wwPDB X-ray Structure Validation Summary Report (i)

Aug 25, 2026 – 03:01 am BST

PDB ID	:	6TB2 / pdb_00006tb2
Title	:	Structure of human haptoglobin-hemoglobin bound to S. aureus IsdH
Authors	:	Mikkelsen, J.H.; Andersen, C.B.F.
Deposited on	:	2019-10-31
Resolution	:	2.90 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 (i) 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 (i)) were used in the production of this report:

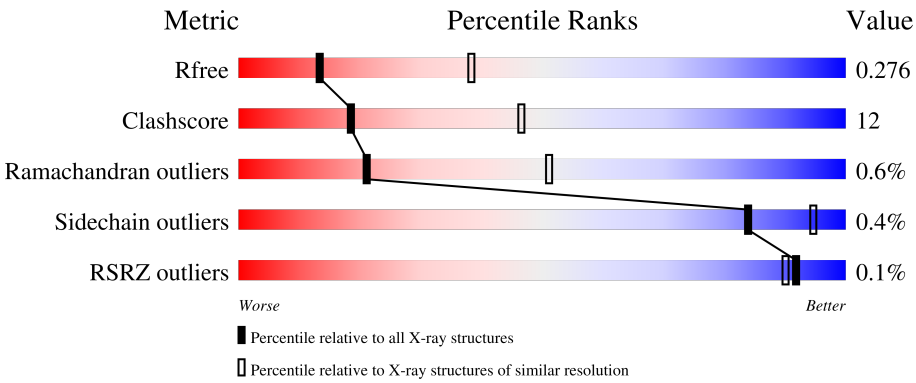
MolProbity	:	4-5-2 with Phenix2.0
Mogul	:	1.8.4, CSD as541be (2020)
Xtriage (Phenix)	:	2.0
EDS	:	3.0
Buster-report	:	wwPDB partial adaption of 1.1.7 (2018)
Percentile statistics	:	20250101.v01 (using entries in the PDB archive January 1st 2025)
CCP4	:	9.0.015 (Gargrove)
Density-Fitness	:	1.0.12
Ideal 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 (i)

The following experimental techniques were used to determine the structure:
X-RAY DIFFRACTION

The reported resolution of this entry is 2.90 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	2481 (2.90-2.90)
Clashscore	190562	2690 (2.90-2.90)
Ramachandran outliers	187476	2623 (2.90-2.90)
Sidechain outliers	187428	2625 (2.90-2.90)
RSRZ outliers	180081	2481 (2.90-2.90)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments of the lower bar indicate the fraction of residues that contain outliers for >=3, 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions <=5% The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density. The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	A	141	78% 22%
2	B	146	76% 23% •
3	C	267	81% 15% •
4	D	354	68% 25% • 6%
4	E	354	65% 29% 6%

2 Entry composition (i)

There are 5 unique types of molecules in this entry. The entry contains 9750 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 Hemoglobin subunit alpha.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	A	141	1069	685	187	194	3	0	0	0

- Molecule 2 is a protein called Hemoglobin subunit beta.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
2	B	146	1123	724	195	201	3	0	0	0

- Molecule 3 is a protein called Haptoglobin.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
3	C	256	1989	1270	333	376	10	0	0	0

There are 12 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
C	140	HIS	-	expression tag	UNP P00738
C	141	HIS	-	expression tag	UNP P00738
C	142	HIS	-	expression tag	UNP P00738
C	143	HIS	-	expression tag	UNP P00738
C	144	HIS	-	expression tag	UNP P00738
C	145	HIS	-	expression tag	UNP P00738
C	146	HIS	-	expression tag	UNP P00738
C	147	HIS	-	expression tag	UNP P00738
C	184	SER	ASN	conflict	UNP P00738
C	207	SER	ASN	conflict	UNP P00738
C	211	SER	ASN	conflict	UNP P00738
C	241	SER	ASN	conflict	UNP P00738

- Molecule 4 is a protein called Cell wall surface anchor family protein.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
4	D	333	2720	1738	440	538	4	0	0	0
4	E	333	2720	1738	440	538	4	0	0	0

