	401	HEC	C1C-NC	-3.41	1.33	1.39
2	A	401	HEC	C3C-C2C	3.34	1.47	1.38
2	A	402	HEC	CHC-C4B	3.31	1.45	1.38
2	A	401	HEC	CHB-C1B	3.26	1.46	1.39
2	A	402	HEC	C3C-C2C	3.26	1.47	1.38
2	A	402	HEC	CHB-C1B	3.25	1.46	1.39
2	B	401	HEC	CHD-C1D	3.23	1.45	1.38

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	402	HEC	C4B-NB	-3.21	1.34	1.40
2	B	401	HEC	C3C-C2C	3.14	1.47	1.38
2	A	402	HEC	C1A-NA	-3.11	1.33	1.39
2	B	402	HEC	CHD-C4C	3.09	1.46	1.39
2	A	401	HEC	CHD-C4C	3.06	1.46	1.39
2	A	402	HEC	C4D-C3D	3.04	1.50	1.45
2	B	401	HEC	C1A-C2A	3.03	1.50	1.45
2	B	402	HEC	C1D-ND	-3.02	1.35	1.40
2	B	401	HEC	C4A-NA	-2.97	1.34	1.39
2	B	401	HEC	CHC-C4B	2.84	1.44	1.38
2	A	402	HEC	C1B-NB	-2.80	1.33	1.38
2	B	401	HEC	C1A-NA	-2.78	1.34	1.39
2	A	401	HEC	C1B-NB	-2.78	1.33	1.38
2	B	401	HEC	C4D-ND	-2.78	1.33	1.38
2	A	401	HEC	C4D-ND	-2.75	1.33	1.38
2	A	401	HEC	C1A-C2A	2.74	1.50	1.45
2	A	401	HEC	C4A-NA	-2.68	1.34	1.39
2	B	402	HEC	C4C-NC	-2.68	1.34	1.39
2	A	402	HEC	CHD-C4C	2.65	1.45	1.39
2	B	402	HEC	C1A-C2A	2.63	1.49	1.45
2	B	401	HEC	CHB-C4A	2.62	1.43	1.38
2	B	401	HEC	C1B-NB	-2.57	1.33	1.38
2	A	401	HEC	C4B-NB	-2.51	1.35	1.40
2	B	401	HEC	C1C-C2C	2.51	1.49	1.43
2	A	402	HEC	C1A-C2A	2.46	1.49	1.45
2	B	402	HEC	C1D-C2D	2.46	1.49	1.44
2	A	402	HEC	C1D-C2D	2.45	1.49	1.44
2	B	401	HEC	C4D-C3D	2.43	1.49	1.45
2	B	402	HEC	C1B-C2B	2.43	1.49	1.44
2	A	401	HEC	C1B-C2B	2.40	1.49	1.44
2	B	401	HEC	CHC-C1C	2.39	1.44	1.39
2	B	401	HEC	CHB-C1B	2.39	1.44	1.39
2	A	402	HEC	C1B-C2B	2.37	1.49	1.44
2	B	402	HEC	C1C-C2C	2.32	1.48	1.43
2	B	402	HEC	C4D-C3D	2.28	1.48	1.45
2	B	401	HEC	C1B-C2B	2.25	1.49	1.44
2	A	401	HEC	C1A-NA	-2.21	1.35	1.39
2	A	402	HEC	CHC-C1C	2.17	1.44	1.39
2	B	401	HEC	CHD-C4C	2.10	1.44	1.39
2	B	402	HEC	C4D-ND	-2.09	1.34	1.38
2	B	402	HEC	C1B-NB	-2.05	1.34	1.38
2	A	401	HEC	C1C-C2C	2.04	1.47	1.43

All (133) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	402	HEC	C1B-C2B-C3B	-7.72	98.86	106.98
2	A	402	HEC	C1B-C2B-C3B	-6.71	99.93	106.98
2	B	401	HEC	C1C-C2C-C3C	-6.34	99.56	106.82
2	B	401	HEC	C2D-C1D-ND	6.24	117.01	109.84
2	B	401	HEC	C1B-C2B-C3B	-6.20	100.46	106.98
2	A	401	HEC	C1C-C2C-C3C	-6.12	99.81	106.82
2	A	402	HEC	C1C-C2C-C3C	-5.95	100.00	106.82
2	A	401	HEC	C1B-C2B-C3B	-5.86	100.81	106.98
2	B	402	HEC	C1C-C2C-C3C	-5.79	100.18	106.82
2	B	402	HEC	C2B-C1B-NB	5.71	116.50	109.90
2	A	402	HEC	C2D-C1D-ND	5.50	116.17	109.84
2	A	401	HEC	CBC-CAC-C3C	5.10	126.24	112.42
2	A	402	HEC	CHB-C1B-NB	-5.08	118.96	124.42
2	B	401	HEC	C3C-C4C-NC	5.06	115.77	110.15
2	B	401	HEC	C1D-C2D-C3D	-5.02	101.70	106.98
2	A	402	HEC	C2B-C1B-NB	4.79	115.44	109.90
2	A	402	HEC	C3B-C4B-NB	4.78	115.41	110.17
2	A	401	HEC	C1D-C2D-C3D	-4.77	101.97	106.98
2	B	402	HEC	C2D-C1D-ND	4.73	115.28	109.84
2	B	401	HEC	CBC-CAC-C3C	4.73	125.23	112.42
2	A	401	HEC	C2D-C1D-ND	4.69	115.23	109.84
2	A	402	HEC	C3D-C4D-ND	4.67	114.86	110.35
2	B	402	HEC	C1D-C2D-C3D	-4.59	102.16	106.98
2	A	402	HEC	C1D-C2D-C3D	-4.56	102.18	106.98
2	B	402	HEC	C3D-C4D-ND	4.51	114.71	110.35
2	A	402	HEC	C2A-C1A-NA	4.43	114.60	110.32
2	A	401	HEC	C2B-C1B-NB	4.38	114.96	109.90
2	B	401	HEC	C2C-C1C-NC	4.13	116.77	110.14
2	B	401	HEC	C2B-C1B-NB	4.12	114.67	109.90
2	A	401	HEC	C3D-C4D-ND	4.10	114.32	110.35
2	B	401	HEC	CBA-CAA-C2A	-4.07	101.29	112.53
2	B	402	HEC	CHB-C1B-NB	-4.06	120.06	124.42
2	A	402	HEC	C2C-C1C-NC	4.05	116.63	110.14
2	B	401	HEC	C3D-C4D-ND	4.03	114.25	110.35
2	B	401	HEC	CAD-C3D-C4D	4.02	131.69	124.70
2	A	401	HEC	C2C-C1C-NC	4.01	116.57	110.14
2	B	401	HEC	CAC-C3C-C2C	4.00	133.21	126.89
2	B	402	HEC	C2A-C1A-NA	3.90	114.08	110.32
2	A	402	HEC	CBD-CAD-C3D	-3.86	101.87	112.53
2	B	401	HEC	C4A-C3A-C2A	-3.81	101.33	106.97
2	A	401	HEC	CBA-CAA-C2A	-3.79	102.05	112.53
2	A	402	HEC	C3C-C4C-NC	3.77	114.33	110.15

