Full wwPDB X-ray Structure Validation Report ⓘ

May 16, 2020 – 04:40 pm BST

PDB ID	:	4FAV
Title	:	Crystal Structure of WT MauG in Complex with Pre-Methylamine Dehydrogenase Aged 50 Days
Authors	:	Yukl, E.T.; Wilmot, C.M.
Deposited on	:	2012-05-22
Resolution	:	2.08 Å(reported)

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

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

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

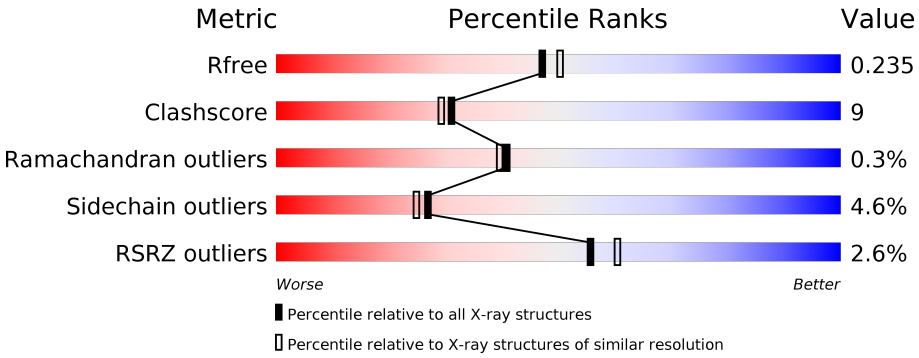
MolProbity	:	4.02b-467
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.11
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber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

1 Overall quality at a glance (i)

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

The reported resolution of this entry is 2.08 Å.

Percentile scores (ranging between 0-100) for global validation metrics of the entry are shown in the following graphic. The table shows the number of entries on which the scores are based.



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	130704	6189 (2.10-2.06)
Clashscore	141614	6738 (2.10-2.06)
Ramachandran outliers	138981	6663 (2.10-2.06)
Sidechain outliers	138945	6664 (2.10-2.06)
RSRZ outliers	127900	6057 (2.10-2.06)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments on the lower bar indicate the fraction of residues that contain outliers for >=3, 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions <=5% The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density. The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	A	373	2% 73% 20% • 5%
1	B	373	% 80% 14% • •
2	C	137	3% 72% 18% • 9%
2	E	137	4% 67% 23% • 9%
3	D	385	5% 73% 23% • •
3	F	385	% 83% 15% • •

2 Entry composition

There are 10 unique types of molecules in this entry. The entry contains 14424 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 Methylamine utilization protein MauG.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	354	Total	C	N	O	S	0	4	0
			2773	1729	503	530	11			
1	B	357	Total	C	N	O	S	0	6	0
			2819	1754	511	542	12			

There are 12 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	368	HIS	-	EXPRESSION TAG	UNP Q51658
A	369	HIS	-	EXPRESSION TAG	UNP Q51658
A	370	HIS	-	EXPRESSION TAG	UNP Q51658
A	371	HIS	-	EXPRESSION TAG	UNP Q51658
A	372	HIS	-	EXPRESSION TAG	UNP Q51658
A	373	HIS	-	EXPRESSION TAG	UNP Q51658
B	368	HIS	-	EXPRESSION TAG	UNP Q51658
B	369	HIS	-	EXPRESSION TAG	UNP Q51658
B	370	HIS	-	EXPRESSION TAG	UNP Q51658
B	371	HIS	-	EXPRESSION TAG	UNP Q51658
B	372	HIS	-	EXPRESSION TAG	UNP Q51658
B	373	HIS	-	EXPRESSION TAG	UNP Q51658

- Molecule 2 is a protein called Methylamine dehydrogenase light chain.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	C	125	Total	C	N	O	S	0	2	0
			966	598	163	191	14			
2	E	125	Total	C	N	O	S	0	4	0
			972	601	162	193	16			

There are 12 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
C	132	HIS	-	EXPRESSION TAG	UNP P22619
C	133	HIS	-	EXPRESSION TAG	UNP P22619
C	134	HIS	-	EXPRESSION TAG	UNP P22619
C	135	HIS	-	EXPRESSION TAG	UNP P22619
C	136	HIS	-	EXPRESSION TAG	UNP P22619
C	137	HIS	-	EXPRESSION TAG	UNP P22619
E	132	HIS	-	EXPRESSION TAG	UNP P22619
E	133	HIS	-	EXPRESSION TAG	UNP P22619
E	134	HIS	-	EXPRESSION TAG	UNP P22619
E	135	HIS	-	EXPRESSION TAG	UNP P22619
E	136	HIS	-	EXPRESSION TAG	UNP P22619
E	137	HIS	-	EXPRESSION TAG	UNP P22619

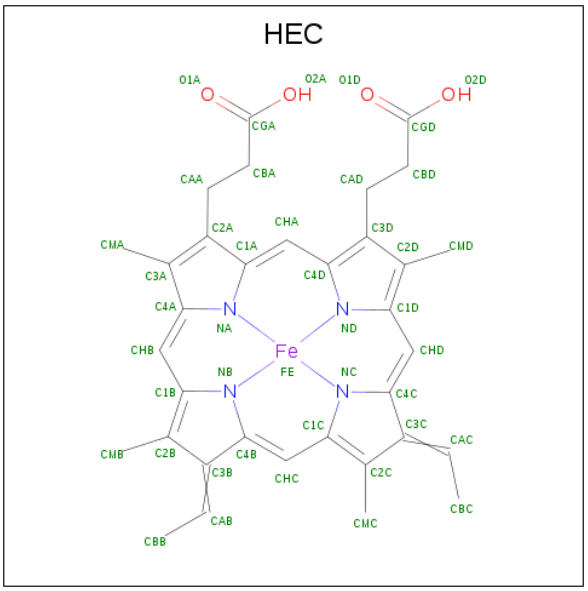
- Molecule 3 is a protein called Methylamine dehydrogenase heavy chain.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	D	376	Total	C	N	O	S	0	3	0
			2945	1865	507	564	9			
3	F	377	Total	C	N	O	S	0	4	0
			2962	1875	512	566	9			

- Molecule 4 is CALCIUM ION (three-letter code: CA) (formula: Ca).

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

- Molecule 5 is HEME C (three-letter code: HEC) (formula: $C_{34}H_{34}FeN_4O_4$).

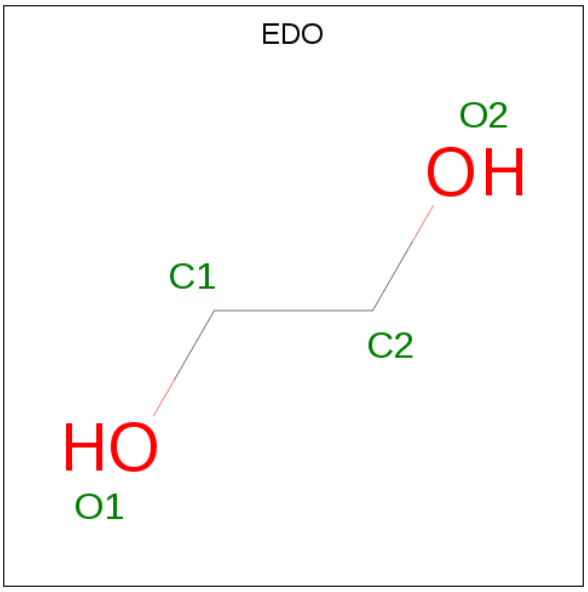


Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
5	A	1	Total	C	Fe	N	O	0	0
			43	34	1	4	4		
5	A	1	Total	C	Fe	N	O	0	0
			43	34	1	4	4		
5	B	1	Total	C	Fe	N	O	0	0
			43	34	1	4	4		
5	B	1	Total	C	Fe	N	O	0	0
			43	34	1	4	4		

- Molecule 6 is SODIUM ION (three-letter code: NA) (formula: Na).

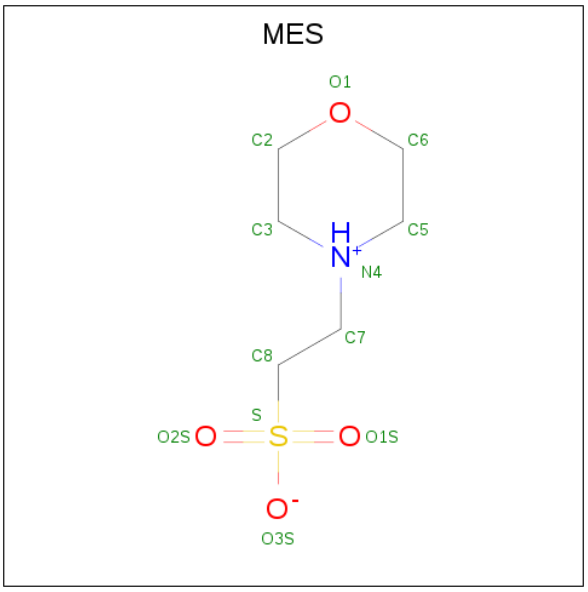
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
6	B	2	Total	Na	0	0
			2	2		

- Molecule 7 is 1,2-ETHANEDIOL (three-letter code: EDO) (formula: $C_2H_6O_2$).



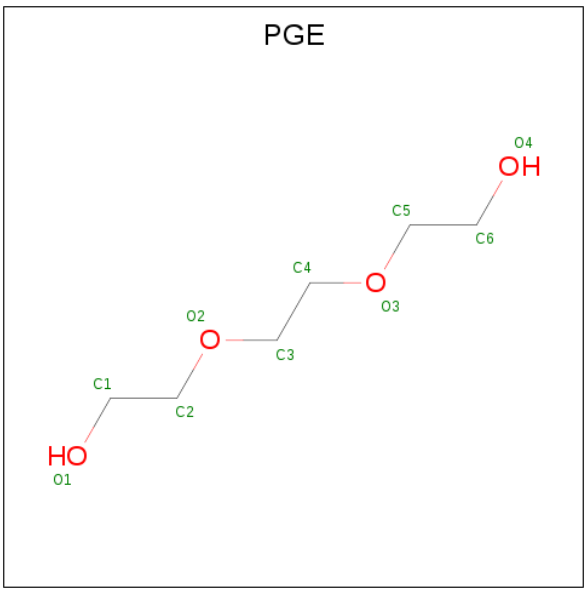
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
7	B	1	Total	C	O	0	0
			4	2	2		

- Molecule 8 is 2-(N-MORPHOLINO)-ETHANESULFONIC ACID (three-letter code: MES) (formula: $C_6H_{13}NO_4S$).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
8	D	1	Total	C	N	O	S	0	0
			12	6	1	4	1		
8	F	1	Total	C	N	O	S	0	0
			12	6	1	4	1		

- Molecule 9 is TRIETHYLENE GLYCOL (three-letter code: PGE) (formula: $C_6H_{14}O_4$).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
9	F	1	Total C O 10 6 4	0	0

