



wwPDB X-ray Structure Validation Summary Report ⓘ

Feb 13, 2017 – 04:45 pm GMT

PDB ID : 1SHR
Title : Crystal structure of ferrocyanide bound human hemoglobin A2 at 1.88Å resolution
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Deposited on : 2004-02-26
Resolution : 1.88 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	:	1.7.2 (RC1), CSD as538be (2017)
Xtriage (Phenix)	:	NOT EXECUTED
EDS	:	NOT EXECUTED
Percentile statistics	:	20161228.v01 (using entries in the PDB archive December 28th 2016)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	recalc28949

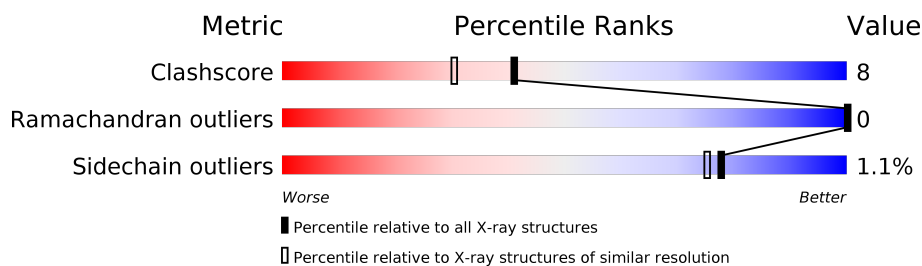
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 1.88 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	112137	8369 (1.90-1.86)
Ramachandran outliers	110173	8279 (1.90-1.86)
Sidechain outliers	110143	8280 (1.90-1.86)

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	141	
1	C	141	
2	B	146	
2	D	146	

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
3	CYN	B	804	-	-	X	-
3	CYN	B	809	-	-	X	-
3	CYN	D	805	-	-	X	-
3	CYN	D	806	-	-	X	-
3	CYN	D	807	-	-	X	-
3	CYN	D	808	-	-	X	-
4	FE	D	802	-	-	X	-

2 Entry composition [i](#)

There are 6 unique types of molecules in this entry. The entry contains 5335 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.

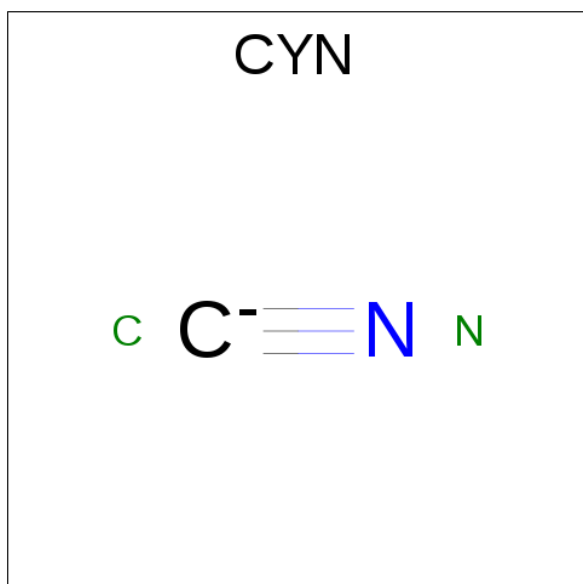
- Molecule 1 is a protein called Hemoglobin alpha chain.

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

- Molecule 2 is a protein called Hemoglobin delta chain.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B	146	Total	C	N	O	S	0	0	0
			1125	721	198	202	4			
2	D	146	Total	C	N	O	S	0	0	0
			1125	721	198	202	4			

- Molecule 3 is CYANIDE ION (three-letter code: CYN) (formula: CN).

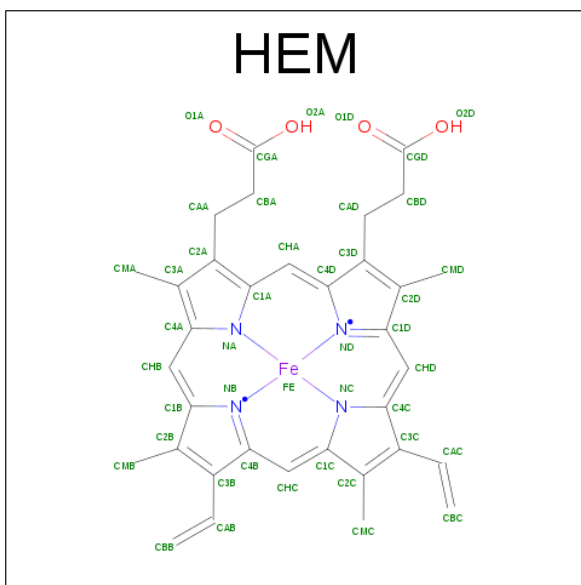


Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	A	1	Total C N 2 1 1	0	0
3	B	1	Total C N 2 1 1	0	0
3	C	1	Total C N 2 1 1	0	0
3	D	1	Total C N 2 1 1	0	0
3	B	1	Total C N 2 1 1	0	0
3	D	1	Total C N 2 1 1	0	0
3	D	1	Total C N 2 1 1	0	0
3	D	1	Total C N 2 1 1	0	0
3	D	1	Total C N 2 1 1	0	0
3	B	1	Total C N 2 1 1	0	0

- Molecule 4 is FE (III) ION (three-letter code: FE) (formula: Fe).