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	401	HEC	CBD-CAD-C3D	-3.76	102.12	112.53
2	B	402	HEC	CHB-C4A-NA	-3.73	120.39	124.45
2	B	402	HEC	CBD-CAD-C3D	-3.73	102.23	112.53
2	B	402	HEC	CBC-CAC-C3C	3.72	122.51	112.42
2	A	402	HEC	C4A-C3A-C2A	-3.71	101.47	106.97
2	A	401	HEC	CBD-CAD-C3D	-3.71	102.29	112.53
2	B	402	HEC	CAD-C3D-C4D	3.70	131.14	124.70
2	B	402	HEC	C1A-C2A-C3A	-3.68	102.26	107.11
2	B	401	HEC	C3A-C4A-NA	3.65	116.38	109.64
2	A	401	HEC	C3B-C4B-NB	3.63	114.15	110.17
2	A	402	HEC	C3A-C4A-NA	3.61	116.32	109.64
2	B	402	HEC	CMC-C2C-C3C	3.61	133.28	125.62
2	A	401	HEC	CHB-C1B-NB	-3.61	120.54	124.42
2	A	401	HEC	CAD-C3D-C4D	3.59	130.95	124.70
2	B	401	HEC	CHB-C1B-NB	-3.53	120.62	124.42
2	B	402	HEC	CMD-C2D-C1D	3.52	130.54	125.03
2	B	401	HEC	C3B-C4B-NB	3.51	114.02	110.17
2	A	402	HEC	CBC-CAC-C3C	3.49	121.88	112.42
2	A	402	HEC	CBA-CAA-C2A	-3.40	103.12	112.53
2	A	401	HEC	C2A-C1A-NA	3.39	113.59	110.32
2	B	401	HEC	CHA-C1A-NA	-3.39	120.77	124.45
2	A	401	HEC	CMC-C2C-C3C	3.35	132.72	125.62
2	B	402	HEC	C3A-C4A-NA	3.33	115.80	109.64
2	A	401	HEC	C1A-C2A-C3A	-3.31	102.75	107.11
2	B	401	HEC	CHA-C4D-ND	-3.30	120.87	124.42
2	A	402	HEC	C1A-C2A-C3A	-3.30	102.77	107.11
2	B	402	HEC	CBB-CAB-C3B	3.24	121.19	112.42
2	A	402	HEC	CMC-C2C-C3C	3.21	132.43	125.62
2	A	402	HEC	CHA-C1A-NA	-3.20	120.97	124.45
2	A	402	HEC	CBB-CAB-C3B	3.18	121.04	112.42
2	A	402	HEC	C4D-C3D-C2D	-3.13	102.34	106.89
2	B	401	HEC	CAA-C2A-C1A	3.11	131.17	124.85
2	A	401	HEC	CAB-C3B-C2B	3.05	133.16	127.56
2	A	402	HEC	CAB-C3B-C2B	3.05	133.16	127.56
2	A	402	HEC	CAC-C3C-C2C	3.02	131.67	126.89
2	B	402	HEC	CAC-C3C-C2C	3.01	131.66	126.89
2	A	401	HEC	C3C-C4C-NC	3.01	113.49	110.15
2	B	402	HEC	C2C-C1C-NC	3.00	114.95	110.14
2	B	401	HEC	C2A-C1A-NA	2.97	113.19	110.32
2	A	402	HEC	CAA-C2A-C1A	2.92	130.79	124.85
2	A	402	HEC	CMB-C2B-C1B	2.86	129.50	125.03
2	A	401	HEC	C3A-C4A-NA	2.85	114.91	109.64

