



# wwPDB X-ray Structure Validation Summary Report ⓘ

Aug 24, 2019 – 06:44 AM EDT

PDB ID : 6E8V  
Title : The crystal structure of bovine ultralong antibody BOV-1  
Authors : Dong, J.; Crowe, J.E.  
Deposited on : 2018-07-31  
Resolution : 3.79 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](mailto: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.

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

MolProbity : 4.02b-467  
Xtriage (Phenix) : 1.13  
EDS : 2.4  
Percentile statistics : 20171227.v01 (using entries in the PDB archive December 27th 2017)  
Refmac : 5.8.0158  
CCP4 : 7.0 (Gargrove)  
Ideal geometry (proteins) : Engh & Huber (2001)  
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)  
Validation Pipeline (wwPDB-VP) : 2.4

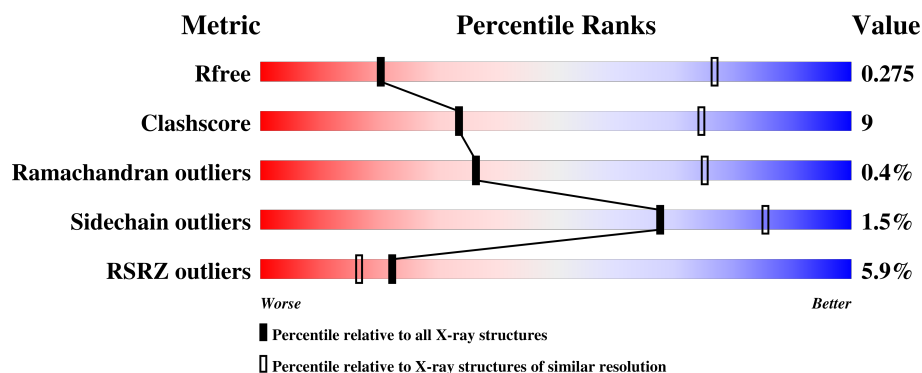
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

The reported resolution of this entry is 3.79 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))
$R_{free}$	111664	1028 (4.02-3.58)
Clashscore	122126	1061 (4.00-3.60)
Ramachandran outliers	120053	1025 (4.00-3.60)
Sidechain outliers	120020	1019 (4.00-3.60)
RSRZ outliers	108989	1021 (4.06-3.54)

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  $\geq 3$ , 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	274	<div> <div>10%</div> <div>62%</div> <div>15%</div> <div>•</div> <div>22%</div> </div>
1	E	274	<div> <div>%</div> <div>76%</div> <div>16%</div> <div>•</div> <div>7%</div> </div>
1	H	274	<div> <div>%</div> <div>78%</div> <div>15%</div> <div>7%</div> </div>
1	J	274	<div> <div>7%</div> <div>59%</div> <div>19%</div> <div>23%</div> </div>
1	O	274	<div> <div>5%</div> <div>64%</div> <div>13%</div> <div>23%</div> </div>

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Mol	Chain	Length	Quality of chain
1	U	274	<div> <div></div> <div>75%</div> <div>18%</div> <div>7%</div> </div>
1	Y	274	<div> <div>14%</div> <div>61%</div> <div>16%</div> <div>22%</div> </div>
1	c	274	<div> <div>3%</div> <div>91%</div> <div>7%</div> </div>
2	B	216	<div> <div>15%</div> <div>74%</div> <div>24%</div> </div>
2	F	216	<div> <div>3%</div> <div>82%</div> <div>17%</div> </div>
2	K	216	<div> <div></div> <div>72%</div> <div>27%</div> </div>
2	L	216	<div> <div></div> <div>77%</div> <div>22%</div> </div>
2	P	216	<div> <div>15%</div> <div>69%</div> <div>26%</div> </div>
2	V	216	<div> <div></div> <div>72%</div> <div>27%</div> </div>
2	Z	216	<div> <div>6%</div> <div>74%</div> <div>22%</div> <div>5%</div> </div>
2	d	216	<div> <div></div> <div>96%</div> </div>

