Full wwPDB X-ray Structure Validation Report (i)

Sep 12, 2023 – 08:25 AM EDT

PDB ID	:	4O1Q
Title	:	Crystal Structure of the Q103N-MauG/pre-Methylamine Dehydrogenase Complex
Authors	:	Yukl, E.T.; Wilmot, C.W.
Deposited on	:	2013-12-16
Resolution	:	2.59 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 (i) 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 (i)) were used in the production of this report:

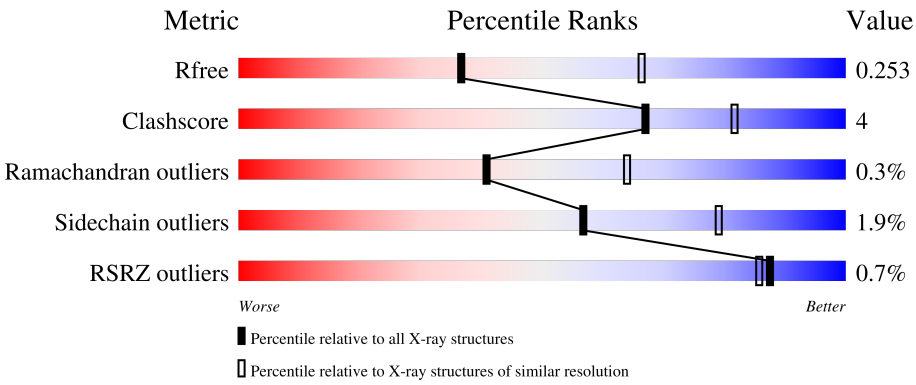
MolProbity	:	4.02b-467
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.35.1
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.35.1

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 2.59 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	3163 (2.60-2.60)
Clashscore	141614	3518 (2.60-2.60)
Ramachandran outliers	138981	3455 (2.60-2.60)
Sidechain outliers	138945	3455 (2.60-2.60)
RSRZ outliers	127900	3104 (2.60-2.60)

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 <=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	% 84% 10% • 5%
1	B	373	% 85% 10% • 5%
2	C	137	% 77% 13% • 9%
2	E	137	81% 9% • 9%
3	D	385	% 90% 8% •

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Mol	Chain	Length	Quality of chain
3	F	385	88% 10% •

2 Entry composition (i)

There are 11 unique types of molecules in this entry. The entry contains 13884 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
			Total	C	N	O	S			
1	A	354	2742	1711	492	528	11	0	1	0
1	B	355	2751	1716	493	531	11	0	1	0

There are 14 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	-5	HIS	-	expression tag	UNP Q51658
A	-4	HIS	-	expression tag	UNP Q51658
A	-3	HIS	-	expression tag	UNP Q51658
A	-2	HIS	-	expression tag	UNP Q51658
A	-1	HIS	-	expression tag	UNP Q51658
A	0	HIS	-	expression tag	UNP Q51658
A	103	ASN	GLN	engineered mutation	UNP Q51658
B	-5	HIS	-	expression tag	UNP Q51658
B	-4	HIS	-	expression tag	UNP Q51658
B	-3	HIS	-	expression tag	UNP Q51658
B	-2	HIS	-	expression tag	UNP Q51658
B	-1	HIS	-	expression tag	UNP Q51658
B	0	HIS	-	expression tag	UNP Q51658
B	103	ASN	GLN	engineered mutation	UNP Q51658

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
2	C	125	955	590	161	191	13	0	0	0
2	E	125	958	592	161	191	14	0	1	0

There are 12 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
C	-5	HIS	-	expression tag	UNP A1BBA0
C	-4	HIS	-	expression tag	UNP A1BBA0
C	-3	HIS	-	expression tag	UNP A1BBA0
C	-2	HIS	-	expression tag	UNP A1BBA0
C	-1	HIS	-	expression tag	UNP A1BBA0
C	0	HIS	-	expression tag	UNP A1BBA0
E	-5	HIS	-	expression tag	UNP A1BBA0
E	-4	HIS	-	expression tag	UNP A1BBA0
E	-3	HIS	-	expression tag	UNP A1BBA0
E	-2	HIS	-	expression tag	UNP A1BBA0
E	-1	HIS	-	expression tag	UNP A1BBA0
E	0	HIS	-	expression tag	UNP A1BBA0

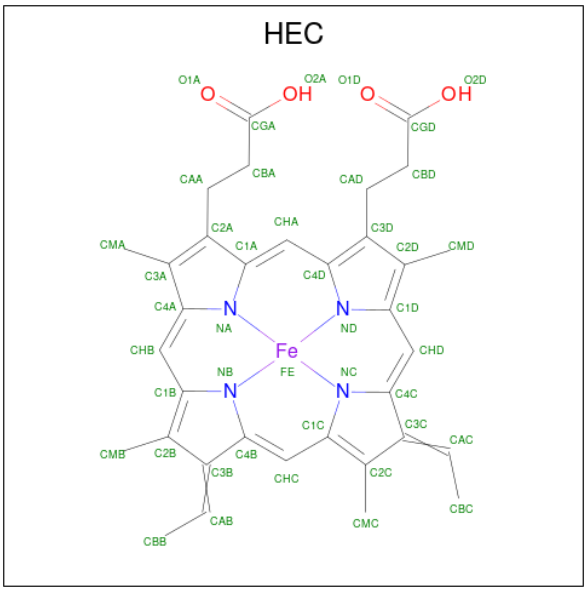
- Molecule 3 is a protein called Methylamine dehydrogenase heavy chain.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
3	D	376	2923	1853	502	560	8	0	0	0
			Total	C	N	O	S			
3	F	376	2931	1857	503	563	8	0	1	0

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

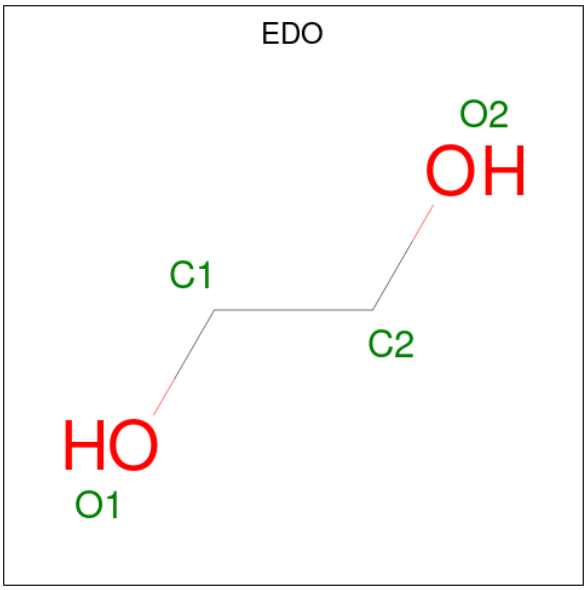
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
			Total	Ca		
4	A	1	1	1	0	0
			Total	Ca		
4	B	1	1	1	0	0

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



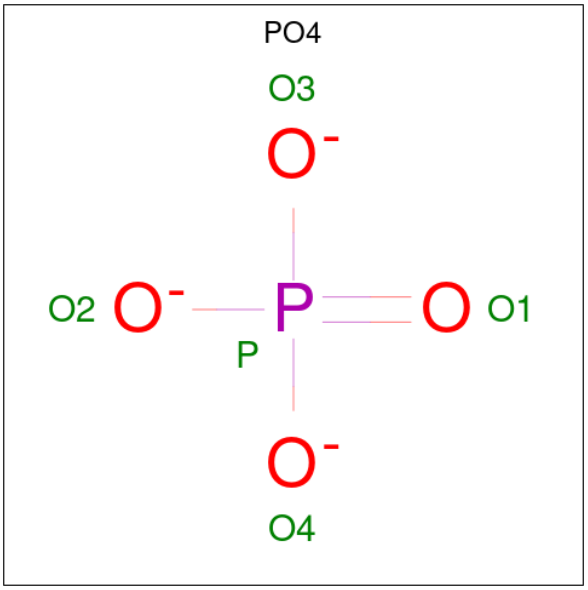
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
			Total	C	Fe	N	O		
5	A	1	43	34	1	4	4	0	0
			Total	C	Fe	N	O		
5	A	1	43	34	1	4	4	0	0
			Total	C	Fe	N	O		
5	B	1	43	34	1	4	4	0	0
			Total	C	Fe	N	O		
5	B	1	43	34	1	4	4	0	0

- Molecule 6 is 1,2-ETHANEDIOL (three-letter code: EDO) (formula: $C_2H_6O_2$).



