Full wwPDB X-ray Structure Validation Report (i)

Aug 28, 2023 – 12:27 PM EDT

PDB ID	:	3L4O
Title	:	Crystal Structure of the MauG/pre-Methylamine Dehydrogenase Complex After Treatment with Hydrogen Peroxide
Authors	:	Jensen, L.M.R.; Wilmot, C.M.
Deposited on	:	2009-12-21
Resolution	:	2.05 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:

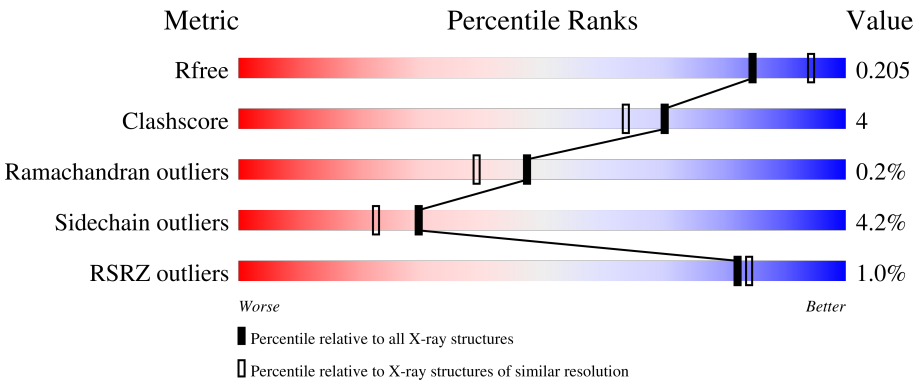
MolProbity	:	4.02b-467
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.35
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.35

1 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 2.05 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	1692 (2.04-2.04)
Clashscore	141614	1773 (2.04-2.04)
Ramachandran outliers	138981	1752 (2.04-2.04)
Sidechain outliers	138945	1752 (2.04-2.04)
RSRZ outliers	127900	1672 (2.04-2.04)

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	.% 83% 10% • 5%
1	B	373	% 84% 10% • 5%
2	C	137	82% 9% • 9%
2	E	137	78% 10% • • 9%
3	D	386	2% 86% 11% • •

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Mol	Chain	Length	Quality of chain
3	F	386	% 87% 10%

2 Entry composition (i)

There are 9 unique types of molecules in this entry. The entry contains 14721 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	353	2735	1708	490	526	11	0	1	0
1	B	355	2749	1716	492	530	11	0	1	0

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
			Total	C	N	O	S			
2	C	125	958	592	161	191	14	0	1	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	132	HIS	-	expression tag	UNP Q51658
C	133	HIS	-	expression tag	UNP Q51658
C	134	HIS	-	expression tag	UNP Q51658
C	135	HIS	-	expression tag	UNP Q51658
C	136	HIS	-	expression tag	UNP Q51658
C	137	HIS	-	expression tag	UNP Q51658
E	132	HIS	-	expression tag	UNP Q51658
E	133	HIS	-	expression tag	UNP Q51658
E	134	HIS	-	expression tag	UNP Q51658
E	135	HIS	-	expression tag	UNP Q51658
E	136	HIS	-	expression tag	UNP Q51658
E	137	HIS	-	expression tag	UNP Q51658

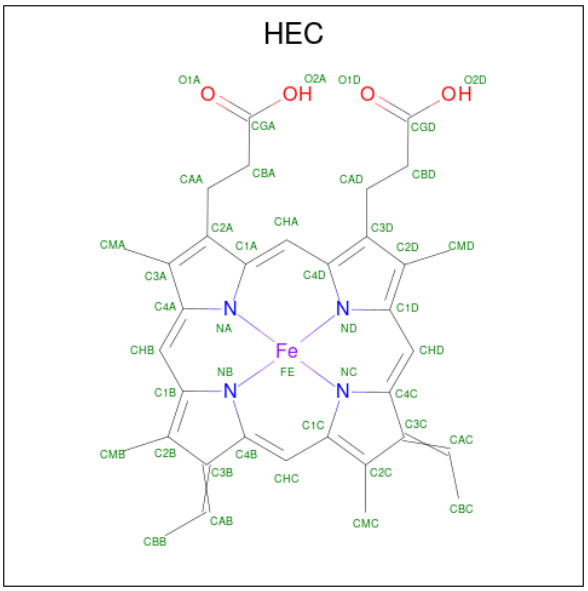
- Molecule 3 is a protein called Methylamine dehydrogenase heavy chain.

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	2923	1853	502	560	8	0	0	0

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

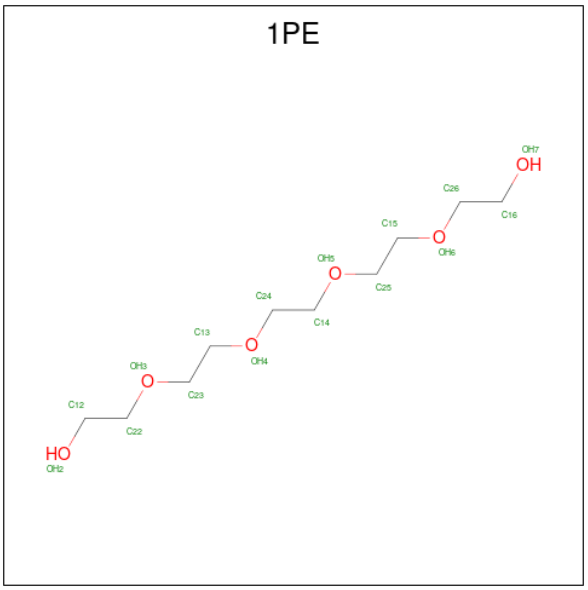
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
			Total	Ca		
4	A	1	1	1	0	0
			Total	Ca		
4	B	1	1	1	0	0

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



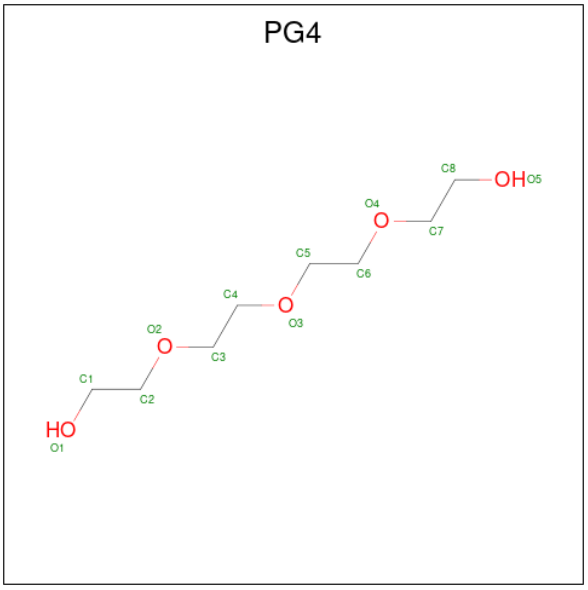
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
			Total	C	Fe	N	O		
5	A	1	43	34	1	4	4	0	0
			Total	C	Fe	N	O		
5	A	1	43	34	1	4	4	0	0
			Total	C	Fe	N	O		
5	B	1	43	34	1	4	4	0	0
			Total	C	Fe	N	O		
5	B	1	43	34	1	4	4	0	0

- Molecule 6 is PENTAETHYLENE GLYCOL (three-letter code: 1PE) (formula: $C_{10}H_{22}O_6$).



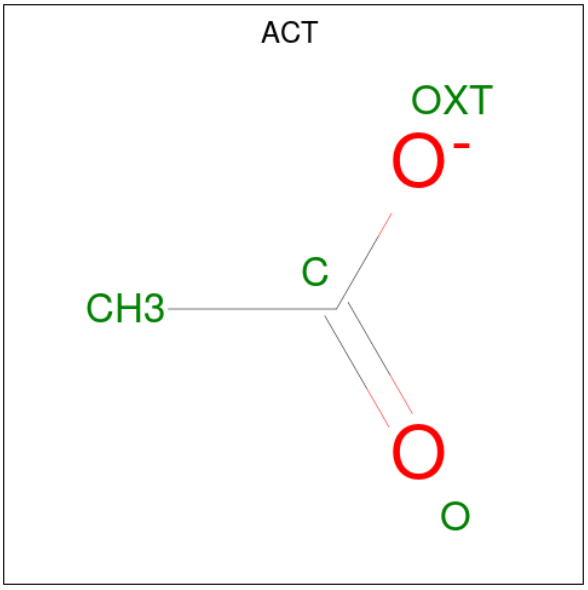
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
			Total	C	O		
6	F	1	16	10	6	0	0

- Molecule 7 is TETRAETHYLENE GLYCOL (three-letter code: PG4) (formula: $C_8H_{18}O_5$).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
			Total	C	O		
7	F	1	13	8	5	0	0

- Molecule 8 is ACETATE ION (three-letter code: ACT) (formula: $C_2H_3O_2$).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
			Total	C	O		
8	F	1	4	2	2	0	0

- Molecule 9 is water.

