wwPDB X-ray Structure Validation Summary Report (i)

Aug 28, 2023 – 03:02 AM EDT

PDB ID	:	3L4M
Title	:	Crystal Structure of the MauG/pre-Methylamine Dehydrogenase Complex.
Authors	:	Jensen, L.M.R.; Wilmot, C.M.
Deposited on	:	2009-12-21
Resolution	:	2.02 Å(reported)

This is a wwPDB X-ray Structure Validation Summary 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:

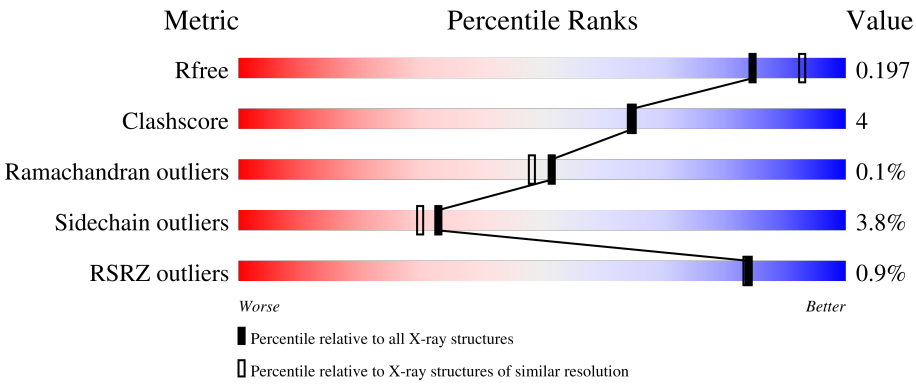
MolProbity	:	4.02b-467
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.35
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (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 2.02 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.



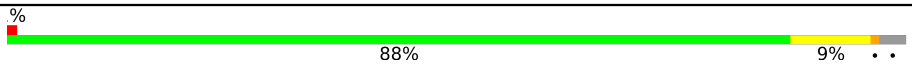
Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	130704	10434 (2.04-2.00)
Clashscore	141614	11643 (2.04-2.00)
Ramachandran outliers	138981	11493 (2.04-2.00)
Sidechain outliers	138945	11492 (2.04-2.00)
RSRZ outliers	127900	10220 (2.04-2.00)

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% 9% • 5%
1	B	373	.% 87% 7% •• 5%
2	C	137	.% 79% 12% • 9%
2	E	137	74% 15% • 9%
3	D	386	2% 87% 10% • •

Continued on next page...

Continued from previous page...

Mol	Chain	Length	Quality of chain
3	F	386	

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

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
2	0AF	C	57	X	-	-	-
2	0AF	E	57	X	-	-	-

2 Entry composition (i)

There are 9 unique types of molecules in this entry. The entry contains 14765 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	2740	1711	491	527	11	0	1	0
1	B	355	2743	1712	491	529	11	0	0	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	957	592	161	190	14	0	1	0
2	E	125	963	596	161	190	16	0	3	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

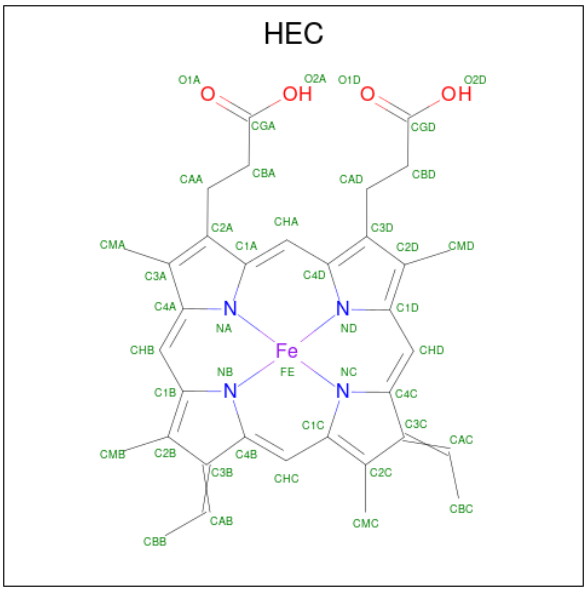
- Molecule 3 is a protein called Methylamine dehydrogenase heavy chain.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
3	D	376	2925	1854	502	560	9	0	1	0
			Total	C	N	O	S			
3	F	376	2926	1855	502	560	9	0	1	0

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

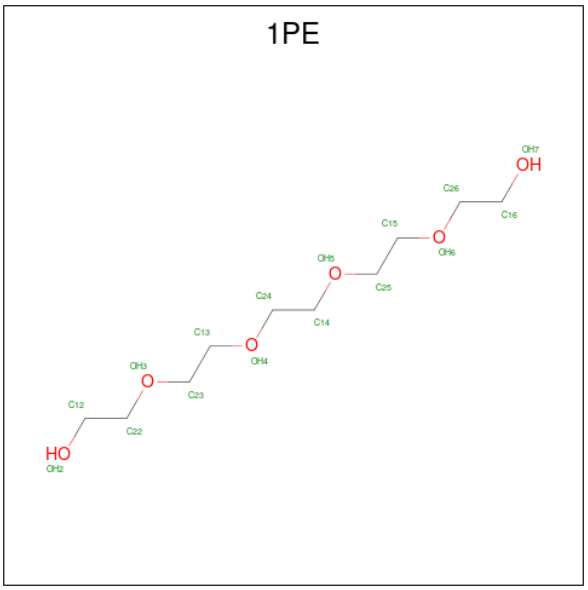
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
			Total	Ca		
4	A	1	1	1	0	0
			Total	Ca		
4	B	1	1	1	0	0

