



# wwPDB X-ray Structure Validation Summary Report ⓘ

May 15, 2020 – 03:49 am BST

PDB ID : 5WHS  
Title : Crystal structure of the catalase-peroxidase from *Neurospora crassa* at 2.6 Å  
Authors : Diaz-Vilchis, A.; Vega-Garcia, V.; Rudino-Pinera, E.; Hansberg, W.  
Deposited on : 2017-07-18  
Resolution : 2.60 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

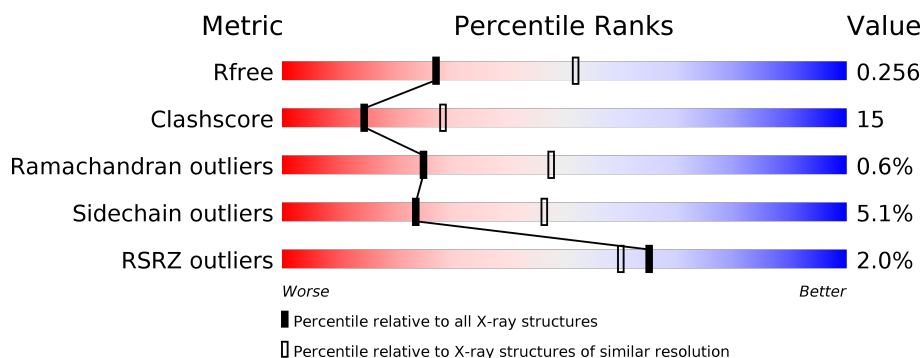
# 1 Overall quality at a glance ⓘ

The following experimental techniques were used to determine the structure:

## *X-RAY DIFFRACTION*

The reported resolution of this entry is 2.60 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	3163 (2.60-2.60)
Clashscore	141614	3518 (2.60-2.60)
Ramachandran outliers	138981	3455 (2.60-2.60)
Sidechain outliers	138945	3455 (2.60-2.60)
RSRZ outliers	127900	3104 (2.60-2.60)

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  $\leq 5\%$ . 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	768	<div> <div>2%</div> <div> <div></div> <div>67%</div> <div>23%</div> <div>• 7%</div> </div> </div>
1	B	768	<div> <div>%</div> <div> <div></div> <div>66%</div> <div>23%</div> <div>• 7%</div> </div> </div>

## 2 Entry composition

There are 3 unique types of molecules in this entry. The entry contains 11962 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-peroxidase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	713	Total	C	N	O	S	0	0	0
			5597	3555	977	1053	12			
1	B	713	Total	C	N	O	S	0	0	0
			5597	3555	977	1053	12			

There are 66 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	-14	MET	-	expression tag	UNP Q8X182
A	-13	ARG	-	expression tag	UNP Q8X182
A	-12	GLY	-	expression tag	UNP Q8X182
A	-11	SER	-	expression tag	UNP Q8X182
A	-10	HIS	-	expression tag	UNP Q8X182
A	-9	HIS	-	expression tag	UNP Q8X182
A	-8	HIS	-	expression tag	UNP Q8X182
A	-7	HIS	-	expression tag	UNP Q8X182
A	-6	HIS	-	expression tag	UNP Q8X182
A	-5	HIS	-	expression tag	UNP Q8X182
A	-4	GLY	-	expression tag	UNP Q8X182
A	-3	SER	-	expression tag	UNP Q8X182
A	-2	ALA	-	expression tag	UNP Q8X182
A	-1	CYS	-	expression tag	UNP Q8X182
A	0	GLU	-	expression tag	UNP Q8X182
A	1	LEU	-	expression tag	UNP Q8X182
A	2	SER	-	expression tag	UNP Q8X182
A	3	GLU	-	expression tag	UNP Q8X182
A	4	CYS	-	expression tag	UNP Q8X182
A	5	PRO	-	expression tag	UNP Q8X182
A	6	VAL	-	expression tag	UNP Q8X182
A	742	LYS	-	expression tag	UNP Q8X182
A	743	GLN	-	expression tag	UNP Q8X182
A	744	GLU	-	expression tag	UNP Q8X182
A	745	GLY	-	expression tag	UNP Q8X182