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
4	B	1	Total Fe 1 1	0	0
4	A	1	Total Fe 1 1	0	0
4	D	1	Total Fe 1 1	0	0

- Molecule 5 is PROTOPORPHYRIN IX CONTAINING FE (three-letter code: HEM) (formula: C₃₄H₃₂FeN₄O₄).



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

- Molecule 6 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
6	A	191	Total O 191 191	0	0
6	B	181	Total O 181 181	0	0
6	C	212	Total O 212 212	0	0
6	D	168	Total O 168 168	0	0

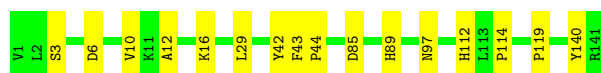
3 Residue-property plots [i](#)

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.


Note EDS was not executed.

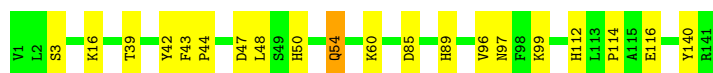
- Molecule 1: Hemoglobin alpha chain

Chain A: 




- Molecule 1: Hemoglobin alpha chain

Chain C: 




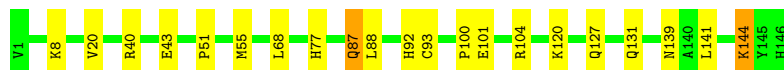
- Molecule 2: Hemoglobin delta chain

Chain B: 



- Molecule 2: Hemoglobin delta chain

Chain D: 



4 Data and refinement statistics

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

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α , β , γ	54.45Å 83.99Å 62.69Å 90.00° 99.86° 90.00°	Depositor
Resolution (Å)	14.89 – 1.88	Depositor
% Data completeness (in resolution range)	98.6 (14.89-1.88)	Depositor
R_{merge}	0.05	Depositor
R_{sym}	(Not available)	Depositor
Refinement program	CNS 1.0	Depositor
R, R_{free}	0.167 , 0.195	Depositor
Estimated twinning fraction	No twinning to report.	Xtriage
Total number of atoms	5335	wwPDB-VP
Average B, all atoms (Å ²)	21.0	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, FE, CYN

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	0.33	0/1097	0.52	0/1491
1	C	0.32	0/1097	0.52	0/1491
2	B	0.30	0/1152	0.50	0/1560
2	D	0.31	0/1152	0.52	0/1560
All	All	0.31	0/4498	0.52	0/6102

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	1069	0	1073	14	0
1	C	1069	0	1073	15	2
2	B	1125	0	1123	17	0
2	D	1125	0	1123	23	0
3	A	2	0	0	1	0
3	B	6	0	0	6	0
3	C	2	0	0	0	0
3	D	10	0	0	9	0
4	A	1	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
4	B	1	0	0	0	0
4	D	1	0	0	0	2
5	A	43	0	30	0	0
5	B	43	0	30	2	0
5	C	43	0	30	0	0
5	D	43	0	30	0	0
6	A	191	0	0	2	0
6	B	181	0	0	6	0
6	C	212	0	0	3	1
6	D	168	0	0	11	1
All	All	5335	0	4512	74	3

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 8.

The worst 5 of 74 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:D:87:GLN:HE21	2:D:87:GLN:H	0.97	0.89
1:C:114:PRO:HG3	6:D:1032:HOH:O	1.80	0.81
2:D:87:GLN:HE21	2:D:87:GLN:N	1.78	0.77
2:D:93:CYS:HB2	6:D:1515:HOH:O	1.89	0.72
2:D:120:LYS:HD3	6:D:1292:HOH:O	1.89	0.72

All (3) 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)
6:C:1150:HOH:O	6:D:1725:HOH:O[2_656]	1.64	0.56
1:C:47:ASP:OD2	4:D:802:FE:FE[2_656]	1.93	0.27
1:C:50:HIS:NE2	4:D:802:FE:FE[2_656]	2.11	0.09

5.3 Torsion angles

5.3.1 Protein backbone

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%)	138 (99%)	1 (1%)	0	100	100
1	C	139/141 (99%)	136 (98%)	3 (2%)	0	100	100
2	B	144/146 (99%)	141 (98%)	3 (2%)	0	100	100
2	D	144/146 (99%)	140 (97%)	4 (3%)	0	100	100
All	All	566/574 (99%)	555 (98%)	11 (2%)	0	100	100

There are no Ramachandran outliers to report.