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



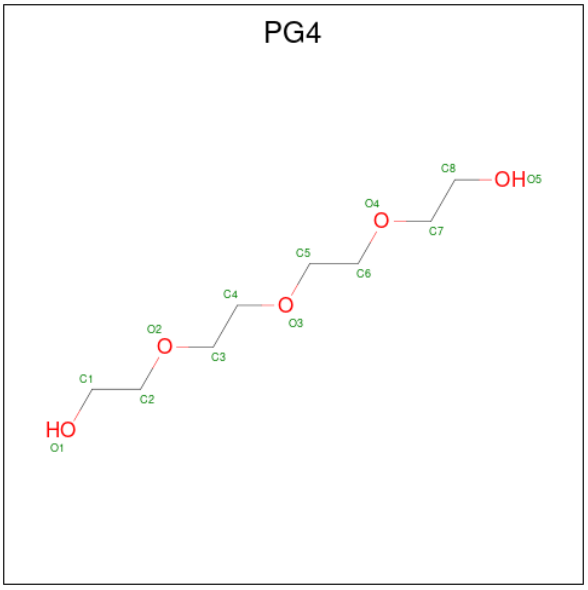
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
			Total	C	Fe	N	O		
5	A	1	43	34	1	4	4	0	0
			Total	C	Fe	N	O		
5	A	1	43	34	1	4	4	0	0
			Total	C	Fe	N	O		
5	B	1	43	34	1	4	4	0	0
			Total	C	Fe	N	O		
5	B	1	43	34	1	4	4	0	0

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



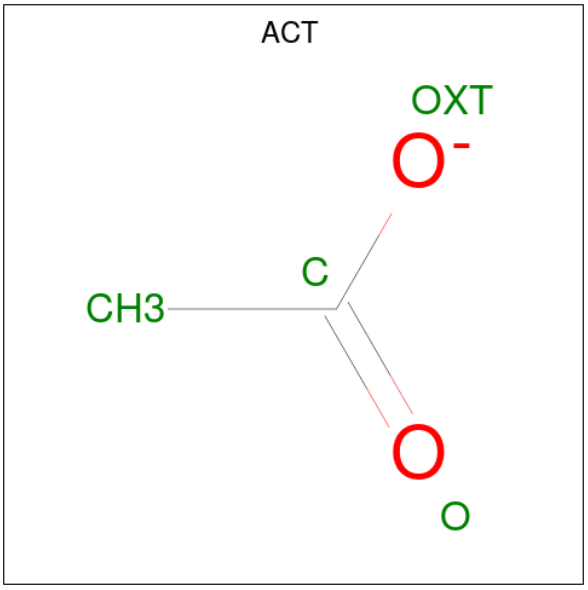
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
			Total	C	O		
6	F	1	16	10	6	0	0

- 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.

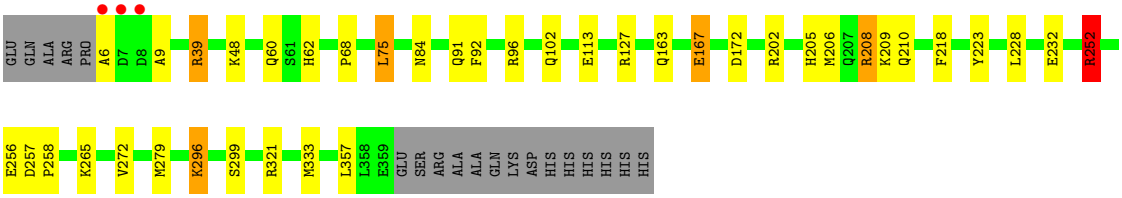
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
			Total	O		
9	A	247	247	247	0	0
			Total	O		
9	B	268	268	268	0	0
			Total	O		
9	C	92	92	92	0	0
			Total	O		
9	D	263	263	263	0	0
			Total	O		
9	E	95	95	95	0	0
			Total	O		
9	F	339	339	339	0	0

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.

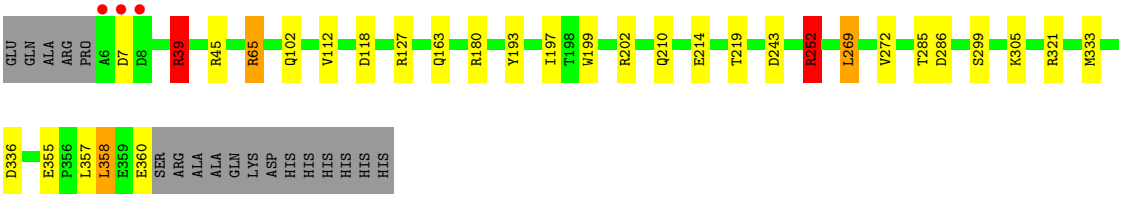
• Molecule 1: Methylamine utilization protein mauG

Chain A:



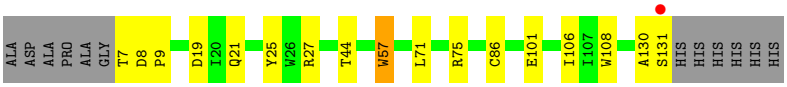
• Molecule 1: Methylamine utilization protein mauG

Chain B:



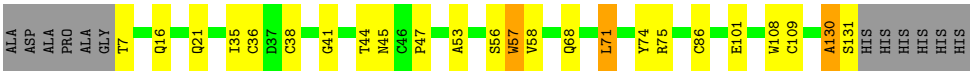
• Molecule 2: Methylamine dehydrogenase light chain

Chain C:



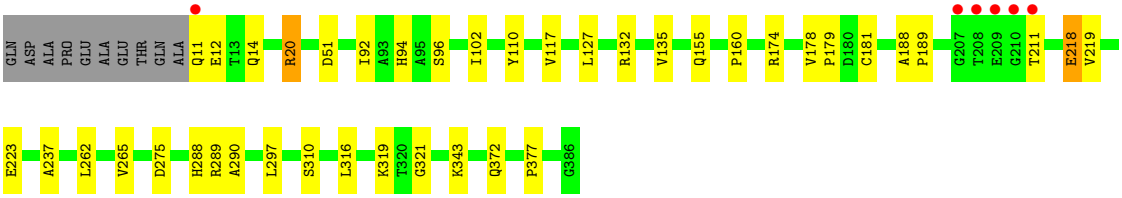
• Molecule 2: Methylamine dehydrogenase light chain

Chain E:



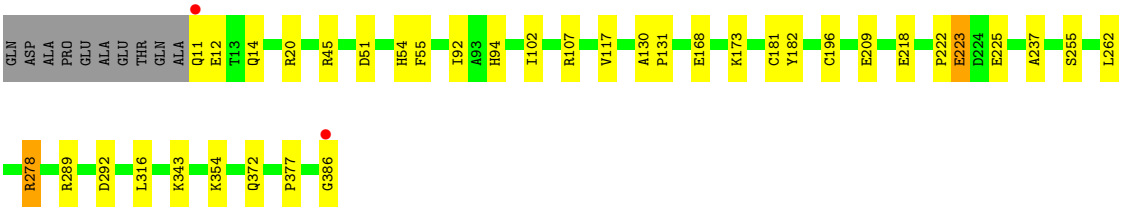
• Molecule 3: Methylamine dehydrogenase heavy chain