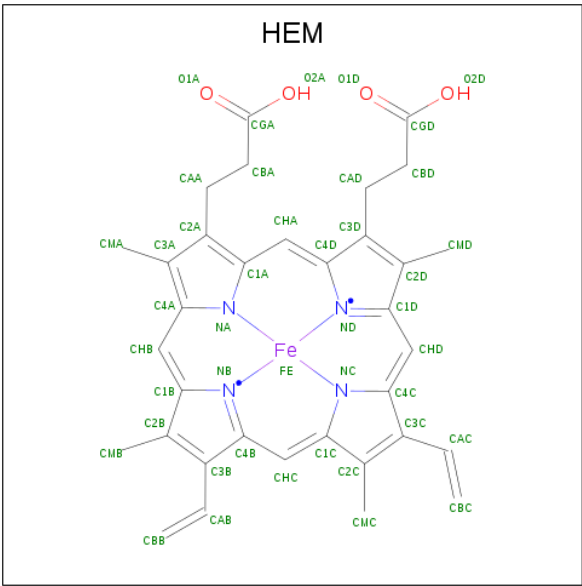
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Chain	Residue	Modelled	Actual	Comment	Reference
A	746	ARG	-	expression tag	UNP Q8X182
A	747	GLY	-	expression tag	UNP Q8X182
A	748	GLN	-	expression tag	UNP Q8X182
A	749	ASN	-	expression tag	UNP Q8X182
A	750	ALA	-	expression tag	UNP Q8X182
A	751	PRO	-	expression tag	UNP Q8X182
A	752	LYS	-	expression tag	UNP Q8X182
A	753	LEU	-	expression tag	UNP Q8X182
B	-14	MET	-	expression tag	UNP Q8X182
B	-13	ARG	-	expression tag	UNP Q8X182
B	-12	GLY	-	expression tag	UNP Q8X182
B	-11	SER	-	expression tag	UNP Q8X182
B	-10	HIS	-	expression tag	UNP Q8X182
B	-9	HIS	-	expression tag	UNP Q8X182
B	-8	HIS	-	expression tag	UNP Q8X182
B	-7	HIS	-	expression tag	UNP Q8X182
B	-6	HIS	-	expression tag	UNP Q8X182
B	-5	HIS	-	expression tag	UNP Q8X182
B	-4	GLY	-	expression tag	UNP Q8X182
B	-3	SER	-	expression tag	UNP Q8X182
B	-2	ALA	-	expression tag	UNP Q8X182
B	-1	CYS	-	expression tag	UNP Q8X182
B	0	GLU	-	expression tag	UNP Q8X182
B	1	LEU	-	expression tag	UNP Q8X182
B	2	SER	-	expression tag	UNP Q8X182
B	3	GLU	-	expression tag	UNP Q8X182
B	4	CYS	-	expression tag	UNP Q8X182
B	5	PRO	-	expression tag	UNP Q8X182
B	6	VAL	-	expression tag	UNP Q8X182
B	742	LYS	-	expression tag	UNP Q8X182
B	743	GLN	-	expression tag	UNP Q8X182
B	744	GLU	-	expression tag	UNP Q8X182
B	745	GLY	-	expression tag	UNP Q8X182
B	746	ARG	-	expression tag	UNP Q8X182
B	747	GLY	-	expression tag	UNP Q8X182
B	748	GLN	-	expression tag	UNP Q8X182
B	749	ASN	-	expression tag	UNP Q8X182
B	750	ALA	-	expression tag	UNP Q8X182
B	751	PRO	-	expression tag	UNP Q8X182
B	752	LYS	-	expression tag	UNP Q8X182
B	753	LEU	-	expression tag	UNP Q8X182

- Molecule 2 is PROTOPORPHYRIN IX CONTAINING FE (three-letter code: HEM) (for-

mula: C<sub>34</sub>H<sub>32</sub>FeN<sub>4</sub>O<sub>4</sub>).



