



wwPDB X-ray Structure Validation Summary Report ⓘ

Aug 5, 2026 – 09:19 PM EDT

PDB ID : 3RLM / pdb_00003rlm
Title : Structure of the W199F MauG/pre-Methylamine Dehydrogenase complex after treatment with hydrogen peroxide
Authors : Yukl, E.T.; Wilmot, C.M.
Deposited on : 2011-04-19
Resolution : 2.13 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 ⓘ 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 : 4-5-2 with Phenix2.0
Mogul : 2022.3.0, CSD as543be (2022)
Xtriage (Phenix) : 2.0
EDS : 3.0
Buster-report : wwPDB partial adaption of 1.1.7 (2018)
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)
CCP4 : 9.0.015 (Gargrove)
Density-Fitness : 1.0.12
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.50

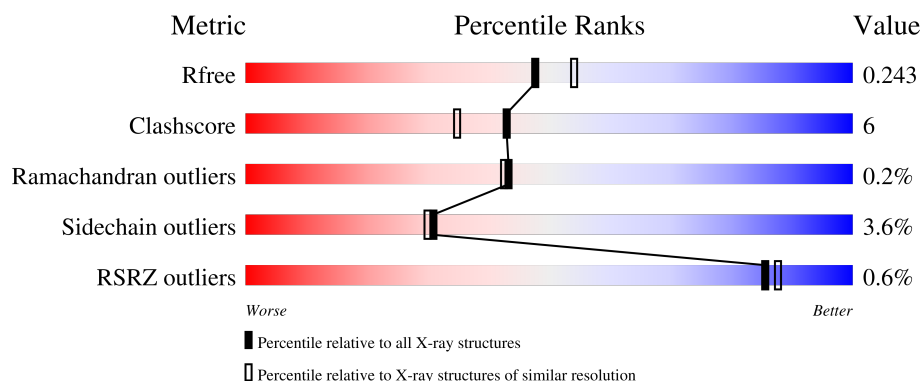
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.13 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}	180053	3689 (2.16-2.12)
Clashscore	190562	3812 (2.16-2.12)
Ramachandran outliers	187476	3773 (2.16-2.12)
Sidechain outliers	187428	3772 (2.16-2.12)
RSRZ outliers	180081	3691 (2.16-2.12)

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 $\leq 5\%$. 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	% 81% 14% 5%
1	B	373	79% 16% 5%
2	C	137	3% 77% 16% ...
2	E	137	67% 23% 9%
3	D	386	% 81% 16% .

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Mol	Chain	Length	Quality of chain
3	F	386	 86% 11%

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
5	HEC	A	500	X	-	-	-
5	HEC	A	600	X	-	-	-
5	HEC	B	500	X	-	-	-
5	HEC	B	600	X	-	-	-

2 Entry composition

There are 8 unique types of molecules in this entry. The entry contains 14548 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	3	0
			2757	1720	495	531	11			
1	B	355	Total	C	N	O	S	0	3	0
			2773	1728	502	532	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	2	0
			1023	632	179	198	14			
2	E	125	Total	C	N	O	S	0	2	0
			960	594	161	190	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

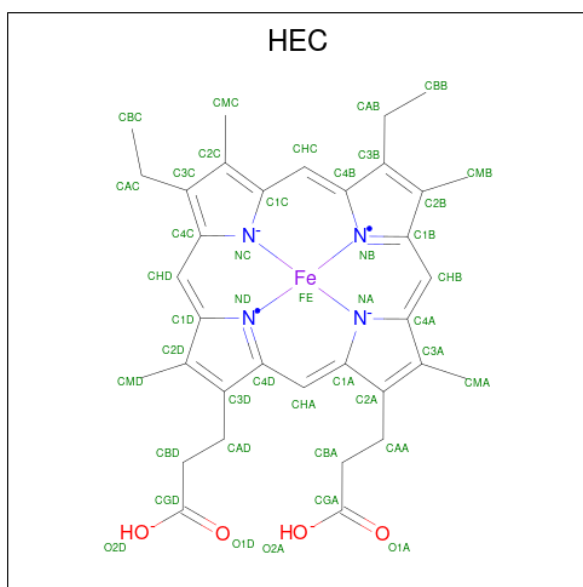
- Molecule 3 is a protein called Methylamine dehydrogenase heavy chain.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	D	376	Total	C	N	O	S	0	1	0
			2934	1859	506	561	8			
3	F	376	Total	C	N	O	S	0	3	0
			2941	1865	504	563	9			

- Molecule 4 is CALCIUM ION (CCD ID: CA) (formula: Ca).

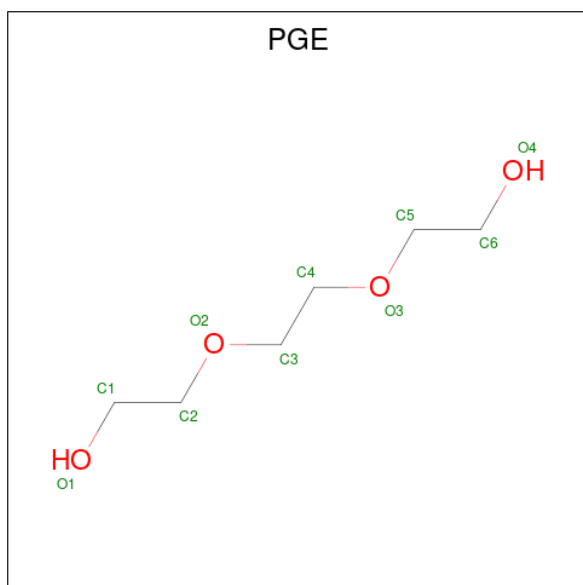
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	1	Total	Ca	0	0
			1	1		
4	B	1	Total	Ca	0	0
			1	1		

- Molecule 5 is HEME C (CCD ID: HEC) (formula: C₃₄H₃₆FeN₄O₄).



