



wwPDB X-ray Structure Validation Summary Report ⓘ

Sep 28, 2016 – 08:43 PM EDT

PDB ID : 5IJV
Title : Crystal structure of bovine Fab E03
Authors : Stanfield, R.L.; Wilson, I.A.
Deposited on : 2016-03-02
Resolution : 2.20 Å(reported)

This is a wwPDB X-ray 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

<http://wwpdb.org/validation/2016/XrayValidationReportHelp>

with specific help available everywhere you see the ⓘ symbol.

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

MolProbity	:	4.02b-467
Mogul	:	unknown
Xtriage (Phenix)	:	1.9-1692
EDS	:	rb-20027939
Percentile statistics	:	20151230.v01 (using entries in the PDB archive December 30th 2015)
Refmac	:	5.8.0135
CCP4	:	6.5.0
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	rb-20027939

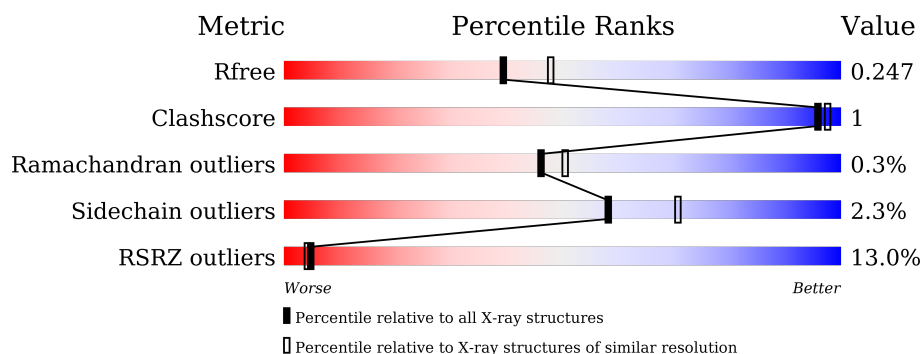
1 Overall quality at a glance ⓘ

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.20 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.




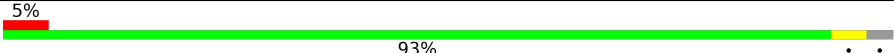
Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	91344	3774 (2.20-2.20)
Clashscore	102246	4477 (2.20-2.20)
Ramachandran outliers	100387	4404 (2.20-2.20)
Sidechain outliers	100360	4405 (2.20-2.20)
RSRZ outliers	91569	3781 (2.20-2.20)

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. 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	A	216	<div> <div></div> <div>94% 5% .</div> </div>
1	C	216	<div> <div>%</div> <div>94% 5% .</div> </div>
1	E	216	<div> <div>29%</div> <div>89% 9% .</div> </div>
1	L	216	<div> <div></div> <div>96% . .</div> </div>
2	B	254	<div> <div>8%</div> <div>93% 5% .</div> </div>
2	D	254	<div> <div>18%</div> <div>93% . .</div> </div>

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Mol	Chain	Length	Quality of chain
2	F	254	 37% 89% 9% .
2	H	254	 5% 93% . .

2 Entry composition [i](#)

There are 3 unique types of molecules in this entry. The entry contains 27068 atoms, of which 13146 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 E03 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			
1	A	213	Total	C	H	N	O	S	0	1	0
			3082	967	1512	263	335	5			
1	C	213	Total	C	H	N	O	S	0	0	0
			3064	959	1503	263	334	5			
1	E	213	Total	C	H	N	O	S	0	0	0
			3064	959	1503	263	334	5			

- Molecule 2 is a protein called bovine Fab E03 heavy chain.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
2	H	246	Total	C	H	N	O	S	0	0	0
			3597	1134	1775	304	374	10			
2	B	248	Total	C	H	N	O	S	0	1	0
			3631	1145	1790	308	377	11			
2	D	247	Total	C	H	N	O	S	0	0	0
			3606	1137	1778	305	375	11			
2	F	249	Total	C	H	N	O	S	0	0	0
			3621	1141	1782	307	380	11			

