

wwPDB X-ray Structure Validation Summary Report (i)

Dec 19, 2023 – 09:01 AM EST

PDB ID	:	1IWH
Title	:	Crystal Structure of Horse Carbonmonoxyhemoglobin-Bezafibrate Complex
		at 1.55A Resolution: A Novel Allosteric Binding Site in R-State Hemoglobin
Authors	:	Shibayama, N.; Miura, S.; Tame, J.R.H.; Yonetani, T.; Park, SY.
Deposited on	:	2002-05-15
Resolution	:	1.55 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 (1)) were used in the production of this report:

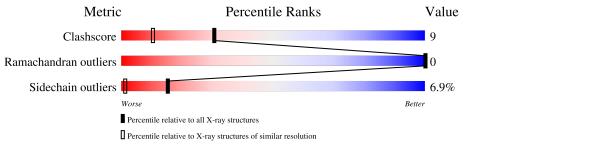
MolProbity	:	4.02b-467
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	NOT EXECUTED
EDS	:	NOT EXECUTED
buster-report	:	1.1.7(2018)
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)		
Validation Pipeline (wwPDB-VP)	:	2.36

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 1.55 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	Similar resolution
Metric	$(\# { m Entries})$	$(\# { m Entries}, { m resolution} { m range}({ m \AA}))$
Clashscore	141614	1529 (1.56-1.56)
Ramachandran outliers	138981	1498 (1.56-1.56)
Sidechain outliers	138945	1495 (1.56-1.56)

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%

Note EDS was not executed.

Mol	Chain	Length	Quality of chain		
1	А	141	87%	9%	•••
2	В	146	83%	14%	•

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
4	CMO	А	143	-	-	Х	-
4	CMO	В	348	-	-	Х	-



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2 Entry composition (i)

There are 6 unique types of molecules in this entry. The entry contains 2613 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.

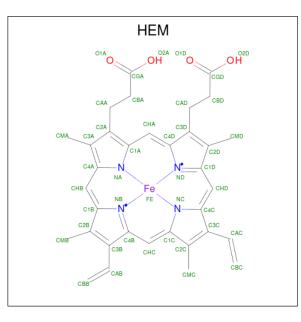
• Molecule 1 is a protein called Hemoglobin alpha chain.

Mol	Chain	Residues		At	oms			ZeroOcc	AltConf	Trace
1	А	141	Total 1069	C 684	N 187	O 196	${ m S} { m 2}$	0	0	0

• Molecule 2 is a protein called Hemoglobin beta chain.

Mol	Chain	Residues		At	oms			ZeroOcc	AltConf	Trace
2	В	146	Total 1134	C 728	N 200	0 204	$\begin{array}{c} \mathrm{S} \\ \mathrm{2} \end{array}$	0	0	0

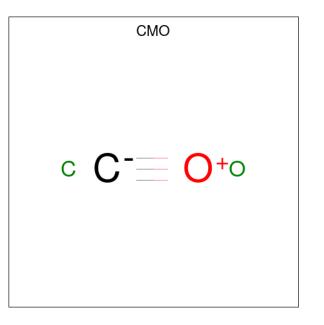
• Molecule 3 is PROTOPORPHYRIN IX CONTAINING FE (three-letter code: HEM) (formula: $C_{34}H_{32}FeN_4O_4$).



Mol	Chain	Residues		Ate	oms			ZeroOcc	AltConf
3	Λ	1	Total	С	Fe	Ν	0	0	0
0	Л	1	43	34	1	4	4	0	0
2	р	1	Total	С	Fe	Ν	Ο	0	0
0	D	1	43	34	1	4	4	0	0

