



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 6, 2026 – 03:40 AM UTC

PDB ID : 5IHU / pdb_00005ihu
Title : Crystal structure of bovine Fab B11
Authors : Stanfield, R.; Wilson, I.
Deposited on : 2016-02-29
Resolution : 2.06 Å(reported)

This is a Full wwPDB X-ray Structure Validation 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 ⓘ 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	:	4-5-2 with Phenix2.0
Xtriage (Phenix)	:	2.0
EDS	:	3.0
Percentile statistics	:	20250101.v01 (using entries in the PDB archive January 1st 2025)
CCP4	:	9.0.010 (Gargrove)
Density-Fitness	:	1.0.12
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.49

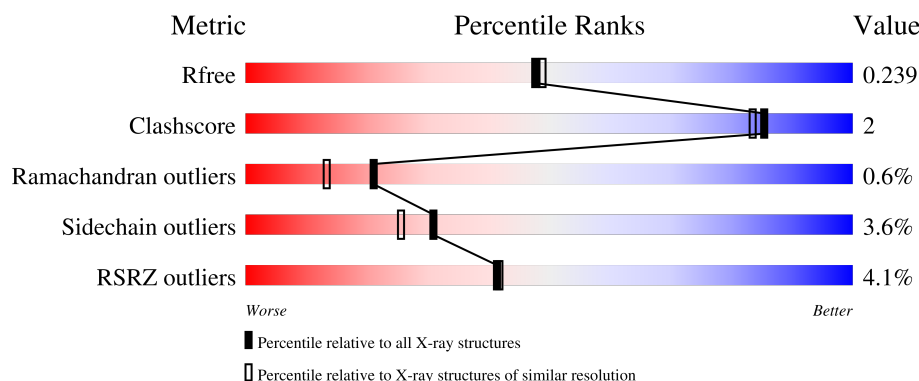
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

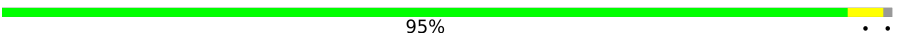
The reported resolution of this entry is 2.06 Å.

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))
R_{free}	180053	3774 (2.08-2.04)
Clashscore	190562	3883 (2.08-2.04)
Ramachandran outliers	187476	3860 (2.08-2.04)
Sidechain outliers	187428	3860 (2.08-2.04)
RSRZ outliers	180081	3775 (2.08-2.04)

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 $\leq 5\%$. 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.

Mol	Chain	Length	Quality of chain
1	L	216	 95%
2	H	273	 7% 90% 8%

2 Entry composition

There are 3 unique types of molecules in this entry. The entry contains 7047 atoms, of which 3430 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 bovine Fab B11 light chain.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
1	L	213	Total	C	H	N	O	S	0	0	0
			3064	959	1503	263	334	5			

- Molecule 2 is a protein called bovine Fab B11 heavy chain.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
2	H	273	Total	C	H	N	O	S	0	2	0
			3928	1239	1927	331	412	19			

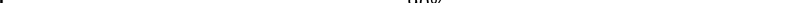
- Molecule 3 is water.

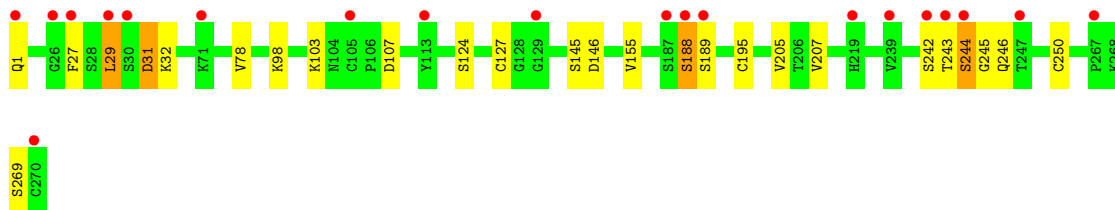
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	L	27	Total	O	0	0
			27	27		
3	H	28	Total	O	0	0
			28	28		

i

- Molecule 1: bovine Fab B11 light chain



- Chain H: 



4 Data and refinement statistics

Property	Value	Source
Space group	C 1 2 1	Depositor
Cell constants a, b, c, α , β , γ	78.41Å 71.46Å 88.32Å 90.00° 97.27° 90.00°	Depositor
Resolution (Å)	38.89 – 2.06 38.89 – 2.06	Depositor EDS
% Data completeness (in resolution range)	95.0 (38.89-2.06) 95.0 (38.89-2.06)	Depositor EDS
R_{merge}	0.05	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	3.05 (at 2.07Å)	Xtriage
Refinement program	PHENIX 1.9_1692	Depositor
R, R_{free}	0.194 , 0.235 0.203 , 0.239	Depositor DCC
R_{free} test set	2372 reflections (7.76%)	wwPDB-VP
Wilson B-factor (Å ²)	44.9	Xtriage
Anisotropy	0.245	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.39 , 52.8	EDS
L-test for twinning ²	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.32$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.97	EDS
Total number of atoms	7047	wwPDB-VP
Average B, all atoms (Å ²)	80.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 5.91% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

²Theoretical values of $\langle |L| \rangle$, $\langle L^2 \rangle$ for acentric reflections are 0.5, 0.333 respectively for untwinned datasets, and 0.375, 0.2 for perfectly twinned datasets.