## 2 Entry composition

There are 2 unique types of molecules in this entry. The entry contains 25749 atoms, of which 0 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 ultralong antibody BOV-1 Heavy chain.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	214	Total	C	N	O	S	0	0	0
			1570	986	258	317	9			
1	E	255	Total	C	N	O	S	0	0	0
			1843	1152	302	375	14			
1	H	255	Total	C	N	O	S	0	0	0
			1870	1171	305	380	14			
1	J	212	Total	C	N	O	S	0	0	0
			1523	955	255	305	8			
1	O	211	Total	C	N	O	S	0	0	0
			1530	958	254	310	8			
1	U	255	Total	C	N	O	S	0	0	0
			1849	1162	299	374	14			
1	Y	213	Total	C	N	O	S	0	0	0
			1540	965	257	310	8			
1	c	254	Total	C	N	O	S	0	0	0
			1837	1152	299	372	14			

- Molecule 2 is a protein called Bovine ultralong antibody BOV-1 light chain.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B	211	Total	C	N	O	S	0	0	0
			1500	922	250	323	5			
2	F	215	Total	C	N	O	S	0	0	0
			1558	956	264	333	5			
2	K	215	Total	C	N	O	S	0	0	0
			1527	941	258	323	5			
2	L	214	Total	C	N	O	S	0	0	0
			1560	959	263	333	5			
2	P	208	Total	C	N	O	S	0	0	0
			1517	932	256	324	5			
2	V	213	Total	C	N	O	S	0	0	0
			1523	939	259	321	4			

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Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	Z	206	Total	C	N	O	S	0	0	0
			1470	895	252	318	5			
2	d	215	Total	C	N	O	S	0	0	0
			1532	939	259	329	5			

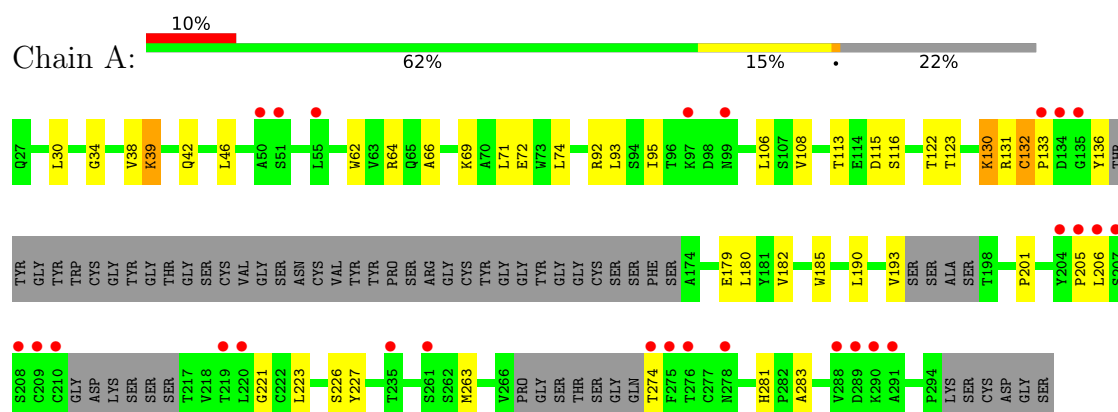
There are 24 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
B	1	GLU	GLN	conflict	UNP Q3T101
B	5	ASN	THR	conflict	UNP Q3T101
B	81	ALA	PRO	conflict	UNP Q3T101
F	1	GLU	GLN	conflict	UNP Q3T101
F	5	ASN	THR	conflict	UNP Q3T101
F	82	ALA	PRO	conflict	UNP Q3T101
K	1	GLU	GLN	conflict	UNP Q3T101
K	5	ASN	THR	conflict	UNP Q3T101
K	82	ALA	PRO	conflict	UNP Q3T101
L	1	GLU	GLN	conflict	UNP Q3T101
L	5	ASN	THR	conflict	UNP Q3T101
L	81	ALA	PRO	conflict	UNP Q3T101
P	1	GLU	GLN	conflict	UNP Q3T101
P	5	ASN	THR	conflict	UNP Q3T101
P	82	ALA	PRO	conflict	UNP Q3T101
V	1	GLU	GLN	conflict	UNP Q3T101
V	5	ASN	THR	conflict	UNP Q3T101
V	82	ALA	PRO	conflict	UNP Q3T101
Z	1	GLU	GLN	conflict	UNP Q3T101
Z	5	ASN	THR	conflict	UNP Q3T101
Z	82	ALA	PRO	conflict	UNP Q3T101
d	1	GLU	GLN	conflict	UNP Q3T101
d	5	ASN	THR	conflict	UNP Q3T101
d	82	ALA	PRO	conflict	UNP Q3T101

