



Full wwPDB X-ray Structure Validation Report ⓘ

May 13, 2020 – 09:35 pm BST

PDB ID : 3OVU
Title : Crystal Structure of Human Alpha-Haemoglobin Complexed with AHSP and the First NEAT Domain of IsdH from Staphylococcus aureus
Authors : Jacques, D.A.; Krishna Kumar, K.; Caradoc-Davies, T.T.; Langley, D.B.; Mackay, J.P.; Guss, J.M.; Gell, D.A.
Deposited on : 2010-09-17
Resolution : 2.83 Å(reported)

This is a Full wwPDB X-ray Structure Validation Report for a publicly released PDB entry.

We welcome your comments at validation@mail.wwpdb.org

A user guide is available at

<https://www.wwpdb.org/validation/2017/XrayValidationReportHelp>

with specific help available everywhere you see the ⓘ symbol.

The 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

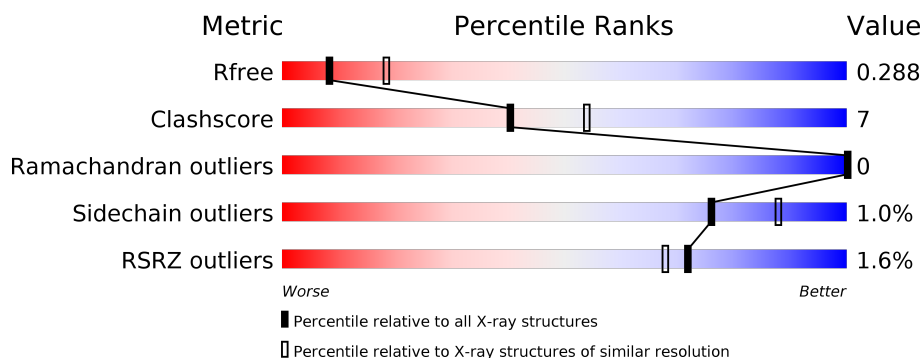
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.83 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	1031 (2.86-2.82)
Clashscore	141614	1078 (2.86-2.82)
Ramachandran outliers	138981	1050 (2.86-2.82)
Sidechain outliers	138945	1051 (2.86-2.82)
RSRZ outliers	127900	1019 (2.86-2.82)

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 ≥ 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	101	<div> <div style="width: 100%; height: 10px; position: relative;"> <div style="position: absolute; top: -10px; left: 0; width: 100%; height: 10px; background-color: red;"></div> <div style="position: absolute; bottom: 0; left: 0; width: 100%; height: 10px;"> <div style="width: 1%; background-color: red;"></div> <div style="width: 74%; background-color: green;"></div> <div style="width: 13%; background-color: yellow;"></div> <div style="width: 12%; background-color: grey;"></div> </div> </div> <div>74% 13% 13%</div> </div>
2	B	164	<div> <div style="width: 100%; height: 10px; position: relative;"> <div style="position: absolute; top: -10px; left: 0; width: 100%; height: 10px; background-color: red;"></div> <div style="position: absolute; bottom: 0; left: 0; width: 100%; height: 10px;"> <div style="width: 1%; background-color: red;"></div> <div style="width: 76%; background-color: green;"></div> <div style="width: 12%; background-color: yellow;"></div> <div style="width: 11%; background-color: grey;"></div> </div> </div> <div>76% 12% 12%</div> </div>
3	C	141	<div> <div style="width: 100%; height: 10px; position: relative;"> <div style="position: absolute; top: -10px; left: 0; width: 100%; height: 10px; background-color: red;"></div> <div style="position: absolute; bottom: 0; left: 0; width: 100%; height: 10px;"> <div style="width: 2%; background-color: red;"></div> <div style="width: 80%; background-color: green;"></div> <div style="width: 18%; background-color: yellow;"></div> <div style="width: 0%; background-color: grey;"></div> </div> </div> <div>80% 18% .</div> </div>