5 Model quality [i](#)

5.1 Standard geometry [i](#)

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	L	0.28	0/1591	0.59	0/2168
2	H	0.29	0/2051	0.63	0/2798
All	All	0.29	0/3642	0.62	0/4966

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	L	1561	1503	1502	2	0
2	H	2001	1927	1927	14	0
3	H	28	0	0	0	0
3	L	27	0	0	0	0
All	All	3617	3430	3429	15	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 2.

All (15) 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:H:188:SER:HB3	2:H:189:SER:HA	1.84	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:H:243:THR:HG22	2:H:244:SER:HA	1.91	0.51
2:H:29:LEU:HD21	2:H:78:VAL:HG23	1.91	0.51
2:H:243:THR:CG2	2:H:244:SER:HA	2.41	0.50
1:L:46:THR:OG1	2:H:155:VAL:O	2.27	0.50
2:H:244:SER:CB	2:H:245:GLY:HA2	2.42	0.50
2:H:207:VAL:HG13	2:H:250[B]:CYS:SG	2.56	0.45
2:H:188:SER:CB	2:H:189:SER:HA	2.46	0.45
2:H:145:SER:OG	2:H:146:ASP:N	2.50	0.45
2:H:107:ASP:N	2:H:107:ASP:OD1	2.51	0.44
2:H:31:ASP:OD1	2:H:31:ASP:N	2.52	0.43
2:H:244:SER:CB	2:H:245:GLY:CA	2.97	0.42
1:L:150:ALA:HB2	1:L:155:ILE:HD11	2.02	0.42
2:H:27:PHE:HE2	2:H:32:LYS:HB2	1.84	0.41
2:H:195[B]:CYS:HG	2:H:250[B]:CYS:HG	1.67	0.41

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	Percentiles	
1	L	211/216 (98%)	200 (95%)	11 (5%)	0	100	100
2	H	273/273 (100%)	256 (94%)	14 (5%)	3 (1%)	11	4
All	All	484/489 (99%)	456 (94%)	25 (5%)	3 (1%)	21	13

All (3) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
2	H	269	SER
2	H	246	GLN
2	H	242	SER

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	L	182/184 (99%)	177 (97%)	5 (3%)	39	35
2	H	232/230 (101%)	222 (96%)	10 (4%)	26	20
All	All	414/414 (100%)	399 (96%)	15 (4%)	31	25

All (15) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	L	18	ARG
1	L	30	ASN
1	L	79	GLN
1	L	108	GLN
1	L	167	GLN
2	H	1	GLN
2	H	29	LEU
2	H	31	ASP
2	H	98	LYS
2	H	103	LYS
2	H	124	SER
2	H	127	CYS
2	H	188	SER
2	H	205	VAL
2	H	244	SER

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (2) such sidechains are listed below:

Mol	Chain	Res	Type
2	H	73	ASN
2	H	101	GLN

5.3.3 RNA ⓘ

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 oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

There are no ligands in this entry.

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

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, 95th 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>	#RSRZ>2			OWAB(Å ²)	Q<0.9
1	L	213/216 (98%)	0.29	0	100	100	39, 74, 120, 145	0
2	H	273/273 (100%)	0.50	20 (7%)	21	21	31, 68, 148, 175	2 (0%)
All	All	486/489 (99%)	0.41	20 (4%)	41	42	31, 71, 140, 175	2 (0%)

All (20) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
2	H	187	SER	3.6
2	H	113	TYR	3.5
2	H	267	PRO	3.2
2	H	219	HIS	3.2
2	H	189	SER	3.1
2	H	243	THR	2.7
2	H	29	LEU	2.6
2	H	239	VAL	2.6
2	H	27	PHE	2.6
2	H	188	SER	2.6
2	H	71	LYS	2.4
2	H	247	THR	2.4
2	H	26	GLY	2.3
2	H	242	SER	2.2
2	H	105	CYS	2.2
2	H	30	SER	2.1
2	H	270	CYS	2.1
2	H	129	GLY	2.0
2	H	244	SER	2.0
2	H	1	GLN	2.0

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 oligosaccharides in this entry.

6.4 Ligands [i](#)

There are no ligands in this entry.

6.5 Other polymers [i](#)

There are no such residues in this entry.