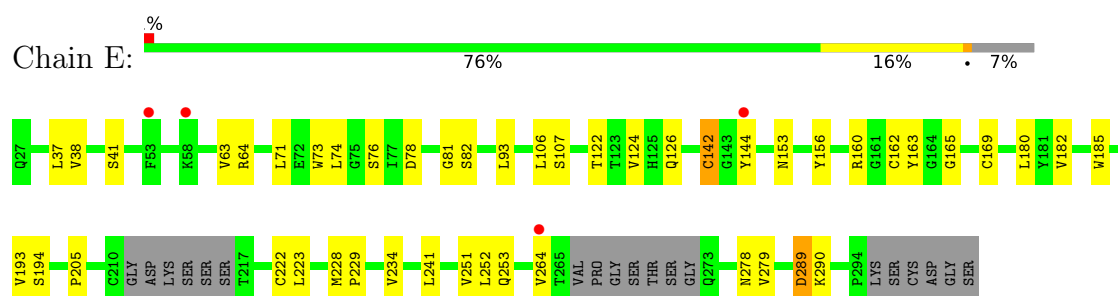
### 3 Residue-property plots [i](#)

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

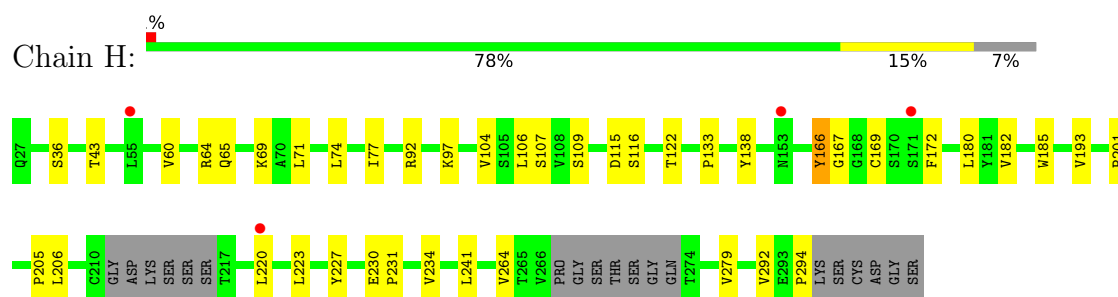
- Molecule 1: Bovine ultralong antibody BOV-1 Heavy chain



- Molecule 1: Bovine ultralong antibody BOV-1 Heavy chain

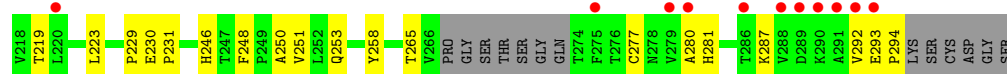
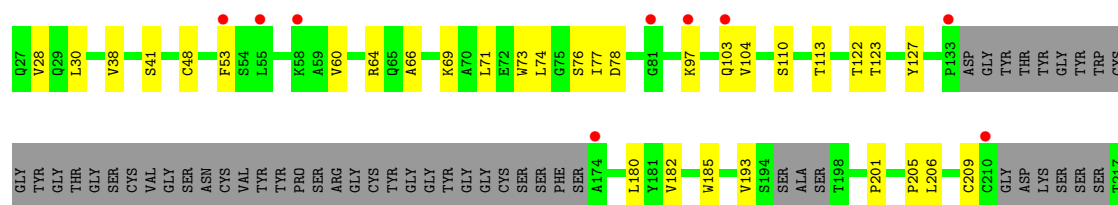


