Full wwPDB X-ray Structure Validation Report ⓘ

Sep 3, 2023 – 03:32 AM EDT

PDB ID	:	3RMZ
Title	:	Crystal Structure of the W199F-MauG/pre-Methylamine Dehydrogenase Complex
Authors	:	Jensen, L.M.R.; Wilmot, C.M.
Deposited on	:	2011-04-21
Resolution	:	1.72 Å(reported)

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

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

The types of validation reports are described at
http://www.wwpdb.org/validation/2017/FAQs#types.

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

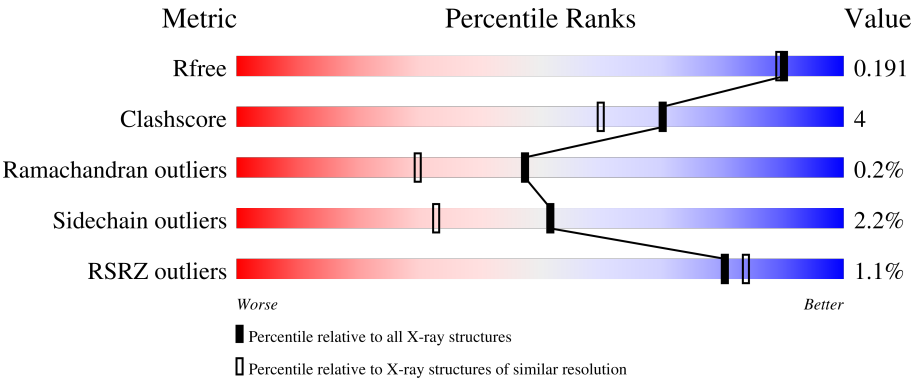
MolProbity	:	4.02b-467
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.35
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (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 1.72 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	5722 (1.74-1.70)
Clashscore	141614	6152 (1.74-1.70)
Ramachandran outliers	138981	6051 (1.74-1.70)
Sidechain outliers	138945	6051 (1.74-1.70)
RSRZ outliers	127900	5629 (1.74-1.70)

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	85% 9% 5%
1	B	373	88% 6% 5%
2	C	137	85% 8%
2	E	137	80% 10% 9%
3	D	386	86% 11%

Continued on next page...

Continued from previous page...

Mol	Chain	Length	Quality of chain
3	F	386	

2 Entry composition (i)

There are 13 unique types of molecules in this entry. The entry contains 15575 atoms, of which 0 are hydrogens and 0 are deuteriums.

In the tables below, the ZeroOcc column contains the number of atoms modelled with zero occupancy, the AltConf column contains the number of residues with at least one atom in alternate conformation and the Trace column contains the number of residues modelled with at most 2 atoms.

- Molecule 1 is a protein called Methylamine utilization protein MauG.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	354	Total	C	N	O	S	0	7	0
			2773	1734	496	532	11			
1	B	355	Total	C	N	O	S	0	3	0
			2757	1721	494	531	11			

There are 14 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	199	PHE	TRP	engineered mutation	UNP Q51658
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	199	PHE	TRP	engineered mutation	UNP Q51658
B	368	HIS	-	expression tag	UNP Q51658
B	369	HIS	-	expression tag	UNP Q51658
B	370	HIS	-	expression tag	UNP Q51658
B	371	HIS	-	expression tag	UNP Q51658
B	372	HIS	-	expression tag	UNP Q51658
B	373	HIS	-	expression tag	UNP Q51658

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	C	131	Total	C	N	O	S	0	5	0
			1032	638	180	199	15			
2	E	124	Total	C	N	O	S	0	4	0
			968	603	161	189	15			

There are 12 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
C	132	HIS	-	expression tag	UNP A1BBA0
C	133	HIS	-	expression tag	UNP A1BBA0
C	134	HIS	-	expression tag	UNP A1BBA0
C	135	HIS	-	expression tag	UNP A1BBA0
C	136	HIS	-	expression tag	UNP A1BBA0
C	137	HIS	-	expression tag	UNP A1BBA0
E	132	HIS	-	expression tag	UNP A1BBA0
E	133	HIS	-	expression tag	UNP A1BBA0
E	134	HIS	-	expression tag	UNP A1BBA0
E	135	HIS	-	expression tag	UNP A1BBA0
E	136	HIS	-	expression tag	UNP A1BBA0
E	137	HIS	-	expression tag	UNP A1BBA0

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	D	376	Total	C	N	O	S	0	7	0
			2957	1882	504	562	9			
3	F	376	Total	C	N	O	S	0	9	0
			2971	1888	507	567	9			

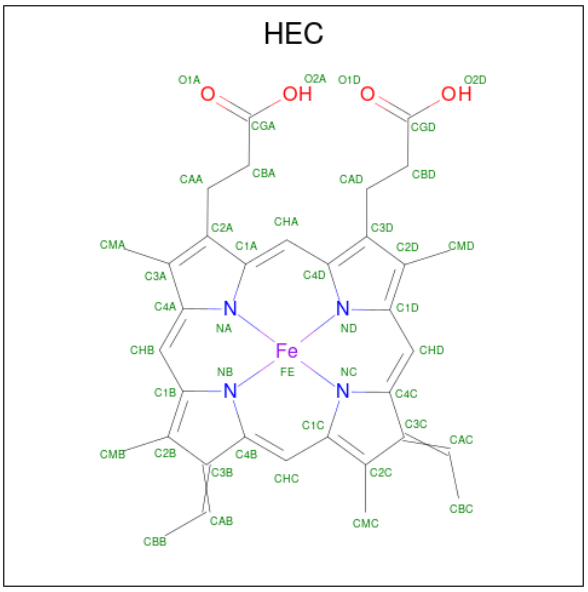
- Molecule 4 is CALCIUM ION (three-letter code: CA) (formula: Ca).

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

- Molecule 5 is SODIUM ION (three-letter code: NA) (formula: Na).

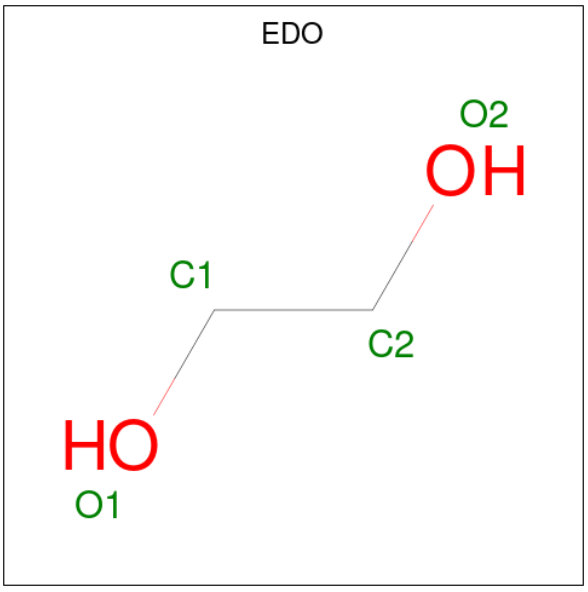
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	A	2	Total	Na	0	0
			2	2		
5	B	2	Total	Na	0	0
			2	2		

- Molecule 6 is HEME C (three-letter code: HEC) (formula: $C_{34}H_{34}FeN_4O_4$).



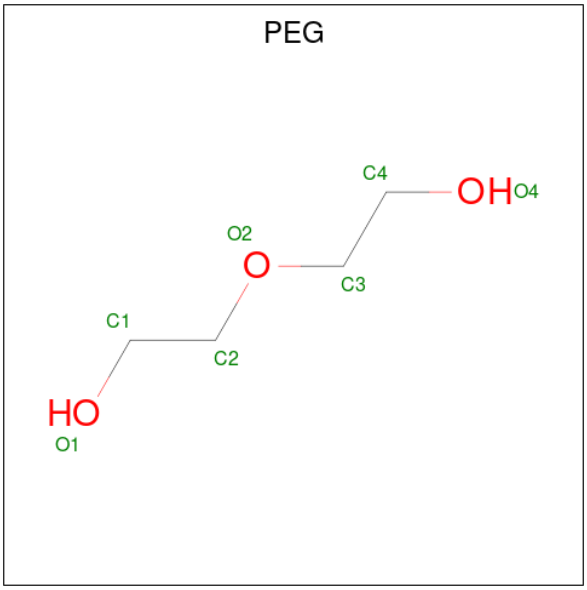
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
6	A	1	Total	C	Fe	N	O	0	0
			43	34	1	4	4		
6	A	1	Total	C	Fe	N	O	0	0
			43	34	1	4	4		
6	B	1	Total	C	Fe	N	O	0	0
			43	34	1	4	4		
6	B	1	Total	C	Fe	N	O	0	0
			43	34	1	4	4		

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



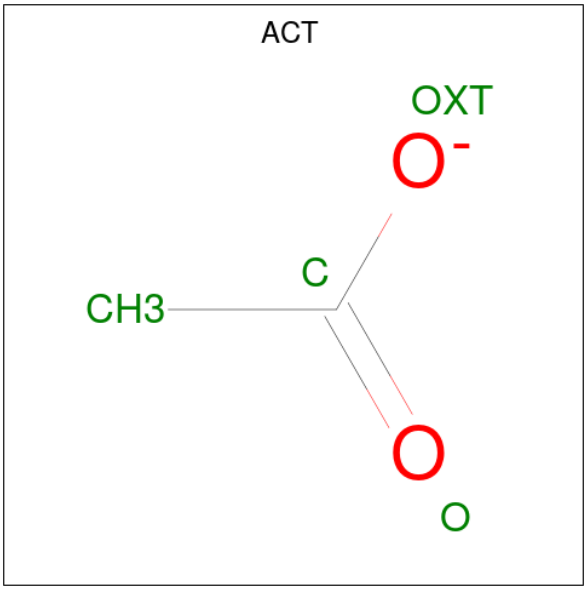
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
7	A	1	Total C O 4 2 2	0	0
7	B	1	Total C O 4 2 2	0	0

- Molecule 8 is DI(HYDROXYETHYL)ETHER (three-letter code: PEG) (formula: $C_4H_{10}O_3$).



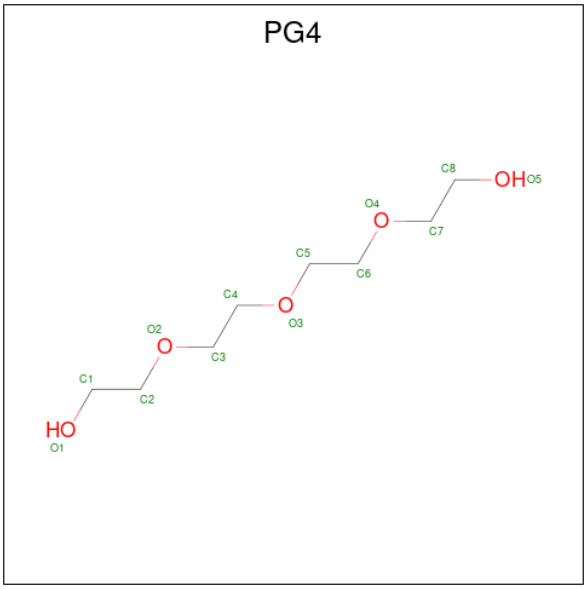
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
8	D	1	Total C O 7 4 3	0	0

- Molecule 9 is ACETATE ION (three-letter code: ACT) (formula: $C_2H_3O_2$).



