



wwPDB X-ray Structure Validation Summary Report

Feb 26, 2014 – 02:29 PM GMT

PDB ID : 1UIW
Title : Crystal Structures of Unliganded and Half-Liganded Human Hemoglobin Derivatives Cross-Linked between Lys 82beta1 and Lys 82beta2
Authors : Park, S.-Y.; Shibayama, N.; Tame, J.R.H.
Deposited on : 2003-07-23
Resolution : 1.50 Å(reported)

This is a wwPDB 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/ValidationPDFNotes.html>

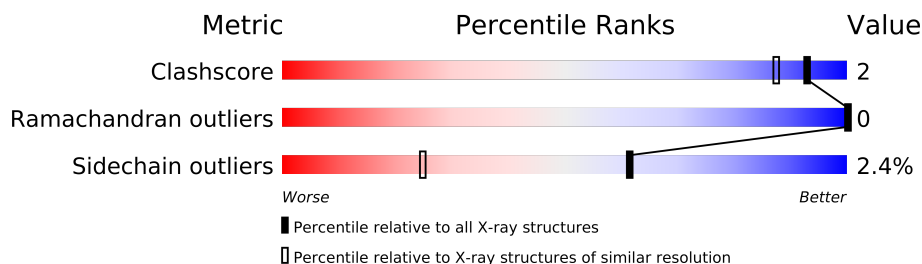
The following versions of software and data (see [references](#)) were used in the production of this report:

MolProbity	:	4.02b-467
Mogul	:	1.15 2013
Xtriage (Phenix)	:	NOT EXECUTED
EDS	:	NOT EXECUTED
Percentile statistics	:	21963
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et. al. (1996)
Validation Pipeline (wwPDB-VP)	:	stable22683

1 Overall quality at a glance

The reported resolution of this entry is 1.50 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	79885	1768 (1.50-1.50)
Ramachandran outliers	78287	1720 (1.50-1.50)
Sidechain outliers	78261	1718 (1.50-1.50)

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. The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density.

Note EDS was not executed.

Mol	Chain	Length	Quality of chain
1	A	141	
1	C	141	
1	E	141	
1	G	141	
2	B	146	
2	D	146	
2	F	146	
2	H	146	

The following table lists non-polymeric compounds that are outliers for geometric or electron-density-fit criteria:

Mol	Type	Chain	Res	Geometry	Electron density
4	2FU	B	2001	X	-
4	2FU	F	2002	X	-

2 Entry composition

There are 5 unique types of molecules in this entry. The entry contains 10985 atoms, of which 0 are hydrogen and 0 are deuterium.

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			
1	E	141	Total	C	N	O	S	0	0	0
			1069	685	187	194	3			
1	G	141	Total	C	N	O	S	0	0	0
			1069	685	187	194	3			

- Molecule 2 is a protein called Hemoglobin beta chain.

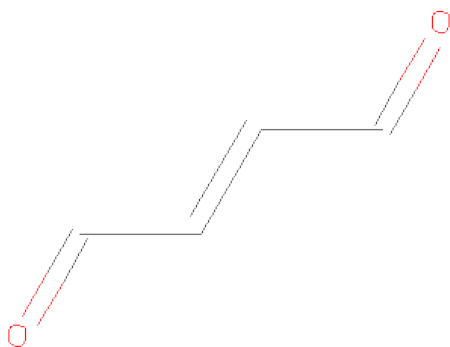
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B	146	Total	C	N	O	S	0	0	0
			1123	724	195	201	3			
2	D	146	Total	C	N	O	S	0	0	0
			1123	724	195	201	3			
2	F	145	Total	C	N	O	S	0	0	0
			1114	719	194	198	3			
2	H	146	Total	C	N	O	S	0	0	0
			1123	724	195	201	3			

- Molecule 3 is PROTOPORPHYRIN IX CONTAINING FE (three-letter code: HEM) (formula: C₃₄H₃₂FeN₄O₄).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
3	A	1	Total	C	Fe	N	O	0	0
			43	34	1	4	4		
3	B	1	Total	C	Fe	N	O	0	0
			43	34	1	4	4		
3	C	1	Total	C	Fe	N	O	0	0
			43	34	1	4	4		
3	D	1	Total	C	Fe	N	O	0	0
			43	34	1	4	4		
3	E	1	Total	C	Fe	N	O	0	0
			43	34	1	4	4		
3	F	1	Total	C	Fe	N	O	0	0
			43	34	1	4	4		
3	G	1	Total	C	Fe	N	O	0	0
			43	34	1	4	4		
3	H	1	Total	C	Fe	N	O	0	0
			43	34	1	4	4		

- Molecule 4 is BUT-2-ENEDIAL (three-letter code: 2FU) (formula: C₄H₄O₂).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
4	B	1	Total	C	O	0	0
			6	4	2		
4	F	1	Total	C	O	0	0
			6	4	2		