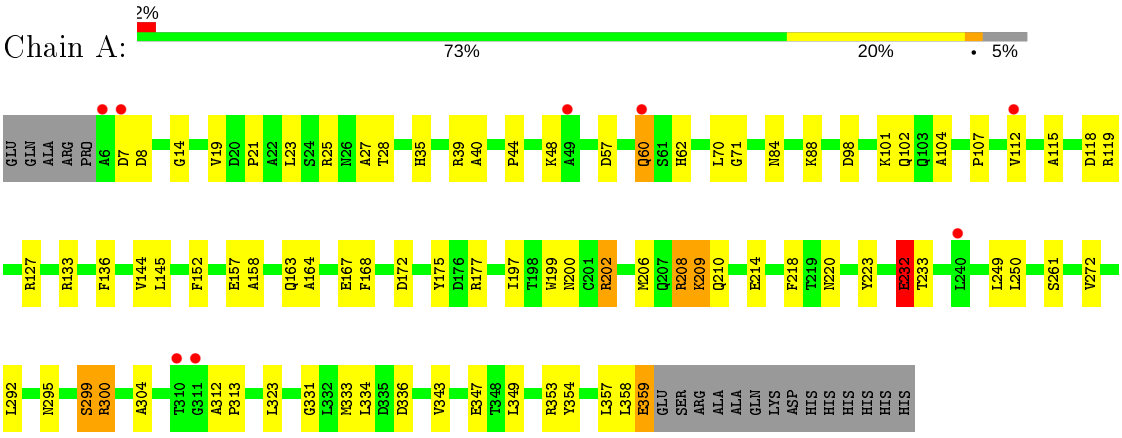
- Molecule 10 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
10	A	96	Total O 99 99	0	3
10	B	209	Total O 210 210	0	1
10	C	41	Total O 41 41	0	0
10	D	116	Total O 117 117	0	1
10	E	72	Total O 72 72	0	0
10	F	233	Total O 234 234	0	1

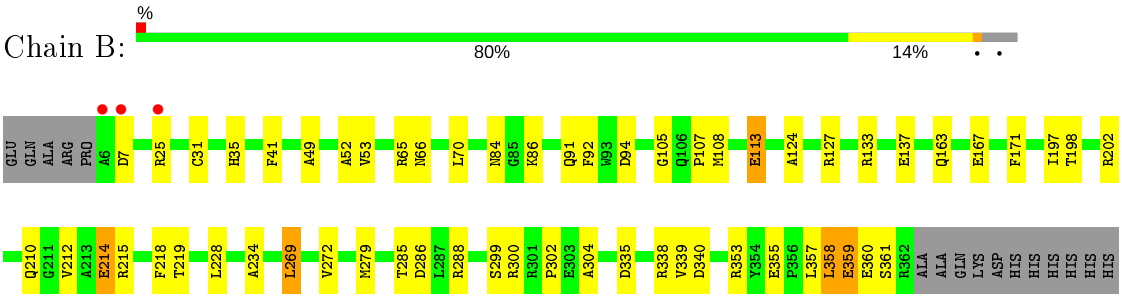
3 Residue-property plots

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

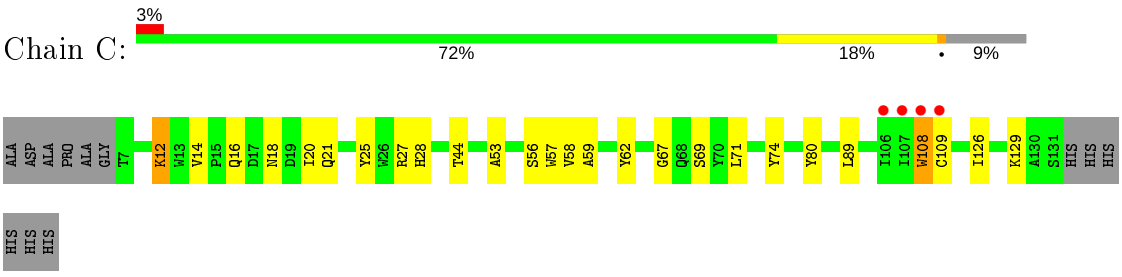
- Molecule 1: Methylamine utilization protein MauG



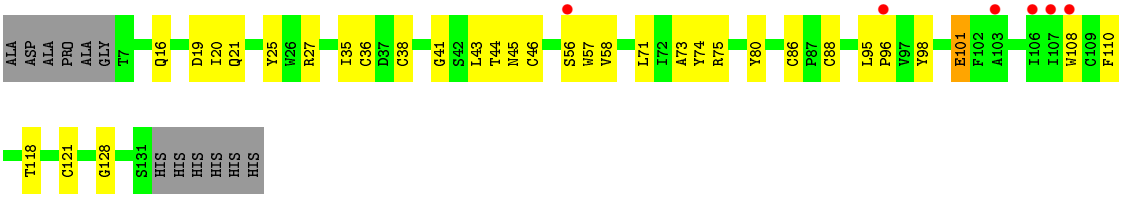
- Molecule 1: Methylamine utilization protein MauG



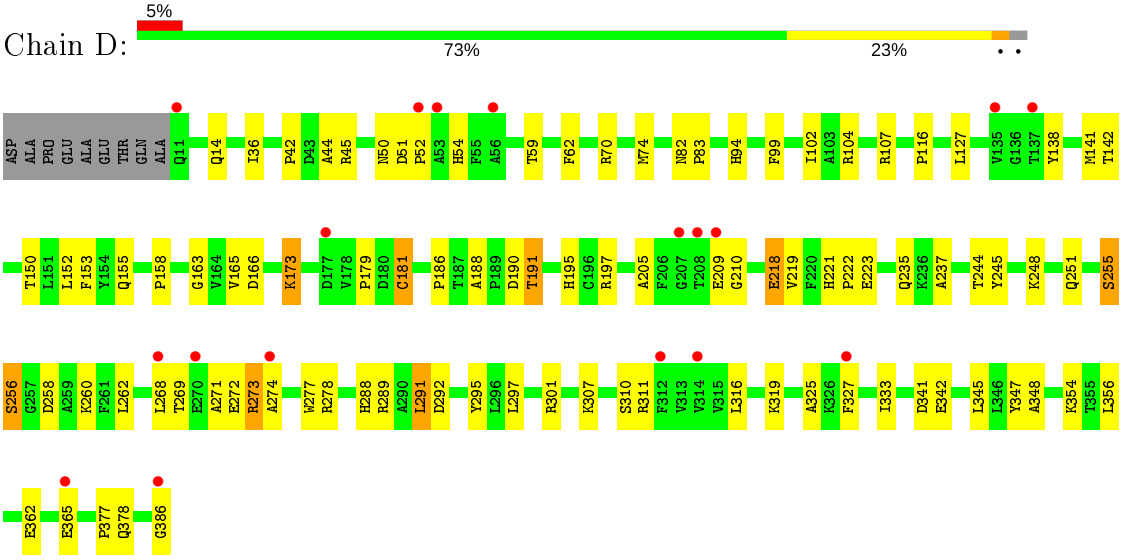
- Molecule 2: Methylamine dehydrogenase light chain



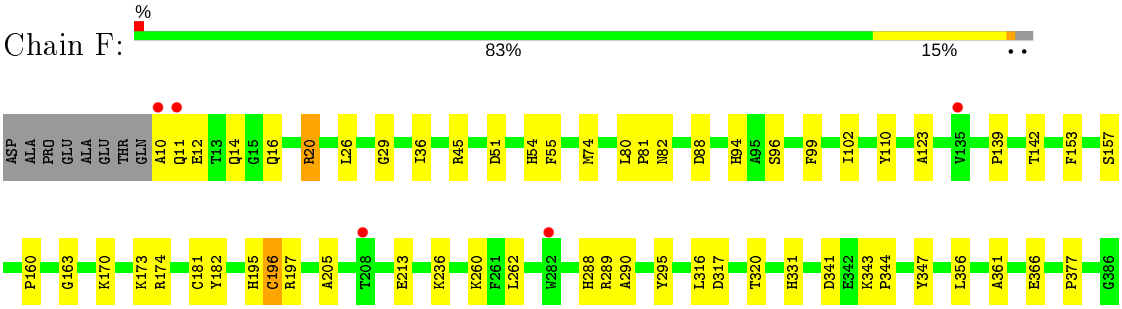
- Molecule 2: Methylamine dehydrogenase light chain



• Molecule 3: Methylamine dehydrogenase heavy chain



• Molecule 3: Methylamine dehydrogenase heavy chain



4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 1	Depositor
Cell constants a, b, c, α, β, γ	55.53Å 83.52Å 107.78Å 109.94° 91.54° 105.78°	Depositor
Resolution (Å)	44.49 – 2.08 44.49 – 2.08	Depositor EDS
% Data completeness (in resolution range)	97.2 (44.49-2.08) 97.2 (44.49-2.08)	Depositor EDS
R_{merge}	0.07	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	2.46 (at 2.08Å)	Xtriage
Refinement program	REFMAC 5.5.0109	Depositor
R, R_{free}	0.163 , 0.224 0.181 , 0.235	Depositor DCC
R_{free} test set	5105 reflections (5.04%)	wwPDB-VP
Wilson B-factor (Å^2)	35.8	Xtriage
Anisotropy	0.056	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.32 , 41.3	EDS
L-test for twinning[2]	$< \|L\| > = 0.50$, $< L^2 > = 0.33$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o,F_c correlation	0.96	EDS
Total number of atoms	14424	wwPDB-VP
Average B, all atoms (Å^2)	45.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.19% of the height of the origin peak. No significant pseudotranslation is detected.*

[1] Intensities estimated from amplitudes.

[2] Theoretical values of $< |L| >$, $< L^2 >$ for acentric reflections are 0.5, 0.333 respectively for untwinned datasets, and 0.375, 0.2 for perfectly twinned datasets.

5 Model quality

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: PGE, 0AF, NA, CA, EDO, MES, 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	0.91	1/2840 (0.0%)	0.89	1/3851 (0.0%)
1	B	1.16	3/2883 (0.1%)	0.94	0/3908
2	C	0.93	0/978	0.93	1/1334 (0.1%)
2	E	1.18	2/990 (0.2%)	1.07	0/1352
3	D	0.89	1/3026 (0.0%)	0.88	3/4122 (0.1%)
3	F	1.14	0/3042	1.02	2/4143 (0.0%)
All	All	1.04	7/13759 (0.1%)	0.95	7/18710 (0.0%)

All (7) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	31	CYS	CB-SG	-5.87	1.72	1.81
1	A	164	ALA	CA-CB	5.64	1.64	1.52
2	E	88[A]	CYS	CB-SG	-5.53	1.72	1.81
2	E	88[B]	CYS	CB-SG	-5.53	1.72	1.81
1	B	113	GLU	CB-CG	5.30	1.62	1.52
1	B	339	VAL	CB-CG2	5.15	1.63	1.52
3	D	62	PHE	CE1-CZ	5.10	1.47	1.37

All (7) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
3	F	289	ARG	NE-CZ-NH1	-5.86	117.37	120.30
3	F	196	CYS	CA-CB-SG	-5.82	103.53	114.00
1	A	208	ARG	NE-CZ-NH2	-5.74	117.43	120.30
3	D	166	ASP	CB-CG-OD2	-5.42	113.42	118.30
3	D	104	ARG	NE-CZ-NH1	5.31	122.95	120.30
2	C	108	TRP	CG-CD2-CE3	-5.20	129.22	133.90
3	D	70	ARG	NE-CZ-NH2	-5.06	117.77	120.30

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts (i)

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	2773	0	2652	63	0
1	B	2819	0	2686	38	0
2	C	966	0	875	22	0
2	E	972	0	880	37	0
3	D	2945	0	2826	62	0
3	F	2962	0	2847	42	0
4	A	1	0	0	0	0
4	B	1	0	0	0	0
5	A	86	0	60	4	0
5	B	86	0	60	5	0
6	B	2	0	0	0	0
7	B	4	0	6	0	0
8	D	12	0	12	0	0
8	F	12	0	12	0	0
9	F	10	0	14	0	0
10	A	99	0	0	6	0
10	B	210	0	0	2	0
10	C	41	0	0	1	0
10	D	117	0	0	6	0
10	E	72	0	0	1	0
10	F	234	0	0	2	0
All	All	14424	0	12930	241	0

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 9.