2 Entry composition

There are 5 unique types of molecules in this entry. The entry contains 2961 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 Alpha-hemoglobin-stabilizing protein.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	88	Total	C	N	O	S	0	0	0
			705	453	117	133	2			

- Molecule 2 is a protein called Iron-regulated surface determinant protein H.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B	144	Total	C	N	O	S	0	0	0
			1168	747	191	229	1			

There are 20 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
B	66	GLY	-	EXPRESSION TAG	UNP Q6G8J7
B	67	SER	-	EXPRESSION TAG	UNP Q6G8J7
B	68	SER	-	EXPRESSION TAG	UNP Q6G8J7
B	69	HIS	-	EXPRESSION TAG	UNP Q6G8J7
B	70	HIS	-	EXPRESSION TAG	UNP Q6G8J7
B	71	HIS	-	EXPRESSION TAG	UNP Q6G8J7
B	72	HIS	-	EXPRESSION TAG	UNP Q6G8J7
B	73	HIS	-	EXPRESSION TAG	UNP Q6G8J7
B	74	HIS	-	EXPRESSION TAG	UNP Q6G8J7
B	75	SER	-	EXPRESSION TAG	UNP Q6G8J7
B	76	SER	-	EXPRESSION TAG	UNP Q6G8J7
B	77	GLY	-	EXPRESSION TAG	UNP Q6G8J7
B	78	LEU	-	EXPRESSION TAG	UNP Q6G8J7
B	79	VAL	-	EXPRESSION TAG	UNP Q6G8J7
B	80	PRO	-	EXPRESSION TAG	UNP Q6G8J7
B	81	ARG	-	EXPRESSION TAG	UNP Q6G8J7
B	82	GLY	-	EXPRESSION TAG	UNP Q6G8J7
B	83	SER	-	EXPRESSION TAG	UNP Q6G8J7
B	84	HIS	-	EXPRESSION TAG	UNP Q6G8J7
B	85	MET	-	EXPRESSION TAG	UNP Q6G8J7

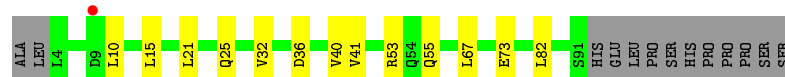
- | Mol | Chain | Residues | Atoms | | | | | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|---------|-------|
| 3 | C | 139 | Total | C | N | O | S | 0 | 0 | 0 |
| | | | 1042 | 669 | 181 | 189 | 3 | | | |

- # HEM

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

- | Mol | Chain | Residues | Atoms | ZeroOcc | AltConf |
|-----|-------|----------|----------------|---------|---------|
| 5 | B | 2 | Total O
2 2 | 0 | 0 |
| 5 | C | 1 | Total O
1 1 | 0 | 0 |

- Molecule 1: Alpha-hemoglobin-stabilizing protein



LEU	GLY
SER	SER
HIS	HIS
HIS	HIS
HIS	HIS
HIS	HIS
SER	SER
SER	SER
LEU	GLY
VAL	LEU
PRO	ARG
GLY	GLY
SER	SER
H84	H84
L90	L90
K91	K91
D92	D92
L99	L99
L116	L116
Y126	Y126
H127	H127
I131	I131
V146	V146
E147	E147
L148	L148
D149	D149
I150	I150
N151	N151
T152	T152
W156	W156
K157	K157
K158	K158
N165	N165
L172	L172
V173	V173
V178	V178
P179	P179
I185	I185
R186	R186
V199	V199
P227	P227

[illegible]

