



wwPDB NMR Structure Validation Summary Report ⓘ

Apr 15, 2026 – 11:35 AM UTC

PDB ID : 2M6Z / pdb_00002m6z
BMRB ID : 7125
Title : Refined solution structure of Human Adult Hemoglobin in the Carbonmonoxy Form
Authors : Fan, J.S.; Yang, D.; Choy, W.Y.
Deposited on : 2013-04-15

This is a wwPDB NMR 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/NMRValidationReportHelp>

with specific help available everywhere you see the ⓘ 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 ⓘ](#)) were used in the production of this report:

MolProbity : **FAILED**
Mogul : 2022.3.0, CSD as543be (2022)
Buster-report : wwPDB partial adaption of 1.1.7 (2018)
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)
wwPDB-RCI : v_1n_11_5_13_A (Berjanski et al., 2005)
PANAV : Wang et al. (2010)
wwPDB-ShiftChecker : v1.2
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.49

1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

SOLUTION NMR

The overall completeness of chemical shifts assignment is 37%.

There are no overall percentile quality scores available for this entry.

The sequence quality summary graphics cannot be shown.

2 Ensemble composition and analysis

This entry contains 20 models. Model 17 is the overall representative, medoid model (most similar to other models). The authors have identified model 1 as representative, based on the following criterion: *lowest energy*.

The following residues are included in the computation of the global validation metrics.

Well-defined (core) protein residues			
Well-defined core	Residue range (total)	Backbone RMSD (Å)	Medoid model
1	A:1-A:138, B:1-B:145 (283)	1.03	17
2	C:1-C:138, D:1-D:146 (284)	1.05	17

Ill-defined regions of proteins are excluded from the global statistics.

Ligands and non-protein polymers are included in the analysis.

The models can be grouped into 2 clusters and 1 single-model cluster was found.

Cluster number	Models
1	3, 4, 7, 9, 10, 11, 12, 13, 14, 15, 16, 17, 19, 20
2	1, 2, 5, 6, 8
Single-model clusters	18

3 Entry composition [i](#)

There are 3 unique types of molecules in this entry. The entry contains 9058 atoms, of which 4502 are hydrogens and 0 are deuteriums.

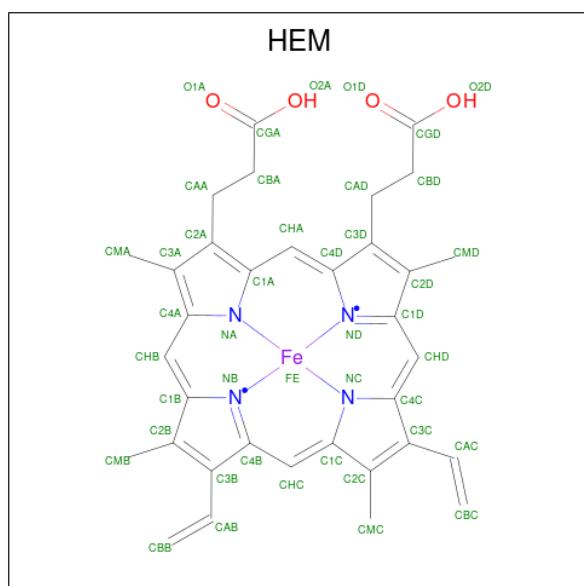
- Molecule 1 is a protein called Hemoglobin subunit alpha.

Mol	Chain	Residues	Atoms						Trace
1	A	141	Total	C	H	N	O	S	0
			2142	685	1073	187	194	3	
1	C	141	Total	C	H	N	O	S	0
			2142	685	1073	187	194	3	

- Molecule 2 is a protein called Hemoglobin subunit beta.

Mol	Chain	Residues	Atoms						Trace
2	B	146	Total	C	H	N	O	S	0
			2241	724	1118	195	201	3	
2	D	146	Total	C	H	N	O	S	0
			2241	724	1118	195	201	3	

- Molecule 3 is PROTOPORPHYRIN IX CONTAINING FE (CCD ID: HEM) (formula: $C_{34}H_{32}FeN_4O_4$).