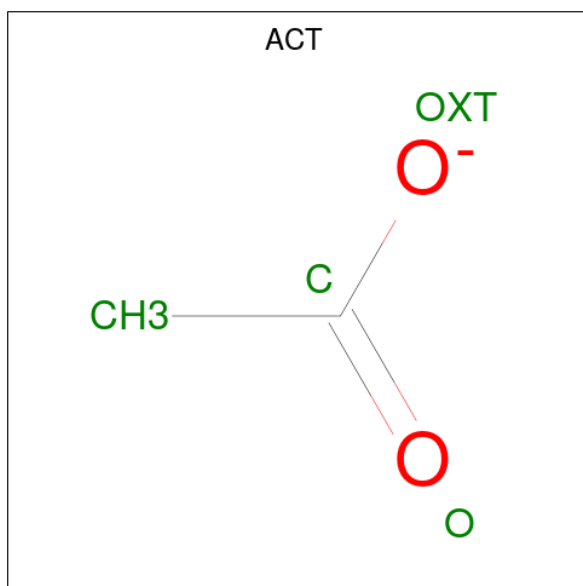
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
5	A	1	Total 43	C 34	Fe 1	N 4	O 4	0	0
5	A	1	Total 43	C 34	Fe 1	N 4	O 4	0	0
5	B	1	Total 43	C 34	Fe 1	N 4	O 4	0	0
5	B	1	Total 43	C 34	Fe 1	N 4	O 4	0	0

- Molecule 6 is TRIETHYLENE GLYCOL (CCD ID: PGE) (formula: $C_6H_{14}O_4$).



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

- Molecule 7 is ACETATE ION (CCD ID: ACT) (formula: $C_2H_3O_2$).



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

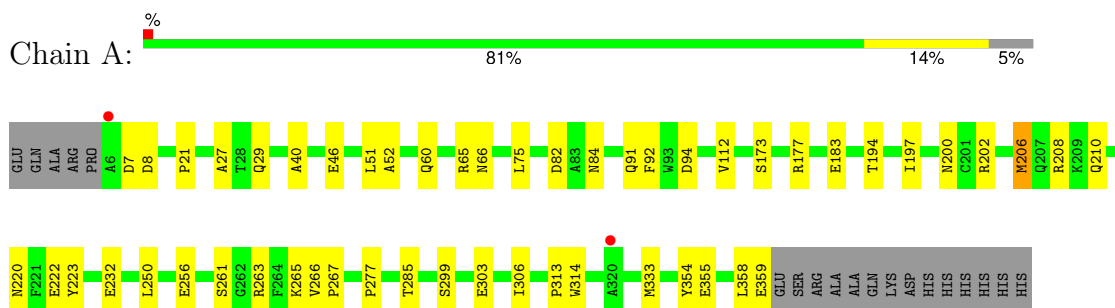
- Molecule 8 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
8	A	146	Total	O	0	1
			147	147		
8	B	219	Total	O	0	1
			220	220		
8	C	59	Total	O	0	0
			59	59		
8	D	168	Total	O	0	0
			168	168		
8	E	80	Total	O	0	0
			80	80		
8	F	294	Total	O	0	0
			294	294		

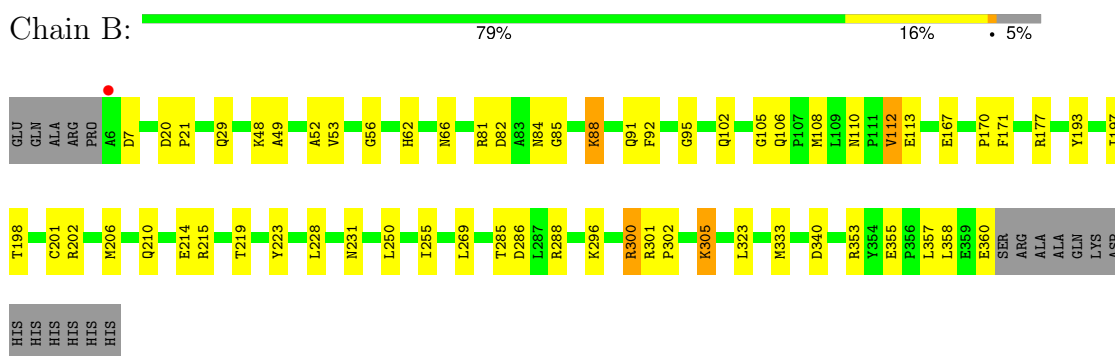
3 Residue-property plots [i](#)

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.

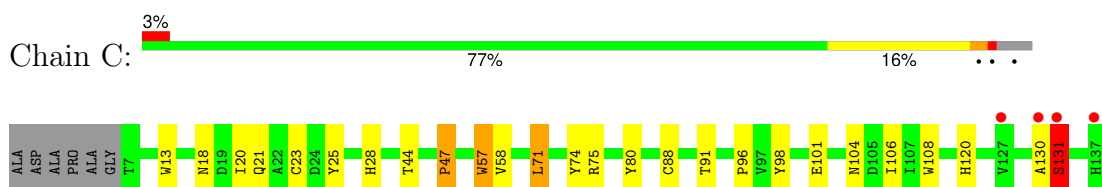
- Molecule 1: Methylamine utilization protein MauG



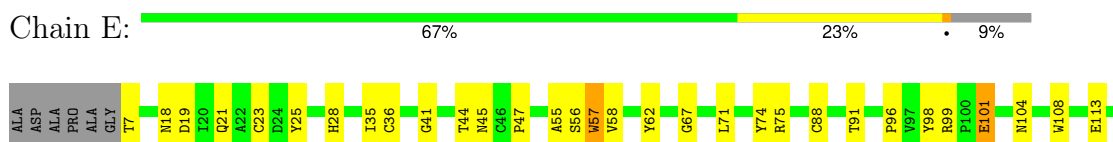
- Molecule 1: Methylamine utilization protein MauG



- Molecule 2: Methylamine dehydrogenase light chain

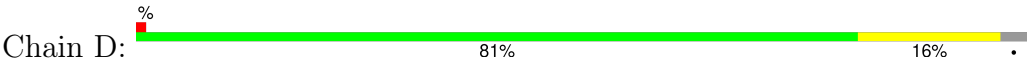


- Molecule 2: Methylamine dehydrogenase light chain



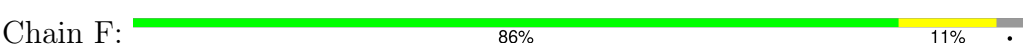
C121	
S131	
HIS	
HIS	
HIS	
HIS	
HIS	

● Molecule 3: Methylamine dehydrogenase heavy chain



GLN	ASP	ALA	PRO	GLU	ALA	GLU	THR	GLN	ALA	Q11	Q14	Q15	Q16	R20	P42	N50	D51	P52	A53	A56	N82	V85	I92	S96	I102	Y110	F114	D115	P116	V117	L127	F133	T137	T142	D177	V178	P179	D180	C181	Y182	G207				
T208	T211	I214	E218	E223	A237	G238	R239	L240	V241	L262	P263	A264	V265	R270	R273	A274	D275	G276	W277	R278	P279	G280	Q283	A286	R289	Y295	L296	L297	Q300	R301	H306	K307	S310	K319	T320	G321	S335	I336	Y347	A348	L349				
L356	P377	Q378	V379	G386																																									