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)	44.49 – 2.02 44.48 – 2.02	Depositor EDS
% Data completeness (in resolution range)	92.7 (44.49-2.02) 92.6 (44.48-2.02)	Depositor EDS
R_{merge}	0.07	Depositor
R_{sym}	0.07	Depositor
$< I/\sigma(I) >$ [1]	2.27 (at 2.01Å)	Xtriage
Refinement program	REFMAC	Depositor
R, R_{free}	0.135 , 0.189 0.144 , 0.197	Depositor DCC
R_{free} test set	5298 reflections (5.03%)	wwPDB-VP
Wilson B-factor (Å^2)	18.5	Xtriage
Anisotropy	0.048	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.36 , 40.9	EDS
L-test for twinning[2]	$< \|L\| > = 0.49$, $< L^2 > = 0.32$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o,F_c correlation	0.96	EDS
Total number of atoms	14765	wwPDB-VP
Average B, all atoms (Å^2)	15.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.75% 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, 0AF, ACT, HEC, 1PE, 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	1.05	0/2807	1.15	14/3809 (0.4%)
1	B	1.08	1/2807 (0.0%)	1.18	15/3809 (0.4%)
2	C	1.03	1/969 (0.1%)	0.91	2/1323 (0.2%)
2	E	1.11	0/981	0.95	0/1340
3	D	1.02	1/3006 (0.0%)	0.88	2/4096 (0.0%)
3	F	1.16	2/3006 (0.1%)	0.94	3/4096 (0.1%)
All	All	1.08	5/13576 (0.0%)	1.02	36/18473 (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	C	1	0
2	E	1	1
All	All	2	3

All (5) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	199	TRP	CB-CG	7.46	1.63	1.50
2	C	101	GLU	CG-CD	5.70	1.60	1.51
3	F	223	GLU	CG-CD	5.54	1.60	1.51
3	D	223	GLU	CG-CD	5.46	1.60	1.51
3	F	209	GLU	CG-CD	5.07	1.59	1.51

The worst 5 of 36 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	B	39	ARG	NE-CZ-NH2	-26.09	107.26	120.30
1	A	39	ARG	NE-CZ-NH2	-24.65	107.98	120.30
1	B	39	ARG	NE-CZ-NH1	22.86	131.73	120.30
1	A	39	ARG	NE-CZ-NH1	22.63	131.61	120.30
1	A	252	ARG	NE-CZ-NH2	-19.45	110.58	120.30

All (2) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
2	C	57	0AF	CA
2	E	57	0AF	CA

All (3) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	252	ARG	Sidechain
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	2740	0	2616	28	0
1	B	2743	0	2614	13	0
2	C	957	0	863	13	0
2	E	963	0	873	22	0
3	D	2925	0	2809	24	0
3	F	2926	0	2813	18	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	3	0
6	F	16	0	22	0	0
7	F	13	0	18	1	0
8	F	4	0	3	0	0
9	A	247	0	0	2	0
9	B	268	0	0	3	0

Continued on next page...

Continued from previous page...

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
9	C	92	0	0	1	0
9	D	263	0	0	1	0
9	E	95	0	0	2	0
9	F	339	0	0	4	0
All	All	14765	0	12751	107	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.

The worst 5 of 107 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:35:ILE:HD12	2:E:86[B]:CYS:SG	1.97	1.05
1:B:285:THR:HG22	1:B:286:ASP:OD1	1.77	0.84
1:A:6:ALA:HA	1:A:9:ALA:HB3	1.59	0.82
2:C:57:0AF:CE3	2:C:108:TRP:CD1	2.63	0.82
3:F:255:SER:HA	7:F:388:PG4:H32	1.66	0.78

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%)	344 (98%)	9 (2%)	0	100	100
1	B	353/373 (95%)	346 (98%)	7 (2%)	0	100	100
2	C	123/137 (90%)	119 (97%)	4 (3%)	0	100	100
2	E	125/137 (91%)	121 (97%)	4 (3%)	0	100	100
3	D	375/386 (97%)	365 (97%)	9 (2%)	1 (0%)	41	36
3	F	375/386 (97%)	363 (97%)	11 (3%)	1 (0%)	41	36

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles
All	All	1704/1792 (95%)	1658 (97%)	44 (3%)	2 (0%)	51 48

All (2) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
3	D	102	ILE
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	277/292 (95%)	266 (96%)	11 (4%)	31 28
1	B	277/292 (95%)	266 (96%)	11 (4%)	31 28
2	C	105/112 (94%)	104 (99%)	1 (1%)	76 80
2	E	107/112 (96%)	102 (95%)	5 (5%)	26 22
3	D	305/311 (98%)	291 (95%)	14 (5%)	27 22
3	F	305/311 (98%)	295 (97%)	10 (3%)	38 36
All	All	1376/1430 (96%)	1324 (96%)	52 (4%)	33 30

5 of 52 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
3	D	160	PRO
3	D	319	LYS
3	F	262	LEU
3	D	174	ARG
3	D	262	LEU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 18 such sidechains are listed below:

Mol	Chain	Res	Type
3	F	54	HIS
3	F	372	GLN
3	F	300	GLN
1	B	163	GLN
3	F	30	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	0AF	E	57	2	13,16,17	1.72	4 (30%)	11,22,24	3.63	4 (36%)
2	0AF	C	57	2	13,16,17	1.43	2 (15%)	11,22,24	3.80	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	1/1/1/2	1/4/6/8	0/2/2/2
2	0AF	C	57	2	1/1/1/2	1/4/6/8	0/2/2/2

The worst 5 of 6 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	E	57	0AF	CB-CA	-3.33	1.46	1.53
2	E	57	0AF	CZ3-CE3	3.02	1.43	1.36
2	E	57	0AF	CH2-CZ2	2.66	1.42	1.37

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	E	57	0AF	CA-N	-2.49	1.40	1.48
2	C	57	0AF	CB-CA	-2.32	1.48	1.53

The worst 5 of 9 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	C	57	0AF	CG-CB-CA	-10.22	98.72	114.53
2	E	57	0AF	CG-CB-CA	-9.63	99.65	114.53
2	E	57	0AF	CB-CA-C	5.77	122.28	111.47
2	C	57	0AF	CB-CA-C	4.34	119.60	111.47
2	C	57	0AF	CB-CG-CD2	3.60	131.86	126.25

All (2) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
2	C	57	0AF	CA
2	E	57	0AF	CA

All (2) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	C	57	0AF	N-CA-CB-CG
2	E	57	0AF	N-CA-CB-CG

There are no ring outliers.

