WORLDWIDE wwPDB PROTEIN DATA BANK

Full wwPDB X-ray Structure Validation Report ⓘ

Aug 26, 2024 – 12:59 PM EDT

PDB ID	:	8VBN
Title	:	Structure of bovine anti-HIV Fab ElsE8
Authors	:	Stanfield, R.L.; Wilson, I.A.
Deposited on	:	2023-12-12
Resolution	:	1.83 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:

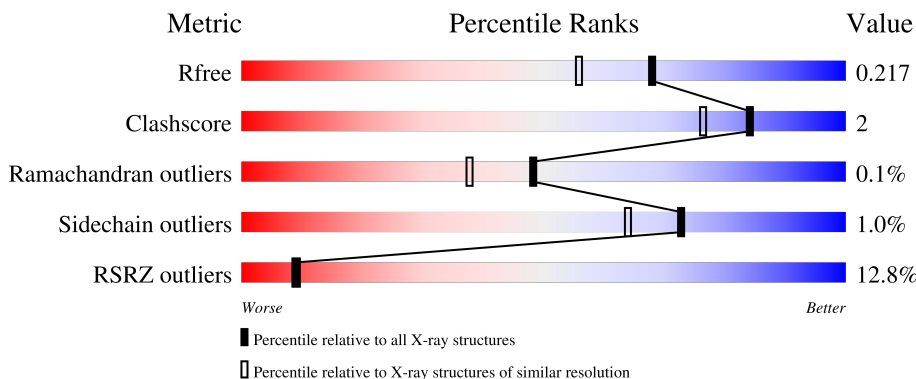|		
MolProbity	:	4.02b-467
Xtriage (Phenix)	:	1.20.1
EDS	:	3.0
Percentile statistics	:	20231227.v01 (using entries in the PDB archive December 27th 2023)
CCP4	:	9.0.002 (Gargrove)
Density-Fitness	:	1.0.11
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)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

1 Overall quality at a glance ⓘ

The following experimental techniques were used to determine the structure:
X-RAY DIFFRACTION

The reported resolution of this entry is 1.83 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	Percentile Ranks	Value
Rfree		0.217
Clashscore		2
Ramachandran outliers		0.1%
Sidechain outliers		1.0%
RSRZ outliers		12.8%

Worse ... *Better*

▌ Percentile relative to all X-ray structures

❚ Percentile relative to X-ray structures of similar resolution

Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	164625	1150 (1.84-1.84)
Clashscore	180529	1248 (1.84-1.84)
Ramachandran outliers	177936	1240 (1.84-1.84)
Sidechain outliers	177891	1240 (1.84-1.84)
RSRZ outliers	164620	1149 (1.84-1.84)

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	A	216	22% / 94% · ·
1	L	216	2% / 97% ·
2	B	265	16% / 90% 8% ·
2	H	265	9% / 79% 6% 15%

2 Entry composition (i)

There are 3 unique types of molecules in this entry. The entry contains 14036 atoms, of which 6592 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 ElsE8 light chain.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
1	L	216	Total 3120	C 979	H 1531	N 270	O 335	S 5	0	1	0
1	A	214	Total 3077	C 968	H 1508	N 265	O 332	S 4	0	0	0

- Molecule 2 is a protein called Bovine Fab ElsE8 heavy chain.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
2	H	225	Total 3322	C 1041	H 1659	N 277	O 338	S 7	0	2	0
2	B	260	Total 3836	C 1216	H 1894	N 320	O 396	S 10	0	2	0

- Molecule 3 is water.

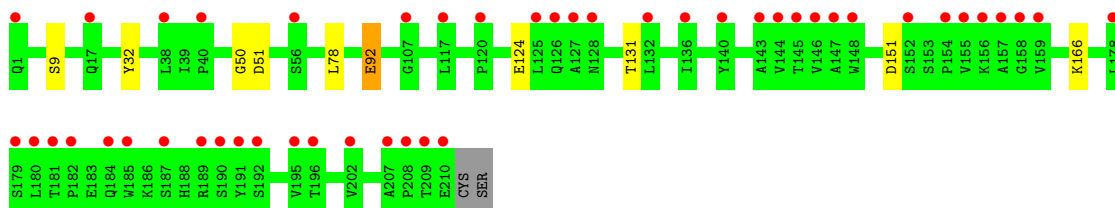| Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	L	249	Total 249	O 249	0	0
3	H	185	Total 185	O 185	0	0
3	B	151	Total 151	O 151	0	0
3	A	96	Total 96	O 96	0	0

