



# wwPDB X-ray Structure Validation Summary Report ⓘ

Jun 14, 2020 – 05:37 am BST

PDB ID : 1QQW  
Title : CRYSTAL STRUCTURE OF HUMAN ERYTHROCYTE CATALASE  
Authors : Ko, T.P.; Safo, M.K.; Musayev, F.N.; Wang, C.; Wu, S.H.; Abraham, D.J.  
Deposited on : 1999-06-09  
Resolution : 2.75 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.

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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 : 1.8.5 (274361), CSD as541be (2020)  
Xtriage (Phenix) : 1.13  
EDS : 2.11  
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) : 2.11

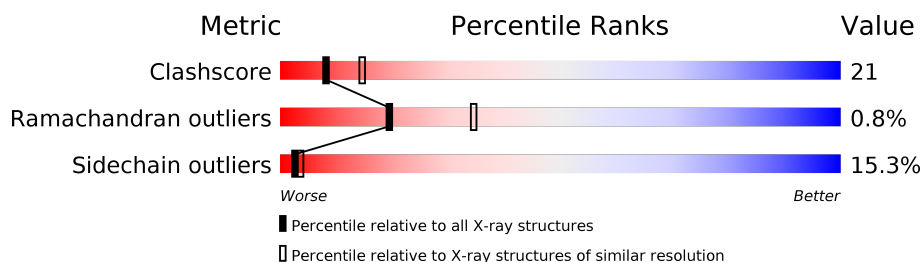
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

The reported resolution of this entry is 2.75 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))
Clashscore	141614	1277 (2.78-2.74)
Ramachandran outliers	138981	1257 (2.78-2.74)
Sidechain outliers	138945	1257 (2.78-2.74)

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 on 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  $\leq 5\%$

Mol	Chain	Length	Quality of chain
1	A	527	
1	B	527	
1	C	527	
1	D	527	

## 2 Entry composition [i](#)

There are 3 unique types of molecules in this entry. The entry contains 16618 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 CATALASE.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	499	Total	C	N	O	S	0	0	0
			4012	2549	712	738	13			
1	B	500	Total	C	N	O	S	0	0	0
			4017	2552	713	739	13			
1	C	499	Total	C	N	O	S	0	0	0
			4012	2549	712	738	13			
1	D	499	Total	C	N	O	S	0	0	0
			4012	2549	712	738	13			

- Molecule 2 is PROTOPORPHYRIN IX CONTAINING FE (three-letter code: HEM) (formula:  $C_{34}H_{32}FeN_4O_4$ ).



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

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Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
2	C	1	Total	C	Fe	N	O	0	0
			43	34	1	4	4		
2	D	1	Total	C	Fe	N	O	0	0
			43	34	1	4	4		

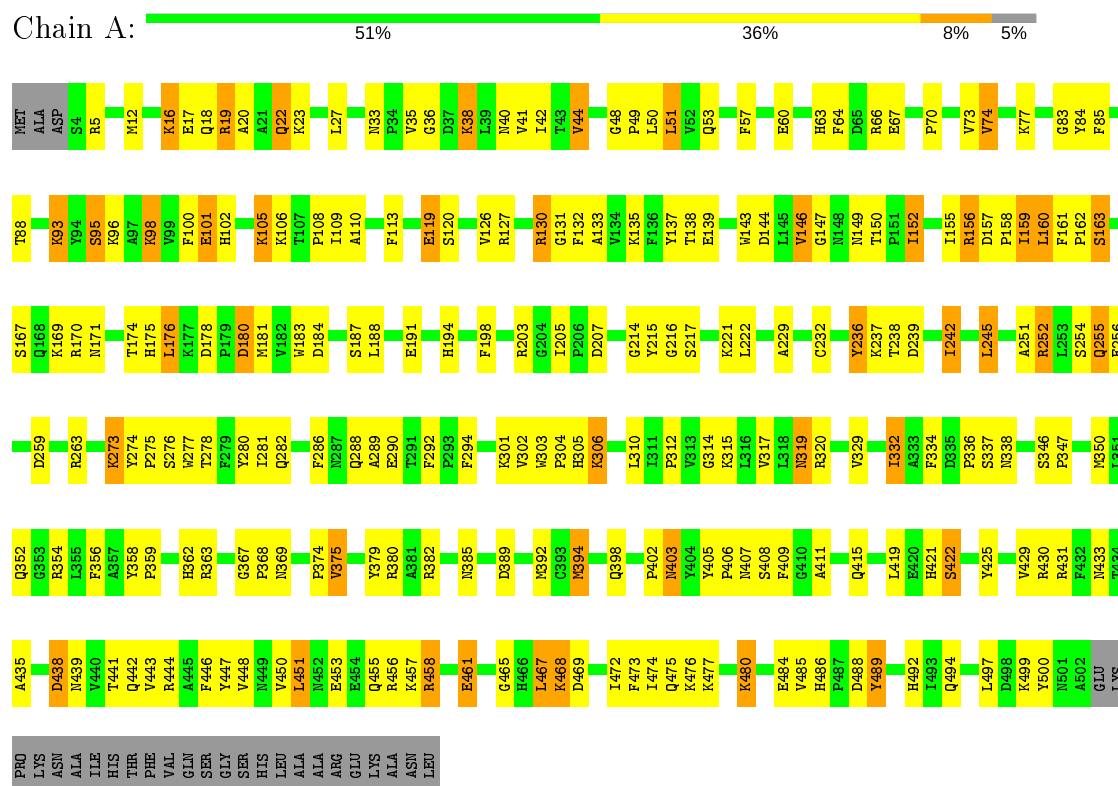
- Molecule 3 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	102	Total	O	0	0
			102	102		
3	B	119	Total	O	0	0
			119	119		
3	C	96	Total	O	0	0
			96	96		
3	D	76	Total	O	0	0
			76	76		