● Molecule 3: Methylamine dehydrogenase heavy chain



GLN	ASP	ALA	PRO	GLU	ALA	GLU	THR	GLN	ALA	Q11	E12	T13	Q14	G15	Q16	R20	R45	D51	N82	I102	A103	D115	P116	V117	T118	L119	T142	F153	P160	G163	R174	P179	Y182	V204	G207	I214	I228	P243	I249																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																														
L254	A259	L262	A267	G280	A286	L297	R301	H306	S310	L316	H331	L345	L346	Y347	K354	T355	L356	E366	P377	G386																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																	</

4 Data and refinement statistics

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 – 2.13 44.49 – 2.13	Depositor EDS
% Data completeness (in resolution range)	95.4 (44.49-2.13) 95.4 (44.49-2.13)	Depositor EDS
R_{merge}	0.07	Depositor
R_{sym}	0.07	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.25 (at 2.14Å)	Xtriage
Refinement program	REFMAC 5.5.0109	Depositor
R, R_{free}	0.181 , 0.237 0.190 , 0.243	Depositor DCC
R_{free} test set	4676 reflections (4.82%)	wwPDB-VP
Wilson B-factor (Å ²)	31.0	Xtriage
Anisotropy	0.115	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.32 , 34.9	EDS
L-test for twinning ²	$\langle L \rangle = 0.50$, $\langle L^2 \rangle = 0.33$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.96	EDS
Total number of atoms	14548	wwPDB-VP
Average B, all atoms (Å ²)	36.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.88% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

²Theoretical values of $\langle |L| \rangle$, $\langle L^2 \rangle$ 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: PGE, CA, HEC, ACT, 0AF

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

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
1	A	0.62	0/2823	0.88	2/3828 (0.1%)
1	B	0.68	0/2836	0.91	0/3844
2	C	0.64	0/1044	0.93	2/1425 (0.1%)
2	E	0.80	0/975	0.92	1/1331 (0.1%)
3	D	0.63	0/3011	0.83	1/4102 (0.0%)
3	F	0.77	0/3024	0.90	0/4119
All	All	0.69	0/13713	0.89	6/18649 (0.0%)

There are no bond length outliers.

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

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	C	47	PRO	O-C-N	5.85	123.90	121.15
2	C	104	ASN	N-CA-C	5.66	120.92	112.94
1	A	200	ASN	N-CA-C	5.61	119.63	112.34
2	E	104	ASN	N-CA-C	5.28	119.28	112.41
3	D	137	THR	N-CA-C	5.15	117.16	109.59

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	2757	0	2632	27	1
1	B	2773	0	2649	39	0
2	C	1023	0	912	23	0
2	E	960	0	869	28	0
3	D	2934	0	2820	37	0
3	F	2941	0	2830	22	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	3	0
6	B	10	0	14	0	0
7	D	4	0	3	0	0
7	F	4	0	3	0	0
8	A	147	0	0	3	0
8	B	220	0	0	10	1
8	C	59	0	0	1	0
8	D	168	0	0	1	0
8	E	80	0	0	4	0
8	F	294	0	0	1	0
All	All	14548	0	12852	163	1

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 6.

The worst 5 of 163 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:C:130:ALA:HA	2:C:131:SER:HB3	1.27	1.09
3:D:273[A]:ARG:HH11	3:D:273[A]:ARG:HG3	1.08	1.07
3:D:273[A]:ARG:HH11	3:D:273[A]:ARG:CG	1.69	1.03
2:E:36[B]:CYS:SG	2:E:41:GLY:HA3	2.08	0.94
2:C:130:ALA:CA	2:C:131:SER:HB3	2.02	0.89

All (1) symmetry-related close contacts are listed below. The label for Atom-2 includes the symmetry operator and encoded unit-cell translations to be applied.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:46[A]:GLU:OE2	8:B:586:HOH:O[1_544]	2.12	0.08

5.3 Torsion angles

5.3.1 Protein backbone

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	355/373 (95%)	345 (97%)	10 (3%)	0	100	100
1	B	356/373 (95%)	345 (97%)	11 (3%)	0	100	100
2	C	130/137 (95%)	119 (92%)	10 (8%)	1 (1%)	16	9
2	E	124/137 (90%)	119 (96%)	5 (4%)	0	100	100
3	D	375/386 (97%)	358 (96%)	15 (4%)	2 (0%)	24	19
3	F	377/386 (98%)	364 (97%)	12 (3%)	1 (0%)	36	33
All	All	1717/1792 (96%)	1650 (96%)	63 (4%)	4 (0%)	43	42

All (4) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
2	C	131	SER
3	D	102	ILE
3	F	102	ILE
3	D	207	GLY

5.3.2 Protein sidechains

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	279/292 (96%)	266 (95%)	13 (5%)	23	19
1	B	280/292 (96%)	266 (95%)	14 (5%)	22	17
2	C	112/112 (100%)	109 (97%)	3 (3%)	39	41

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
2	E	106/112 (95%)	103 (97%)	3 (3%)	38	39
3	D	305/311 (98%)	293 (96%)	12 (4%)	28	26
3	F	307/311 (99%)	301 (98%)	6 (2%)	48	53
All	All	1389/1430 (97%)	1338 (96%)	51 (4%)	31	29

5 of 51 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
2	C	71	LEU
3	D	218	GLU
3	F	316	LEU
2	C	131	SER
3	D	127	LEU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 23 such sidechains are listed below:

Mol	Chain	Res	Type
3	D	359	HIS
3	F	11	GLN
2	E	68	GLN
3	F	14	GLN
1	B	91	GLN

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

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	15,16,17	1.17	1 (6%)	14,22,24	1.07	0
2	0AF	C	57	2	15,16,17	1.34	3 (20%)	14,22,24	0.98	1 (7%)

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	0AF	E	57	2	-	0/5/6/8	0/2/2/2
2	0AF	C	57	2	-	1/5/6/8	0/2/2/2

All (4) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	C	57	0AF	CD2-CG	-2.92	1.39	1.44
2	C	57	0AF	CD2-CE2	-2.43	1.38	1.41
2	E	57	0AF	CD2-CE2	-2.22	1.38	1.41
2	C	57	0AF	CE2-NE1	-2.07	1.34	1.37

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	C	57	0AF	CE3-CD2-CG	-2.24	130.51	133.85

There are no chirality outliers.