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		

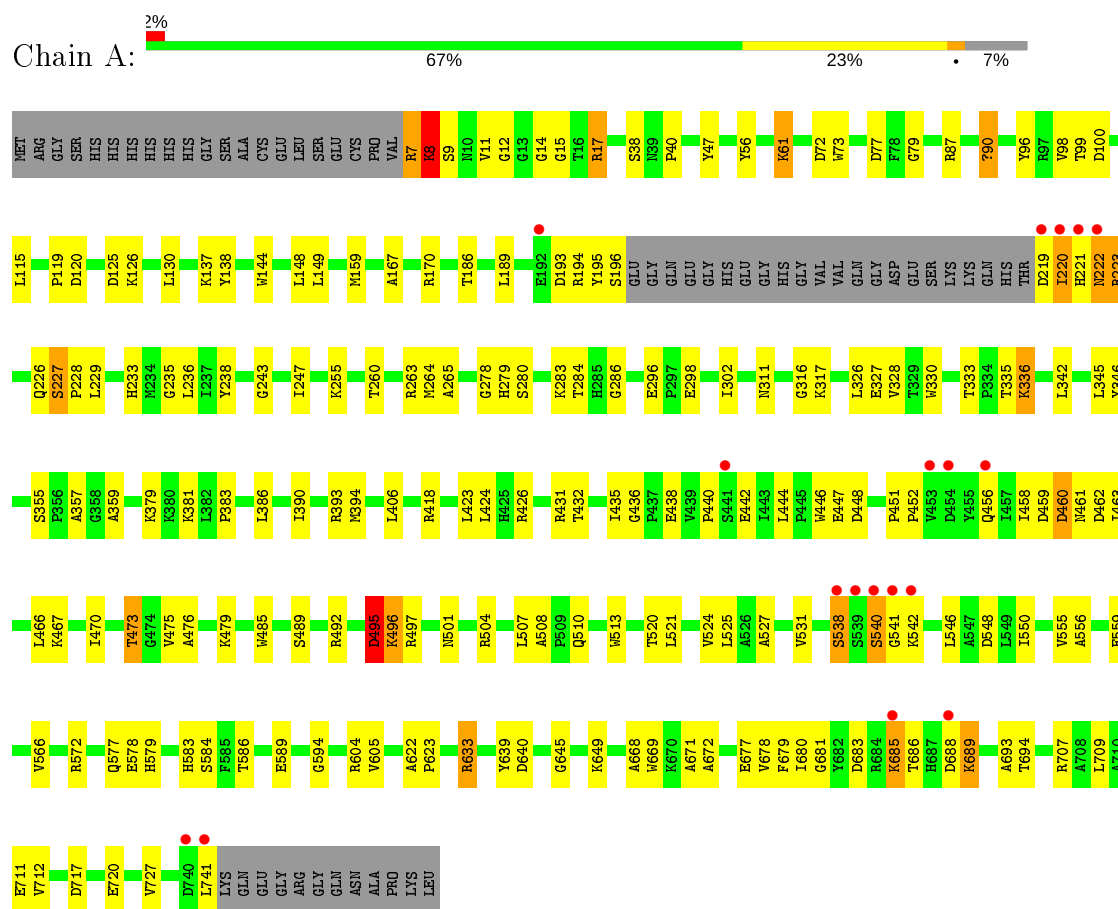
- Molecule 3 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	314	Total	O	0	0
			314	314		
3	B	368	Total	O	0	0
			368	368		

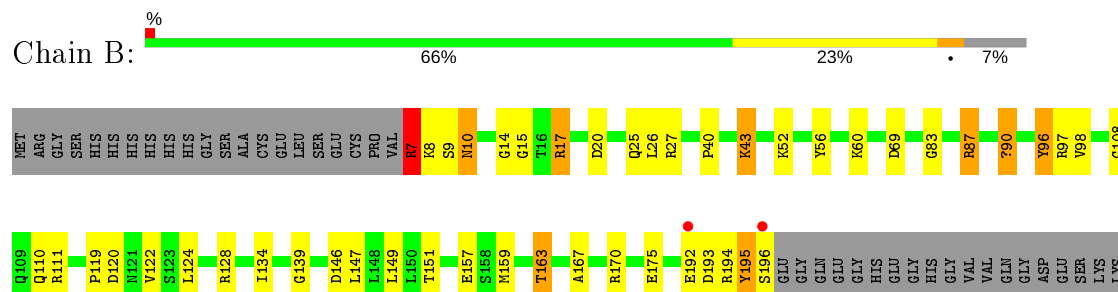
### 3 Residue-property plots [i](#)

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 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: Catalase-peroxidase



#### • Molecule 1: Catalase-peroxidase



K690	V566	E447	V328	GLN
G701	D448	D454	T329	HIS
R707	A575	Q455	W330	THR
A708	E578	Y456	T335	D219
L709	Q456	I457	K347	I220
A710	H583	I458	F348	H221
E711	S584	I463	E351	N222
V712	F585	K467	K361	R223
F726	T586	I470	W362	D224
V727	F595	T473	K365	S231
V733	Y598	I481	W366	S232
F739	K600	I485	I371	H233
D740	K603	A488	K381	K234
L741	R604	S489	L382	G235
LYS	V605	S490	K385	L236
GLN	R614	S491	L386	I237
GLY	A622	R492	D889	Y238
ARG	P623	D495	T390	D245
GLY	I629	R504	A391	V251
GLN	G630	T505	I401	A252
ASN	G631	R506	C402	S253
ALA	L632	Q510	R403	A254
PRO	R633	V515	D404	T260
LYS	V634	L521	K411	M264
LEU	L635	L525	R418	A265
	L635	A526	A419	K266
	Y639	A527	W420	N267
	D640	N665	I423	D268
	L647	N666	L424	E269
	T648	W669	P430	E270
	T665	K670	R431	G277
	N666	A671	T432	Q278
		A672	R433	H279
		D673	W434	S280
		N674	I435	K283
		E675	E438	T284
		V678	V439	H292
		I680	P440	K295
		K685	S441	A299
		T686	E442	W309
		H687	I443	A310
			L444	N311
			W446	S312
				F313
				G316
				L326
				E327