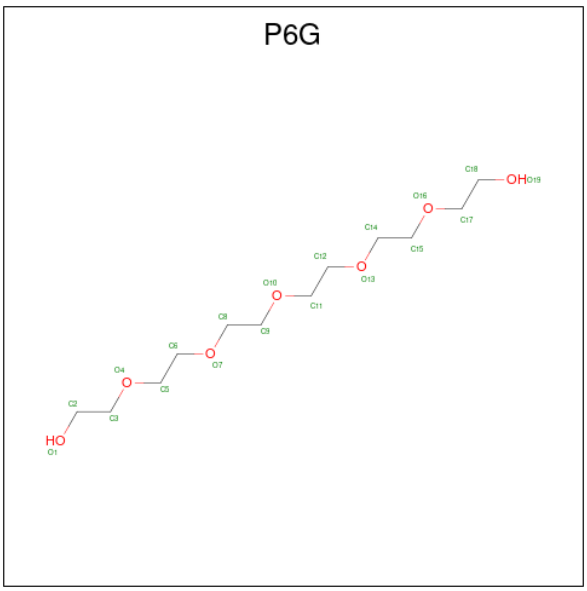
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
9	D	1	Total C O 4 2 2	0	0

- Molecule 10 is TETRAETHYLENE GLYCOL (three-letter code: PG4) (formula: $C_8H_{18}O_5$).



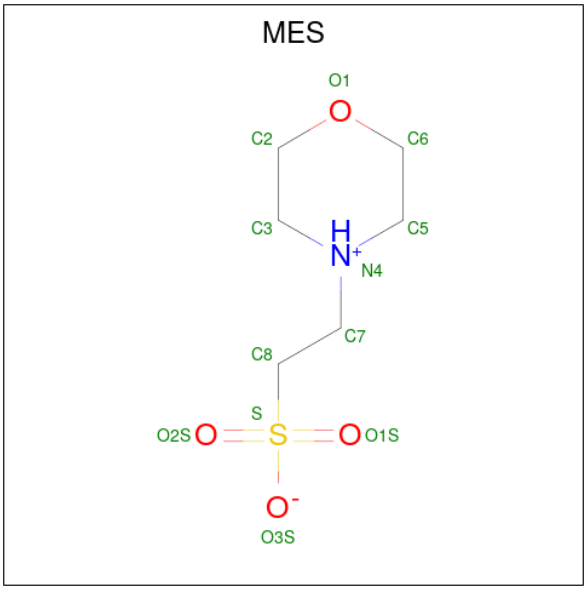
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
10	F	1	Total C O 13 8 5	0	0

- Molecule 11 is HEXAETHYLENE GLYCOL (three-letter code: P6G) (formula: $C_{12}H_{26}O_7$).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
11	F	1	Total C O 19 12 7	0	0

- Molecule 12 is 2-(N-MORPHOLINO)-ETHANESULFONIC ACID (three-letter code: MES) (formula: $C_6H_{13}NO_4S$).



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

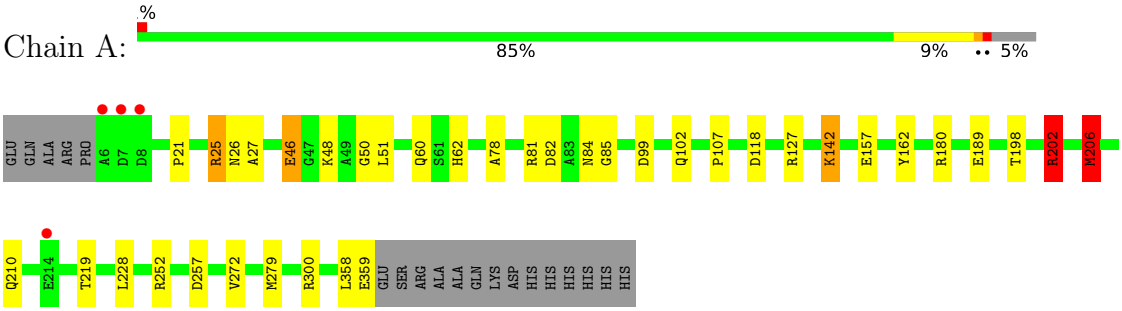
- Molecule 13 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
13	A	381	Total O 381 381	0	0
13	B	387	Total O 387 387	0	0
13	C	134	Total O 134 134	0	0
13	D	371	Total O 371 371	0	0
13	E	132	Total O 132 132	0	0
13	F	471	Total O 471 471	0	0

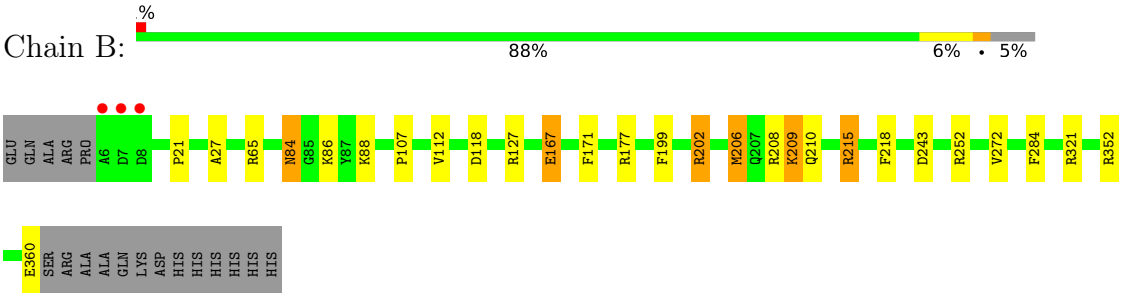
3 Residue-property plots (i)

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.

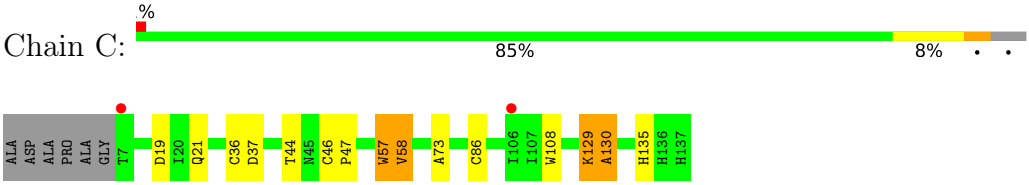
• Molecule 1: Methylamine utilization protein MauG



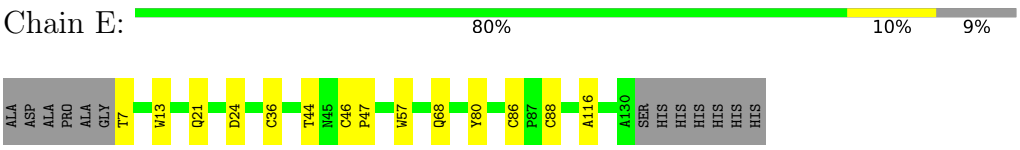
• Molecule 1: Methylamine utilization protein MauG



• Molecule 2: Methylamine dehydrogenase light chain

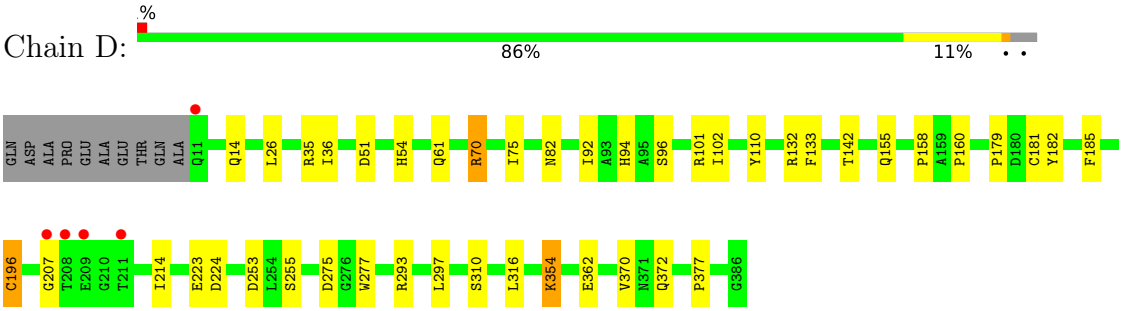


• Molecule 2: Methylamine dehydrogenase light chain



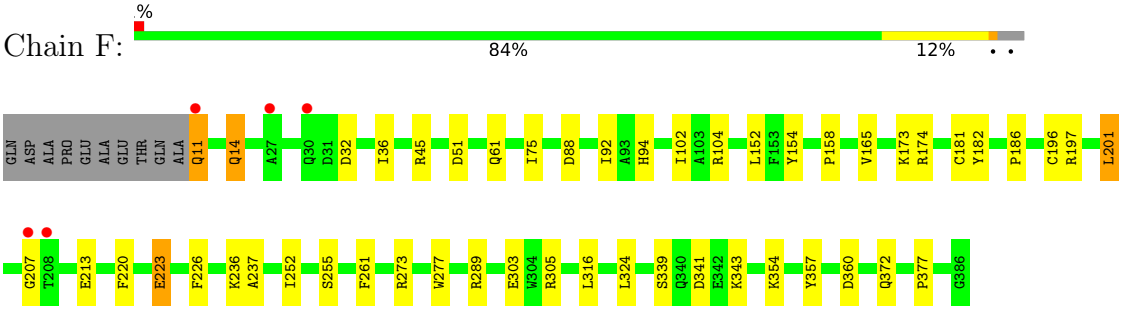
• Molecule 3: Methylamine dehydrogenase heavy chain

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)	39.58 – 1.72 39.57 – 1.72	Depositor EDS
% Data completeness (in resolution range)	94.8 (39.58-1.72) 94.8 (39.57-1.72)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	0.06	Depositor
$< I/\sigma(I) >$ [1]	1.27 (at 1.72Å)	Xtriage
Refinement program	REFMAC 5.5.0109	Depositor
R, R_{free}	0.138 , 0.181 0.149 , 0.191	Depositor DCC
R_{free} test set	8789 reflections (5.05%)	wwPDB-VP
Wilson B-factor (Å^2)	17.3	Xtriage
Anisotropy	0.058	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.35 , 39.1	EDS
L-test for twinning[2]	$< \|L\| > = 0.49$, $< L^2 > = 0.33$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o,F_c correlation	0.97	EDS
Total number of atoms	15575	wwPDB-VP
Average B, all atoms (Å^2)	20.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.44% 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, CA, ACT, 0AF, HEC, NA, PG4, P6G, EDO, PEG

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	1.21	5/2854 (0.2%)	1.14	15/3870 (0.4%)
1	B	1.26	7/2826 (0.2%)	1.13	12/3833 (0.3%)
2	C	1.20	0/1063	1.14	3/1447 (0.2%)
2	E	1.27	3/990 (0.3%)	1.14	1/1351 (0.1%)
3	D	1.19	4/3055 (0.1%)	1.11	12/4163 (0.3%)
3	F	1.33	8/3075 (0.3%)	1.19	16/4189 (0.4%)
All	All	1.25	27/13863 (0.2%)	1.14	59/18853 (0.3%)