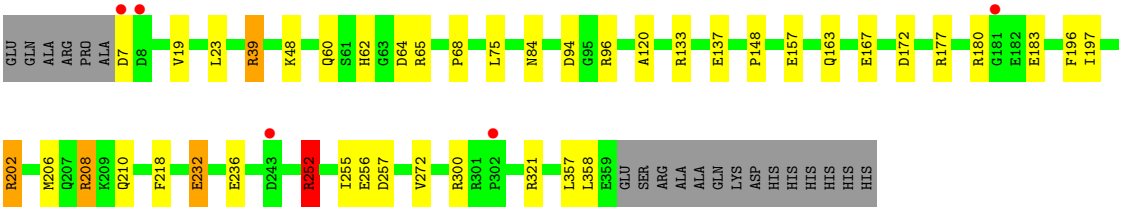
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
			Total	O		
9	A	227	227	227	0	0
			Total	O		
9	B	288	288	288	0	0
			Total	O		
9	C	85	85	85	0	0
			Total	O		
9	D	228	228	228	0	0
			Total	O		
9	E	107	107	107	0	0
			Total	O		
9	F	333	333	333	0	0

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.

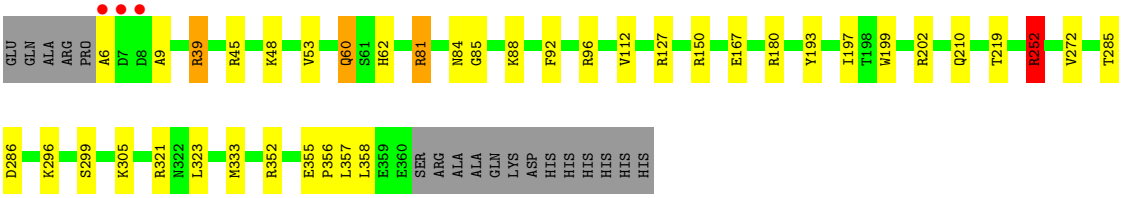
• Molecule 1: Methylamine utilization protein mauG

Chain A:



• Molecule 1: Methylamine utilization protein mauG

Chain B:



• Molecule 2: Methylamine dehydrogenase light chain

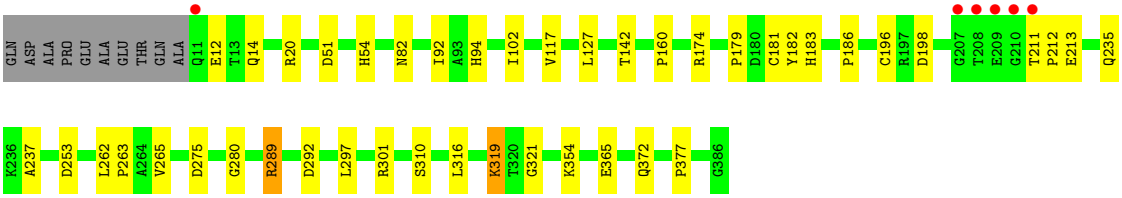
Chain C:

• Molecule 2: Methylamine dehydrogenase light chain

Chain E:

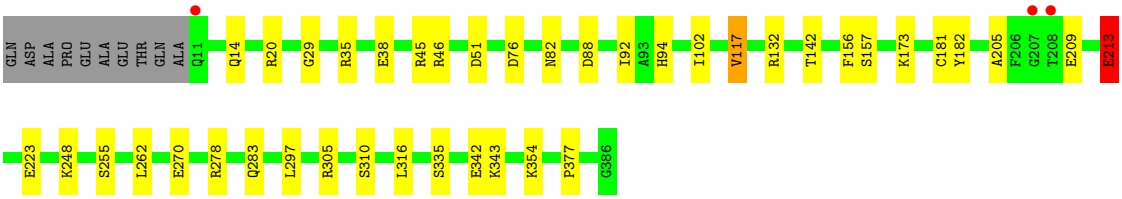
• Molecule 3: Methylamine dehydrogenase heavy chain

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)	38.20 – 2.05 38.20 – 2.05	Depositor EDS
% Data completeness (in resolution range)	97.0 (38.20-2.05) 97.1 (38.20-2.05)	Depositor EDS
R_{merge}	0.07	Depositor
R_{sym}	0.07	Depositor
$< I/\sigma(I) >$ [1]	2.49 (at 2.05Å)	Xtriage
Refinement program	REFMAC	Depositor
R, R_{free}	0.142 , 0.194 0.156 , 0.205	Depositor DCC
R_{free} test set	5304 reflections (4.99%)	wwPDB-VP
Wilson B-factor (Å^2)	27.8	Xtriage
Anisotropy	0.038	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.34 , 39.1	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	0.97	EDS
Total number of atoms	14721	wwPDB-VP
Average B, all atoms (Å^2)	21.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.67% 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: PG4, 1PE, HEC, ACT, TRQ, CA

The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 5$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	$\#\|Z\|>5$	RMSZ	$\#\|Z\|>5$
1	A	1.02	1/2802 (0.0%)	1.03	13/3802 (0.3%)
1	B	1.12	3/2816 (0.1%)	1.16	13/3821 (0.3%)
2	C	0.98	0/969	0.91	1/1323 (0.1%)
2	E	1.17	0/969	0.95	2/1323 (0.2%)
3	D	0.96	0/3000	0.85	2/4088 (0.0%)
3	F	1.20	4/3000 (0.1%)	0.94	9/4088 (0.2%)
All	All	1.08	8/13556 (0.1%)	0.99	40/18445 (0.2%)

Chiral center outliers are detected by calculating the chiral volume of a chiral center and verifying if the center is modelled as a planar moiety or with the opposite hand.A planarity outlier is detected by checking planarity of atoms in a peptide group, atoms in a mainchain group or atoms of a sidechain that are expected to be planar.

Mol	Chain	#Chirality outliers	#Planarity outliers
1	A	0	1
1	B	0	1
2	E	0	1
All	All	0	3

All (8) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	199	TRP	CB-CG	7.75	1.64	1.50
3	F	223	GLU	CG-CD	6.97	1.62	1.51
3	F	213	GLU	CG-CD	6.32	1.61	1.51
1	A	19	VAL	CB-CG2	5.46	1.64	1.52
1	B	53	VAL	CB-CG1	5.29	1.64	1.52
1	B	92	PHE	CE1-CZ	5.09	1.47	1.37
3	F	156	PHE	CD2-CE2	5.04	1.49	1.39
3	F	342	GLU	CG-CD	5.03	1.59	1.51

All (40) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	B	39	ARG	NE-CZ-NH2	-22.57	109.01	120.30
1	B	252	ARG	NE-CZ-NH2	-21.51	109.55	120.30
1	B	39	ARG	NE-CZ-NH1	19.15	129.88	120.30
1	B	252	ARG	NE-CZ-NH1	18.05	129.33	120.30
1	A	39	ARG	NE-CZ-NH2	-16.85	111.88	120.30
1	A	252	ARG	NE-CZ-NH2	-15.68	112.46	120.30
1	A	39	ARG	NE-CZ-NH1	13.31	126.96	120.30
1	A	252	ARG	NE-CZ-NH1	12.17	126.39	120.30
1	B	39	ARG	CD-NE-CZ	9.57	137.00	123.60
1	A	208	ARG	NE-CZ-NH2	-8.18	116.21	120.30
1	B	252	ARG	CD-NE-CZ	8.07	134.90	123.60
1	B	180	ARG	NE-CZ-NH2	-7.46	116.57	120.30
3	D	198	ASP	CB-CG-OD1	6.91	124.52	118.30
3	F	305	ARG	NE-CZ-NH2	-6.72	116.94	120.30
1	B	127	ARG	NE-CZ-NH2	-6.68	116.96	120.30
1	B	252	ARG	CG-CD-NE	-6.63	97.88	111.80
3	F	278	ARG	NE-CZ-NH1	6.37	123.49	120.30
2	C	19	ASP	CB-CG-OD1	6.05	123.75	118.30
1	B	45	ARG	NE-CZ-NH2	-6.01	117.30	120.30
1	A	208	ARG	NE-CZ-NH1	5.95	123.28	120.30
1	B	321	ARG	NE-CZ-NH2	-5.84	117.38	120.30
1	B	150	ARG	NE-CZ-NH1	5.84	123.22	120.30
3	F	76	ASP	CB-CG-OD1	5.81	123.53	118.30
1	A	39	ARG	CD-NE-CZ	5.71	131.60	123.60
1	A	39	ARG	CG-CD-NE	-5.68	99.88	111.80
1	A	257	ASP	CB-CG-OD2	-5.64	113.22	118.30
3	F	305	ARG	NE-CZ-NH1	5.62	123.11	120.30
3	F	35	ARG	NE-CZ-NH2	-5.58	117.51	120.30
1	A	64	ASP	CB-CG-OD1	5.57	123.31	118.30
2	E	58	VAL	CB-CA-C	-5.43	101.08	111.40
1	B	39	ARG	CG-CD-NE	-5.41	100.44	111.80
3	F	46	ARG	NE-CZ-NH1	-5.33	117.63	120.30
3	F	278	ARG	NE-CZ-NH2	-5.25	117.67	120.30
1	A	180	ARG	NE-CZ-NH1	5.18	122.89	120.30
3	D	289	ARG	NE-CZ-NH2	-5.18	117.71	120.30
1	A	252	ARG	CG-CD-NE	-5.14	101.00	111.80
3	F	88	ASP	CB-CG-OD1	5.11	122.90	118.30
2	E	71	LEU	CB-CG-CD1	5.11	119.68	111.00
1	A	252	ARG	CD-NE-CZ	5.04	130.66	123.60
3	F	132	ARG	NE-CZ-NH1	5.01	122.80	120.30