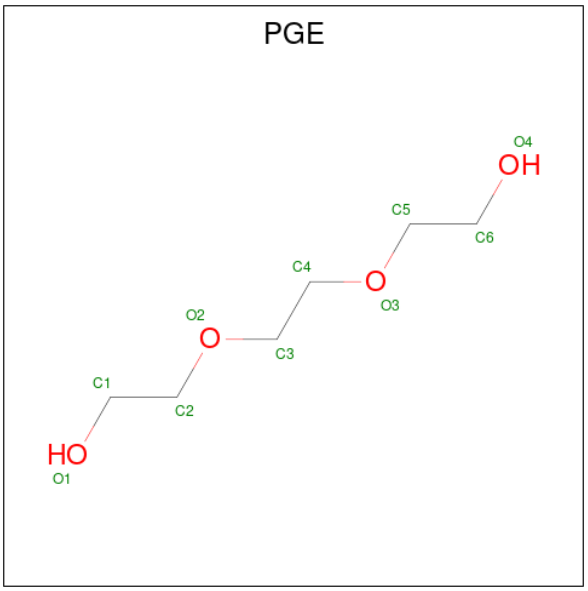
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
			Total	C	O		
6	A	1	4	2	2	0	0
			Total	C	O		
6	A	1	4	2	2	0	0
			Total	C	O		
6	B	1	4	2	2	0	0

- Molecule 7 is PHOSPHATE ION (three-letter code: PO4) (formula: O_4P).



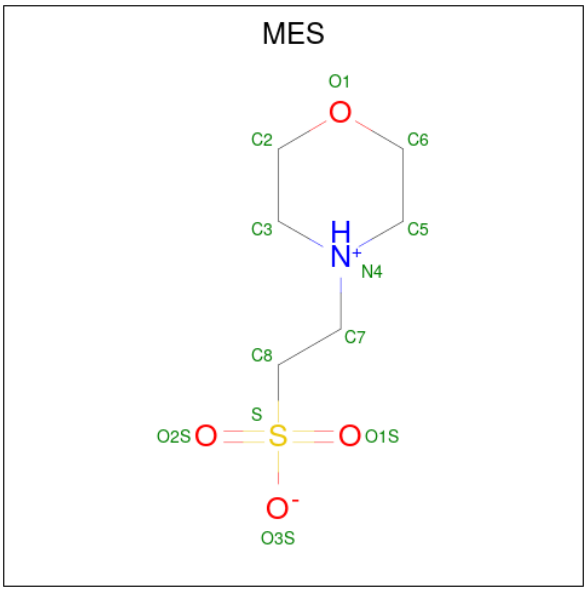
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
			Total	O	P		
7	B	1	5	4	1	0	0

- Molecule 8 is TRIETHYLENE GLYCOL (three-letter code: PGE) (formula: $C_6H_{14}O_4$).



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

- Molecule 9 is 2-(N-MORPHOLINO)-ETHANESULFONIC ACID (three-letter code: MES) (formula: $C_6H_{13}NO_4S$).



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

- Molecule 10 is SODIUM ION (three-letter code: NA) (formula: Na).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
			Total	Na		
10	F	1	1	1	0	0

- Molecule 11 is water.

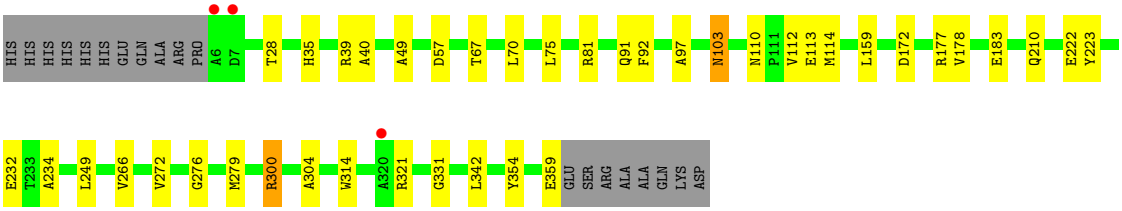
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
			Total	O		
11	A	63	63	63	0	0
			Total	O		
11	B	97	97	97	0	0
			Total	O		
11	C	29	29	29	0	0
			Total	O		
11	D	65	65	65	0	0
			Total	O		
11	E	27	27	27	0	0
			Total	O		
11	F	116	117	117	0	1

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.

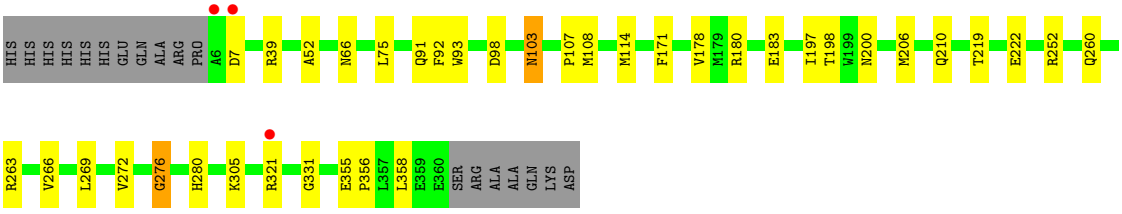
• Molecule 1: Methylamine utilization protein MauG

Chain A:



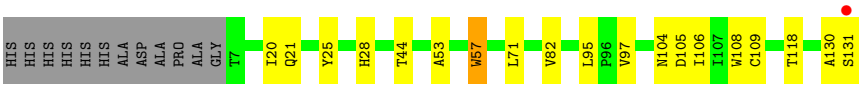
• Molecule 1: Methylamine utilization protein MauG

Chain B:



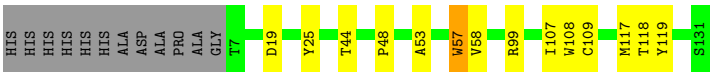
• Molecule 2: Methylamine dehydrogenase light chain

Chain C:



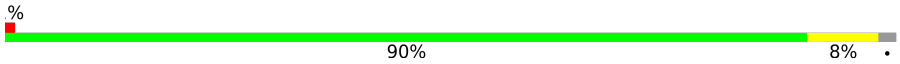
• Molecule 2: Methylamine dehydrogenase light chain

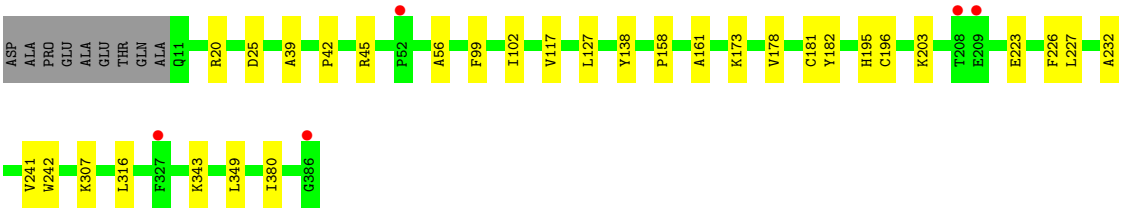
Chain E:



• Molecule 3: Methylamine dehydrogenase heavy chain

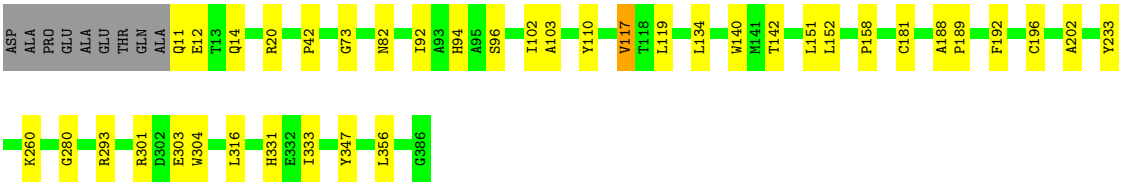
Chain D:





- Molecule 3: Methylamine dehydrogenase heavy chain

Chain F:



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 – 2.59 44.49 – 2.59	Depositor EDS
% Data completeness (in resolution range)	98.2 (44.49-2.59) 98.2 (44.49-2.59)	Depositor EDS
R_{merge}	0.12	Depositor
R_{sym}	0.12	Depositor
$< I/\sigma(I) >$ [1]	2.45 (at 2.58Å)	Xtriage
Refinement program	REFMAC 5.7.0029	Depositor
R, R_{free}	0.198 , 0.254 0.195 , 0.253	Depositor DCC
R_{free} test set	2653 reflections (5.00%)	wwPDB-VP
Wilson B-factor (Å^2)	40.2	Xtriage
Anisotropy	0.545	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.30 , 30.7	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	0.94	EDS
Total number of atoms	13884	wwPDB-VP
Average B, all atoms (Å^2)	52.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.02% 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 (i)

5.1 Standard geometry (i)

Bond lengths and bond angles in the following residue types are not validated in this section: MES, NA, HEC, CA, PO4, PGE, 0AF, EDO

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	0.32	0/2806	0.51	0/3808
1	B	0.33	0/2815	0.52	0/3820
2	C	0.32	0/964	0.51	0/1315
2	E	0.31	0/970	0.52	0/1323
3	D	0.29	0/3000	0.51	0/4088
3	F	0.31	0/3008	0.54	0/4099
All	All	0.31	0/13563	0.52	0/18453

There are no bond length outliers.