## 4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	71.81Å 142.35Å 183.11Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	112.38 – 2.60 56.50 – 2.60	Depositor EDS
% Data completeness (in resolution range)	99.9 (112.38-2.60) 99.9 (56.50-2.60)	Depositor EDS
$R_{merge}$	0.07	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	2.32 (at 2.61Å)	Xtriage
Refinement program	REFMAC 5.8.0107	Depositor
R, $R_{free}$	0.209 , 0.254 0.212 , 0.256	Depositor DCC
$R_{free}$ test set	2000 reflections (3.42%)	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	28.4	Xtriage
Anisotropy	0.058	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.33 , 41.3	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	0.92	EDS
Total number of atoms	11962	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	28.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.74% 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, TOX

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	1.13	2/5734 (0.0%)	0.86	2/7791 (0.0%)
1	B	1.37	6/5734 (0.1%)	0.98	10/7791 (0.1%)
All	All	1.26	8/11468 (0.1%)	0.92	12/15582 (0.1%)

Chiral center outliers are detected by calculating the chiral volume of a chiral center and verifying if the center is modelled as a planar moiety or with the opposite hand. A planarity outlier is detected by checking planarity of atoms in a peptide group, atoms in a mainchain group or atoms of a sidechain that are expected to be planar.

Mol	Chain	#Chirality outliers	#Planarity outliers
1	A	0	1
1	B	0	1
All	All	0	2

The worst 5 of 8 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	327	GLU	CD-OE1	-6.08	1.19	1.25
1	B	195	TYR	CE1-CZ	-5.49	1.31	1.38
1	B	584	SER	CB-OG	-5.37	1.35	1.42
1	B	96	TYR	CE1-CZ	-5.17	1.31	1.38
1	A	47	TYR	CE1-CZ	-5.13	1.31	1.38

The worst 5 of 12 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	100	ASP	CB-CG-OD1	6.49	124.14	118.30
1	B	629	ILE	CG1-CB-CG2	-6.19	97.78	111.40
1	B	418	ARG	NE-CZ-NH1	6.16	123.38	120.30
1	B	69	ASP	CB-CG-OD1	6.06	123.75	118.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	27	ARG	NE-CZ-NH2	6.01	123.31	120.30

There are no chirality outliers.

All (2) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	90	TOX	Mainchain
1	B	90	TOX	Mainchain

## 5.2 Too-close contacts ⓘ

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	5597	0	5411	189	0
1	B	5597	0	5411	162	0
2	A	43	0	30	5	0
2	B	43	0	30	7	0
3	A	314	0	0	12	2
3	B	368	0	0	10	2
All	All	11962	0	10882	342	2

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 15.

The worst 5 of 342 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:284:THR:OG1	1:A:326:LEU:O	1.62	1.17
1:B:431:ARG:NH2	1:B:440:PRO:O	1.85	1.08
1:A:219:ASP:O	1:A:220:ILE:HG13	1.55	1.06
1:B:267:ASN:OD1	1:B:270:GLU:HG3	1.56	1.04
1:A:8:LYS:HA	1:A:15:GLY:H	1.21	1.01

All (2) 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)
3:A:1179:HOH:O	3:B:949:HOH:O[3_555]	2.14	0.06
3:A:1200:HOH:O	3:B:1177:HOH:O[3_555]	2.15	0.05

## 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	708/768 (92%)	672 (95%)	33 (5%)	3 (0%)	34 57
1	B	708/768 (92%)	682 (96%)	21 (3%)	5 (1%)	22 43
All	All	1416/1536 (92%)	1354 (96%)	54 (4%)	8 (1%)	25 47

5 of 8 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	8	LYS
1	A	220	ILE
1	A	460	ASP
1	B	220	ILE
1	B	10	ASN

### 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	577/621 (93%)	546 (95%)	31 (5%)	22 44
1	B	577/621 (93%)	549 (95%)	28 (5%)	25 48

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
All	All	1154/1242 (93%)	1095 (95%)	59 (5%)	24 46

5 of 59 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	688	ASP
1	B	60	LYS
1	B	629	ILE
1	A	689	LYS
1	A	727	VAL

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 14 such sidechains are listed below:

Mol	Chain	Res	Type
1	A	638	ASN
1	B	221	HIS
1	B	533	GLN
1	A	577	GLN
1	B	510	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
1	TOX	B	90	1	10,17,18	2.65	3 (30%)	10,23,25	1.35	1 (10%)
1	TOX	A	90	1	10,17,18	2.67	4 (40%)	10,23,25	1.51	3 (30%)