There are no chirality outliers.

All (3) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	7	ASP	Peptide
1	B	39	ARG	Sidechain
2	E	130	ALA	Peptide

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	2735	0	2611	23	0
1	B	2749	0	2622	19	0
2	C	958	0	862	12	0
2	E	958	0	862	12	0
3	D	2923	0	2808	20	0
3	F	2923	0	2808	17	0
4	A	1	0	0	0	0
4	B	1	0	0	0	0
5	A	86	0	60	2	0
5	B	86	0	60	2	0
6	F	16	0	22	0	0
7	F	13	0	18	1	0
8	F	4	0	3	0	0
9	A	227	0	0	2	0
9	B	288	0	0	2	0
9	C	85	0	0	1	0
9	D	228	0	0	0	0
9	E	107	0	0	0	0
9	F	333	0	0	1	0
All	All	14721	0	12736	94	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 (94) 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:B:48:LYS:H	1:B:62:HIS:HE1	1.13	0.93

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:210:GLN:HE22	2:C:44:THR:HG21	1.42	0.85
1:B:48:LYS:H	1:B:62:HIS:CE1	1.96	0.81
1:A:206:MET:HA	1:A:206:MET:HE2	1.60	0.81
1:B:285:THR:HG22	1:B:286:ASP:OD1	1.80	0.80
3:F:20:ARG:HG2	3:F:20:ARG:HH11	1.50	0.77
3:F:255:SER:HA	7:F:388:PG4:H32	1.68	0.74
3:D:292:ASP:OD2	3:D:319:LYS:HD2	1.88	0.72
3:D:14:GLN:HE21	2:E:21:GLN:HE22	1.37	0.71
2:C:57:TRQ:HB2	2:C:108:TRP:NE1	2.06	0.71
3:D:262:LEU:HB3	3:D:263:PRO:HD2	1.77	0.66
1:B:299:SER:HB2	1:B:333:MET:HG3	1.78	0.65
1:B:197:ILE:O	1:B:202:ARG:CD	2.45	0.64
2:E:56:SER:HB3	2:E:74:TYR:O	1.98	0.64
2:E:57:TRQ:HB2	2:E:108:TRP:NE1	2.12	0.64
1:B:197:ILE:O	1:B:202:ARG:HD2	1.98	0.63
3:D:237:ALA:HB2	3:D:289:ARG:HG3	1.80	0.63
1:A:252:ARG:HD3	9:A:859:HOH:O	1.99	0.63
1:B:81:ARG:HD3	1:B:85:GLY:HA2	1.79	0.63
5:B:600:HEC:HBC3	5:B:600:HEC:HMC1	1.82	0.61
3:D:372:GLN:HE22	2:E:86:CYS:H	1.46	0.61
3:F:205:ALA:HB3	3:F:213:GLU:HG3	1.83	0.61
2:E:56:SER:CB	2:E:74:TYR:O	2.49	0.60
3:D:297:LEU:HD22	3:D:310:SER:HB2	1.82	0.60
3:D:253:ASP:HB2	3:D:262:LEU:HD11	1.84	0.58
1:B:202:ARG:HH21	2:E:75:ARG:HD2	1.68	0.58
2:C:23:CYS:HB3	2:C:88[B]:CYS:SG	2.44	0.58
1:B:6:ALA:HA	1:B:9:ALA:HB3	1.85	0.58
2:E:71:LEU:HD22	2:E:129:LYS:O	2.06	0.55
3:F:20:ARG:HG2	3:F:20:ARG:NH1	2.20	0.55
1:A:48:LYS:H	1:A:62:HIS:HE1	1.55	0.54
1:A:208:ARG:NH2	3:F:29:GLY:O	2.33	0.54
2:C:57:TRQ:HZ3	2:C:108:TRP:HB2	1.89	0.54
1:A:206:MET:CE	1:A:218:PHE:CD2	2.91	0.53
1:A:133:ARG:O	1:A:137:GLU:HG3	2.09	0.53
1:A:210:GLN:NE2	2:C:44:THR:HG21	2.19	0.53
3:D:211:THR:HG22	3:D:212:PRO:HD2	1.92	0.52
3:F:51:ASP:HA	3:F:377:PRO:HA	1.92	0.51
1:B:197:ILE:O	1:B:202:ARG:HD3	2.10	0.51
2:C:21:GLN:HE22	3:F:14:GLN:HE21	1.59	0.50
3:D:186:PRO:HB2	3:D:235:GLN:NE2	2.27	0.50
3:D:186:PRO:HB2	3:D:235:GLN:HE21	1.77	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:210:GLN:HE22	2:E:44:THR:HG21	1.76	0.50
1:B:252:ARG:HD3	9:B:855:HOH:O	2.12	0.50
1:A:48:LYS:H	1:A:62:HIS:CE1	2.31	0.48
3:F:45:ARG:NH2	3:F:343:LYS:O	2.46	0.48
1:A:206:MET:HE3	1:A:218:PHE:CD2	2.48	0.48
2:C:23:CYS:CB	2:C:88[B]:CYS:SG	3.02	0.48
3:F:205:ALA:HB3	3:F:213:GLU:CG	2.44	0.47
1:A:272:VAL:HG21	5:A:600:HEC:HMA3	1.96	0.47
1:A:252:ARG:HD2	1:A:255:ILE:HG12	1.96	0.47
3:D:372:GLN:NE2	2:E:86:CYS:H	2.12	0.47
1:B:96:ARG:HA	1:B:252:ARG:HG3	1.96	0.47
1:A:206:MET:HE2	1:A:206:MET:CA	2.38	0.46
2:C:130:ALA:O	2:C:131:SER:HB2	2.15	0.46
3:F:248:LYS:CE	9:F:927:HOH:O	2.63	0.46
3:D:211:THR:CG2	3:D:212:PRO:HD2	2.45	0.46
1:B:60:GLN:O	1:B:62:HIS:HD2	1.99	0.46
3:D:182:TYR:O	3:D:183:HIS:HB2	2.16	0.46
2:C:23:CYS:SG	2:C:88[B]:CYS:SG	3.13	0.45
1:A:120:ALA:HA	1:A:148:PRO:HB3	1.98	0.45
9:C:1185:HOH:O	3:D:54:HIS:HD2	2.00	0.45
1:A:163:GLN:HE22	5:A:500:HEC:HMA1	1.81	0.45
3:D:181:CYS:HA	3:D:196:CYS:HA	1.98	0.45
1:A:60:GLN:O	1:A:62:HIS:CD2	2.70	0.45
3:F:297:LEU:HD22	3:F:310:SER:HB2	1.99	0.45
1:B:272:VAL:HG21	5:B:600:HEC:HMA3	1.97	0.44
1:B:305:LYS:HE3	9:B:605:HOH:O	2.18	0.44
3:D:51:ASP:HA	3:D:377:PRO:HA	1.99	0.44
3:D:280:GLY:HA3	3:D:301:ARG:CZ	2.47	0.44
3:D:12:GLU:CD	3:D:20:ARG:HH21	2.20	0.44
2:C:57:TRQ:HB2	2:C:108:TRP:HE1	1.81	0.44
2:E:57:TRQ:HZ3	2:E:108:TRP:HB2	1.99	0.44
1:B:48:LYS:N	1:B:62:HIS:HE1	1.95	0.43
3:F:181:CYS:C	3:F:182:TYR:CD1	2.91	0.43
3:F:82:ASN:HB3	3:F:142:THR:HB	2.01	0.43
2:C:130:ALA:O	2:C:131:SER:CB	2.67	0.42
2:E:94:GLU:HG2	2:E:102:PHE:O	2.19	0.42
1:A:196:PHE:HE2	1:A:206:MET:HE3	1.84	0.42
3:F:38:GLU:HB3	3:F:117:VAL:HG23	2.01	0.42
1:A:232:GLU:HB2	9:A:939:HOH:O	2.19	0.42
1:A:177:ARG:NE	1:A:183:GLU:OE1	2.45	0.42
1:B:193:TYR:O	1:B:197:ILE:HG12	2.19	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:D:82:ASN:HB3	3:D:142:THR:HB	2.03	0.41
2:C:96:PRO:HB2	2:C:98:TYR:CE1	2.55	0.41
1:A:65:ARG:HH12	1:A:94:ASP:CG	2.24	0.41
2:E:110:PHE:CE1	3:F:157:SER:HB2	2.56	0.41
3:F:209:GLU:HA	3:F:209:GLU:OE1	2.20	0.41
3:F:283:GLN:HB2	3:F:335:SER:HB3	2.03	0.41
1:A:172:ASP:O	1:A:177:ARG:NH1	2.55	0.40
1:A:197:ILE:HA	1:A:202:ARG:HB3	2.04	0.40
1:B:355:GLU:N	1:B:356:PRO:CD	2.85	0.40
1:A:96:ARG:HA	1:A:252:ARG:HG3	2.04	0.40
3:D:265:VAL:CG2	3:D:321:GLY:HA3	2.51	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	352/373 (94%)	342 (97%)	10 (3%)	0	100	100
1	B	354/373 (95%)	347 (98%)	7 (2%)	0	100	100
2	C	123/137 (90%)	119 (97%)	4 (3%)	0	100	100
2	E	123/137 (90%)	120 (98%)	3 (2%)	0	100	100
3	D	374/386 (97%)	356 (95%)	16 (4%)	2 (0%)	29	18
3	F	374/386 (97%)	361 (96%)	12 (3%)	1 (0%)	41	31
All	All	1700/1792 (95%)	1645 (97%)	52 (3%)	3 (0%)	47	39