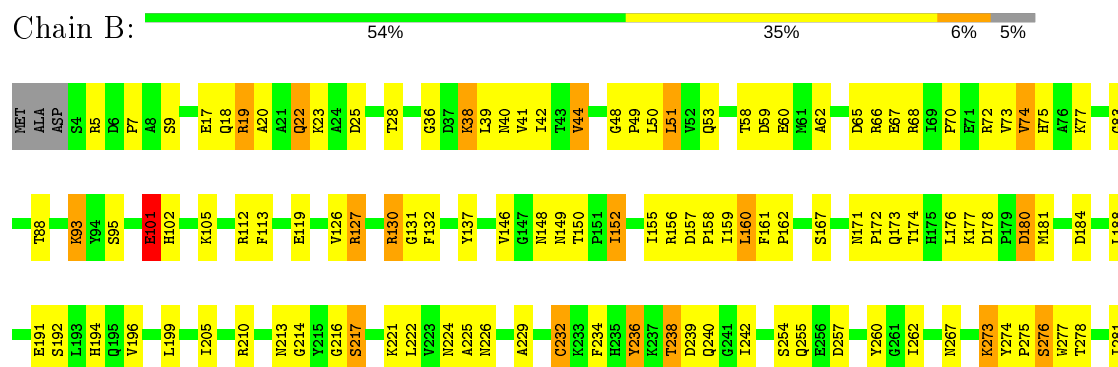
### 3 Residue-property plots

These plots are drawn for all protein, RNA and DNA 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. 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. 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: CATALASE



#### • Molecule 1: CATALASE





LYS	A345	Y724
ASN	S946	P275
ALA	R430	S276
ILE	N350	H277
HIS	N350	T278
THR	R354	F279
PHE	Y358	T280
VAL	P359	I281
GLN	D437	Q282
SER	D438	
GLY	N439	T285
SER		F286
HIS	Q442	H287
LEU	Y443	Q288
ALA	R444	A289
ALA	A445	E290
ARG	F446	T291
ARG	Y447	F292
GLU		F293
LYS	L451	F294
ALA	N452	N295
ASN	D453	
LEU	E454	D298
	Q455	L299
	R456	T300
	K457	K301
	D458	V302
		N303
	E461	K306
	L467	L310
	K468	
		V313
	L472	G314
	F473	G315
	L474	V315
	Q475	L316
	K476	V317
	K477	L318
	A478	N319
	Y479	R320
	R480	N321
	N481	
	E484	N324
	L485	V325
	R486	V326
	F487	A327
	D488	V328
	Y489	E329
	Q490	E330
	S491	Q331
		I332
	Q494	A333
		F334
		D335
		P336
	N501	S337
	A502	N338
GLU	L422	N339
LYS	Q424	
TRP	Y425	

## 4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	84.90Å 141.67Å 232.46Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	40.00 – 2.75 232.46 – 2.73	Depositor EDS
% Data completeness (in resolution range)	(Not available) (40.00-2.75) 80.7 (232.46-2.73)	Depositor EDS
$R_{merge}$	0.12	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	1.20 (at 2.73Å)	Xtriage
Refinement program	X-PLOR 3.851	Depositor
R, $R_{free}$	0.206 , 0.272 0.262 , (Not available)	Depositor DCC
$R_{free}$ test set	No test flags present.	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	17.3	Xtriage
Anisotropy	0.626	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.29 , 36.3	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.48$ , $\langle L^2 \rangle = 0.31$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
$F_o, F_c$ correlation	0.80	EDS
Total number of atoms	16618	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	12.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.65% 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: HEM

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	0.32	0/4131	0.49	0/5613
1	B	0.31	0/4136	0.49	0/5620
1	C	0.32	0/4131	0.49	0/5613
1	D	0.31	0/4131	0.48	0/5613
All	All	0.32	0/16529	0.49	0/22459

There are no bond length outliers.

There are no bond angle outliers.