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	401	HEC	C4D-C3D-C2D	-2.85	102.74	106.89
2	A	401	HEC	CHA-C4D-ND	-2.83	121.38	124.42
2	A	402	HEC	CHD-C1D-ND	-2.81	120.89	124.37
2	A	401	HEC	CHC-C4B-C3B	-2.80	120.06	125.23
2	B	401	HEC	CBB-CAB-C3B	2.77	119.93	112.42
2	B	401	HEC	CHC-C4B-C3B	-2.76	120.13	125.23
2	B	402	HEC	C3B-C4B-NB	2.75	113.18	110.17
2	A	402	HEC	CHC-C4B-C3B	-2.72	120.21	125.23
2	B	402	HEC	C3C-C4C-NC	2.72	113.17	110.15
2	A	401	HEC	C4A-C3A-C2A	-2.69	102.98	106.97
2	B	401	HEC	CMA-C3A-C4A	2.69	129.46	124.73
2	B	402	HEC	C4A-C3A-C2A	-2.68	103.00	106.97
2	B	402	HEC	CBA-CAA-C2A	-2.67	105.15	112.53
2	B	402	HEC	CMB-C2B-C3B	2.62	133.24	126.15
2	B	401	HEC	CMB-C2B-C1B	2.62	129.12	125.03
2	B	401	HEC	CHD-C1D-ND	-2.62	121.13	124.37
2	B	401	HEC	O1A-CGA-CBA	-2.61	114.82	123.09
2	B	401	HEC	CMC-C2C-C1C	2.59	129.36	125.42
2	B	401	HEC	CMC-C2C-C3C	2.57	131.08	125.62
2	A	402	HEC	CAD-C3D-C4D	2.57	129.17	124.70
2	A	402	HEC	O2D-CGD-CBD	2.57	122.11	114.00
2	B	402	HEC	O1A-CGA-CBA	-2.52	115.09	123.09
2	A	401	HEC	CHA-C1A-NA	-2.46	121.78	124.45
2	A	401	HEC	CHC-C1C-C2C	-2.46	120.29	127.43
2	A	401	HEC	CMD-C2D-C1D	2.42	128.82	125.03
2	B	401	HEC	C1A-C2A-C3A	-2.42	103.93	107.11
2	B	402	HEC	CAB-C3B-C4B	-2.39	121.69	124.79
2	A	402	HEC	CHB-C4A-NA	-2.36	121.88	124.45
2	B	402	HEC	CAB-C3B-C2B	2.36	131.89	127.56
2	A	401	HEC	C4D-C3D-C2D	-2.34	103.49	106.89
2	A	401	HEC	CBB-CAB-C3B	2.31	118.68	112.42
2	B	402	HEC	O2A-CGA-CBA	2.29	121.23	114.00
2	B	402	HEC	C4D-C3D-C2D	-2.28	103.58	106.89
2	A	401	HEC	CAA-CBA-CGA	2.28	119.70	113.67
2	B	401	HEC	O2A-CGA-CBA	2.26	121.15	114.00
2	B	401	HEC	CHD-C1D-C2D	-2.21	120.67	126.95
2	B	401	HEC	CMD-C2D-C1D	2.20	128.47	125.03
2	A	402	HEC	CMA-C3A-C4A	2.20	128.60	124.73
2	A	402	HEC	CHC-C1C-C2C	-2.18	121.09	127.43
2	B	401	HEC	CAB-C3B-C2B	2.13	131.48	127.56
2	B	402	HEC	CAA-C2A-C1A	2.13	129.18	124.85
2	A	401	HEC	CMB-C2B-C3B	2.13	131.90	126.15

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	401	HEC	CHB-C4A-C3A	-2.12	121.07	125.49
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
2	A	401	HEC	CAC-C3C-C2C	2.04	130.12	126.89
2	A	401	HEC	CAB-C3B-C4B	-2.02	122.16	124.79
2	B	401	HEC	CHC-C1C-NC	-2.01	120.22	123.86
2	B	401	HEC	C1A-CHA-C4D	2.00	130.27	126.02

All (4) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
2	A	401	HEC	NA
2	A	402	HEC	NA
2	B	401	HEC	NA
2	B	402	HEC	NA

All (28) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	A	401	HEC	C4C-C3C-CAC-CBC
2	A	402	HEC	C4C-C3C-CAC-CBC
2	B	401	HEC	C4C-C3C-CAC-CBC
2	B	402	HEC	C4C-C3C-CAC-CBC
2	A	401	HEC	C4B-C3B-CAB-CBB
2	A	402	HEC	C4B-C3B-CAB-CBB
2	B	401	HEC	C4B-C3B-CAB-CBB
2	B	402	HEC	C4B-C3B-CAB-CBB
2	A	401	HEC	C2B-C3B-CAB-CBB
2	B	402	HEC	C2B-C3B-CAB-CBB
2	B	401	HEC	C2B-C3B-CAB-CBB
2	A	402	HEC	C2B-C3B-CAB-CBB
2	A	401	HEC	C2C-C3C-CAC-CBC
2	A	402	HEC	C2C-C3C-CAC-CBC
2	B	401	HEC	C2C-C3C-CAC-CBC
2	B	402	HEC	C2C-C3C-CAC-CBC
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
2	B	401	HEC	CAA-CBA-CGA-O1A

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Mol	Chain	Res	Type	Atoms
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

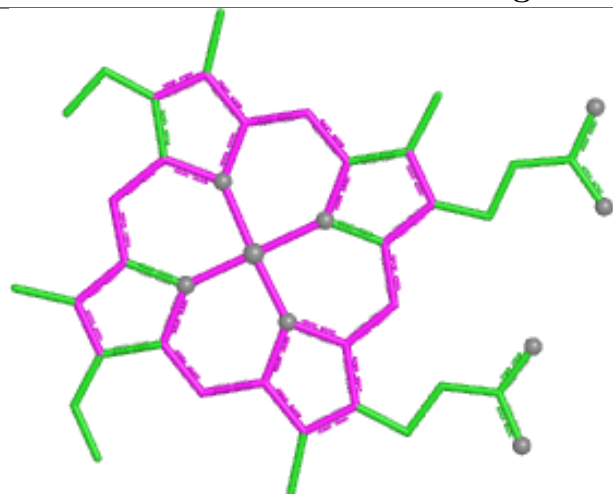
There are no ring outliers.