All (3) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
3	D	102	ILE

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Mol	Chain	Res	Type
3	F	102	ILE
3	D	179	PRO

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%)	261 (94%)	16 (6%)	20	11
1	B	278/292 (95%)	265 (95%)	13 (5%)	26	18
2	C	105/112 (94%)	103 (98%)	2 (2%)	57	53
2	E	105/112 (94%)	99 (94%)	6 (6%)	20	12
3	D	304/311 (98%)	292 (96%)	12 (4%)	32	25
3	F	304/311 (98%)	295 (97%)	9 (3%)	41	34
All	All	1373/1430 (96%)	1315 (96%)	58 (4%)	30	22

All (58) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	23	LEU
1	A	39	ARG
1	A	68	PRO
1	A	75	LEU
1	A	84	ASN
1	A	157	GLU
1	A	167	GLU
1	A	202	ARG
1	A	232	GLU
1	A	236	GLU
1	A	252	ARG
1	A	256	GLU
1	A	300	ARG
1	A	321	ARG
1	A	357	LEU
1	A	358	LEU

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Mol	Chain	Res	Type
1	B	60	GLN
1	B	81	ARG
1	B	84	ASN
1	B	88	LYS
1	B	112	VAL
1	B	167	GLU
1	B	219	THR
1	B	252	ARG
1	B	296	LYS
1	B	323	LEU
1	B	352	ARG
1	B	357	LEU
1	B	358	LEU
2	C	71	LEU
2	C	129	LYS
3	D	92	ILE
3	D	94	HIS
3	D	117	VAL
3	D	127	LEU
3	D	160	PRO
3	D	174	ARG
3	D	213	GLU
3	D	275	ASP
3	D	316	LEU
3	D	319	LYS
3	D	354	LYS
3	D	365	GLU
2	E	16	GLN
2	E	58	VAL
2	E	68	GLN
2	E	71	LEU
2	E	129	LYS
2	E	131	SER
3	F	92	ILE
3	F	94	HIS
3	F	117	VAL
3	F	173	LYS
3	F	213	GLU
3	F	262	LEU
3	F	270	GLU
3	F	316	LEU
3	F	354	LYS

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (19) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	26	ASN
1	A	29	GLN
1	A	62	HIS
1	A	91	GLN
1	A	163	GLN
1	A	210	GLN
1	B	16	GLN
1	B	29	GLN
1	B	60	GLN
1	B	62	HIS
1	B	91	GLN
1	B	163	GLN
1	B	210	GLN
3	D	14	GLN
3	D	30	GLN
3	D	372	GLN
3	F	14	GLN
3	F	216	HIS
3	F	300	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)

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	TRQ	C	57	2	13,17,18	2.15	2 (15%)	14,24,26	3.05	7 (50%)
2	TRQ	E	57	2	13,17,18	1.70	3 (23%)	14,24,26	2.76	6 (42%)

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	TRQ	C	57	2	-	0/4/19/21	0/2/2/2
2	TRQ	E	57	2	-	0/4/19/21	0/2/2/2

All (5) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	C	57	TRQ	CH2-CZ2	-5.44	1.47	1.54
2	C	57	TRQ	CZ3-CE3	4.56	1.42	1.34
2	E	57	TRQ	CZ3-CE3	3.64	1.40	1.34
2	E	57	TRQ	CH2-CZ2	-3.20	1.50	1.54
2	E	57	TRQ	CD1-NE1	-2.65	1.32	1.36

All (13) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	E	57	TRQ	CZ2-CE2-NE1	8.11	132.89	119.94
2	C	57	TRQ	CZ2-CE2-NE1	7.80	132.40	119.94
2	C	57	TRQ	O6-CH2-CZ2	-4.58	115.39	118.51
2	E	57	TRQ	CB-CG-CD1	-3.35	123.83	127.97
2	E	57	TRQ	CE2-CD2-CE3	3.16	123.09	119.15
2	C	57	TRQ	CB-CG-CD1	-3.10	124.14	127.97
2	C	57	TRQ	CE2-CD2-CE3	3.06	122.96	119.15
2	C	57	TRQ	O7-CZ2-CE2	2.97	124.98	121.84
2	C	57	TRQ	CB-CA-C	2.54	116.23	111.47
2	E	57	TRQ	CB-CA-C	2.49	116.14	111.47
2	C	57	TRQ	CG-CB-CA	-2.48	110.70	114.53
2	E	57	TRQ	O7-CZ2-CH2	2.12	121.49	119.00
2	E	57	TRQ	O6-CH2-CZ2	2.01	119.87	118.51

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

2 monomers are involved in 5 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	C	57	TRQ	3	0
2	E	57	TRQ	2	0

5.5 Carbohydrates (i)

There are no monosaccharides in this entry.

5.6 Ligand geometry (i)

Of 9 ligands modelled in this entry, 2 are monoatomic - leaving 7 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	$\#\|Z\| > 2$
6	1PE	F	387	-	15,15,15	0.66	0	14,14,14	0.43	0
5	HEC	A	600	1	32,50,50	1.55	6 (18%)	24,82,82	2.71	9 (37%)
5	HEC	B	500	1	32,50,50	1.62	9 (28%)	24,82,82	2.29	11 (45%)
8	ACT	F	389	-	3,3,3	0.85	0	3,3,3	1.38	0
5	HEC	B	600	1	32,50,50	1.55	5 (15%)	24,82,82	2.80	12 (50%)
5	HEC	A	500	1	32,50,50	1.71	9 (28%)	24,82,82	2.52	12 (50%)
7	PG4	F	388	-	12,12,12	0.66	0	11,11,11	0.50	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
6	1PE	F	387	-	-	4/13/13/13	-
5	HEC	A	600	1	-	2/10/54/54	-
5	HEC	B	500	1	-	2/10/54/54	-
5	HEC	B	600	1	-	2/10/54/54	-
5	HEC	A	500	1	-	1/10/54/54	-
7	PG4	F	388	-	-	7/10/10/10	-

