Full wwPDB X-ray Structure Validation Report (i)

Jun 24, 2024 – 08:32 PM 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 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:

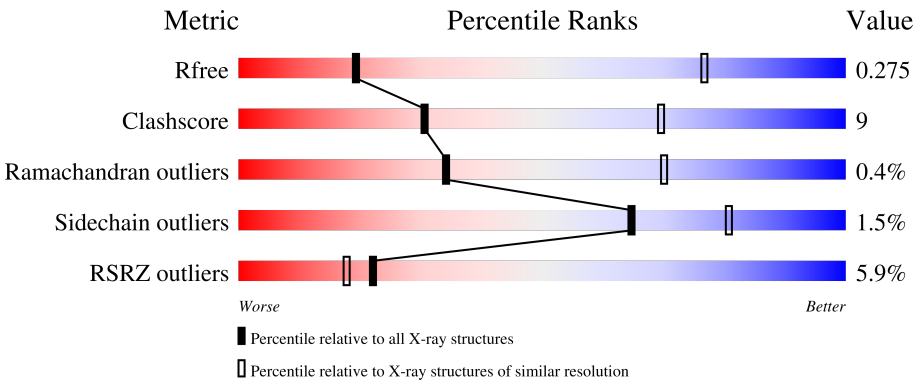
MolProbity	:	4.02b-467
Xtriage (Phenix)	:	1.13
EDS	:	2.37.1
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.37.1

1 Overall quality at a glance (i)

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}	130704	1212 (4.00-3.60)
Clashscore	141614	1288 (4.00-3.60)
Ramachandran outliers	138981	1243 (4.00-3.60)
Sidechain outliers	138945	1237 (4.00-3.60)
RSRZ outliers	127900	1121 (4.00-3.60)

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	274	10%, 62%, 15%, •, 22%
1	E	274	%, 76%, 16%, •, 7%
1	H	274	%, 78%, 15%, 7%
1	J	274	7%, 59%, 19%, 23%
1	O	274	5%, 64%, 13%, 23%

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

2 Entry composition (i)

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

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

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

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

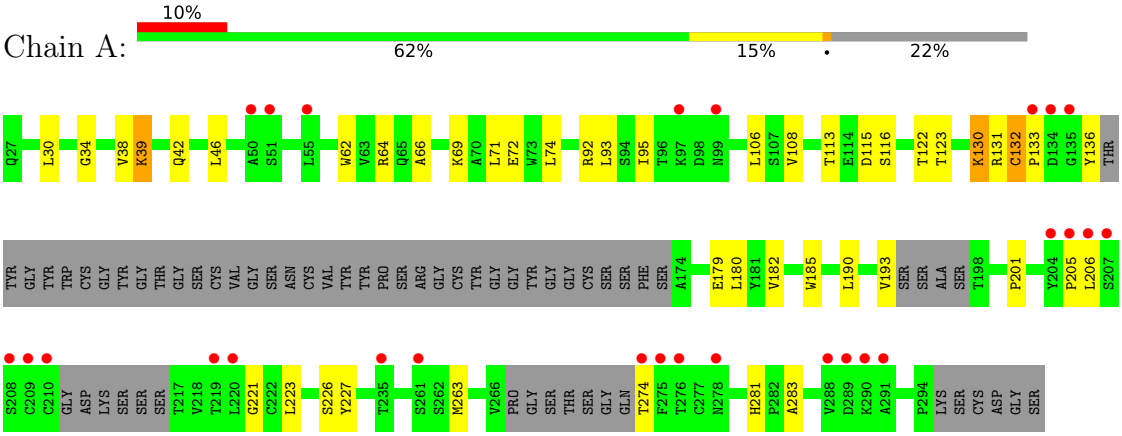
There are 24 discrepancies between the modelled and reference sequences:

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

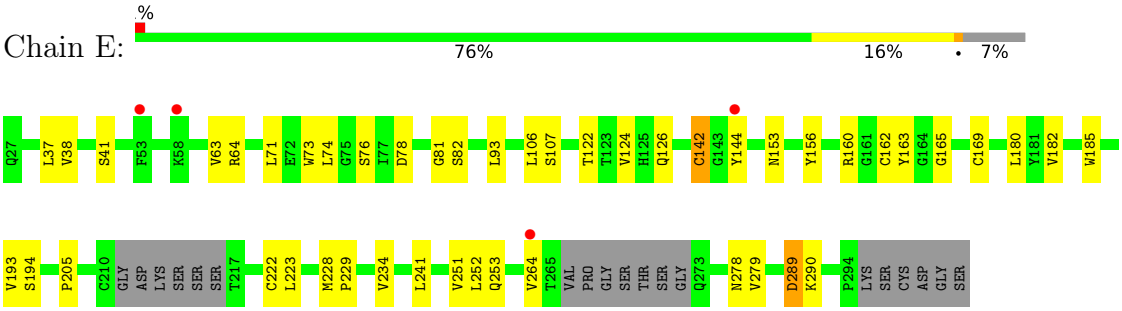
3 Residue-property plots (i)

These plots are drawn for all protein, RNA, 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.

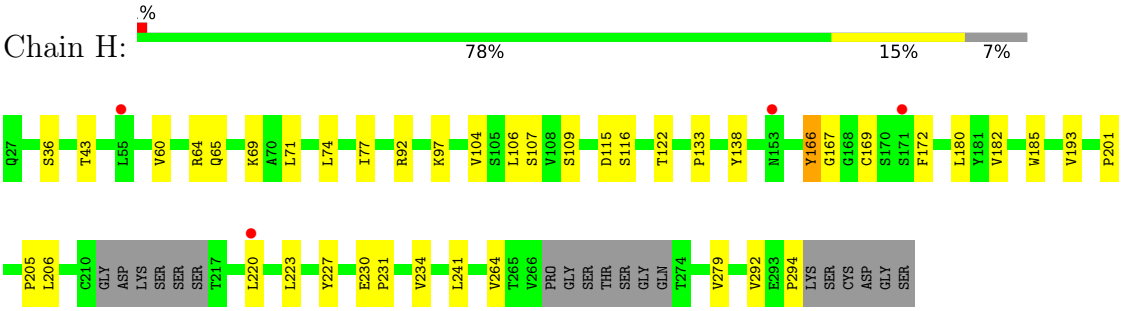
• Molecule 1: Bovine ultralong antibody BOV-1 Heavy chain



