

wwPDB X-ray Structure Validation Summary Report (i)

Jun 14, 2020 – 10:36 am BST

PDB ID : 2HMQ

Title : THE STRUCTURES OF MET AND AZIDOMET HEMERYTHRIN AT 1.66

ANGSTROMS RESOLUTION

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 $Deposited \ on \quad : \quad 1990\text{-}10\text{-}18$

Resolution : 1.66 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 following versions of software and data (see references (1)) 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

Percentile statistics : 20191225.v01 (using entries in the PDB archive December 25th 2019)

Refmac: 5.8.0158

CCP4 : 7.0.044 (Gargrove) roteins) : Engh & Huber (2001)

Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)

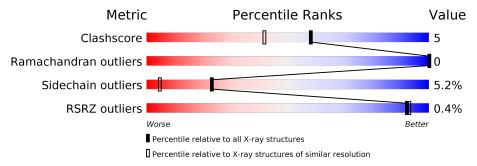
Validation Pipeline (wwPDB-VP) : 2.11

1 Overall quality at a glance (i)

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

The reported resolution of this entry is 1.66 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	$\begin{array}{c} \text{Whole archive} \\ (\#\text{Entries}) \end{array}$	$\begin{array}{c} {\rm Similar \; resolution} \\ (\#{\rm Entries, \; resolution \; range(\AA)}) \end{array}$
Clashscore	141614	1931 (1.66-1.66)
Ramachandran outliers	138981	1891 (1.66-1.66)
Sidechain outliers	138945	1891 (1.66-1.66)
RSRZ outliers	127900	1791 (1.66-1.66)

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 <=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	114	69%	27%	•
1	В	114	80%	16%	• •
1	С	114	74%	25%	
1	D	114	75%	23%	•



2 Entry composition (i)

There are 4 unique types of molecules in this entry. The entry contains 4153 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 HEMERYTHRIN.

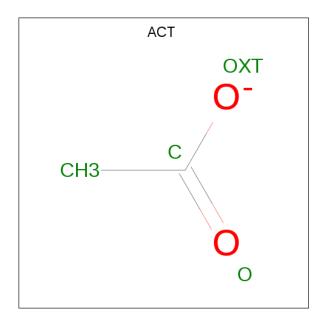
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf	Trace		
1	Α	113	Total	С	N	О	S	0	7	0
1	A	110	965	619	166	177	3	0	1	0
1	В	113	Total	С	N	О	S	0	3	0
1	Б		960	616	164	177	3	U	ა	U
1	С	113	Total	С	N	О	S	0	1	0
1		110	952	612	163	174	3	0	1	U
1	1 D	119	Total	С	N	О	S	0	2	0
	113	955	613	164	175	3	0	2	U	

There are 4 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	21	ILE	VAL	MICROHETEROGENEITY	UNP P02246
В	21	ILE	VAL	MICROHETEROGENEITY	UNP P02246
С	21	ILE	VAL	MICROHETEROGENEITY	UNP P02246
D	21	ILE	VAL	MICROHETEROGENEITY	UNP P02246

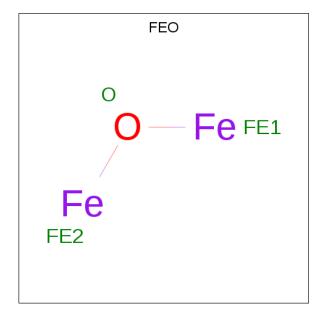
• Molecule 2 is ACETATE ION (three-letter code: ACT) (formula: C₂H₃O₂).





Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
2	A	1	Total C O 4 2 2	0	0
2	В	1	Total C O 4 2 2	0	0
2	С	1	Total C O 4 2 2	0	0
2	D	1	Total C O 4 2 2	0	0

 \bullet Molecule 3 is MU-OXO-DIIRON (three-letter code: FEO) (formula: Fe₂O).





Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	A	1	Total Fe O 3 2 1	0	0
3	В	1	Total Fe O 3 2 1	0	0
3	С	1	Total Fe O 3 2 1	0	0
3	D	1	Total Fe O 3 2 1	0	0

• Molecule 4 is water.

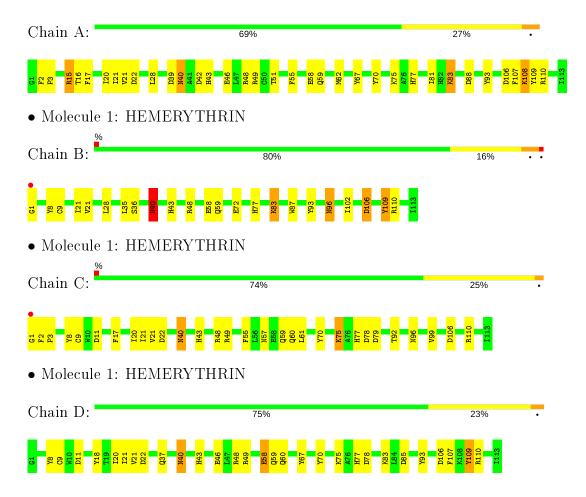
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
4	A	69	Total O 69 69	0	0
4	В	70	Total O 70 70	0	0
4	С	66	Total O 66 66	0	0
4	D	88	Total O 88 88	0	0