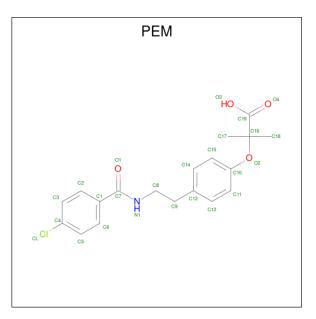


• Molecule 4 is CARBON MONOXIDE (three-letter code: CMO) (formula: CO).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
4	А	1	$\begin{array}{ccc} \text{Total} & \text{C} & \text{O} \\ 2 & 1 & 1 \end{array}$	0	0
4	В	1	$\begin{array}{ccc} \text{Total} \text{C} \text{O} \\ 2 1 1 \end{array}$	0	0

• Molecule 5 is 2-[P-[2-P-CHLOROBENZAMIDO)ETHYL]PHENOXY]-2-METHYLPROPI ONIC ACID (three-letter code: PEM) (formula: C₁₉H₂₀ClNO₄).





Mol	Chain	Residues		Ate	oms			ZeroOcc	AltConf
5	А	1	Total 25		Cl 1	N 1	0 4	0	0

• Molecule 6 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
6	А	148	Total O 148 148	0	0
6	В	147	Total O 147 147	0	0

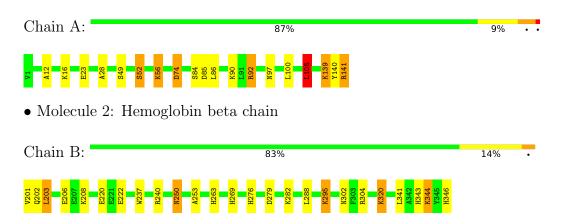


3 Residue-property plots (i)

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. 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. 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.

Note EDS was not executed.

• Molecule 1: Hemoglobin alpha chain





4 Data and refinement statistics (i)

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

Property	Value	Source
Space group	C 2 2 21	Depositor
Cell constants	62.40Å 107.50Å 86.75Å	Depositor
a, b, c, α , β , γ	90.00° 90.00° 90.00°	Depositor
Resolution (Å)	20.00 - 1.55	Depositor
% Data completeness	89.7 (20.00-1.55)	Depositor
(in resolution range)	05.1 (20.00-1.00)	Depositor
R_{merge}	0.06	Depositor
R _{sym}	(Not available)	Depositor
Refinement program	SHELXL-97	Depositor
R, R_{free}	0.174 , 0.233	Depositor
Estimated twinning fraction	No twinning to report.	Xtriage
Total number of atoms	2613	wwPDB-VP
Average B, all atoms $(Å^2)$	17.0	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, CMO, PEM

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		
	Ullaili	RMSZ	# Z > 5	RMSZ	# Z > 5	
1	А	0.44	0/1096	1.04	4/1487~(0.3%)	
2	В	0.43	0/1162	1.12	4/1572~(0.3%)	
All	All	0.44	0/2258	1.08	8/3059~(0.3%)	

There are no bond length outliers.

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

Mol	Chain	Res	Type	Atoms	Ζ	$\mathbf{Observed}(^{o})$	$Ideal(^{o})$
2	В	288	LEU	CB-CG-CD2	6.88	122.69	111.00
2	В	240	ARG	NE-CZ-NH1	6.74	123.67	120.30
1	А	105	LEU	CA-CB-CG	6.51	130.28	115.30
2	В	304	ARG	NE-CZ-NH2	6.43	123.52	120.30
1	А	141	ARG	NE-CZ-NH1	-5.85	117.37	120.30

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	А	1069	0	1073	13	0
2	В	1134	0	1121	16	0
3	А	43	0	30	4	0
3	В	43	0	30	5	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
4	А	2	0	0	4	0
4	В	2	0	0	4	0
5	А	25	0	19	2	0
6	А	148	0	0	4	0
6	В	147	0	0	3	0
All	All	2613	0	2273	39	0

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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 9.