All (29) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
5	A	500	HEC	C3C-C4C	3.94	1.50	1.43
5	B	500	HEC	C3C-C4C	3.89	1.50	1.43
5	A	600	HEC	C3C-C4C	3.70	1.49	1.43
5	A	500	HEC	C2A-C1A	3.61	1.50	1.42
5	B	500	HEC	C2A-C1A	3.49	1.50	1.42
5	A	500	HEC	C4B-C3B	3.29	1.49	1.43
5	A	600	HEC	C2A-C1A	3.27	1.50	1.42
5	B	600	HEC	C3C-C2C	-3.13	1.37	1.40
5	B	600	HEC	C4B-C3B	3.10	1.48	1.43
5	B	500	HEC	C3A-C4A	2.97	1.49	1.42
5	A	500	HEC	C3A-C4A	2.97	1.49	1.42
5	B	600	HEC	C4D-CHA	2.89	1.49	1.41
5	B	500	HEC	C4B-C3B	2.86	1.48	1.43
5	A	600	HEC	C4D-CHA	2.81	1.48	1.41
5	B	500	HEC	C1D-CHD	2.74	1.48	1.41
5	B	600	HEC	C2A-C1A	2.69	1.48	1.42
5	A	500	HEC	C1C-CHC	2.57	1.48	1.41
5	B	500	HEC	C1B-CHB	2.50	1.47	1.41
5	A	500	HEC	C1D-CHD	2.50	1.47	1.41
5	A	500	HEC	C1B-CHB	2.48	1.47	1.41
5	A	500	HEC	CBA-CGA	2.46	1.56	1.50
5	A	600	HEC	C3A-C4A	2.44	1.48	1.42
5	B	600	HEC	C3A-C4A	2.38	1.48	1.42
5	B	500	HEC	O2A-CGA	-2.25	1.23	1.30
5	A	600	HEC	C1C-CHC	2.24	1.47	1.41
5	A	500	HEC	C4D-CHA	2.22	1.47	1.41
5	A	600	HEC	C1C-NC	-2.08	1.31	1.36
5	B	500	HEC	C1C-CHC	2.03	1.46	1.41
5	B	500	HEC	CBA-CGA	2.01	1.55	1.50

All (44) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
5	B	600	HEC	CBD-CAD-C3D	-6.69	101.21	112.62
5	A	600	HEC	CBD-CAD-C3D	-6.43	101.65	112.62
5	A	500	HEC	CBD-CAD-C3D	-5.69	102.92	112.62
5	A	600	HEC	CMC-C2C-C3C	5.52	132.32	125.82
5	B	600	HEC	C1D-C2D-C3D	-5.46	103.20	107.00
5	B	500	HEC	CBD-CAD-C3D	-5.45	103.31	112.62
5	B	600	HEC	CBA-CAA-C2A	-4.69	104.70	112.60
5	B	600	HEC	CMB-C2B-C3B	4.57	131.19	125.82
5	B	500	HEC	CMC-C2C-C3C	4.34	130.93	125.82
5	A	500	HEC	C4C-C3C-C2C	-4.30	101.71	106.35

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
5	A	600	HEC	C4C-C3C-C2C	-4.06	101.97	106.35
5	A	600	HEC	CBA-CAA-C2A	-3.91	106.02	112.60
5	A	500	HEC	C1D-C2D-C3D	-3.67	104.44	107.00
5	B	500	HEC	CMB-C2B-C3B	3.65	130.11	125.82
5	A	600	HEC	CMA-C3A-C2A	3.51	131.56	124.94
5	B	600	HEC	CMC-C2C-C3C	3.48	129.91	125.82
5	A	600	HEC	C1D-C2D-C3D	-3.47	104.58	107.00
5	A	500	HEC	CMB-C2B-C3B	3.34	129.75	125.82
5	A	500	HEC	O2A-CGA-CBA	3.27	124.54	114.03
5	A	600	HEC	CMC-C2C-C1C	-3.18	123.58	128.46
5	A	600	HEC	CMB-C2B-C3B	3.17	129.54	125.82
5	B	500	HEC	C1D-C2D-C3D	-2.81	105.04	107.00
5	A	500	HEC	CMA-C3A-C2A	2.77	130.17	124.94
5	B	500	HEC	C4C-C3C-C2C	-2.77	103.36	106.35
5	A	500	HEC	C2B-C3B-C4B	-2.76	103.37	106.35
5	A	500	HEC	CMC-C2C-C3C	2.72	129.02	125.82
5	B	500	HEC	CMA-C3A-C2A	2.60	129.84	124.94
5	B	600	HEC	CMA-C3A-C2A	2.59	129.83	124.94
5	B	500	HEC	C3C-C4C-NC	2.56	115.78	110.94
5	A	600	HEC	C3C-C4C-NC	2.48	115.63	110.94
5	B	600	HEC	O1D-CGD-CBD	-2.48	115.11	123.08
5	A	500	HEC	CAD-CBD-CGD	-2.39	107.05	113.76
5	A	500	HEC	C3C-C4C-NC	2.39	115.46	110.94
5	B	600	HEC	CAD-CBD-CGD	-2.30	107.30	113.76
5	B	600	HEC	CMD-C2D-C3D	2.22	129.13	124.94
5	B	600	HEC	CMC-C2C-C1C	-2.19	125.10	128.46
5	B	600	HEC	O2A-CGA-O1A	-2.18	117.86	123.30
5	B	600	HEC	O2D-CGD-CBD	2.12	120.84	114.03
5	B	500	HEC	O2A-CGA-CBA	2.09	120.74	114.03
5	A	500	HEC	O2A-CGA-O1A	-2.08	118.11	123.30
5	B	500	HEC	CMD-C2D-C3D	2.06	128.82	124.94
5	B	500	HEC	C2B-C3B-C4B	-2.05	104.13	106.35
5	B	500	HEC	CMC-C2C-C1C	-2.04	125.33	128.46
5	A	500	HEC	C3B-C4B-NB	2.04	114.79	110.94

There are no chirality outliers.

All (18) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
7	F	388	PG4	O2-C3-C4-O3
7	F	388	PG4	O3-C5-C6-O4
6	F	387	1PE	OH7-C16-C26-OH6

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Mol	Chain	Res	Type	Atoms
6	F	387	1PE	OH2-C12-C22-OH3
7	F	388	PG4	O1-C1-C2-O2
6	F	387	1PE	OH5-C14-C24-OH4
7	F	388	PG4	C1-C2-O2-C3
7	F	388	PG4	C8-C7-O4-C6
7	F	388	PG4	O4-C7-C8-O5
7	F	388	PG4	C3-C4-O3-C5
5	B	500	HEC	CAA-CBA-CGA-O2A
5	B	600	HEC	CAD-CBD-CGD-O2D
5	A	600	HEC	CAD-CBD-CGD-O2D
5	A	600	HEC	CAD-CBD-CGD-O1D
5	B	500	HEC	CAA-CBA-CGA-O1A
5	B	600	HEC	CAD-CBD-CGD-O1D
6	F	387	1PE	C23-C13-OH4-C24
5	A	500	HEC	CAD-CBD-CGD-O1D

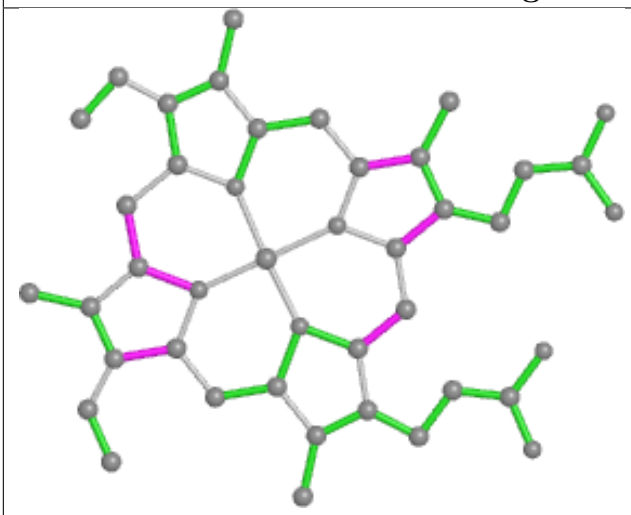
There are no ring outliers.

4 monomers are involved in 5 short contacts:

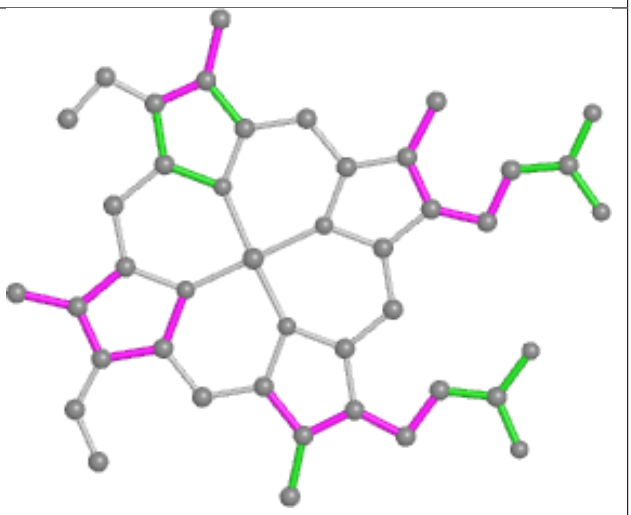
Mol	Chain	Res	Type	Clashes	Symm-Clashes
5	A	600	HEC	1	0
5	B	600	HEC	2	0
5	A	500	HEC	1	0
7	F	388	PG4	1	0

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.