2 monomers are involved in 6 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	E	57	0AF	3	0
2	C	57	0AF	3	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	$\#\|Z\| > 2$
5	HEC	A	500	1	32,50,50	1.72	9 (28%)	24,82,82	2.42	14 (58%)
5	HEC	A	600	1	32,50,50	1.45	4 (12%)	24,82,82	2.80	13 (54%)
7	PG4	F	388	-	12,12,12	0.59	0	11,11,11	0.45	0
6	1PE	F	387	-	15,15,15	0.64	0	14,14,14	0.61	0
5	HEC	B	600	1	32,50,50	1.51	5 (15%)	24,82,82	3.05	10 (41%)
8	ACT	F	389	-	3,3,3	1.00	0	3,3,3	1.57	1 (33%)
5	HEC	B	500	1	32,50,50	1.40	7 (21%)	24,82,82	2.24	11 (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
5	HEC	A	500	1	-	0/10/54/54	-
5	HEC	A	600	1	-	2/10/54/54	-
7	PG4	F	388	-	-	8/10/10/10	-
6	1PE	F	387	-	-	5/13/13/13	-
5	HEC	B	600	1	-	2/10/54/54	-
5	HEC	B	500	1	-	3/10/54/54	-

The worst 5 of 25 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
5	A	600	HEC	C4B-C3B	3.49	1.49	1.43
5	A	500	HEC	C1D-CHD	3.21	1.49	1.41
5	A	500	HEC	C3C-C4C	3.20	1.48	1.43
5	A	500	HEC	CBA-CGA	3.16	1.57	1.50
5	A	500	HEC	C4B-C3B	3.15	1.48	1.43

The worst 5 of 49 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
5	B	600	HEC	CBD-CAD-C3D	-7.28	100.20	112.62
5	A	600	HEC	CBD-CAD-C3D	-6.83	100.97	112.62
5	B	600	HEC	C1D-C2D-C3D	-5.89	102.90	107.00
5	A	500	HEC	CBD-CAD-C3D	-5.46	103.30	112.62
5	B	500	HEC	CMB-C2B-C3B	5.44	132.21	125.82

There are no chirality outliers.

5 of 20 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
7	F	388	PG4	O1-C1-C2-O2
6	F	387	1PE	OH4-C13-C23-OH3
6	F	387	1PE	OH7-C16-C26-OH6

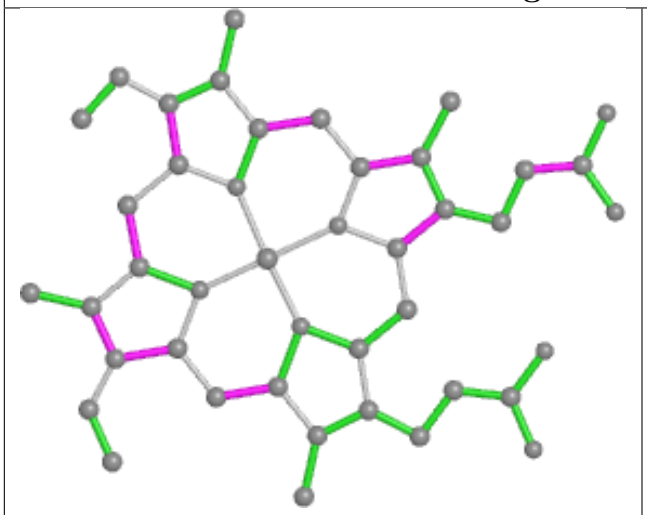
There are no ring outliers.

5 monomers are involved in 8 short contacts:

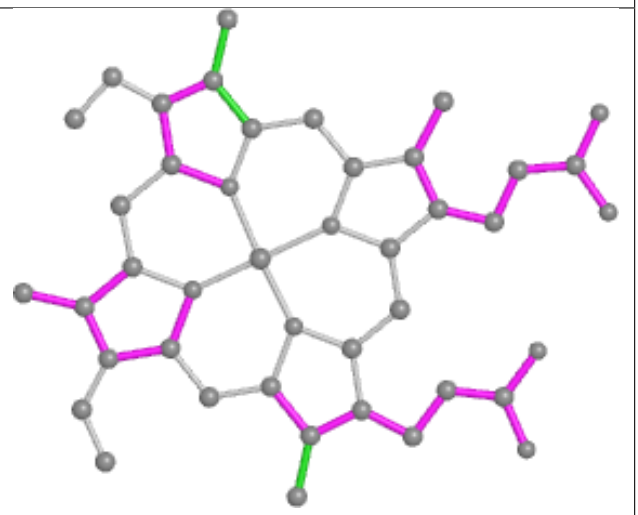
Mol	Chain	Res	Type	Clashes	Symm-Clashes
5	A	500	HEC	3	0
5	A	600	HEC	1	0
7	F	388	PG4	1	0
5	B	600	HEC	2	0
5	B	500	HEC	1	0

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.