3 Residue-property plots ⓘ

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.
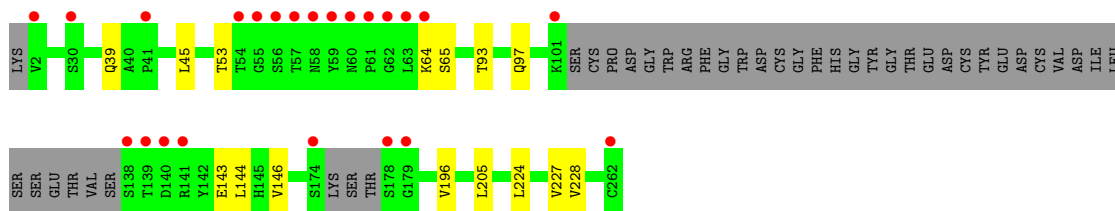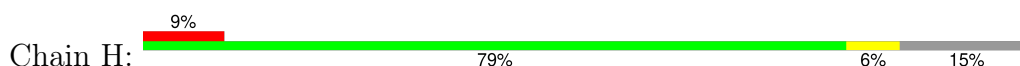
• Molecule 1: Bovine Fab ElsE8 light chain

Chain L:
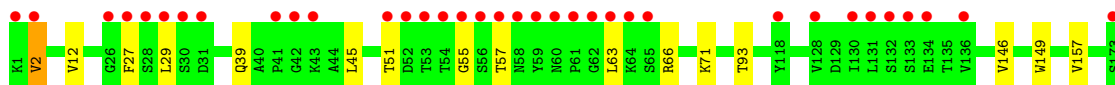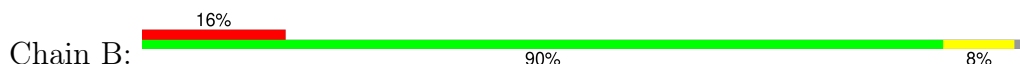
• Molecule 1: Bovine Fab ElsE8 light chain

Chain A:

• Molecule 2: Bovine Fab ElsE8 heavy chain

Chain H:

• Molecule 2: Bovine Fab ElsE8 heavy chain

Chain B:

SER LYS SER T177 S178 G179 G180 V196 L205 H210 L224 V228 T229 T251 P259 K260 SER CYS

4 Data and refinement statistics ⓘ

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α, β, γ	59.22Å 120.27Å 150.30Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	46.95 – 1.83 46.95 – 1.83	Depositor EDS
% Data completeness (in resolution range)	99.6 (46.95-1.83) 99.8 (46.95-1.83)	Depositor EDS
R_{merge}	0.12	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	1.39 (at 1.83Å)	Xtriage
Refinement program	PHENIX 1.19.2_4158	Depositor
R, R_{free}	0.196 , 0.218 0.196 , 0.217	Depositor DCC
R_{free} test set	1972 reflections (2.07%)	wwPDB-VP
Wilson B-factor (Å²)	26.3	Xtriage
Anisotropy	0.100	Xtriage
Bulk solvent k_{sol}(e/Å³), B_{sol}(Å²)	0.38 , 40.3	EDS
L-test for twinning [2]	$< |L| > = 0.49, < L^2 > = 0.32$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o,F_c correlation	0.95	EDS
Total number of atoms	14036	wwPDB-VP
Average B, all atoms (Å²)	42.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.48% of the height of the origin peak. No significant pseudotranslation is detected.*

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[1]Intensities estimated from amplitudes.
[2]Theoretical values of $< |L| >$, $< L^2 >$ for acentric reflections are 0.5, 0.333 respectively for untwinned datasets, and 0.375, 0.2 for perfectly twinned datasets.

5 Model quality ⓘ

5.1 Standard geometry ⓘ

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	0.28	0/1602	0.50	0/2188
1	L	0.30	0/1625	0.54	0/2218
2	B	0.27	0/1991	0.51	0/2717
2	H	0.29	0/1701	0.53	0/2320
All	All	0.29	0/6919	0.52	0/9443

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 ⓘ

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	1569	1508	1508	4	0
1	L	1589	1531	1530	4	0
2	B	1942	1894	1893	14	0
2	H	1663	1659	1659	9	0
3	A	96	0	0	1	0
3	B	151	0	0	1	0
3	H	185	0	0	1	0
3	L	249	0	0	1	0
All	All	7444	6592	6590	29	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.