- Molecule 1: Bovine ultralong antibody BOV-1 Heavy chain

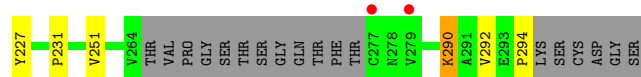
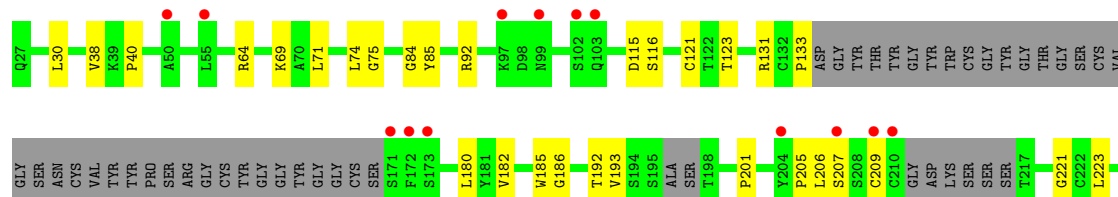


- Molecule 1: Bovine ultralong antibody BOV-1 Heavy chain

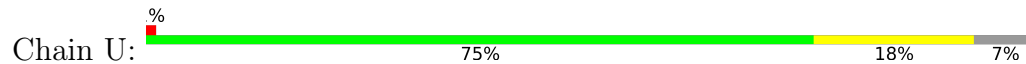




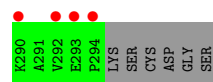
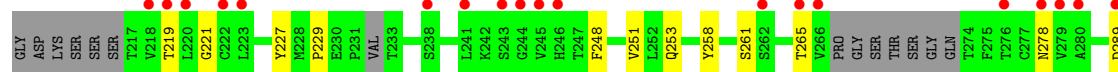
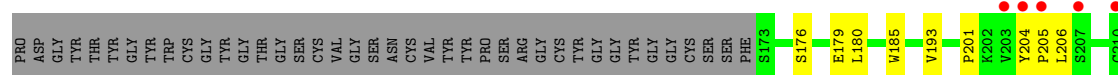
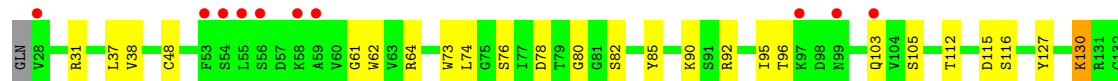
• Molecule 1: Bovine ultralong antibody BOV-1 Heavy chain



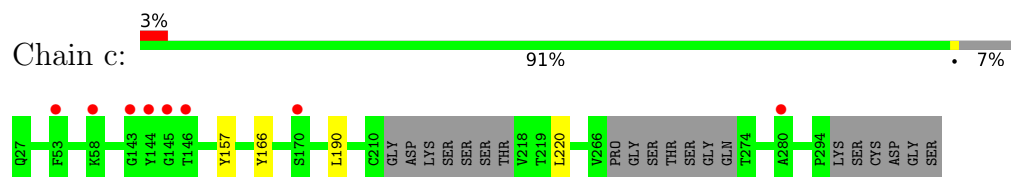
• Molecule 1: Bovine ultralong antibody BOV-1 Heavy chain