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
1	TOX	B	90	1	-	2/4/8/10	0/2/2/2
1	TOX	A	90	1	-	2/4/8/10	0/2/2/2

The worst 5 of 7 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	90	TOX	CD1-NE1	-5.18	1.34	1.39
1	B	90	TOX	O-C	5.10	1.40	1.19
1	A	90	TOX	O-C	5.09	1.40	1.19
1	B	90	TOX	CD1-NE1	-5.00	1.34	1.39
1	B	90	TOX	CE3-CD2	-2.83	1.36	1.42

All (4) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	90	TOX	CZ3-CH2-CZ2	-2.66	116.71	120.44
1	A	90	TOX	CZ3-CH2-CZ2	-2.54	116.88	120.44
1	A	90	TOX	CZ3-CE3-CD2	-2.40	117.56	120.89
1	A	90	TOX	CE3-CD2-CG	-2.01	130.72	134.42

There are no chirality outliers.

All (4) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
1	B	90	TOX	N-CA-CB-CG
1	B	90	TOX	C-CA-CB-CG
1	A	90	TOX	N-CA-CB-CG
1	A	90	TOX	C-CA-CB-CG

There are no ring outliers.

2 monomers are involved in 4 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
1	B	90	TOX	2	0
1	A	90	TOX	2	0

## 5.5 Carbohydrates

There are no carbohydrates in this entry.

## 5.6 Ligand geometry

2 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	B	800	1	27,50,50	0.75	1 (3%)	17,82,82	1.17	1 (5%)
2	HEM	A	800	1	27,50,50	0.84	1 (3%)	17,82,82	1.21	1 (5%)

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	B	800	1	-	0/6/54/54	-
2	HEM	A	800	1	-	0/6/54/54	-

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	800	HEM	C3B-C2B	-2.83	1.36	1.40
2	B	800	HEM	C3B-C2B	-2.45	1.37	1.40

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	A	800	HEM	CAD-CBD-CGD	-2.09	109.16	112.67
2	B	800	HEM	CAA-CBA-CGA	-2.08	109.17	112.67

There are no chirality outliers.

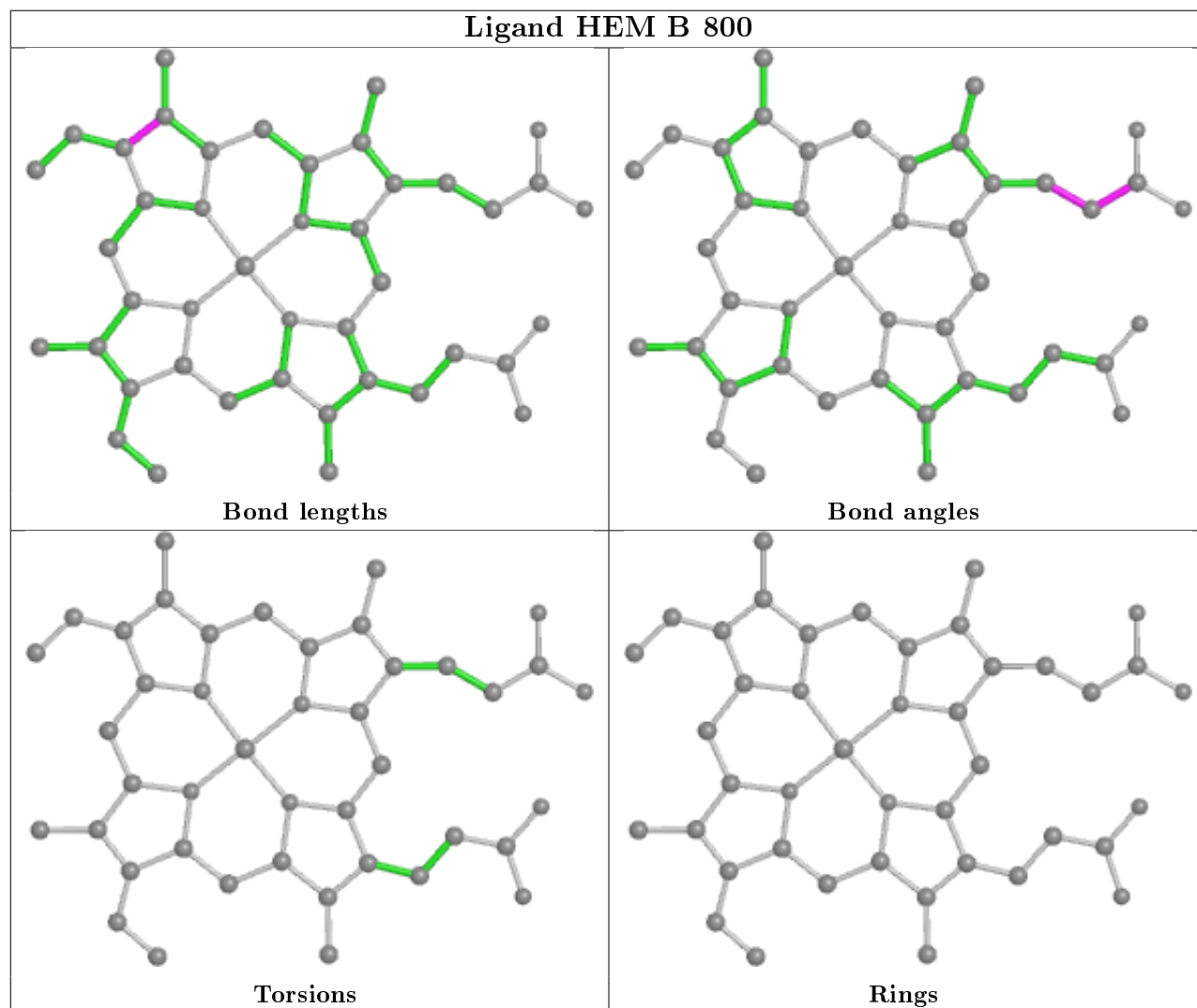
There are no torsion outliers.