All (1) torsion outliers are listed below:

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

There are no ring outliers.

2 monomers are involved in 3 short contacts:

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

5.5 Carbohydrates [i](#)

There are no oligosaccharides 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	8,1	50,50,50	2.65	27 (54%)	68,82,82	1.93	24 (35%)
5	HEC	B	500	8,1	50,50,50	2.64	25 (50%)	68,82,82	1.99	24 (35%)
7	ACT	F	387	-	3,3,3	0.74	0	3,3,3	1.49	0
7	ACT	D	387	-	3,3,3	0.88	0	3,3,3	1.39	0
5	HEC	B	600	1	50,50,50	2.44	22 (44%)	68,82,82	2.01	23 (33%)
6	PGE	B	374	-	9,9,9	0.55	0	8,8,8	0.46	0
5	HEC	A	600	1	50,50,50	2.63	23 (46%)	68,82,82	1.92	23 (33%)

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	8,1	1/1/3/7	3/14/54/54	-
5	HEC	B	500	8,1	1/1/3/7	4/14/54/54	-
5	HEC	B	600	1	1/1/3/7	4/14/54/54	-
6	PGE	B	374	-	-	5/7/7/7	-
5	HEC	A	600	1	1/1/3/7	4/14/54/54	-

The worst 5 of 97 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
5	B	500	HEC	FE-ND	5.38	2.11	1.94

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
5	B	500	HEC	CHA-C1A	5.31	1.48	1.38
5	A	600	HEC	CHC-C4B	5.23	1.49	1.38
5	B	500	HEC	CHD-C1D	5.21	1.48	1.38
5	A	500	HEC	CHC-C4B	5.19	1.48	1.38

The worst 5 of 94 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	B	500	HEC	C3D-C4D-ND	5.10	115.28	110.35
5	B	600	HEC	C3C-C4C-NC	4.93	115.62	110.15
5	B	600	HEC	C2D-C1D-ND	4.61	115.14	109.84
5	B	500	HEC	C3B-C4B-NB	4.46	115.06	110.17
5	A	500	HEC	C2D-C1D-ND	4.35	114.83	109.84

All (4) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
5	A	500	HEC	NA
5	A	600	HEC	NA
5	B	500	HEC	NA
5	B	600	HEC	NA

5 of 20 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
6	B	374	PGE	C1-C2-O2-C3
5	B	600	HEC	C2C-C3C-CAC-CBC
5	B	600	HEC	C4C-C3C-CAC-CBC
5	A	500	HEC	C2C-C3C-CAC-CBC
6	B	374	PGE	O3-C5-C6-O4

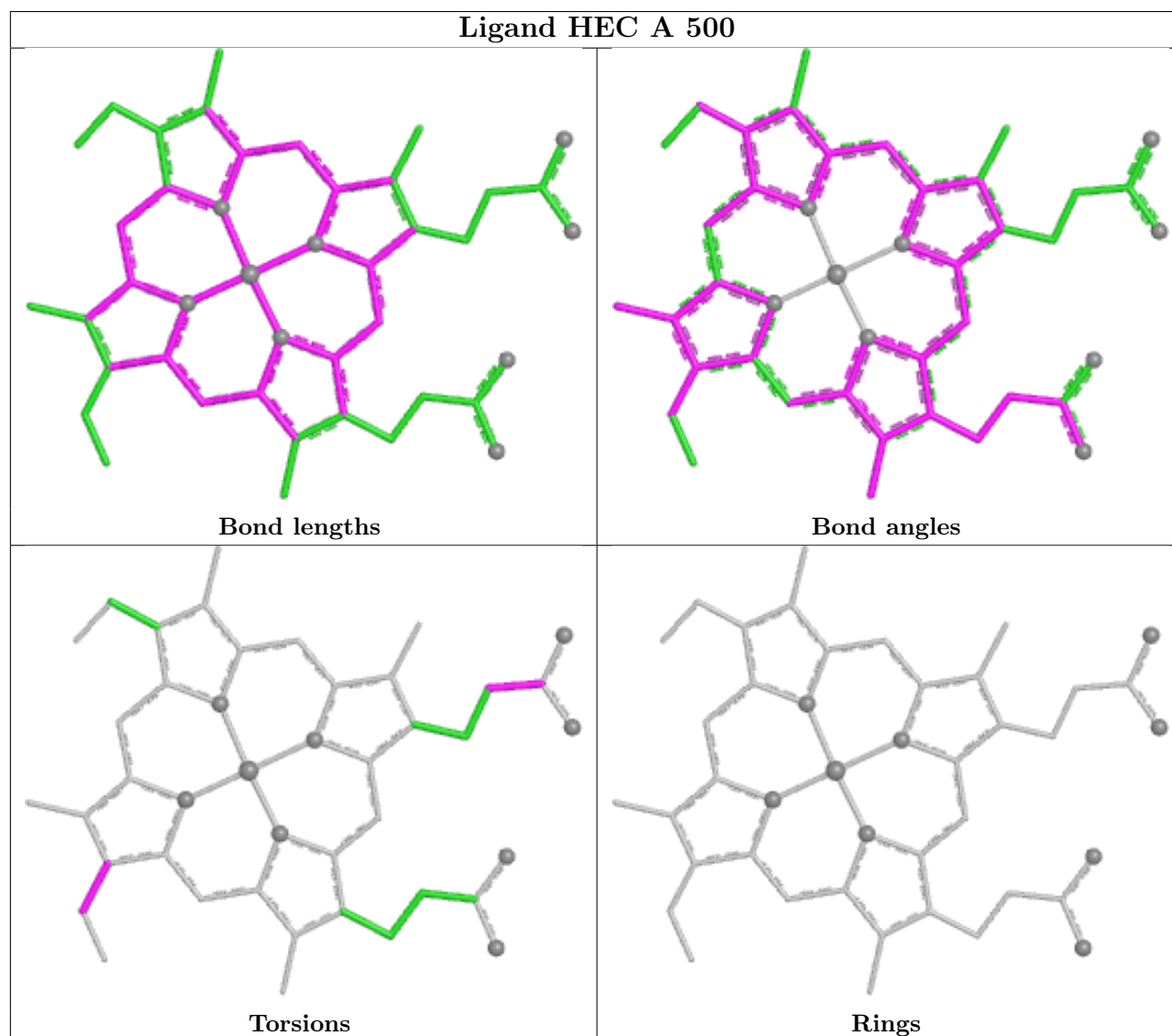
There are no ring outliers.