4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α , β , γ	68.64Å 71.66Å 82.06Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	49.57 – 2.83 49.57 – 2.82	Depositor EDS
% Data completeness (in resolution range)	97.9 (49.57-2.83) 97.8 (49.57-2.82)	Depositor EDS
R_{merge}	0.16	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.16 (at 2.81Å)	Xtriage
Refinement program	REFMAC	Depositor
R, R_{free}	0.252 , 0.280 0.255 , 0.288	Depositor DCC
R_{free} test set	483 reflections (4.81%)	wwPDB-VP
Wilson B-factor (Å ²)	62.4	Xtriage
Anisotropy	0.184	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.30 , 54.4	EDS
L-test for twinning ²	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.32$	Xtriage
Estimated twinning fraction	0.034 for k,h,-l	Xtriage
F_o, F_c correlation	0.90	EDS
Total number of atoms	2961	wwPDB-VP
Average B, all atoms (Å ²)	67.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 6.41% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

²Theoretical values of $\langle |L| \rangle$, $\langle L^2 \rangle$ for acentric reflections are 0.5, 0.333 respectively for untwinned datasets, and 0.375, 0.2 for perfectly twinned datasets.

5 Model quality [i](#)

5.1 Standard geometry [i](#)

Bond lengths and bond angles in the following residue types are not validated in this section: 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	0.29	0/718	0.36	0/974
2	B	0.26	0/1198	0.39	0/1629
3	C	0.27	0/1070	0.37	0/1458
All	All	0.27	0/2986	0.38	0/4061

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	705	0	682	11	0
2	B	1168	0	1114	16	0
3	C	1042	0	1033	20	0
4	C	43	0	30	3	0
5	B	2	0	0	0	0
5	C	1	0	0	0	0
All	All	2961	0	2859	42	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 7.

All (42) 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:B:131:ILE:HD12	2:B:150:ILE:HD12	1.47	0.95
3:C:80:LEU:HD13	3:C:132:VAL:HG23	1.73	0.68
2:B:131:ILE:HD12	2:B:150:ILE:CD1	2.23	0.66
3:C:80:LEU:CD1	3:C:132:VAL:HG23	2.26	0.65
2:B:178:VAL:HG13	2:B:179:PRO:HA	1.80	0.63
1:A:41:VAL:HG21	1:A:82:LEU:HD21	1.85	0.59
3:C:32:MET:SD	3:C:39:THR:HG21	2.45	0.57
1:A:32:VAL:HG22	1:A:36:ASP:HB2	1.87	0.57
2:B:116:LEU:HD13	2:B:127:HIS:HB3	1.87	0.57
2:B:131:ILE:CD1	2:B:150:ILE:HD12	2.27	0.56
3:C:101:LEU:HD23	4:C:142:HEM:HHC	1.87	0.56
3:C:93:VAL:HG22	4:C:142:HEM:CAC	2.38	0.53
2:B:173:VAL:HG11	2:B:186:ARG:HD2	1.91	0.53
1:A:10:LEU:HD21	1:A:55:GLN:CB	2.39	0.52
1:A:15:LEU:HD21	1:A:73:GLU:CB	2.40	0.52
2:B:172:LEU:HD12	2:B:185:ILE:HG22	1.90	0.52
1:A:53:ARG:HD3	1:A:67:LEU:HD13	1.92	0.51
1:A:10:LEU:HD21	1:A:55:GLN:HB2	1.94	0.50
3:C:106:LEU:HD11	3:C:126:ASP:HA	1.94	0.50
1:A:40:VAL:HG13	3:C:103:HIS:CE1	2.46	0.50
3:C:86:LEU:HD23	3:C:89:HIS:CE1	2.47	0.49
3:C:129:LEU:O	3:C:132:VAL:HG12	2.12	0.49
2:B:158:LYS:NZ	2:B:199:VAL:HG12	2.28	0.48
2:B:126:TYR:OH	3:C:8:THR:HG23	2.13	0.48
3:C:93:VAL:HG22	4:C:142:HEM:HAC	1.95	0.48
2:B:152:THR:CG2	3:C:11:LYS:HZ1	2.27	0.47
3:C:13:ALA:CB	3:C:125:LEU:HD11	2.44	0.46
3:C:17:VAL:HG13	3:C:24:TYR:CE2	2.50	0.46
2:B:148:LEU:HB3	2:B:150:ILE:HD11	1.98	0.45
3:C:86:LEU:HD23	3:C:89:HIS:ND1	2.32	0.44
1:A:21:LEU:HD23	1:A:25:GLN:HE21	1.82	0.43
2:B:99:LEU:N	2:B:99:LEU:HD12	2.34	0.42
3:C:39:THR:HG23	3:C:97:ASN:CG	2.40	0.42
2:B:146:VAL:HG12	2:B:148:LEU:CD1	2.50	0.42
2:B:158:LYS:HZ2	2:B:199:VAL:HG12	1.84	0.42
1:A:21:LEU:HD11	3:C:122:HIS:CE1	2.55	0.42
3:C:6:ASP:O	3:C:10:VAL:HG23	2.20	0.42
3:C:76:MET:N	3:C:77:PRO:CD	2.83	0.42
1:A:21:LEU:O	1:A:21:LEU:HD23	2.19	0.41
2:B:152:THR:HG23	3:C:11:LYS:HZ1	1.84	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:36:ASP:O	1:A:40:VAL:HG23	2.21	0.41
2:B:90:LEU:CD2	2:B:172:LEU:HD11	2.51	0.40