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: HEMERYTHRIN





4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 4	Depositor
Cell constants	86.60Å 86.60Å 80.80Å	Depositor
a, b, c, α , β , γ	90.00° 90.00° 90.00°	Depositor
Resolution (Å)	10.00 - 1.66	Depositor
Resolution (A)	86.60 - 1.66	EDS
% Data completeness	(Not available) (10.00-1.66)	Depositor
(in resolution range)	91.9 (86.60-1.66)	EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) > 1$	$0.98 \; ({\rm at} \; 1.66 {\rm \AA})$	Xtriage
Refinement program	PROFFT	Depositor
R, R_{free}	0.189 , (Not available)	Depositor
$\Pi,\ \Pi free$	0.167 , (Not available)	DCC
R_{free} test set	No test flags present.	wwPDB-VP
Wilson B-factor (Å ²)	17.8	Xtriage
Anisotropy	0.211	Xtriage
Bulk solvent $k_{sol}(e/Å^3)$, $B_{sol}(Å^2)$	0.29 , 58.0	EDS
L-test for twinning ²	$< L >=0.51, < L^2>=0.35$	Xtriage
Estimated twinning fraction	0.033 for h,-k,-l	Xtriage
F_o, F_c correlation	0.97	EDS
Total number of atoms	4153	wwPDB-VP
Average B, all atoms (Å ²)	19.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: The largest off-origin peak in the Patterson function is 3.69% of the height of the origin peak. No significant pseudotranslation is detected.

²Theoretical 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.



¹Intensities estimated from amplitudes.

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: FEO, ACT

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).

Mal	Mol Chain	Boı	nd lengths	Bond angles		
MIOI		RMSZ	# Z > 5	RMSZ	# Z > 5	
1	A	1.25	1/1030 (0.1%)	1.91	32/1390~(2.3%)	
1	В	1.20	1/996 (0.1%)	1.76	15/1346 (1.1%)	
1	С	1.18	$2/979 \ (0.2\%)$	1.72	$18/1323 \ (1.4\%)$	
1	D	1.25	1/987 (0.1%)	1.90	30/1334~(2.2%)	
All	All	1.22	5/3992 (0.1%)	1.83	95/5393~(1.8%)	

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 maintain group or atoms of a sidechain that are expected to be planar.

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

All (5) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	$\operatorname{Observed}(\operatorname{\AA})$	Ideal(A)
1	D	58	GLU	CD-OE2	-6.96	1.18	1.25
1	С	1	GLY	N-CA	5.93	1.54	1.46
1	В	1	GLY	N-CA	5.68	1.54	1.46
1	A	46	GLU	CD-OE1	-5.60	1.19	1.25
1	С	92	THR	CB-OG1	5.13	1.53	1.43

The worst 5 of 95 bond angle outliers are listed below:

N	Mol	Chain	Res	Type	${f Atoms}$	\mathbf{Z}	$\mathbf{Observed}(^o)$	$\operatorname{Ideal}({}^o)$
	1	A	110	ARG	NE-CZ-NH2	-19.10	110.75	120.30
	1	В	106	ASP	CB-CG-OD1	18.25	134.73	118.30

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Mol	Chain	Res	Type	${f Atoms}$	\mathbf{Z}	$\mathbf{Observed}(^o)$	$\operatorname{Ideal}({}^{o})$
1	D	110	ARG	NE-CZ-NH2	-16.09	112.26	120.30
1	D	106	ASP	CB-CG-OD1	15.36	132.12	118.30
1	С	11	ASP	CB-CG-OD1	11.07	128.26	118.30

There are no chirality outliers.

All (2) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	15	ARG	Sidechain
1	В	9	CYS	Mainchain

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	965	0	910	11	0
1	В	960	0	910	8	0
1	С	952	0	906	8	0
1	D	955	0	908	7	0
2	A	4	0	3	0	0
2	В	4	0	3	0	0
2	С	4	0	3	0	0
2	D	4	0	3	0	0
3	A	3	0	0	1	0
3	В	3	0	0	0	0
3	С	3	0	0	0	0
3	D	3	0	0	0	0
4	A	69	0	0	0	0
4	В	70	0	0	0	0
4	С	66	0	0	2	0
4	D	88	0	0	1	0
All	All	4153	0	3646	35	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 5.

The worst 5 of 35 close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.