There are no bond angle outliers.

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	2742	0	2613	26	0
1	B	2751	0	2619	23	0
2	C	955	0	859	15	0
2	E	958	0	863	10	0
3	D	2923	0	2808	17	0
3	F	2931	0	2810	22	0
4	A	1	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
4	B	1	0	0	0	0
5	A	86	0	60	9	0
5	B	86	0	60	5	0
6	A	8	0	12	0	0
6	B	4	0	6	0	0
7	B	5	0	0	0	0
8	C	10	0	14	0	0
9	D	12	0	13	0	0
9	F	12	0	13	0	0
10	F	1	0	0	0	0
11	A	63	0	0	1	0
11	B	97	0	0	3	0
11	C	29	0	0	1	0
11	D	65	0	0	1	0
11	E	27	0	0	1	0
11	F	117	0	0	1	0
All	All	13884	0	12750	101	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 4.

All (101) 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)
5:B:403:HEC:HBC3	5:B:403:HEC:HMC1	1.75	0.68
1:B:39:ARG:NH2	1:B:276:GLY:O	2.31	0.63
1:B:103:ASN:ND2	11:B:597:HOH:O	2.32	0.62
3:F:82:ASN:HB3	3:F:142:THR:HB	1.81	0.61
2:E:107:ILE:HD12	2:E:119:TYR:HB2	1.83	0.61
5:A:403:HEC:HMC1	5:A:403:HEC:HBC3	1.83	0.60
1:B:210:GLN:HE22	2:E:44:THR:HG21	1.67	0.60
1:A:172:ASP:O	1:A:177:ARG:NH1	2.35	0.59
3:F:96:SER:HB3	3:F:110:TYR:CZ	2.38	0.59
1:A:210:GLN:HE22	2:C:44:THR:HG21	1.68	0.57
1:B:107:PRO:CG	11:B:597:HOH:O	2.52	0.57
1:B:197:ILE:HG22	1:B:206:MET:CE	2.36	0.55
5:B:402:HEC:HBC3	5:B:402:HEC:HMC1	1.88	0.54
2:C:104:ASN:OD1	3:D:307:LYS:NZ	2.42	0.52
1:B:266:VAL:HG22	5:B:403:HEC:HMD3	1.91	0.52
2:C:105:ASP:HB2	3:D:138:TYR:OH	2.08	0.52
3:F:196:CYS:SG	3:F:202:ALA:HB2	2.50	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:260:GLN:HA	1:B:263:ARG:HD2	1.93	0.51
3:D:232:ALA:HB3	3:D:241:VAL:HB	1.93	0.51
1:A:40:ALA:HA	1:A:354:TYR:CE2	2.47	0.50
2:C:21:GLN:HE22	3:F:14:GLN:HE21	1.58	0.50
1:A:178:VAL:HA	1:A:183:GLU:O	2.12	0.50
2:E:99:ARG:NH1	11:E:212:HOH:O	2.38	0.50
2:E:118:THR:HG21	3:F:103:ALA:HB1	1.94	0.49
2:C:20:ILE:HG22	2:C:25:TYR:CE2	2.47	0.49
3:F:73:GLY:HA3	3:F:119:LEU:HD11	1.94	0.49
1:B:91:GLN:O	1:B:92:PHE:HB2	2.13	0.48
1:A:67:THR:OG1	5:A:402:HEC:HMD3	2.14	0.48
2:C:82:VAL:HG12	3:D:56:ALA:HA	1.96	0.48
2:C:20:ILE:HG22	2:C:25:TYR:CZ	2.48	0.47
1:B:272:VAL:HG21	5:B:403:HEC:HMA3	1.95	0.47
3:F:142:THR:CG2	3:F:151:LEU:HD21	2.45	0.47
2:C:95:LEU:HD22	3:D:226:PHE:CE1	2.49	0.47
1:A:114:MET:CG	5:A:402:HEC:HMC2	2.46	0.47
3:F:347:TYR:HB3	3:F:356:LEU:HD11	1.97	0.46
1:B:198:THR:HG22	2:E:58:VAL:HG13	1.97	0.46
3:F:293:ARG:NH2	11:F:565:HOH:O	2.46	0.46
1:A:28:THR:OG1	1:A:57:ASP:OD1	2.34	0.46
1:A:159:LEU:HD13	5:A:402:HEC:HBB3	1.98	0.46
3:F:151:LEU:HD23	3:F:151:LEU:C	2.36	0.46
1:A:91:GLN:O	1:A:92:PHE:HB2	2.15	0.46
3:D:181:CYS:HA	3:D:196:CYS:HA	1.97	0.46
1:A:49:ALA:CB	1:A:234:ALA:HA	2.46	0.46
1:B:197:ILE:HG22	1:B:206:MET:HE2	1.97	0.46
1:B:200:ASN:O	5:B:403:HEC:HMC3	2.14	0.46
2:C:25:TYR:HB3	2:C:28:HIS:CD2	2.51	0.46
1:B:52:ALA:O	1:B:66:ASN:HA	2.16	0.46
1:B:331:GLY:O	3:F:158:PRO:HA	2.15	0.45
2:E:117:MET:HB3	3:F:134:LEU:HD12	1.98	0.45
1:A:39:ARG:NH2	1:A:276:GLY:O	2.50	0.45
3:D:42:PRO:HD3	3:D:117:VAL:HG12	1.96	0.45
1:A:272:VAL:HG21	5:A:403:HEC:HMA3	1.98	0.45
1:B:178:VAL:HA	1:B:183:GLU:O	2.16	0.45
2:C:130:ALA:O	2:C:131:SER:CB	2.65	0.45
1:A:67:THR:HG23	5:A:402:HEC:C1D	2.47	0.45
1:A:342:LEU:HD13	5:A:403:HEC:HMB1	1.99	0.45
1:B:108:MET:HA	1:B:114:MET:HB2	1.99	0.45
2:C:97:VAL:HG23	2:C:106:ILE:HD11	1.99	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:E:53:ALA:HB2	2:E:109:CYS:HA	1.99	0.44
2:C:118:THR:HG23	3:D:99:PHE:CZ	2.52	0.44
1:A:110:ASN:HB3	1:A:113:GLU:HB2	1.99	0.44
1:B:171:PHE:O	1:B:180:ARG:NH2	2.49	0.44
1:A:110:ASN:OD1	1:A:112:VAL:HG22	2.18	0.44
3:F:12:GLU:OE1	3:F:20:ARG:NH1	2.50	0.44
3:F:188:ALA:HB1	3:F:189:PRO:HD2	2.00	0.44
3:D:45:ARG:NH2	3:D:343:LYS:O	2.51	0.44
1:B:222:GLU:O	1:B:266:VAL:HG23	2.18	0.43
1:A:266:VAL:HG22	5:A:403:HEC:HMD3	2.00	0.43
3:D:39:ALA:HB2	2:E:48:PRO:HG3	1.98	0.43
2:E:57:0AF:CE3	2:E:108:TRP:CD1	3.01	0.43
3:F:331:HIS:HB2	3:F:333:ILE:HD11	2.00	0.43
1:B:98:ASP:OD1	1:B:252:ARG:NH2	2.52	0.43
1:A:91:GLN:HB2	1:A:97:ALA:HB3	2.00	0.43
3:F:140:TRP:CE2	3:F:233:TYR:HB3	2.54	0.42
2:C:53:ALA:HB2	2:C:109:CYS:HA	2.01	0.42
3:D:161:ALA:HA	3:D:178:VAL:HG22	2.02	0.42
3:F:42:PRO:HD3	3:F:117:VAL:HG12	2.00	0.42
3:F:303:GLU:HG3	3:F:304:TRP:CD1	2.55	0.42
3:D:349:LEU:HB2	3:D:380:ILE:HD11	2.02	0.42
3:F:280:GLY:HA3	3:F:301:ARG:CZ	2.49	0.42
2:E:19:ASP:O	2:E:25:TYR:HB2	2.19	0.42
1:A:222:GLU:O	1:A:266:VAL:HG23	2.20	0.42
1:B:107:PRO:CD	11:B:597:HOH:O	2.68	0.42
3:D:227:LEU:HB3	3:D:242:TRP:CD1	2.54	0.42
3:F:142:THR:HG23	3:F:151:LEU:HD21	2.01	0.42
3:F:181:CYS:HA	3:F:196:CYS:HA	2.01	0.41
1:A:300:ARG:HD3	3:D:158:PRO:HG3	2.03	0.41
3:D:182:TYR:N	3:D:195:HIS:O	2.50	0.41
1:B:197:ILE:HG22	1:B:206:MET:HE1	2.01	0.41
1:A:103:ASN:ND2	11:A:563:HOH:O	2.50	0.41
2:C:130:ALA:HB1	11:C:303:HOH:O	2.20	0.41
1:A:304:ALA:O	1:A:314:TRP:NE1	2.47	0.41
1:B:93:TRP:CE2	1:B:280:HIS:HA	2.56	0.41
1:B:355:GLU:N	1:B:356:PRO:CD	2.84	0.41
3:D:25:ASP:HA	11:D:546:HOH:O	2.21	0.41
2:C:57:0AF:CE3	2:C:108:TRP:CD1	3.04	0.41
1:A:35:HIS:CE1	1:A:70:LEU:HD21	2.56	0.40
1:A:279:MET:SD	5:A:403:HEC:HBD1	2.62	0.40
1:A:331:GLY:O	3:D:158:PRO:HA	2.20	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:F:152:LEU:HD13	3:F:192:PHE:CD2	2.57	0.40
1:A:223:TYR:CG	1:A:249:LEU:HD22	2.57	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	353/373 (95%)	339 (96%)	13 (4%)	1 (0%)	41	64
1	B	354/373 (95%)	342 (97%)	10 (3%)	2 (1%)	25	47
2	C	122/137 (89%)	115 (94%)	7 (6%)	0	100	100
2	E	123/137 (90%)	116 (94%)	7 (6%)	0	100	100
3	D	374/385 (97%)	356 (95%)	17 (4%)	1 (0%)	41	64
3	F	375/385 (97%)	356 (95%)	18 (5%)	1 (0%)	41	64
All	All	1701/1790 (95%)	1624 (96%)	72 (4%)	5 (0%)	41	64