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	86/101 (85%)	85 (99%)	1 (1%)	0	100	100
2	B	142/164 (87%)	130 (92%)	12 (8%)	0	100	100
3	C	137/141 (97%)	134 (98%)	3 (2%)	0	100	100
All	All	365/406 (90%)	349 (96%)	16 (4%)	0	100	100

There are no Ramachandran outliers to report.

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	75/93 (81%)	75 (100%)	0	100	100
2	B	128/150 (85%)	127 (99%)	1 (1%)	81	90
3	C	109/113 (96%)	107 (98%)	2 (2%)	59	78
All	All	312/356 (88%)	309 (99%)	3 (1%)	76	88

All (3) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
2	B	92	ASP
3	C	43	PHE
3	C	117	PHE

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (8) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	25	GLN
1	A	46	ASN
1	A	72	GLN
1	A	75	ASN
2	B	127	HIS
2	B	225	ASN
3	C	9	ASN
3	C	97	ASN

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 carbohydrates in this entry.

5.6 Ligand geometry [i](#)

1 ligand is 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
4	HEM	C	142	3	27,50,50	2.21	5 (18%)	17,82,82	1.36	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
4	HEM	C	142	3	-	0/6/54/54	-

All (5) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	C	142	HEM	C3D-C2D	5.50	1.54	1.37
4	C	142	HEM	C3C-C2C	-4.70	1.33	1.40
4	C	142	HEM	C3B-C2B	-4.70	1.33	1.40
4	C	142	HEM	C3C-CAC	3.51	1.55	1.47
4	C	142	HEM	C3B-CAB	3.39	1.54	1.47

There are no bond angle outliers.

There are no chirality outliers.

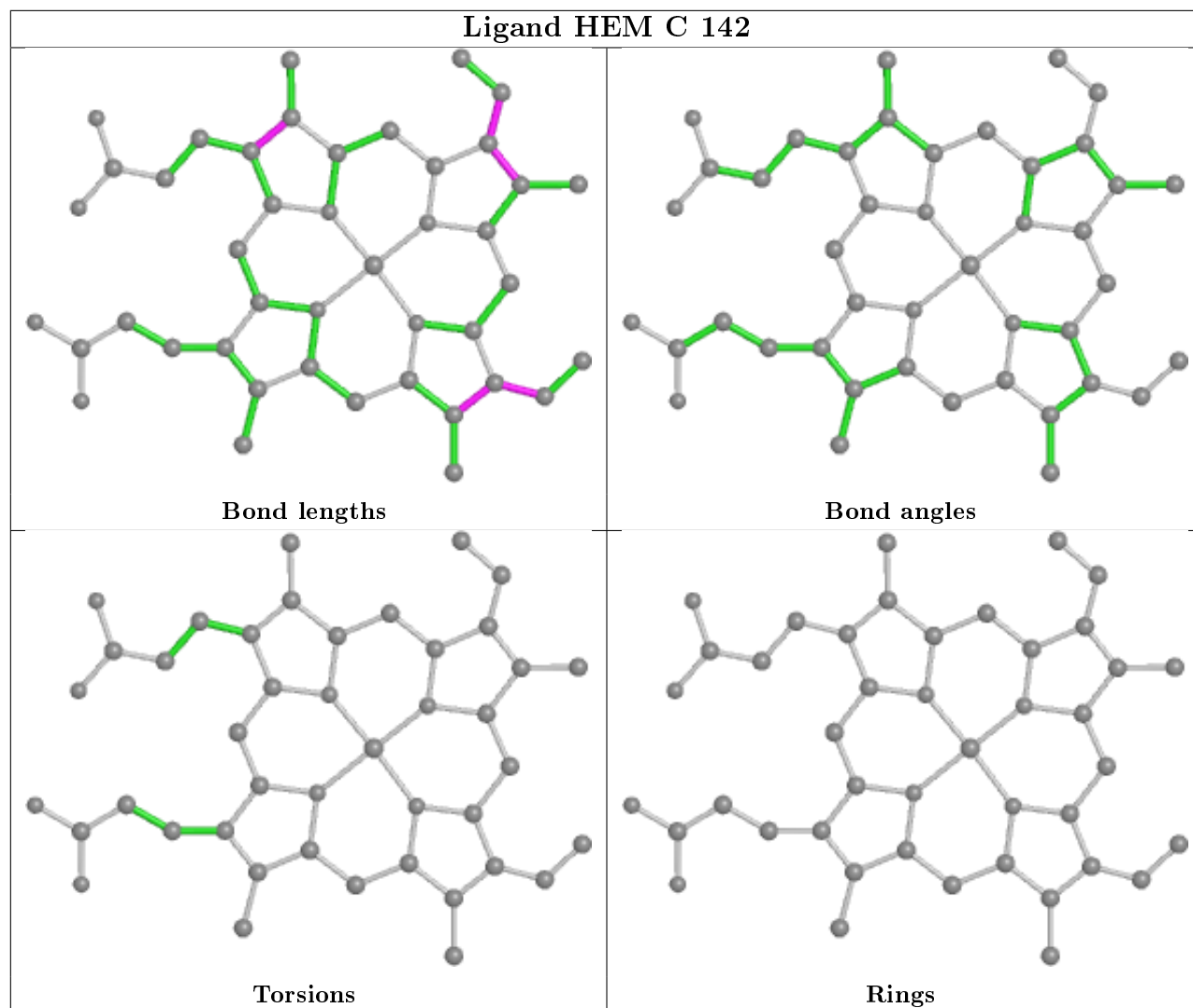
There are no torsion outliers.

There are no ring outliers.

1 monomer is involved in 3 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	C	142	HEM	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.



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 ⓘ

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	88/101 (87%)	0.16	1 (1%) 80 78	49, 71, 93, 110	0
2	B	144/164 (87%)	0.19	2 (1%) 75 71	49, 65, 82, 108	0
3	C	139/141 (98%)	0.13	3 (2%) 62 57	49, 63, 82, 96	0
All	All	371/406 (91%)	0.16	6 (1%) 72 68	49, 66, 87, 110	0

All (6) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
3	C	85	ASP	3.4
1	A	9	ASP	3.2
3	C	44	PRO	2.5
2	B	165	ASN	2.4
2	B	156	TRP	2.4
3	C	140	TYR	2.1