- Molecule 3 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	L	54	Total	O	0	0
			54	54		
3	H	54	Total	O	0	0
			54	54		
3	A	83	Total	O	0	0
			83	83		
3	B	39	Total	O	0	0
			39	39		

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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	C	32	Total 32	O 32	0	0
3	D	33	Total 33	O 33	0	0
3	E	23	Total 23	O 23	0	0
3	F	21	Total 21	O 21	0	0

3 Residue-property plots [i](#)

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.

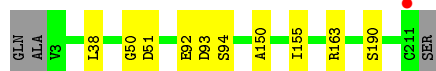
- Molecule 1: bovine Fab E03 light chain

Chain L:  96% ..



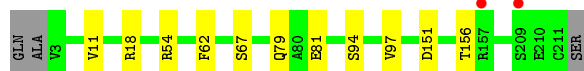
- Molecule 1: bovine Fab E03 light chain

Chain A:  94% 5% ..




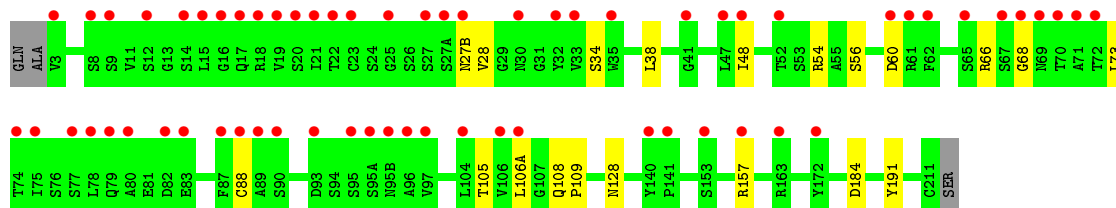
- Molecule 1: bovine Fab E03 light chain

Chain C:  94% 5% ..



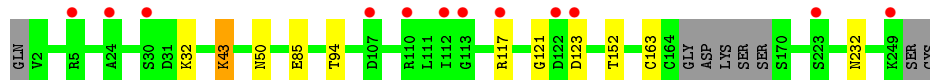
- Molecule 1: bovine Fab E03 light chain

Chain E:  29% 89% 9% ..

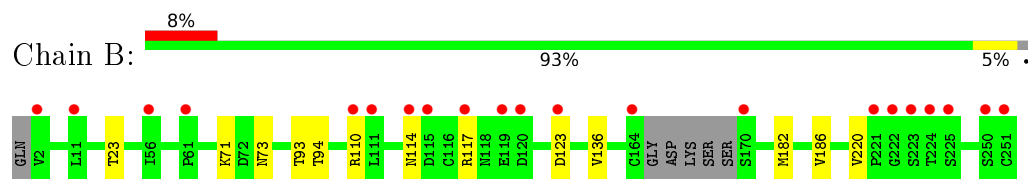


- Molecule 2: bovine Fab E03 heavy chain

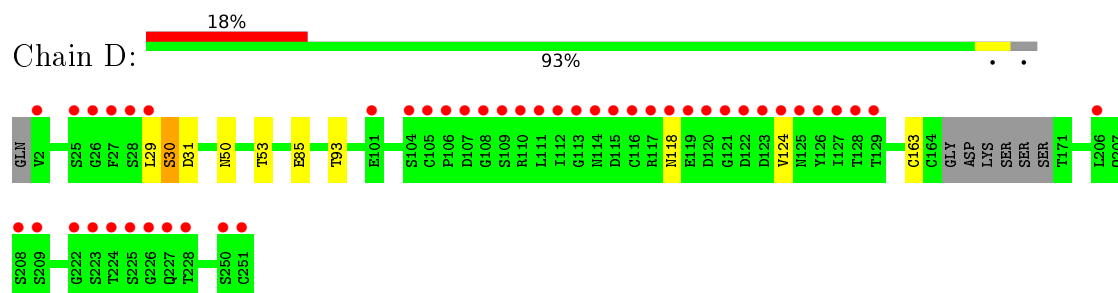
Chain H:  5% 93% ..