4 monomers are involved in 37 short contacts:

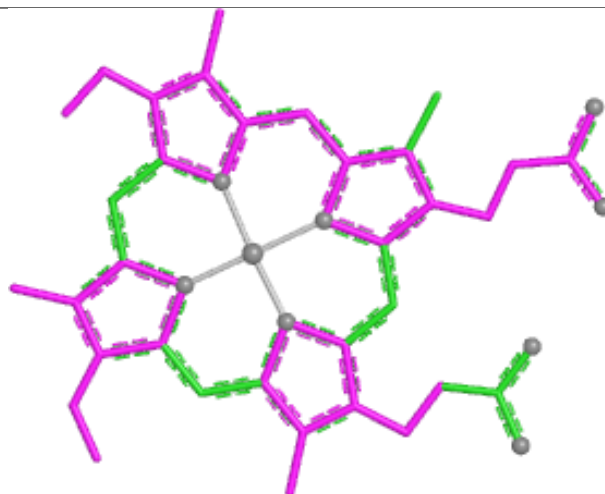
Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	B	402	HEC	10	0
2	B	401	HEC	6	0
2	A	402	HEC	7	0
2	A	401	HEC	14	0

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.

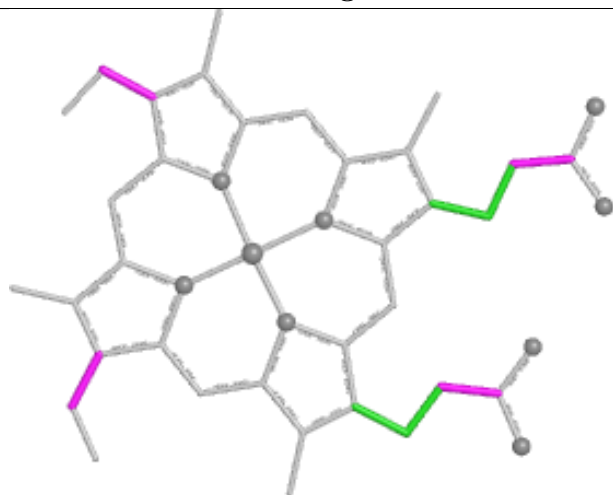
Ligand HEC B 402



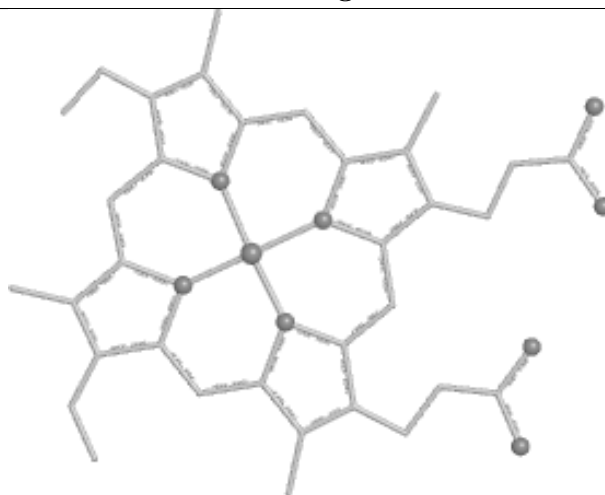
Bond lengths



Bond angles

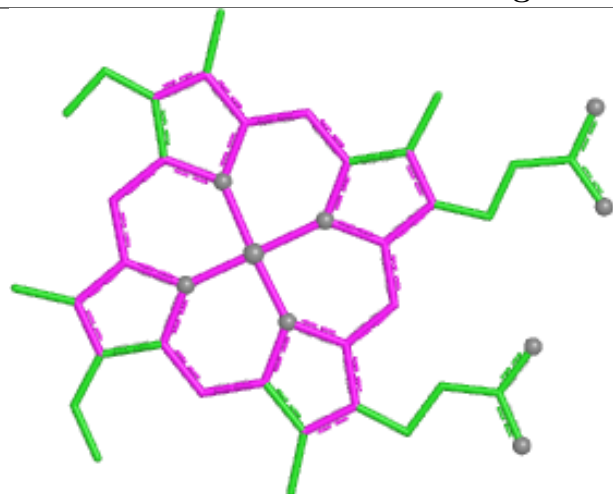


Torsions

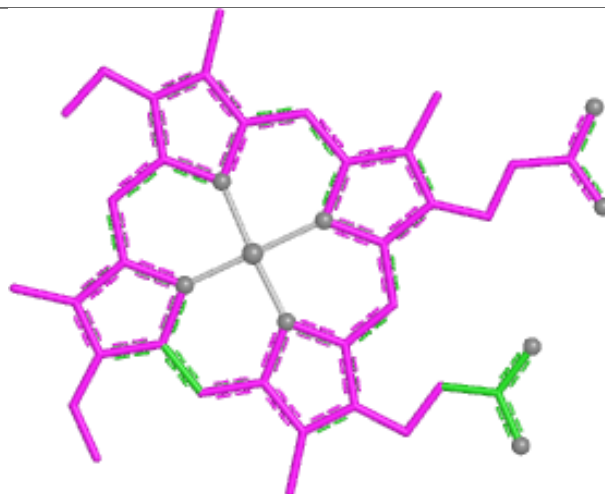


Rings