All (5) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	B	276	GLY
1	B	358	LEU
3	F	102	ILE
1	A	232	GLU
3	D	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	277/292 (95%)	271 (98%)	6 (2%)	52	76
1	B	278/292 (95%)	271 (98%)	7 (2%)	47	73
2	C	104/112 (93%)	103 (99%)	1 (1%)	76	90
2	E	105/112 (94%)	105 (100%)	0	100	100
3	D	304/310 (98%)	298 (98%)	6 (2%)	55	78
3	F	305/310 (98%)	299 (98%)	6 (2%)	55	78
All	All	1373/1428 (96%)	1347 (98%)	26 (2%)	57	79

All (26) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	75	LEU
1	A	81	ARG
1	A	103	ASN
1	A	300	ARG
1	A	321	ARG
1	A	359	GLU
1	B	7	ASP
1	B	75	LEU
1	B	103	ASN
1	B	219	THR
1	B	269	LEU
1	B	305	LYS
1	B	321	ARG
2	C	71	LEU
3	D	20	ARG
3	D	127	LEU
3	D	173	LYS
3	D	203	LYS
3	D	223	GLU
3	D	316	LEU
3	F	11	GLN
3	F	92	ILE
3	F	94	HIS
3	F	117	VAL
3	F	260	LYS
3	F	316	LEU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (15) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	60	GLN
1	A	84	ASN
1	A	91	GLN
1	A	103	ASN
1	A	163	GLN
1	A	210	GLN
1	B	91	GLN
1	B	103	ASN
1	B	163	GLN
1	B	210	GLN
3	D	30	GLN
2	E	21	GLN
2	E	68	GLN
3	F	14	GLN
3	F	331	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	1.51	1 (7%)	11,22,24	0.99	0
2	0AF	C	57	2	13,16,17	1.38	1 (7%)	11,22,24	0.94	1 (9%)

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 (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	E	57	0AF	CZ2-CE2	4.39	1.49	1.42
2	C	57	0AF	CZ2-CE2	3.59	1.48	1.42

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	C	57	0AF	CB-CA-C	2.08	115.37	111.47

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

2 monomers are involved in 2 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	E	57	0AF	1	0
2	C	57	0AF	1	0

5.5 Carbohydrates (i)

There are no monosaccharides in this entry.

5.6 Ligand geometry (i)

Of 14 ligands modelled in this entry, 3 are monoatomic - leaving 11 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	32,50,50	2.38	12 (37%)	24,82,82	2.40	8 (33%)
5	HEC	B	403	1	32,50,50	2.33	11 (34%)	24,82,82	2.65	7 (29%)
5	HEC	A	403	1	32,50,50	2.27	12 (37%)	24,82,82	2.17	7 (29%)
9	MES	D	401	-	12,12,12	2.02	1 (8%)	14,16,16	6.86	8 (57%)
6	EDO	B	404	-	3,3,3	0.47	0	2,2,2	0.28	0
9	MES	F	401	-	12,12,12	2.19	1 (8%)	14,16,16	6.57	5 (35%)
5	HEC	A	402	1	32,50,50	2.37	12 (37%)	24,82,82	2.72	8 (33%)
8	PGE	C	201	-	9,9,9	0.51	0	8,8,8	0.28	0
6	EDO	A	404	-	3,3,3	0.50	0	2,2,2	0.23	0
7	PO4	B	405	-	4,4,4	0.90	0	6,6,6	0.38	0
6	EDO	A	405	-	3,3,3	0.48	0	2,2,2	0.28	0

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	-	0/10/54/54	-
5	HEC	B	403	1	-	2/10/54/54	-
5	HEC	A	403	1	-	4/10/54/54	-
9	MES	D	401	-	-	2/6/14/14	0/1/1/1
6	EDO	B	404	-	-	1/1/1/1	-
9	MES	F	401	-	-	3/6/14/14	0/1/1/1
5	HEC	A	402	1	-	0/10/54/54	-
8	PGE	C	201	-	-	1/7/7/7	-
6	EDO	A	404	-	-	1/1/1/1	-
6	EDO	A	405	-	-	0/1/1/1	-

All (49) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
5	B	403	HEC	C2B-C3B	7.67	1.48	1.40
5	A	402	HEC	C2B-C3B	7.17	1.48	1.40
9	F	401	MES	C8-S	-7.14	1.67	1.77
5	B	402	HEC	C2B-C3B	7.14	1.48	1.40
5	A	403	HEC	C2B-C3B	6.52	1.47	1.40
9	D	401	MES	C8-S	-6.34	1.68	1.77
5	A	403	HEC	C3C-C2C	6.14	1.47	1.40
5	B	402	HEC	C3C-C2C	6.01	1.47	1.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
5	B	403	HEC	C3C-C2C	5.72	1.46	1.40
5	A	402	HEC	C3C-C2C	5.55	1.46	1.40
5	A	402	HEC	C3C-C4C	3.77	1.49	1.43
5	A	403	HEC	C2A-C3A	3.43	1.47	1.37
5	A	402	HEC	C2A-C3A	3.40	1.47	1.37
5	B	402	HEC	C3C-C4C	3.37	1.49	1.43
5	B	402	HEC	C3D-C2D	3.34	1.47	1.37
5	B	403	HEC	C2A-C3A	3.32	1.47	1.37
5	B	402	HEC	C2A-C3A	3.19	1.47	1.37
5	A	403	HEC	C3D-C2D	3.01	1.46	1.37
5	A	402	HEC	C3D-C2D	3.00	1.46	1.37
5	A	402	HEC	C2A-C1A	2.98	1.49	1.42
5	A	402	HEC	C1D-CHD	2.98	1.49	1.41
5	B	402	HEC	C4B-C3B	2.88	1.48	1.43
5	B	403	HEC	C2A-C1A	2.87	1.49	1.42
5	B	403	HEC	C3D-C2D	2.83	1.46	1.37
5	B	403	HEC	C3A-C4A	2.83	1.49	1.42
5	A	403	HEC	C1B-CHB	2.81	1.48	1.41
5	A	403	HEC	C3A-C4A	2.81	1.48	1.42
5	B	402	HEC	C1D-CHD	2.79	1.48	1.41
5	A	403	HEC	C3C-C4C	2.78	1.48	1.43
5	B	402	HEC	C1B-CHB	2.74	1.48	1.41
5	B	402	HEC	C3A-C4A	2.73	1.48	1.42
5	A	402	HEC	C3A-C4A	2.72	1.48	1.42
5	A	403	HEC	C2A-C1A	2.66	1.48	1.42
5	B	403	HEC	C3C-C4C	2.65	1.47	1.43
5	B	403	HEC	C4B-C3B	2.65	1.47	1.43
5	A	402	HEC	C4B-C3B	2.63	1.47	1.43
5	B	402	HEC	C2A-C1A	2.56	1.48	1.42
5	B	403	HEC	C1B-CHB	2.55	1.48	1.41
5	A	402	HEC	C4D-CHA	2.54	1.48	1.41
5	A	402	HEC	C1B-CHB	2.48	1.47	1.41
5	A	403	HEC	C4B-C3B	2.46	1.47	1.43
5	B	402	HEC	C1C-CHC	2.41	1.47	1.41
5	B	403	HEC	C4D-CHA	2.31	1.47	1.41
5	A	403	HEC	C4D-CHA	2.30	1.47	1.41
5	B	402	HEC	C4D-CHA	2.23	1.47	1.41
5	A	403	HEC	C1D-CHD	2.17	1.47	1.41
5	A	403	HEC	C1C-CHC	2.14	1.47	1.41
5	B	403	HEC	C1C-CHC	2.04	1.46	1.41
5	A	402	HEC	C1C-CHC	2.01	1.46	1.41