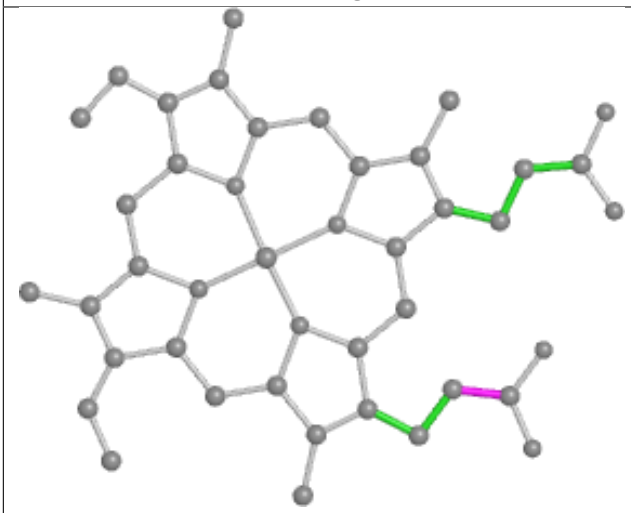
Ligand HEC A 600



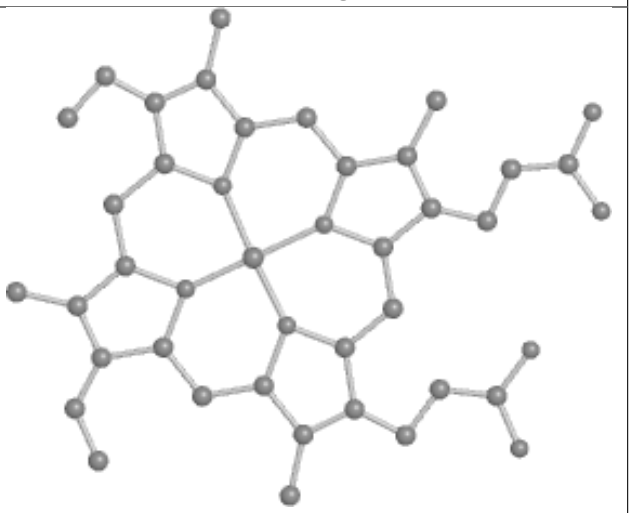
Bond lengths



Bond angles

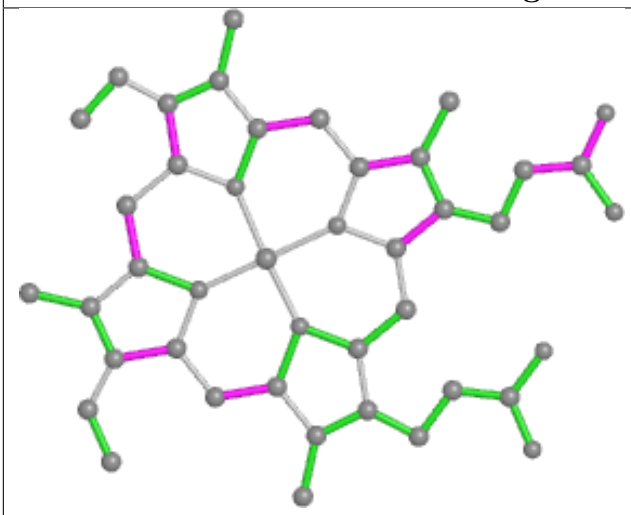


Torsions

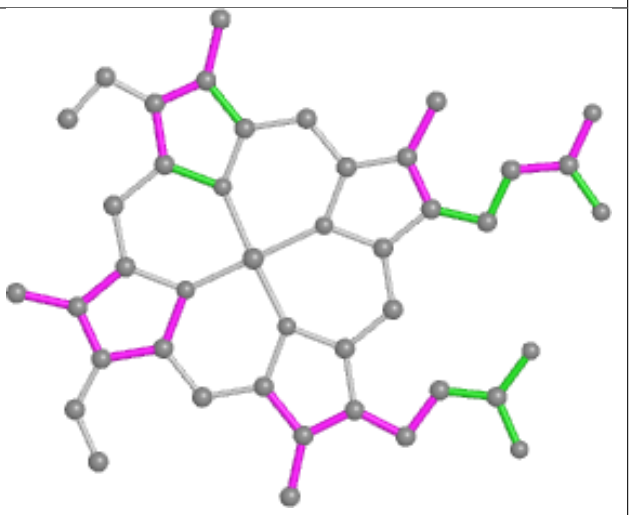


Rings

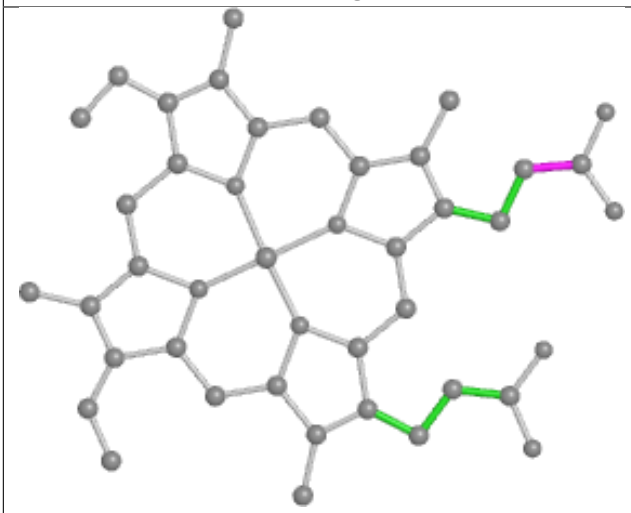
Ligand HEC B 500



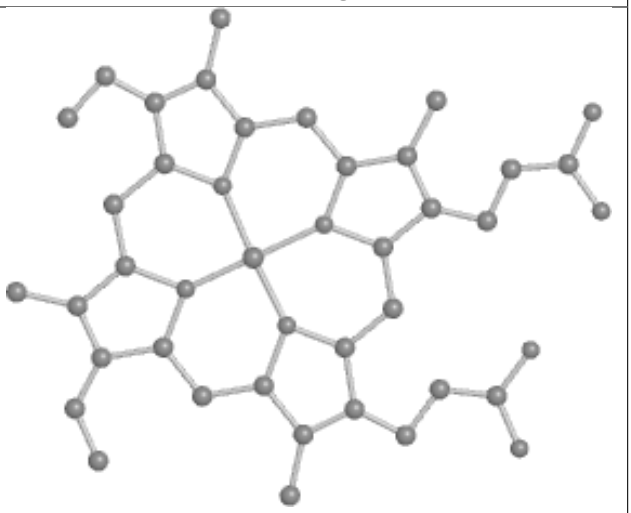
Bond lengths



Bond angles

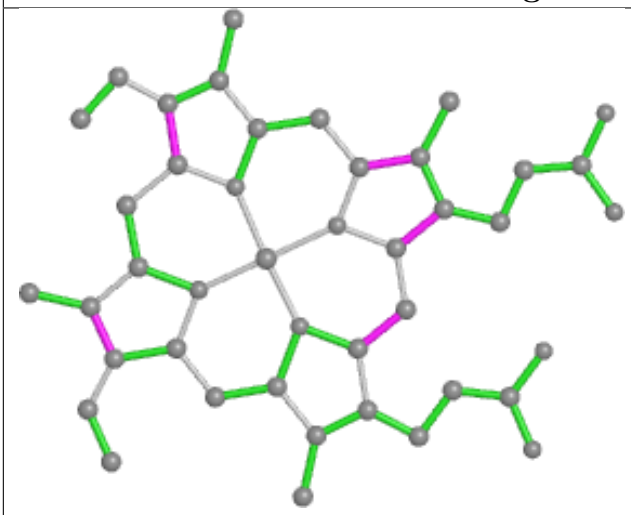


Torsions

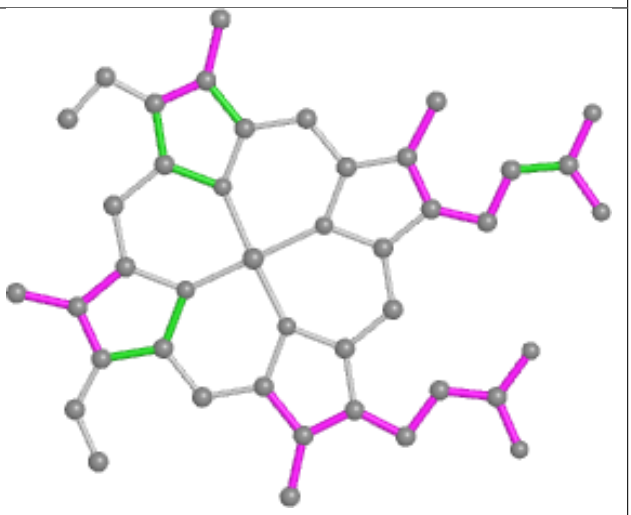


Rings

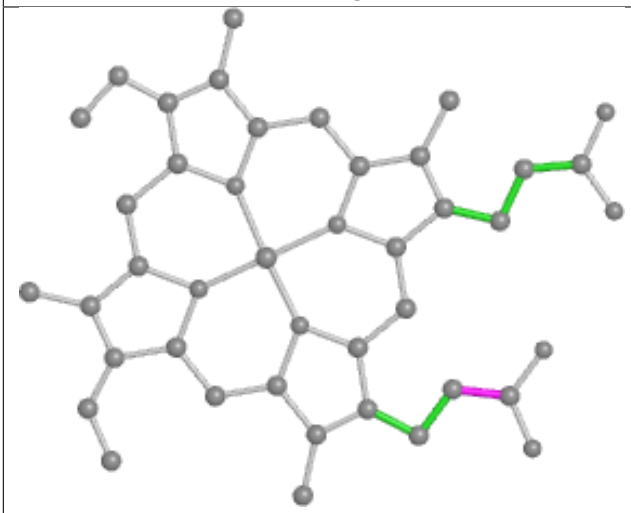
Ligand HEC B 600



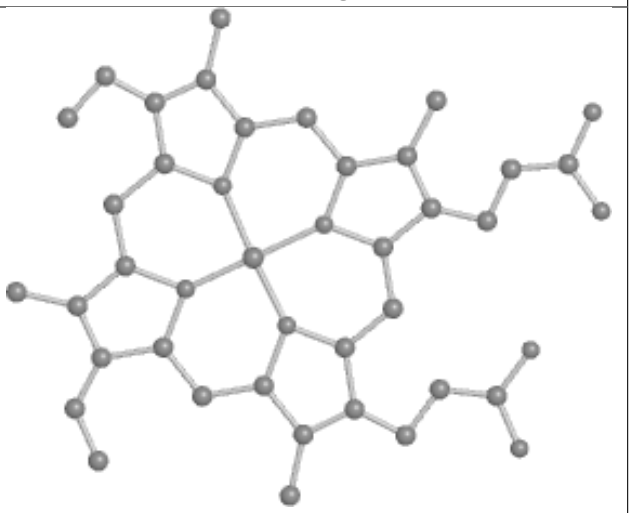
Bond lengths



Bond angles

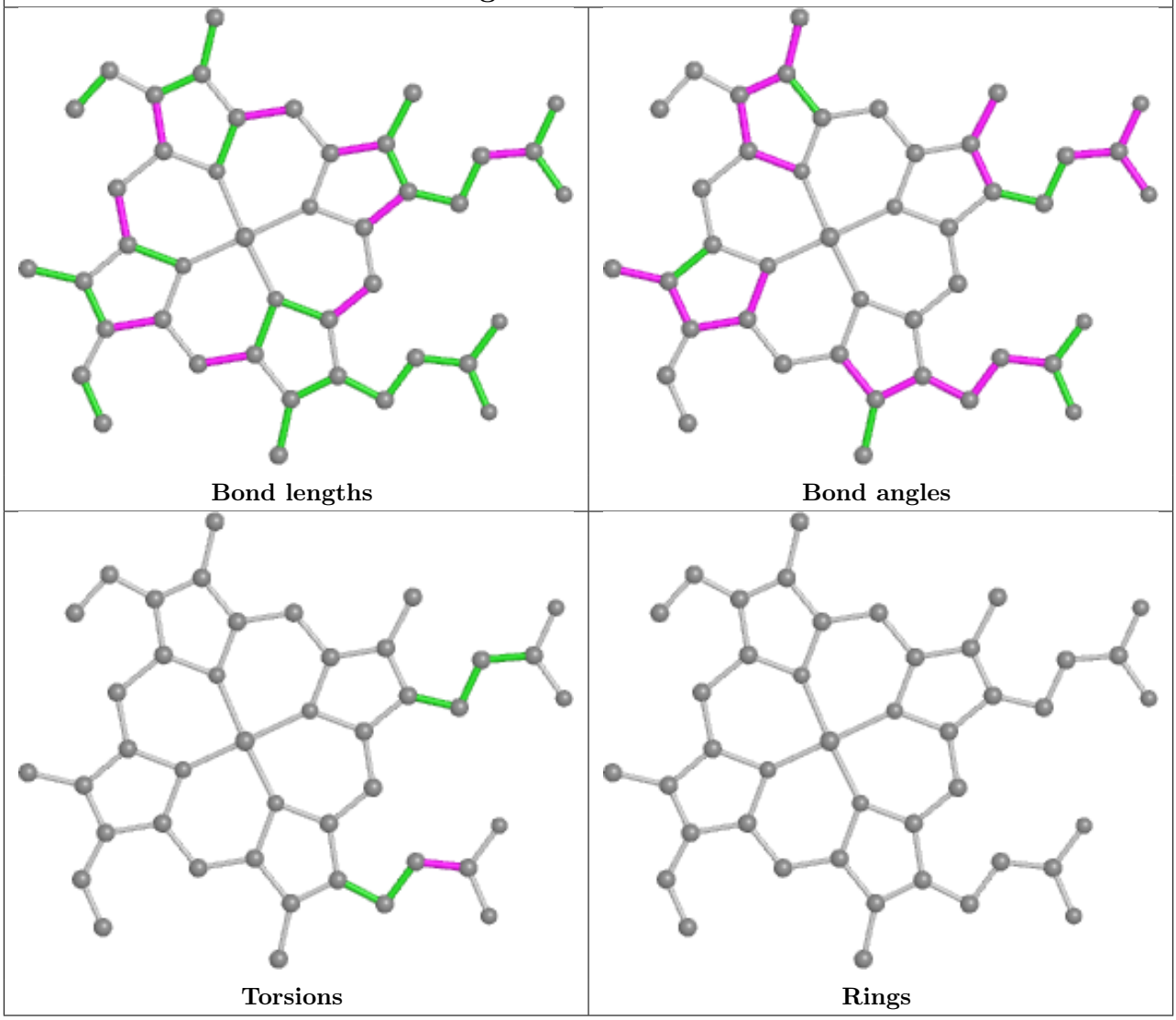


Torsions



Rings

Ligand HEC A 500



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	353/373 (94%)	-0.43	5 (1%) 75 78	14, 21, 32, 48	0
1	B	355/373 (95%)	-0.49	3 (0%) 86 88	14, 20, 34, 55	0