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All (29) 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:97:GLN:HG2	2:H:144:LEU:HD13	1.72	0.69
1:A:92:GLU:OE2	3:A:301:HOH:O	2.14	0.65
2:H:205:LEU:HD21	2:H:228:VAL:HG21	1.86	0.57
2:B:229:THR:HG23	3:B:334:HOH:O	2.06	0.55
2:B:29:LEU:HD21	2:B:71:LYS:HD2	1.92	0.52
2:B:12:VAL:CG1	2:B:157:VAL:HG22	2.43	0.48
2:B:51:THR:HG23	2:B:51:THR:O	2.13	0.48
1:L:135:LEU:CD1	2:H:227:VAL:HG21	2.44	0.48
1:L:18[B]:ARG:NH2	3:L:303:HOH:O	2.37	0.47
2:B:39:GLN:HB2	2:B:45:LEU:HD23	1.97	0.47
2:B:224:LEU:HD12	2:B:224:LEU:C	2.34	0.47
2:B:55:GLY:O	2:B:57:THR:HG23	2.15	0.46
1:L:32:TYR:CD1	2:H:143:GLU:HG2	2.50	0.46
2:B:12:VAL:HG13	2:B:157:VAL:HG22	1.96	0.46
2:H:53:THR:HG23	3:H:394:HOH:O	2.15	0.45
1:A:50:GLY:O	1:A:51:ASP:HB2	2.18	0.44
2:B:93:THR:HB	2:B:146:VAL:HG13	2.00	0.43
2:H:64:LYS:O	2:H:65:SER:OG	2.30	0.43
2:H:93:THR:HB	2:H:146:VAL:HG13	2.01	0.42
2:B:146:VAL:HG11	2:B:149:TRP:CE2	2.54	0.42
2:B:51:THR:HA	2:B:57:THR:HG22	2.00	0.42
2:H:39:GLN:HB2	2:H:45:LEU:HD23	2.00	0.42
2:B:63:LEU:O	2:B:66:ARG:N	2.45	0.42
1:L:185:TRP:CZ2	1:L:208:PRO:HA	2.55	0.41
1:A:32:TYR:HA	1:A:50:GLY:HA2	2.02	0.41
2:B:2:VAL:HG23	2:B:27:PHE:CE1	2.56	0.41
2:H:224:LEU:C	2:H:224:LEU:HD12	2.40	0.41
1:A:124:GLU:OE2	1:A:131:THR:OG1	2.28	0.41
2:B:205:LEU:HD21	2:B:228:VAL:HG21	2.03	0.40

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	212/216 (98%)	204 (96%)	7 (3%)	1 (0%)	25	12
1	L	215/216 (100%)	210 (98%)	5 (2%)	0	100	100
2	B	258/265 (97%)	249 (96%)	9 (4%)	0	100	100
2	H	221/265 (83%)	213 (96%)	8 (4%)	0	100	100
All	All	906/962 (94%)	876 (97%)	29 (3%)	1 (0%)	48	38

All (1) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	151	ASP

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	178/180 (99%)	174 (98%)	4 (2%)	47	31
1	L	181/180 (101%)	180 (99%)	1 (1%)	84	79
2	B	227/230 (99%)	225 (99%)	2 (1%)	75	67
2	H	197/230 (86%)	196 (100%)	1 (0%)	86	83
All	All	783/820 (96%)	775 (99%)	8 (1%)	73	64

All (8) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	L	1	GLN
2	H	196	VAL
2	B	2	VAL
2	B	210	HIS
1	A	9	SER
1	A	78	LEU
1	A	92	GLU

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Mol	Chain	Res	Type
1	A	166	LYS

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

5.3.3   RNA ⓘ

There are no RNA molecules 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 oligosaccharides in this entry.

5.6   Ligand geometry ⓘ

There are no ligands in this entry.