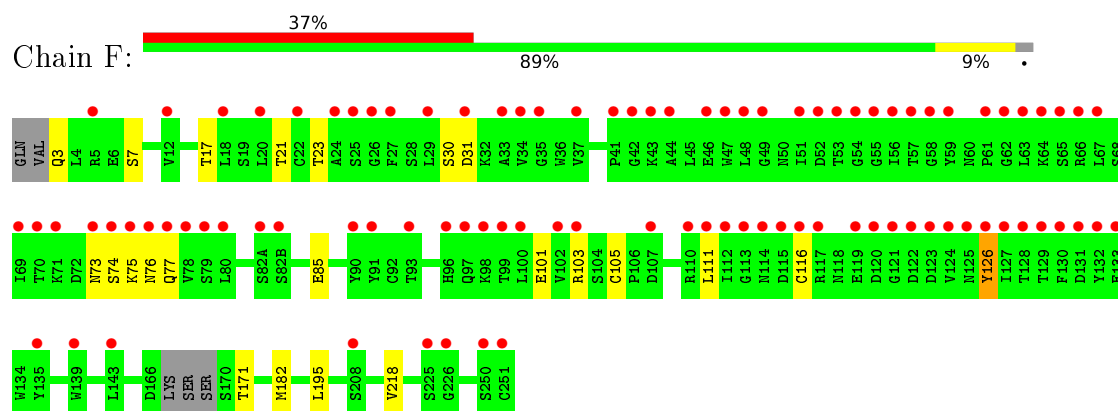
- Molecule 2: bovine Fab E03 heavy chain



- Molecule 2: bovine Fab E03 heavy chain



- Molecule 2: bovine Fab E03 heavy chain



4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α , β , γ	62.24Å 221.74Å 67.95Å 90.00° 104.81° 90.00°	Depositor
Resolution (Å)	49.10 – 2.20 49.10 – 2.20	Depositor EDS
% Data completeness (in resolution range)	98.8 (49.10-2.20) 98.8 (49.10-2.20)	Depositor EDS
R_{merge}	0.09	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.55 (at 2.20Å)	Xtriage
Refinement program	PHENIX (1.10 _2155: ???)	Depositor
R, R_{free}	0.204 , 0.247 0.203 , 0.247	Depositor DCC
R_{free} test set	3805 reflections (4.29%)	DCC
Wilson B-factor (Å ²)	36.9	Xtriage
Anisotropy	0.511	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.36 , 40.9	EDS
L-test for twinning ²	$\langle L \rangle = 0.50$, $\langle L^2 \rangle = 0.33$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.95	EDS
Total number of atoms	27068	wwPDB-VP
Average B, all atoms (Å ²)	65.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 10.85% 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	A	0.29	0/1604	0.50	0/2186
1	C	0.28	0/1591	0.48	0/2168
1	E	0.27	0/1591	0.48	0/2168
1	L	0.28	0/1591	0.49	0/2168
2	B	0.30	0/1882	0.52	0/2569
2	D	0.29	0/1865	0.51	0/2546
2	F	0.29	0/1876	0.52	0/2560
2	H	0.29	0/1859	0.50	0/2538
All	All	0.29	0/13859	0.50	0/18903

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	A	1570	1512	1511	3	0
1	C	1561	1503	1502	3	0
1	E	1561	1503	1502	7	0
1	L	1561	1503	1502	3	0
2	B	1841	1790	1790	4	0
2	D	1828	1778	1778	4	0
2	F	1839	1782	1781	11	0
2	H	1822	1775	1775	5	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
3	A	83	0	0	0	0
3	B	39	0	0	1	0
3	C	32	0	0	1	0
3	D	33	0	0	0	0
3	E	23	0	0	1	0
3	F	21	0	0	1	0
3	H	54	0	0	0	0
3	L	54	0	0	0	0
All	All	13922	13146	13141	39	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 1.