All (241) 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)
2:E:36[B]:CYS:HB2	2:E:121:CYS:SG	1.76	1.24
1:A:299:SER:HB2	1:A:333:MET:HG3	1.27	1.12

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:F:174[B]:ARG:HG2	3:F:174[B]:ARG:HH21	1.19	1.03
2:E:36[B]:CYS:HB2	2:E:121:CYS:HG	1.10	0.93
1:B:107:PRO:HG3	10:B:652[A]:HOH:O	1.72	0.89
3:F:174[B]:ARG:CG	3:F:174[B]:ARG:HH21	1.86	0.88
10:C:230:HOH:O	3:F:36:ILE:HD11	1.73	0.88
2:E:35:ILE:HD12	2:E:86[B]:CYS:SG	2.16	0.85
1:B:210:GLN:HE22	2:E:44:THR:HG21	1.40	0.84
2:C:21:GLN:HE22	3:F:14:GLN:HE21	1.24	0.83
1:A:48:LYS:H	1:A:62:HIS:HE1	1.27	0.82
1:A:210:GLN:HE22	2:C:44:THR:HG21	1.45	0.81
1:A:300:ARG:HD2	1:A:300:ARG:H	1.47	0.79
1:B:105:GLY:HA2	1:B:108:MET:HE3	1.64	0.78
1:B:300[B]:ARG:O	1:B:300[B]:ARG:HG2	1.82	0.78
3:D:237:ALA:HB2	3:D:289:ARG:HG3	1.65	0.78
3:F:181[B]:CYS:HB3	3:F:196:CYS:SG	2.25	0.76
3:D:209:GLU:HG2	3:D:210:GLY:N	2.00	0.76
3:D:342[B]:GLU:HA	10:D:590:HOH:O	1.86	0.75
1:A:300:ARG:CD	1:A:300:ARG:H	1.98	0.75
3:D:14:GLN:HE21	2:E:21:GLN:HE22	1.34	0.75
2:E:38:CYS:SG	2:E:86[B]:CYS:HB2	2.27	0.74
1:A:353[B]:ARG:HD3	1:A:354:TYR:CZ	2.22	0.73
3:F:236:LYS:NZ	10:F:728[A]:HOH:O	2.23	0.72
3:D:342[A]:GLU:HA	10:D:590:HOH:O	1.90	0.71
1:A:343:VAL:O	1:A:347:GLU:HG3	1.89	0.71
1:A:299:SER:CB	1:A:333:MET:HG3	2.16	0.71
1:A:163:GLN:HE22	5:A:402:HEC:HMA1	1.55	0.70
1:A:299:SER:HB2	1:A:333:MET:CG	2.14	0.70
1:B:197:ILE:O	1:B:202:ARG:CD	2.39	0.70
1:B:198:THR:HG22	2:E:58:VAL:HG13	1.73	0.69
1:A:48:LYS:H	1:A:62:HIS:CE1	2.11	0.69
3:D:54:HIS:HD2	10:D:607:HOH:O	1.74	0.69
2:E:56:SER:CB	2:E:74:TYR:O	2.42	0.67
3:F:123:ALA:HB2	3:F:170:LYS:HE2	1.76	0.67
1:B:105:GLY:HA2	1:B:108:MET:CE	2.25	0.66
1:B:197:ILE:O	1:B:202:ARG:HD2	1.94	0.66
2:C:58:VAL:HG22	2:C:59:ALA:N	2.10	0.66
1:B:214:GLU:HG3	1:B:215[A]:ARG:HG3	1.78	0.65
2:C:57:0AF:HBC1	2:C:108:TRP:NE1	2.12	0.65
3:D:44:ALA:HB1	3:D:341:ASP:HB3	1.79	0.64
2:E:57:0AF:HBC1	2:E:108:TRP:NE1	2.12	0.64
2:E:21:GLN:O	2:E:86[B]:CYS:SG	2.57	0.63