The worst 5 of 39 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)	
5:A:501:PEM:O2	5:A:501:PEM:C10	1.66	1.42	
3:A:142:HEM:NC	4:A:143:CMO:C	2.36	0.88	
3:B:347:HEM:NB	4:B:348:CMO:C	2.40	0.85	
3:A:142:HEM:NB	4:A:143:CMO:C	2.40	0.84	
3:A:142:HEM:ND	4:A:143:CMO:C	2.45	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	Perce	ntiles
1	А	139/141~(99%)	138 (99%)	1 (1%)	0	100	100
2	В	144/146~(99%)	141 (98%)	3~(2%)	0	100	100
All	All	283/287~(99%)	279~(99%)	4 (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	А	115/115~(100%)	109~(95%)	6~(5%)	23 3		
2	В	118/118 (100%)	108 (92%)	10 (8%)	10 1		
All	All	233/233~(100%)	217~(93%)	16 (7%)	15 1		

5 of 16 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
2	В	341	LEU
2	В	320	LYS
2	В	206	GLU
2	В	295	LYS
2	В	203	LEU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 7 such sidechains are listed below:

Mol	Chain	Res	Type
2	В	269	HIS
2	В	276	HIS
2	В	343	HIS
2	В	302	ASN
2	В	250	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 monosaccharides in this entry.

5.6 Ligand geometry (i)

5 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	Turne	ype Chain Res		Link	B	gths	Bond angles			
	Type	Unam	nes	LIIIK	Counts	RMSZ	# Z >2	Counts	RMSZ	# Z >2
3	HEM	В	347	4,2	41,50,50	2.80	9 (21%)	45,82,82	2.86	22 (48%)
4	CMO	А	143	3	$0,\!1,\!1$	-	-	-		
4	CMO	В	348	3	0,1,1	-	-	-		
5	PEM	А	501	-	26,26,26	2.40	9 (34%)	36,36,36	2.65	15 (41%)
3	HEM	А	142	4,1	41,50,50	2.58	10 (24%)	45,82,82	3.03	19 (42%)

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	PEM	А	501	-	-	2/21/21/21	0/2/2/2
3	HEM	В	347	4,2	-	6/12/54/54	-
3	HEM	А	142	4,1	-	4/12/54/54	-

The worst 5 of 28 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	А	142	HEM	CMD-C2D	10.62	1.73	1.50
3	В	347	HEM	C3C-CAC	9.88	1.68	1.47
5	А	501	PEM	O2-C10	8.35	1.66	1.41
3	В	347	HEM	CMC-C2C	7.01	1.68	1.51
3	В	347	HEM	CAB-C3B	-6.34	1.30	1.47



Mol	Chain	Res	Type	Atoms	Z	$Observed(^{o})$	$Ideal(^{o})$
3	А	142	HEM	CMA-C3A-C4A	-7.12	117.51	128.46
3	А	142	HEM	CHA-C4D-ND	6.48	132.39	124.38
3	А	142	HEM	C3B-C2B-C1B	-6.38	101.75	106.49
3	А	142	HEM	CMA-C3A-C2A	6.34	136.89	124.94
5	А	501	PEM	C9-C13-C14	-6.21	105.52	121.23

The worst 5 of 56 bond angle outliers are listed below:

There are no chirality outliers.

5 of 12 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	В	347	HEM	C2B-C3B-CAB-CBB
3	В	347	HEM	C3A-C2A-CAA-CBA
5	А	501	PEM	O2-C16-C19-O3
5	А	501	PEM	C17-C16-C19-O3
3	А	142	HEM	CAD-CBD-CGD-O2D