2	C	124/137 (90%)	-0.15	0 100 100	17, 21, 31, 53	0
2	E	124/137 (90%)	-0.33	0 100 100	12, 17, 27, 51	0
3	D	376/386 (97%)	-0.36	6 (1%) 72 74	13, 20, 30, 54	0
3	F	376/386 (97%)	-0.43	3 (0%) 86 88	13, 17, 28, 50	0
All	All	1708/1792 (95%)	-0.40	17 (0%) 82 84	12, 20, 31, 55	0

All (17) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	6	ALA	6.5
3	D	208	THR	4.6
1	B	7	ASP	4.5
3	F	208	THR	3.6
3	F	11	GLN	3.5
1	A	7	ASP	3.1
3	F	207	GLY	3.0
1	A	302	PRO	2.9
3	D	209	GLU	2.9
3	D	207	GLY	2.6
3	D	210	GLY	2.6
3	D	11	GLN	2.6
1	B	8	ASP	2.3
1	A	8	ASP	2.2
1	A	243	ASP	2.2
3	D	211	THR	2.2
1	A	181	GLY	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, 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	TRQ	C	57	16/17	0.96	0.12	24,29,36,44	0
2	TRQ	E	57	16/17	0.96	0.15	20,25,35,37	0

6.3 Carbohydrates (i)

There are no monosaccharides in this entry.