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:D:251:GLN:O	3:D:262:LEU:HB2	1.99	0.63
3:D:218:GLU:HG2	3:D:219:VAL:O	2.00	0.62
3:D:288:HIS:ND1	3:D:291:LEU:HB2	2.15	0.62
1:B:133:ARG:O	1:B:137:GLU:HG3	2.00	0.62
1:A:21:PRO:O	1:A:27:ALA:HA	1.99	0.62
2:C:12[A]:LYS:HE2	2:C:14:VAL:HG23	1.81	0.61
2:C:12[A]:LYS:HE2	2:C:14:VAL:CG2	2.29	0.61
2:E:101[A]:GLU:OE1	3:F:197:ARG:NH2	2.28	0.61
1:A:232:GLU:CG	1:A:233:THR:H	2.15	0.60
1:B:288[B]:ARG:NH2	1:B:340:ASP:OD1	2.33	0.60
3:D:255:SER:O	3:D:256:SER:HB3	2.03	0.59
5:A:403:HEC:HBC3	5:A:403:HEC:HMC1	1.85	0.59
1:A:272:VAL:HG21	5:A:403:HEC:HMA3	1.85	0.59
3:D:188:ALA:HB3	3:D:191:THR:HG23	1.85	0.59
3:F:82:ASN:HB3	3:F:142:THR:HB	1.84	0.58
1:B:285:THR:HG22	1:B:286:ASP:OD1	2.04	0.58
1:A:101:LYS:NZ	1:A:157:GLU:OE2	2.30	0.58
2:E:75:ARG:HA	10:E:249:HOH:O	2.03	0.58
1:B:197:ILE:O	1:B:202:ARG:HD3	2.02	0.57
3:D:155:GLN:NE2	10:D:614:HOH:O	2.30	0.57
10:A:554:HOH:O	3:D:197:ARG:HD2	2.03	0.57
3:D:44:ALA:CB	3:D:341:ASP:HB3	2.35	0.57
3:D:269:THR:O	3:D:273[A]:ARG:HD3	2.05	0.57
3:F:88:ASP:HB3	10:F:728[B]:HOH:O	2.02	0.57
1:B:113:GLU:HG2	5:B:402:HEC:HBC2	1.86	0.56
3:D:245:TYR:HB2	10:D:580:HOH:O	2.05	0.56
3:D:347:TYR:HB3	3:D:356:LEU:HD11	1.87	0.56
1:A:172:ASP:O	1:A:177:ARG:NH1	2.39	0.56
1:A:359:GLU:H	1:A:359:GLU:CD	2.09	0.55
2:E:56:SER:HB2	2:E:74:TYR:O	2.05	0.55
3:F:51:ASP:HA	3:F:377:PRO:HA	1.89	0.55
3:D:181[A]:CYS:HB3	3:D:195:HIS:O	2.06	0.55
1:B:198:THR:CG2	2:E:58:VAL:HG13	2.36	0.55
3:F:174[B]:ARG:NH2	3:F:174[B]:ARG:HG2	2.04	0.55
3:D:52:PRO:HG2	3:D:378:GLN:OE1	2.06	0.55
1:A:104:ALA:O	1:A:107:PRO:HD2	2.07	0.55
3:D:297:LEU:HD22	3:D:310:SER:HB2	1.88	0.54
3:F:45:ARG:NH2	3:F:343:LYS:O	2.41	0.54
3:D:190:ASP:OD1	3:D:191:THR:HG22	2.08	0.54
3:D:51:ASP:O	3:D:59:THR:HB	2.08	0.54
1:B:300[B]:ARG:O	1:B:300[B]:ARG:CG	2.52	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:F:153:PHE:CZ	3:F:163:GLY:HA3	2.44	0.53
3:D:268:LEU:HD22	3:D:277:TRP:HB3	1.91	0.53
1:B:288[B]:ARG:NH1	1:B:340:ASP:OD1	2.42	0.52
1:A:40:ALA:HA	1:A:354:TYR:CZ	2.45	0.52
1:A:39[A]:ARG:HD2	1:A:44:PRO:HB3	1.91	0.52
1:A:197:ILE:C	1:A:202:ARG:HG2	2.31	0.52
1:A:39[B]:ARG:O	1:A:39[B]:ARG:HG2	2.10	0.52
3:F:174[B]:ARG:CG	3:F:174[B]:ARG:NH2	2.57	0.52
2:E:38:CYS:SG	2:E:86[B]:CYS:CB	2.94	0.51
1:A:353[B]:ARG:HD3	1:A:354:TYR:CE2	2.45	0.51
2:C:58:VAL:CG2	2:C:59:ALA:N	2.73	0.51
1:A:210:GLN:NE2	2:C:44:THR:HG21	2.21	0.51
2:C:80:TYR:HE2	3:F:74:MET:O	1.93	0.51
1:B:91:GLN:O	1:B:92:PHE:HB2	2.10	0.50
1:A:295:ASN:HD21	1:A:334:LEU:H	1.59	0.50
2:E:36[B]:CYS:SG	2:E:41:GLY:HA3	2.51	0.50
3:D:74:MET:O	2:E:80:TYR:HE2	1.93	0.50
1:A:136:PHE:HB3	1:A:144:VAL:CG1	2.42	0.50
3:F:347:TYR:HB3	3:F:356:LEU:HD11	1.92	0.50
3:D:195:HIS:NE2	3:D:221:HIS:HE1	2.09	0.50
1:A:300:ARG:HG3	3:D:158:PRO:CG	2.42	0.50
3:D:244:THR:HG23	3:D:248:LYS:O	2.12	0.50
3:D:51:ASP:HA	3:D:377:PRO:HA	1.93	0.50
3:F:331:HIS:HE1	3:F:366:GLU:OE1	1.94	0.50
1:A:202:ARG:HB2	1:A:206:MET:HG3	1.93	0.50
1:B:163:GLN:HE22	5:B:402:HEC:HMA1	1.77	0.50
3:D:362:GLU:OE1	3:D:362:GLU:HA	2.12	0.50
3:F:173:LYS:O	3:F:174[B]:ARG:HB3	2.12	0.49
2:E:96:PRO:HB2	2:E:98:TYR:CE1	2.48	0.49
3:D:36:ILE:HD13	2:E:46:CYS:HB2	1.93	0.49
1:A:353[B]:ARG:HD3	1:A:354:TYR:CE1	2.47	0.49
2:E:57:0AF:HBC1	2:E:108:TRP:HE1	1.78	0.49
2:C:20:ILE:HG22	2:C:25:TYR:CZ	2.48	0.49
1:A:353[B]:ARG:HG2	10:A:585:HOH:O	2.12	0.48
1:A:331:GLY:O	3:D:158:PRO:HA	2.13	0.48
3:F:205:ALA:HB3	3:F:213[B]:GLU:HB3	1.95	0.48
1:B:272:VAL:HG21	5:B:403:HEC:HMA3	1.95	0.48
3:F:341:ASP:OD1	3:F:341:ASP:N	2.47	0.48
2:E:110:PHE:CE1	3:F:157:SER:HB2	2.48	0.48
1:A:19:VAL:HG13	10:A:567:HOH:O	2.12	0.48
1:A:300:ARG:HG3	3:D:158:PRO:HG3	1.96	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:E:74:TYR:O	2:E:75:ARG:HG3	2.14	0.48
1:B:52:ALA:O	1:B:66:ASN:HA	2.13	0.48
1:A:359:GLU:N	1:A:359:GLU:CD	2.66	0.47
1:B:359:GLU:OE1	1:B:359:GLU:N	2.46	0.47
3:D:45:ARG:HD3	3:D:345:LEU:HD11	1.96	0.47
2:C:62:TYR:CE1	2:C:67:GLY:HA2	2.49	0.47
3:F:213[A]:GLU:HG2	3:F:213[A]:GLU:O	2.13	0.47
2:C:12[A]:LYS:N	2:C:12[A]:LYS:HD3	2.30	0.47
1:B:212:VAL:HG22	2:E:128:GLY:HA2	1.96	0.47
1:B:299:SER:HB3	1:B:304:ALA:CB	2.45	0.47
3:D:325:ALA:HB1	3:D:327:PHE:CE1	2.50	0.47
1:B:210:GLN:NE2	2:E:44:THR:HG21	2.18	0.47
2:E:56:SER:HB3	2:E:74:TYR:O	2.15	0.47
1:A:209:LYS:HD2	10:A:591:HOH:O	2.14	0.47
2:C:18:ASN:O	3:F:16:GLN:HA	2.14	0.47
3:D:292:ASP:OD2	3:D:319:LYS:HG3	2.15	0.47
2:E:20:ILE:HG22	2:E:25:TYR:CZ	2.50	0.47
3:F:344:PRO:HG2	3:F:361:ALA:HB3	1.95	0.47
1:A:28:THR:OG1	1:A:57:ASP:OD1	2.31	0.46
2:C:57:0AF:HBC1	2:C:108:TRP:HE1	1.78	0.46
3:D:99:PHE:CE2	3:D:107:ARG:HB2	2.50	0.46
2:C:126:ILE:CD1	3:F:26:LEU:HD13	2.45	0.46
2:C:53:ALA:HB2	2:C:109:CYS:HA	1.98	0.46
3:D:255:SER:O	3:D:256:SER:CB	2.63	0.46
3:D:272:GLU:HA	10:D:525:HOH:O	2.15	0.46
1:A:208:ARG:NH2	3:F:29:GLY:O	2.28	0.46
3:D:191:THR:HB	3:D:205:ALA:HA	1.98	0.46
1:A:175:TYR:CZ	1:A:218:PHE:HZ	2.33	0.46
1:A:312:ALA:HB1	1:A:313:PRO:HD2	1.98	0.46
1:A:197:ILE:HA	1:A:202:ARG:HG2	1.97	0.46
3:D:50:ASN:CG	3:D:83:PRO:HG3	2.36	0.46
1:A:232:GLU:HG3	1:A:233:THR:HG23	1.98	0.46
3:D:295:TYR:N	3:D:295:TYR:CD1	2.83	0.46
2:E:36[A]:CYS:SG	2:E:121:CYS:C	2.95	0.46
3:F:181[B]:CYS:HB3	3:F:196:CYS:HA	1.98	0.46
3:F:80:LEU:N	3:F:81:PRO:CD	2.79	0.45
1:A:136:PHE:HB3	1:A:144:VAL:HG11	1.99	0.45
1:B:335:ASP:OD1	1:B:338:ARG:NH1	2.45	0.45
1:B:49:ALA:HB3	1:B:53:VAL:HG22	1.99	0.45
1:B:35:HIS:CE1	1:B:70:LEU:HD21	2.52	0.45
3:D:152:LEU:HA	3:D:163:GLY:O	2.16	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:14:GLY:N	1:A:158:ALA:HB1	2.32	0.45
2:C:12[A]:LYS:O	2:C:12[A]:LYS:HG2	2.16	0.45
2:C:56:SER:CB	2:C:74:TYR:O	2.65	0.44
3:D:74:MET:O	2:E:80:TYR:CE2	2.70	0.44
2:E:118:THR:HG23	3:F:99:PHE:CE1	2.53	0.44
3:F:317:ASP:OD1	3:F:320:THR:HG23	2.17	0.44
3:D:153:PHE:CE1	3:D:163:GLY:HA3	2.52	0.44
2:E:36[B]:CYS:SG	2:E:45:ASN:O	2.75	0.44
1:A:353[B]:ARG:CD	1:A:354:TYR:CZ	2.99	0.44
1:B:86:LYS:HD3	10:B:695:HOH:O	2.18	0.44
2:E:36[B]:CYS:CB	2:E:121:CYS:SG	2.65	0.43
1:A:163:GLN:HA	1:A:168:PHE:CD1	2.53	0.43
1:A:292:LEU:HA	1:A:292:LEU:HD23	1.90	0.43
5:B:403:HEC:HBC3	5:B:403:HEC:HMC1	2.01	0.43
1:A:98:ASP:N	1:A:102[B]:GLN:OE1	2.51	0.43
1:A:175:TYR:CB	1:A:349:LEU:HD23	2.48	0.43
1:B:355:GLU:O	1:B:358:LEU:HB2	2.17	0.43
2:C:80:TYR:CE2	3:F:74:MET:O	2.70	0.43
2:C:89:LEU:HD11	3:D:307:LYS:HD2	1.99	0.43
2:E:19:ASP:O	2:E:25:TYR:HB2	2.18	0.43
1:A:304:ALA:HA	10:A:505[B]:HOH:O	2.17	0.43
1:A:35:HIS:CE1	1:A:70:LEU:HD21	2.53	0.43
3:D:36:ILE:CD1	2:E:46:CYS:HB2	2.49	0.43
3:D:289:ARG:NH2	3:D:386:GLY:O	2.52	0.43
1:A:223:TYR:CG	1:A:249:LEU:HD22	2.54	0.43
1:A:200:ASN:O	5:A:403:HEC:HMC3	2.19	0.43
3:F:10:ALA:HA	3:F:11:GLN:HA	1.75	0.42
3:F:288:HIS:CE1	3:F:290:ALA:HB3	2.54	0.42
1:B:218:PHE:HB3	1:B:269:LEU:HB2	2.01	0.42
3:F:12:GLU:OE1	3:F:20:ARG:NH1	2.50	0.42
2:E:98:TYR:CE1	3:F:195:HIS:HE1	2.37	0.42
3:F:54:HIS:O	3:F:55:PHE:HB2	2.20	0.42
1:A:127[B]:ARG:HG2	1:A:145:LEU:HB3	2.02	0.42
3:D:173:LYS:HA	3:D:173:LYS:HD2	1.53	0.42
3:D:82:ASN:HB3	3:D:142:THR:HB	2.02	0.42
1:A:206:MET:O	1:A:220:ASN:HB3	2.20	0.42
1:B:49:ALA:HB2	1:B:234:ALA:HA	2.00	0.42
3:D:268:LEU:HD13	3:D:277:TRP:O	2.20	0.42
1:A:250:LEU:HD22	1:A:261:SER:HB2	2.01	0.42
2:E:58:VAL:HG12	2:E:73:ALA:HA	2.01	0.42
3:F:288:HIS:HE1	3:F:290:ALA:HB3	1.85	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:60:GLN:O	1:A:62:HIS:HD2	2.03	0.41
3:D:311:ARG:HB2	3:D:311:ARG:HE	1.68	0.41
1:B:65:ARG:HH12	1:B:94:ASP:CG	2.23	0.41
3:D:260:LYS:HB3	3:D:260:LYS:HE2	1.93	0.41
3:D:333:ILE:HG21	3:D:348:ALA:HB1	2.02	0.41
2:E:27:ARG:HD2	2:E:43:LEU:HD21	2.02	0.41
1:A:199:TRP:HH2	1:A:333:MET:O	2.03	0.41
3:D:278:ARG:O	3:D:301:ARG:NH1	2.53	0.41
3:D:45:ARG:HD3	3:D:345:LEU:CD1	2.50	0.41
1:A:71:GLY:HA2	1:A:168:PHE:O	2.20	0.41
1:B:218:PHE:CB	1:B:269:LEU:HB2	2.51	0.41
2:C:25:TYR:CE2	2:C:27:ARG:HG3	2.56	0.41
3:D:271:ALA:O	3:D:274:ALA:HB3	2.20	0.41
3:F:295:TYR:N	3:F:295:TYR:CD1	2.89	0.41
1:B:41:PHE:HE2	1:B:353:ARG:HH21	1.69	0.41
3:D:150:THR:HA	3:D:165:VAL:O	2.21	0.41
2:E:95:LEU:HB3	2:E:96:PRO:CD	2.51	0.41
1:A:25:ARG:HB2	1:A:115:ALA:O	2.21	0.41
1:B:228:LEU:HD13	1:B:279:MET:HB3	2.02	0.41
1:A:175:TYR:HB2	1:A:349:LEU:HD23	2.02	0.41
3:D:138:TYR:HB2	3:D:141:MET:HG2	2.03	0.41
3:D:186:PRO:HB2	3:D:235:GLN:NE2	2.36	0.41
2:C:25:TYR:HB3	2:C:28:HIS:CD2	2.55	0.41
1:A:353[B]:ARG:CG	10:A:585:HOH:O	2.69	0.40
1:B:124:ALA:HA	1:B:127:ARG:NH1	2.36	0.40
3:F:20:ARG:HB3	3:F:20:ARG:CZ	2.51	0.40
1:B:171:PHE:CZ	1:B:215[A]:ARG:HB3	2.56	0.40
3:D:42:PRO:HG3	3:D:116:PRO:HB2	2.03	0.40
1:A:300:ARG:N	1:A:300:ARG:CD	2.71	0.40
3:D:221:HIS:HD2	3:D:222:PRO:O	2.04	0.40
3:F:96:SER:HB3	3:F:110:TYR:CZ	2.57	0.40
1:A:119:ARG:HG2	1:A:152:PHE:CD1	2.57	0.40
5:B:402:HEC:HBB3	5:B:402:HEC:HMB1	2.03	0.40

There are no symmetry-related clashes.

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	356/373 (95%)	344 (97%)	11 (3%)	1 (0%)	41 39
1	B	361/373 (97%)	351 (97%)	10 (3%)	0	100 100
2	C	124/137 (90%)	120 (97%)	4 (3%)	0	100 100
2	E	126/137 (92%)	124 (98%)	2 (2%)	0	100 100
3	D	377/385 (98%)	360 (96%)	14 (4%)	3 (1%)	19 14
3	F	379/385 (98%)	367 (97%)	11 (3%)	1 (0%)	41 39
All	All	1723/1790 (96%)	1666 (97%)	52 (3%)	5 (0%)	41 39

All (5) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	232	GLU
3	D	256	SER
3	D	102	ILE
3	D	179	PRO
3	F	102	ILE

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	280/292 (96%)	259 (92%)	21 (8%)	13 9
1	B	285/292 (98%)	272 (95%)	13 (5%)	27 25
2	C	106/112 (95%)	100 (94%)	6 (6%)	20 17

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
2	E	108/112 (96%)	104 (96%)	4 (4%)	34 34
3	D	307/310 (99%)	291 (95%)	16 (5%)	23 20
3	F	308/310 (99%)	301 (98%)	7 (2%)	50 53
All	All	1394/1428 (98%)	1327 (95%)	67 (5%)	27 23

All (67) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	7	ASP
1	A	8	ASP
1	A	23	LEU
1	A	60	GLN
1	A	84	ASN
1	A	88	LYS
1	A	112	VAL
1	A	118	ASP
1	A	133	ARG
1	A	167	GLU
1	A	202	ARG
1	A	209	LYS
1	A	214	GLU
1	A	232	GLU
1	A	299	SER
1	A	300	ARG
1	A	323	LEU
1	A	336	ASP
1	A	357	LEU
1	A	358	LEU
1	A	359	GLU
1	B	7	ASP
1	B	25	ARG
1	B	84	ASN
1	B	167	GLU
1	B	214	GLU
1	B	219	THR
1	B	269	LEU
1	B	302	PRO
1	B	357	LEU
1	B	358	LEU
1	B	359	GLU
1	B	360	GLU

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Mol	Chain	Res	Type
1	B	361	SER
2	C	12[A]	LYS
2	C	12[B]	LYS
2	C	16	GLN
2	C	69	SER
2	C	71	LEU
2	C	129	LYS
3	D	94	HIS
3	D	127	LEU
3	D	173	LYS
3	D	181[A]	CYS
3	D	181[B]	CYS
3	D	191	THR
3	D	218	GLU
3	D	223	GLU
3	D	255	SER
3	D	258	ASP
3	D	273[A]	ARG
3	D	273[B]	ARG
3	D	291	LEU
3	D	316	LEU
3	D	354	LYS
3	D	365	GLU
2	E	16	GLN
2	E	71	LEU
2	E	101[A]	GLU
2	E	101[B]	GLU
3	F	20	ARG
3	F	94	HIS
3	F	139	PRO
3	F	160	PRO
3	F	260	LYS
3	F	262	LEU
3	F	316	LEU

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (18) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	26	ASN
1	A	29	GLN
1	A	62	HIS
1	A	163	GLN

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Mol	Chain	Res	Type
1	A	210	GLN
1	A	295	ASN
1	B	16	GLN
1	B	29	GLN
1	B	84	ASN
1	B	91	GLN
1	B	163	GLN
1	B	210	GLN
3	D	14	GLN
3	D	30	GLN
3	D	221	HIS
3	F	14	GLN
3	F	30	GLN
3	F	54	HIS

5.3.3 RNA (i)

There are no RNA molecules in this entry.