All (43) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
9	F	401	MES	O3S-S-C8	-12.65	85.30	105.77
9	D	401	MES	O3S-S-C8	-12.26	85.93	105.77
9	D	401	MES	O3S-S-O2S	-11.74	82.58	111.27
9	F	401	MES	O3S-S-O2S	-11.53	83.10	111.27
9	D	401	MES	O3S-S-O1S	-11.05	84.27	111.27
9	D	401	MES	O2S-S-C8	10.79	119.91	106.92
9	F	401	MES	O3S-S-O1S	-10.74	85.04	111.27
9	F	401	MES	O2S-S-C8	10.18	119.17	106.92
9	D	401	MES	O1S-S-C8	9.46	118.31	106.92
9	F	401	MES	O1S-S-C8	9.25	118.05	106.92
5	B	403	HEC	CBD-CAD-C3D	-7.55	99.74	112.62
5	A	402	HEC	CBD-CAD-C3D	-7.26	100.23	112.62
5	B	403	HEC	C1D-C2D-C3D	-6.98	102.14	107.00
5	A	402	HEC	C1D-C2D-C3D	-6.85	102.23	107.00
5	A	403	HEC	C1D-C2D-C3D	-6.59	102.41	107.00
5	B	402	HEC	CBD-CAD-C3D	-5.68	102.93	112.62
5	B	402	HEC	C1D-C2D-C3D	-5.25	103.34	107.00
5	A	402	HEC	C2B-C3B-C4B	-4.58	101.41	106.35
9	D	401	MES	C6-C5-N4	4.36	116.71	110.10
5	B	402	HEC	CBA-CAA-C2A	-4.23	105.48	112.60
5	A	403	HEC	CBD-CAD-C3D	-4.03	105.74	112.62
5	B	402	HEC	C2B-C3B-C4B	-3.91	102.13	106.35
5	A	403	HEC	C2B-C3B-C4B	-3.64	102.43	106.35
5	B	403	HEC	C2B-C3B-C4B	-3.43	102.65	106.35
5	B	403	HEC	CMB-C2B-C3B	3.34	129.74	125.82
9	D	401	MES	C2-C3-N4	3.21	114.98	110.10
5	A	402	HEC	C3B-C4B-NB	3.21	117.01	110.94
5	B	402	HEC	C4C-C3C-C2C	-3.20	102.89	106.35
9	D	401	MES	C5-N4-C3	3.14	115.91	108.83
5	A	402	HEC	C4C-C3C-C2C	-3.12	102.98	106.35
5	A	402	HEC	CBA-CAA-C2A	-2.87	107.76	112.60
5	A	402	HEC	CMC-C2C-C3C	2.83	129.14	125.82
5	B	403	HEC	C4C-C3C-C2C	-2.81	103.32	106.35
5	B	402	HEC	CMB-C2B-C3B	2.78	129.09	125.82
5	B	402	HEC	C3B-C4B-NB	2.62	115.89	110.94
5	A	402	HEC	CMB-C2B-C3B	2.44	128.69	125.82
5	A	403	HEC	CMC-C2C-C3C	2.43	128.68	125.82
5	A	403	HEC	C3B-C4B-NB	2.35	115.38	110.94
5	B	402	HEC	CMC-C2C-C3C	2.31	128.53	125.82
5	A	403	HEC	C4C-C3C-C2C	-2.24	103.93	106.35
5	B	403	HEC	C3B-C4B-NB	2.14	114.99	110.94
5	B	403	HEC	C3C-C4C-NC	2.12	114.94	110.94
5	A	403	HEC	CMB-C2B-C3B	2.02	128.19	125.82

There are no chirality outliers.

All (14) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
5	A	403	HEC	C3D-CAD-CBD-CGD
9	F	401	MES	C7-C8-S-O1S
9	F	401	MES	C7-C8-S-O2S
9	F	401	MES	N4-C7-C8-S
6	B	404	EDO	O1-C1-C2-O2
6	A	404	EDO	O1-C1-C2-O2
9	D	401	MES	C7-C8-S-O2S
8	C	201	PGE	C3-C4-O3-C5
5	A	403	HEC	C2A-CAA-CBA-CGA
9	D	401	MES	C7-C8-S-O3S
5	A	403	HEC	CAD-CBD-CGD-O2D
5	B	403	HEC	CAD-CBD-CGD-O1D
5	A	403	HEC	CAD-CBD-CGD-O1D
5	B	403	HEC	CAD-CBD-CGD-O2D

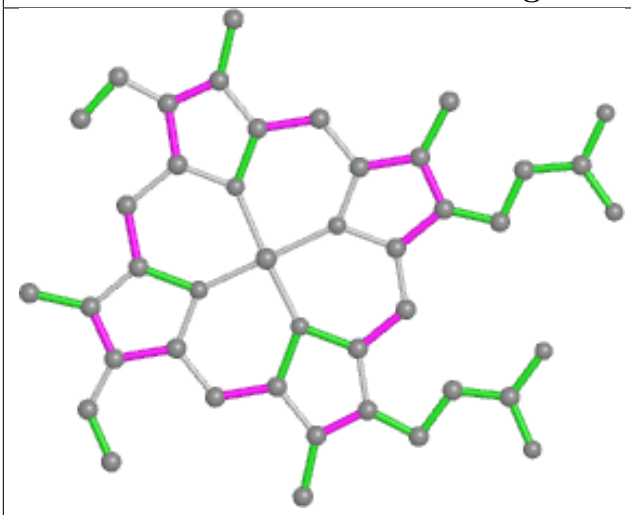
There are no ring outliers.

4 monomers are involved in 14 short contacts:

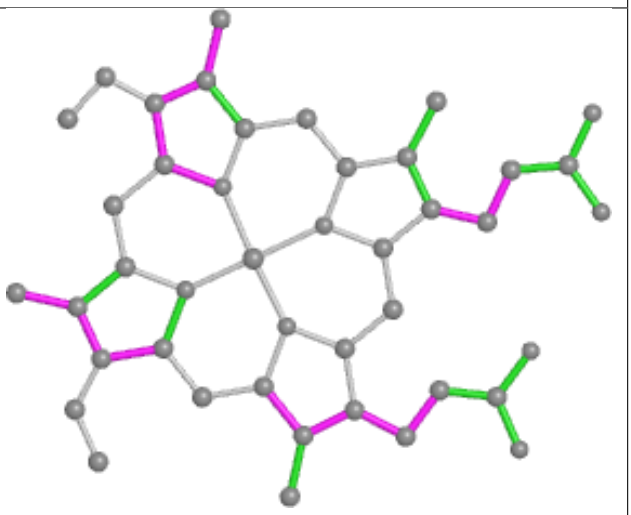
Mol	Chain	Res	Type	Clashes	Symm-Clashes
5	B	402	HEC	1	0
5	B	403	HEC	4	0
5	A	403	HEC	5	0
5	A	402	HEC	4	0

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.