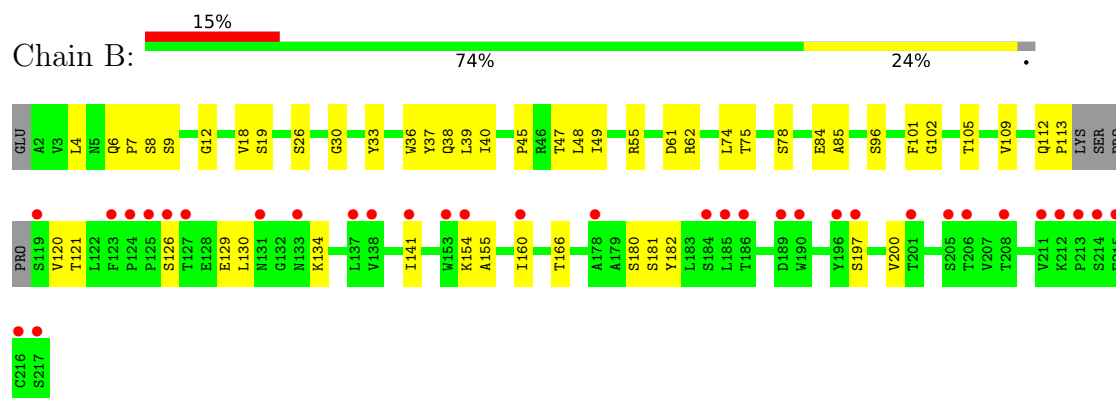
• Molecule 1: Bovine ultralong antibody BOV-1 Heavy chain



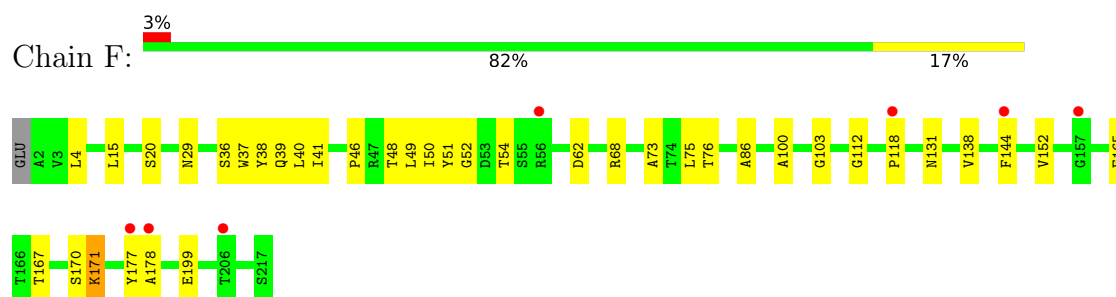
- Molecule 1: Bovine ultralong antibody BOV-1 Heavy chain



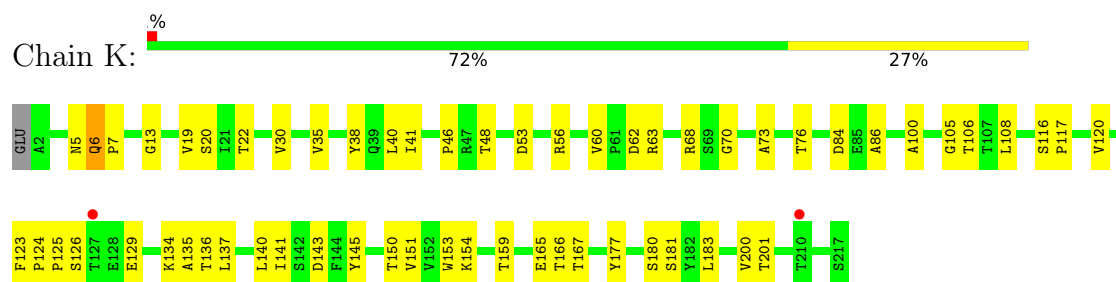
- Molecule 2: Bovine ultralong antibody BOV-1 light chain



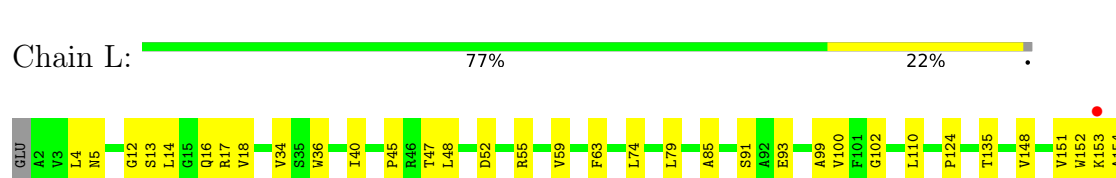
- Molecule 2: Bovine ultralong antibody BOV-1 light chain



