

# Full wwPDB X-ray Structure Validation Report (i)

#### Aug 26, 2024 – 12:58 PM EDT

PDB ID	:	8VBQ
Title	:	Structure of bovine anti-HIV Fab Bess7
Authors	:	Stanfield, R.L.; Wilson, I.A.
Deposited on		
Resolution	:	2.10  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 (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:

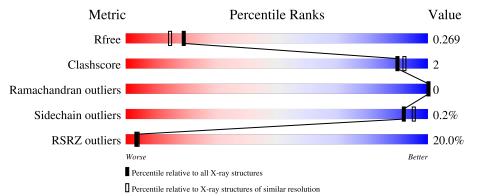
MolProbity	:	4.02b-467
Xtriage (Phenix)	:	1.20.1
$\mathrm{EDS}$	:	3.0
Percentile statistics	:	20231227.v01 (using entries in the PDB archive December 27th 2023)
CCP4	:	9.0.002 (Gargrove)
Density-Fitness	:	1.0.11
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.38.3

# 1 Overall quality at a glance (i)

The following experimental techniques were used to determine the structure:  $X\text{-}RAY \, DIFFRACTION$ 

The reported resolution of this entry is 2.10 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	$\begin{array}{c} \textbf{Whole archive} \\ \textbf{(\#Entries)} \end{array}$	${f Similar\ resolution}\ (\#{ m Entries,\ resolution\ range}({ m \AA}))$
$R_{free}$	164625	6234 (2.10-2.10)
Clashscore	180529	6893 (2.10-2.10)
Ramachandran outliers	177936	6839 (2.10-2.10)
Sidechain outliers	177891	6840 (2.10-2.10)
RSRZ outliers	164620	6234 (2.10-2.10)

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% 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	Н	272	93%	7%
2	L	216	98%	•



# 2 Entry composition (i)

There are 3 unique types of molecules in this entry. The entry contains 7134 atoms, of which 3423 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 Bess7 heavy chain.

Mol	Chain	Residues		Atoms				ZeroOcc	AltConf	Trace	
1	Н	271	Total 3910	C 1243	Н 1916	N 329	O 409	S 13	0	0	0

• Molecule 2 is a protein called Bovine Fab Bess7 light chain.

Mol	Chain	Residues			Atom	IS			ZeroOcc	AltConf	Trace
2	T	215	Total	С	Η	Ν	Ο	$\mathbf{S}$	0	0	0
		215	3082	971	1507	266	333	5	0	0	0

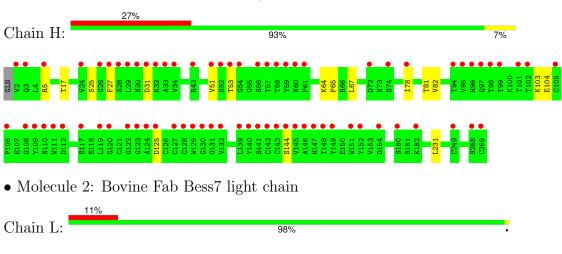
• Molecule 3 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	Н	78	Total         O           78         78	0	0
3	L	64	$\begin{array}{cc} \text{Total} & \text{O} \\ 64 & 64 \end{array}$	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 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.



• Molecule 1: Bovine Fab Bess7 heavy chain



## 4 Data and refinement statistics (i)

Property	Value	Source
Space group	C 1 2 1	Depositor
Cell constants	83.00Å 69.78Å 87.52Å	Depositor
a, b, c, $\alpha$ , $\beta$ , $\gamma$	$90.00^{\circ}$ $103.52^{\circ}$ $90.00^{\circ}$	Depositor
Resolution (Å)	48.29 - 2.10	Depositor
Resolution (A)	48.29 - 2.10	EDS
% Data completeness	98.8 (48.29-2.10)	Depositor
(in resolution range)	98.7 (48.29-2.10)	EDS
R <sub>merge</sub>	0.15	Depositor
$R_{sym}$	(Not available)	Depositor
$< I/\sigma(I) > 1$	$1.34 (at 2.10 \text{\AA})$	Xtriage
Refinement program	PHENIX 1.19.2_4158	Depositor
D D.	0.232 , $0.268$	Depositor
$R, R_{free}$	0.232 , $0.269$	DCC
$R_{free}$ test set	1370 reflections $(4.80\%)$	wwPDB-VP
Wilson B-factor $(Å^2)$	31.8	Xtriage
Anisotropy	0.463	Xtriage
Bulk solvent $k_{sol}(e/Å^3)$ , $B_{sol}(Å^2)$	0.40,36.0	EDS
L-test for twinning <sup>2</sup>	$ \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	0.93	EDS
Total number of atoms	7134	wwPDB-VP
Average B, all atoms $(Å^2)$	50.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: The largest off-origin peak in the Patterson function is 5.76% of the height of the origin peak. No significant pseudotranslation is detected.

<sup>&</sup>lt;sup>2</sup>Theoretical 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.



<sup>&</sup>lt;sup>1</sup>Intensities estimated from amplitudes.