Mol	Chain	Residues	Atoms					
3	A	1	Total	C	Fe	H	N	O
			73	34	1	30	4	4
3	B	1	Total	C	Fe	H	N	O
			73	34	1	30	4	4

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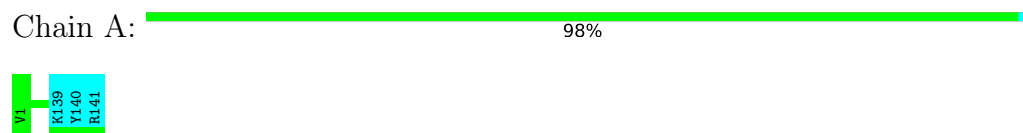
Mol	Chain	Residues	Atoms					
			Total	C	Fe	H	N	O
3	C	1	73	34	1	30	4	4
3	D	1	73	34	1	30	4	4

4 Residue-property plots

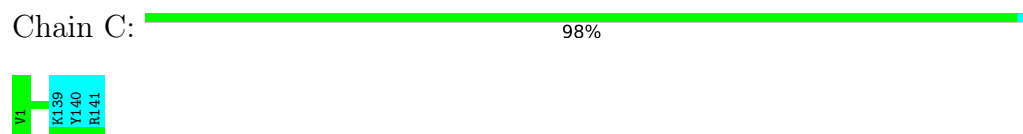
4.1 Average score per residue in the NMR ensemble

These plots are provided for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic is the same as shown in the summary in section 1 of this report. The second graphic shows the sequence where residues are colour-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 outliers are shown as green connectors. Residues which are classified as ill-defined in the NMR ensemble, are shown in cyan with an underline colour-coded according to the previous scheme. Residues which were present in the experimental sample, but not modelled in the final structure are shown in grey.

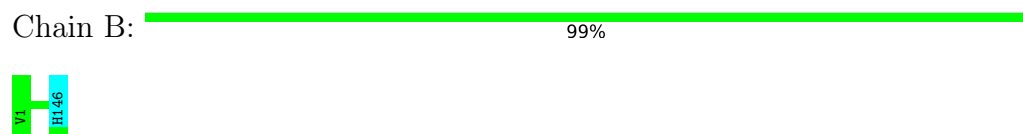
- Molecule 1: Hemoglobin subunit alpha



- Molecule 1: Hemoglobin subunit alpha



- Molecule 2: Hemoglobin subunit beta



- Molecule 2: Hemoglobin subunit beta



There are no outlier residues in this chain.

4.2 Residue scores for the representative (medoid) model from the NMR ensemble

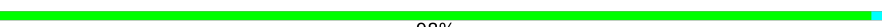
The representative model is number 17. Colouring as in section 4.1 above.

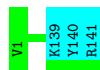
- Molecule 1: Hemoglobin subunit alpha





- Molecule 1: Hemoglobin subunit alpha

Chain C:  98% .

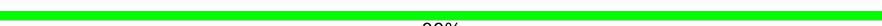


- Molecule 2: Hemoglobin subunit beta

Chain B:  98% ..



- Molecule 2: Hemoglobin subunit beta

Chain D:  99% .



5 Refinement protocol and experimental data overview

The models were refined using the following method: *torsion angle dynamics*.

Of the 100 calculated structures, 20 were deposited, based on the following criterion: *structures with the least restraint violations*.

The following table shows the software used for structure solution, optimisation and refinement.

Software name	Classification	Version
X-PLOR NIH	structure solution	2.30
X-PLOR NIH	refinement	2.30

The following table shows chemical shift validation statistics as aggregates over all chemical shift files. Detailed validation can be found in section 7 of this report.

Chemical shift file(s)	working_cs.cif
Number of chemical shift lists	1
Total number of shifts	2761
Number of shifts mapped to atoms	2760
Number of unparsed shifts	0
Number of shifts with mapping errors	1
Number of shifts with mapping warnings	0
Assignment completeness (well-defined parts)	37%

6 Model quality [i](#)

6.1 Standard geometry [i](#)

MolProbity failed to run properly - this section will have to be empty.