- Molecule 2: Bovine ultralong antibody BOV-1 light chain



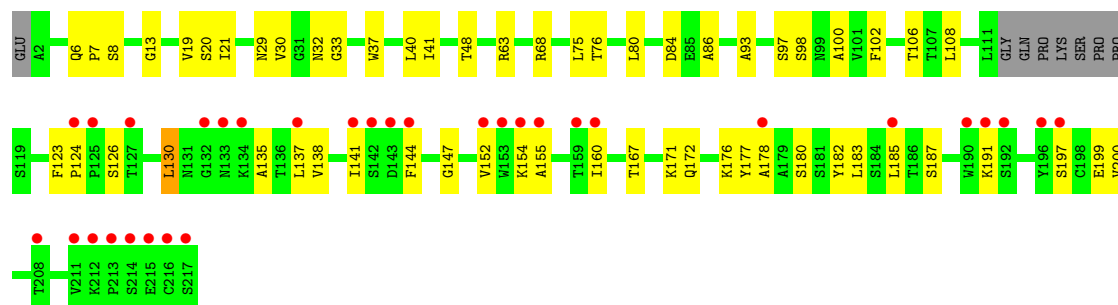
- Molecule 2: Bovine ultralong antibody BOV-1 light chain



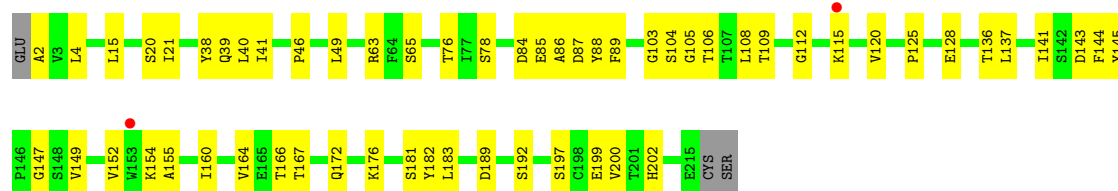




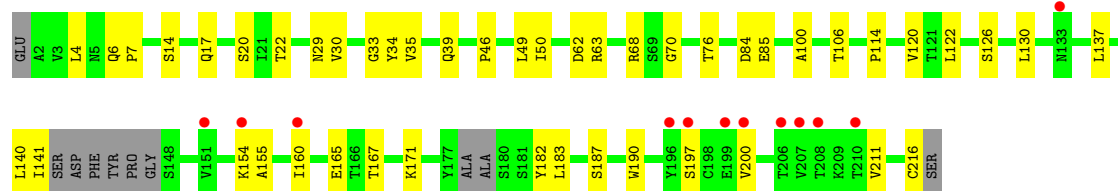
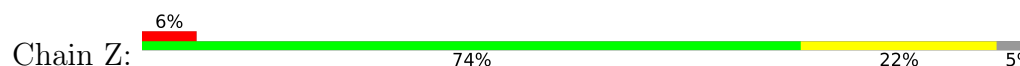
• Molecule 2: Bovine ultralong antibody BOV-1 light chain



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• Molecule 2: Bovine ultralong antibody BOV-1 light chain



• Molecule 2: Bovine ultralong antibody BOV-1 light chain



## 4 Data and refinement statistics

Property	Value	Source
Space group	P 42 21 2	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	308.22Å 308.22Å 133.75Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	49.20 – 3.79 49.20 – 3.79	Depositor EDS
% Data completeness (in resolution range)	99.7 (49.20-3.79) 100.0 (49.20-3.79)	Depositor EDS
$R_{merge}$	0.22	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	3.33 (at 3.77Å)	Xtriage
Refinement program	PHENIX (1.14_3260: ???)	Depositor
R, $R_{free}$	0.218 , 0.275 0.218 , 0.275	Depositor DCC
$R_{free}$ test set	3256 reflections (5.07%)	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	92.8	Xtriage
Anisotropy	0.925	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.30 , 84.1	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.46$ , $\langle L^2 \rangle = 0.29$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
$F_o, F_c$ correlation	0.90	EDS
Total number of atoms	25749	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	114.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 10.28% of the height of the origin peak. No significant pseudotranslation is detected.*

<sup>1</sup>Intensities estimated from amplitudes.