There are 40 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
D	302	HIS	-	expression tag	UNP A0A0E8IWL6
D	303	HIS	-	expression tag	UNP A0A0E8IWL6
D	304	HIS	-	expression tag	UNP A0A0E8IWL6
D	305	HIS	-	expression tag	UNP A0A0E8IWL6
D	306	HIS	-	expression tag	UNP A0A0E8IWL6
D	307	HIS	-	expression tag	UNP A0A0E8IWL6
D	308	SER	-	expression tag	UNP A0A0E8IWL6
D	309	SER	-	expression tag	UNP A0A0E8IWL6
D	310	GLY	-	expression tag	UNP A0A0E8IWL6
D	311	LEU	-	expression tag	UNP A0A0E8IWL6
D	312	VAL	-	expression tag	UNP A0A0E8IWL6
D	313	PRO	-	expression tag	UNP A0A0E8IWL6
D	314	ARG	-	expression tag	UNP A0A0E8IWL6
D	315	GLY	-	expression tag	UNP A0A0E8IWL6
D	316	SER	-	expression tag	UNP A0A0E8IWL6
D	317	HIS	-	expression tag	UNP A0A0E8IWL6
D	318	MET	-	expression tag	UNP A0A0E8IWL6
D	319	LEU	-	expression tag	UNP A0A0E8IWL6
D	320	GLU	-	expression tag	UNP A0A0E8IWL6
D	642	ALA	TYR	conflict	UNP A0A0E8IWL6
E	302	HIS	-	expression tag	UNP A0A0E8IWL6
E	303	HIS	-	expression tag	UNP A0A0E8IWL6
E	304	HIS	-	expression tag	UNP A0A0E8IWL6
E	305	HIS	-	expression tag	UNP A0A0E8IWL6
E	306	HIS	-	expression tag	UNP A0A0E8IWL6
E	307	HIS	-	expression tag	UNP A0A0E8IWL6
E	308	SER	-	expression tag	UNP A0A0E8IWL6
E	309	SER	-	expression tag	UNP A0A0E8IWL6
E	310	GLY	-	expression tag	UNP A0A0E8IWL6
E	311	LEU	-	expression tag	UNP A0A0E8IWL6
E	312	VAL	-	expression tag	UNP A0A0E8IWL6
E	313	PRO	-	expression tag	UNP A0A0E8IWL6
E	314	ARG	-	expression tag	UNP A0A0E8IWL6
E	315	GLY	-	expression tag	UNP A0A0E8IWL6
E	316	SER	-	expression tag	UNP A0A0E8IWL6

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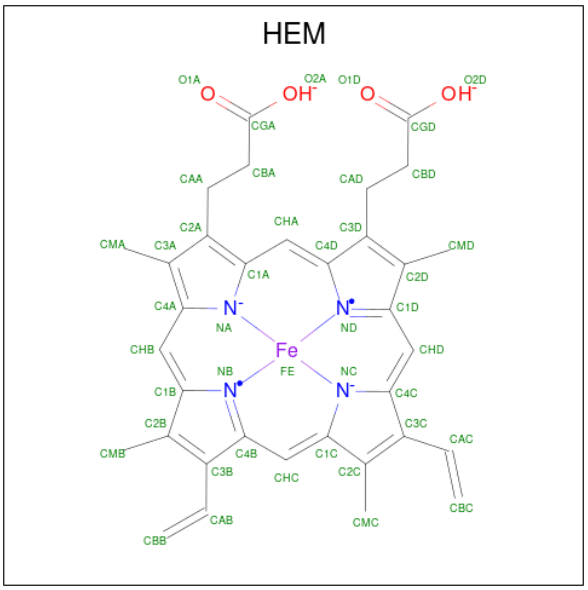
Chain	Residue	Modelled	Actual	Comment	Reference
E	317	HIS	-	expression tag	UNP A0A0E8IWL6
E	318	MET	-	expression tag	UNP A0A0E8IWL6
E	319	LEU	-	expression tag	UNP A0A0E8IWL6
E	320	GLU	-	expression tag	UNP A0A0E8IWL6
E	642	ALA	TYR	conflict	UNP A0A0E8IWL6

- Molecule 5 is PROTOPORPHYRIN IX CONTAINING FE (CCD ID: HEM) (formula: $C_{34}H_{32}FeN_4O_4$) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
			Total	C	Fe	N	O		
5	A	1	43	34	1	4	4	0	0
			Total	C	Fe	N	O		
5	B	1	86	68	2	8	8	0	1

3 Residue-property plots (i)

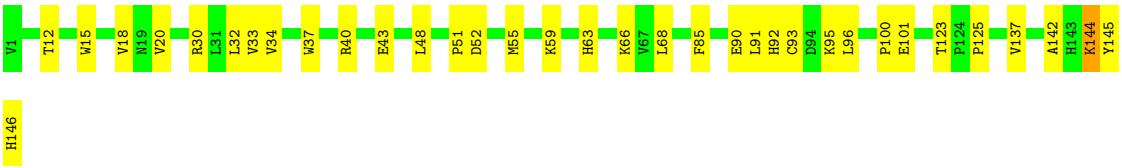
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. 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: Hemoglobin subunit alpha

Chain A:

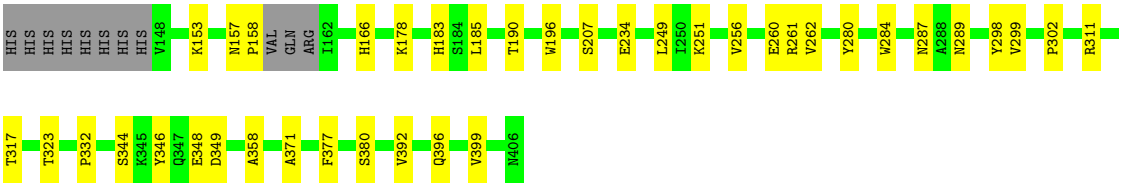
- Molecule 2: Hemoglobin subunit beta

Chain B:



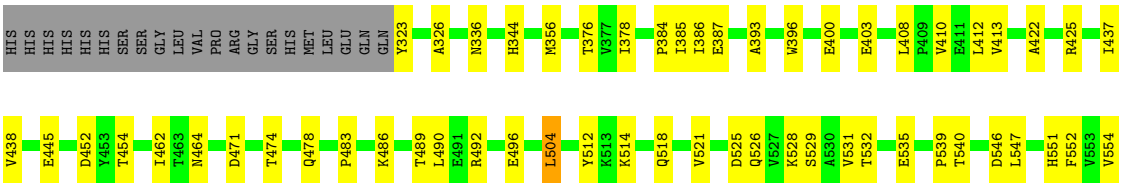
- Molecule 3: Haptoglobin

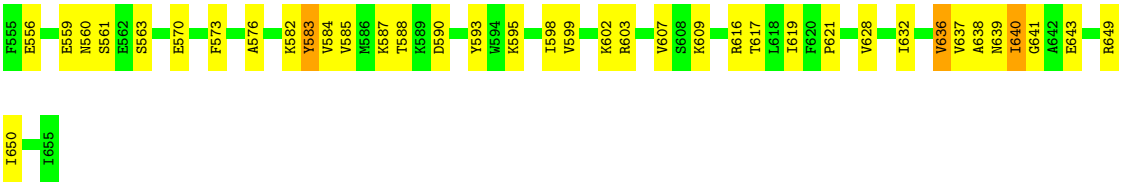
Chain C:



- Molecule 4: Cell wall surface anchor family protein

Chain D:





• Molecule 4: Cell wall surface anchor family protein

Chain E:

4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α, β, γ	84.10Å 86.77Å 217.95Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	78.46 – 2.90 78.46 – 2.90	Depositor EDS
% Data completeness (in resolution range)	99.2 (78.46-2.90) 99.4 (78.46-2.90)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	1.41 (at 2.91Å)	Xtriage
Refinement program	PHENIX 1.16_3549	Depositor
R, R_{free}	0.235 , 0.270 0.243 , 0.276	Depositor DCC
R_{free} test set	1994 reflections (5.50%)	wwPDB-VP
Wilson B-factor (Å^2)	117.5	Xtriage
Anisotropy	0.030	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.32 , 87.6	EDS
L-test for twinning[2]	$< \|L\| > = 0.48$, $< L^2 > = 0.31$	Xtriage
Estimated twinning fraction	0.022 for k,h,-l	Xtriage
F_o,F_c correlation	0.95	EDS
Total number of atoms	9750	wwPDB-VP
Average B, all atoms (Å^2)	134.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.54% of the height of the origin peak. No significant pseudotranslation is detected.*

[1]Intensities estimated from amplitudes.

[2]Theoretical values of $< |L| >$, $< L^2 >$ for acentric reflections are 0.5, 0.333 respectively for untwinned datasets, and 0.375, 0.2 for perfectly twinned datasets.

5 Model quality (i)

5.1 Standard geometry (i)

Bond lengths and bond angles in the following residue types are not validated in this section: 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	0/1097	0.69	0/1491
2	B	0.29	0/1153	0.66	0/1566
3	C	0.30	0/2037	0.68	0/2767
4	D	0.25	0/2783	0.53	0/3779
4	E	0.26	0/2783	0.56	3/3779 (0.1%)
All	All	0.28	0/9853	0.61	3/13382 (0.0%)

There are no bond length outliers.

All (3) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
4	E	419	LYS	CB-CG-CD	9.47	133.08	111.30
4	E	419	LYS	CA-CB-CG	-8.09	97.93	114.10
4	E	419	LYS	CD-CE-NZ	-5.95	92.87	111.90

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	1069	0	1073	25	0
2	B	1123	0	1118	35	0
3	C	1989	0	1966	28	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
4	D	2720	0	2655	69	0
4	E	2720	0	2655	84	0
5	A	43	0	30	1	0
5	B	86	0	60	14	0
All	All	9750	0	9557	232	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 12.