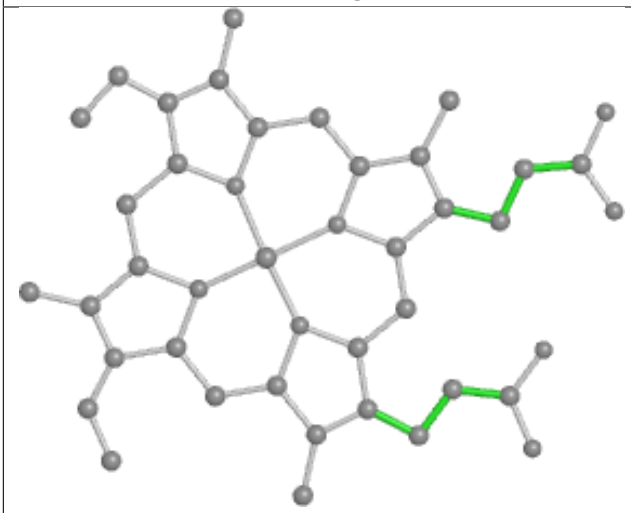
Ligand HEC B 402



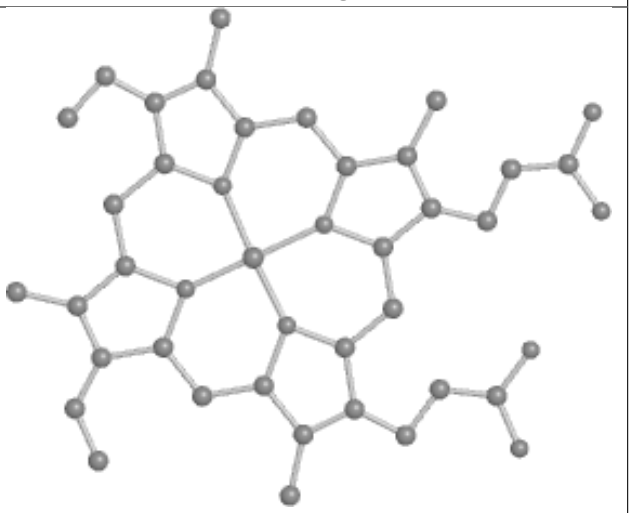
Bond lengths



Bond angles

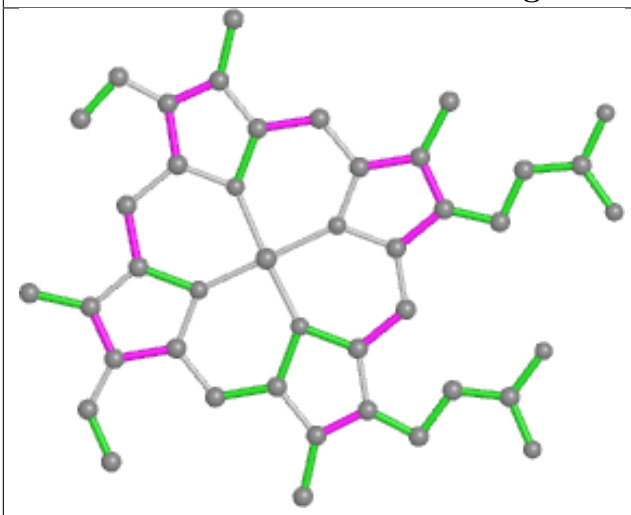


Torsions

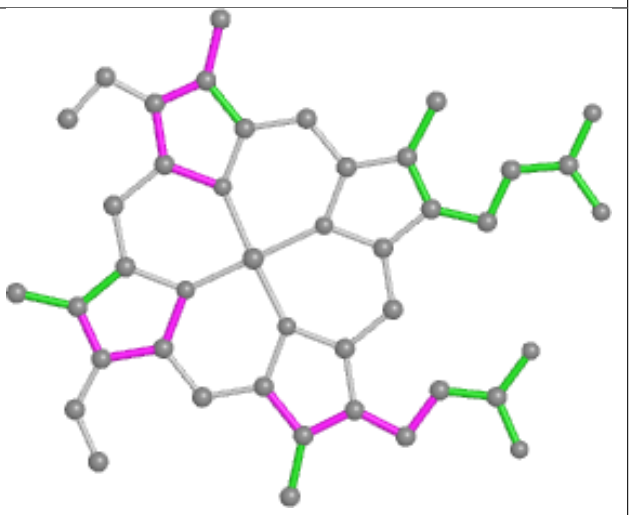


Rings

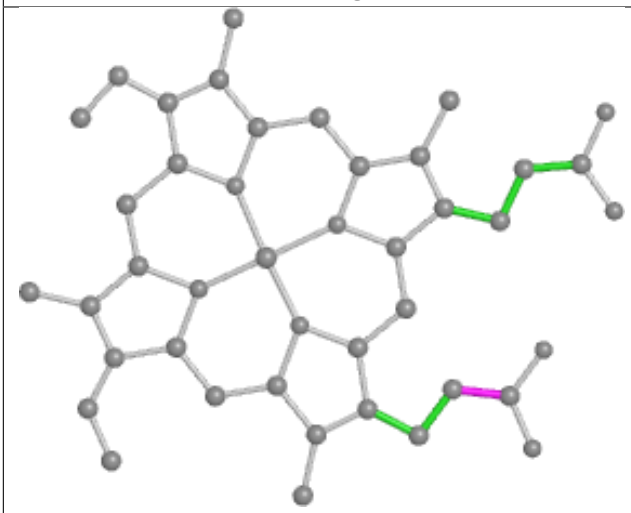
Ligand HEC B 403



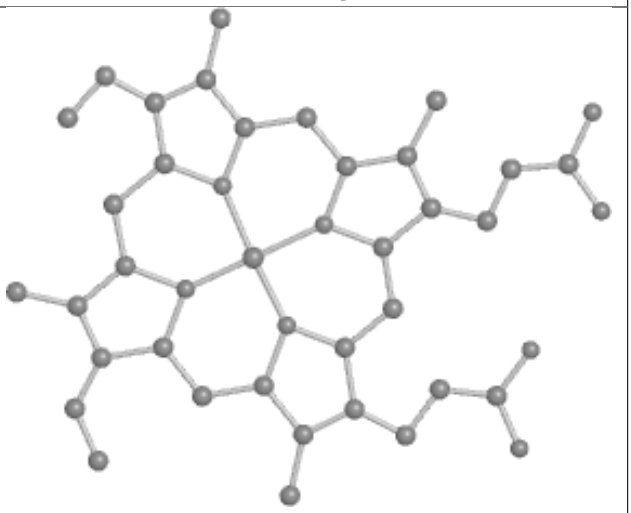
Bond lengths



Bond angles

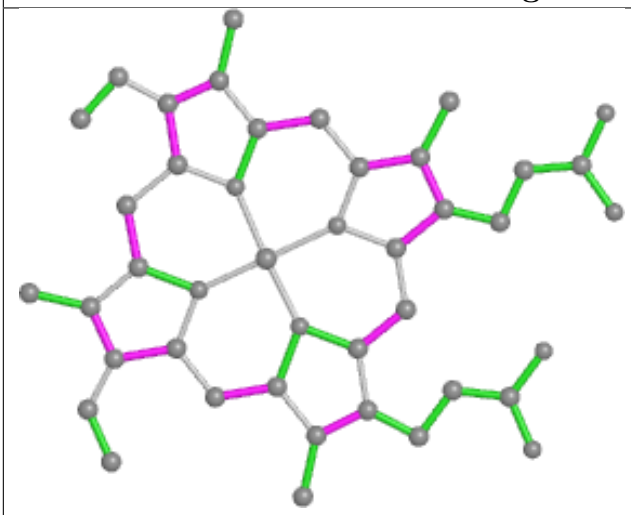


Torsions

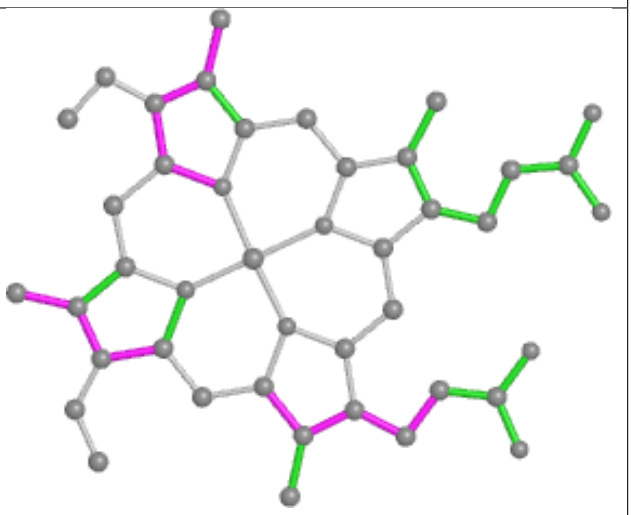


Rings

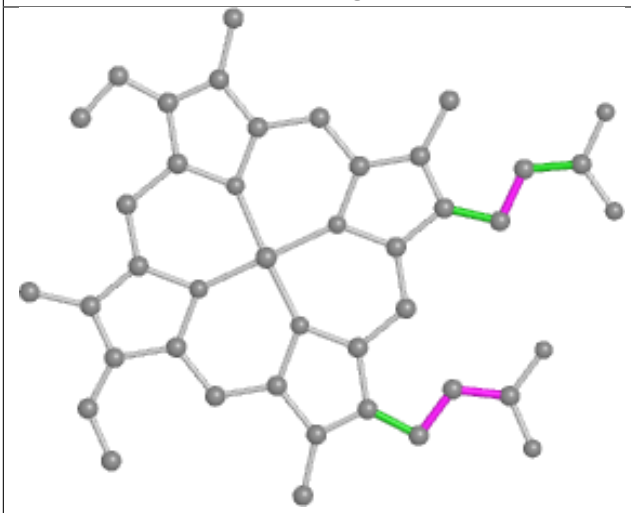
Ligand HEC A 403



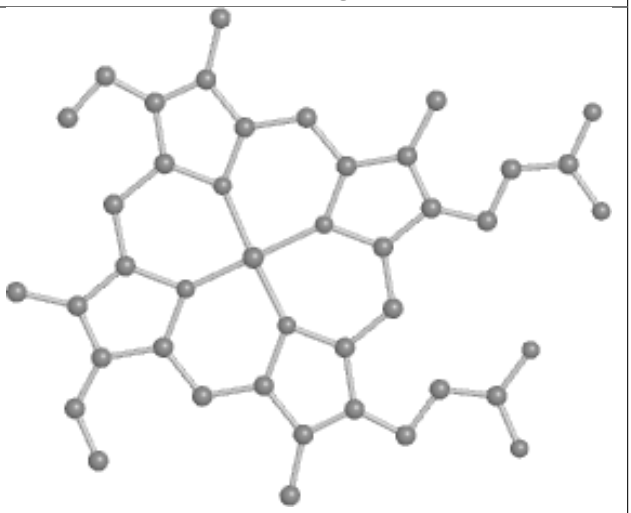
Bond lengths



Bond angles

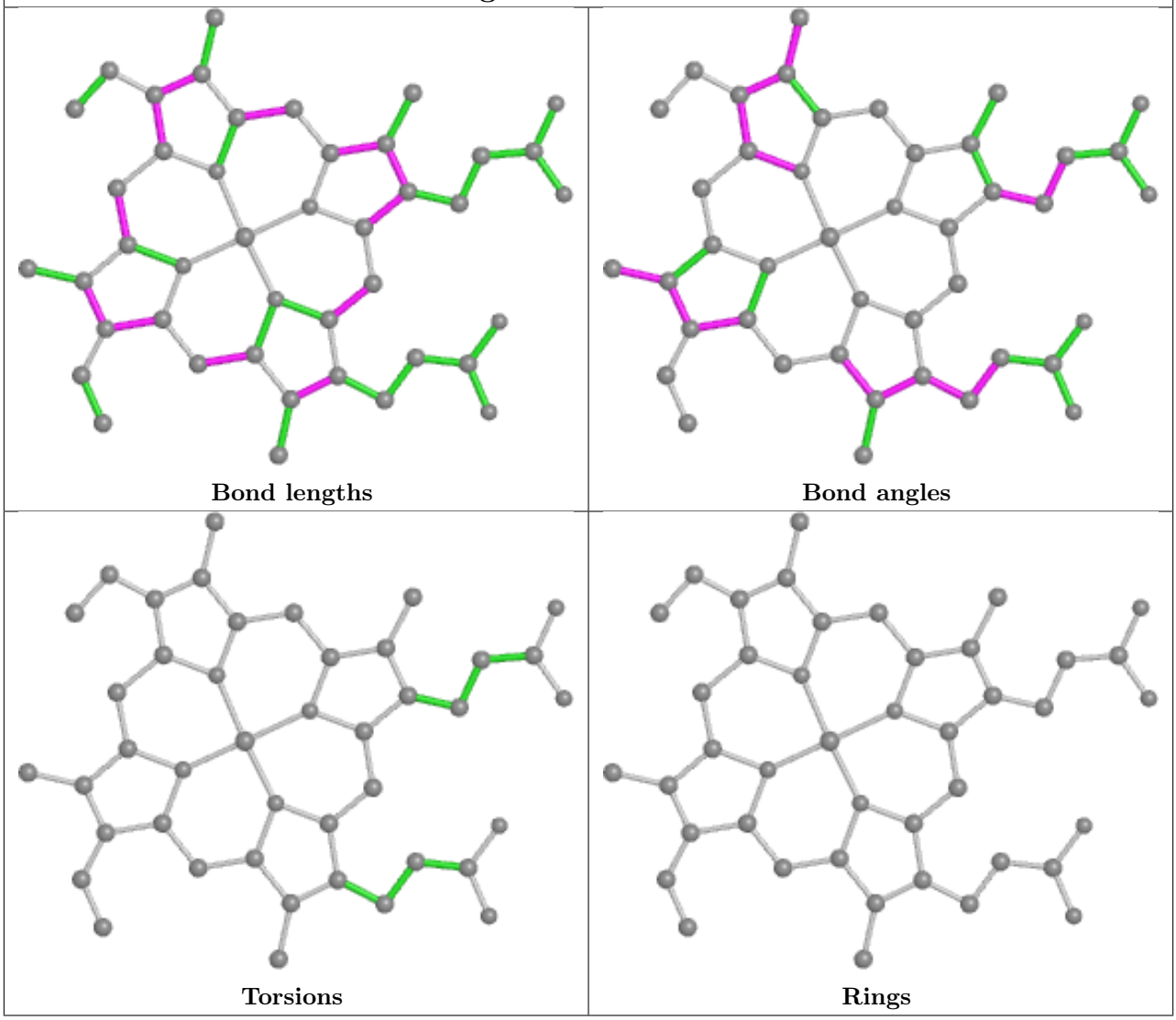


Torsions



Rings

Ligand HEC A 402



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 (i)

6.1 Protein, DNA and RNA chains (i)

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	354/373 (94%)	-0.30	3 (0%)	86	84	43, 55, 70, 81	0
1	B	355/373 (95%)	-0.36	3 (0%)	86	84	36, 47, 62, 75	0
2	C	124/137 (90%)	-0.06	1 (0%)	86	84	39, 50, 73, 86	0
2	E	124/137 (90%)	-0.01	0	100	100	37, 46, 58, 83	0
3	D	376/385 (97%)	-0.13	5 (1%)	77	73	38, 59, 86, 102	0
3	F	376/385 (97%)	-0.31	0	100	100	35, 46, 63, 73	0
All	All	1709/1790 (95%)	-0.24	12 (0%)	87	86	35, 51, 76, 102	0

All (12) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	6	ALA	6.7