There are no ring outliers.

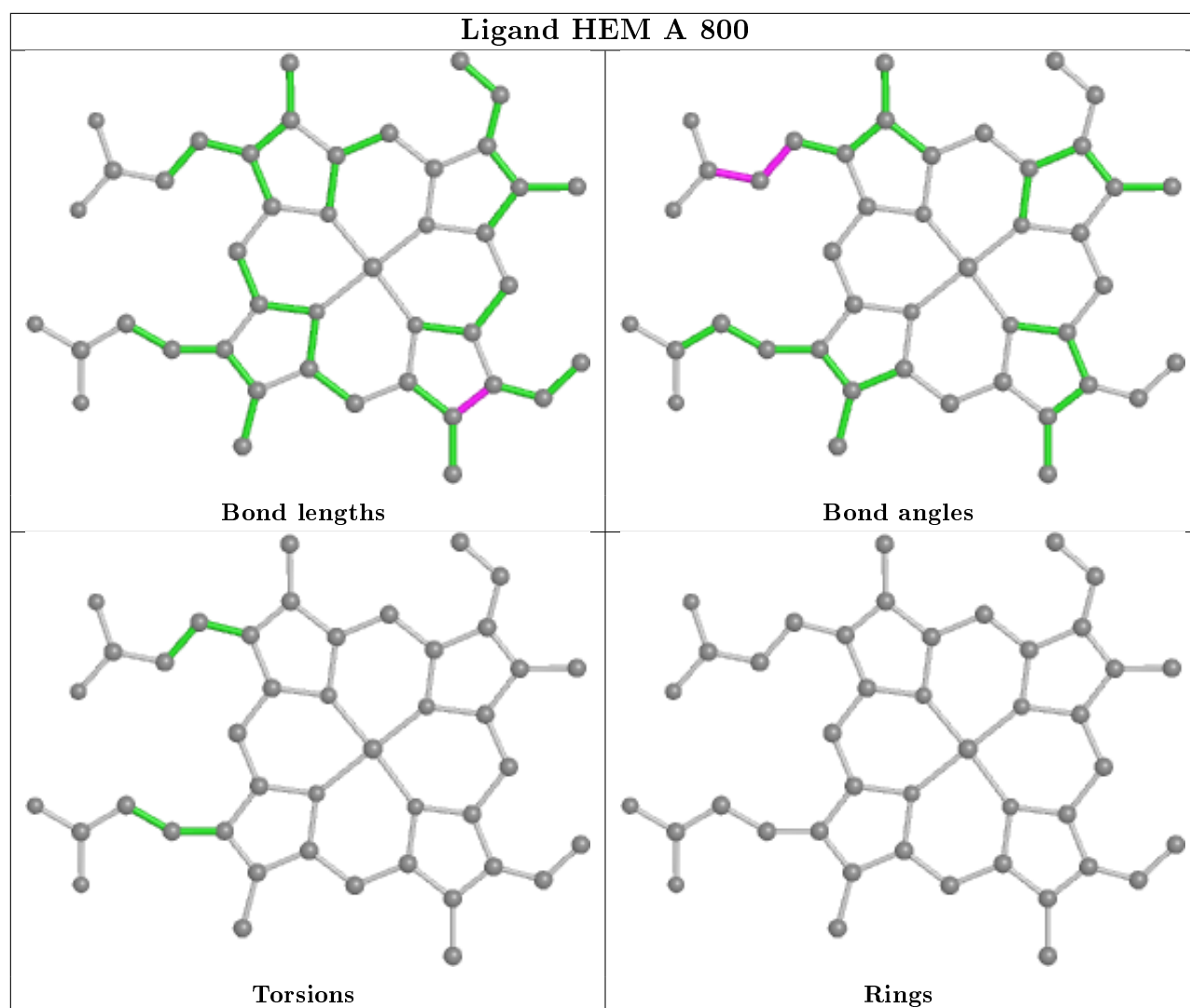
2 monomers are involved in 12 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	B	800	HEM	7	0
2	A	800	HEM	5	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 [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	712/768 (92%)	-0.17	18 (2%) 57 51	14, 29, 49, 91	0
1	B	712/768 (92%)	-0.26	11 (1%) 73 70	13, 24, 47, 106	0
All	All	1424/1536 (92%)	-0.21	29 (2%) 65 60	13, 27, 48, 106	0