4 monomers are involved in 5 short contacts:

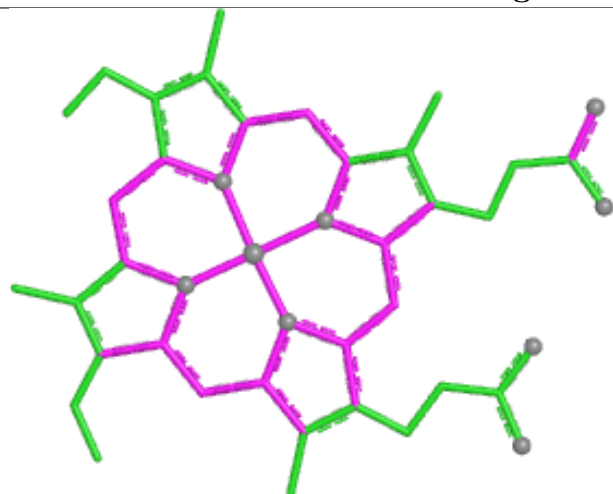
Mol	Chain	Res	Type	Clashes	Symm-Clashes
5	A	500	HEC	1	0
5	B	500	HEC	2	0
5	B	600	HEC	1	0
5	A	600	HEC	1	0

The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths,

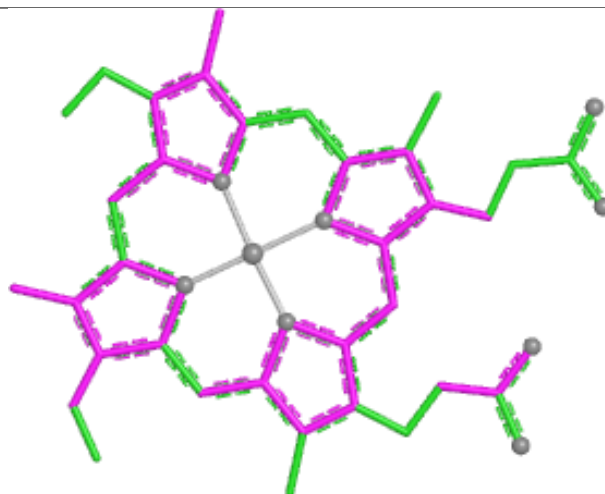
bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. For torsion angles, if less than 5% of the Mogul distribution of torsion angles is within 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.