The worst 5 of 232 close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:C:234:GLU:OE1	3:C:251:LYS:NZ	2.11	0.84
1:A:76:MET:HE1	1:A:132:VAL:HG22	1.60	0.83
4:D:540:THR:HG22	4:D:607:VAL:HA	1.61	0.83
1:A:7:LYS:NZ	1:A:74:ASP:OD1	2.11	0.82
4:E:403:GLU:HG2	4:E:408:LEU:HD11	1.63	0.79

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	139/141 (99%)	137 (99%)	2 (1%)	0	100 100
2	B	144/146 (99%)	139 (96%)	4 (3%)	1 (1%)	18 48
3	C	252/267 (94%)	240 (95%)	12 (5%)	0	100 100
4	D	331/354 (94%)	303 (92%)	24 (7%)	4 (1%)	10 34
4	E	331/354 (94%)	306 (92%)	23 (7%)	2 (1%)	21 51
All	All	1197/1262 (95%)	1125 (94%)	65 (5%)	7 (1%)	21 51

5 of 7 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
2	B	144	LYS
4	D	636	VAL
4	E	546	ASP
4	D	546	ASP
4	D	640	ILE

5.3.2 Protein sidechains (i)

In the following table, the Percentiles column shows the percent sidechain outliers of the chain as a percentile score with respect to all X-ray entries followed by that with respect to entries of similar resolution.

The Analysed column shows the number of residues for which the sidechain conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	113/113 (100%)	113 (100%)	0	100	100
2	B	118/118 (100%)	118 (100%)	0	100	100
3	C	219/230 (95%)	217 (99%)	2 (1%)	70	90
4	D	302/321 (94%)	301 (100%)	1 (0%)	86	96
4	E	302/321 (94%)	301 (100%)	1 (0%)	86	96
All	All	1054/1103 (96%)	1050 (100%)	4 (0%)	84	94

All (4) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
3	C	299	VAL
3	C	323	THR
4	D	583	TYR
4	E	419	LYS

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 10 such sidechains are listed below:

Mol	Chain	Res	Type
4	D	639	ASN
4	E	331	GLN
4	E	653	GLN
2	B	143	HIS
3	C	331	GLN

5.3.3 RNA (i)

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates (i)

There are no oligosaccharides in this entry.

5.6 Ligand geometry (i)

3 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	$\#\|Z\| > 2$
5	HEM	B	201[B]	2	50,50,50	1.53	9 (18%)	66,82,82	1.55	11 (16%)
5	HEM	A	201	1	50,50,50	1.50	5 (10%)	66,82,82	1.17	4 (6%)
5	HEM	B	201[A]	2	50,50,50	1.53	6 (12%)	66,82,82	1.34	8 (12%)

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	HEM	B	201[B]	2	-	6/14/54/54	-
5	HEM	A	201	1	-	3/14/54/54	-
5	HEM	B	201[A]	2	-	4/14/54/54	-

The worst 5 of 20 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
5	A	201	HEM	FE-ND	5.52	2.12	1.94
5	A	201	HEM	FE-NA	4.73	2.11	1.95
5	B	201[A]	HEM	FE-ND	4.65	2.09	1.94
5	B	201[B]	HEM	FE-ND	4.25	2.08	1.94
5	B	201[A]	HEM	FE-NB	4.15	2.07	1.94

The worst 5 of 23 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
5	B	201[B]	HEM	CAD-CBD-CGD	-4.42	104.09	113.60
5	B	201[B]	HEM	CAD-C3D-C2D	-3.75	120.90	127.88
5	B	201[A]	HEM	C3B-C2B-C1B	3.56	109.13	106.49
5	B	201[A]	HEM	CHC-C1C-NC	3.18	127.87	124.44
5	B	201[B]	HEM	C3B-C2B-C1B	3.17	108.84	106.49

There are no chirality outliers.

5 of 13 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
5	B	201[B]	HEM	C3D-CAD-CBD-CGD
5	A	201	HEM	C2A-CAA-CBA-CGA
5	B	201[A]	HEM	C4B-C3B-CAB-CBB
5	B	201[B]	HEM	C1A-C2A-CAA-CBA
5	B	201[B]	HEM	C4B-C3B-CAB-CBB

There are no ring outliers.

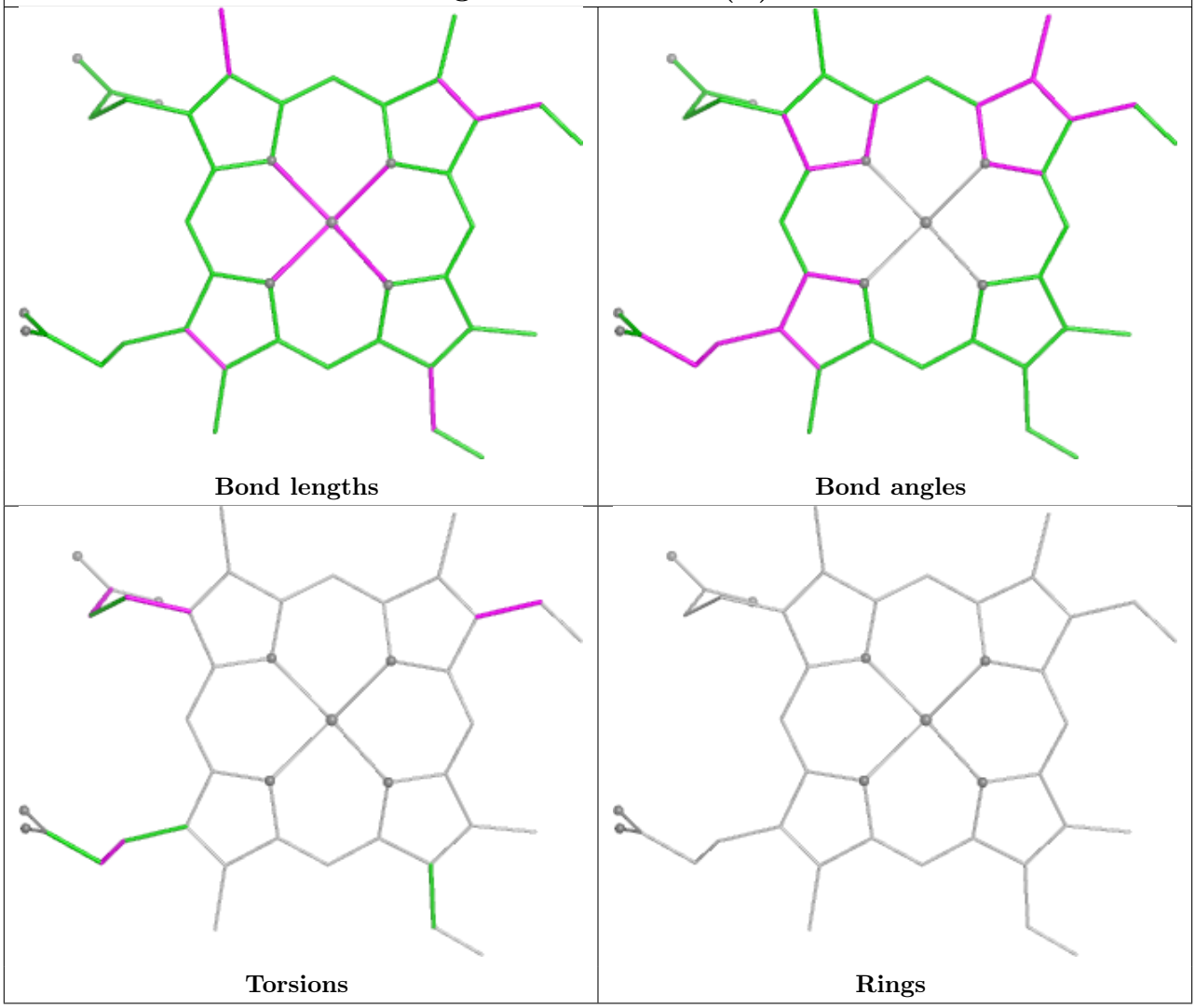
3 monomers are involved in 15 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
5	B	201[B]	HEM	8	0
5	A	201	HEM	1	0
5	B	201[A]	HEM	6	0

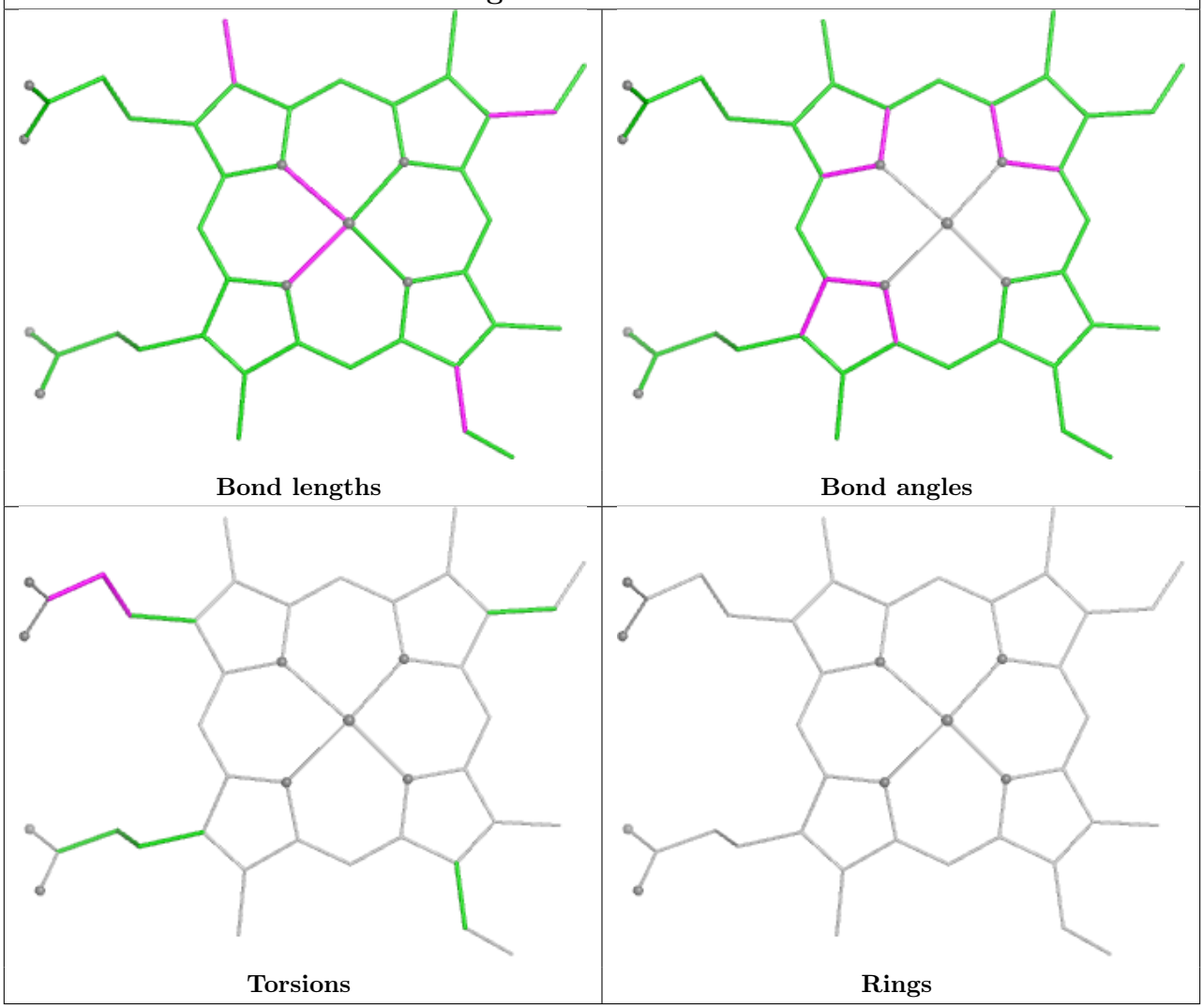
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. For torsion angles, if less then 5% of the Mogul distribution of torsion angles is within 10 degrees of the torsion angle in question, then that torsion angle is considered an outlier. Any bond that is central to one or more torsion angles identified as an outlier by Mogul will be highlighted in the graph. For rings, the root-mean-square deviation (RMSD) between the ring in question and similar rings identified by Mogul is calculated over all ring torsion angles. If the average RMSD is greater than 60 degrees and the minimal RMSD between the ring in question and any Mogul-identified rings is also greater than 60 degrees, then that ring is considered an outlier.

The outliers are highlighted in purple. The color gray indicates Mogul did not find sufficient equivalents in the CSD to analyse the geometry.

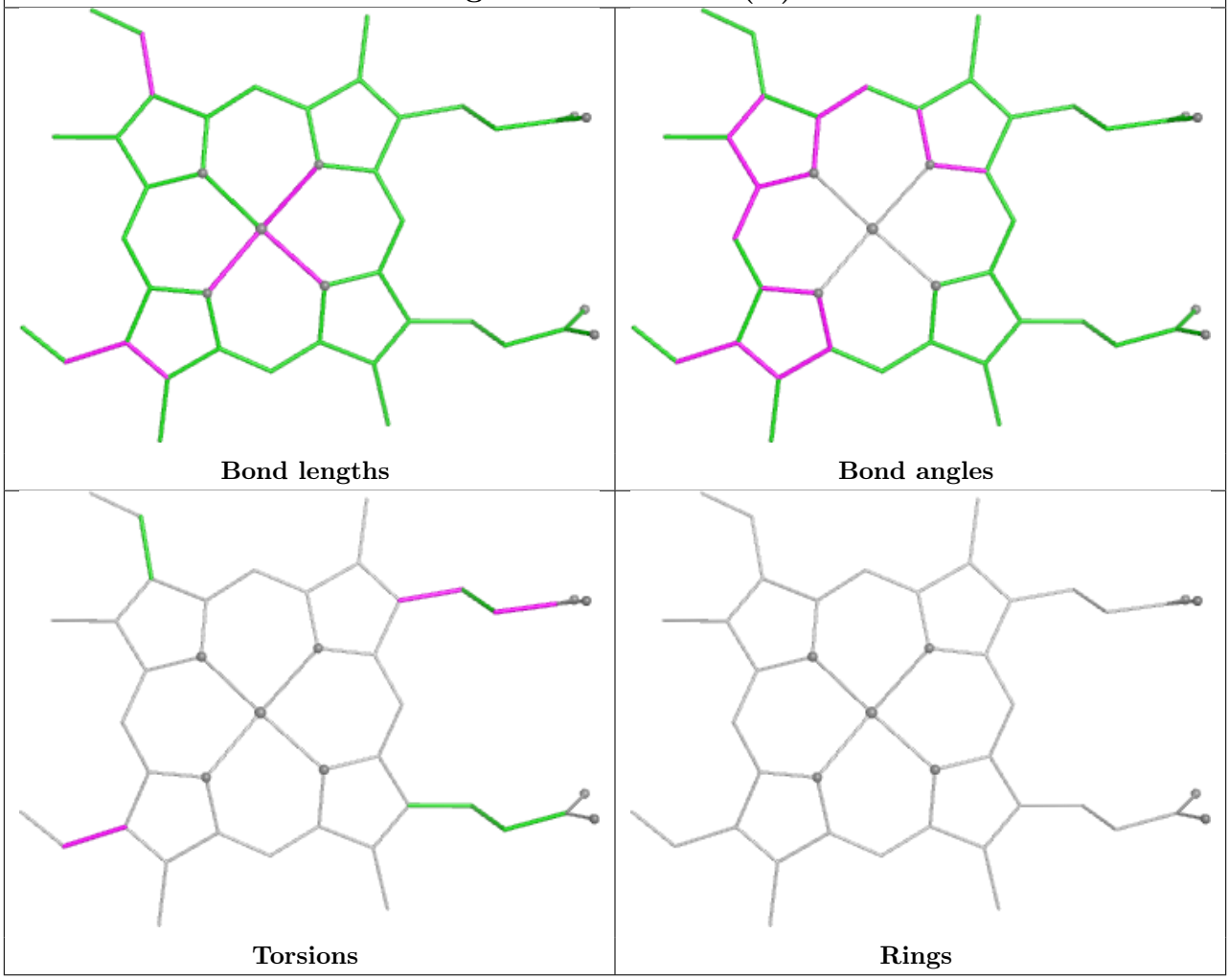
Ligand HEM B 201 (B)



Ligand HEM A 201



Ligand HEM B 201 (A)



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	141/141 (100%)	-0.47	0	100	100	85, 104, 135, 154	0
2	B	146/146 (100%)	-0.32	0	100	100	91, 121, 155, 178	0
3	C	256/267 (95%)	-0.39	0	100	100	85, 111, 136, 149	0
4	D	333/354 (94%)	-0.47	0	100	100	97, 131, 167, 176	0
4	E	333/354 (94%)	-0.40	1 (0%)	90	87	112, 158, 234, 255	0
All	All	1209/1262 (95%)	-0.41	1 (0%)	92	90	85, 127, 209, 255	0

All (1) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
4	E	452	ASP	2.9

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

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

6.3 Carbohydrates (i)

There are no oligosaccharides in this entry.

6.4 Ligands (i)

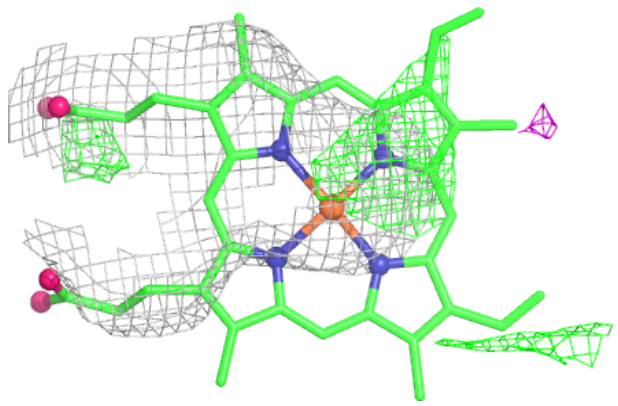
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists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

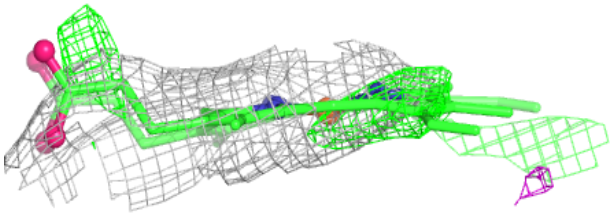
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
5	HEM	B	201[A]	43/43	0.96	0.22	132,134,143,152	43
5	HEM	B	201[B]	43/43	0.96	0.22	132,134,143,152	43
5	HEM	A	201	43/43	0.97	0.07	96,100,105,109	0

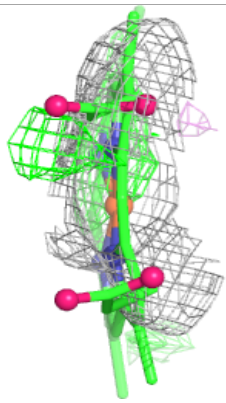
The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation to approximate a three-dimensional view.