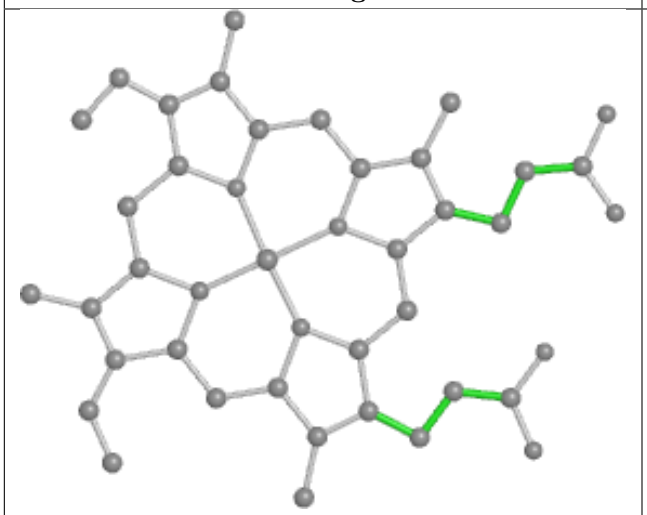
Ligand HEC A 500



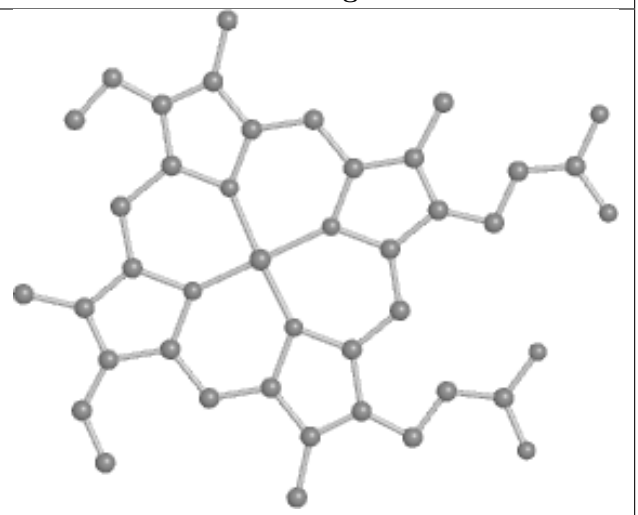
Bond lengths



Bond angles

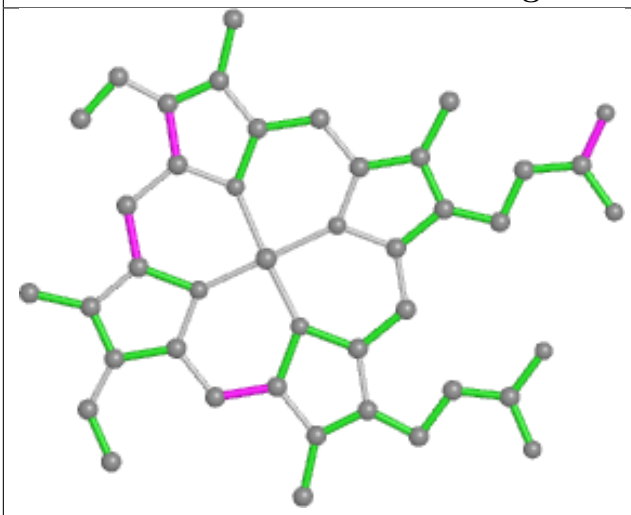


Torsions

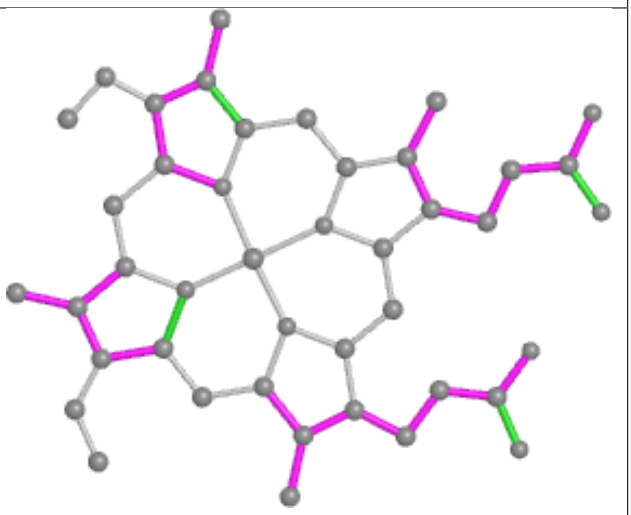


Rings

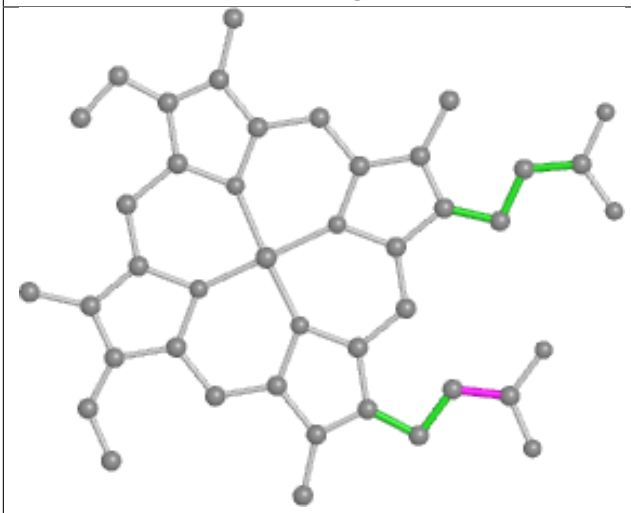
Ligand HEC A 600



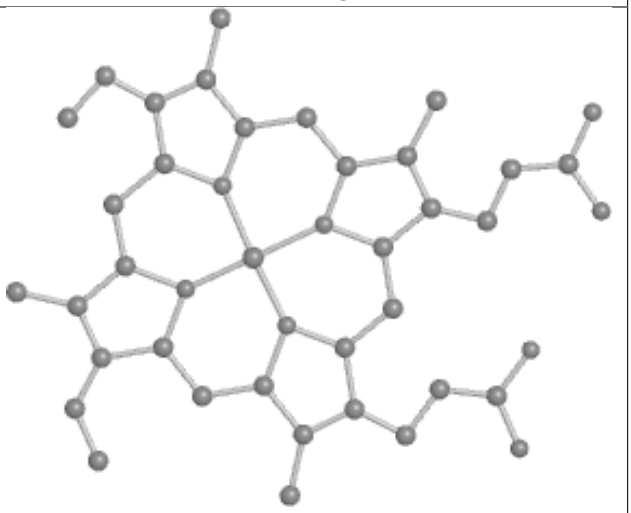
Bond lengths



Bond angles

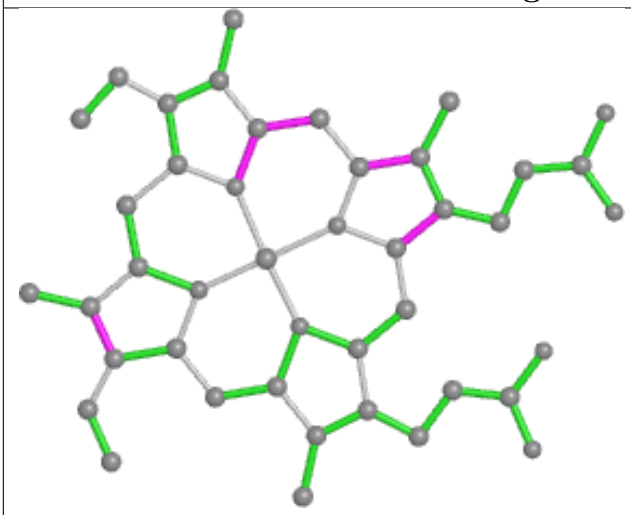


Torsions

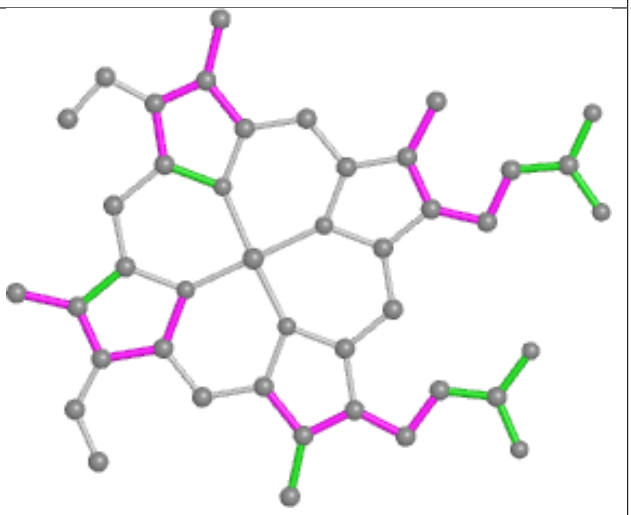


Rings

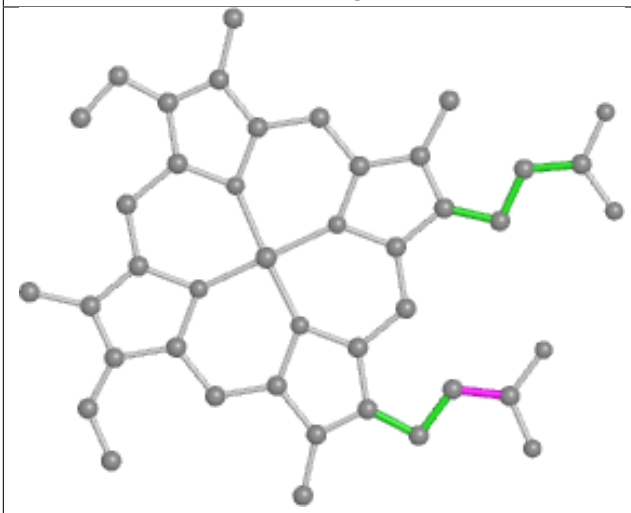
Ligand HEC B 600



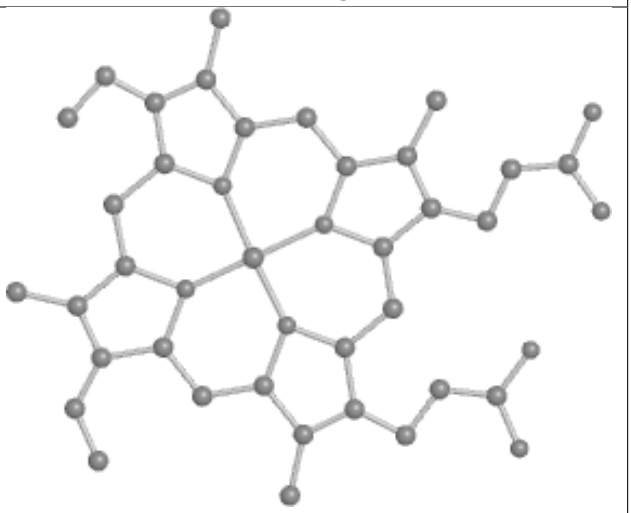
Bond lengths



Bond angles

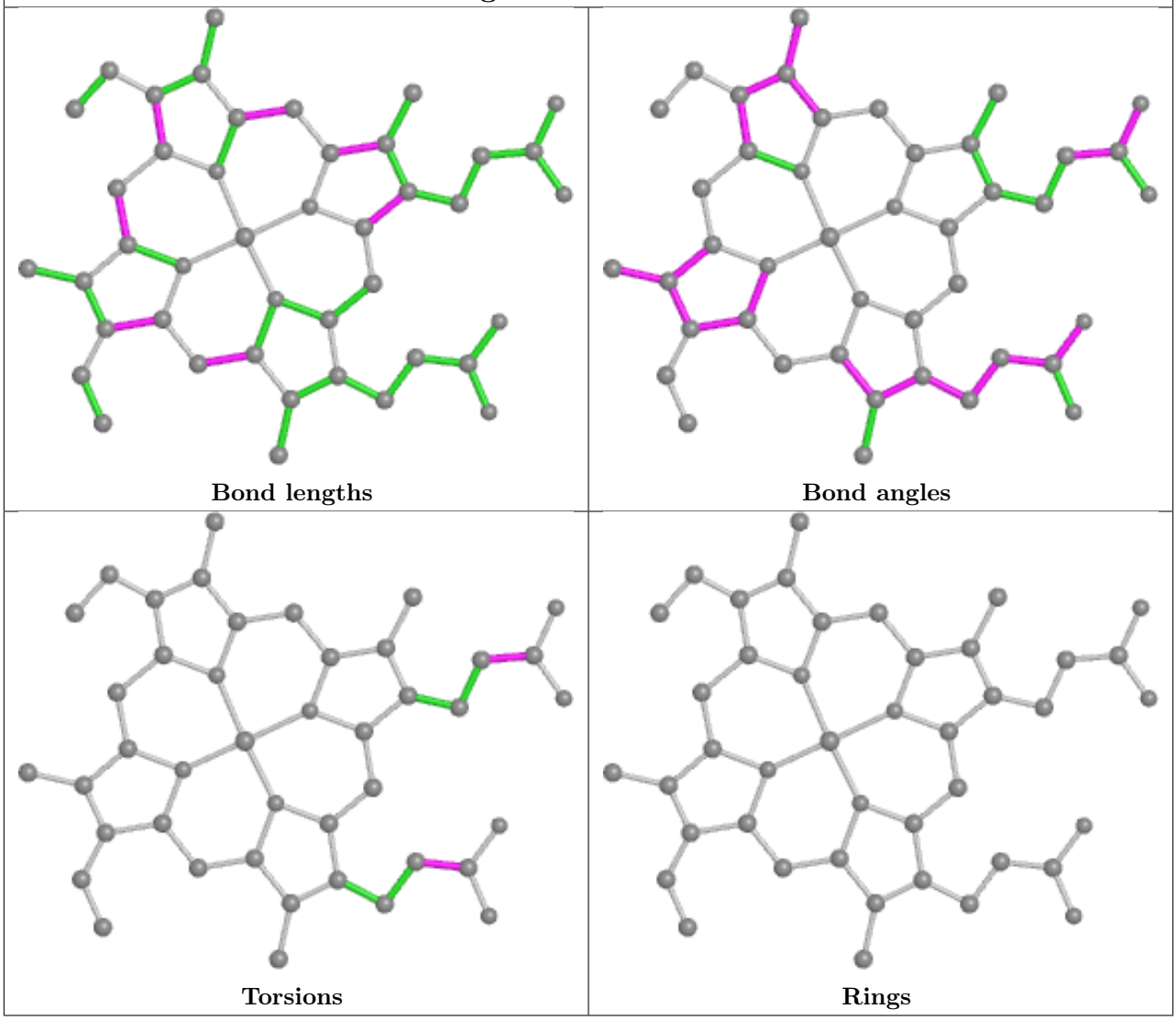


Torsions



Rings

Ligand HEC B 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	354/373 (94%)	-0.71	3 (0%)	86	85	8, 13, 26, 49	0