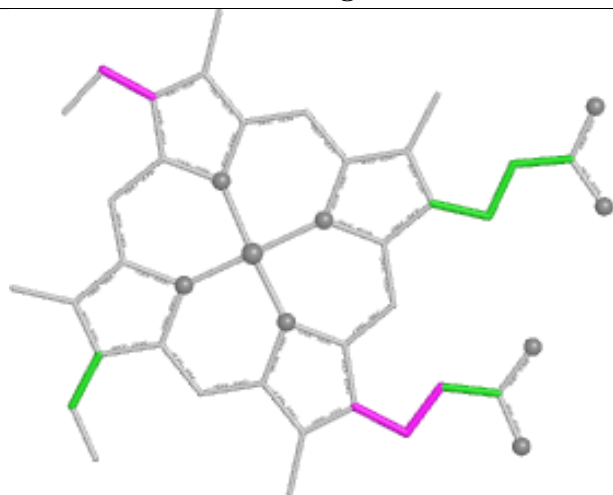
Ligand HEC B 500



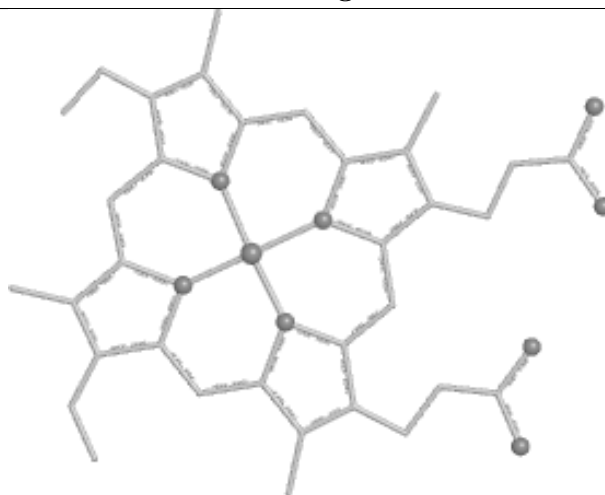
Bond lengths



Bond angles

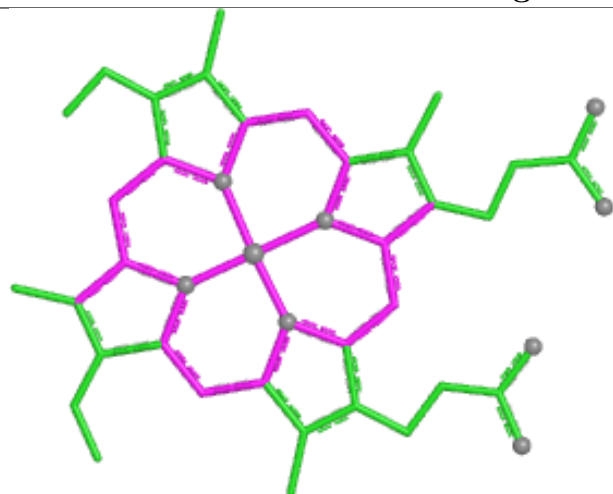


Torsions

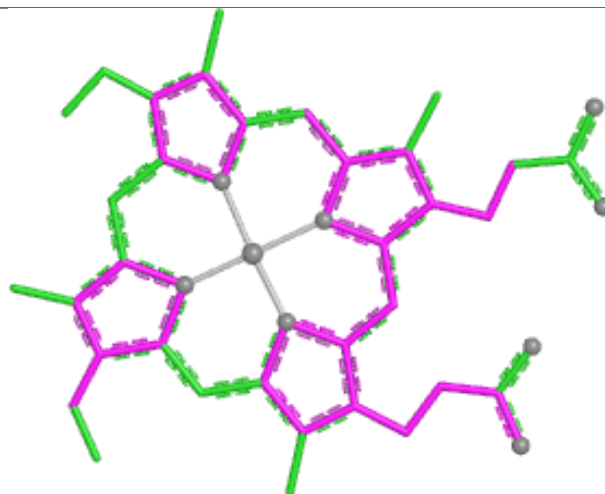


Rings

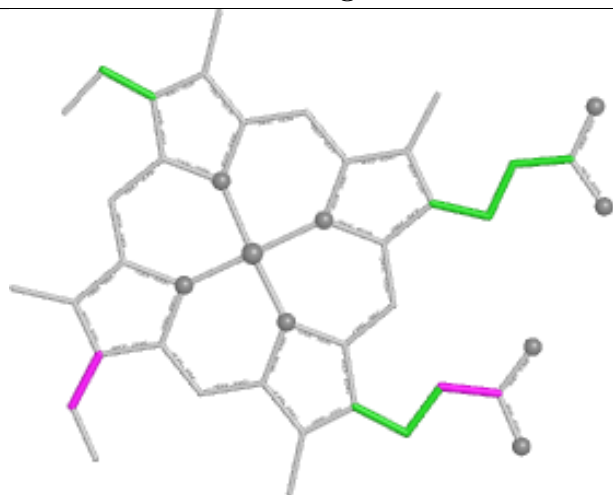
Ligand HEC B 600



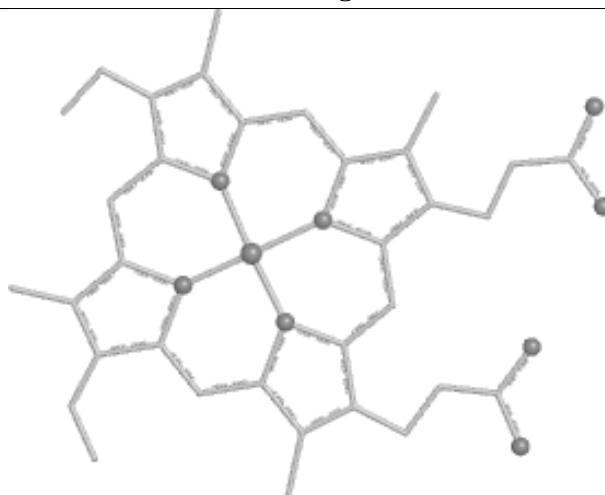
Bond lengths



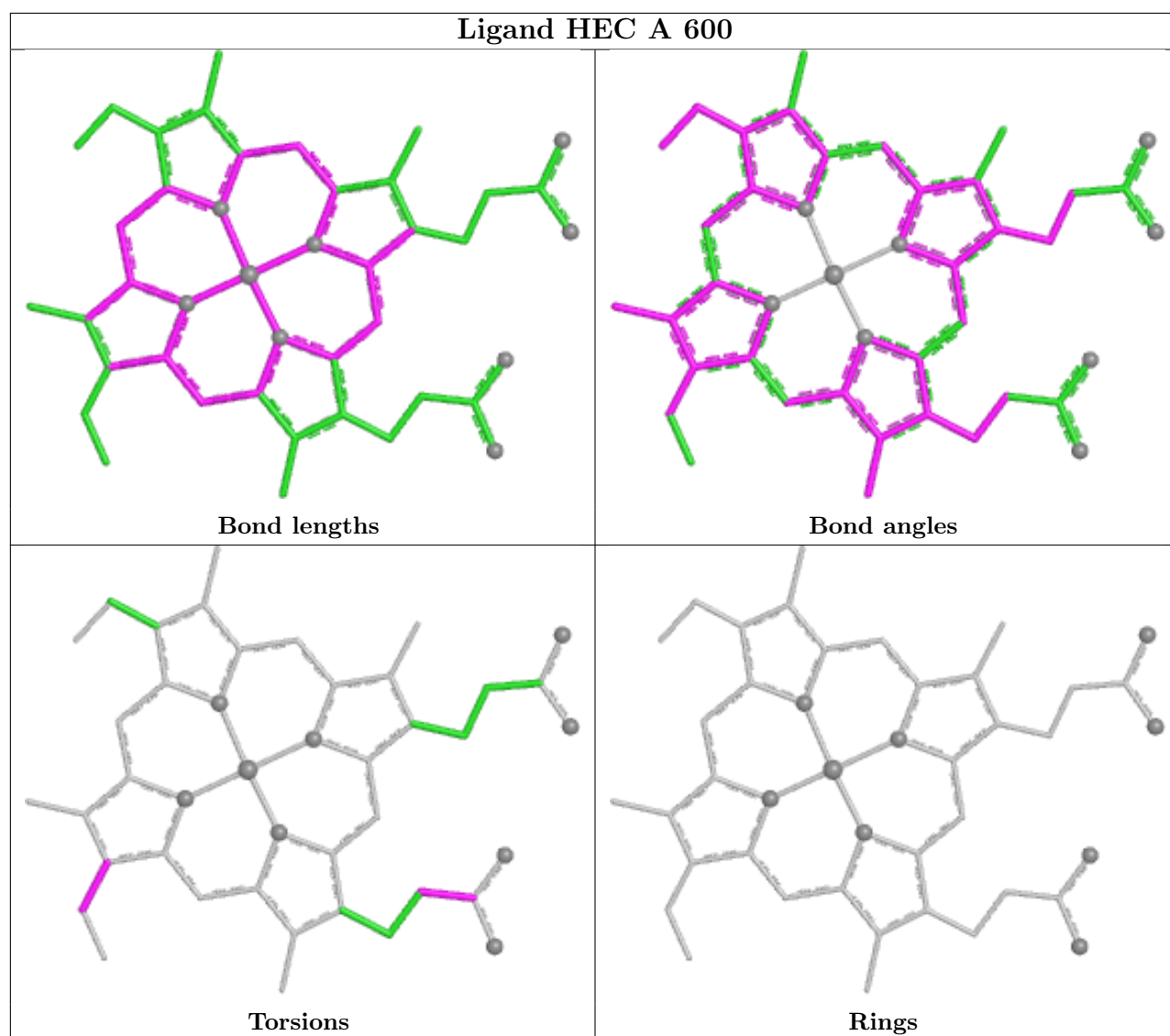
Bond angles



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 [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%)	0.09	2 (0%) 85 88	21, 41, 57, 66	3 (0%)
1	B	355/373 (95%)	-0.12	1 (0%) 90 92	16, 35, 50, 65	3 (0%)
2	C	130/137 (94%)	0.08	4 (3%) 51 55	22, 35, 62, 73	2 (1%)
2	E	124/137 (90%)	-0.24	0 100 100	18, 28, 38, 59	2 (1%)
3	D	376/386 (97%)	0.13	3 (0%) 82 85	26, 42, 66, 75	1 (0%)
3	F	376/386 (97%)	-0.31	0 100 100	18, 29, 43, 57	3 (0%)
All	All	1715/1792 (95%)	-0.06	10 (0%) 85 88	16, 36, 58, 75	14 (0%)

