



# wwPDB X-ray Structure Validation Summary Report ⓘ

Oct 29, 2024 – 08:15 AM EDT

PDB ID : 3RLM  
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](mailto: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>.

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

MolProbity	:	4.02b-467
Mogul	:	2022.3.0, CSD as543be (2022)
Xtriage (Phenix)	:	1.20.1
EDS	:	3.0
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20231227.v01 (using entries in the PDB archive December 27th 2023)
CCP4	:	9.0.003 (Gargrove)
Density-Fitness	:	1.0.11
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.39

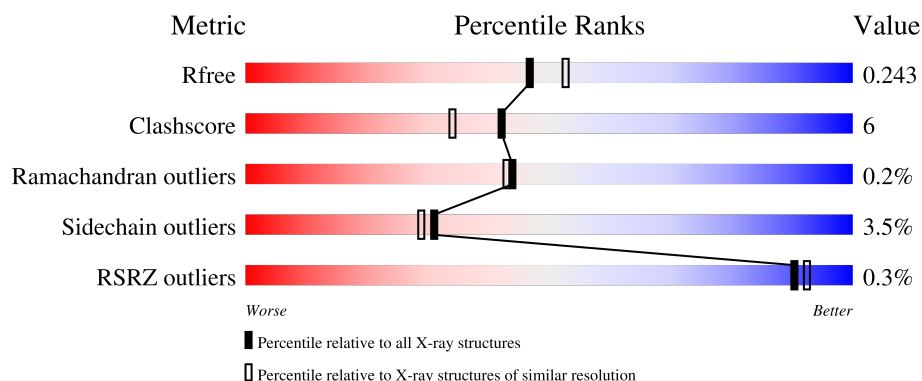
# 1 Overall quality at a glance ⓘ

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))
$R_{free}$	164625	3336 (2.16-2.12)
Clashscore	180529	3585 (2.16-2.12)
Ramachandran outliers	177936	3554 (2.16-2.12)
Sidechain outliers	177891	3553 (2.16-2.12)
RSRZ outliers	164620	3337 (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  $\geq 3$ , 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	<div> <div>%</div> <div> <div></div> <div>81%</div> <div>13%</div> <div>5%</div> </div> </div>
1	B	373	<div> <div></div> <div>79%</div> <div>16%</div> <div>5%</div> </div>
2	C	137	<div> <div>%</div> <div> <div></div> <div>77%</div> <div>16%</div> <div>• • •</div> </div> </div>
2	E	137	<div> <div></div> <div>68%</div> <div>23%</div> <div>• 9%</div> </div>
3	D	386	<div> <div>%</div> <div> <div></div> <div>82%</div> <div>16%</div> <div>•</div> </div> </div>

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Mol	Chain	Length	Quality of chain
3	F	386	 A horizontal bar chart showing the quality of chain F. The bar is divided into three segments: a green segment representing 86%, a yellow segment representing 11%, and a small grey segment at the end. A small black dot is located at the end of the grey segment.

## 2 Entry composition [i](#)

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

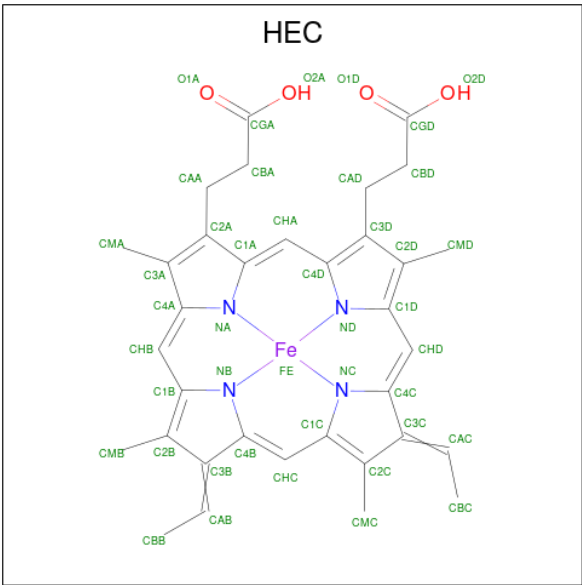
- Molecule 3 is a protein called Methylamine dehydrogenase heavy chain.

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 (three-letter code: CA) (formula: Ca).

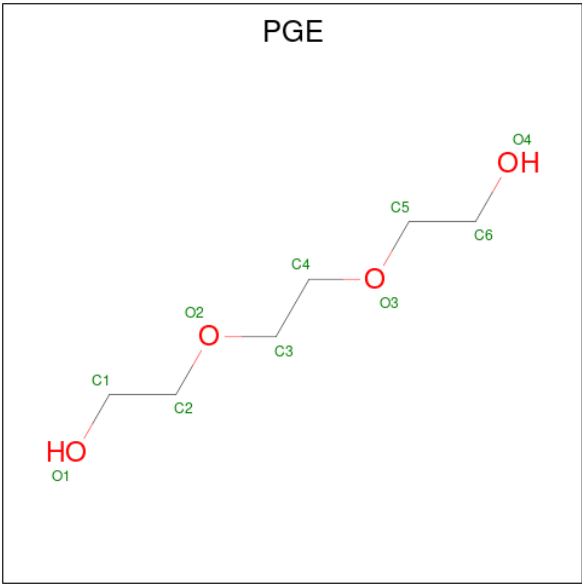
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	1	Total	Ca	0	0
			1	1		
4	B	1	Total	Ca	0	0
			1	1		

- Molecule 5 is HEME C (three-letter code: HEC) (formula: C<sub>34</sub>H<sub>34</sub>FeN<sub>4</sub>O<sub>4</sub>).



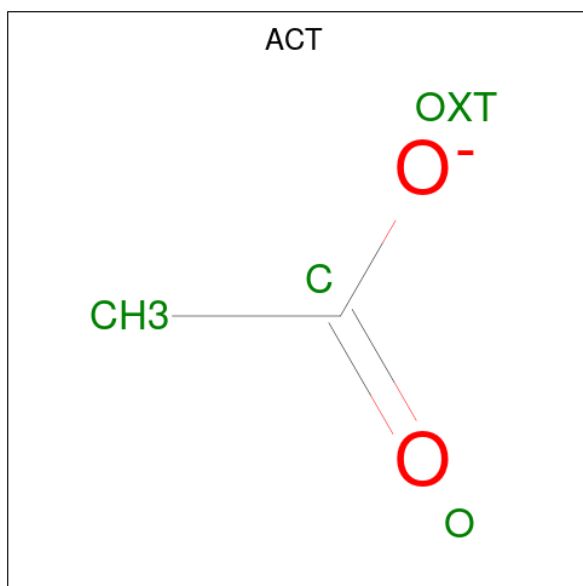
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
5	A	1	Total 43	C 34	Fe 1	N 4	O 4	0	0
5	A	1	Total 43	C 34	Fe 1	N 4	O 4	0	0
5	B	1	Total 43	C 34	Fe 1	N 4	O 4	0	0
5	B	1	Total 43	C 34	Fe 1	N 4	O 4	0	0

- Molecule 6 is TRIETHYLENE GLYCOL (three-letter code: PGE) (formula: C<sub>6</sub>H<sub>14</sub>O<sub>4</sub>).



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

- Molecule 7 is ACETATE ION (three-letter code: 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		







## 4 Data and refinement statistics

Property	Value	Source
Space group	P 1	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	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
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	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 (5.05%)	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	31.0	Xtriage
Anisotropy	0.115	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.32 , 34.9	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.50$ , $\langle L^2 \rangle = 0.33$	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 <sup>2</sup> )	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.*

<sup>1</sup>Intensities estimated from amplitudes.

<sup>2</sup>Theoretical 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: OAF, HEC, PGE, CA, ACT

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	0.50	0/2823	0.64	2/3828 (0.1%)
1	B	0.56	0/2836	0.66	1/3844 (0.0%)
2	C	0.54	0/1044	0.70	0/1425
2	E	0.70	0/975	0.74	0/1331
3	D	0.51	0/3011	0.62	0/4102
3	F	0.62	0/3024	0.71	0/4119
All	All	0.56	0/13713	0.67	3/18649 (0.0%)

There are no bond length outliers.

All (3) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	252	ARG	NE-CZ-NH2	-6.41	117.10	120.30
1	A	39	ARG	NE-CZ-NH2	-5.21	117.69	120.30
1	A	252	ARG	NE-CZ-NH2	-5.11	117.75	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	2757	0	2632	27	1
1	B	2773	0	2649	38	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
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	4	0
5	B	86	0	60	6	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	10
2	E	124/137 (90%)	119 (96%)	5 (4%)	0	100	100
3	D	375/386 (97%)	358 (96%)	15 (4%)	2 (0%)	25	20
3	F	377/386 (98%)	364 (97%)	12 (3%)	1 (0%)	37	33
All	All	1717/1792 (96%)	1650 (96%)	63 (4%)	4 (0%)	44	43

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%)	22	18
1	B	280/292 (96%)	267 (95%)	13 (5%)	23	19
2	C	112/112 (100%)	109 (97%)	3 (3%)	40	40

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
2	E	106/112 (95%)	104 (98%)	2 (2%)	52	56
3	D	305/311 (98%)	293 (96%)	12 (4%)	27	25
3	F	307/311 (99%)	301 (98%)	6 (2%)	50	53
All	All	1389/1430 (97%)	1340 (96%)	49 (4%)	31	29

5 of 49 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
2	C	131	SER
3	D	223	GLU
3	D	20	ARG
3	D	177	ASP
3	D	273[A]	ARG

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 16 such sidechains are listed below:

Mol	Chain	Res	Type
3	F	14	GLN
3	F	11	GLN
1	B	210	GLN
2	E	68	GLN
1	B	163	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	C	57	2	13,16,17	1.06	0	9,22,24	1.17	1 (11%)
2	0AF	E	57	2	13,16,17	1.22	1 (7%)	9,22,24	1.65	2 (22%)

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	-	1/4/6/8	0/2/2/2
2	0AF	E	57	2	-	0/4/6/8	0/2/2/2

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	E	57	0AF	CZ3-CE3	2.27	1.41	1.36

All (3) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	E	57	0AF	CB-CG-CD1	-3.74	123.34	127.97
2	E	57	0AF	CB-CG-CD2	2.28	129.80	126.25
2	C	57	0AF	CE3-CD2-CG	-2.13	130.51	134.42

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	C	57	0AF	2	0
2	E	57	0AF	1	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
7	ACT	F	387	-	3,3,3	0.74	0	3,3,3	1.49	0
5	HEC	A	500	8,1	32,50,50	1.59	8 (25%)	30,82,82	2.72	10 (33%)
5	HEC	A	600	1	32,50,50	1.63	9 (28%)	30,82,82	3.25	11 (36%)
5	HEC	B	500	8,1	32,50,50	1.60	9 (28%)	30,82,82	2.75	12 (40%)
6	PGE	B	374	-	9,9,9	0.55	0	8,8,8	0.46	0
5	HEC	B	600	1	32,50,50	1.45	4 (12%)	30,82,82	3.07	13 (43%)
7	ACT	D	387	-	3,3,3	0.88	0	3,3,3	1.39	0

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
5	HEC	A	500	8,1	-	1/10/54/54	-
5	HEC	A	600	1	-	2/10/54/54	-
5	HEC	B	500	8,1	-	1/10/54/54	-
6	PGE	B	374	-	-	5/7/7/7	-
5	HEC	B	600	1	-	2/10/54/54	-

The worst 5 of 30 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
5	B	500	HEC	C3C-C4C	3.44	1.49	1.43
5	A	600	HEC	C3C-C4C	3.37	1.49	1.43

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
5	A	500	HEC	C3A-C4A	3.17	1.49	1.42
5	B	500	HEC	C2A-C1A	3.10	1.49	1.42
5	A	500	HEC	C3C-C4C	3.06	1.48	1.43

The worst 5 of 46 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	A	600	HEC	CBB-CAB-C3B	-9.00	106.44	127.49
5	B	600	HEC	CBB-CAB-C3B	-8.40	107.84	127.49
5	B	500	HEC	CBB-CAB-C3B	-7.63	109.63	127.49
5	A	500	HEC	CBB-CAB-C3B	-7.42	110.12	127.49
5	B	600	HEC	CBC-CAC-C3C	-7.29	110.43	127.49

There are no chirality outliers.

5 of 11 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
6	B	374	PGE	C1-C2-O2-C3
6	B	374	PGE	O3-C5-C6-O4
6	B	374	PGE	O1-C1-C2-O2
5	B	500	HEC	C3D-CAD-CBD-CGD
6	B	374	PGE	C6-C5-O3-C4

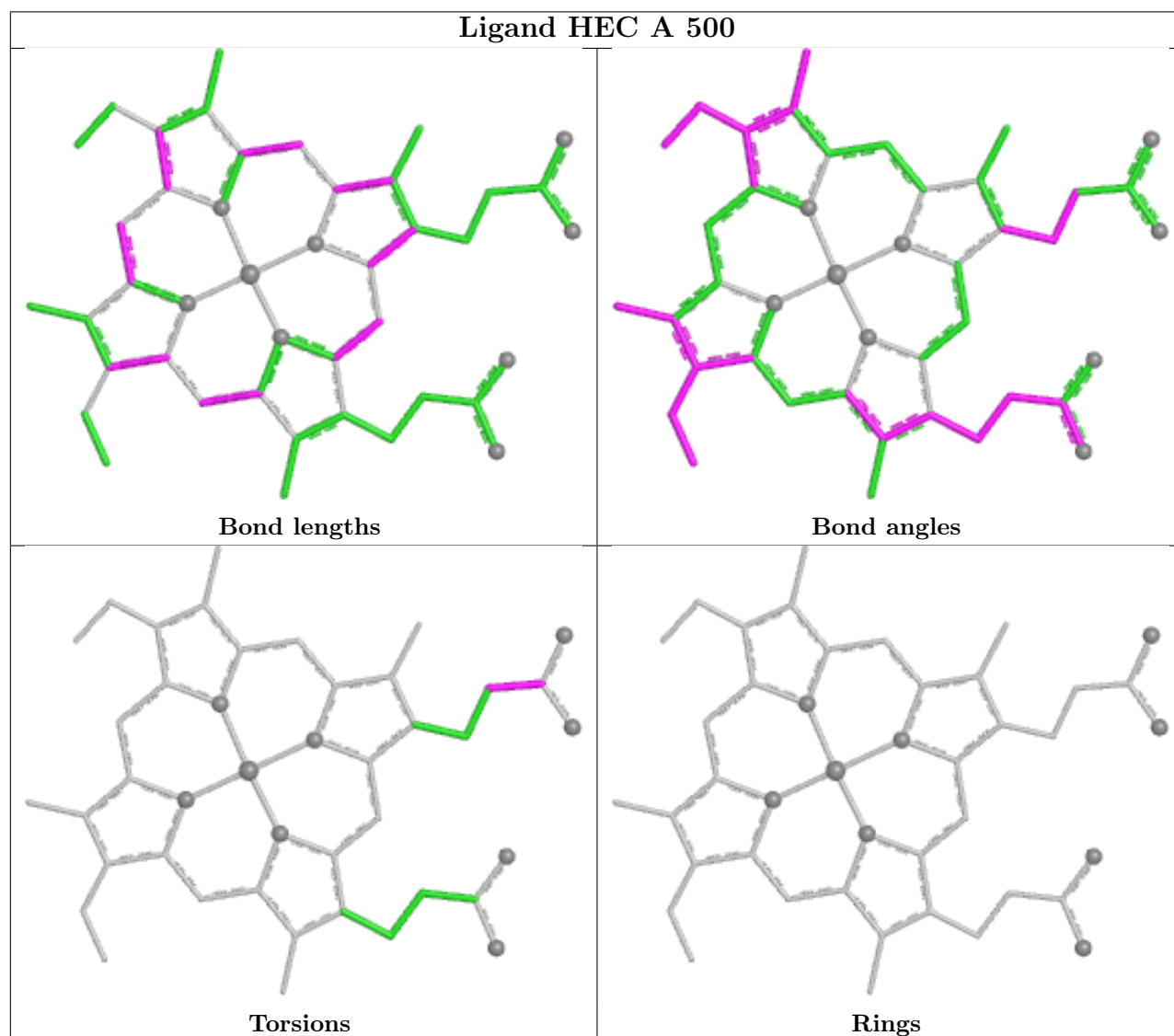
There are no ring outliers.

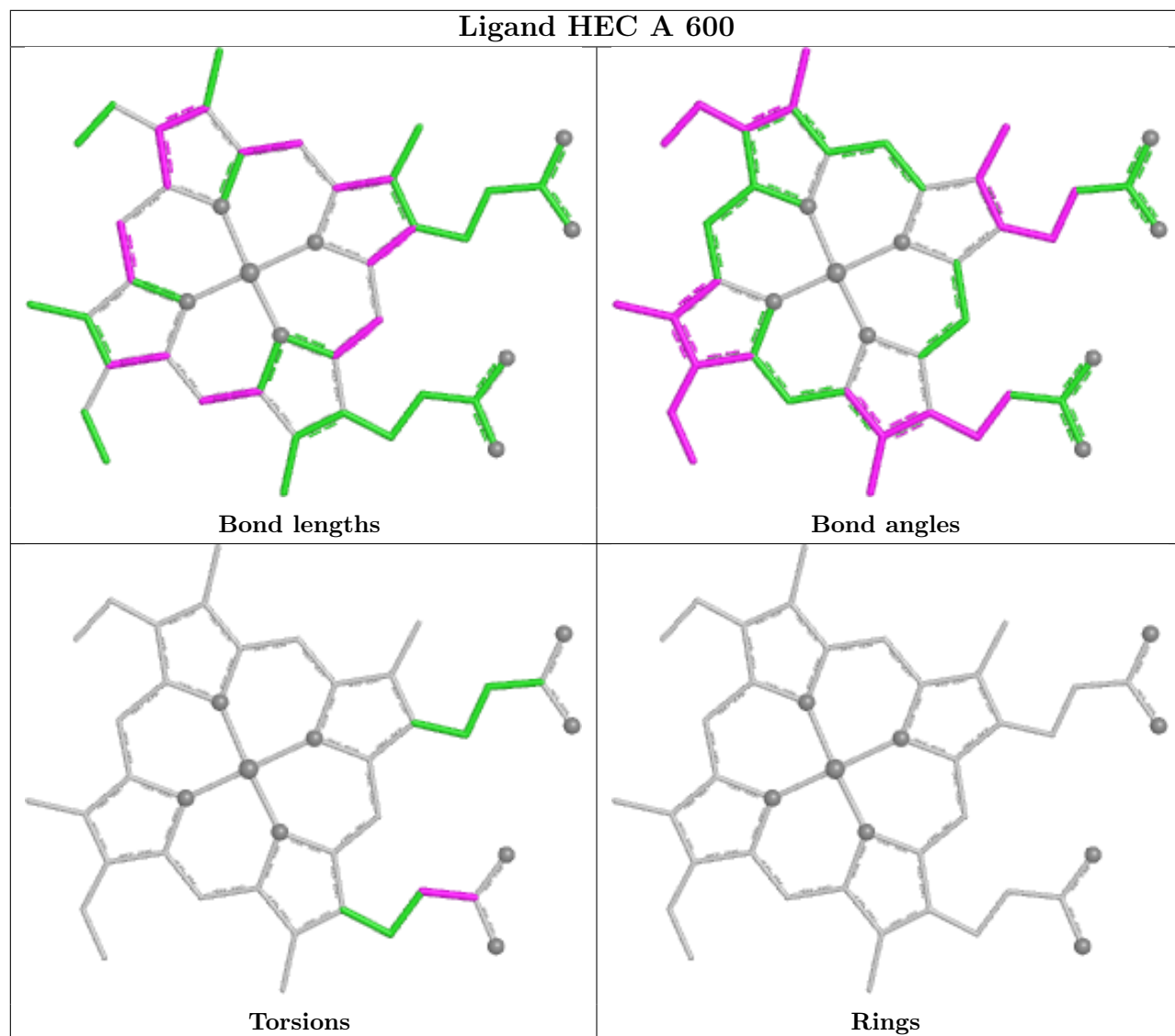
4 monomers are involved in 10 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
5	A	500	HEC	2	0
5	A	600	HEC	2	0
5	B	500	HEC	3	0
5	B	600	HEC	3	0

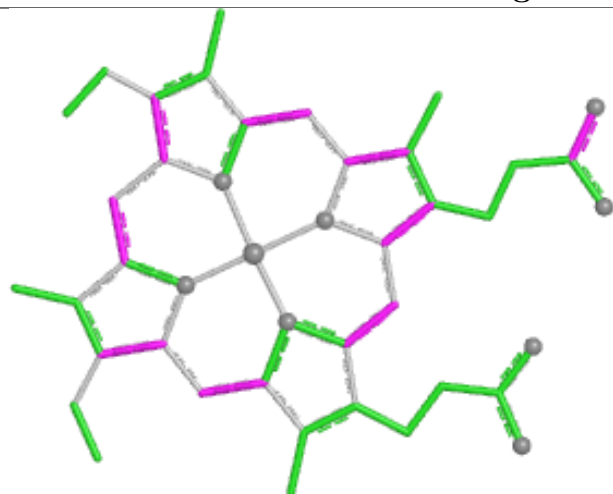
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included.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

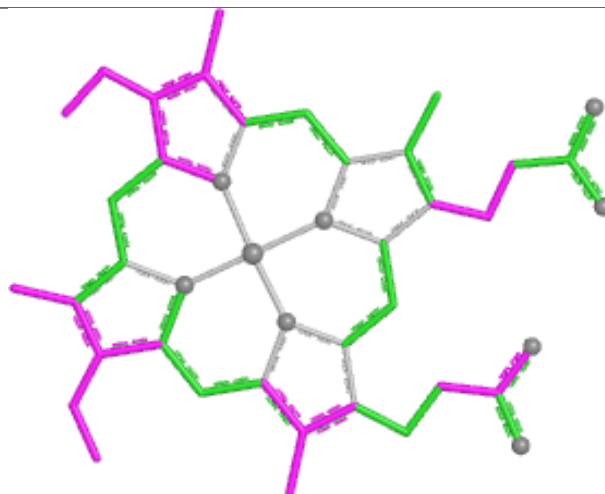




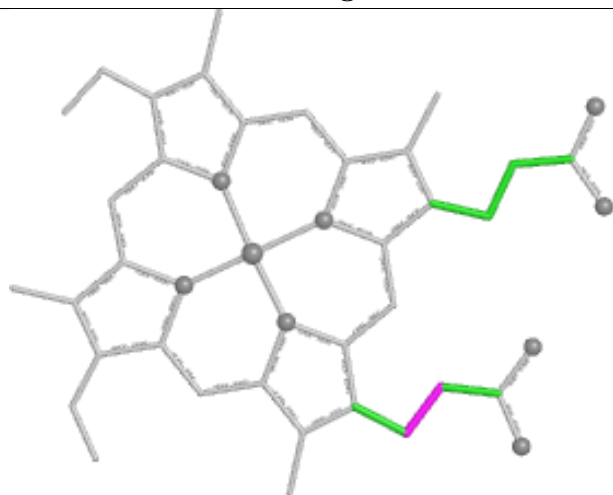
## Ligand HEC B 500



Bond lengths



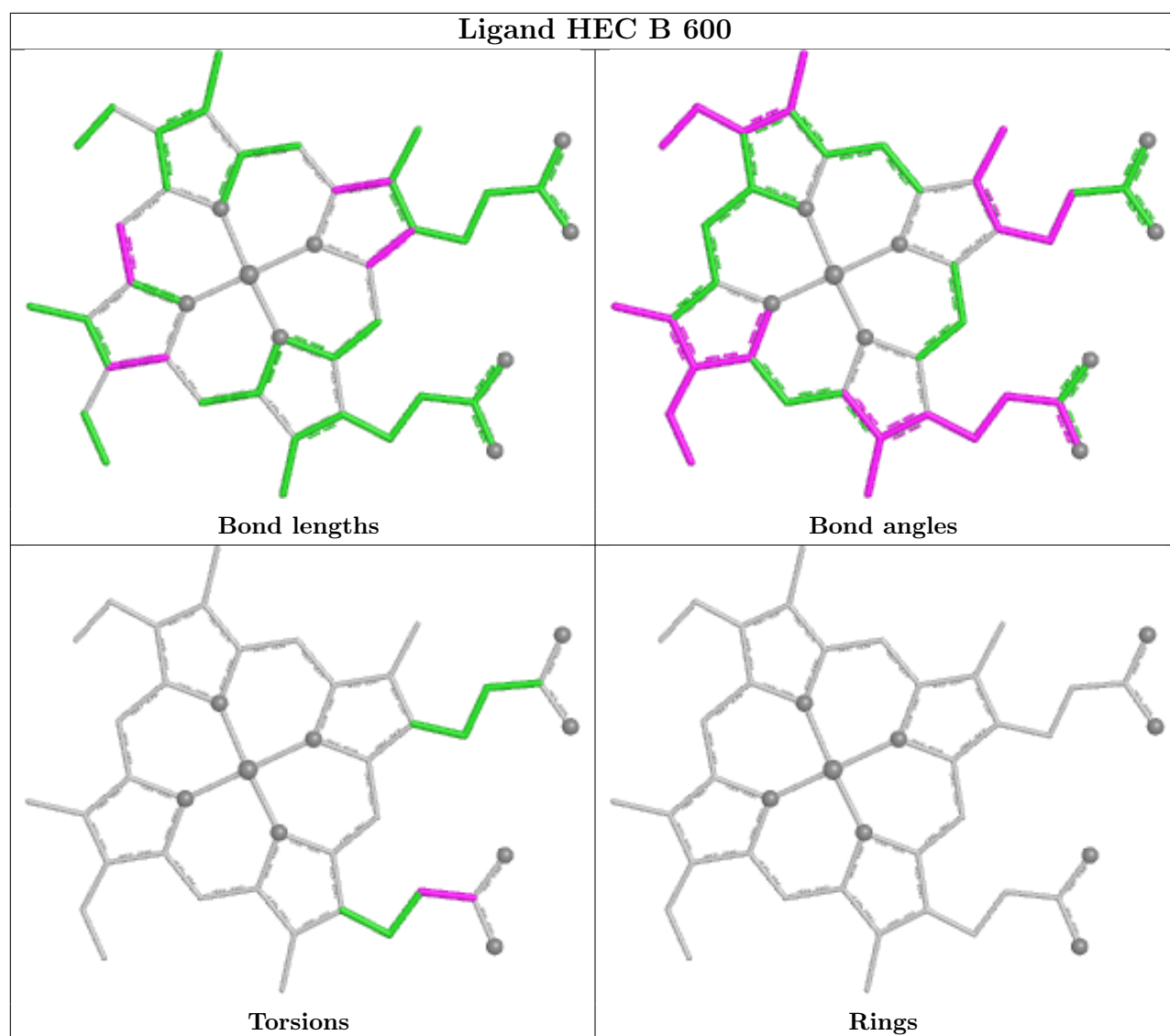
Bond angles



Torsions



Rings



## 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, 95<sup>th</sup> 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 <sup>2</sup> )	Q<0.9
1	A	354/373 (94%)	-0.02	2 (0%) 85 88	21, 41, 57, 66	3 (0%)
1	B	355/373 (95%)	-0.22	0 100 100	16, 35, 50, 65	3 (0%)
2	C	130/137 (94%)	-0.02	2 (1%) 71 75	22, 35, 62, 73	2 (1%)
2	E	124/137 (90%)	-0.35	0 100 100	18, 28, 38, 59	2 (1%)
3	D	376/386 (97%)	0.02	2 (0%) 87 89	26, 42, 66, 75	1 (0%)
3	F	376/386 (97%)	-0.41	0 100 100	18, 29, 43, 57	3 (0%)
All	All	1715/1792 (95%)	-0.16	6 (0%) 90 92	16, 36, 58, 75	14 (0%)

The worst 5 of 6 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
3	D	208	THR	2.9
1	A	320	ALA	2.7
3	D	207	GLY	2.6
2	C	137	HIS	2.5
1	A	6	ALA	2.5

### 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<sup>th</sup> 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 <sup>2</sup> )	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 monosaccharides in this entry.

## 6.4 Ligands [i](#)

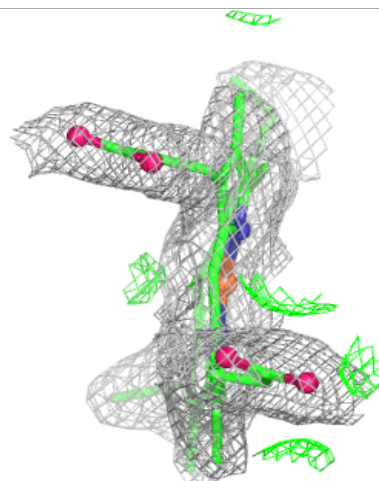
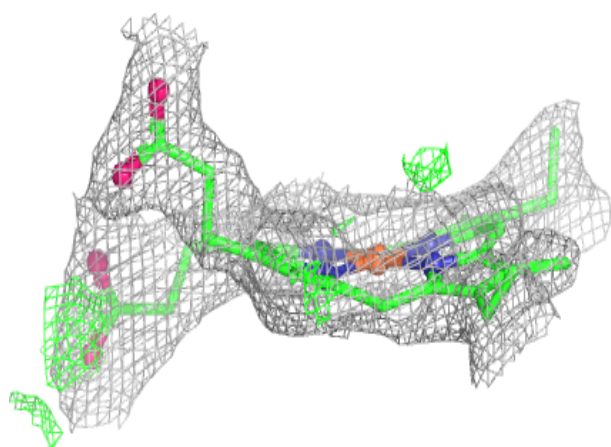
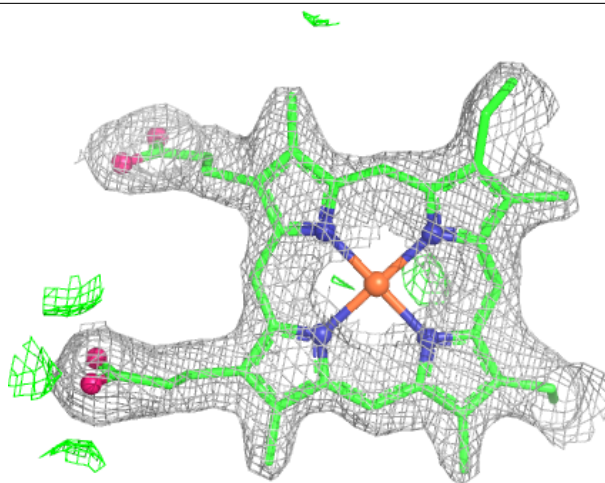
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95<sup>th</sup> percentile and maximum values of B factors of atoms in the group. The column labelled 'Q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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å <sup>2</sup> )	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	0.03	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:**

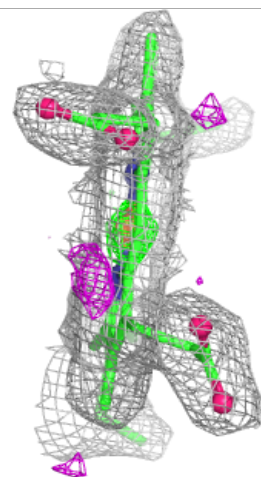
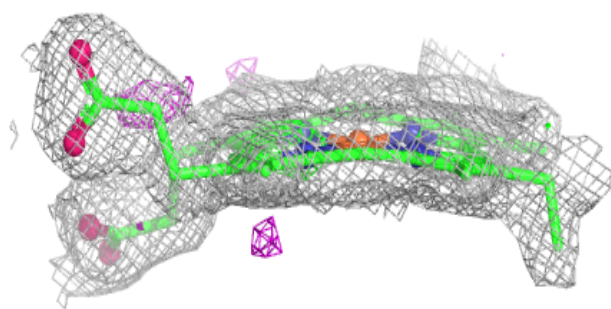
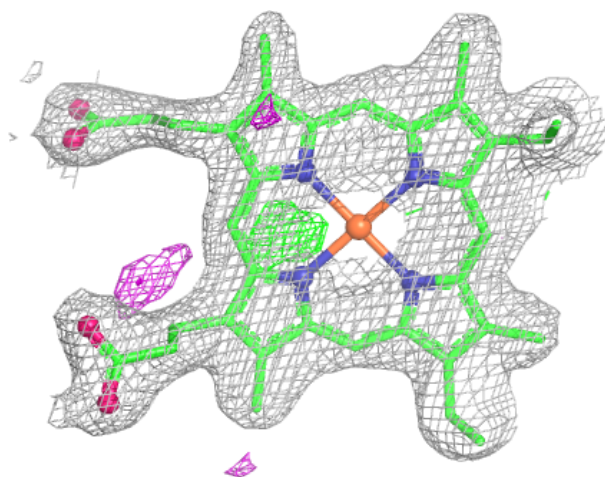
$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)





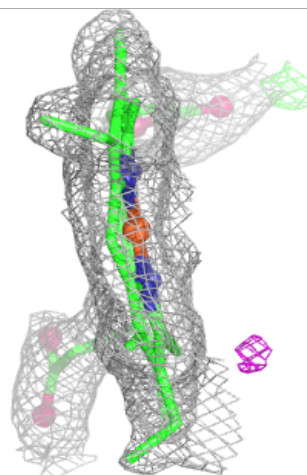
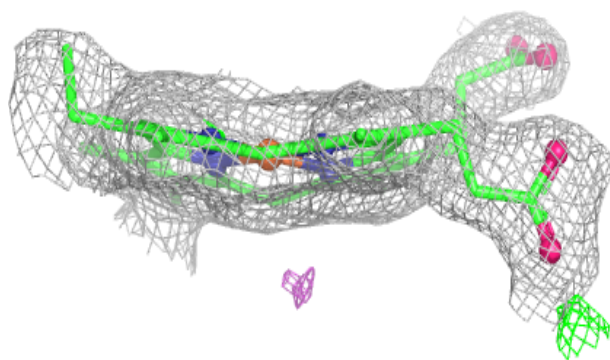
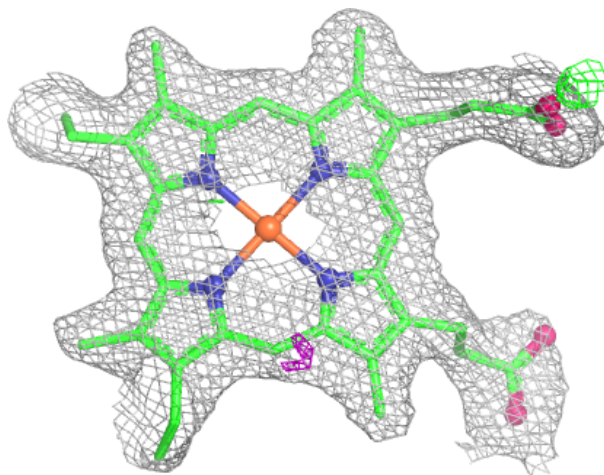
**Electron density around HEC B 600:**

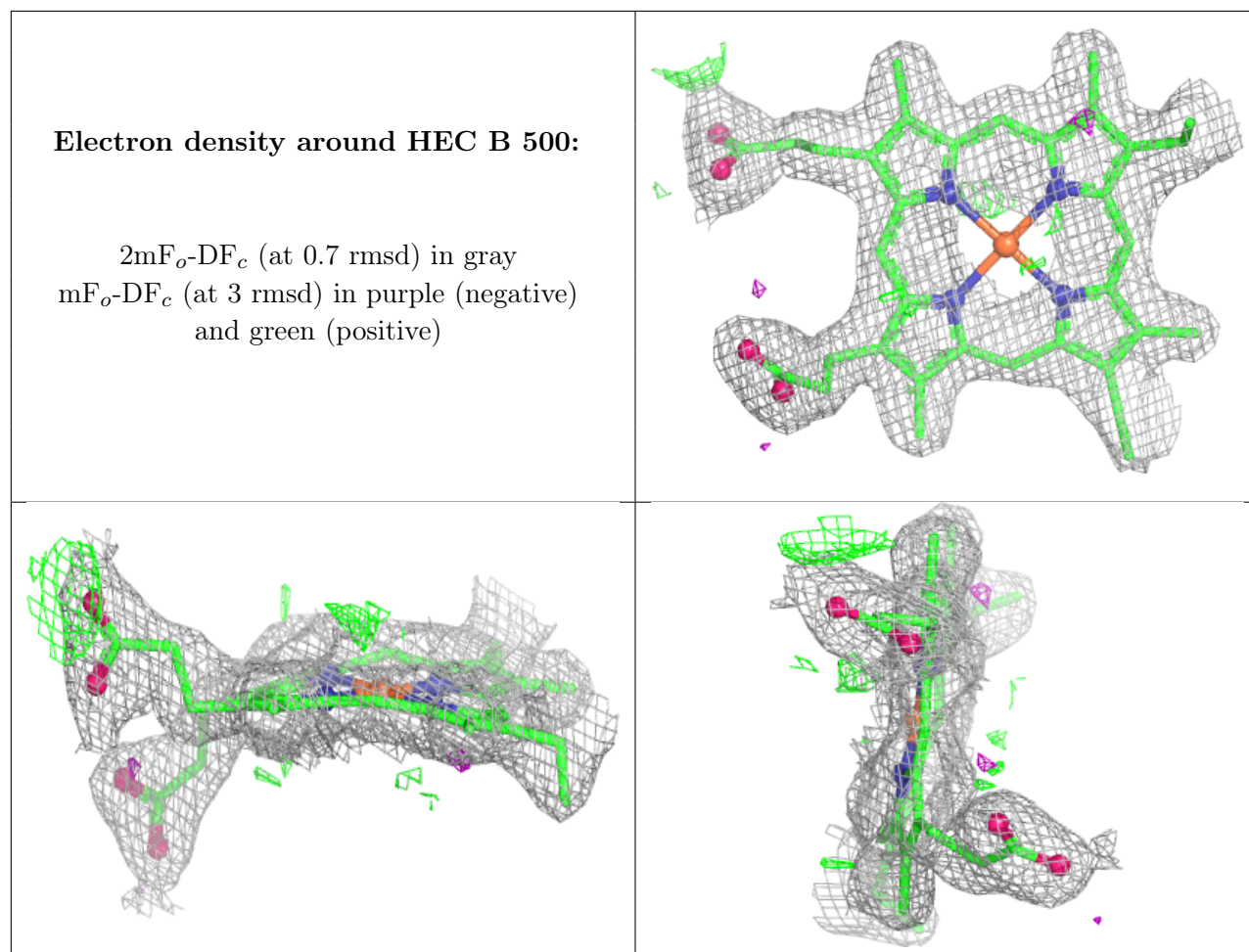
$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)



**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.