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	4012	0	3843	204	0
1	B	4017	0	3846	178	0
1	C	4012	0	3844	192	0
1	D	4012	0	3844	193	0
2	A	43	0	30	2	0
2	B	43	0	30	3	0
2	C	43	0	30	2	0
2	D	43	0	30	1	0
3	A	102	0	0	10	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
3	B	119	0	0	9	0
3	C	96	0	0	5	0
3	D	76	0	0	7	0
All	All	16618	0	15497	672	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 21.

The worst 5 of 672 close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:402:PRO:HG2	1:A:411:ALA:HB2	1.42	1.01
1:B:403:ASN:HD22	1:B:403:ASN:H	1.03	0.99
1:B:156:ARG:HH22	1:B:439:ASN:HD21	1.06	0.99
1:D:156:ARG:HH22	1:D:439:ASN:HD21	1.13	0.96
1:C:156:ARG:HH22	1:C:439:ASN:HD21	1.14	0.95

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	497/527 (94%)	443 (89%)	51 (10%)	3 (1%)	25	42
1	B	498/527 (94%)	445 (89%)	48 (10%)	5 (1%)	15	27
1	C	497/527 (94%)	445 (90%)	47 (10%)	5 (1%)	15	27
1	D	497/527 (94%)	455 (92%)	39 (8%)	3 (1%)	25	42
All	All	1989/2108 (94%)	1788 (90%)	185 (9%)	16 (1%)	19	34

5 of 16 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	20	ALA
1	C	20	ALA
1	D	20	ALA
1	B	20	ALA
1	B	101	GLU

### 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	429/451 (95%)	358 (83%)	71 (17%)	2	3
1	B	429/451 (95%)	370 (86%)	59 (14%)	3	5
1	C	429/451 (95%)	366 (85%)	63 (15%)	3	4
1	D	429/451 (95%)	360 (84%)	69 (16%)	2	3
All	All	1716/1804 (95%)	1454 (85%)	262 (15%)	2	4

5 of 262 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	B	451	LEU
1	C	105	LYS
1	D	395	GLN
1	B	461	GLU
1	C	22	GLN

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 78 such sidechains are listed below:

Mol	Chain	Res	Type
1	B	433	ASN
1	C	40	ASN
1	D	439	ASN
1	B	436	ASN
1	B	475	GLN

### 5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

There are no non-standard protein/DNA/RNA residues in this entry.

## 5.5 Carbohydrates ⓘ

There are no carbohydrates in this entry.

## 5.6 Ligand geometry ⓘ

4 ligands 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	HEM	A	600	1	27,50,50	1.67	7 (25%)	17,82,82	0.75	0
2	HEM	B	600	1	27,50,50	1.78	7 (25%)	17,82,82	0.90	1 (5%)
2	HEM	C	600	1	27,50,50	1.77	7 (25%)	17,82,82	1.04	1 (5%)
2	HEM	D	600	1	27,50,50	1.75	6 (22%)	17,82,82	0.98	2 (11%)

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	HEM	A	600	1	-	0/6/54/54	-
2	HEM	B	600	1	-	0/6/54/54	-
2	HEM	C	600	1	-	0/6/54/54	-
2	HEM	D	600	1	-	1/6/54/54	-

The worst 5 of 27 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	600	HEM	C3C-CAC	-3.85	1.39	1.47
2	C	600	HEM	C3B-CAB	-3.74	1.40	1.47
2	B	600	HEM	C3B-CAB	-3.74	1.40	1.47
2	A	600	HEM	C3C-CAC	-3.64	1.40	1.47
2	D	600	HEM	C3B-CAB	-3.63	1.40	1.47

All (4) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	D	600	HEM	C3B-C4B-NB	2.33	112.22	109.21
2	C	600	HEM	C3B-C4B-NB	2.33	112.22	109.21
2	B	600	HEM	C3B-C4B-NB	2.13	111.97	109.21
2	D	600	HEM	C4C-C3C-C2C	-2.07	105.45	106.90

There are no chirality outliers.

All (1) torsion outliers are listed below:

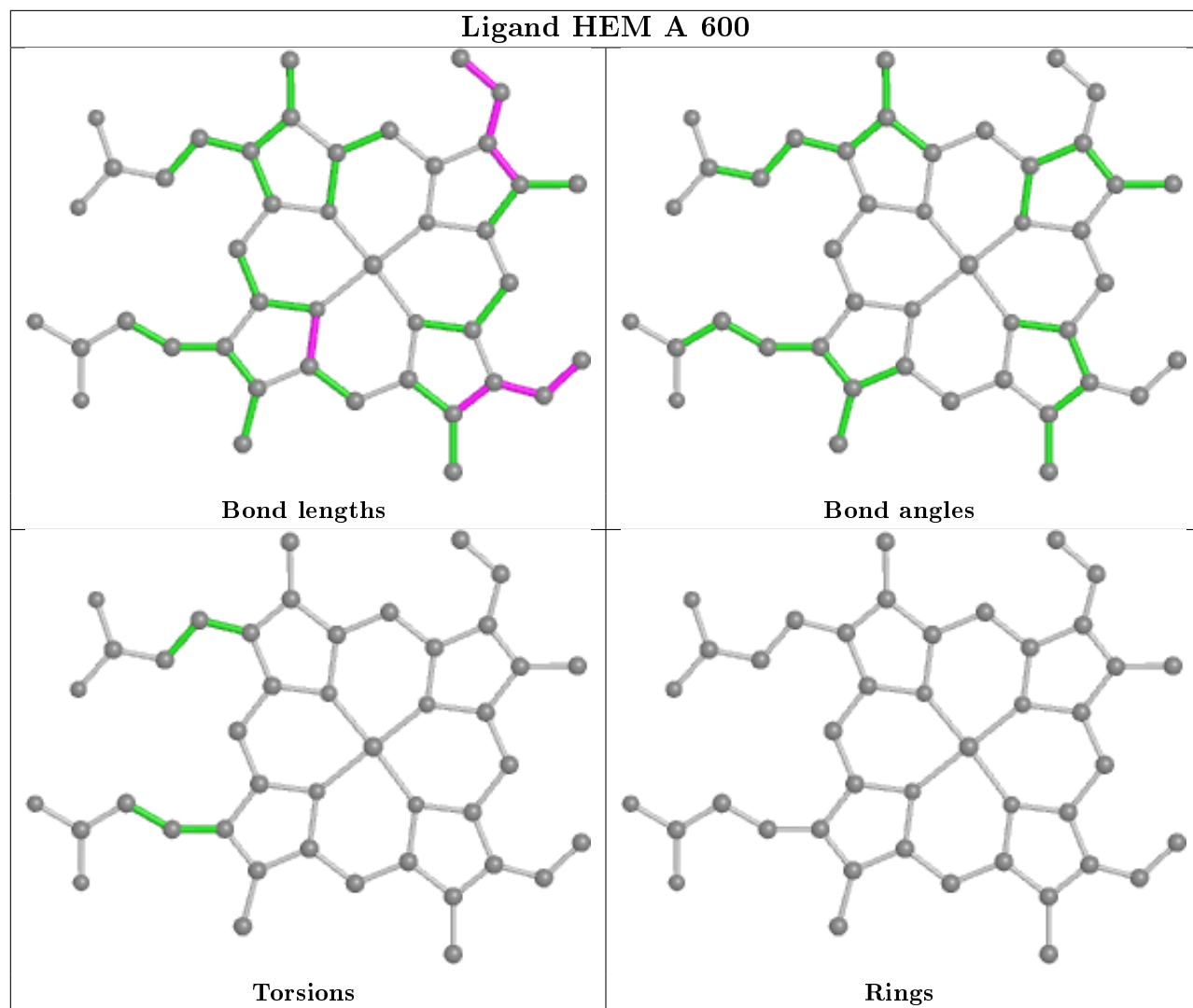
Mol	Chain	Res	Type	Atoms
2	D	600	HEM	C3D-CAD-CBD-CGD