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

2 non-standard protein/DNA/RNA residues 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	0AF	E	57	2	13,16,17	1.36	1 (7%)	11,22,24	3.03	5 (45%)
2	0AF	C	57	2	13,16,17	1.09	0	11,22,24	3.28	5 (45%)

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	0AF	E	57	2	-	0/4/6/8	0/2/2/2
2	0AF	C	57	2	-	0/4/6/8	0/2/2/2

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	E	57	0AF	CZ3-CE3	2.02	1.41	1.36

All (10) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	C	57	0AF	CB-CG-CD1	-7.83	118.30	127.97
2	E	57	0AF	CB-CG-CD1	-7.40	118.83	127.97
2	E	57	0AF	CB-CG-CD2	4.86	133.82	126.25
2	C	57	0AF	CB-CG-CD2	4.81	133.74	126.25
2	C	57	0AF	CB-CA-C	4.40	119.72	111.47
2	C	57	0AF	CZ3-CH2-CZ2	-2.66	116.92	120.28
2	E	57	0AF	CE3-CD2-CG	2.63	139.24	134.42
2	E	57	0AF	CZ3-CH2-CZ2	-2.61	116.98	120.28
2	E	57	0AF	CH2-CZ2-CE2	2.18	122.72	120.12
2	C	57	0AF	CE3-CD2-CG	2.13	138.33	134.42

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

2 monomers are involved in 4 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	E	57	0AF	2	0
2	C	57	0AF	2	0

5.5 Carbohydrates (i)

There are no carbohydrates in this entry.

5.6 Ligand geometry (i)

Of 12 ligands modelled in this entry, 4 are monoatomic - leaving 8 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	$\#\|Z\| > 2$
5	HEC	B	402	1,10	26,50,50	1.59	7 (26%)	18,82,82	2.74	12 (66%)
8	MES	F	401	-	12,12,12	2.15	1 (8%)	14,16,16	3.12	8 (57%)
5	HEC	A	403	1	26,50,50	1.64	6 (23%)	18,82,82	3.24	8 (44%)
5	HEC	B	403	1	26,50,50	1.54	4 (15%)	18,82,82	3.45	12 (66%)
7	EDO	B	406	-	3,3,3	0.29	0	2,2,2	0.49	0
9	PGE	F	402	-	9,9,9	0.56	0	8,8,8	0.33	0
8	MES	D	401	-	12,12,12	1.94	1 (8%)	14,16,16	2.75	8 (57%)
5	HEC	A	402	1	26,50,50	1.65	9 (34%)	18,82,82	2.24	8 (44%)

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral centers analysed, the number of these observed in the model and the number defined in the Chemical Component Dictionary. Similar counts are reported in the Torsion and Rings columns. '-' means no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
5	HEC	B	402	1,10	-	0/6/54/54	-
8	MES	F	401	-	-	5/6/14/14	0/1/1/1
5	HEC	A	403	1	-	0/6/54/54	-
5	HEC	B	403	1	-	0/6/54/54	-
7	EDO	B	406	-	-	1/1/1/1	-
9	PGE	F	402	-	-	6/7/7/7	-
8	MES	D	401	-	-	4/6/14/14	0/1/1/1
5	HEC	A	402	1	-	0/6/54/54	-

All (28) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
8	F	401	MES	C8-S	-7.32	1.67	1.77
8	D	401	MES	C8-S	-6.17	1.68	1.77
5	B	403	HEC	C3C-C4C	3.88	1.50	1.43
5	A	403	HEC	C4A-C3A	3.54	1.50	1.42
5	B	402	HEC	C4D-CHA	3.06	1.49	1.41
5	B	402	HEC	C1B-NB	-2.98	1.30	1.36
5	A	402	HEC	C3C-C4C	2.87	1.48	1.43

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
5	A	403	HEC	C3C-C4C	2.84	1.48	1.43
5	A	402	HEC	C1B-CHB	2.77	1.48	1.41
5	A	403	HEC	C3C-C2C	-2.76	1.37	1.40
5	B	403	HEC	C3C-C2C	-2.72	1.37	1.40
5	A	402	HEC	C4A-C3A	2.71	1.48	1.42
5	A	403	HEC	C1A-C2A	2.63	1.48	1.42
5	A	402	HEC	C1A-C2A	2.62	1.48	1.42
5	B	403	HEC	C4D-ND	-2.61	1.30	1.36
5	B	403	HEC	C4A-C3A	2.61	1.48	1.42
5	A	402	HEC	C4D-CHA	2.53	1.48	1.41
5	B	402	HEC	C3C-C4C	2.53	1.47	1.43
5	A	403	HEC	C1D-CHD	2.42	1.47	1.41
5	B	402	HEC	C4A-C3A	2.39	1.48	1.42
5	A	402	HEC	C1C-CHC	2.38	1.47	1.41
5	A	402	HEC	C3B-C4B	2.32	1.47	1.43
5	A	402	HEC	C1D-ND	-2.25	1.31	1.36
5	B	402	HEC	C1B-CHB	2.24	1.47	1.41
5	A	403	HEC	C3B-C2B	-2.13	1.38	1.40
5	B	402	HEC	C3B-C4B	2.09	1.46	1.43
5	A	402	HEC	C1B-NB	-2.06	1.31	1.36
5	B	402	HEC	C3C-C2C	-2.01	1.38	1.40

All (56) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
5	A	403	HEC	CBD-CAD-C3D	-7.47	98.70	112.49
5	B	403	HEC	CMB-C2B-C3B	7.23	134.32	125.82
8	F	401	MES	C5-N4-C3	6.25	122.89	108.83
5	B	403	HEC	CBD-CAD-C3D	-6.19	101.07	112.49
5	A	403	HEC	C1D-C2D-C3D	-5.81	102.95	107.00
8	F	401	MES	O3S-S-C8	5.77	115.10	105.77
5	B	403	HEC	CMC-C2C-C3C	5.29	132.05	125.82
5	A	403	HEC	CMC-C2C-C3C	5.28	132.03	125.82
5	A	402	HEC	C1D-C2D-C3D	-5.18	103.39	107.00
8	F	401	MES	C6-C5-N4	-4.93	102.62	110.10
5	B	402	HEC	CMB-C2B-C3B	4.88	131.56	125.82
8	D	401	MES	C5-N4-C3	4.69	119.38	108.83
5	B	402	HEC	C4B-C3B-C2B	-4.44	101.56	106.35
8	D	401	MES	C2-C3-N4	-4.38	103.47	110.10
5	B	402	HEC	CMC-C2C-C3C	4.24	130.80	125.82
5	B	403	HEC	C4C-C3C-C2C	-4.20	101.82	106.35
5	B	403	HEC	CMC-C2C-C1C	-3.86	122.53	128.46

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
5	A	403	HEC	CMB-C2B-C3B	3.79	130.28	125.82
8	D	401	MES	C7-N4-C3	3.77	120.87	111.23
8	D	401	MES	C6-C5-N4	-3.74	104.44	110.10
5	A	403	HEC	CBA-CAA-C2A	-3.50	106.03	112.48
5	A	403	HEC	CMC-C2C-C1C	-3.46	123.15	128.46
5	B	403	HEC	CMD-C2D-C3D	3.37	131.29	124.94
8	D	401	MES	C7-N4-C5	3.32	119.73	111.23
5	B	402	HEC	CAA-CBA-CGA	-3.32	107.11	112.67
5	B	403	HEC	CMD-C2D-C1D	-3.17	123.59	128.46
8	F	401	MES	C7-N4-C5	3.17	119.34	111.23
5	B	403	HEC	C1D-C2D-C3D	-3.11	104.83	107.00
5	B	402	HEC	C1D-C2D-C3D	-3.08	104.85	107.00
5	B	402	HEC	CMB-C2B-C1B	-3.05	123.78	128.46
5	A	402	HEC	C4C-C3C-C2C	-2.99	103.13	106.35
5	A	402	HEC	CMC-C2C-C3C	2.95	129.28	125.82
5	B	403	HEC	CAD-CBD-CGD	-2.87	107.86	112.67
5	A	402	HEC	CMA-C3A-C2A	2.85	130.32	124.94
5	B	403	HEC	CMB-C2B-C1B	-2.81	124.15	128.46
8	F	401	MES	C2-C3-N4	-2.80	105.86	110.10
5	A	402	HEC	CBA-CAA-C2A	-2.79	107.34	112.48
5	B	402	HEC	CBD-CAD-C3D	-2.77	107.38	112.49
5	B	403	HEC	CBA-CAA-C2A	-2.73	107.44	112.48
8	D	401	MES	O3S-S-C8	2.67	110.09	105.77
5	A	402	HEC	C4B-C3B-C2B	-2.67	103.47	106.35
5	A	403	HEC	CAA-CBA-CGA	-2.65	108.22	112.67
5	B	402	HEC	C3B-C4B-NB	2.63	115.90	110.94
8	F	401	MES	C7-N4-C3	2.55	117.77	111.23
5	B	402	HEC	CMD-C2D-C3D	2.55	129.75	124.94
8	D	401	MES	O1S-S-C8	2.51	109.94	106.92
5	A	403	HEC	C4C-C3C-C2C	-2.50	103.66	106.35
8	F	401	MES	O1-C2-C3	-2.46	106.37	111.80
8	D	401	MES	C6-O1-C2	2.44	118.05	109.89
5	A	402	HEC	CMD-C2D-C3D	2.34	129.35	124.94
5	B	402	HEC	CMD-C2D-C1D	-2.30	124.94	128.46
5	B	402	HEC	CBA-CAA-C2A	-2.14	108.54	112.48
5	B	402	HEC	C4C-C3C-C2C	-2.07	104.12	106.35
5	A	402	HEC	C3C-C4C-NC	2.05	114.81	110.94
5	B	403	HEC	C3C-C4C-NC	2.04	114.79	110.94
8	F	401	MES	O1-C6-C5	-2.01	107.38	111.80

There are no chirality outliers.

All (16) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
8	F	401	MES	N4-C7-C8-S
8	F	401	MES	C7-C8-S-O1S
8	D	401	MES	C7-C8-S-O2S
8	D	401	MES	C7-C8-S-O3S
9	F	402	PGE	O3-C5-C6-O4
8	F	401	MES	C7-C8-S-O3S
7	B	406	EDO	O1-C1-C2-O2
8	F	401	MES	C8-C7-N4-C3
9	F	402	PGE	C4-C3-O2-C2
9	F	402	PGE	C1-C2-O2-C3
8	F	401	MES	C7-C8-S-O2S
8	D	401	MES	C7-C8-S-O1S
9	F	402	PGE	C6-C5-O3-C4
9	F	402	PGE	O2-C3-C4-O3
8	D	401	MES	C8-C7-N4-C3
9	F	402	PGE	O1-C1-C2-O2

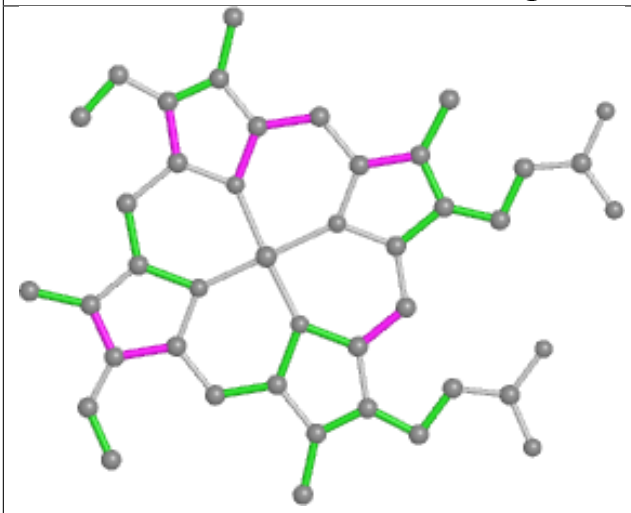
There are no ring outliers.