1	B	355/373 (95%)	-0.70	3 (0%)	86	85	8, 14, 27, 50	0
2	C	124/137 (90%)	-0.44	1 (0%)	86	85	10, 14, 24, 52	0
2	E	124/137 (90%)	-0.44	0	100	100	6, 11, 23, 53	0
3	D	376/386 (97%)	-0.56	6 (1%)	72	71	6, 13, 24, 53	0
3	F	376/386 (97%)	-0.65	2 (0%)	91	91	6, 11, 23, 48	0
All	All	1709/1792 (95%)	-0.62	15 (0%)	84	83	6, 13, 25, 53	0

The worst 5 of 15 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	7	ASP	5.3
1	A	7	ASP	4.9
3	D	208	THR	4.6
1	A	6	ALA	4.4
1	B	6	ALA	4.1

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	E	57	15/16	0.96	0.14	10,14,22,22	0
2	0AF	C	57	15/16	0.97	0.11	17,19,26,26	0

6.3 Carbohydrates (i)

There are no monosaccharides in this entry.

6.4 Ligands (i)

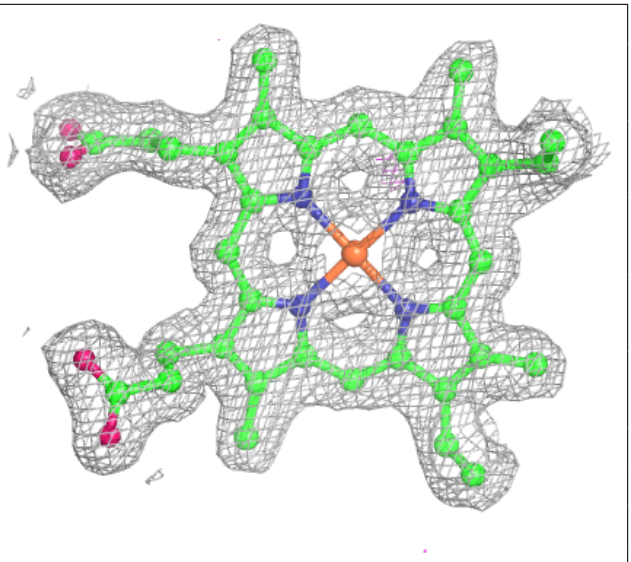