<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.

## 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	0.26	0/1602	0.49	0/2187
1	E	0.27	0/1887	0.48	0/2577
1	H	0.27	0/1915	0.49	0/2613
1	J	0.26	0/1553	0.48	0/2120
1	O	0.27	0/1560	0.49	0/2128
1	U	0.27	0/1894	0.49	0/2589
1	Y	0.26	0/1569	0.48	0/2141
1	c	0.28	0/1881	0.49	0/2570
2	B	0.27	0/1527	0.48	0/2089
2	F	0.28	0/1588	0.49	0/2166
2	K	0.28	0/1557	0.49	0/2131
2	L	0.29	0/1590	0.48	0/2169
2	P	0.27	0/1543	0.48	0/2100
2	V	0.27	0/1552	0.48	0/2120
2	Z	0.26	0/1491	0.47	0/2031
2	d	0.27	0/1560	0.49	0/2130
All	All	0.27	0/26269	0.48	0/35861

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	0	1524	32	0
1	E	1843	0	1727	29	0
1	H	1870	0	1779	24	0
1	J	1523	0	1441	33	0
1	O	1530	0	1469	28	0
1	U	1849	0	1744	30	0
1	Y	1540	0	1476	30	0
1	c	1837	0	1731	0	0
2	B	1500	0	1382	37	0
2	F	1558	0	1471	25	0
2	K	1527	0	1402	45	0
2	L	1560	0	1491	27	0
2	P	1517	0	1445	45	0
2	V	1523	0	1421	38	0
2	Z	1470	0	1383	33	0
2	d	1532	0	1422	0	0
All	All	25749	0	24308	401	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 9.

The worst 5 of 401 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:P:171:LYS:HA	2:P:177:TYR:HA	1.62	0.81
2:Z:120:VAL:HG21	2:Z:200:VAL:HG11	1.64	0.80
2:P:8:SER:HB3	2:V:2:ALA:HB2	1.64	0.79
2:Z:14:SER:HB3	2:Z:17:GLN:HG3	1.67	0.77
1:Y:92:ARG:NH1	1:Y:115:ASP:OD2	2.18	0.77

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	204/274 (74%)	196 (96%)	7 (3%)	1 (0%)	31	71
1	E	249/274 (91%)	240 (96%)	9 (4%)	0	100	100
1	H	249/274 (91%)	234 (94%)	13 (5%)	2 (1%)	21	62
1	J	202/274 (74%)	191 (95%)	9 (4%)	2 (1%)	17	58
1	O	201/274 (73%)	188 (94%)	12 (6%)	1 (0%)	31	71
1	U	249/274 (91%)	236 (95%)	12 (5%)	1 (0%)	36	75
1	Y	203/274 (74%)	195 (96%)	7 (3%)	1 (0%)	31	71
1	c	248/274 (90%)	237 (96%)	11 (4%)	0	100	100
2	B	207/216 (96%)	190 (92%)	17 (8%)	0	100	100
2	F	213/216 (99%)	202 (95%)	11 (5%)	0	100	100
2	K	213/216 (99%)	193 (91%)	19 (9%)	1 (0%)	31	71
2	L	212/216 (98%)	192 (91%)	20 (9%)	0	100	100
2	P	204/216 (94%)	189 (93%)	15 (7%)	0	100	100
2	V	211/216 (98%)	197 (93%)	14 (7%)	0	100	100
2	Z	200/216 (93%)	183 (92%)	16 (8%)	1 (0%)	31	71
2	d	213/216 (99%)	193 (91%)	17 (8%)	3 (1%)	12	52
All	All	3478/3920 (89%)	3256 (94%)	209 (6%)	13 (0%)	36	75