The worst 5 of 29 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	538	SER	5.9
1	B	221	HIS	4.8
1	B	219	ASP	4.6
1	B	222	ASN	4.6
1	A	219	ASP	3.9

### 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
1	TOX	A	90	16/17	0.95	0.16	21,23,28,33	0
1	TOX	B	90	16/17	0.96	0.14	12,14,19,23	0

### 6.3 Carbohydrates [i](#)

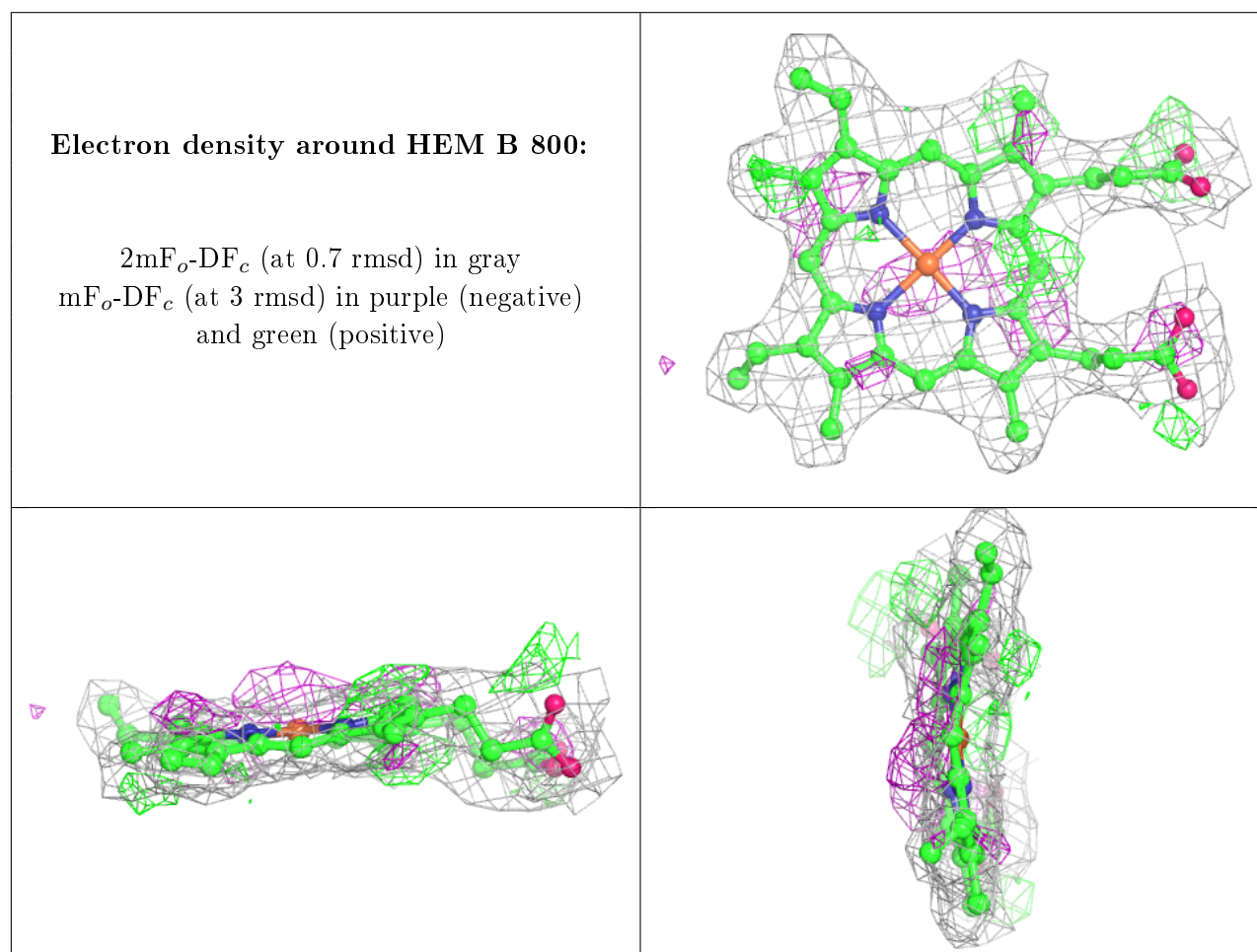
There are no carbohydrates in this entry.