- Molecule 5 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	A	280	Total	O	0	0
			280	280		
5	B	253	Total	O	0	0
			253	253		
5	C	256	Total	O	0	0
			256	256		
5	D	211	Total	O	0	0
			211	211		
5	E	200	Total	O	0	0
			200	200		
5	F	206	Total	O	0	0
			206	206		
5	G	270	Total	O	0	0
			270	270		
5	H	194	Total	O	0	0
			194	194		

3 Residue-property plots

These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of errors 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: 



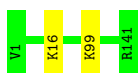
- Molecule 1: Hemoglobin alpha chain

Chain C: 



- Molecule 1: Hemoglobin alpha chain

Chain E: 



- Molecule 1: Hemoglobin alpha chain

Chain G: 



- Molecule 2: Hemoglobin beta chain

Chain B: 



- Molecule 2: Hemoglobin beta chain

Chain D: 



- Molecule 2: Hemoglobin beta chain

Chain F: 



- Molecule 2: Hemoglobin beta chain

Chain H: 



4 Data and refinement statistics

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

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α , β , γ	66.14Å 96.34Å 102.48Å 90.00° 101.79° 90.00°	Depositor
Resolution (Å)	29.11 – 1.50	Depositor
% Data completeness (in resolution range)	100.0 (29.11-1.50)	Depositor
R_{merge}	0.05	Depositor
R_{sym}	(Not available)	Depositor
Refinement program	REFMAC 5.1.22	Depositor
R, R_{free}	0.172 , 0.205	Depositor
Estimated twinning fraction	No twinning to report.	Xtriage
Total number of atoms	10985	wwPDB-VP
Average B, all atoms (Å ²)	16.0	wwPDB-VP

5 Model quality

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: HEM, 2FU

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	0.82	0/1097	0.76	1/1491 (0.1%)
1	C	0.71	0/1097	0.72	0/1491
1	E	0.80	0/1097	0.71	0/1491
1	G	0.78	0/1097	0.70	0/1491
2	B	0.80	0/1153	0.76	3/1566 (0.2%)
2	D	0.76	0/1153	0.75	3/1566 (0.2%)
2	F	0.71	0/1143	0.71	2/1551 (0.1%)
2	H	0.81	0/1153	0.73	0/1566
All	All	0.78	0/8990	0.73	9/12213 (0.1%)

There are no bond length outliers.

The worst 5 of 9 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	D	52	ASP	CB-CG-OD2	6.30	123.97	118.30
2	B	99	ASP	CB-CG-OD1	5.80	123.52	118.30
2	D	94	ASP	CB-CG-OD2	5.41	123.17	118.30
2	B	79	ASP	CB-CG-OD2	5.34	123.11	118.30
2	D	99	ASP	CB-CG-OD1	5.33	123.09	118.30

There are no chirality outliers.

There are no planarity outliers.

5.2 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 hydrogens added by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, and the number in parentheses is this value normalized per 1000 atoms of the molecule in the

chain. The Symm-Clashes column gives symmetry related clashes, in the same way as for the Clashes column.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	1069	0	1073	4	0
1	C	1069	0	1073	2	0
1	E	1069	0	1073	1	0
1	G	1069	0	1073	3	0
2	B	1123	0	1116	3	0
2	D	1123	0	1115	11	0
2	F	1114	0	1108	2	0
2	H	1123	0	1116	6	0
3	A	43	0	30	0	0
3	B	43	0	30	0	0
3	C	43	0	30	0	0
3	D	43	0	30	0	0
3	E	43	0	30	0	0
3	F	43	0	30	0	0
3	G	43	0	30	0	0
3	H	43	0	30	0	0
4	B	6	0	2	0	0
4	F	6	0	2	0	0
5	A	280	0	0	2	0
5	B	253	0	0	3	0
5	C	256	0	0	2	0
5	D	211	0	0	2	0
5	E	200	0	0	1	0
5	F	206	0	0	1	0
5	G	270	0	0	2	0
5	H	194	0	0	2	0
All	All	10985	0	8991	30	0

Clashscore is defined as the number of clashes calculated for the entry per 1000 atoms (including hydrogens) of the entry. The overall clashscore for this entry is 2.

The worst 5 of 30 close contacts within the same asymmetric unit are listed below.

Atom-1	Atom-2	Distance(Å)	Clash(Å)
2:F:139:ASN:HB3	5:F:2115:HOH:O	1.69	0.92
2:D:14:LEU:HD21	2:D:118:PHE:CE2	2.11	0.85
1:A:56:LYS:HG2	5:A:192:HOH:O	1.89	0.72
1:E:99:LYS:HG3	5:E:214:HOH:O	1.93	0.68
2:H:104:ARG:HG3	2:H:104:ARG:HH21	1.59	0.66

There are no symmetry-related clashes.

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%)	136 (98%)	3 (2%)	0	100	100
1	C	139/141 (99%)	137 (99%)	2 (1%)	0	100	100
1	E	139/141 (99%)	135 (97%)	4 (3%)	0	100	100
1	G	139/141 (99%)	137 (99%)	2 (1%)	0	100	100
2	B	144/146 (99%)	143 (99%)	1 (1%)	0	100	100
2	D	144/146 (99%)	142 (99%)	2 (1%)	0	100	100
2	F	141/146 (97%)	140 (99%)	1 (1%)	0	100	100
2	H	144/146 (99%)	142 (99%)	2 (1%)	0	100	100
All	All	1129/1148 (98%)	1112 (98%)	17 (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%)	112 (99%)	1 (1%)	87	69
1	C	113/113 (100%)	112 (99%)	1 (1%)	87	69
1	E	113/113 (100%)	112 (99%)	1 (1%)	87	69
1	G	113/113 (100%)	112 (99%)	1 (1%)	87	69
2	B	118/118 (100%)	116 (98%)	2 (2%)	73	41
2	D	118/118 (100%)	113 (96%)	5 (4%)	40	8
2	F	117/118 (99%)	111 (95%)	6 (5%)	33	6
2	H	118/118 (100%)	113 (96%)	5 (4%)	40	8

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
All	All	923/924 (100%)	901 (98%)	22 (2%)	61 25

5 of 22 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	E	16	LYS
2	F	68	LEU
2	H	104	ARG
2	F	1	VAL
2	F	50	THR

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 27 such sidechains are listed below:

Mol	Chain	Res	Type
2	D	117	HIS
1	E	89	HIS
2	H	102	ASN
2	D	139	ASN
2	B	102	ASN

5.3.3 RNA ⓘ

There are no RNA chains in this entry.

5.4 Non-standard residues in protein, DNA, RNA chains ⓘ

There are no non-standard protein/DNA/RNA residues in this entry.

5.5 Carbohydrates ⓘ

There are no carbohydrates in this entry.

5.6 Ligand geometry ⓘ

10 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	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
3	HEM	A	142	1	49,50,50	3.22	21 (42%)	46,82,82	1.98	9 (19%)
3	HEM	B	147	2	49,50,50	2.64	19 (38%)	46,82,82	2.05	9 (19%)
4	2FU	B	2001	2	5,5,5	0.88	0	4,4,4	2.92	3 (75%)
3	HEM	C	142	1	49,50,50	2.97	19 (38%)	46,82,82	2.08	9 (19%)
3	HEM	D	147	2	49,50,50	2.80	20 (40%)	46,82,82	2.14	11 (23%)
3	HEM	E	142	1	49,50,50	2.77	24 (48%)	46,82,82	2.21	9 (19%)
3	HEM	F	147	2	49,50,50	3.04	20 (40%)	46,82,82	2.18	11 (23%)
4	2FU	F	2002	2	5,5,5	1.25	1 (20%)	4,4,4	6.86	3 (75%)
3	HEM	G	142	1	49,50,50	2.94	21 (42%)	46,82,82	2.31	11 (23%)
3	HEM	H	147	2	49,50,50	2.69	21 (42%)	46,82,82	2.17	13 (28%)

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
3	HEM	A	142	1	-	0/14/114/114	0/0/8/8
3	HEM	B	147	2	-	0/14/114/114	0/0/8/8
4	2FU	B	2001	2	-	2/3/3/3	0/0/0/0
3	HEM	C	142	1	-	0/14/114/114	0/0/8/8
3	HEM	D	147	2	-	0/14/114/114	0/0/8/8
3	HEM	E	142	1	-	0/14/114/114	0/0/8/8
3	HEM	F	147	2	-	0/14/114/114	0/0/8/8
4	2FU	F	2002	2	-	2/3/3/3	0/0/0/0
3	HEM	G	142	1	-	0/14/114/114	0/0/8/8
3	HEM	H	147	2	-	0/14/114/114	0/0/8/8

The worst 5 of 166 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	F	147	HEM	C2B-C1B	10.56	1.47	1.44
3	A	142	HEM	C2B-C1B	10.16	1.47	1.44
3	A	142	HEM	C3D-C4D	9.19	1.46	1.44
3	C	142	HEM	C2B-C1B	8.63	1.46	1.44

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	H	147	HEM	C3D-C4D	7.21	1.46	1.44

The worst 5 of 88 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	F	2002	2FU	C5-C1-C2	10.73	132.84	121.62
3	G	142	HEM	C3B-C4B-NB	-9.18	107.43	114.00
3	E	142	HEM	C3B-C4B-NB	-8.76	107.73	114.00
3	F	147	HEM	C3B-C4B-NB	-8.27	108.08	114.00
3	C	142	HEM	C3B-C4B-NB	-8.08	108.22	114.00

There are no chirality outliers.

All (4) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
4	B	2001	2FU	O3-C2-C1-C5
4	F	2002	2FU	O8-C7-C5-C1
4	B	2001	2FU	O8-C7-C5-C1
4	F	2002	2FU	O3-C2-C1-C5

There are no ring outliers.

5.7 Other polymers ⓘ

There are no such residues in this entry.

5.8 Polymer linkage issues

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 will therefore be empty.

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

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

6.3 Carbohydrates ⓘ

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

6.4 Ligands ⓘ

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

6.5 Other polymers ⓘ

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