1	A	6	ALA	3.6
1	A	7	ASP	3.1
3	D	386	GLY	3.1
1	A	320	ALA	3.1
3	D	208	THR	2.8
1	B	7	ASP	2.7
3	D	52	PRO	2.4
1	B	321	ARG	2.3
3	D	209	GLU	2.3
2	C	131	SER	2.2
3	D	327	PHE	2.1

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, 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
2	0AF	C	57	15/16	0.91	0.20	46,49,52,52	0
2	0AF	E	57	15/16	0.96	0.21	44,46,48,48	0

6.3 Carbohydrates (i)

There are no monosaccharides in this entry.

6.4 Ligands (i)

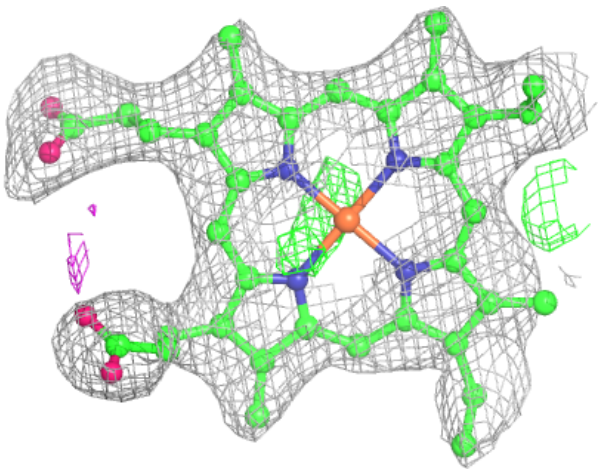
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists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

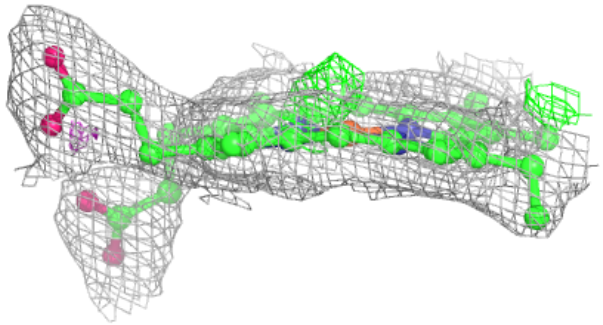
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
8	PGE	C	201	10/10	0.66	0.26	60,69,74,74	0
9	MES	D	401	12/12	0.80	0.32	105,111,112,113	0
6	EDO	A	404	4/4	0.84	0.32	61,62,62,63	0
6	EDO	A	405	4/4	0.86	0.15	60,60,60,61	0
9	MES	F	401	12/12	0.88	0.31	88,96,101,101	0
10	NA	F	402	1/1	0.90	0.08	52,52,52,52	0
6	EDO	B	404	4/4	0.93	0.12	59,59,59,60	0
4	CA	A	401	1/1	0.94	0.10	61,61,61,61	0
7	PO4	B	405	5/5	0.96	0.14	76,77,78,78	0
5	HEC	A	402	43/43	0.97	0.12	44,48,52,54	0
5	HEC	A	403	43/43	0.97	0.14	44,45,46,47	0
5	HEC	B	402	43/43	0.97	0.13	39,41,44,46	0
5	HEC	B	403	43/43	0.97	0.15	36,37,38,39	0
4	CA	B	401	1/1	0.99	0.08	33,33,33,33	0