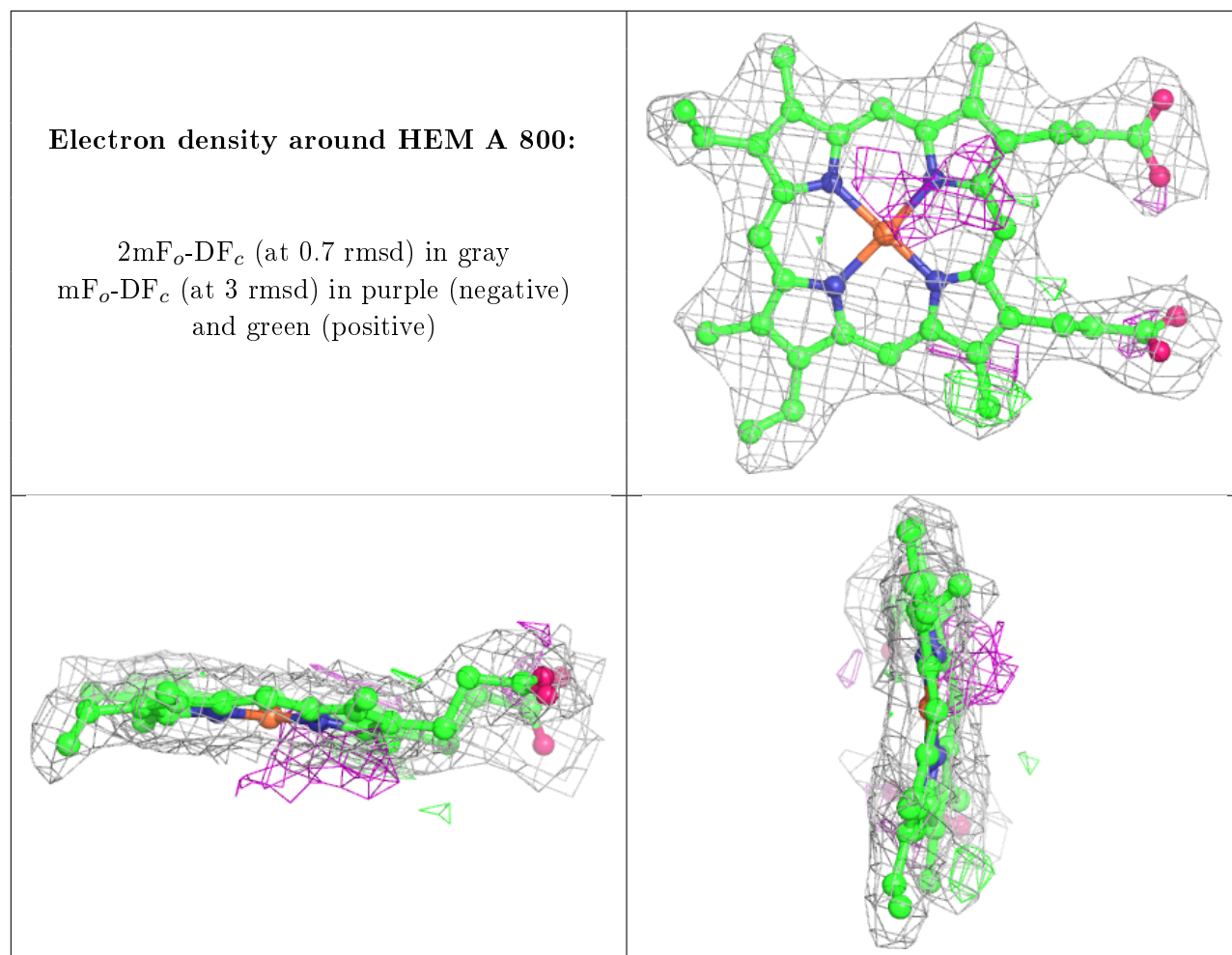
## 6.4 Ligands ⓘ

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	HEM	B	800	43/43	0.91	0.19	16,18,19,20	0
2	HEM	A	800	43/43	0.93	0.18	22,24,28,31	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.





## 6.5 Other polymers ⓘ

There are no such residues in this entry.