6.2 Too-close contacts [i](#)

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6.3 Torsion angles [i](#)

6.3.1 Protein backbone [i](#)

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6.3.2 Protein sidechains [i](#)

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6.3.3 RNA [i](#)

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

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6.5 Carbohydrates [i](#)

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6.6 Ligand geometry [i](#)

MolProbity failed to run properly - this section will have to be empty.

6.7 Other polymers [i](#)

MolProbity failed to run properly - this section will have to be empty.

6.8 Polymer linkage issues ⓘ

There are no chain breaks in this entry.

7 Chemical shift validation

The completeness of assignment taking into account all chemical shift lists is 37% for the well-defined parts and 36% for the entire structure.

7.1 Chemical shift list 1

File name: working_cs.cif

Chemical shift list name: *assigned_chem_shift_list_1*

7.1.1 Bookkeeping

The following table shows the results of parsing the chemical shift list and reports the number of nuclei with statistically unusual chemical shifts.

Total number of shifts	2761
Number of shifts mapped to atoms	2760
Number of unparsed shifts	0
Number of shifts with mapping errors	1
Number of shifts with mapping warnings	0
Number of shift outliers (ShiftChecker)	29

The following assigned chemical shifts were not mapped to the molecules present in the coordinate file.

- No matching atom found in the structure. All 1 occurrences are reported below.

List ID	Chain	Res	Type	Atom	Shift Data		
					Value	Uncertainty	Ambiguity
1	A	103	HIS	HE2	12.08	0.009	1

7.1.2 Chemical shift referencing

The following table shows the suggested chemical shift referencing corrections.

Nucleus	# values	Correction $\pm$ precision, ppm	Suggested action
$^{13}\text{C}_\alpha$	275	-0.93 ± 0.08	Should be checked
$^{13}\text{C}_\beta$	228	0.20 ± 0.07	None needed (< 0.5 ppm)
$^{13}\text{C}'$	0	—	None (insufficient data)
^{15}N	259	0.54 ± 0.18	Should be applied

7.1.3 Completeness of resonance assignments ⓘ

The following table shows the completeness of the chemical shift assignments for the well-defined regions of the structure. The overall completeness is 37%, i.e. 2740 atoms were assigned a chemical shift out of a possible 7487. 0 out of 134 assigned methyl groups (LEU and VAL) were assigned stereospecifically.

	Total	¹ H	¹³ C	¹⁵ N
Backbone	1069/2819 (38%)	539/1146 (47%)	273/1134 (24%)	257/539 (48%)
Sidechain	1514/3945 (38%)	1007/2608 (39%)	503/1237 (41%)	4/100 (4%)
Aromatic	157/723 (22%)	78/374 (21%)	72/304 (24%)	7/45 (16%)
Overall	2740/7487 (37%)	1624/4128 (39%)	848/2675 (32%)	268/684 (39%)

7.1.4 Statistically unusual chemical shifts ⓘ

The following table lists the statistically unusual chemical shifts. These are statistical measures, and large deviations from the mean do not necessarily imply incorrect assignments. Molecules containing paramagnetic centres or hemes are expected to give rise to anomalous chemical shifts.

List Id	Chain	Res	Type	Atom	Shift, ppm	Expected range, ppm	Z-score
1	B	92	HIS	HD2	0.89	4.65 – 9.35	-13.0
1	A	87	HIS	HD2	1.00	4.65 – 9.35	-12.8
1	B	92	HIS	HE1	1.41	5.13 – 10.76	-11.6
1	A	87	HIS	HE1	1.44	5.13 – 10.76	-11.6
1	B	67	VAL	HG11	-1.83	-0.48 – 2.12	-10.2
1	B	67	VAL	HG12	-1.83	-0.48 – 2.12	-10.2
1	B	67	VAL	HG13	-1.83	-0.48 – 2.12	-10.2
1	A	62	VAL	HG11	-1.76	-0.48 – 2.12	-9.9
1	A	62	VAL	HG12	-1.76	-0.48 – 2.12	-9.9
1	A	62	VAL	HG13	-1.76	-0.48 – 2.12	-9.9
1	B	141	LEU	HD21	-1.05	-0.65 – 2.13	-6.4
1	B	141	LEU	HD22	-1.05	-0.65 – 2.13	-6.4
1	B	141	LEU	HD23	-1.05	-0.65 – 2.13	-6.4
1	B	141	LEU	HD11	-0.83	-0.61 – 2.12	-5.8
1	B	141	LEU	HD12	-0.83	-0.61 – 2.12	-5.8
1	B	141	LEU	HD13	-0.83	-0.61 – 2.12	-5.8
1	A	29	LEU	HD21	-0.85	-0.65 – 2.13	-5.7
1	A	29	LEU	HD22	-0.85	-0.65 – 2.13	-5.7
1	A	29	LEU	HD23	-0.85	-0.65 – 2.13	-5.7
1	B	28	LEU	HD11	-0.72	-0.61 – 2.12	-5.4
1	B	28	LEU	HD12	-0.72	-0.61 – 2.12	-5.4
1	B	28	LEU	HD13	-0.72	-0.61 – 2.12	-5.4
1	A	58	HIS	HD2	4.50	4.65 – 9.35	-5.3
1	B	141	LEU	HB3	-0.36	-0.26 – 3.31	-5.3