Electron density around HEM B 201 (A):

2mF$_o$-DF$_c$ (at 0.7 rmsd) in gray
mF$_o$-DF$_c$ (at 3 rmsd) in purple (negative)
and green (positive)

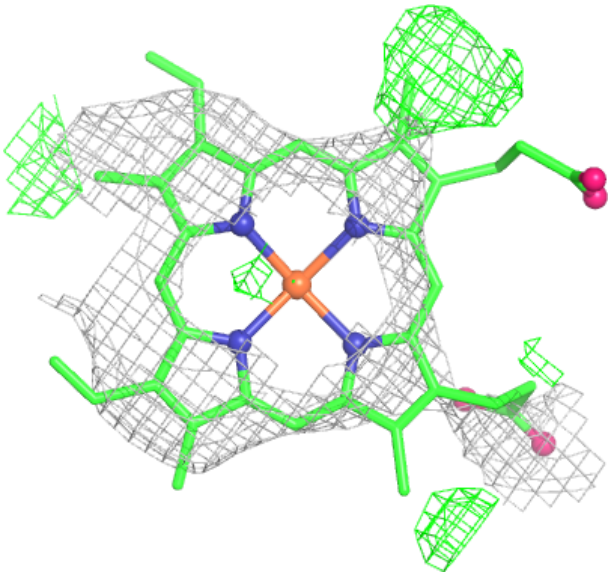


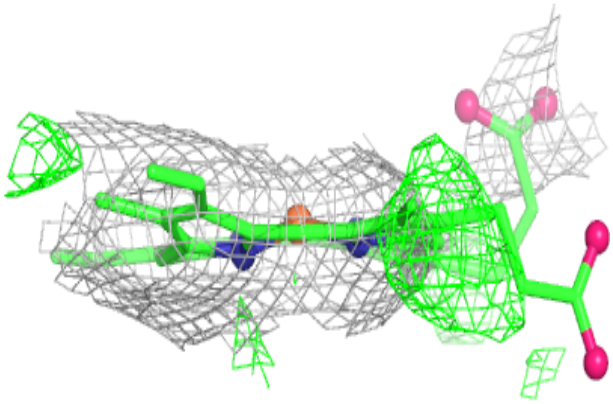


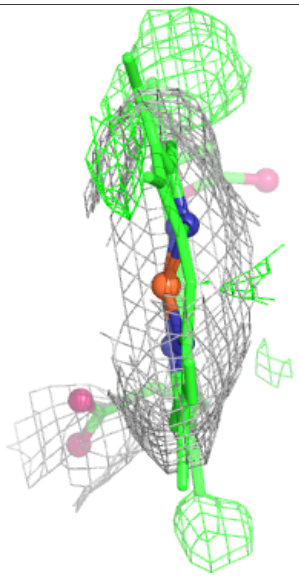


Electron density around HEM B 201 (B):

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

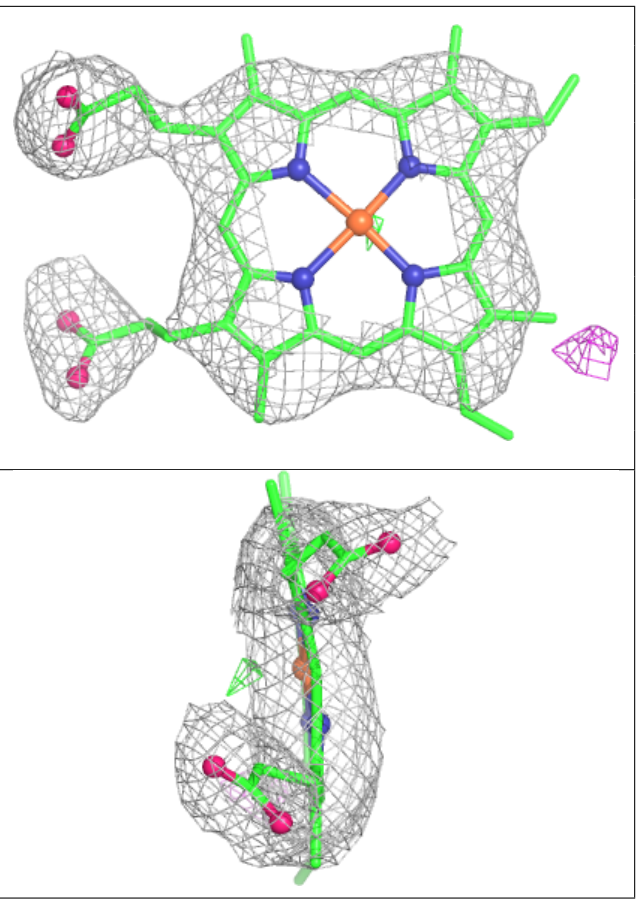






Electron density around HEM A 201:

$2mF_o$-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.