4 monomers are involved in 9 short contacts:

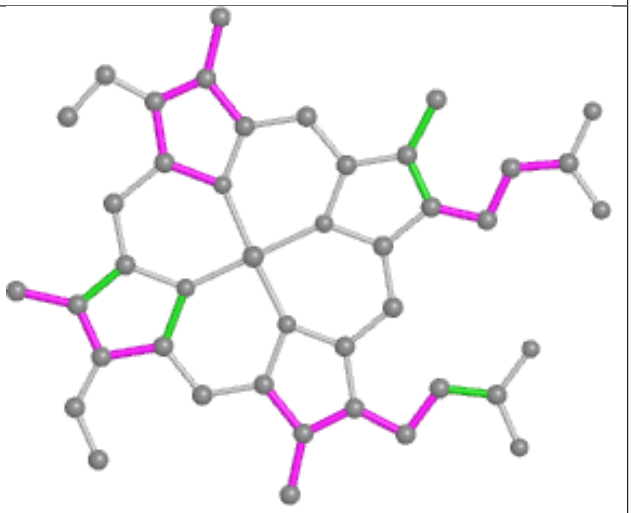
Mol	Chain	Res	Type	Clashes	Symm-Clashes
5	B	402	HEC	3	0
5	A	403	HEC	3	0
5	B	403	HEC	2	0
5	A	402	HEC	1	0

The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. For torsion angles, if less then 5% of the Mogul distribution of torsion angles is within 10 degrees of the torsion angle in question, then that torsion angle is considered an outlier. Any bond that is central to one or more torsion angles identified as an outlier by Mogul will be highlighted in the graph. For rings, the root-mean-square deviation (RMSD) between the ring in question and similar rings identified by Mogul is calculated over all ring torsion angles. If the average RMSD is greater than 60 degrees and the minimal RMSD between the ring in question and any Mogul-identified rings is also greater than 60 degrees, then that ring is considered an outlier. The outliers are highlighted in purple. The color gray indicates Mogul did not find sufficient equivalents in the CSD to analyse the geometry.

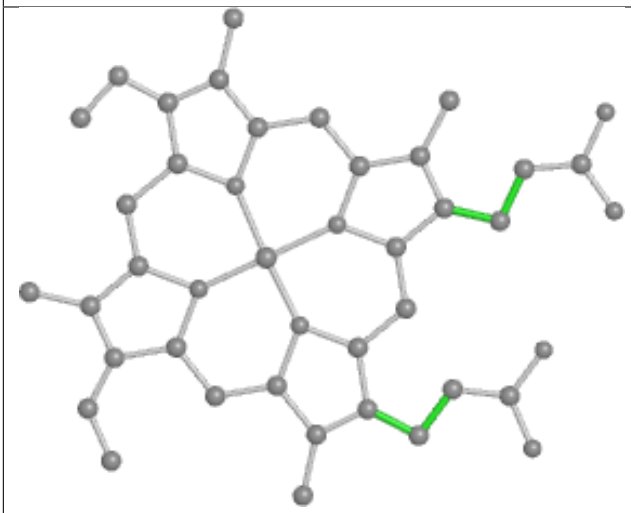
Ligand HEC B 402



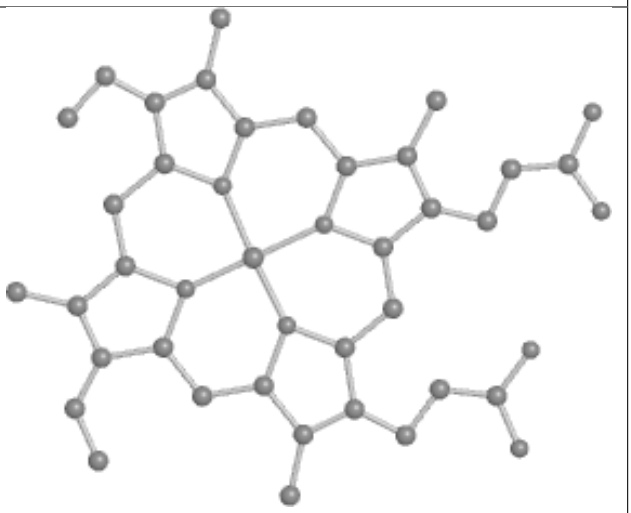
Bond lengths



Bond angles

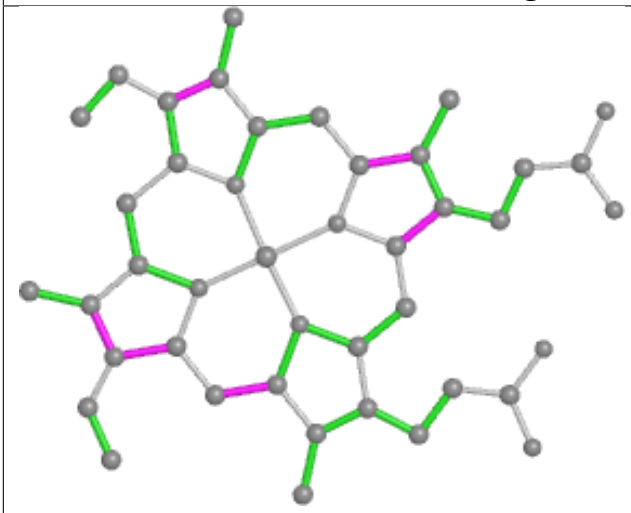


Torsions



Rings

Ligand HEC A 403



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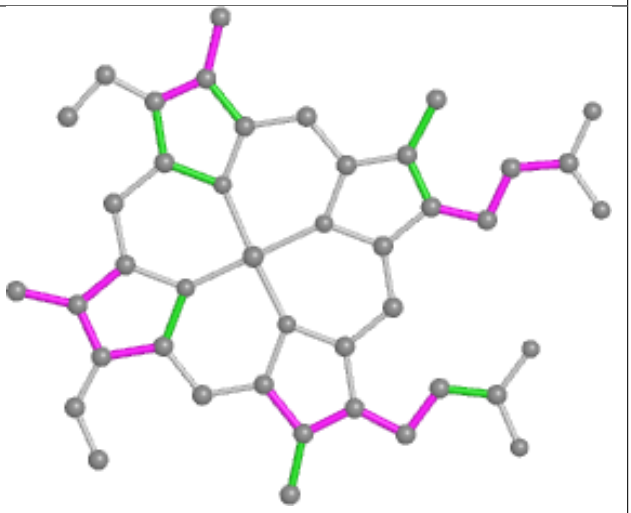

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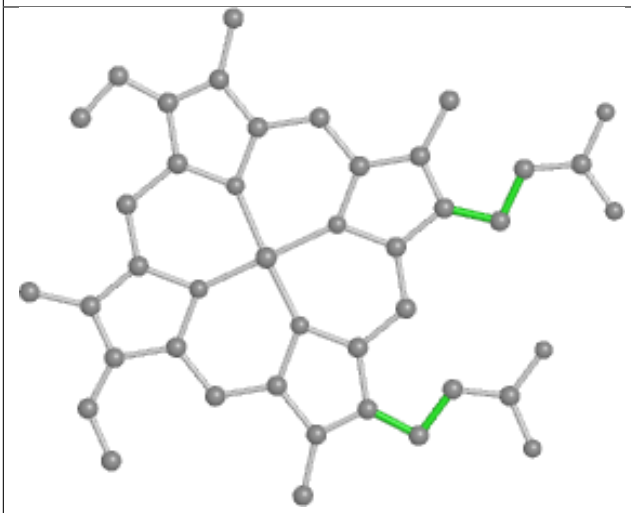

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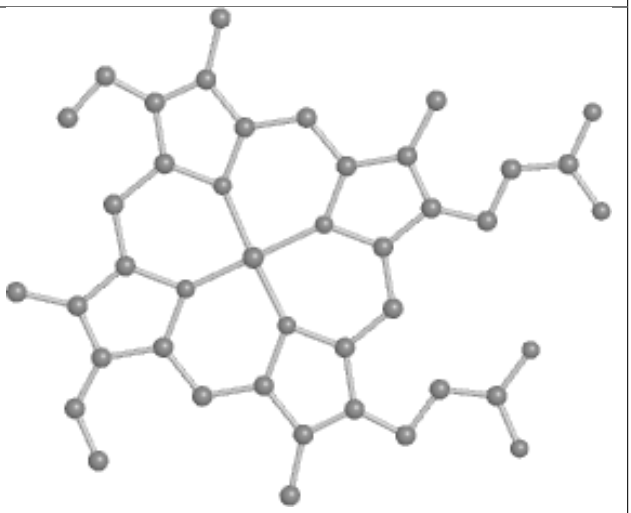
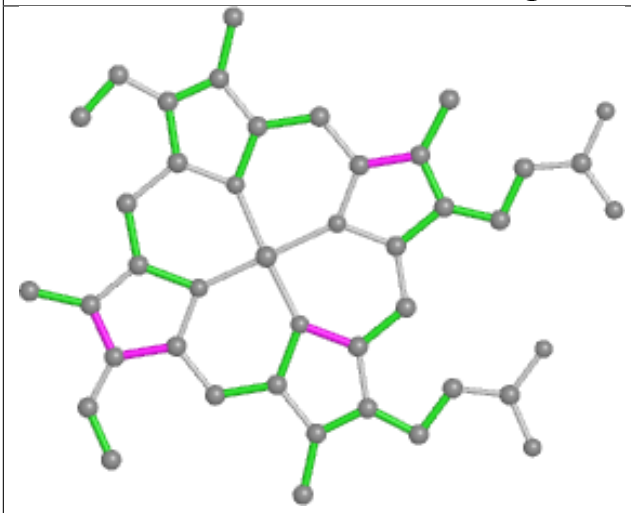
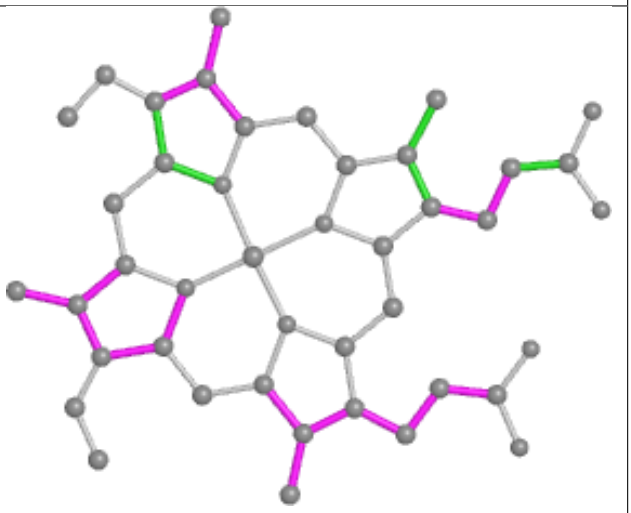


Rings

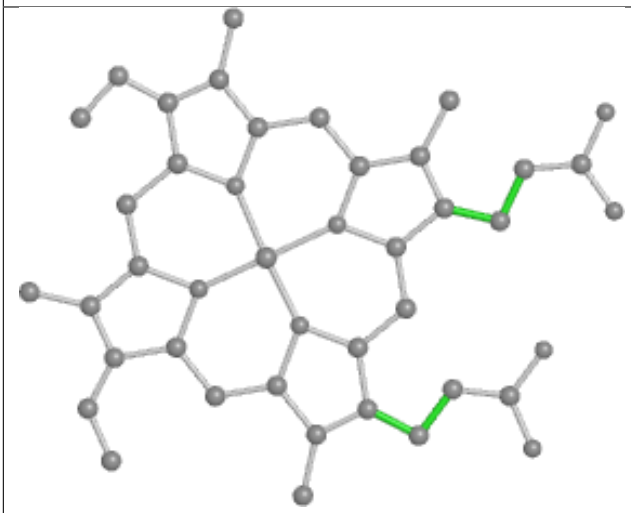
Ligand HEC B 403



Bond lengths



Bond angles



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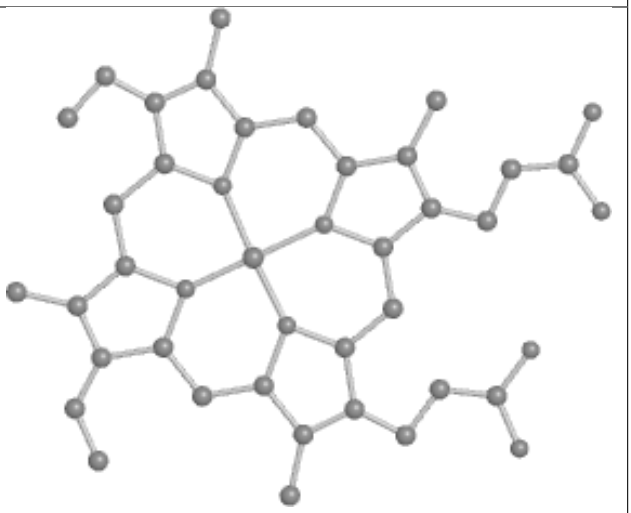
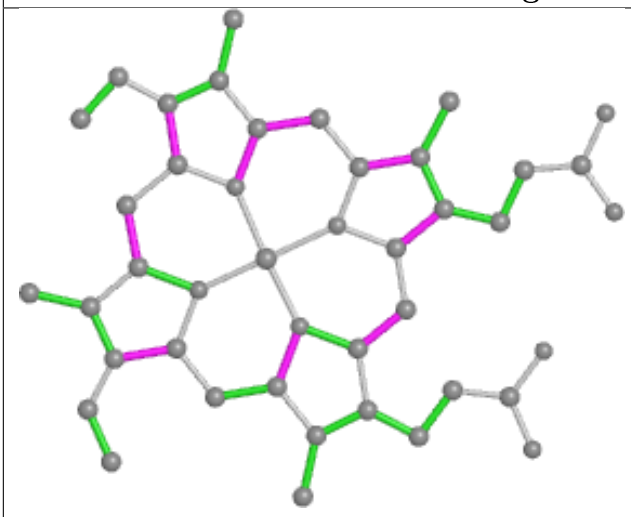
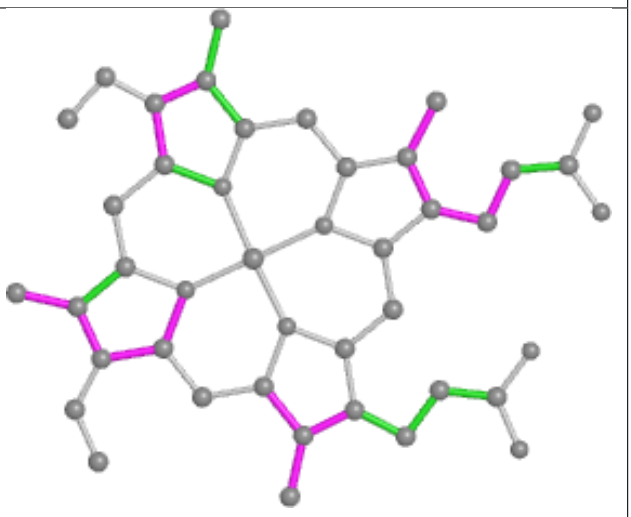


Rings

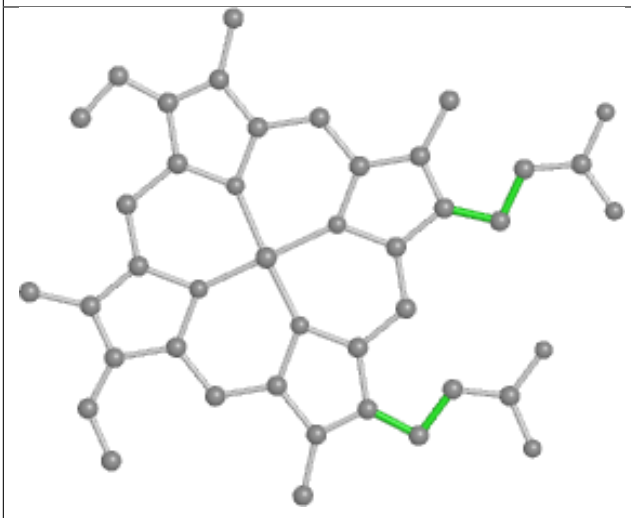
Ligand HEC A 402



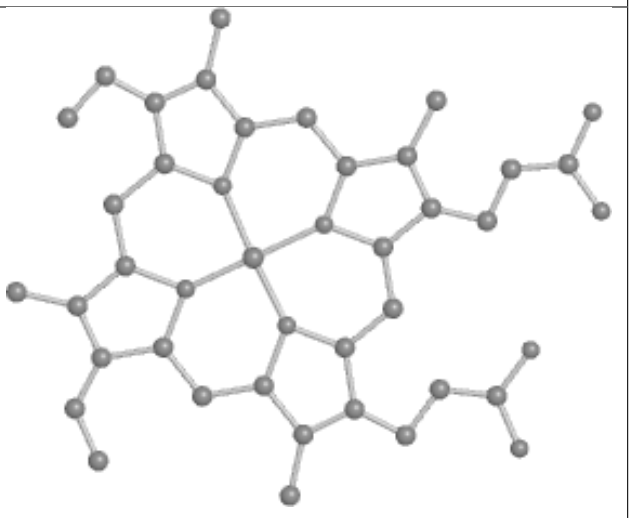
Bond lengths



Bond angles



Torsions



Rings

5.7 Other polymers

There are no such residues in this entry.

5.8 Polymer linkage issues

There are no chain breaks in this entry.

6 Fit of model and data

6.1 Protein, DNA and RNA chains

In the following table, the column labelled '#RSRZ> 2' contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 95^{th} percentile and maximum values of the occupancy-weighted average B-factor per residue. The column labelled 'Q< 0.9' lists the number of (and percentage) of residues with an average occupancy less than 0.9.

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å^2)	Q<0.9
1	A	354/373 (94%)	-0.03	8 (2%) 60 64	35, 51, 75, 85	0
1	B	357/373 (95%)	-0.26	3 (0%) 86 87	23, 37, 58, 85	0
2	C	124/137 (90%)	0.33	4 (3%) 47 53	29, 46, 67, 87	0
2	E	124/137 (90%)	0.31	6 (4%) 30 35	25, 33, 46, 73	0
3	D	376/385 (97%)	0.23	18 (4%) 30 35	30, 55, 88, 97	0
3	F	377/385 (97%)	-0.08	5 (1%) 77 79	24, 35, 55, 80	0
All	All	1712/1790 (95%)	0.02	44 (2%) 56 60	23, 43, 76, 97	0

All (44) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	6	ALA	6.5
1	B	6	ALA	6.1
1	B	7	ASP	5.4
3	F	10	ALA	4.7
3	D	208	THR	4.4
3	D	386	GLY	4.4
3	F	11	GLN	3.9
1	A	7	ASP	3.7
2	C	106	ILE	3.7
1	A	240	LEU	3.6
2	C	108	TRP	3.5
3	D	312	PHE	3.1
2	E	108	TRP	3.0
3	D	209	GLU	3.0
3	F	208	THR	3.0
2	E	103	ALA	2.8
3	D	56	ALA	2.8
2	C	107	ILE	2.7
3	D	135	VAL	2.6

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Mol	Chain	Res	Type	RSRZ
3	D	11	GLN	2.6
3	D	177	ASP	2.6
1	A	112	VAL	2.6
2	E	107	ILE	2.6
3	D	274	ALA	2.5
1	A	311	GLY	2.5
3	F	135	VAL	2.5
1	A	49	ALA	2.5
3	D	270	GLU	2.4
1	A	310	THR	2.4
2	E	106	ILE	2.4
1	A	60	GLN	2.3
2	E	96	PRO	2.3
3	D	207	GLY	2.3
3	F	282	TRP	2.2
2	C	109	CYS	2.2
3	D	327	PHE	2.1
1	B	25	ARG	2.1
3	D	137	THR	2.1
3	D	52	PRO	2.1
3	D	365	GLU	2.0
3	D	53	ALA	2.0
2	E	56	SER	2.0
3	D	268	LEU	2.0
3	D	314	VAL	2.0

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

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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
2	0AF	C	57	15/16	0.92	0.29	51,68,72,74	0
2	0AF	E	57	15/16	0.94	0.31	34,47,54,59	0

6.3 Carbohydrates (i)

There are no carbohydrates in this entry.

6.4 Ligands (i)

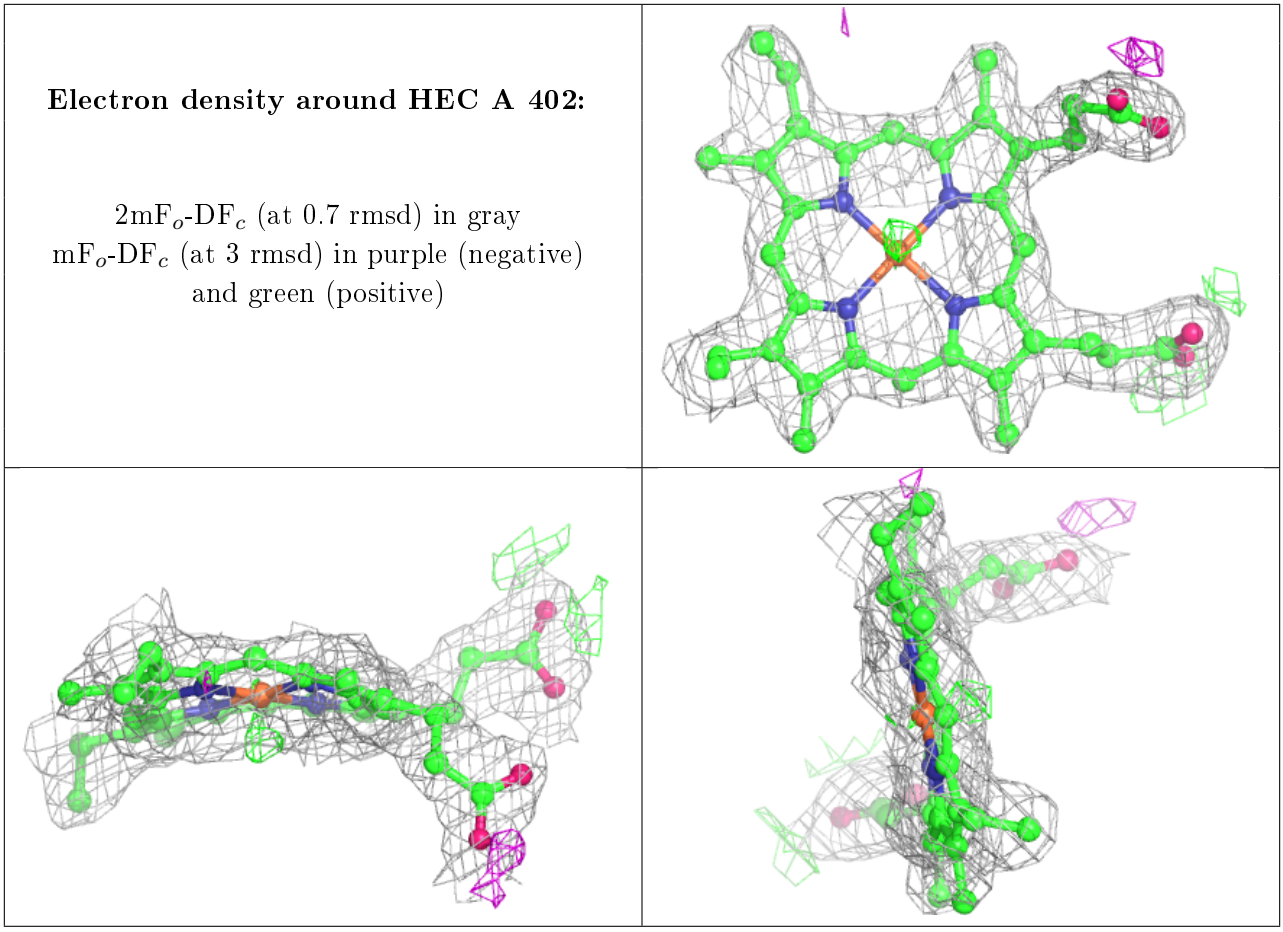
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95^{th} percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9'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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
9	PGE	F	402	10/10	0.64	0.26	95,100,103,103	0
8	MES	D	401	12/12	0.90	0.30	81,92,97,97	0
8	MES	F	401	12/12	0.94	0.24	33,46,48,50	12
7	EDO	B	406	4/4	0.95	0.14	55,56,58,61	0
6	NA	B	405	1/1	0.96	0.06	41,41,41,41	0
4	CA	A	401	1/1	0.97	0.08	47,47,47,47	0
5	HEC	A	402	43/43	0.97	0.10	34,43,48,49	0
5	HEC	B	402	43/43	0.98	0.10	24,31,35,36	0
6	NA	B	404	1/1	0.98	0.07	44,44,44,44	0
5	HEC	A	403	43/43	0.99	0.10	38,40,44,46	0
5	HEC	B	403	43/43	0.99	0.11	16,22,25,27	0
4	CA	B	401	1/1	0.99	0.12	26,26,26,26	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.