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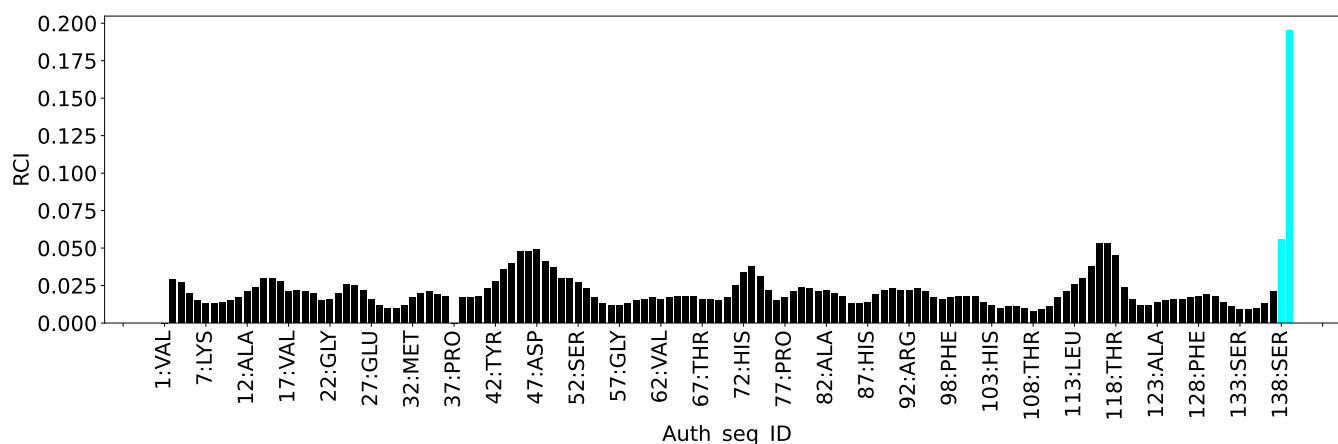
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List Id	Chain	Res	Type	Atom	Shift, ppm	Expected range, ppm	Z-score
1	B	63	HIS	HD2	4.57	4.65 – 9.35	-5.2
1	B	96	LEU	HD21	-0.69	-0.65 – 2.13	-5.1
1	B	96	LEU	HD22	-0.69	-0.65 – 2.13	-5.1
1	B	96	LEU	HD23	-0.69	-0.65 – 2.13	-5.1
1	A	86	LEU	HG	-0.15	-0.13 – 3.16	-5.0

7.1.5 Random Coil Index (RCI) plots [i](#)

The image below reports *random coil index* values for the protein chains in the structure. The height of each bar gives a probability of a given residue to be disordered, as predicted from the available chemical shifts and the amino acid sequence. A value above 0.2 is an indication of significant predicted disorder. The colour of the bar shows whether the residue is in the well-defined core (black) or in the ill-defined residue ranges (cyan), as described in section 2 on ensemble composition. If well-defined core and ill-defined regions are not identified then it is shown as gray bars.

Random coil index (RCI) for chain A:



Random coil index (RCI) for chain B:

