



wwPDB X-ray Structure Validation Summary Report ⓘ

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PDB ID : 1MBS
Title : X-RAY CRYSTALLOGRAPHIC STUDIES OF SEAL MYOGLOBIN. THE
MOLECULE AT 2.5 ANGSTROMS RESOLUTION
Authors : Scouloudi, H.
Deposited on : 1979-03-22
Resolution : 2.50 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
<http://wwpdb.org/validation/2016/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 : 1.7 (RC4), CSD as536be (2015)
Xtriage (Phenix) : **NOT EXECUTED**
EDS : **NOT EXECUTED**
Percentile statistics : 20151230.v01 (using entries in the PDB archive December 30th 2015)
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : trunk26865

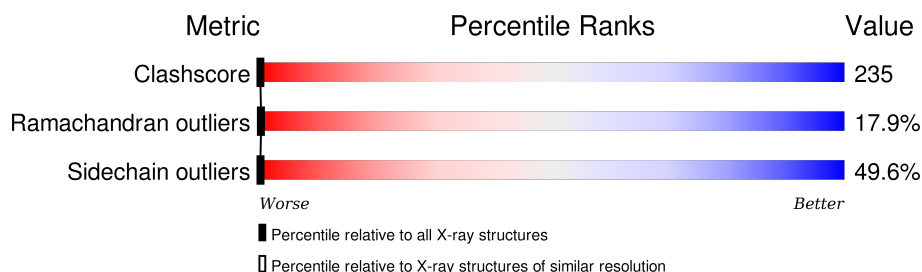
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.50 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	102246	4242 (2.50-2.50)
Ramachandran outliers	100387	4156 (2.50-2.50)
Sidechain outliers	100360	4158 (2.50-2.50)

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. 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.

Note EDS was not executed.

Mol	Chain	Length	Quality of chain
1	A	153	

The following table lists non-polymeric compounds, carbohydrate monomers and non-standard residues in protein, DNA, RNA chains that are outliers for geometric or electron-density-fit criteria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
2	HEM	A	154	-	-	X	-

2 Entry composition [i](#)

There are 2 unique types of molecules in this entry. The entry contains 1266 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 MYOGLOBIN.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	153	Total	C	N	O	S	0	0	0
			1223	783	221	217	2			

- 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		

Note EDS was not executed.

- Chain A:** 6% 47% 35% 12%

E122	F123	G124	A125	D126	A127	Q128	A129	A130	M131	K132	K133	A134	L135	A136	L137	F138	K139	M140	D141	I142	A143	A144	K145	Y146	K147	A148	L149	G150	F151	H152	G153																											
L61	R62	K63	H64	G65	R66	T67	V68	L69	T70	A71	L72	G73	G74	R75	L76	K77	K78	K79	G80	H81	R82	R83	A84	B85	L86	Q86	P88	L89	A90	Q91	S92	R93	A94	T95	K96	H97	K98	R99	P100	T101	K102	Y103	L104	E105	F106	I107	S108	E109	L112	H113	V114	L115	H116	S117	K118	H119	P120	L121

4 Data and refinement statistics

Xtriage (Phenix) and EDS were not executed - this section will therefore be incomplete.

Property	Value	Source
Space group	A 2	Depositor
Cell constants a, b, c, α , β , γ	57.81Å 29.70Å 106.09Å 90.00° 101.99° 90.00°	Depositor
Resolution (Å)	(Not available) – 2.50	Depositor
% Data completeness (in resolution range)	(Not available) ((Not available)-2.50)	Depositor
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
Refinement program	unknown	Depositor
R, R_{free}	(Not available) , (Not available)	Depositor
Estimated twinning fraction	No twinning to report.	Xtriage
Total number of atoms	1266	wwPDB-VP
Average B, all atoms (Å ²)	0.0	wwPDB-VP

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	1.42	6/1252 (0.5%)	1.31	7/1679 (0.4%)

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	1	0

The worst 5 of 6 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	153	GLY	C-O	-36.80	0.64	1.23
1	A	62	ARG	NE-CZ	11.17	1.47	1.33
1	A	57	ARG	NE-CZ	11.00	1.47	1.33
1	A	31	ARG	NE-CZ	10.88	1.47	1.33
1	A	56	ARG	NE-CZ	10.85	1.47	1.33

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

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	62	ARG	CD-NE-CZ	-10.18	109.35	123.60
1	A	31	ARG	CD-NE-CZ	-9.11	110.85	123.60
1	A	57	ARG	CD-NE-CZ	-8.96	111.06	123.60
1	A	56	ARG	CD-NE-CZ	-8.16	112.17	123.60
1	A	123	PHE	CB-CG-CD1	-6.88	115.98	120.80

All (1) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
1	A	123	PHE	CA

There are no planarity outliers.

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	1223	0	1236	573	167
2	A	43	0	30	30	0
All	All	1266	0	1266	596	167

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 235.

The worst 5 of 596 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:128:GLN:HA	1:A:131:MET:SD	1.35	1.65
2:A:154:HEM:CMA	2:A:154:HEM:C3A	1.82	1.62
1:A:82:HIS:CE1	1:A:137:LEU:HD21	1.37	1.58
1:A:102:LYS:HB3	1:A:106:PHE:CZ	1.01	1.53
1:A:102:LYS:CB	1:A:106:PHE:CZ	1.94	1.50

The worst 5 of 167 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:90:ALA:O	1:A:149:LEU:C[2_555]	0.36	1.84
1:A:145:LYS:CG	1:A:151:PHE:CZ[2_555]	0.42	1.78
1:A:104:LEU:CD2	1:A:148:GLU:OE1[2_555]	0.49	1.71
1:A:146:TYR:N	1:A:146:TYR:CB[2_555]	0.58	1.62
1:A:145:LYS:C	1:A:146:TYR:CG[2_555]	0.59	1.61

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	151/153 (99%)	76 (50%)	48 (32%)	27 (18%)	0 0

5 of 27 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	2	LEU
1	A	3	SER
1	A	19	THR
1	A	78	LYS
1	A	84	ALA

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	127/127 (100%)	64 (50%)	63 (50%)	0 0

5 of 63 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	62	ARG
1	A	82	HIS
1	A	141	ASP
1	A	66	ASN
1	A	70	THR

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 7 such

sidechains are listed below:

Mol	Chain	Res	Type
1	A	66	ASN
1	A	152	HIS
1	A	93	HIS
1	A	48	HIS
1	A	113	HIS

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	$\# Z > 2$
2	HEM	A	154	-	30,50,50	5.76	15 (50%)	24,82,82	4.10	17 (70%)

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	154	-	-	0/10/54/54	0/0/8/8

The worst 5 of 15 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	154	HEM	C3D-C4D	-15.90	1.31	1.51
2	A	154	HEM	C3B-C4B	-12.83	1.40	1.51
2	A	154	HEM	C2C-C1C	-7.77	1.37	1.52
2	A	154	HEM	CHC-C1C	-7.55	1.19	1.36
2	A	154	HEM	CMD-C2D	-7.11	1.36	1.53

The worst 5 of 17 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	A	154	HEM	C3C-CAC-CBC	-7.11	113.55	124.46
2	A	154	HEM	C1D-CHD-C4C	-7.08	113.99	125.82
2	A	154	HEM	CMA-C3A-C4A	-5.64	119.03	128.36
2	A	154	HEM	CBA-CAA-C2A	-5.52	102.63	112.53
2	A	154	HEM	C3B-C4B-NB	-4.75	102.55	111.63

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

1 monomer is involved in 30 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	A	154	HEM	30	0

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](#)

EDS was not executed - this section will therefore be empty.

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

EDS was not executed - this section will therefore be empty.

6.3 Carbohydrates [i](#)

EDS was not executed - this section will therefore be empty.

6.4 Ligands [i](#)

EDS was not executed - this section will therefore be empty.

6.5 Other polymers [i](#)

EDS was not executed - this section will therefore be empty.