The worst 5 of 39 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:C:79:GLN:NE2	1:C:81:GLU:OE2	2.15	0.79
2:F:23:THR:OG1	2:F:77:GLN:OE1	2.04	0.76
2:B:117:ARG:NH1	2:B:123:ASP:OD1	2.19	0.76
2:F:73:ASN:O	2:F:75:LYS:N	2.25	0.70
1:C:151:ASP:OD1	3:C:301:HOH:O	2.10	0.68

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	A	212/216 (98%)	205 (97%)	6 (3%)	1 (0%)	34	35
1	C	211/216 (98%)	202 (96%)	9 (4%)	0	100	100
1	E	211/216 (98%)	199 (94%)	12 (6%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	L	211/216 (98%)	204 (97%)	7 (3%)	0	100	100
2	B	245/254 (96%)	239 (98%)	6 (2%)	0	100	100
2	D	243/254 (96%)	231 (95%)	11 (4%)	1 (0%)	39	42
2	F	245/254 (96%)	232 (95%)	9 (4%)	4 (2%)	12	8
2	H	242/254 (95%)	237 (98%)	5 (2%)	0	100	100
All	All	1820/1880 (97%)	1749 (96%)	65 (4%)	6 (0%)	46	50

5 of 6 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
2	D	30	SER
2	F	76	ASN
2	F	31	ASP
2	F	74	SER
1	A	93	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	183/184 (100%)	180 (98%)	3 (2%)	70	82
1	C	182/184 (99%)	176 (97%)	6 (3%)	45	56
1	E	182/184 (99%)	175 (96%)	7 (4%)	40	49
1	L	182/184 (99%)	181 (100%)	1 (0%)	92	96
2	B	214/218 (98%)	208 (97%)	6 (3%)	51	63
2	D	212/218 (97%)	208 (98%)	4 (2%)	65	77
2	F	213/218 (98%)	208 (98%)	5 (2%)	58	71
2	H	211/218 (97%)	206 (98%)	5 (2%)	57	69
All	All	1579/1608 (98%)	1542 (98%)	37 (2%)	58	71

5 of 37 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	C	18	ARG
1	C	156	THR
2	F	126	TYR
1	C	67	SER
1	C	94	SER

Some 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 carbohydrates 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	A	213/216 (98%)	0.05	1 (0%) 91 91	22, 35, 57, 106	0
1	C	213/216 (98%)	0.23	2 (0%) 85 85	29, 53, 79, 100	0
1	E	213/216 (98%)	1.39	63 (29%) 1 0	34, 86, 138, 169	0
1	L	213/216 (98%)	0.02	1 (0%) 91 91	27, 43, 62, 78	0
2	B	248/254 (97%)	0.46	21 (8%) 13 12	24, 49, 99, 169	0
2	D	247/254 (97%)	1.17	45 (18%) 2 2	28, 45, 144, 212	0
2	F	249/254 (98%)	1.94	94 (37%) 0 0	28, 94, 152, 185	0
2	H	246/254 (96%)	0.32	12 (4%) 33 33	28, 44, 91, 152	0
All	All	1842/1880 (97%)	0.72	239 (12%) 5 4	22, 49, 128, 212	0

The worst 5 of 239 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
2	F	130	PHE	14.3
2	F	113	GLY	10.4
2	F	99	THR	9.7
2	D	226	GLY	9.0
2	D	225	SER	8.5

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

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

6.3 Carbohydrates ⓘ

There are no carbohydrates in this entry.

6.4 Ligands

There are no ligands in this entry.

6.5 Other polymers

There are no such residues in this entry.