5 of 13 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	H	166	TYR
1	J	229	PRO
1	O	231	PRO
2	Z	114	PRO
2	d	117	PRO

### 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	180/229 (79%)	174 (97%)	6 (3%)	41	72
1	E	204/229 (89%)	199 (98%)	5 (2%)	50	77
1	H	212/229 (93%)	209 (99%)	3 (1%)	69	86
1	J	166/229 (72%)	163 (98%)	3 (2%)	62	83
1	O	173/229 (76%)	172 (99%)	1 (1%)	87	94
1	U	206/229 (90%)	202 (98%)	4 (2%)	60	82
1	Y	171/229 (75%)	169 (99%)	2 (1%)	74	88
1	c	205/229 (90%)	201 (98%)	4 (2%)	58	81
2	B	165/184 (90%)	165 (100%)	0	100	100
2	F	176/184 (96%)	174 (99%)	2 (1%)	76	88
2	K	163/184 (89%)	161 (99%)	2 (1%)	74	88
2	L	179/184 (97%)	176 (98%)	3 (2%)	63	84
2	P	173/184 (94%)	172 (99%)	1 (1%)	87	94
2	V	164/184 (89%)	163 (99%)	1 (1%)	87	94
2	Z	166/184 (90%)	165 (99%)	1 (1%)	87	94
2	d	168/184 (91%)	164 (98%)	4 (2%)	52	77
All	All	2871/3304 (87%)	2829 (98%)	42 (2%)	67	85

5 of 42 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	J	277	CYS
2	L	215	CYS
2	d	36	SER
2	K	6	GLN
2	L	91	SER

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (1) such sidechains are listed below:

Mol	Chain	Res	Type
1	c	253	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 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, 95<sup>th</sup> 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 <sup>2</sup> )	Q<0.9
1	A	214/274 (78%)	0.78	27 (12%) 3 4	76, 132, 199, 289	0
1	E	255/274 (93%)	0.06	4 (1%) 72 62	74, 101, 150, 191	0
1	H	255/274 (93%)	0.01	4 (1%) 72 62	70, 89, 135, 178	0
1	J	212/274 (77%)	0.44	20 (9%) 8 7	75, 112, 208, 249	0
1	O	211/274 (77%)	0.52	15 (7%) 16 12	73, 117, 178, 230	0
1	U	255/274 (93%)	0.01	4 (1%) 72 62	72, 100, 145, 180	0
1	Y	213/274 (77%)	0.74	38 (17%) 1 1	74, 119, 210, 330	0
1	c	254/274 (92%)	0.02	8 (3%) 49 38	71, 98, 143, 166	0
2	B	211/216 (97%)	0.63	33 (15%) 2 2	69, 121, 242, 284	0
2	F	215/216 (99%)	0.16	7 (3%) 46 36	70, 112, 175, 279	0
2	K	215/216 (99%)	-0.06	2 (0%) 84 77	69, 99, 150, 179	0
2	L	214/216 (99%)	0.01	1 (0%) 90 86	67, 99, 142, 160	0
2	P	208/216 (96%)	0.65	32 (15%) 2 2	68, 112, 218, 261	0
2	V	213/216 (98%)	0.03	2 (0%) 84 77	69, 105, 150, 180	0
2	Z	206/216 (95%)	0.25	12 (5%) 23 17	69, 115, 182, 227	0
2	d	215/216 (99%)	0.04	0 100 100	69, 103, 167, 198	0
All	All	3566/3920 (90%)	0.26	209 (5%) 22 17	67, 105, 187, 330	0

The worst 5 of 209 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	O	210	CYS	8.8
1	Y	218	VAL	7.3
2	B	124	PRO	7.2
1	A	209	CYS	6.7
2	B	185	LEU	6.0



## 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 carbohydrates 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.