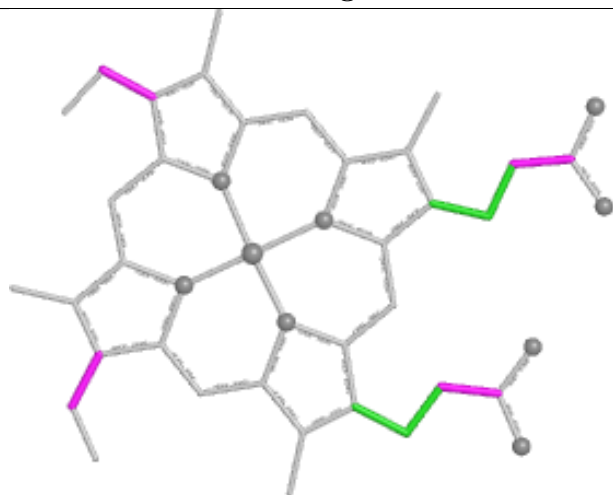
Ligand HEC B 401



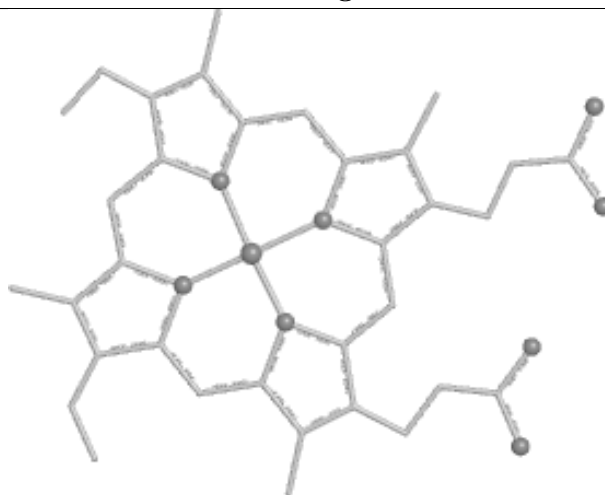
Bond lengths



Bond angles

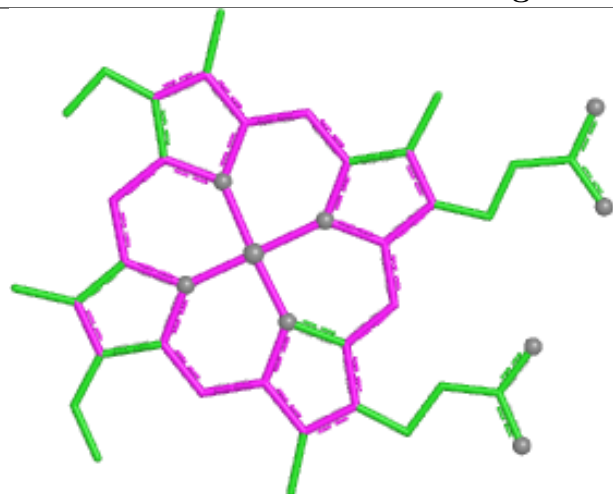


Torsions

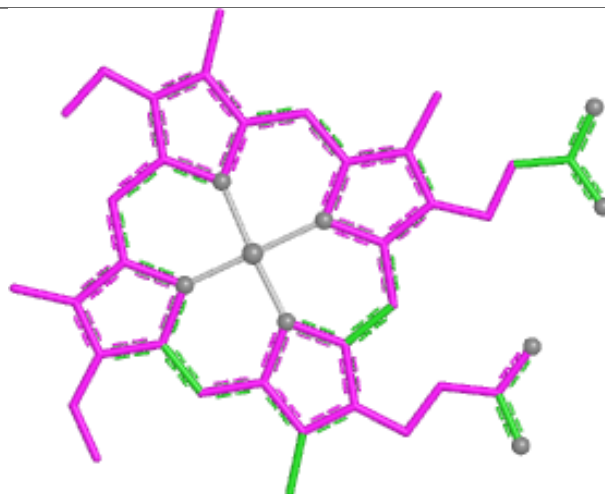


Rings

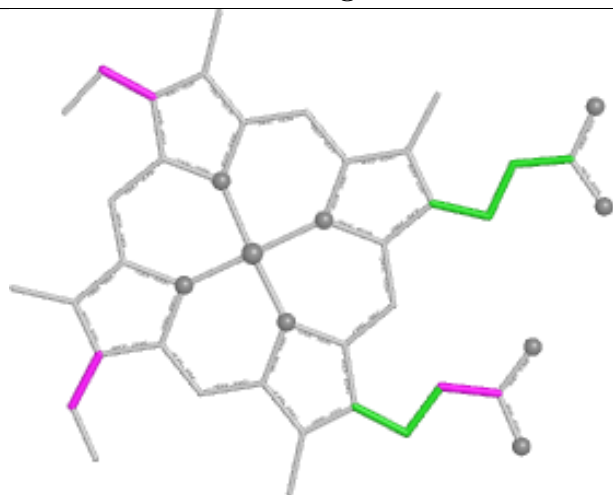
Ligand HEC A 402



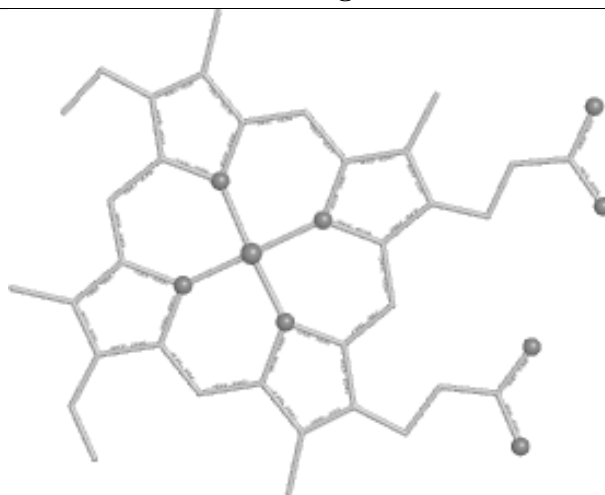
Bond lengths



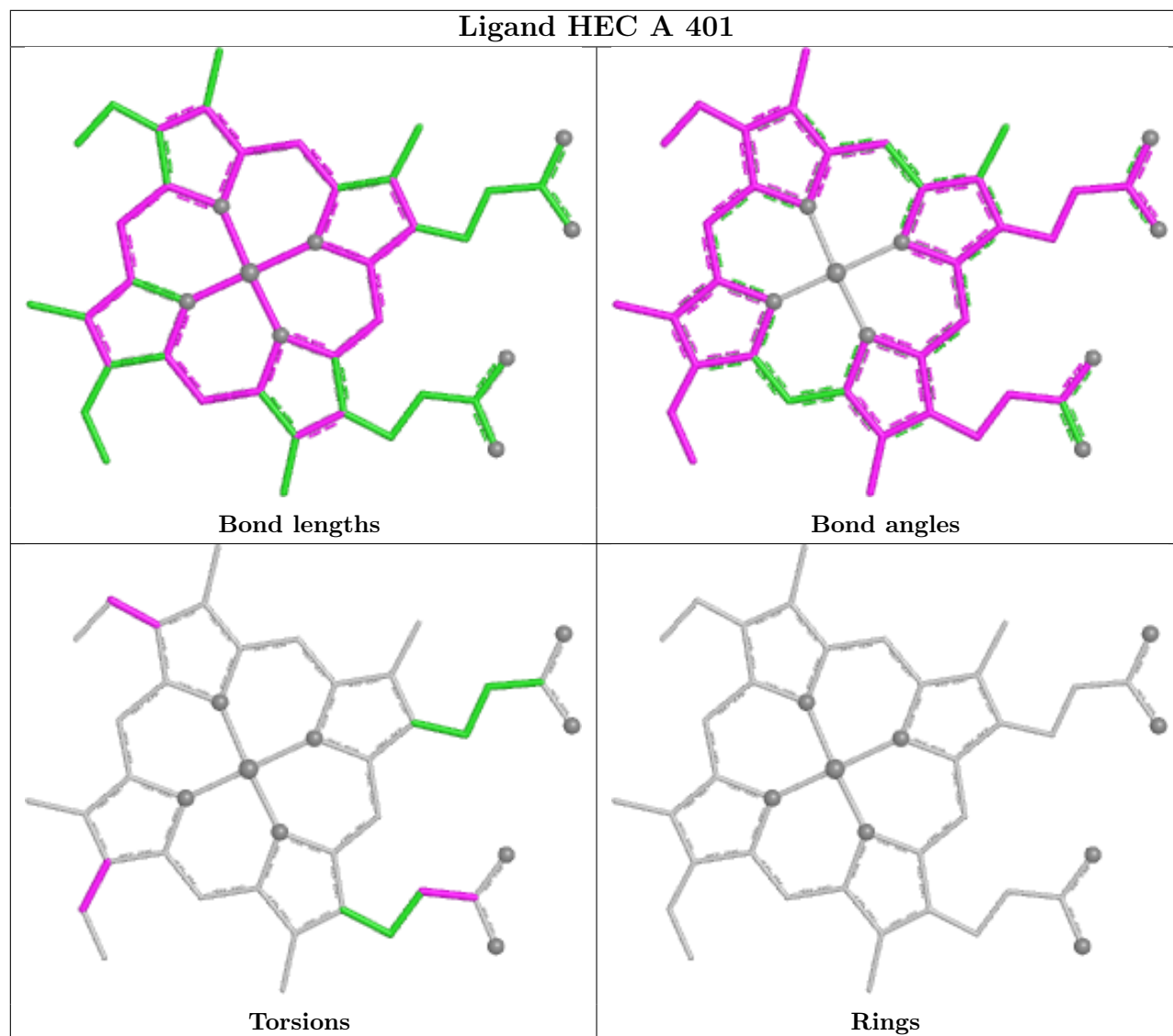
Bond angles



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%)	0.15	12 (3%) 48 43	5, 22, 47, 66	0
1	B	323/388 (83%)	0.73	43 (13%) 7 5	7, 32, 63, 87	0
All	All	673/776 (86%)	0.43	55 (8%) 17 14	5, 26, 59, 87	0

All (55) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	142	ALA	7.0
1	B	132	ALA	5.9
1	B	172	ILE	5.9
1	B	25	ALA	5.6
1	B	342	ASP	4.5
1	B	141	ASP	4.5
1	B	146	GLU	4.2
1	B	374	ARG	4.0
1	B	140	SER	3.9
1	B	203	ALA	3.7
1	B	341	ILE	3.6
1	B	41	VAL	3.6
1	B	133	ASP	3.5
1	A	25	ALA	3.5
1	A	133	ASP	3.4
1	B	139	ALA	3.3
1	B	339	VAL	3.2
1	A	321	SER	3.2
1	B	145	ALA	3.1
1	B	258	GLY	3.1
1	A	202	GLU	3.0
1	B	201	GLY	3.0
1	A	342	ASP	2.9
1	B	321	SER	2.8