All (27) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	F	213	GLU	CD-OE1	8.11	1.34	1.25
1	A	162	TYR	CD2-CE2	6.42	1.49	1.39
1	B	360	GLU	CB-CG	6.31	1.64	1.52
1	B	360	GLU	CG-CD	6.21	1.61	1.51
1	B	199	PHE	CD2-CE2	6.19	1.51	1.39
3	F	220	PHE	CD2-CE2	6.15	1.51	1.39
3	D	133	PHE	CE1-CZ	5.80	1.48	1.37
3	F	165	VAL	CB-CG1	5.79	1.65	1.52
3	D	185	PHE	CE1-CZ	5.70	1.48	1.37
2	E	88[A]	CYS	CB-SG	-5.66	1.72	1.81
2	E	88[B]	CYS	CB-SG	-5.66	1.72	1.81
1	B	209	LYS	CD-CE	5.61	1.65	1.51
3	D	277	TRP	C-O	5.56	1.33	1.23
3	F	154	TYR	CE1-CZ	5.55	1.45	1.38
1	B	167	GLU	CG-CD	5.55	1.60	1.51
1	A	46[A]	GLU	CB-CG	5.52	1.62	1.52
1	A	46[B]	GLU	CB-CG	5.52	1.62	1.52
1	B	284	PHE	CE2-CZ	5.47	1.47	1.37
3	F	357	TYR	CD2-CE2	5.36	1.47	1.39
3	F	339	SER	CB-OG	5.32	1.49	1.42

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	F	277	TRP	CZ3-CH2	5.29	1.48	1.40
1	A	78	ALA	CA-CB	5.19	1.63	1.52
2	E	116	ALA	CA-CB	-5.17	1.41	1.52
3	D	370	VAL	CB-CG2	5.13	1.63	1.52
1	A	189	GLU	CB-CG	5.10	1.61	1.52
1	B	218	PHE	CE2-CZ	5.09	1.47	1.37
3	F	223	GLU	CG-CD	5.01	1.59	1.51

All (59) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	B	206	MET	CG-SD-CE	-15.39	75.58	100.20
1	A	206	MET	CG-SD-CE	-9.45	85.08	100.20
3	D	70	ARG	NE-CZ-NH1	9.31	124.95	120.30
3	F	197	ARG	NE-CZ-NH1	-8.81	115.90	120.30
1	B	208	ARG	NE-CZ-NH1	-8.62	115.99	120.30
3	D	132	ARG	NE-CZ-NH2	-8.28	116.16	120.30
1	A	127	ARG	NE-CZ-NH2	8.17	124.39	120.30
1	A	118	ASP	CB-CG-OD1	7.79	125.31	118.30
3	D	101	ARG	NE-CZ-NH2	-7.76	116.42	120.30
3	F	174	ARG	NE-CZ-NH2	-7.27	116.67	120.30
1	A	252	ARG	NE-CZ-NH2	-7.16	116.72	120.30
3	D	354	LYS	CD-CE-NZ	-6.99	95.62	111.70
1	B	252	ARG	NE-CZ-NH2	-6.97	116.81	120.30
1	A	99	ASP	CB-CG-OD2	6.95	124.55	118.30
1	A	127	ARG	NE-CZ-NH1	-6.92	116.84	120.30
1	B	321	ARG	NE-CZ-NH1	-6.72	116.94	120.30
1	A	180	ARG	NE-CZ-NH1	6.51	123.56	120.30
1	A	257	ASP	CB-CG-OD2	-6.35	112.58	118.30
3	F	14	GLN	CA-CB-CG	6.34	127.36	113.40
1	A	202	ARG	NE-CZ-NH2	-6.32	117.14	120.30
1	A	257	ASP	CB-CG-OD1	6.29	123.96	118.30
1	A	25	ARG	NE-CZ-NH2	-6.22	117.19	120.30
2	C	19	ASP	CB-CG-OD1	6.19	123.87	118.30
1	A	82	ASP	CB-CG-OD2	6.08	123.77	118.30
3	F	236	LYS	CD-CE-NZ	6.08	125.68	111.70
3	D	253	ASP	CB-CG-OD1	6.06	123.75	118.30
3	F	104	ARG	NE-CZ-NH1	6.05	123.33	120.30
1	A	142	LYS	CD-CE-NZ	6.03	125.56	111.70
3	D	35	ARG	NE-CZ-NH1	5.98	123.29	120.30
1	B	65	ARG	NE-CZ-NH1	-5.91	117.35	120.30
1	B	127	ARG	NE-CZ-NH1	5.86	123.23	120.30

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	B	177	ARG	NE-CZ-NH1	5.81	123.20	120.30
3	D	70	ARG	NE-CZ-NH2	-5.76	117.42	120.30
3	F	104	ARG	NE-CZ-NH2	-5.74	117.43	120.30
3	F	32	ASP	CB-CG-OD2	5.73	123.45	118.30
3	F	341	ASP	CB-CG-OD1	5.72	123.45	118.30
3	F	226	PHE	CB-CG-CD1	-5.72	116.80	120.80
1	B	243	ASP	CB-CG-OD1	5.71	123.44	118.30
2	C	37	ASP	CB-CG-OD2	5.69	123.42	118.30
1	A	82	ASP	CB-CG-OD1	-5.63	113.23	118.30
3	F	14	GLN	N-CA-CB	-5.59	100.54	110.60
3	D	253	ASP	CB-CG-OD2	-5.51	113.34	118.30
3	F	201	LEU	CB-CG-CD1	-5.49	101.67	111.00
1	B	118	ASP	CB-CG-OD1	5.49	123.24	118.30
2	E	24	ASP	CB-CG-OD1	5.44	123.19	118.30
3	D	293	ARG	NE-CZ-NH2	-5.40	117.60	120.30
3	D	224	ASP	CB-CG-OD1	5.39	123.15	118.30
1	A	180	ARG	NE-CZ-NH2	-5.35	117.63	120.30
3	F	324	LEU	CB-CG-CD1	-5.33	101.94	111.00
3	D	196	CYS	CA-CB-SG	-5.32	104.43	114.00
2	C	37	ASP	CB-CG-OD1	-5.26	113.56	118.30
1	B	321	ARG	NE-CZ-NH2	5.23	122.92	120.30
3	F	305[A]	ARG	NE-CZ-NH1	-5.22	117.69	120.30
3	F	305[B]	ARG	NE-CZ-NH1	-5.22	117.69	120.30
3	F	88	ASP	CB-CG-OD1	5.14	122.92	118.30
1	B	127	ARG	NE-CZ-NH2	-5.11	117.75	120.30
1	B	215	ARG	NE-CZ-NH2	-5.09	117.75	120.30
3	D	26	LEU	CB-CG-CD2	-5.08	102.37	111.00
3	F	273	ARG	NE-CZ-NH1	5.02	122.81	120.30

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts (i)

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	2773	0	2664	23	0

Continued on next page...

Continued from previous page...

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	B	2757	0	2636	13	0
2	C	1032	0	918	15	0
2	E	968	0	880	8	0
3	D	2957	0	2871	27	0
3	F	2971	0	2881	19	0
4	A	1	0	0	0	0
4	B	1	0	0	0	0
5	A	2	0	0	0	0
5	B	2	0	0	0	0
6	A	86	0	60	2	0
6	B	86	0	60	2	0
7	A	4	0	6	0	0
7	B	4	0	6	0	0
8	D	7	0	10	3	0
9	D	4	0	3	0	0
10	F	13	0	18	3	0
11	F	19	0	26	6	0
12	F	12	0	12	0	0
13	A	381	0	0	3	0
13	B	387	0	0	4	0
13	C	134	0	0	2	0
13	D	371	0	0	4	0
13	E	132	0	0	1	0
13	F	471	0	0	7	0
All	All	15575	0	13051	96	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 (96) 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)
3:D:372[A]:GLN:OE1	13:D:1255:HOH:O	1.83	0.94
11:F:388:P6G:H21	13:F:903:HOH:O	1.70	0.90
3:F:255:SER:HA	10:F:387:PG4:H32	1.56	0.86
3:D:255:SER:HB2	8:D:387:PEG:H22	1.58	0.85
1:B:107:PRO:HG3	13:B:1931:HOH:O	1.81	0.81
3:F:360[B]:ASP:OD1	13:F:830:HOH:O	2.00	0.79
3:D:255:SER:HA	8:D:387:PEG:H32	1.66	0.78
1:B:84:ASN:HD22	1:B:86:LYS:NZ	1.84	0.75
3:D:372[A]:GLN:HE22	2:E:86:CYS:H	1.33	0.75

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:D:297[B]:LEU:HG	3:D:310:SER:HB2	1.71	0.72
3:D:207:GLY:HA2	13:D:1859:HOH:O	1.88	0.72
3:D:14[A]:GLN:HE21	2:E:21:GLN:HE22	1.39	0.70
2:C:135:HIS:HD2	13:C:351:HOH:O	1.75	0.69
3:D:255:SER:CB	8:D:387:PEG:H22	2.20	0.69
1:A:210:GLN:HE22	2:C:44:THR:HG21	1.57	0.69
1:B:84:ASN:HD22	1:B:86:LYS:HZ2	1.40	0.69
1:A:107:PRO:HG3	13:A:1962:HOH:O	1.93	0.68
1:A:48:LYS:H	1:A:62:HIS:HE1	1.43	0.67
1:A:300[B]:ARG:HH22	3:D:155:GLN:HE22	1.44	0.66
1:B:210:GLN:HE22	2:E:44:THR:HG21	1.63	0.64
1:B:202:ARG:HB2	1:B:206:MET:HG3	1.80	0.63
1:A:48:LYS:H	1:A:62:HIS:CE1	2.18	0.62
6:B:600:HEC:HBC3	6:B:600:HEC:HMC1	1.82	0.62
2:E:13[B]:TRP:HB3	13:E:1444:HOH:O	2.01	0.61
2:C:86:CYS:H	3:F:372[A]:GLN:HE22	1.49	0.60
2:C:135:HIS:HE1	13:C:702:HOH:O	1.82	0.60
3:F:51:ASP:HA	3:F:377:PRO:HA	1.84	0.60
2:E:36[B]:CYS:SG	2:E:47:PRO:HD3	2.42	0.59
11:F:388:P6G:H81	13:F:903:HOH:O	2.02	0.59
2:C:21:GLN:HE22	3:F:14:GLN:HE21	1.50	0.59
1:A:202:ARG:HB2	1:A:206:MET:HG3	1.86	0.58
3:F:207:GLY:HA3	13:F:771:HOH:O	2.03	0.58
3:D:75[B]:ILE:HD11	3:D:92:ILE:HD11	1.86	0.57
3:D:179:PRO:HD3	3:D:214:ILE:HD13	1.85	0.57
2:C:129[B]:LYS:O	2:C:130:ALA:CB	2.53	0.57
3:F:11:GLN:HG2	3:F:11:GLN:O	2.07	0.55
1:A:46[B]:GLU:OE2	1:A:51:LEU:HD11	2.06	0.54
3:D:14[B]:GLN:HG3	13:D:401:HOH:O	2.06	0.54
1:B:88:LYS:NZ	13:B:814:HOH:O	2.40	0.54
3:D:372[A]:GLN:NE2	2:E:86:CYS:H	2.03	0.53
1:A:300[B]:ARG:HH22	3:D:155:GLN:NE2	2.04	0.53
11:F:388:P6G:H52	13:F:903:HOH:O	2.09	0.53
1:A:198:THR:HG22	2:C:58[B]:VAL:HG23	1.91	0.53
10:F:387:PG4:H42	13:F:990:HOH:O	2.09	0.53
1:A:81:ARG:CZ	1:A:85:GLY:HA2	2.39	0.53
3:D:51:ASP:HA	3:D:377:PRO:HA	1.91	0.52
1:A:46[A]:GLU:CD	1:A:50:GLY:HA2	2.30	0.52
3:F:255:SER:HB2	10:F:387:PG4:H22	1.91	0.52
2:C:129[B]:LYS:O	2:C:130:ALA:HB2	2.10	0.51
3:D:181[B]:CYS:HB3	3:D:196:CYS:SG	2.50	0.51