The worst 5 of 10 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
3	D	208	THR	3.0
1	A	320	ALA	2.9
3	D	207	GLY	2.8
1	A	6	ALA	2.6
2	C	137	HIS	2.6

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

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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
2	0AF	C	57	15/16	0.91	0.10	40,42,43,45	0
2	0AF	E	57	15/16	0.93	0.07	32,33,34,36	0

6.3 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

6.4 Ligands [i](#)

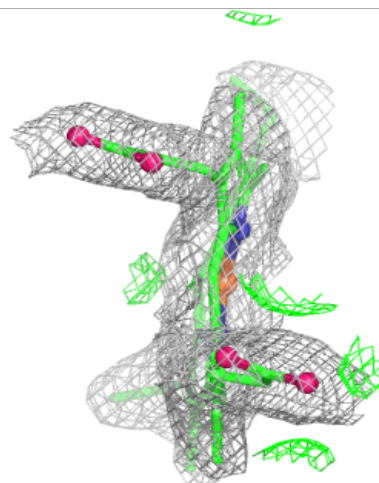
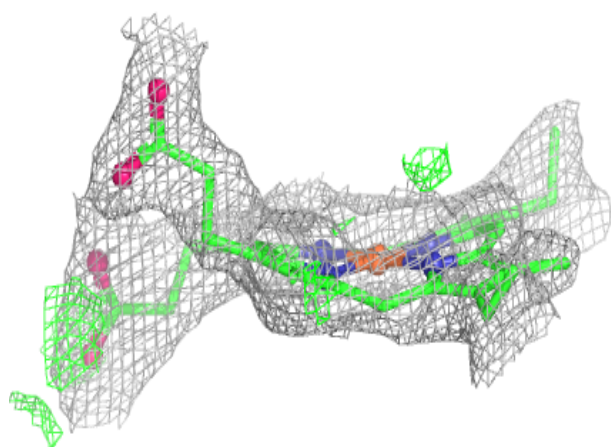
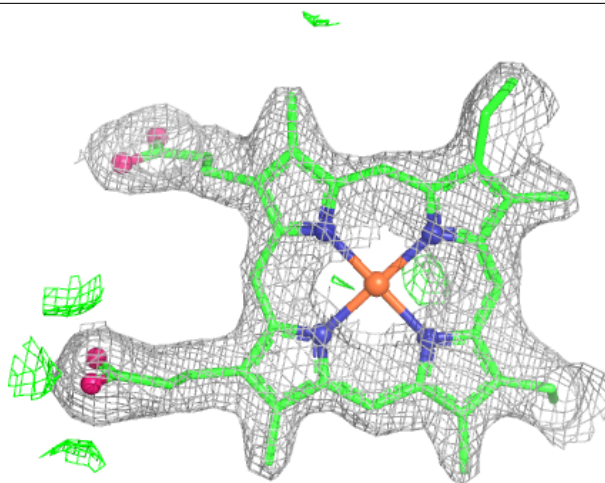
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists 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	PGE	B	374	10/10	0.79	0.17	71,74,76,77	0
7	ACT	F	387	4/4	0.89	0.12	49,49,50,50	0
7	ACT	D	387	4/4	0.92	0.12	40,41,41,41	0
5	HEC	A	500	43/43	0.97	0.08	31,37,39,40	0
5	HEC	B	600	43/43	0.98	0.07	18,24,26,29	0
4	CA	A	400	1/1	0.98	0.03	40,40,40,40	0
5	HEC	A	600	43/43	0.98	0.07	30,33,37,41	0
5	HEC	B	500	43/43	0.98	0.07	22,26,28,31	0
4	CA	B	400	1/1	0.99	0.02	24,24,24,24	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.

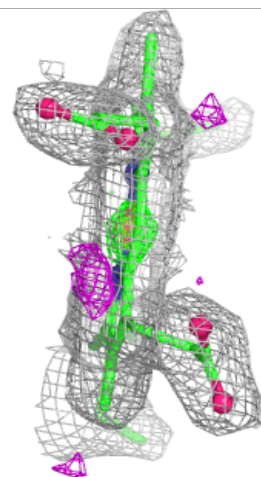
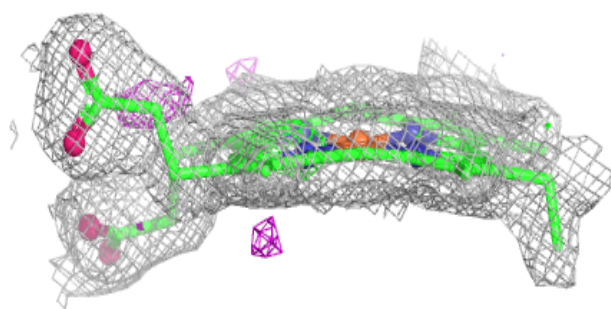
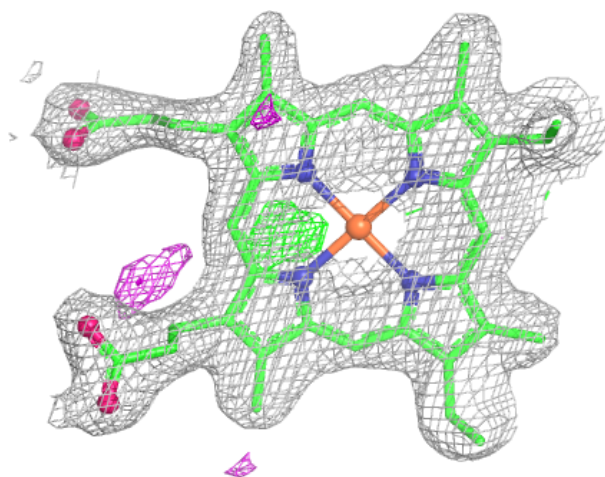
Electron density around HEC A 500:

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



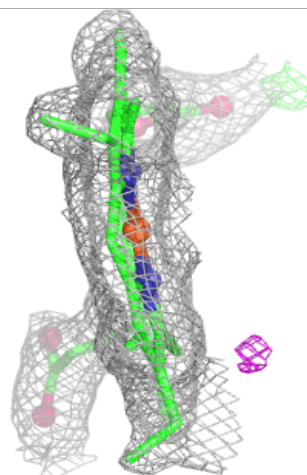
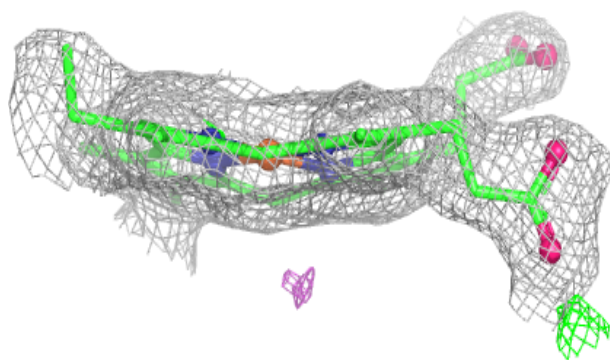
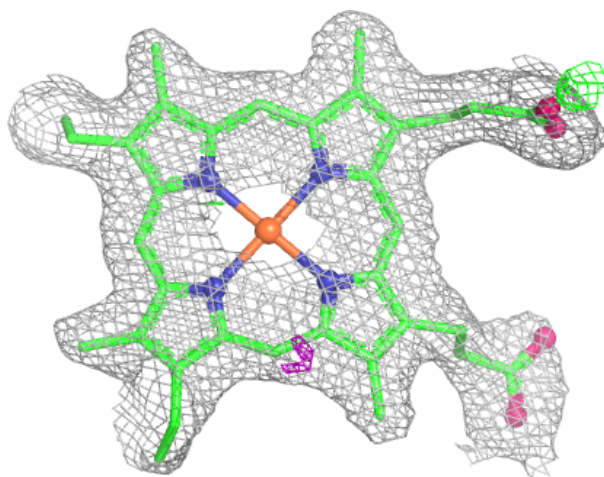
Electron density around HEC B 600:

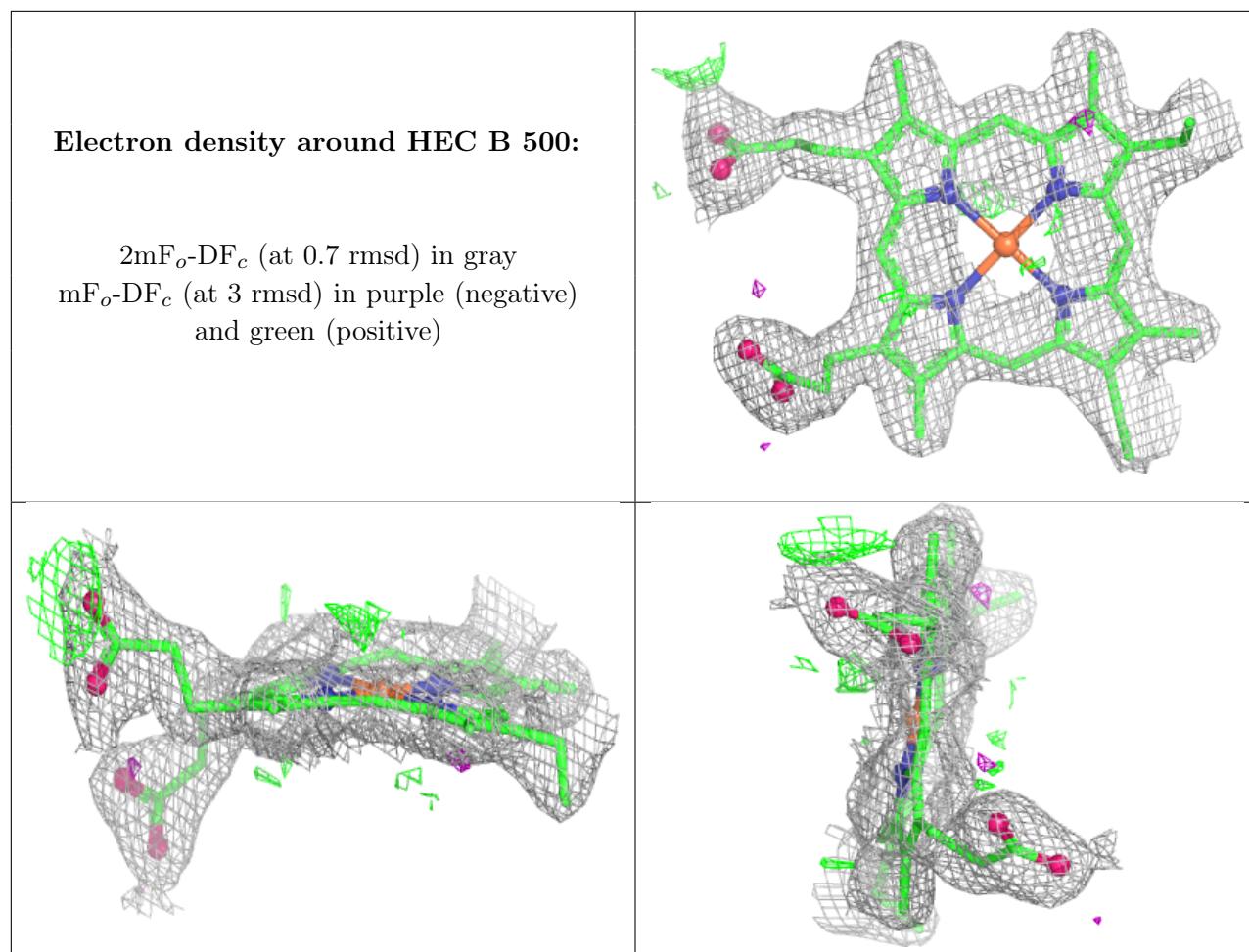
$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)



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)





6.5 Other polymers [i](#)

There are no such residues in this entry.