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Mol	Chain	Res	Type	RSRZ
1	B	143	ASN	2.7
1	B	131	GLY	2.7
1	B	256	ILE	2.7
1	B	243	GLU	2.6
1	B	42	ASP	2.6
1	A	341	ILE	2.6
1	B	43	ASN	2.6
1	B	239	ALA	2.6
1	A	243	GLU	2.5
1	B	347	GLU	2.5
1	B	38	ARG	2.5
1	B	204	GLN	2.5
1	B	40	PRO	2.5
1	B	234	ASP	2.4
1	B	174	PHE	2.4
1	B	330	ALA	2.4
1	B	272	ILE	2.4
1	B	257	ASP	2.4
1	B	120	THR	2.3
1	B	245	GLU	2.3
1	A	208	ALA	2.2
1	B	270	PHE	2.2
1	B	202	GLU	2.2
1	A	132	ALA	2.1
1	A	141	ASP	2.1
1	B	130	PHE	2.1
1	A	245	GLU	2.1
1	B	225	HIS	2.0
1	A	361	GLU	2.0
1	B	271	ASP	2.0
1	B	173	SER	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](#)

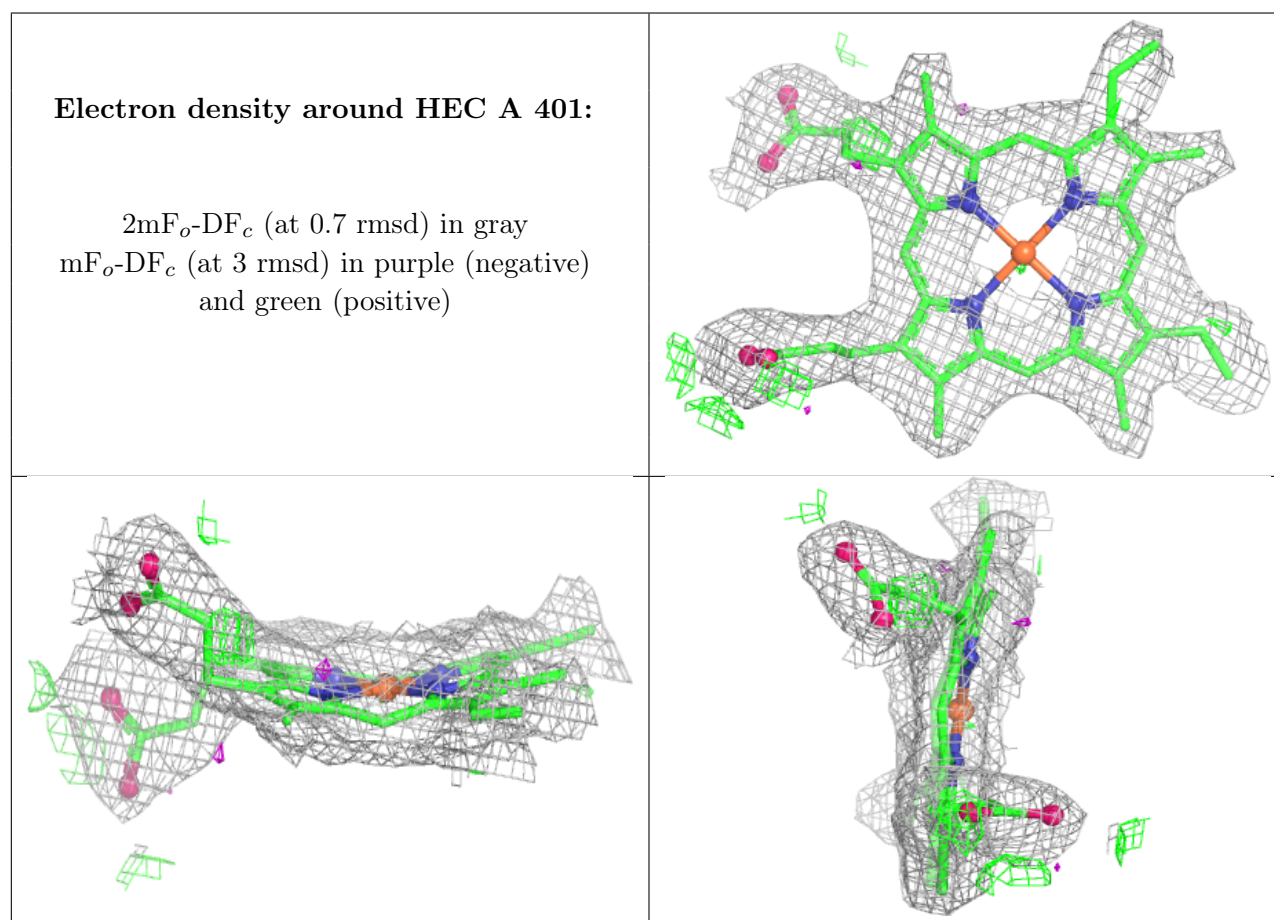
There are no oligosaccharides in this entry.

6.4 Ligands ⓘ

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.