# 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		
	Ullaill	RMSZ	# Z  > 5	RMSZ	# Z  > 5	
1	Н	0.24	0/2041	0.48	0/2790	
2	L	0.26	0/1608	0.48	0/2196	
All	All	0.25	0/3649	0.48	0/4986	

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	Н	1994	1916	1918	10	0
2	L	1575	1507	1513	2	0
3	Н	78	0	0	0	0
3	L	64	0	0	0	0
All	All	3711	3423	3431	12	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 (12) 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)
1:H:31:ASP:HA	1:H:53:THR:HG22	1.72	0.70

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Atom-1	Atom-2	Interatomic	Clash
Atom-1	Atom-2	distance $(Å)$	overlap (Å)
1:H:67:LEU:CD2	1:H:82:VAL:HG22	2.33	0.58
1:H:51:VAL:HG12	1:H:78:ILE:HD12	1.86	0.58
2:L:210:GLU:N	2:L:210:GLU:OE1	2.42	0.53
1:H:17:THR:HG23	1:H:81:THR:HG23	1.94	0.49
1:H:103:LYS:NZ	1:H:125:ASP:OD2	2.47	0.48
1:H:231:LEU:HD12	1:H:231:LEU:C	2.34	0.48
2:L:37:GLN:HB2	2:L:47:LEU:HD11	1.96	0.48
1:H:104:GLU:O	1:H:144:SER:N	2.50	0.45
1:H:17:THR:CG2	1:H:81:THR:HG23	2.49	0.42
1:H:64:LYS:N	1:H:65:PRO:CD	2.83	0.41
1:H:5:ARG:NH2	1:H:25:SER:OG	2.50	0.41

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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	Н	269/272~(99%)	255~(95%)	14~(5%)	0	100 100
2	L	213/216~(99%)	204 (96%)	9 (4%)	0	100 100
All	All	482/488~(99%)	459 (95%)	23~(5%)	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	Н	230/231~(100%)	229 (100%)	1 (0%)	89 93
2	L	179/180~(99%)	179~(100%)	0	100 100
All	All	409/411 (100%)	408 (100%)	1 (0%)	92 95

All (1) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	Н	27	PHE

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. There are no such sidechains identified.

#### 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 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 (i)

## 6.1 Protein, DNA and RNA chains (i)

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,  $95^{th}$  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	$\langle RSRZ \rangle$	#RSRZ>2	$OWAB(Å^2)$	Q < 0.9
1	Н	271/272 (99%)	1.06	74 (27%) 2 2	25, 43, 109, 121	0
2	L	215/216~(99%)	0.71	23 (10%) 12 13	23, 43, 78, 106	0
All	All	486/488 (99%)	0.91	97 (19%) 3 4	23, 43, 103, 121	0

All (97) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	Н	27	PHE	5.8
1	Н	29	LEU	5.3
1	Н	145	VAL	5.3
1	Н	2	VAL	5.1
1	Н	96	HIS	4.9
1	Н	149	TYR	4.8
1	Н	146	ALA	4.8
1	Н	111	TRP	4.8
2	L	25	GLY	4.6
1	Н	33	ALA	4.4
2	L	211	CYS	4.2
1	Н	101	THR	4.2
1	Н	269	CYS	4.0
1	Н	51	VAL	3.8
1	Н	249	CYS	3.8
1	Н	152	TYR	3.7
1	Н	53	THR	3.7
1	Н	99	THR	3.7
1	Н	108	GLY	3.6
2	L	27(B)	ASN	3.6
1	Н	140	TYR	3.6
1	Н	97	GLN	3.5
1	Н	32	LYS	3.5
1	Н	30	ASN	3.5

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Mol	nued fron Chain	Res	Type	RSRZ
1	Н	130	GLY	3.5
1	Н	102	THR	3.5
2	L	2	ALA	3.4
1	Н	28	SER	3.4
1	Н	131	GLY	3.4
1	Н	151	TRP	3.3
1	Н	124	ALA	3.3
1	Н	132	VAL	3.3
1	Н	129	TRP	3.2
1	Н	117	SER	3.2
1	Н	119	LEU	3.2
1	Н	147	HIS	3.2
2	L	95(A)	SER	3.2
1	Н	78	ILE	3.2
1	Н	144	SER	3.1
1	Н	143	CYS	3.1
1	Н	109	TYR	3.1
1	Н	59	TYR	3.1
1	Н	56	SER	3.1
2	L	1	GLN	3.0
2	L	91	ALA	3.0
1	Н	57	THR	3.0
1	Н	98	THR	3.0
1	Н	60	ASN	3.0
2	L	187	SER	3.0
1	Н	148	THR	3.0
1	Н	123	GLY	3.0
1	Н	31	ASP	2.9
1	Н	95	VAL	2.9
2	L	95(B)	ASN	2.9
2	L	31	GLY	2.9
2	L	209	THR	2.8
1	Н	106	PRO	2.8
1	Н	127	CYS	2.8
1	Н	182	LYS	2.8
1	Н	94	THR	2.8
1	Н	58	THR	2.7
1	Н	52	SER	2.7
1	Н	54	GLY	2.7
2	L	26	SER	2.6
2	L	152	SER	2.6
2	L	4	LEU	2.6

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Mol	Chain	Res	Type	RSRZ
1	Н	268	SER	2.6
2	L	94	SER	2.6
2	L	32	TYR	2.6
2	L	96	ALA	2.5
1	Н	105	CYS	2.5
1	Н	61	PRO	2.5
1	Н	5	ARG	2.4
1	Н	125	ASP	2.4
1	Н	74	SER	2.3
2	L	60	ASP	2.3
1	Н	139	LEU	2.3
2	L	155	VAL	2.3
1	Н	122	GLY	2.3
2	L	17	GLN	2.3
1	Н	154	ASP	2.2
1	Н	34	VAL	2.2
1	Н	72	ASP	2.2
1	Н	110	ASN	2.2
1	Н	24	VAL	2.2
1	Н	128	CYS	2.1
1	Н	142	CYS	2.1
2	L	106(A)	LEU	2.1
1	Н	180	SER	2.1
1	Н	26	GLY	2.1
2	L	208	PRO	2.1
1	Н	141	SER	2.1
1	Н	43	ARG	2.1
1	Н	112	ASP	2.0
1	Н	3	GLN	2.0
1	Н	120	GLY	2.0
2	L	210	GLU	2.0

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### 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 monosaccharides 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.