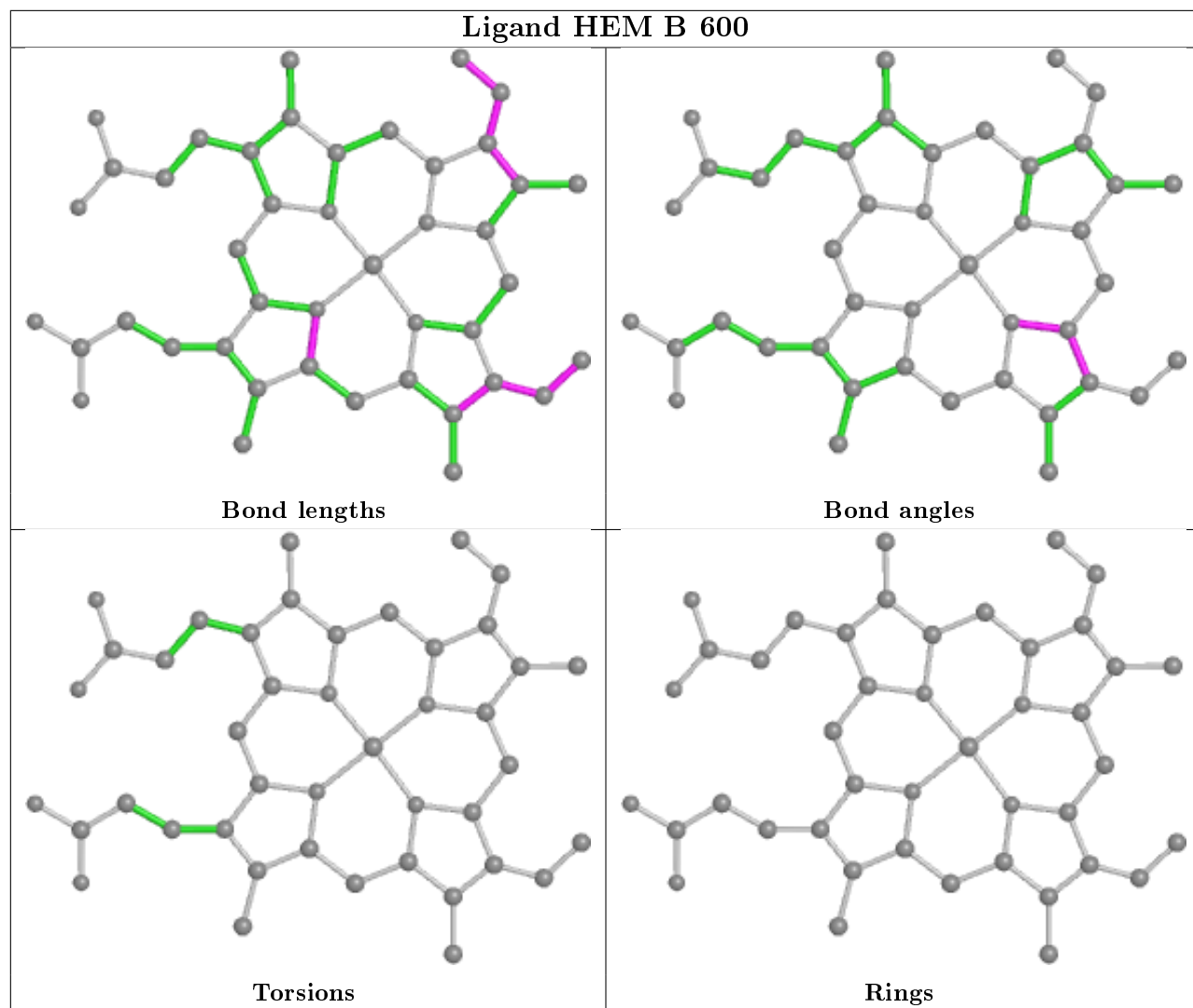
There are no ring outliers.

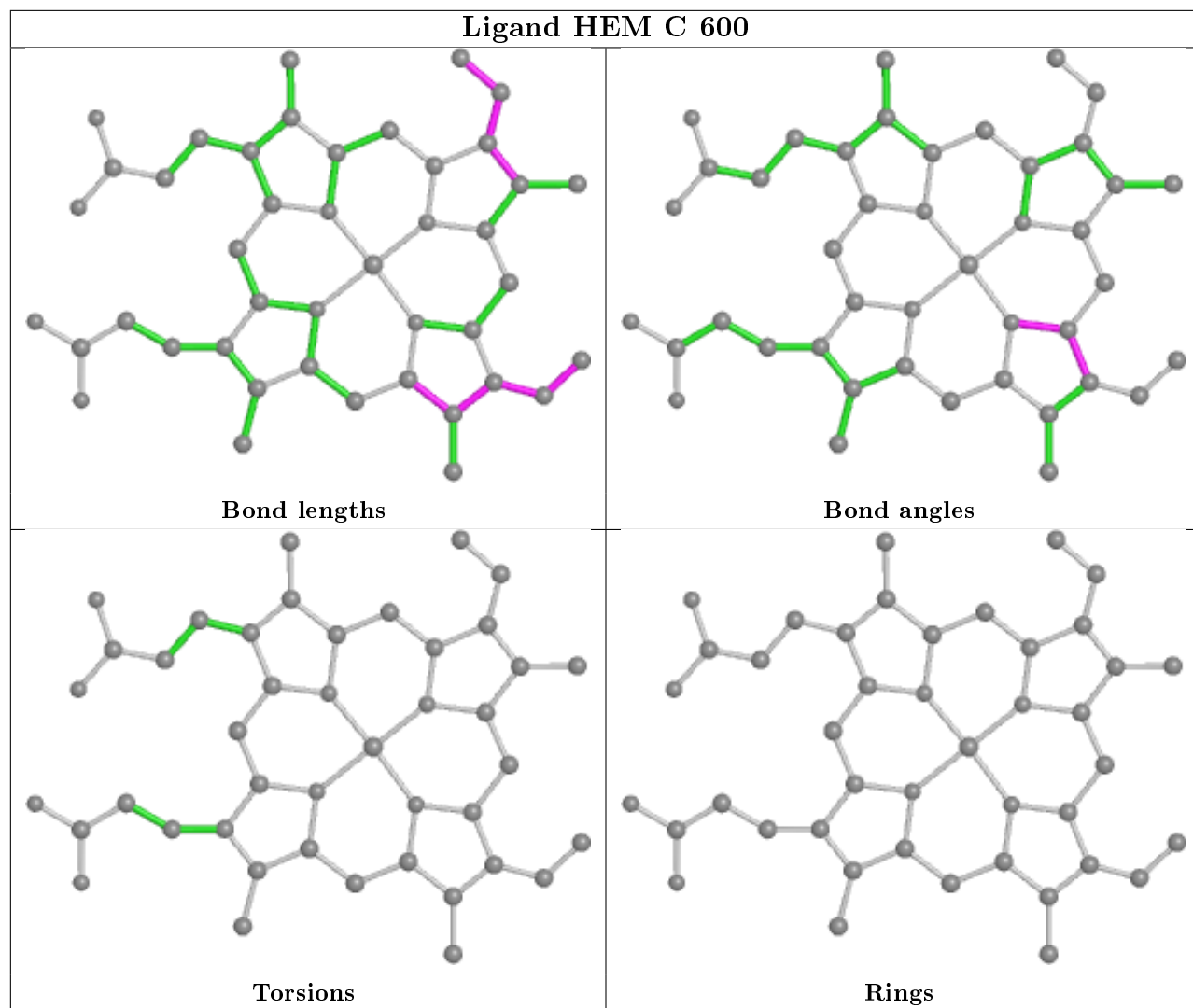
4 monomers are involved in 8 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	A	600	HEM	2	0
2	B	600	HEM	3	0
2	C	600	HEM	2	0
2	D	600	HEM	1	0

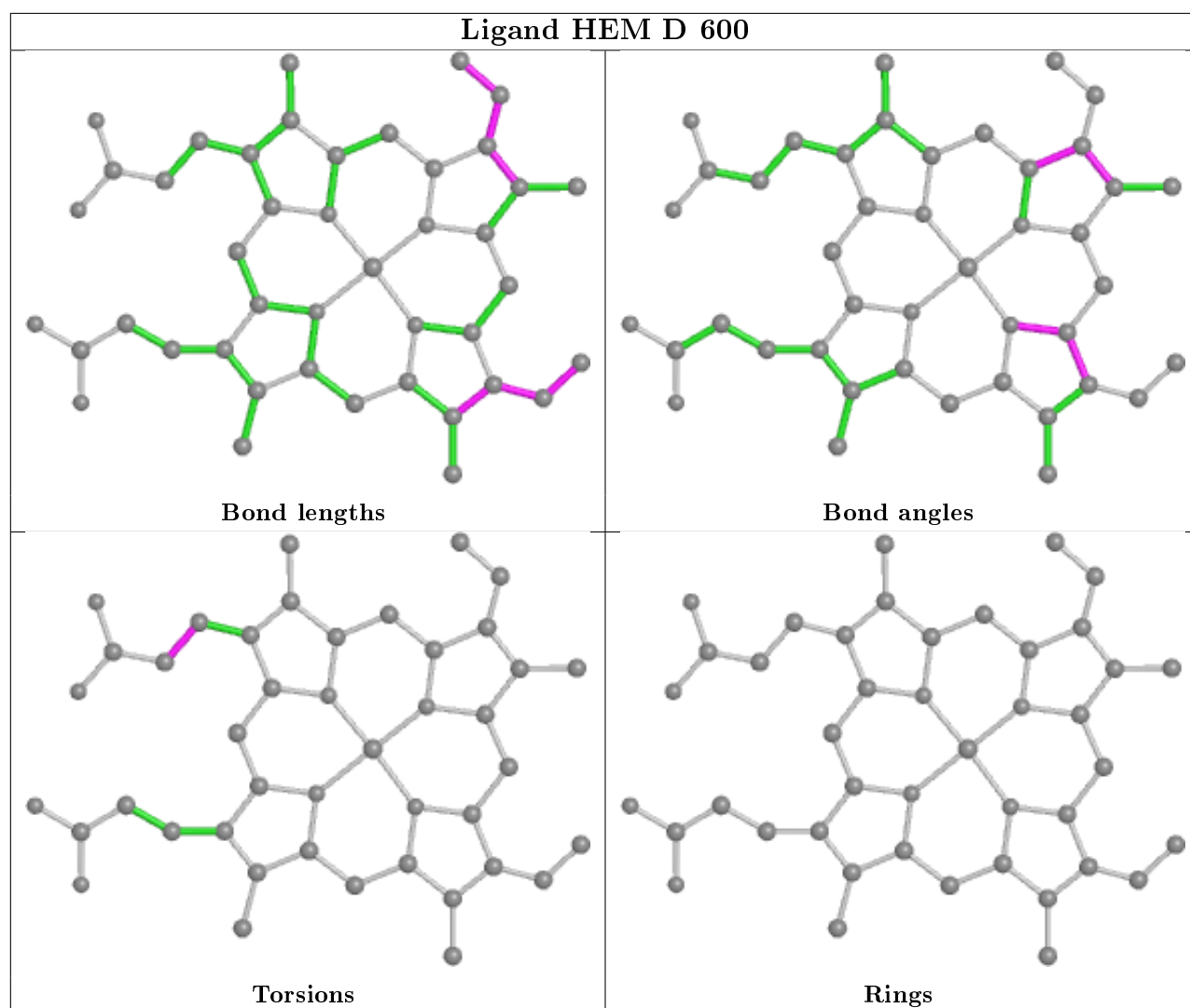
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included.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











## 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 ⓘ

Unable to reproduce the depositors R factor - this section is therefore empty.