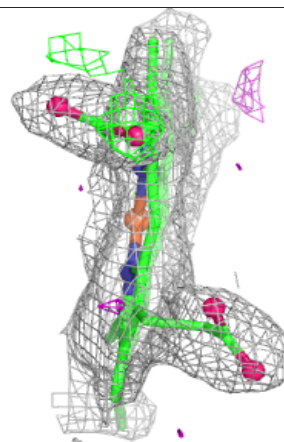
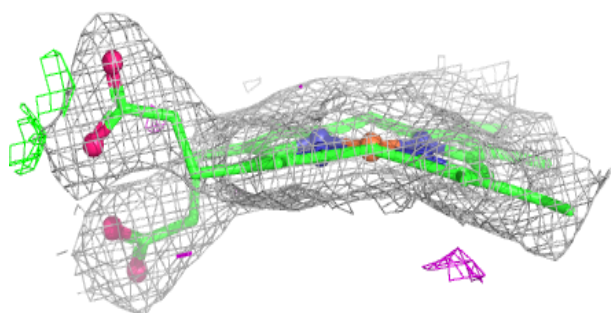
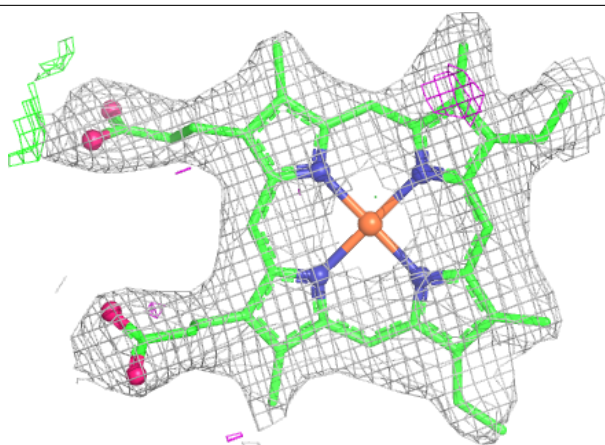
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
3	CA	A	403	1/1	0.80	0.03	5,5,5,5	0
2	HEC	A	401	43/43	0.94	0.10	9,12,15,16	0
2	HEC	B	402	43/43	0.95	0.10	15,18,22,26	0
2	HEC	B	401	43/43	0.95	0.11	14,17,28,33	0
2	HEC	A	402	43/43	0.96	0.09	9,9,17,22	0
3	CA	B	403	1/1	0.97	0.06	11,11,11,11	0

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.



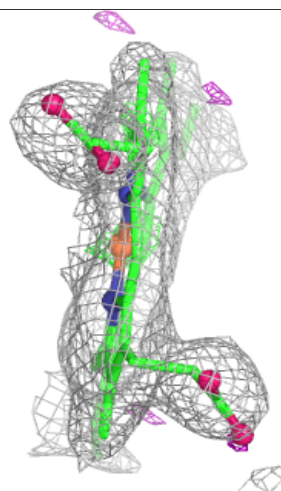
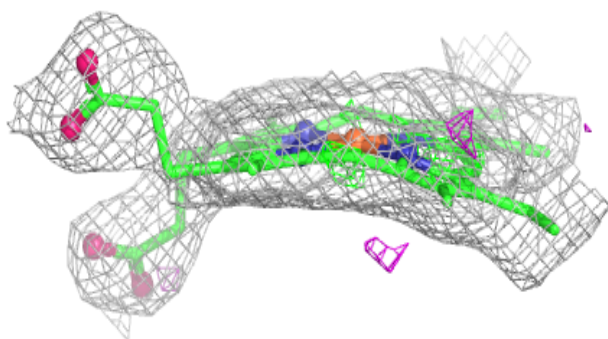
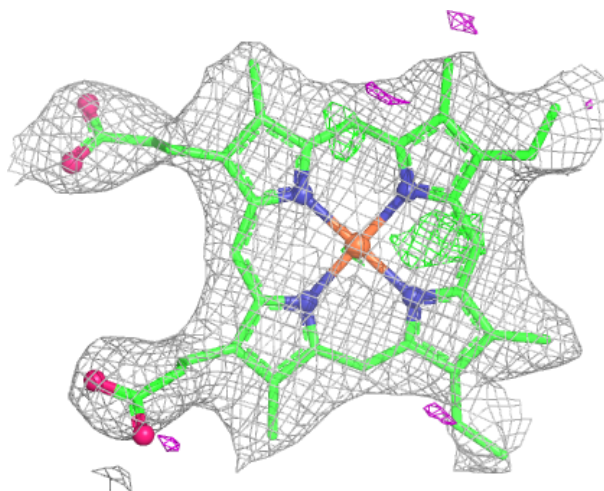
Electron density around HEC B 402:

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



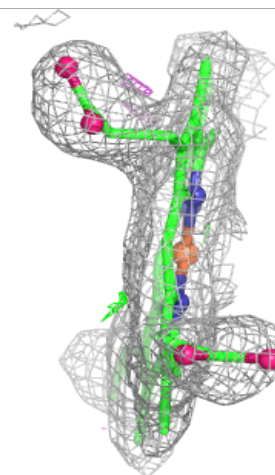
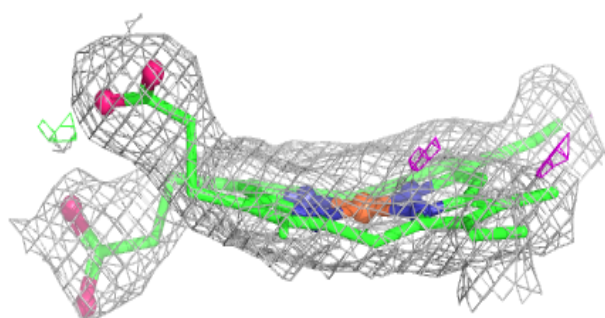
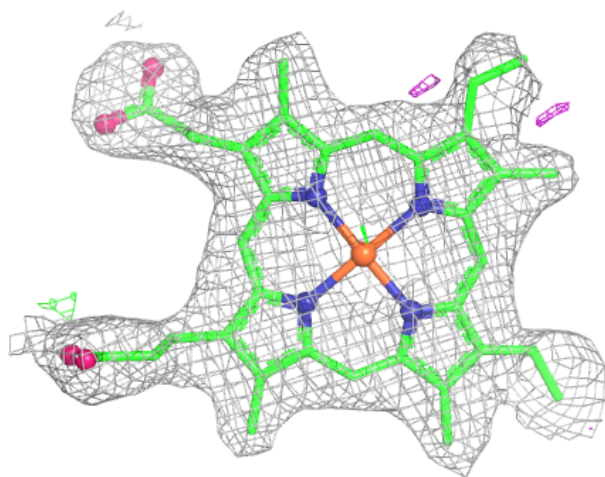
Electron density around HEC B 401:

$2mF_o-DF_c$ (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.