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

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

6.3 Carbohydrates ⓘ

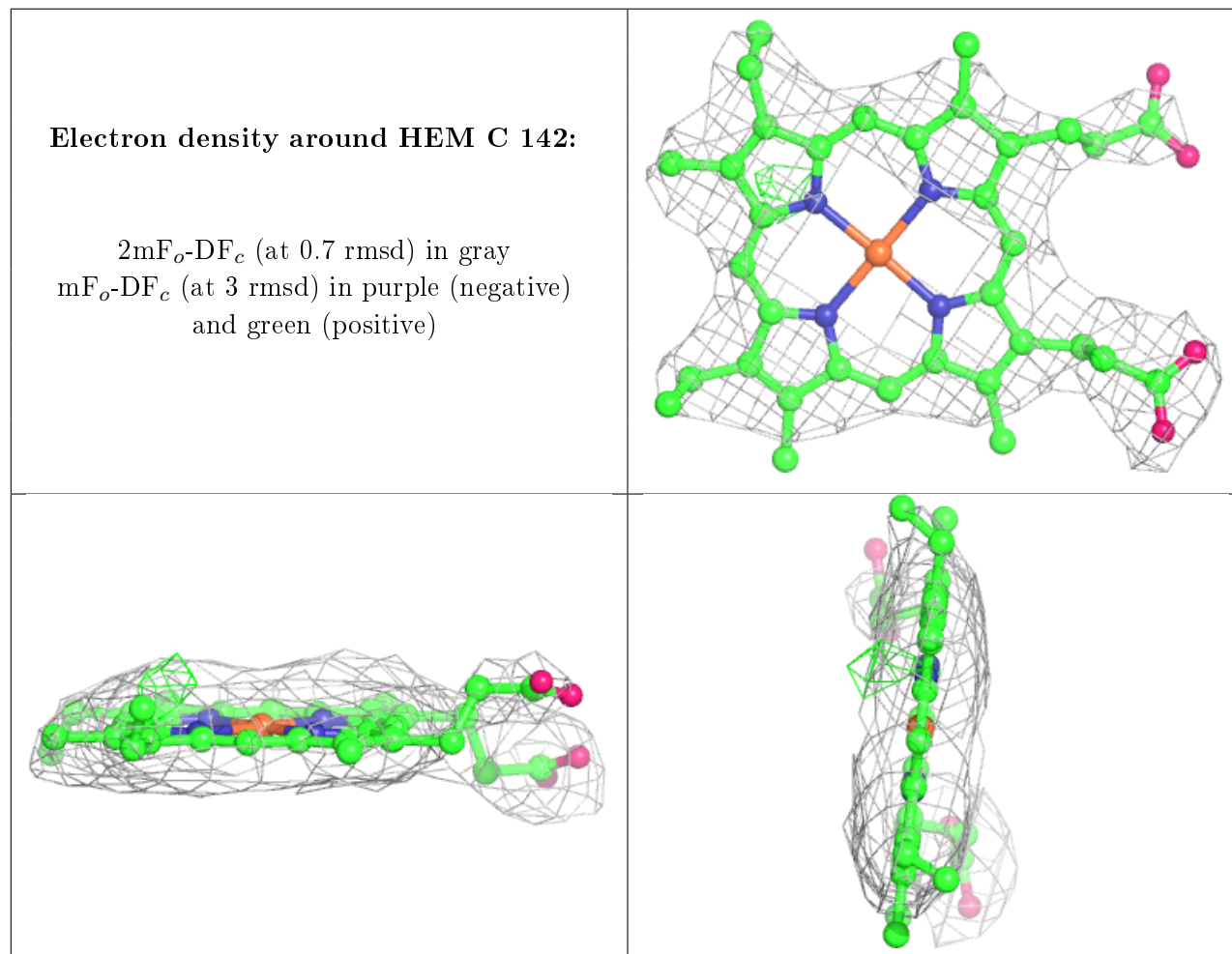
There are no carbohydrates in this entry.

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, 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(\AA^2)	Q<0.9
4	HEM	C	142	43/43	0.93	0.21	64,65,68,69	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 [i](#)

There are no such residues in this entry.