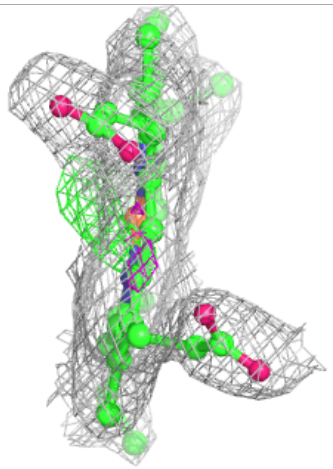
The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation 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)

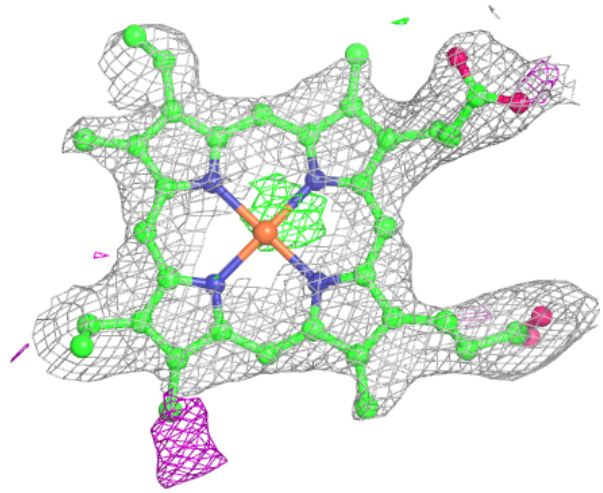


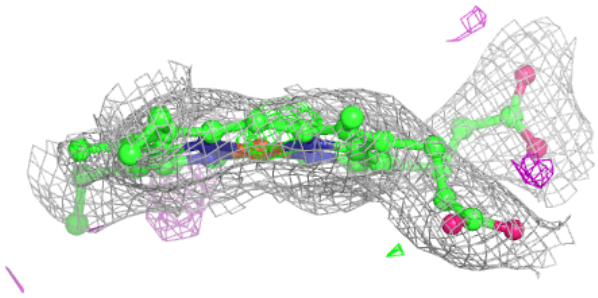


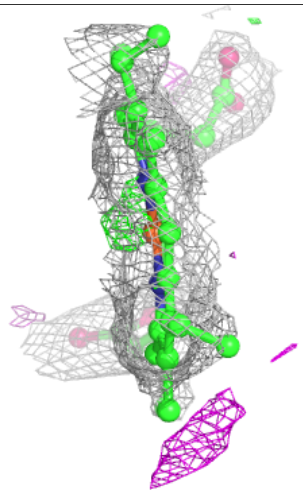


Electron density around HEC A 403:

2mF$_o$-DF$_c$ (at 0.7 rmsd) in gray
mF$_o$-DF$_c$ (at 3 rmsd) in purple (negative)
and green (positive)

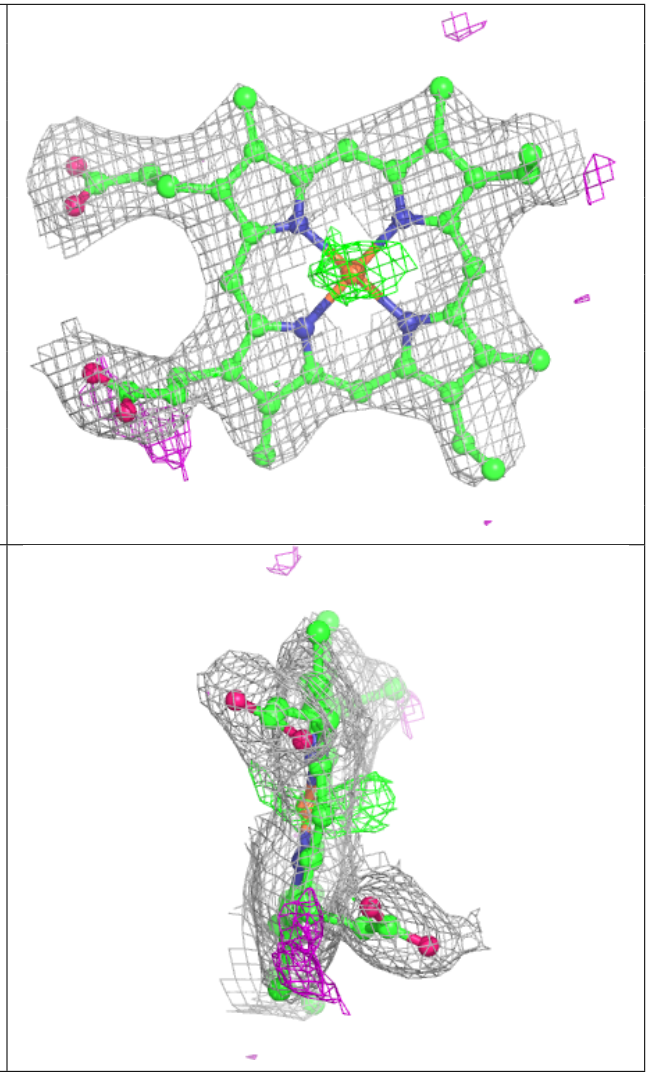


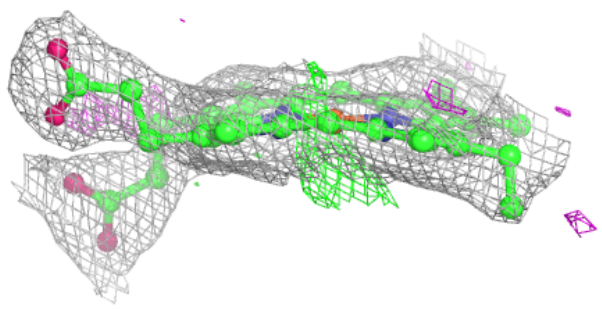




Electron density around HEC B 402:

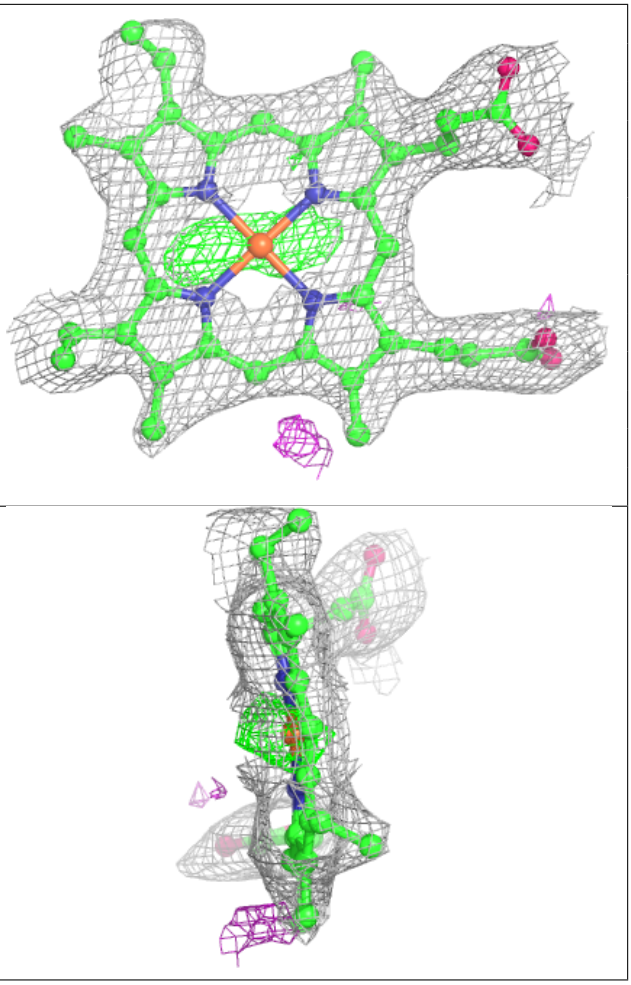
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)





Electron density around HEC B 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 (i)

There are no such residues in this entry.