Atom-1	Atom-2	$egin{array}{c} ext{Interatomic} \ ext{distance} \ (ext{Å}) \end{array}$	$egin{array}{c} ext{Clash} \ ext{overlap } (ext{Å}) \end{array}$
1:D:59:GLN:HE21	1:D:77:HIS:HD1	1.07	1.03
1:B:59:GLN:HE21	1:B:77:HIS:HD1	1.06	1.01
1:A:59:GLN:HE21	1:A:77:HIS:HD1	1.11	0.98
1:C:59:GLN:HE21	1:C:77:HIS:HD1	1.08	0.98
1:A:2:PHE:HB3	1:A:3:PRO:HD2	1.74	0.70

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	Perce	$_{ m ntiles}$
1	A	$116/114 \; (102\%)$	114 (98%)	2 (2%)	0	100	100
1	В	112/114~(98%)	109 (97%)	3 (3%)	0	100	100
1	С	110/114 (96%)	109 (99%)	1 (1%)	0	100	100
1	D	111/114 (97%)	111 (100%)	0	0	100	100
All	All	449/456 (98%)	443 (99%)	6 (1%)	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	107/101 (106%)	101 (94%)	6 (6%)	21 4		
1	В	103/101 (102%)	96 (93%)	7 (7%)	16 2		

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles		
1	С	101/101 (100%)	96 (95%)	5 (5%)	24 5		
1	D	102/101 (101%)	97 (95%)	5 (5%)	25 5		
All	All	413/404 (102%)	390 (94%)	23 (6%)	23 4		

5 of 23 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	В	83	LYS
1	В	109	TYR
1	D	83	LYS
1	В	96	ASN
1	С	9	CYS

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 22 such sidechains are listed below:

Mol	Chain	Res	Type
1	В	59	GLN
1	С	45	ASN
1	D	59	GLN
1	С	37	GLN
1	С	40	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)

8 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	Trens	Chain	Res	Link	Bond lengths			Bond angles		
10101	Type	Chain	nes	LIIIK	Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
2	ACT	D	114	1	1,3,3	8.17	1 (100%)	0,3,3	0.00	-
3	FEO	В	115	1	0,2,2	0.00	-	-		
2	ACT	В	114	1	1,3,3	6.35	1 (100%)	0,3,3	0.00	-
3	FEO	D	115	1	0,2,2	0.00	-	-		
3	FEO	A	115	1,4	0,2,2	0.00	ı	-		
2	ACT	С	114	1	1,3,3	7.86	1 (100%)	0,3,3	0.00	-
3	FEO	С	115	1,4	0,2,2	0.00	-	-		
2	ACT	A	114	1	1,3,3	8.02	1 (100%)	0,3,3	0.00	-

All (4) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	$\mathbf{Observed}(\mathbf{\mathring{A}})$	$Ideal(\AA)$
2	D	114	ACT	СН3-С	8.17	1.59	1.48
2	A	114	ACT	СН3-С	8.02	1.59	1.48
2	С	114	ACT	СН3-С	7.86	1.58	1.48
2	В	114	ACT	СН3-С	6.35	1.56	1.48

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 1 short contact:

Mol	Chain	${f Res}$	Type	Clashes	Symm-Clashes
3	A	115	FEO	1	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)

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^{th} 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 $>$	$\#\mathrm{RSRZ}{>}2$	$\mathbf{OWAB}(\mathbf{\mathring{A}}^2)$	Q < 0.9
1	A	114/114 (100%)	-0.70	0 100 100	7, 15, 30, 49	2 (1%)
1	В	114/114 (100%)	-0.52	1 (0%) 84 86	11, 21, 35, 59	2 (1%)
1	С	114/114 (100%)	-0.65	1 (0%) 84 86	10, 17, 35, 63	2 (1%)
1	D	114/114 (100%)	-0.76	0 100 100	7, 14, 28, 37	2 (1%)
All	All	456/456 (100%)	-0.66	2 (0%) 92 93	7, 17, 34, 63	8 (1%)

All (2) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	С	1	GLY	2.9
1	В	1	GLY	2.7

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 carbohydrates 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, 95^{th} 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	$\mathbf{B} ext{-}\mathbf{factors}(\mathbf{\mathring{A}}^2)$	Q < 0.9
2	ACT	D	114	4/4	0.87	0.13	14,18,19,20	4
2	ACT	В	114	4/4	0.89	0.12	17,19,20,21	4
2	ACT	A	114	4/4	0.89	0.16	13,14,16,20	4
2	ACT	С	114	4/4	0.95	0.10	18,19,21,22	4
3	FEO	A	115	3/3	0.99	0.07	5,5,12,13	0
3	FEO	В	115	3/3	0.99	0.07	12,12,18,19	0
3	FEO	С	115	3/3	0.99	0.07	8,8,14,17	0
3	FEO	D	115	3/3	0.99	0.08	6,6,11,13	0

6.5 Other polymers (i)

There are no such residues in this entry.