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 ⓘ

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	A	214/216 (99%)	1.02	47 (21%)	3	2	19, 49, 92, 123	0
1	L	216/216 (100%)	-0.38	5 (2%)	61	66	17, 25, 48, 76	1 (0%)
2	B	260/265 (98%)	0.80	42 (16%)	5	5	19, 41, 107, 144	2 (0%)
2	H	225/265 (84%)	0.18	23 (10%)	13	14	13, 31, 86, 123	2 (0%)
All	All	915/962 (95%)	0.42	117 (12%)	9	9	13, 35, 89, 144	5 (0%)

All (117) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
2	B	61	PRO	6.4
2	B	60	ASN	5.2
2	B	130	ILE	5.1
2	B	131	LEU	5.1
2	H	30	SER	4.8
2	H	59	TYR	4.8
2	H	174	SER	4.7
2	B	58	ASN	4.7
2	B	29	LEU	4.5
1	A	157	ALA	4.4
2	B	63	LEU	4.3
2	B	52	ASP	4.1
2	B	64	LYS	4.1
2	B	62	GLY	4.0
2	B	59	TYR	4.0
2	H	179	GLY	3.9
2	B	56	SER	3.8
1	A	148	TRP	3.8
2	B	179	GLY	3.7
1	A	155	VAL	3.7
2	B	54	THR	3.7

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Mol	Chain	Res	Type	RSRZ
2	B	118	TYR	3.6
2	H	58	ASN	3.6
1	A	195	VAL	3.6
2	H	61	PRO	3.5
2	H	2	VAL	3.5
1	L	156	LYS	3.5
1	A	159	VAL	3.4
2	B	53	THR	3.3
2	H	139	THR	3.3
2	H	262	CYS	3.3
2	H	62	GLY	3.3
2	H	56	SER	3.2
2	B	41	PRO	3.2
2	H	101	LYS	3.2
2	B	180	GLY	3.2
1	L	211	CYS	3.2
2	B	57	THR	3.2
2	H	64	LYS	3.2
1	A	185	TRP	3.2
2	B	128	VAL	3.1
1	A	158	GLY	3.1
1	A	187	SER	3.1
1	L	212	SER	3.1
1	A	209	THR	3.1
2	B	177	THR	3.1
2	B	26	GLY	3.1
1	A	152	SER	3.1
2	B	260	LYS	3.0
1	A	128	ASN	3.0
2	B	196	VAL	3.0
2	H	138	SER	2.9
1	A	178	LEU	2.9
2	B	2	VAL	2.9
2	H	41	PRO	2.9
2	B	43	LYS	2.8
1	A	207	ALA	2.8
1	A	154	PRO	2.8
2	B	65	SER	2.8
2	B	133	SER	2.8
1	A	179	SER	2.7
2	B	259	PRO	2.7
2	B	31	ASP	2.7

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Mol	Chain	Res	Type	RSRZ
1	A	191	TYR	2.7
1	A	196	THR	2.7
2	H	57	THR	2.7
2	B	55	GLY	2.7
1	A	146	VAL	2.7
2	H	60	ASN	2.7
1	A	117	LEU	2.7
2	B	28	SER	2.6
1	A	182	PRO	2.6
1	A	38	LEU	2.6
1	A	120	PRO	2.6
1	A	145	THR	2.6
1	A	202	VAL	2.6
1	A	40	PRO	2.6
1	A	126	GLN	2.6
1	A	127	ALA	2.6
1	A	156	LYS	2.5
2	B	27	PHE	2.5
1	A	140	TYR	2.5
1	A	192	SER	2.5
1	A	125	LEU	2.5
2	H	55	GLY	2.5
1	A	181	THR	2.5
2	B	134	GLU	2.5
1	A	144	VAL	2.5
2	H	178	SER	2.4
2	B	42	GLY	2.4
2	H	63	LEU	2.4
1	A	147	ALA	2.4
1	A	189	ARG	2.4
1	A	180	LEU	2.4
2	B	136	VAL	2.4
1	A	17	GLN	2.4
1	A	210	GLU	2.4
1	A	1	GLN	2.4
1	A	132	LEU	2.3
2	H	140	ASP	2.3
2	B	51	THR	2.3
2	B	30	SER	2.3
1	L	1	GLN	2.3
2	B	132	SER	2.3
1	A	143	ALA	2.2

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Mol	Chain	Res	Type	RSRZ
1	A	208	PRO	2.2
2	H	54	THR	2.2
2	H	141	ARG	2.2
2	B	251	THR	2.2
1	A	184	GLN	2.1
1	L	41	GLY	2.1
2	B	1	LYS	2.1
1	A	136	ILE	2.1
1	A	190	SER	2.1
1	A	56	SER	2.0
1	A	107	GLY	2.0
2	B	173	SER	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 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.