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:300[B]:ARG:HH12	3:D:155:GLN:HE22	1.57	0.50
1:B:352:ARG:HD2	13:B:1503:HOH:O	2.11	0.50
1:B:21:PRO:O	1:B:27:ALA:HA	2.12	0.49
1:A:102[B]:GLN:NE2	13:A:1853:HOH:O	2.46	0.49
3:D:14[B]:GLN:HE22	3:D:70:ARG:HB2	1.77	0.48
2:C:86:CYS:H	3:F:372[A]:GLN:NE2	2.11	0.48
1:A:300[B]:ARG:NH2	3:D:155:GLN:HE22	2.11	0.48
3:F:45:ARG:NH2	3:F:343:LYS:O	2.47	0.48
1:B:171:PHE:CZ	1:B:215:ARG:HB3	2.49	0.47
3:D:36:ILE:HD13	2:E:46:CYS:HB2	1.96	0.47
3:D:61:GLN:HB3	3:D:75[A]:ILE:HB	1.98	0.46
1:B:84:ASN:HD22	1:B:86:LYS:HZ3	1.62	0.46
2:C:58[B]:VAL:HG22	2:C:73:ALA:HA	1.99	0.45
3:F:181[B]:CYS:HB3	3:F:196:CYS:SG	2.55	0.45
3:F:252[B]:ILE:HD11	3:F:261:PHE:HE2	1.82	0.45
1:A:25:ARG:HH11	1:A:26:ASN:HD21	1.64	0.44
3:D:36:ILE:CD1	2:E:46:CYS:HB2	2.48	0.44
1:B:84:ASN:OD1	1:B:84:ASN:N	2.51	0.43
1:A:198:THR:CG2	2:C:58[B]:VAL:HG23	2.48	0.43
11:F:388:P6G:H112	11:F:388:P6G:H82	1.76	0.43
2:C:46:CYS:HB2	3:F:36:ILE:HD13	2.01	0.43
1:A:358:LEU:O	1:A:359:GLU:HB2	2.19	0.43
6:A:600:HEC:HBC3	6:A:600:HEC:HMC1	2.01	0.43
3:D:54:HIS:HD2	13:D:1757:HOH:O	2.02	0.43
1:A:21:PRO:O	1:A:27:ALA:HA	2.19	0.42
1:A:228:LEU:HD13	1:A:279:MET:HB3	2.02	0.42
1:A:60:GLN:O	1:A:62:HIS:HD2	2.02	0.42
1:B:272:VAL:HG21	6:B:600:HEC:HMA3	2.01	0.42
2:C:36[B]:CYS:SG	2:C:47:PRO:HD3	2.60	0.42
1:A:272:VAL:HG21	6:A:600:HEC:HMA3	2.02	0.42
3:D:82:ASN:HB3	3:D:142:THR:HB	2.02	0.42
3:D:362:GLU:HA	3:D:362:GLU:OE1	2.19	0.42
2:C:57:0AF:CE3	2:C:108:TRP:CD1	3.02	0.41
3:D:96:SER:HB3	3:D:110:TYR:CZ	2.55	0.41
2:C:46:CYS:HB2	3:F:36:ILE:CD1	2.51	0.41
3:F:61:GLN:HB3	3:F:75[B]:ILE:HB	2.02	0.41
3:F:152:LEU:HD12	3:F:186:PRO:HG3	2.03	0.41
1:B:209:LYS:NZ	13:B:751:HOH:O	2.44	0.41
3:F:237:ALA:HB2	3:F:289:ARG:HG3	2.02	0.41
3:F:201:LEU:HD11	3:F:252[B]:ILE:HD13	2.03	0.41
11:F:388:P6G:H141	11:F:388:P6G:H111	1.88	0.41

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:46[B]:GLU:CD	1:A:51:LEU:HD11	2.42	0.40
11:F:388:P6G:C8	13:F:903:HOH:O	2.67	0.40
1:A:157:GLU:HG3	13:A:410:HOH:O	2.20	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	359/373 (96%)	349 (97%)	10 (3%)	0	100 100
1	B	356/373 (95%)	346 (97%)	10 (3%)	0	100 100
2	C	133/137 (97%)	128 (96%)	4 (3%)	1 (1%)	19 6
2	E	125/137 (91%)	122 (98%)	3 (2%)	0	100 100
3	D	381/386 (99%)	366 (96%)	13 (3%)	2 (0%)	29 13
3	F	383/386 (99%)	370 (97%)	12 (3%)	1 (0%)	41 24
All	All	1737/1792 (97%)	1681 (97%)	52 (3%)	4 (0%)	47 30

All (4) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
2	C	130	ALA
3	D	102[A]	ILE
3	D	102[B]	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	282/292 (97%)	277 (98%)	5 (2%)	59	41
1	B	279/292 (96%)	275 (99%)	4 (1%)	67	52
2	C	115/112 (103%)	111 (96%)	4 (4%)	36	16
2	E	107/112 (96%)	104 (97%)	3 (3%)	43	23
3	D	311/311 (100%)	304 (98%)	7 (2%)	50	31
3	F	313/311 (101%)	303 (97%)	10 (3%)	39	18
All	All	1407/1430 (98%)	1374 (98%)	33 (2%)	52	31

All (33) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	84	ASN
1	A	142	LYS
1	A	202	ARG
1	A	206	MET
1	A	219	THR
1	B	84	ASN
1	B	112	VAL
1	B	167	GLU
1	B	202	ARG
2	C	58[A]	VAL
2	C	58[B]	VAL
2	C	129[A]	LYS
2	C	129[B]	LYS
3	D	94	HIS
3	D	158	PRO
3	D	160	PRO
3	D	223	GLU
3	D	275	ASP
3	D	316	LEU
3	D	354	LYS
2	E	7	THR
2	E	68	GLN
2	E	80	TYR
3	F	11	GLN
3	F	92	ILE
3	F	94	HIS

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
3	F	158	PRO
3	F	173	LYS
3	F	223	GLU
3	F	303[A]	GLU
3	F	303[B]	GLU
3	F	316	LEU
3	F	354	LYS

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (14) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	26	ASN
1	A	62	HIS
1	A	210	GLN
1	B	16	GLN
1	B	26	ASN
1	B	29	GLN
1	B	84	ASN
1	B	91	GLN
1	B	210	GLN
2	C	135	HIS
2	C	136	HIS
3	D	30	GLN
3	D	155	GLN
3	F	14	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	C	57	2	13,16,17	1.92	4 (30%)	11,22,24	2.75	6 (54%)
2	0AF	E	57	2	13,16,17	1.96	5 (38%)	11,22,24	1.99	2 (18%)

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

All (9) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	C	57	0AF	CB-CA	-3.36	1.46	1.53
2	E	57	0AF	CA-N	-3.19	1.38	1.48
2	C	57	0AF	CA-N	-3.09	1.38	1.48
2	C	57	0AF	CZ3-CE3	3.00	1.43	1.36
2	E	57	0AF	CZ3-CE3	2.78	1.43	1.36
2	E	57	0AF	CZ2-CE2	-2.48	1.38	1.42
2	E	57	0AF	CB-CA	-2.45	1.48	1.53
2	C	57	0AF	CZ2-CE2	-2.41	1.38	1.42
2	E	57	0AF	CH2-CZ2	2.12	1.41	1.37

All (8) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	C	57	0AF	CB-CG-CD1	-4.38	122.56	127.97
2	C	57	0AF	CG-CB-CA	-4.16	108.09	114.53
2	E	57	0AF	CB-CG-CD2	4.08	132.59	126.25
2	E	57	0AF	CB-CG-CD1	-3.64	123.47	127.97
2	C	57	0AF	CH2-CZ2-CE2	3.40	124.17	120.12
2	C	57	0AF	CB-CA-C	3.34	117.74	111.47
2	C	57	0AF	CB-CG-CD2	3.29	131.37	126.25
2	C	57	0AF	CZ3-CH2-CZ2	-2.43	117.21	120.28

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

1 monomer is involved in 1 short contact:

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

5.5 Carbohydrates (i)

There are no monosaccharides in this entry.

5.6 Ligand geometry (i)

Of 17 ligands modelled in this entry, 6 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	$\#\|Z\| > 2$
10	PG4	F	387	-	12,12,12	0.56	0	11,11,11	0.50	0
11	P6G	F	388	-	18,18,18	0.61	0	17,17,17	0.77	0
6	HEC	B	600	1	32,50,50	1.29	4 (12%)	24,82,82	2.66	9 (37%)
12	MES	F	389	-	12,12,12	1.35	1 (8%)	14,16,16	3.80	8 (57%)
7	EDO	A	374	-	3,3,3	0.45	0	2,2,2	0.35	0
7	EDO	B	374	-	3,3,3	0.50	0	2,2,2	0.05	0
9	ACT	D	388	-	3,3,3	0.46	0	3,3,3	1.69	1 (33%)
8	PEG	D	387	-	6,6,6	0.64	0	5,5,5	0.64	0
6	HEC	A	500	1,13	32,50,50	1.41	5 (15%)	24,82,82	2.49	10 (41%)
6	HEC	A	600	1	32,50,50	1.51	5 (15%)	24,82,82	3.36	10 (41%)
6	HEC	B	500	1,13	32,50,50	1.93	8 (25%)	24,82,82	2.02	9 (37%)

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
10	PG4	F	387	-	-	7/10/10/10	-

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
11	P6G	F	388	-	-	10/16/16/16	-
6	HEC	B	600	1	-	2/10/54/54	-
12	MES	F	389	-	-	1/6/14/14	0/1/1/1
7	EDO	A	374	-	-	1/1/1/1	-
7	EDO	B	374	-	-	1/1/1/1	-
8	PEG	D	387	-	-	3/4/4/4	-
6	HEC	A	500	1,13	-	4/10/54/54	-
6	HEC	A	600	1	-	2/10/54/54	-
6	HEC	B	500	1,13	-	2/10/54/54	-

All (23) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
6	B	500	HEC	C2B-C3B	-6.16	1.34	1.40
12	F	389	MES	C8-S	-4.43	1.71	1.77
6	B	500	HEC	C3C-C2C	-3.49	1.37	1.40
6	A	600	HEC	C3C-C2C	-3.46	1.37	1.40
6	B	600	HEC	C2B-C3B	-3.30	1.37	1.40
6	B	500	HEC	C1D-CHD	3.22	1.49	1.41
6	B	500	HEC	C3A-C4A	3.11	1.49	1.42
6	B	500	HEC	C1B-CHB	2.91	1.49	1.41
6	A	500	HEC	C3A-C4A	2.86	1.49	1.42
6	A	500	HEC	C1D-CHD	2.72	1.48	1.41
6	B	600	HEC	C1C-CHC	2.65	1.48	1.41
6	A	600	HEC	C2B-C3B	-2.63	1.38	1.40
6	B	500	HEC	C3C-C4C	2.61	1.47	1.43
6	A	600	HEC	O1D-CGD	2.59	1.30	1.22
6	B	500	HEC	C1B-NB	-2.59	1.30	1.36
6	B	500	HEC	O2A-CGA	-2.47	1.22	1.30
6	A	600	HEC	C2A-C1A	2.46	1.48	1.42
6	A	600	HEC	C3C-C4C	2.41	1.47	1.43
6	A	500	HEC	C4B-C3B	2.32	1.47	1.43
6	A	500	HEC	O2D-CGD	-2.17	1.23	1.30
6	B	600	HEC	C2A-C1A	2.14	1.47	1.42
6	B	600	HEC	CBB-CAB	2.14	1.57	1.49
6	A	500	HEC	C1C-CHC	2.03	1.46	1.41

All (47) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
6	A	600	HEC	CBD-CAD-C3D	-9.27	96.80	112.62

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
12	F	389	MES	O1S-S-C8	8.00	116.54	106.92
6	A	600	HEC	C1D-C2D-C3D	-7.69	101.65	107.00
6	B	600	HEC	CBD-CAD-C3D	-6.19	102.06	112.62
12	F	389	MES	C5-N4-C3	6.13	122.62	108.83
12	F	389	MES	C2-C3-N4	-5.85	101.23	110.10
6	B	600	HEC	C1D-C2D-C3D	-5.83	102.94	107.00
6	A	600	HEC	CBA-CAA-C2A	-5.77	102.88	112.60
6	A	500	HEC	C2B-C3B-C4B	-4.95	101.01	106.35
6	A	600	HEC	CMD-C2D-C3D	4.88	134.14	124.94
6	A	600	HEC	CMC-C2C-C3C	4.63	131.27	125.82
6	A	500	HEC	CMC-C2C-C3C	4.59	131.22	125.82
6	B	600	HEC	CMB-C2B-C3B	4.48	131.09	125.82
6	A	500	HEC	CMB-C2B-C1B	-4.46	121.60	128.46
6	A	500	HEC	CMB-C2B-C3B	4.26	130.83	125.82
12	F	389	MES	C6-C5-N4	-4.06	103.94	110.10
6	B	500	HEC	CBD-CAD-C3D	-3.98	105.82	112.62
12	F	389	MES	O1-C2-C3	-3.93	103.13	111.80
6	B	600	HEC	CBA-CAA-C2A	-3.64	106.46	112.60
6	B	500	HEC	CBA-CAA-C2A	-3.48	106.74	112.60
6	B	500	HEC	CMB-C2B-C1B	-3.48	123.12	128.46
12	F	389	MES	O3S-S-O2S	-3.40	102.96	111.27
6	A	600	HEC	CAD-CBD-CGD	-3.37	104.31	113.76
6	B	600	HEC	O1D-CGD-CBD	-3.31	112.44	123.08
6	A	500	HEC	CMC-C2C-C1C	-3.26	123.45	128.46
6	A	500	HEC	CBD-CAD-C3D	-3.19	107.17	112.62
12	F	389	MES	C7-N4-C5	3.13	119.23	111.23
6	B	600	HEC	CMC-C2C-C3C	2.99	129.34	125.82
6	A	500	HEC	CMA-C3A-C2A	2.89	130.39	124.94
6	B	500	HEC	CMB-C2B-C3B	2.81	129.12	125.82
6	B	500	HEC	CMA-C3A-C2A	2.80	130.22	124.94
6	B	500	HEC	CMC-C2C-C3C	2.79	129.10	125.82
6	A	600	HEC	CMD-C2D-C1D	-2.77	124.21	128.46
6	B	600	HEC	CMB-C2B-C1B	-2.75	124.23	128.46
6	A	500	HEC	C3B-C4B-NB	2.74	116.11	110.94
12	F	389	MES	C7-N4-C3	2.70	118.14	111.23
6	B	500	HEC	C2B-C3B-C4B	-2.55	103.59	106.35
6	B	600	HEC	O2D-CGD-O1D	2.41	129.31	123.30
9	D	388	ACT	OXT-C-CH3	2.31	124.73	115.18
6	A	600	HEC	CMC-C2C-C1C	-2.26	124.98	128.46
6	B	500	HEC	O1D-CGD-CBD	-2.25	115.85	123.08
6	A	600	HEC	CMB-C2B-C3B	2.22	128.43	125.82
6	A	500	HEC	C4C-C3C-C2C	-2.22	103.96	106.35

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
6	B	500	HEC	O2A-CGA-CBA	2.18	121.03	114.03
6	B	600	HEC	CMD-C2D-C3D	2.16	129.01	124.94
6	A	600	HEC	CMA-C3A-C2A	2.11	128.91	124.94
6	A	500	HEC	C1D-C2D-C3D	-2.10	105.54	107.00

There are no chirality outliers.

All (33) torsion outliers are listed below:

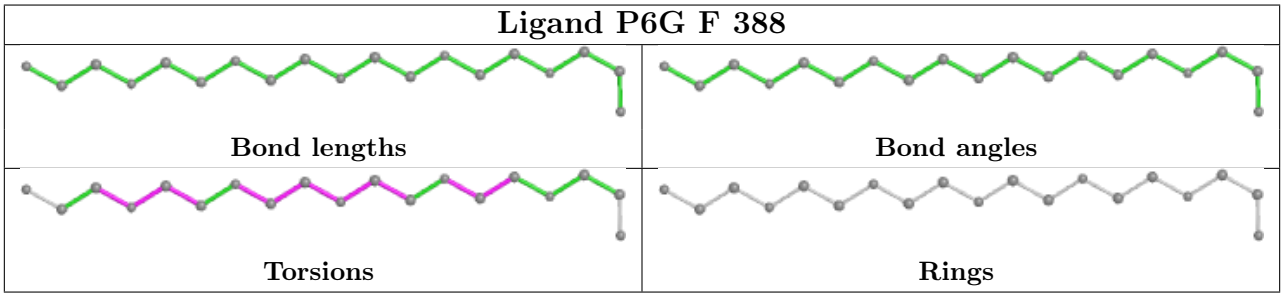
Mol	Chain	Res	Type	Atoms
11	F	388	P6G	C11-C12-O13-C14
11	F	388	P6G	C8-C9-O10-C11
10	F	387	PG4	O2-C3-C4-O3
11	F	388	P6G	O10-C11-C12-O13
8	D	387	PEG	O2-C3-C4-O4
10	F	387	PG4	O1-C1-C2-O2
10	F	387	PG4	O3-C5-C6-O4
11	F	388	P6G	C14-C15-O16-C17
7	A	374	EDO	O1-C1-C2-O2
7	B	374	EDO	O1-C1-C2-O2
12	F	389	MES	C8-C7-N4-C5
11	F	388	P6G	C5-C6-O7-C8
10	F	387	PG4	C3-C4-O3-C5
11	F	388	P6G	C18-C17-O16-C15
11	F	388	P6G	C12-C11-O10-C9
8	D	387	PEG	C1-C2-O2-C3
10	F	387	PG4	C1-C2-O2-C3
11	F	388	P6G	O7-C8-C9-O10
6	A	500	HEC	CAD-CBD-CGD-O2D
6	A	500	HEC	CAA-CBA-CGA-O2A
6	A	500	HEC	CAD-CBD-CGD-O1D
6	B	600	HEC	CAD-CBD-CGD-O2D
6	B	500	HEC	CAD-CBD-CGD-O1D
11	F	388	P6G	O13-C14-C15-O16
8	D	387	PEG	C4-C3-O2-C2
6	A	600	HEC	CAD-CBD-CGD-O1D
6	B	600	HEC	CAD-CBD-CGD-O1D
6	B	500	HEC	CAA-CBA-CGA-O2A
10	F	387	PG4	C6-C5-O3-C4
6	A	600	HEC	CAD-CBD-CGD-O2D
11	F	388	P6G	O4-C5-C6-O7
6	A	500	HEC	CAA-CBA-CGA-O1A
10	F	387	PG4	C8-C7-O4-C6

There are no ring outliers.

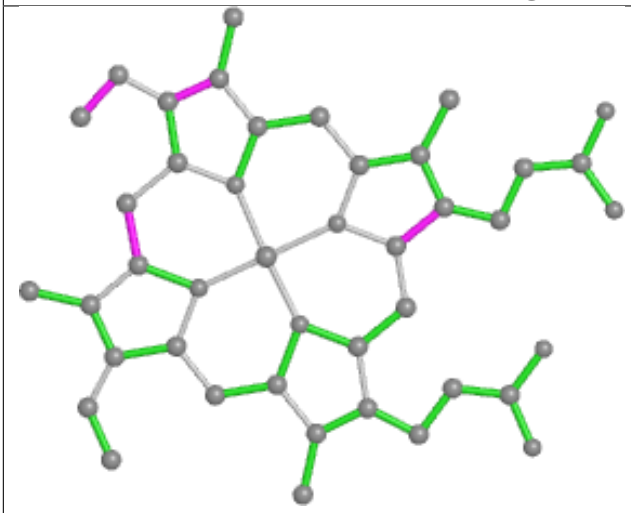
5 monomers are involved in 16 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
10	F	387	PG4	3	0
11	F	388	P6G	6	0
6	B	600	HEC	2	0
8	D	387	PEG	3	0
6	A	600	HEC	2	0

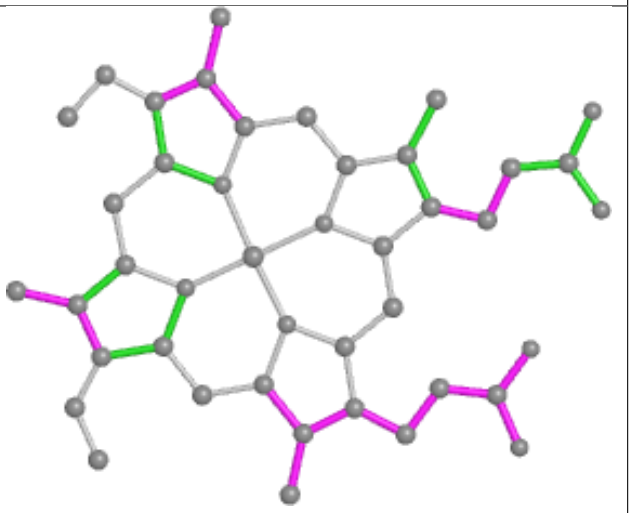
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. 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.



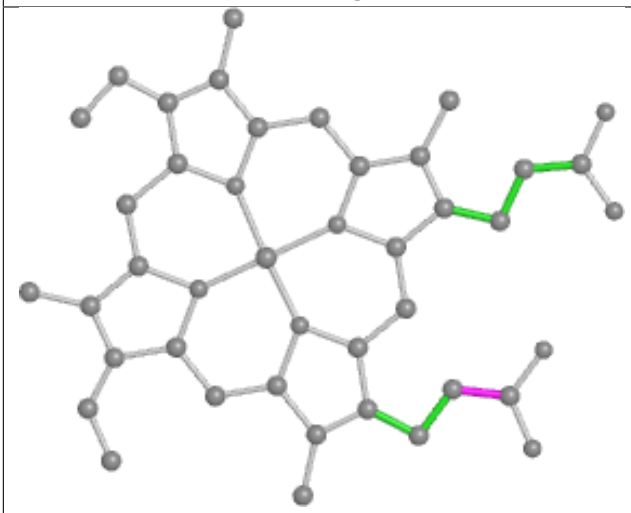
Ligand HEC B 600



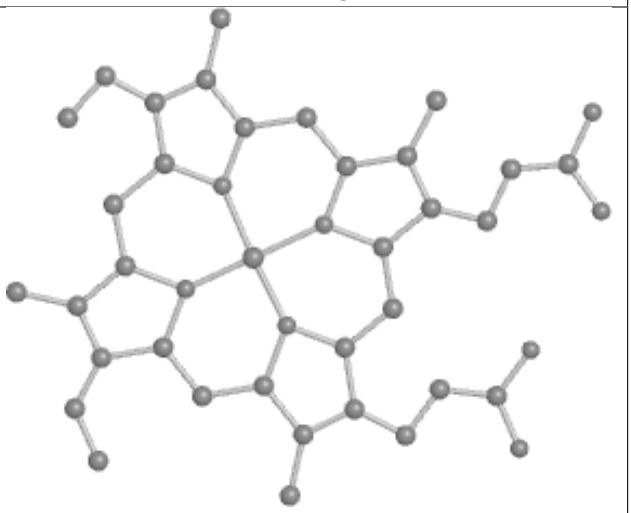
Bond lengths



Bond angles

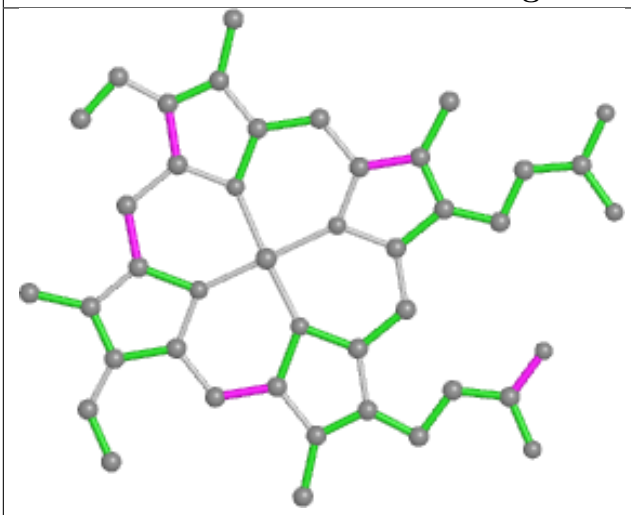


Torsions

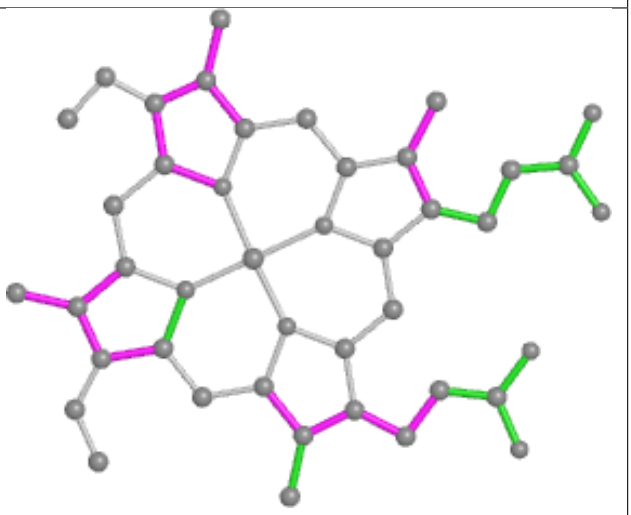


Rings

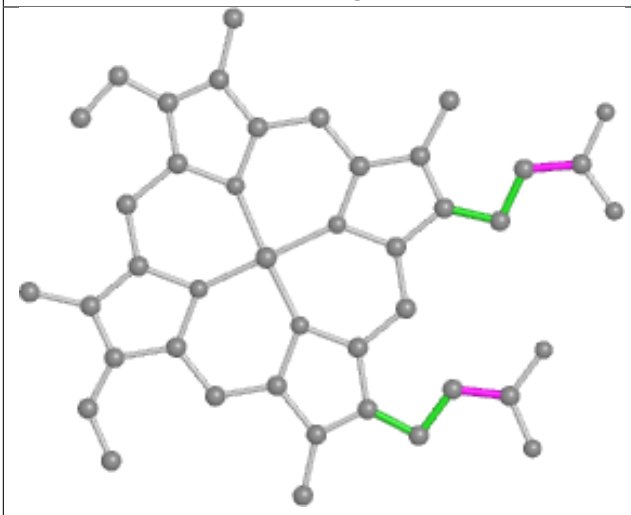
Ligand HEC A 500



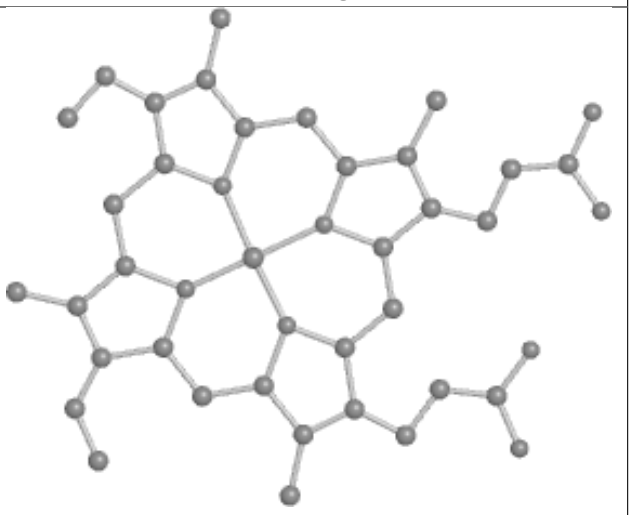
Bond lengths



Bond angles

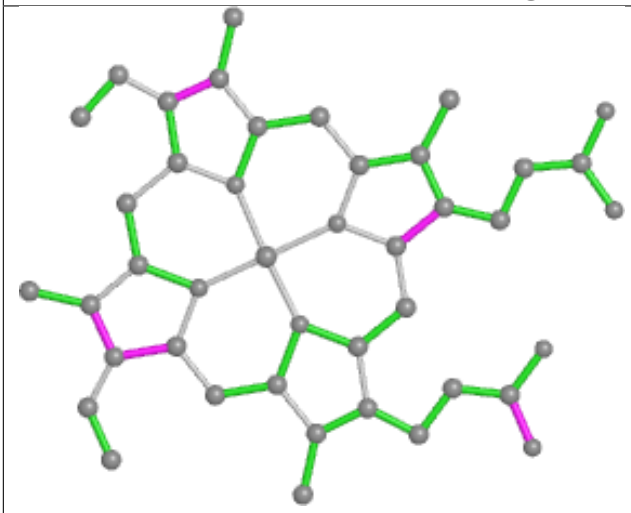


Torsions

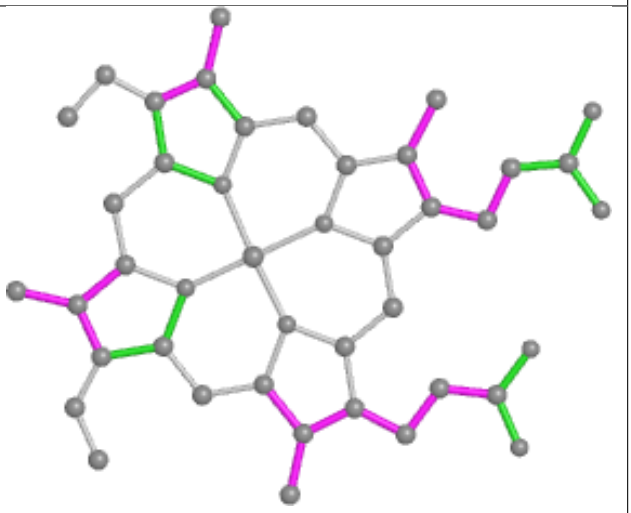


Rings

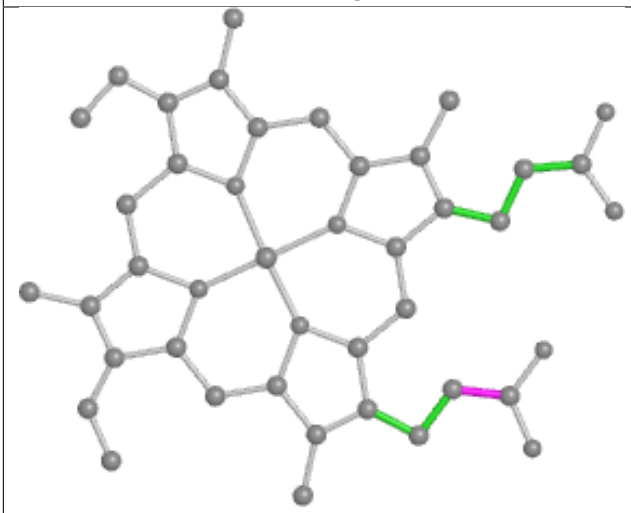
Ligand HEC A 600



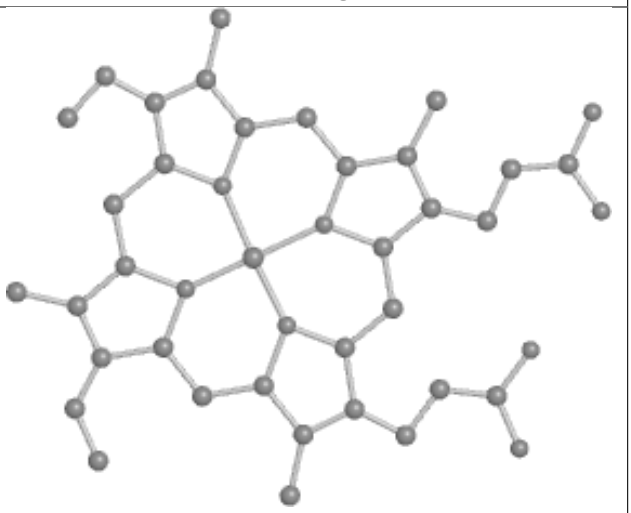
Bond lengths



Bond angles

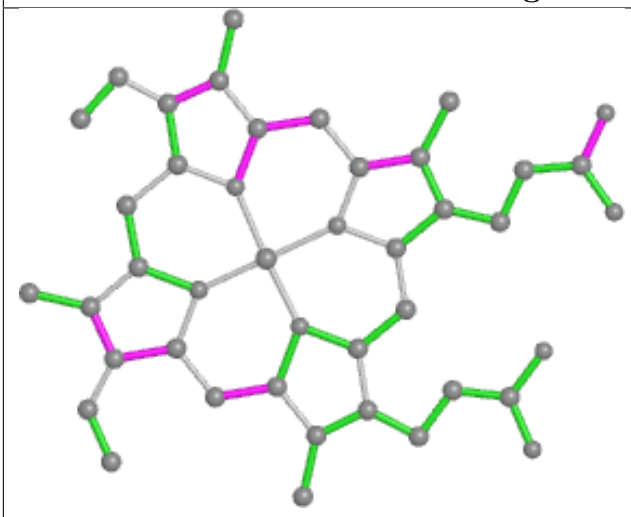


Torsions

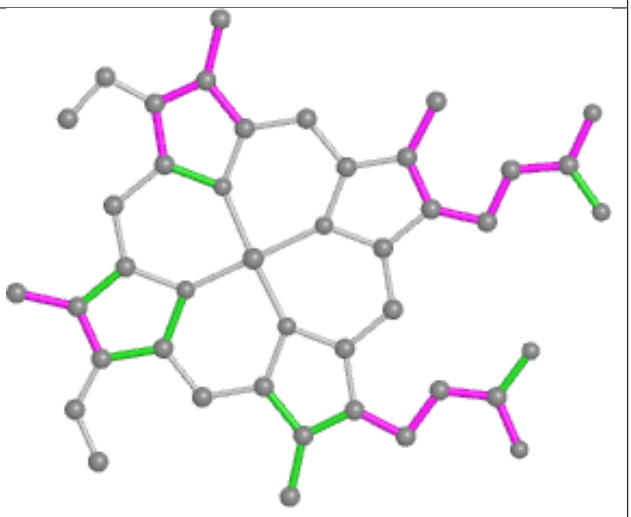


Rings

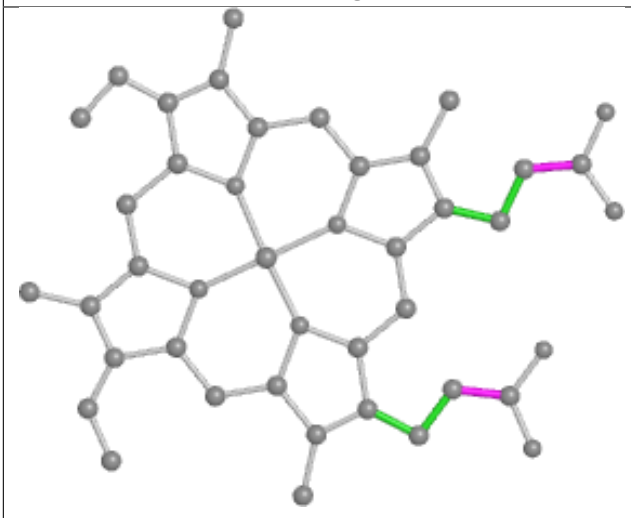
Ligand HEC B 500



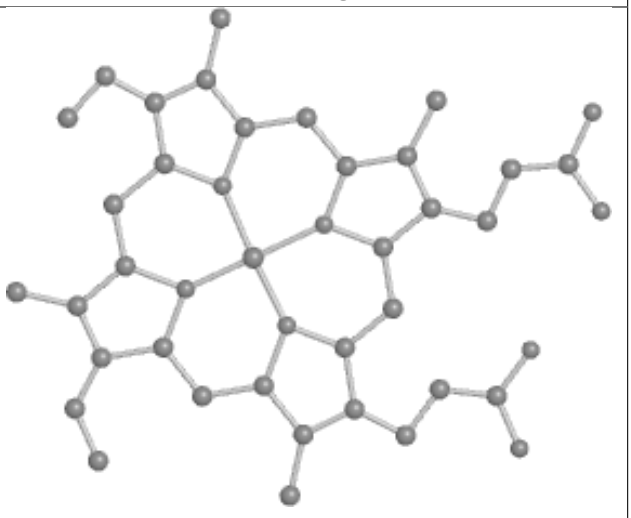
Bond lengths



Bond angles



Torsions



Rings

5.7 Other polymers (i)

There are no such residues in this entry.

5.8 Polymer linkage issues (i)

There are no chain breaks in this entry.

6 Fit of model and data

6.1 Protein, DNA and RNA chains

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

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å^2)	Q<0.9
1	A	354/373 (94%)	-0.53	4 (1%) 80 84	12, 19, 32, 52	0
1	B	355/373 (95%)	-0.48	3 (0%) 86 89	11, 20, 34, 56	0
2	C	130/137 (94%)	-0.18	2 (1%) 73 78	12, 17, 31, 44	0
2	E	123/137 (89%)	-0.29	0 100 100	11, 15, 25, 40	0
3	D	376/386 (97%)	-0.41	5 (1%) 77 81	12, 20, 36, 60	0
3	F	376/386 (97%)	-0.45	5 (1%) 77 81	10, 15, 28, 49	0
All	All	1714/1792 (95%)	-0.43	19 (1%) 80 84	10, 18, 33, 60	0

All (19) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	6	ALA	6.8
1	A	7	ASP	5.2
1	B	6	ALA	5.2
3	D	208	THR	5.1
1	B	7	ASP	4.8
3	D	11	GLN	3.9
3	F	11	GLN	3.2
3	D	207	GLY	3.1
1	B	8	ASP	2.8
3	D	209	GLU	2.6
3	F	207	GLY	2.5
2	C	7	THR	2.5
3	D	211	THR	2.4
1	A	214	GLU	2.1
3	F	30	GLN	2.1
1	A	8	ASP	2.1
2	C	106	ILE	2.1
3	F	27	ALA	2.0
3	F	208	THR	2.0

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

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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
2	0AF	C	57	15/16	0.97	0.11	17,19,22,23	0
2	0AF	E	57	15/16	0.98	0.10	13,15,18,20	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, 95^{th} percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

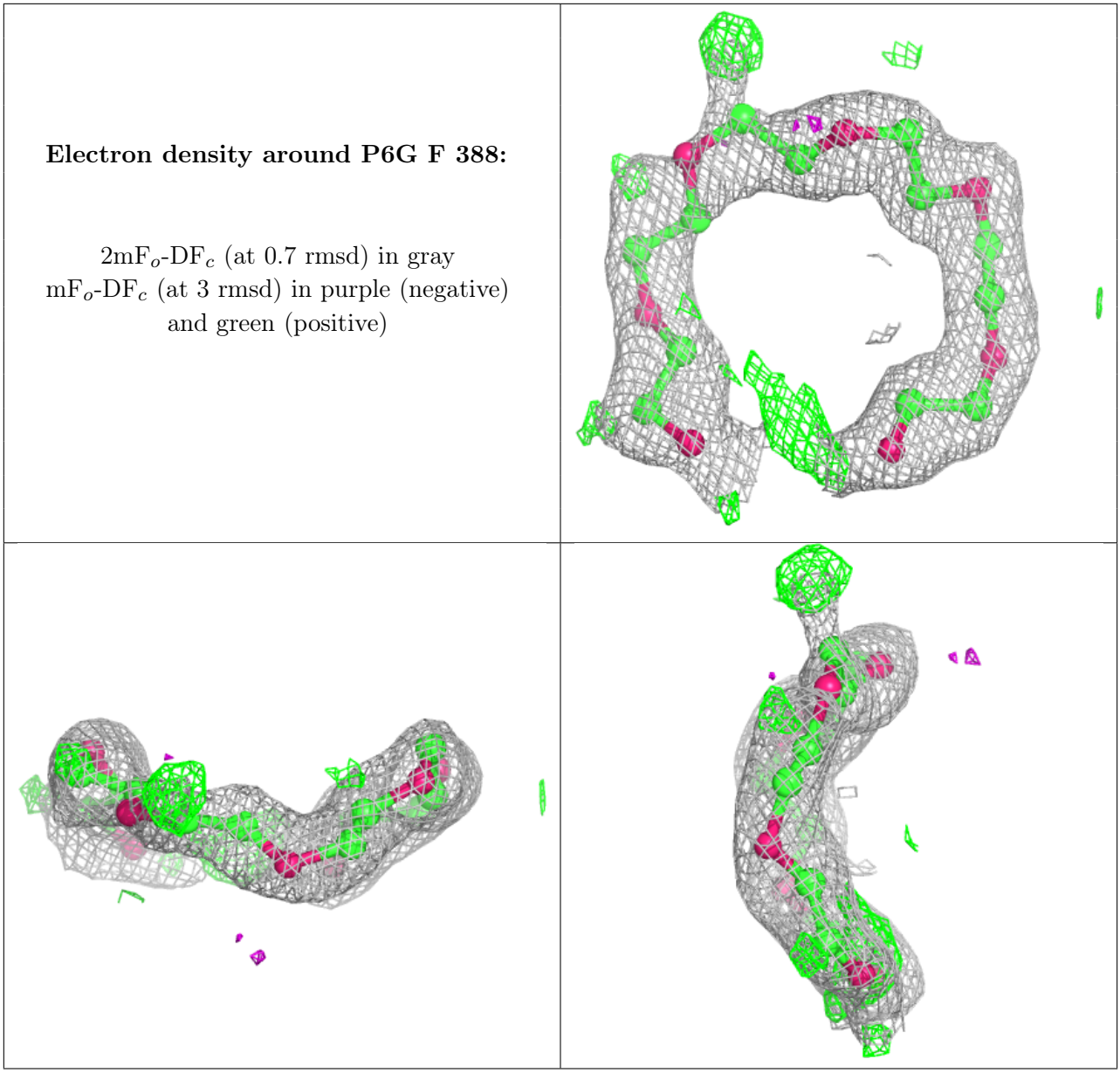
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
8	PEG	D	387	7/7	0.83	0.12	53,54,55,56	0
10	PG4	F	387	13/13	0.87	0.12	51,55,62,63	0
7	EDO	A	374	4/4	0.91	0.12	40,43,43,46	0
7	EDO	B	374	4/4	0.92	0.07	36,40,41,43	0
11	P6G	F	388	19/19	0.92	0.10	20,33,52,53	0
12	MES	F	389	12/12	0.93	0.15	14,31,38,38	12
9	ACT	D	388	4/4	0.97	0.07	26,27,30,31	0
6	HEC	B	500	43/43	0.98	0.07	11,14,17,19	0
5	NA	A	402	1/1	0.99	0.08	26,26,26,26	0
5	NA	B	401	1/1	0.99	0.03	22,22,22,22	0
5	NA	B	402	1/1	0.99	0.06	24,24,24,24	0
6	HEC	A	500	43/43	0.99	0.06	11,15,18,21	0
6	HEC	A	600	43/43	0.99	0.08	9,12,15,16	0
5	NA	A	401	1/1	0.99	0.05	23,23,23,23	0
6	HEC	B	600	43/43	0.99	0.08	7,11,14,16	0
4	CA	B	400	1/1	1.00	0.07	13,13,13,13	0
4	CA	A	400	1/1	1.00	0.08	14,14,14,14	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.

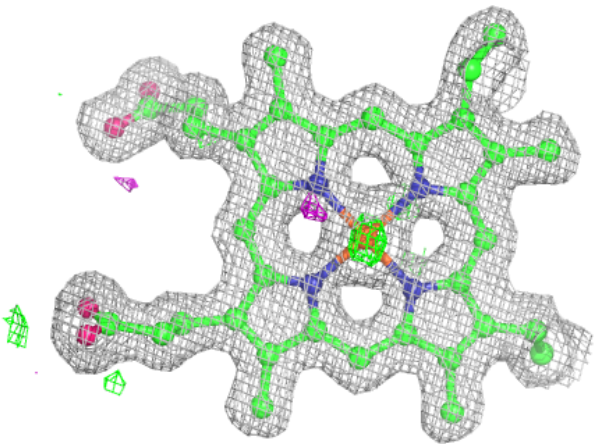
Electron density around P6G F 388:

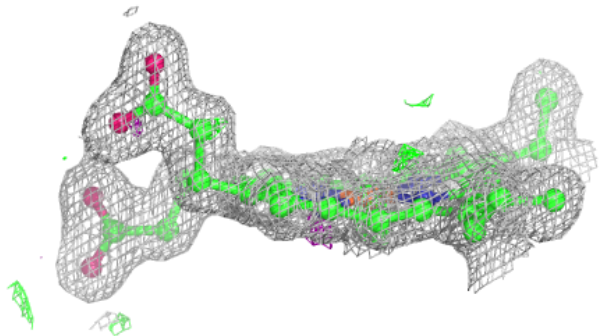
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

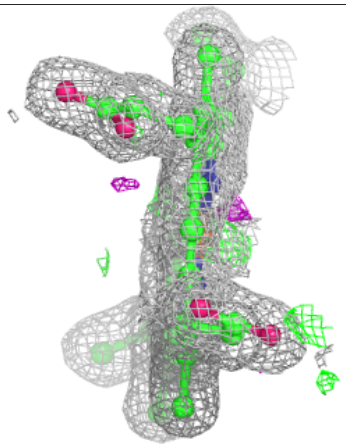


Electron density around HEC B 500:

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

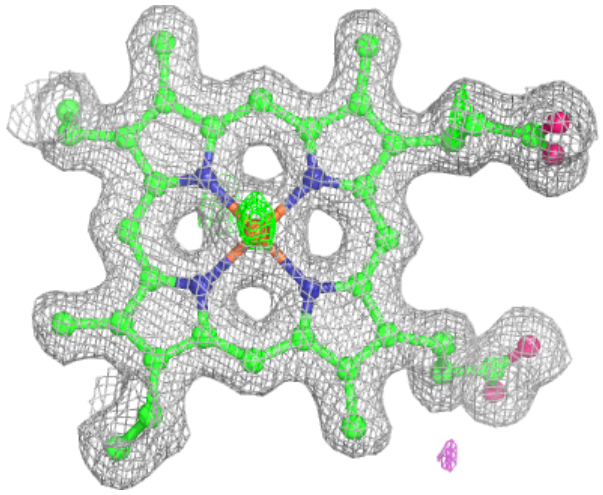


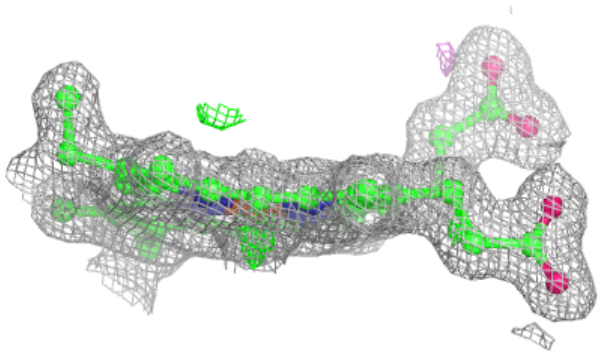


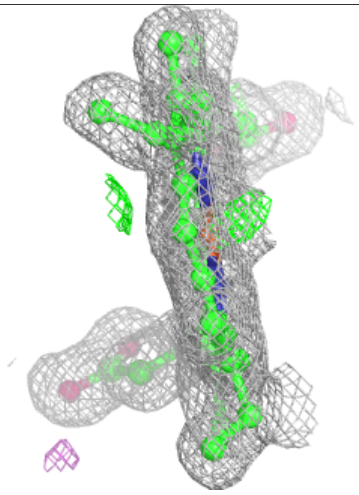


Electron density around HEC A 500:

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

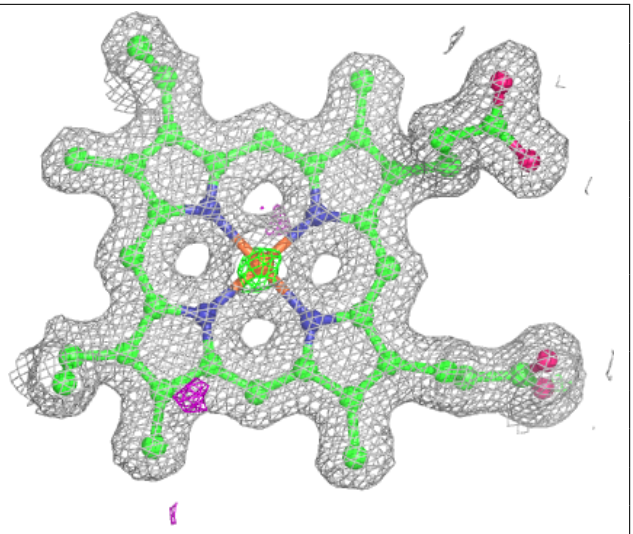


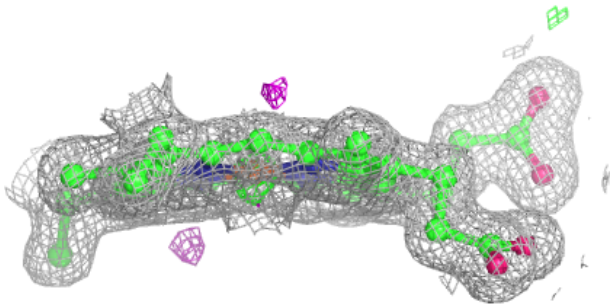


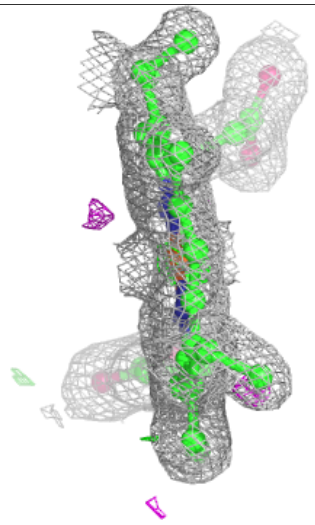


Electron density around HEC A 600:

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

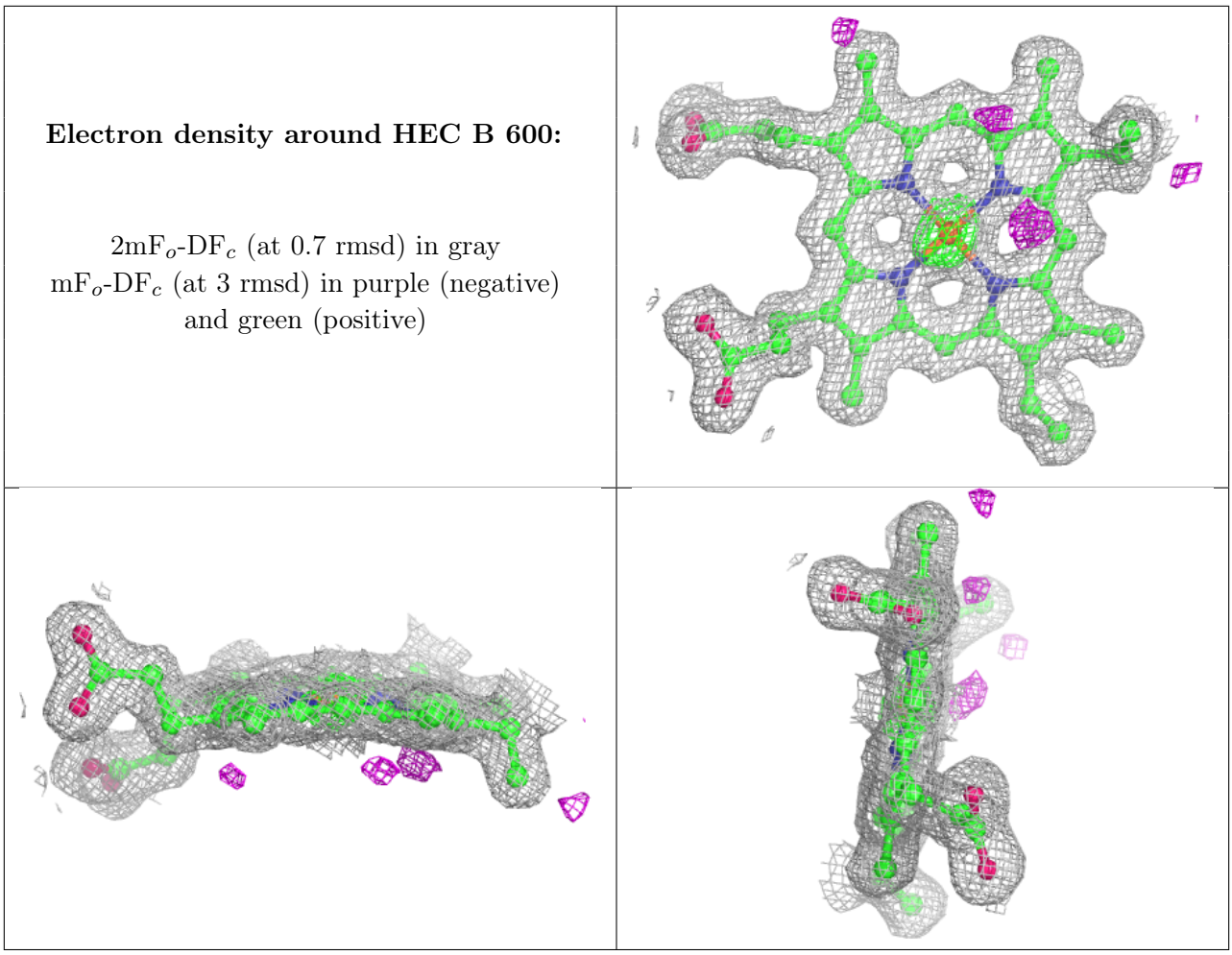






Electron density around HEC B 600:

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



6.5 Other polymers

There are no such residues in this entry.