6.4 Ligands (i)

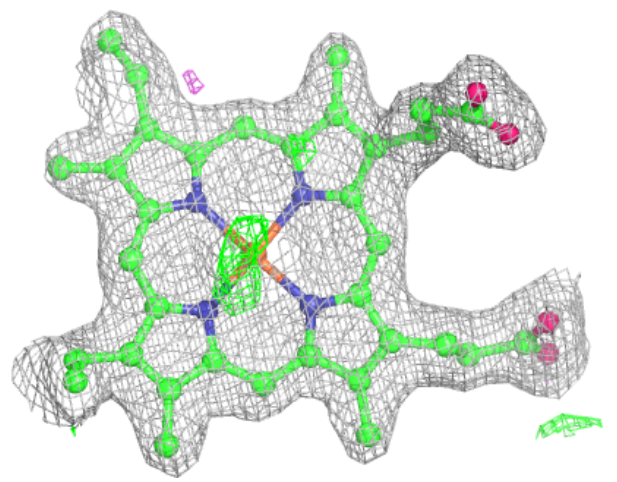
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists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

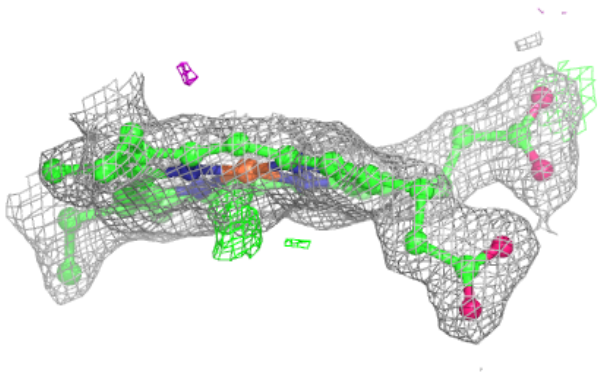
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
7	PG4	F	388	13/13	0.85	0.16	52,57,68,69	0
6	1PE	F	387	16/16	0.87	0.14	39,48,61,63	0
8	ACT	F	389	4/4	0.96	0.10	36,39,40,40	0
5	HEC	A	500	43/43	0.98	0.08	23,26,28,29	0
5	HEC	B	600	43/43	0.99	0.11	13,18,21,22	0
4	CA	A	400	1/1	0.99	0.10	25,25,25,25	0
5	HEC	A	600	43/43	0.99	0.10	21,26,28,30	0
5	HEC	B	500	43/43	0.99	0.08	17,22,25,26	0
4	CA	B	400	1/1	1.00	0.10	20,20,20,20	0

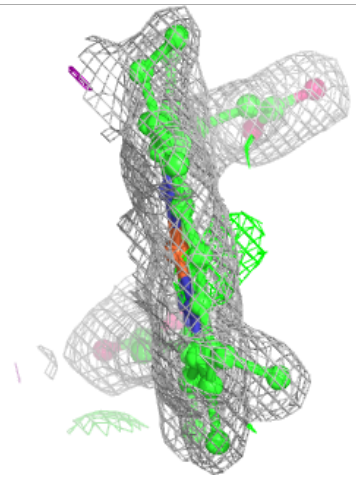
The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation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

Electron density around HEC A 500:

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

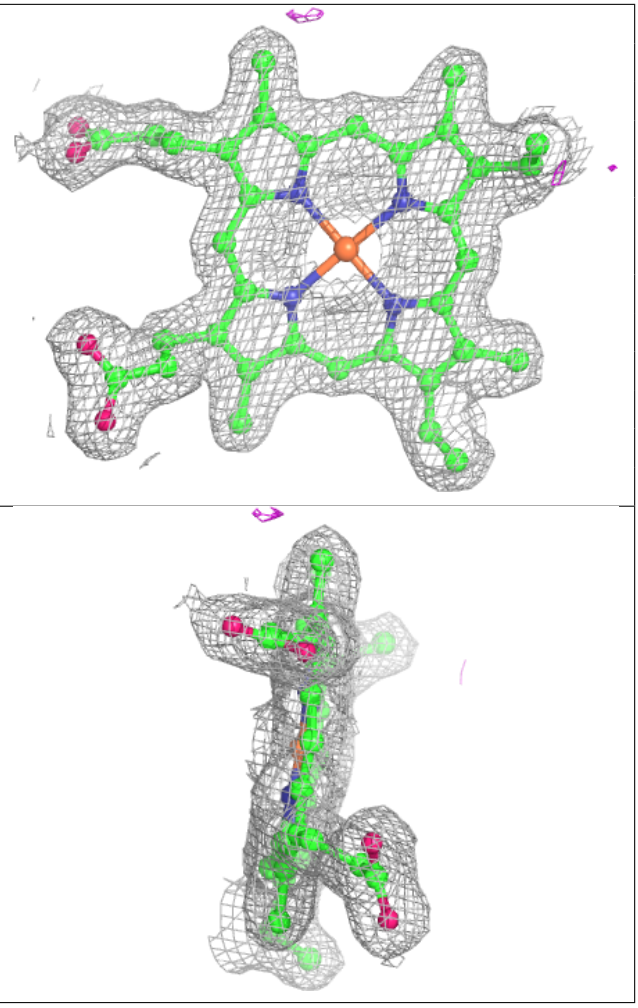






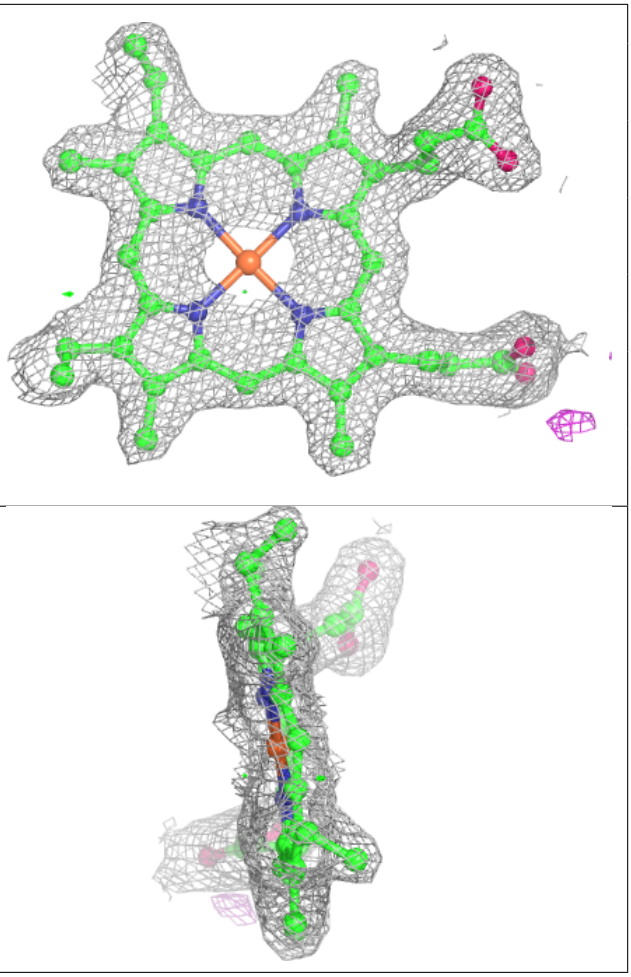
Electron density around HEC B 600:

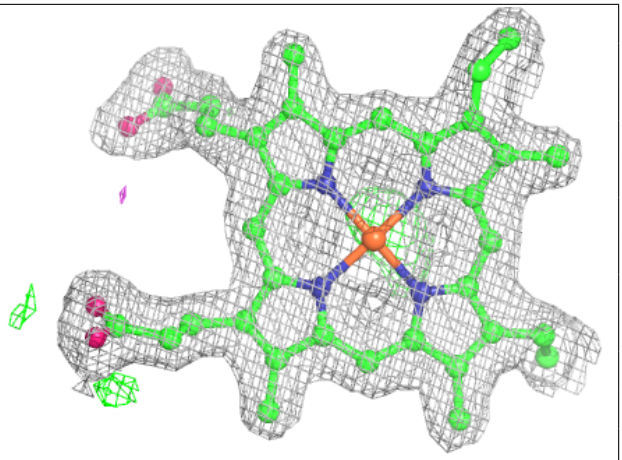
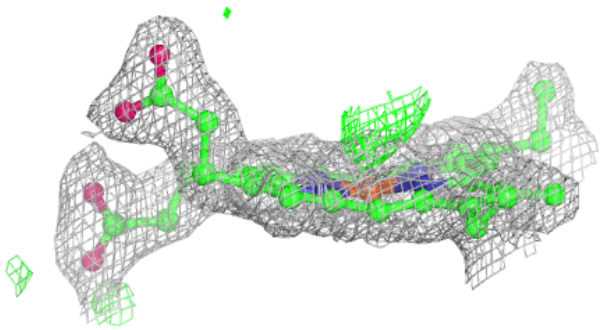
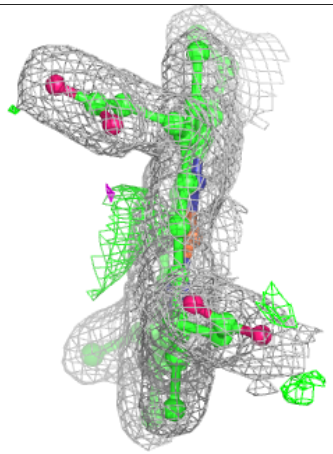
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)



Electron density around HEC A 600:

$2mF_o$-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 500: 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.