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

Unable to reproduce the depositors R factor - this section is therefore empty.

### 6.3 Carbohydrates ⓘ

Unable to reproduce the depositors R factor - this section is therefore empty.

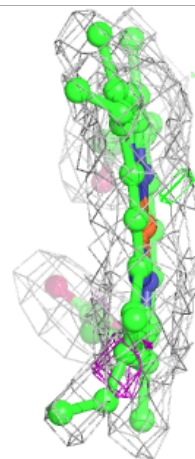
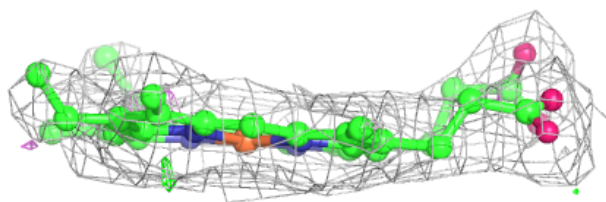
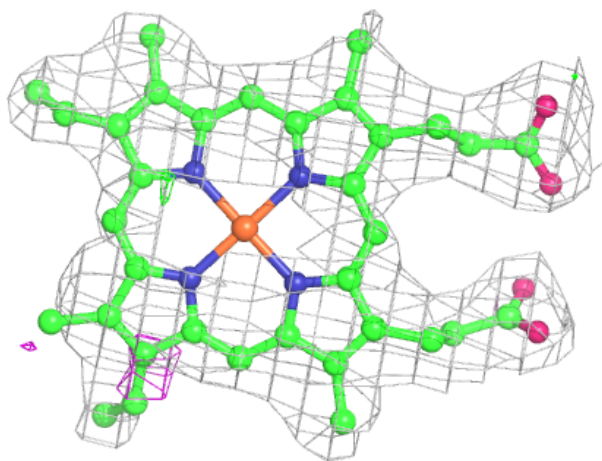
### 6.4 Ligands ⓘ

Unable to reproduce the depositors R factor - this section is therefore empty.

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.

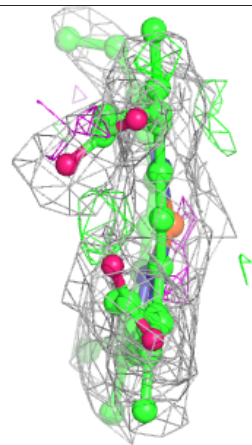
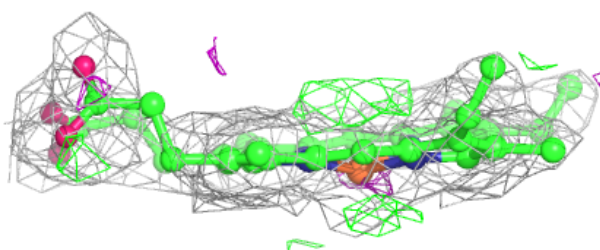
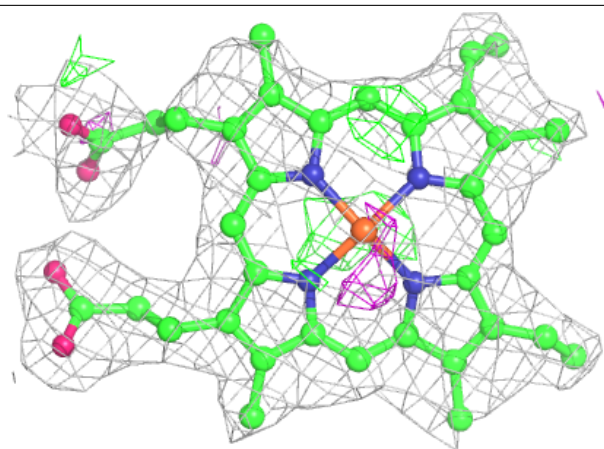
**Electron density around HEM A 600:**

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



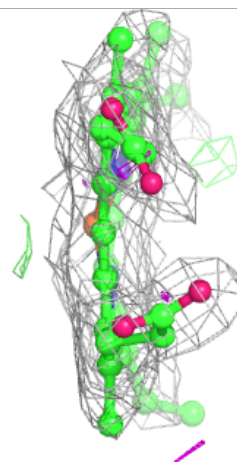
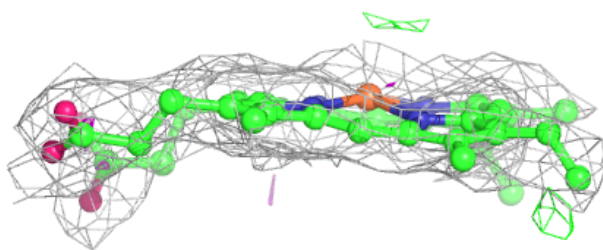
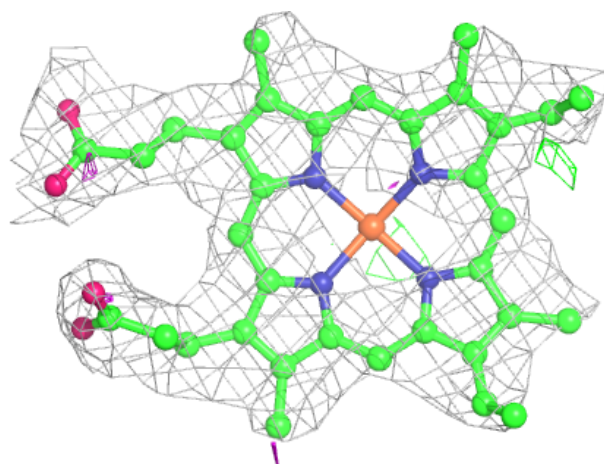
**Electron density around HEM B 600:**

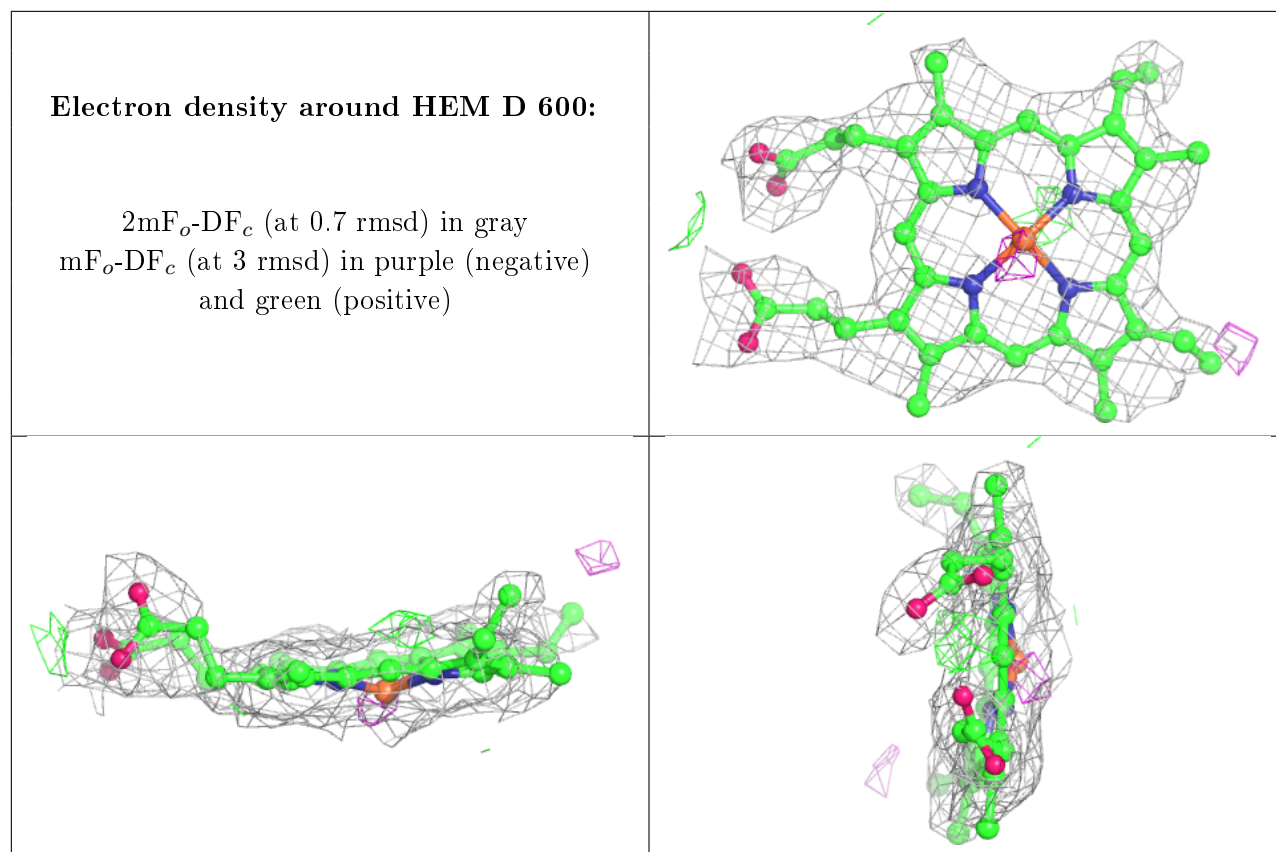
$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)



**Electron density around HEM C 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](#)

Unable to reproduce the depositor's R factor - this section is therefore empty.