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists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

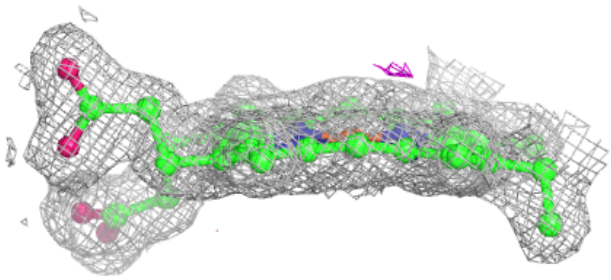
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
6	1PE	F	387	16/16	0.89	0.10	29,38,47,47	0
7	PG4	F	388	13/13	0.93	0.10	41,45,55,55	0
8	ACT	F	389	4/4	0.96	0.10	34,36,38,38	0
5	HEC	B	600	43/43	0.99	0.06	3,9,10,11	0
5	HEC	A	500	43/43	0.99	0.05	4,9,12,16	0
5	HEC	A	600	43/43	0.99	0.06	4,9,12,14	0
5	HEC	B	500	43/43	0.99	0.05	7,11,14,20	0
4	CA	B	400	1/1	1.00	0.04	10,10,10,10	0
4	CA	A	400	1/1	1.00	0.03	9,9,9,9	0

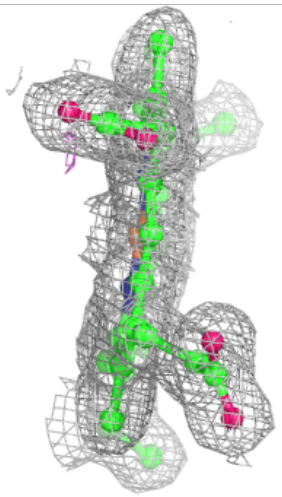
The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation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

Electron density around HEC B 600:

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

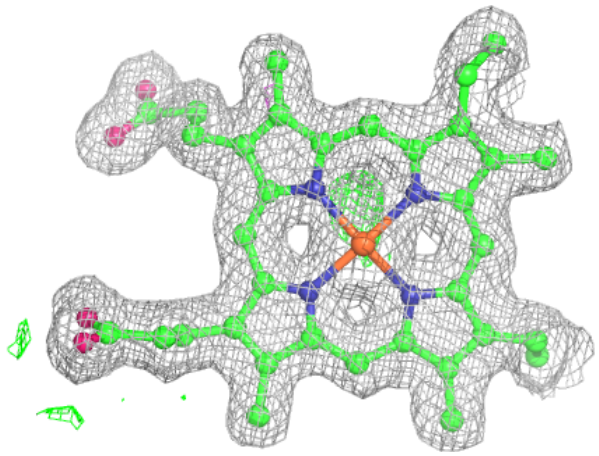


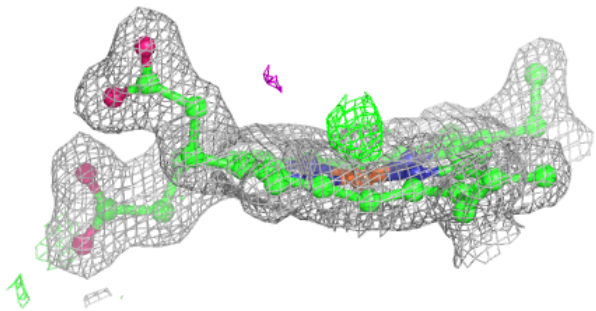


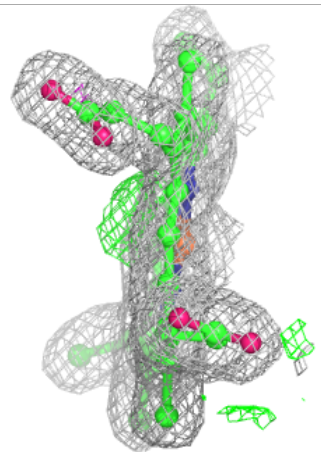


Electron density around HEC A 500:

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

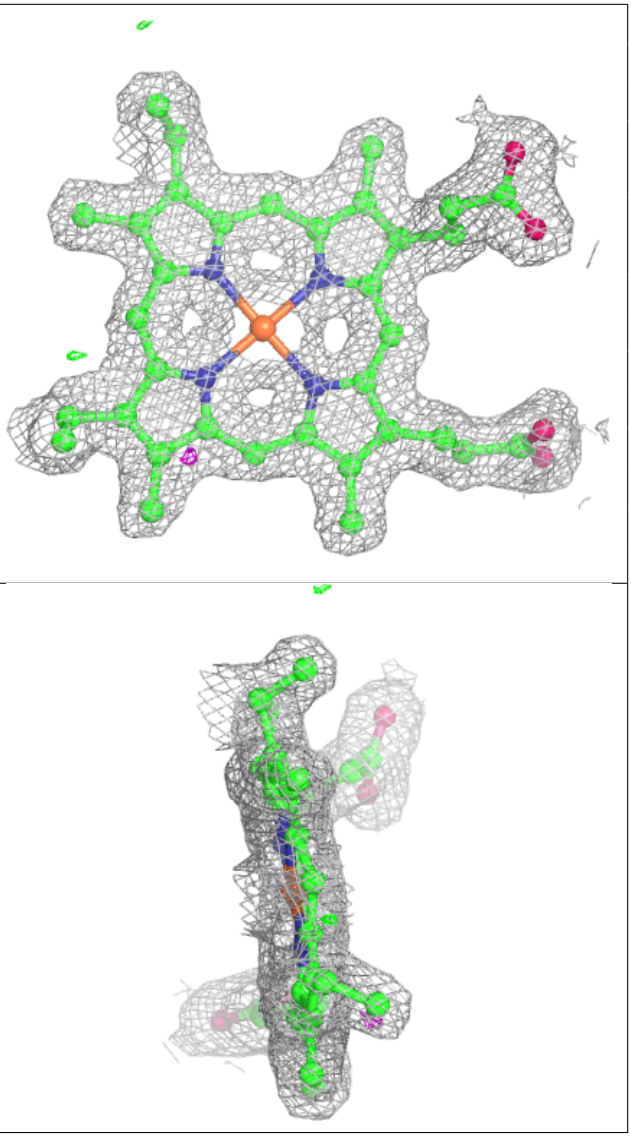


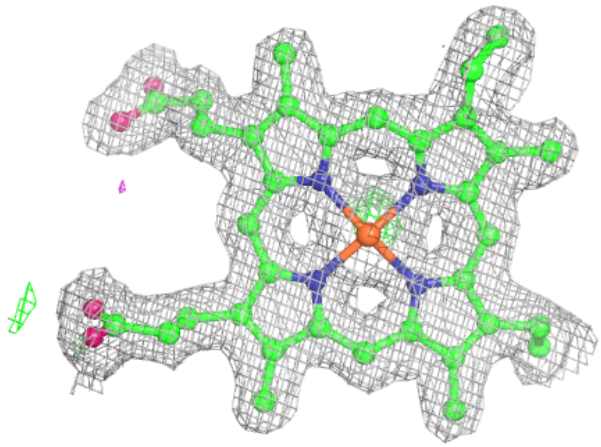
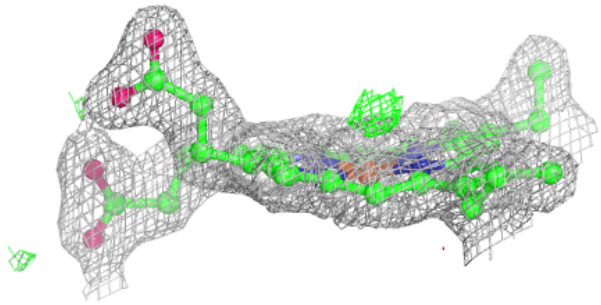
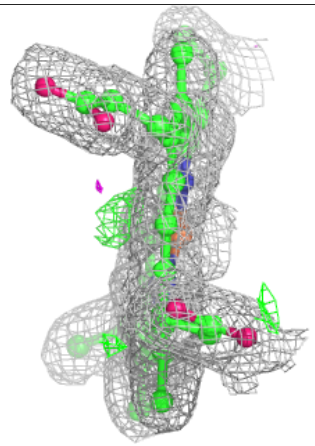




Electron density around HEC A 600:

$2mF_o$-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.