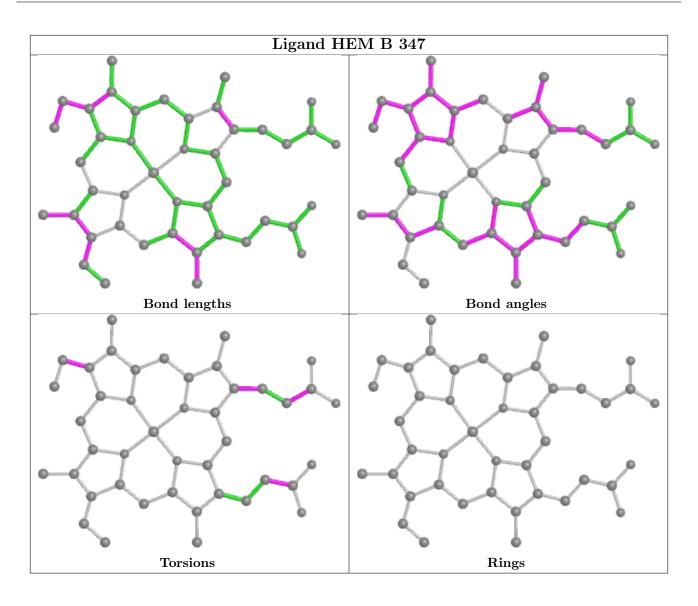
There are no ring outliers.

5 monomers are involved in 11 short contacts:

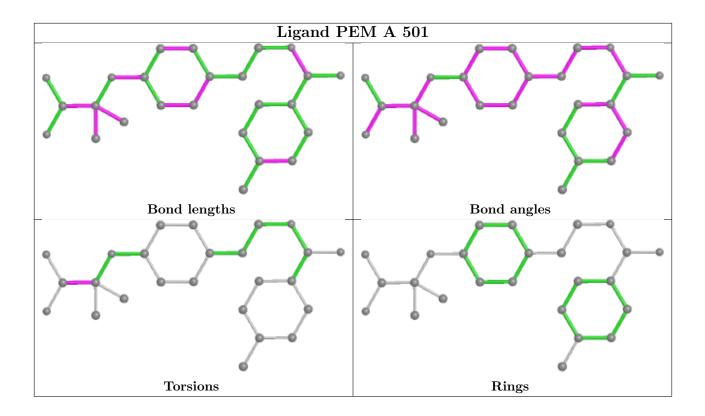
Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	В	347	HEM	5	0
4	А	143	CMO	4	0
4	В	348	CMO	4	0
5	А	501	PEM	2	0
3	А	142	HEM	4	0

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.



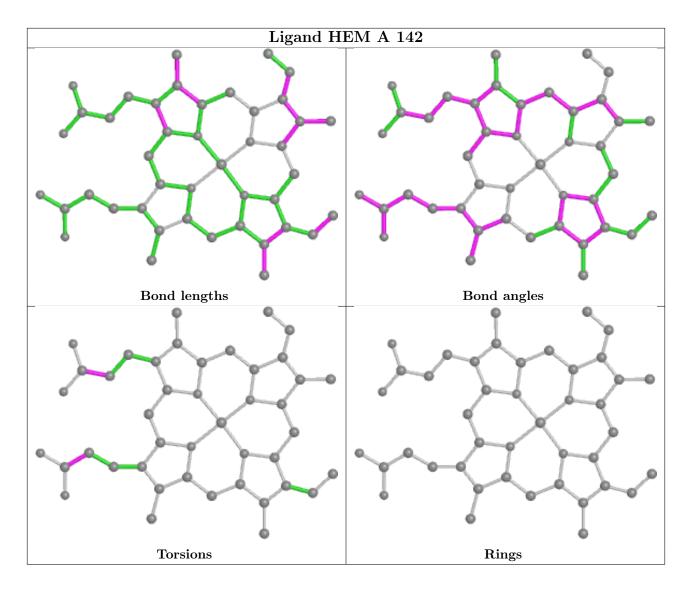












5.7 Other polymers (i)

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 is therefore empty.

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

EDS was not executed - this section is therefore empty.

6.3 Carbohydrates (i)

EDS was not executed - this section is therefore empty.

6.4 Ligands (i)

EDS was not executed - this section is therefore empty.

6.5 Other polymers (i)

EDS was not executed - this section is therefore empty.