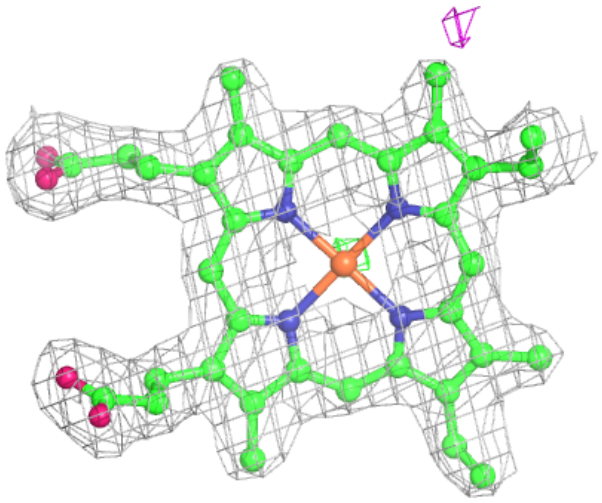
Electron density around HEC A 402:

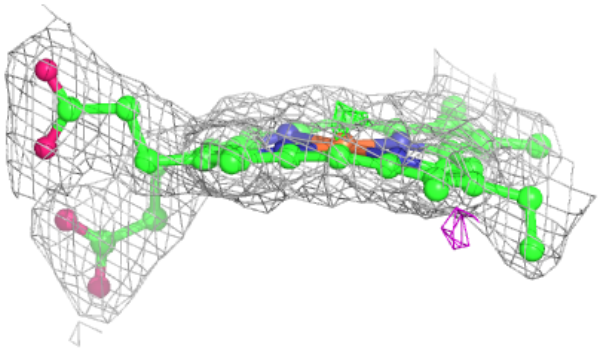
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

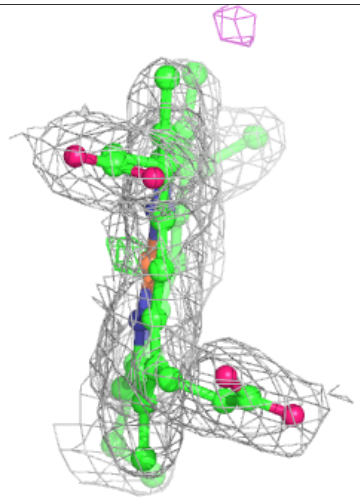


Electron density around HEC B 402:

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

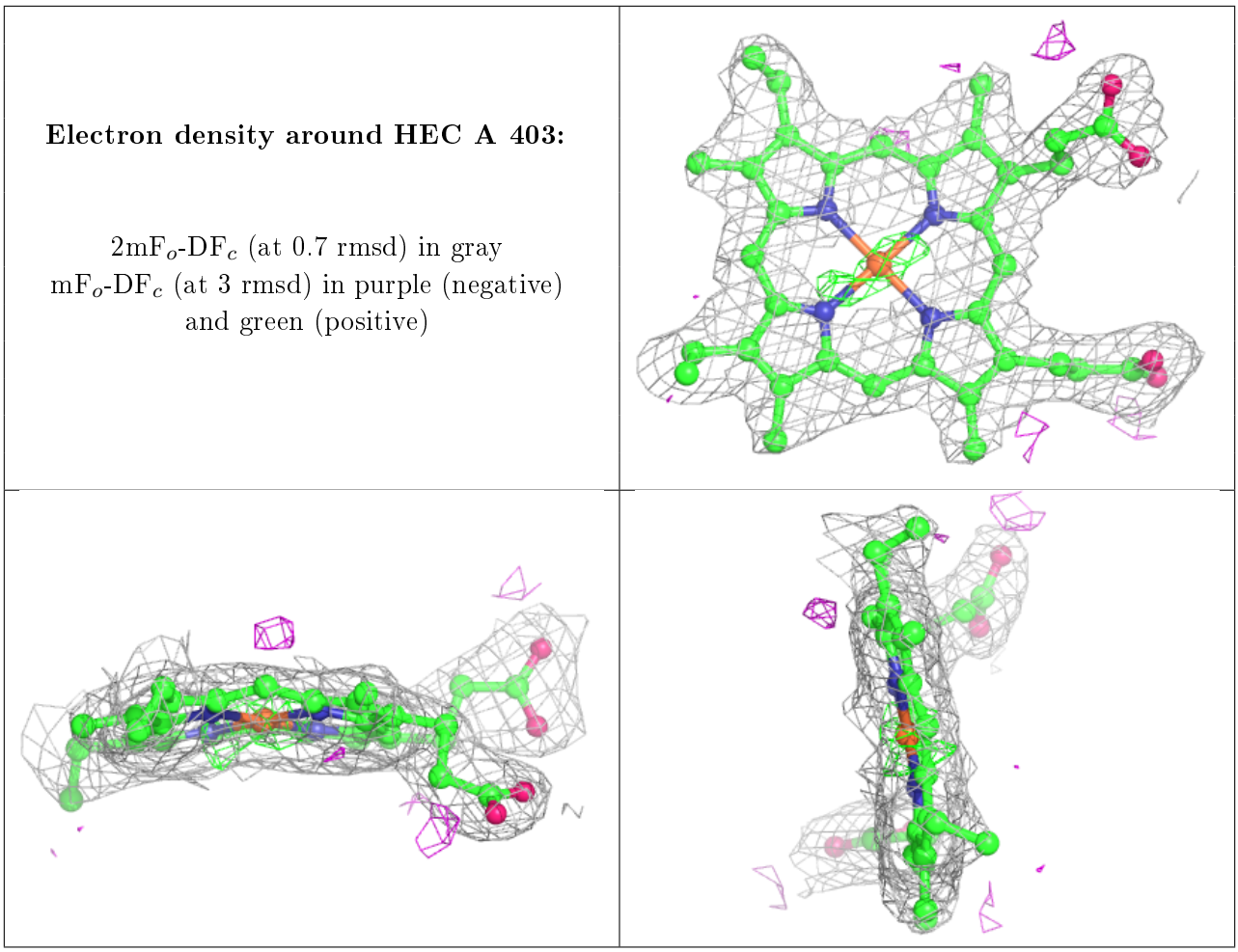






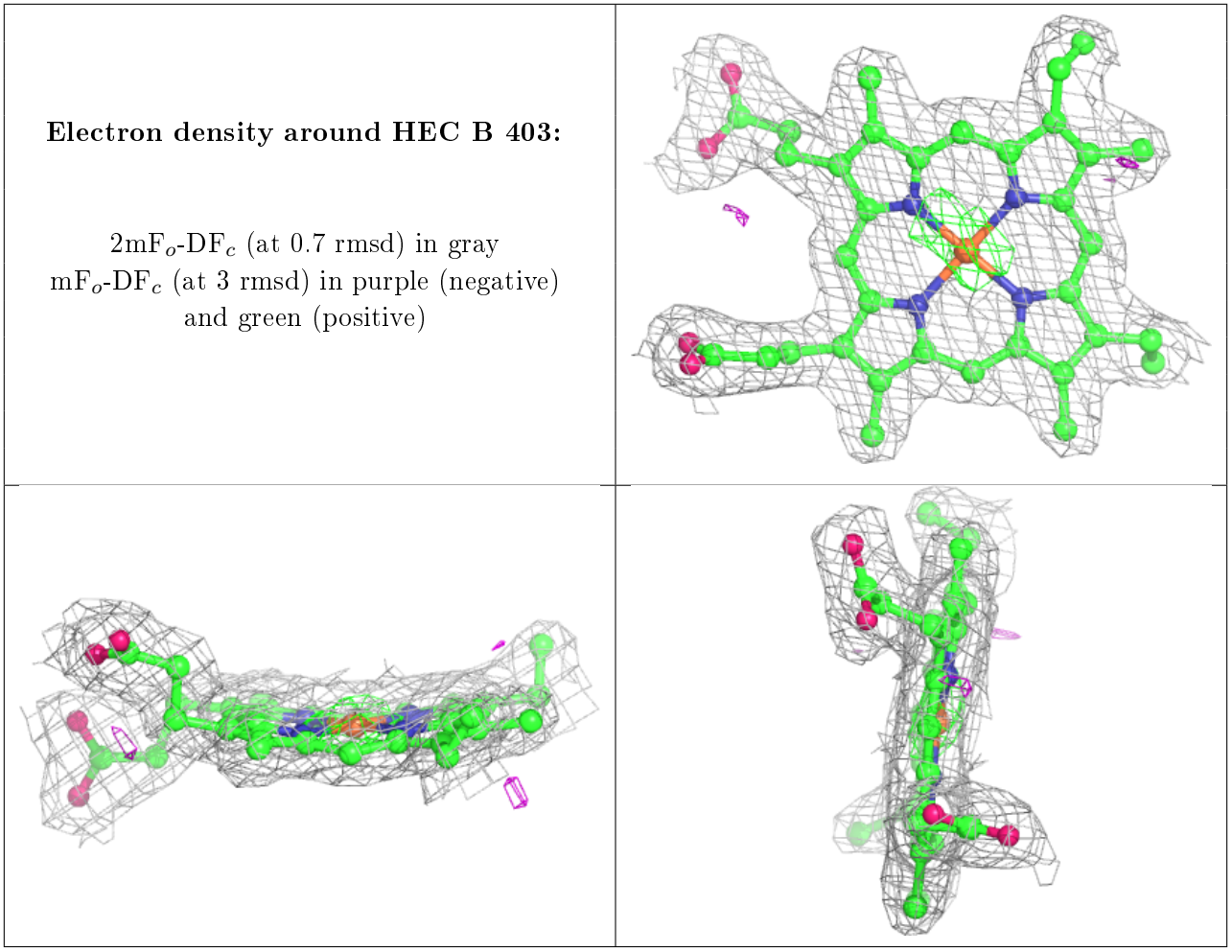
Electron density around HEC A 403:

$2mF_o$-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 403:

$2mF_o$-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

There are no such residues in this entry.