5.3.2 Protein sidechains ⓘ

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
1	C	113/113 (100%)	112 (99%)	1 (1%)	82	81
2	B	118/118 (100%)	117 (99%)	1 (1%)	85	84
2	D	118/118 (100%)	115 (98%)	3 (2%)	53	42
All	All	462/462 (100%)	457 (99%)	5 (1%)	78	75

All (5) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
2	B	95	LYS
1	C	54	GLN
2	D	87	GLN
2	D	139	ASN
2	D	144	LYS

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 12 such sidechains are listed below:

Mol	Chain	Res	Type
1	C	9	ASN
1	C	54	GLN
1	C	97	ASN
2	B	139	ASN
1	C	89	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](#)

Of 17 ligands modelled in this entry, 3 are monoatomic - leaving 14 for Mogul analysis.

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	A	142	1,3	28,50,50	1.38	4 (14%)	17,82,82	1.91	3 (17%)
3	CYN	A	143	5	0,1,1	0.00	-	0,0,0	0.00	-
5	HEM	B	347	3,2	28,50,50	1.32	4 (14%)	17,82,82	1.80	4 (23%)
3	CYN	B	348	5	0,1,1	0.00	-	0,0,0	0.00	-
3	CYN	B	804	-	0,1,1	0.00	-	0,0,0	0.00	-
3	CYN	B	809	4	0,1,1	0.00	-	0,0,0	0.00	-
5	HEM	C	542	1,3	28,50,50	1.39	4 (14%)	17,82,82	1.91	4 (23%)
3	CYN	C	543	5	0,1,1	0.00	-	0,0,0	0.00	-
5	HEM	D	747	3,2	28,50,50	1.33	4 (14%)	17,82,82	1.83	4 (23%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
3	CYN	D	748	5	0,1,1	0.00	-	0,0,0	0.00	-
3	CYN	D	805	-	0,1,1	0.00	-	0,0,0	0.00	-
3	CYN	D	806	-	0,1,1	0.00	-	0,0,0	0.00	-
3	CYN	D	807	-	0,1,1	0.00	-	0,0,0	0.00	-
3	CYN	D	808	4	0,1,1	0.00	-	0,0,0	0.00	-

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	A	142	1,3	-	0/6/54/54	0/0/8/8
3	CYN	A	143	5	-	0/0/0/0	0/0/0/0
5	HEM	B	347	3,2	-	0/6/54/54	0/0/8/8
3	CYN	B	348	5	-	0/0/0/0	0/0/0/0
3	CYN	B	804	-	-	0/0/0/0	0/0/0/0
3	CYN	B	809	4	-	0/0/0/0	0/0/0/0
5	HEM	C	542	1,3	-	0/6/54/54	0/0/8/8
3	CYN	C	543	5	-	0/0/0/0	0/0/0/0
5	HEM	D	747	3,2	-	0/6/54/54	0/0/8/8
3	CYN	D	748	5	-	0/0/0/0	0/0/0/0
3	CYN	D	805	-	-	0/0/0/0	0/0/0/0
3	CYN	D	806	-	-	0/0/0/0	0/0/0/0
3	CYN	D	807	-	-	0/0/0/0	0/0/0/0
3	CYN	D	808	4	-	0/0/0/0	0/0/0/0

The worst 5 of 16 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
5	A	142	HEM	C3C-CAC	-4.43	1.38	1.47
5	C	542	HEM	C3C-CAC	-4.36	1.39	1.47
5	B	347	HEM	C3C-CAC	-3.77	1.40	1.47
5	D	747	HEM	C3C-CAC	-3.68	1.40	1.47
5	B	347	HEM	C3B-C2B	-2.50	1.37	1.40

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

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	D	747	HEM	CBD-CAD-C3D	-3.45	105.89	112.47
5	C	542	HEM	CMA-C3A-C4A	-3.23	123.50	128.46
5	B	347	HEM	CMA-C3A-C4A	-3.15	123.62	128.46

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	B	347	HEM	CBD-CAD-C3D	-3.13	106.50	112.47
5	D	747	HEM	CMA-C3A-C4A	-3.07	123.75	128.46

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

8 monomers are involved in 13 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	A	143	CYN	1	0
5	B	347	HEM	2	0
3	B	804	CYN	3	0
3	B	809	CYN	4	0
3	D	805	CYN	2	0
3	D	806	CYN	3	0
3	D	807	CYN	4	0
3	D	808	CYN	4	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

6.1 Protein, DNA and RNA chains

EDS was not executed - this section is therefore empty.

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

EDS was not executed - this section is therefore empty.

6.3 Carbohydrates

EDS was not executed - this section is therefore empty.

6.4 Ligands

EDS was not executed - this section is therefore empty.

6.5 Other polymers

EDS was not executed - this section is therefore empty.