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

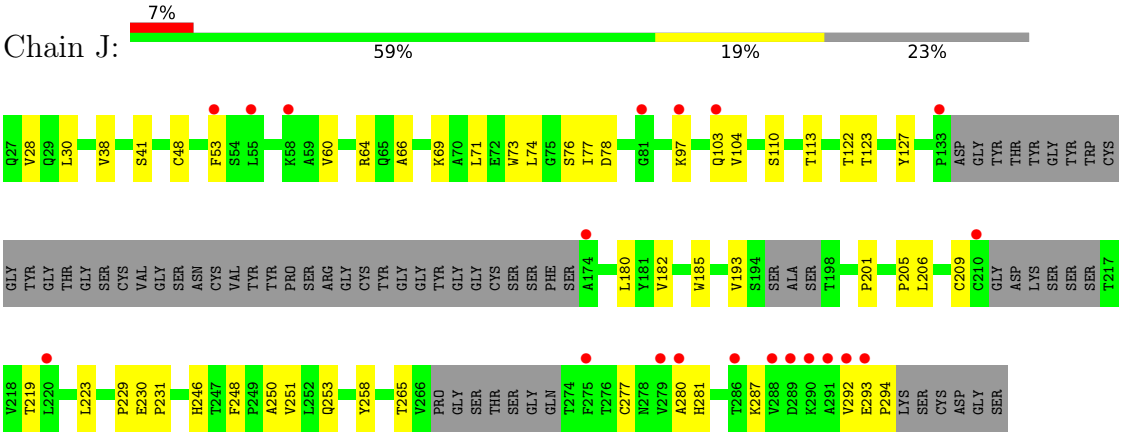


• Molecule 1: Bovine ultralong antibody BOV-1 Heavy chain



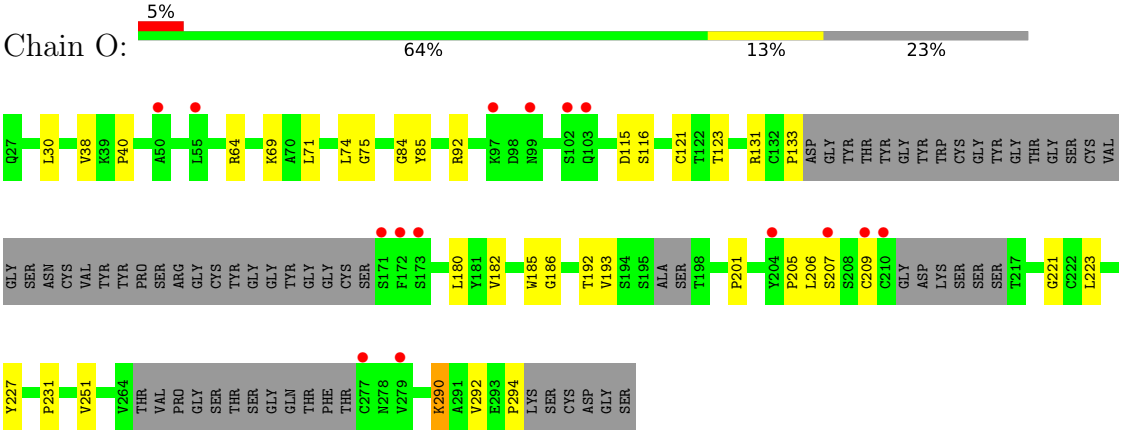
• Molecule 1: Bovine ultralong antibody BOV-1 Heavy chain

Chain J:



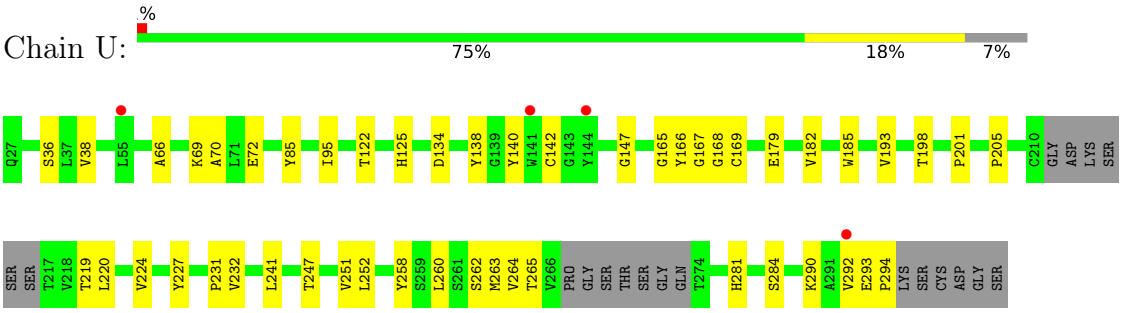
• Molecule 1: Bovine ultralong antibody BOV-1 Heavy chain

Chain O:



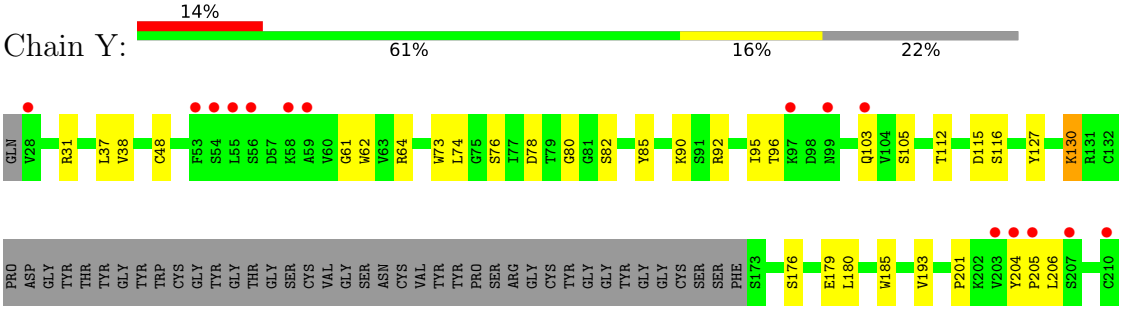
• Molecule 1: Bovine ultralong antibody BOV-1 Heavy chain

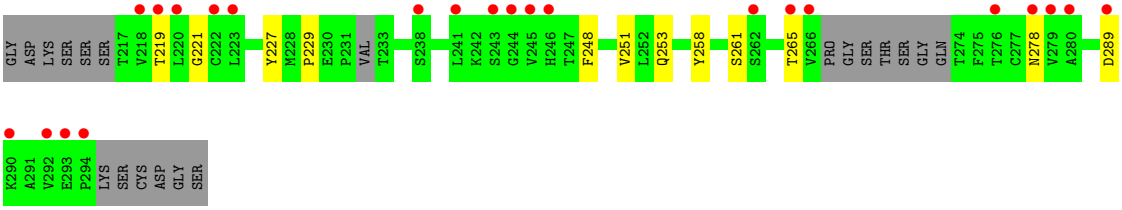
Chain U:



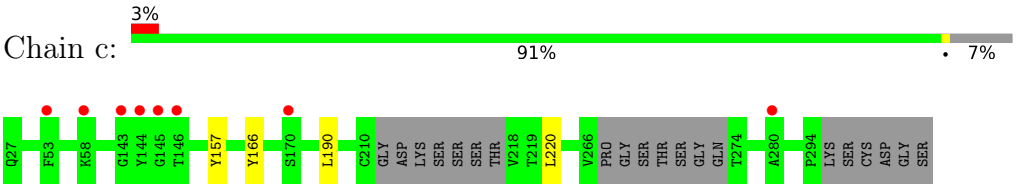
• Molecule 1: Bovine ultralong antibody BOV-1 Heavy chain

Chain Y:

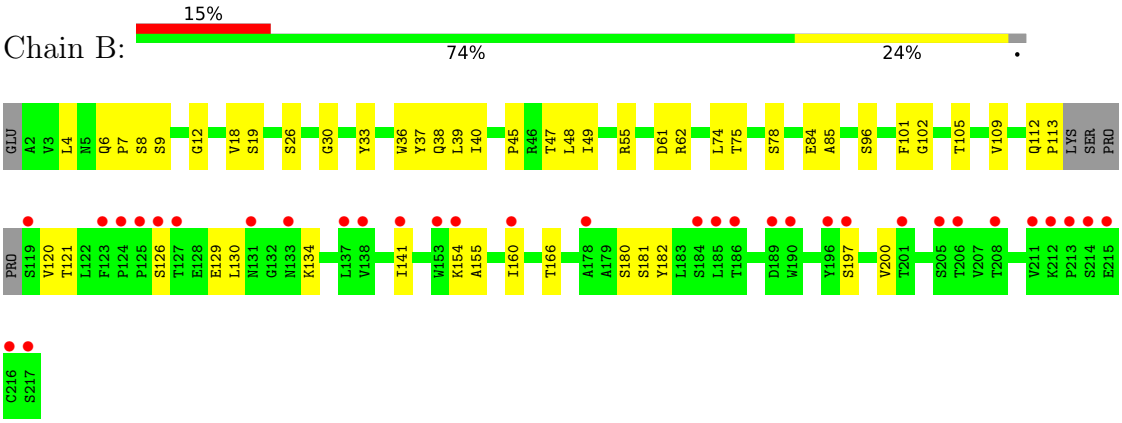




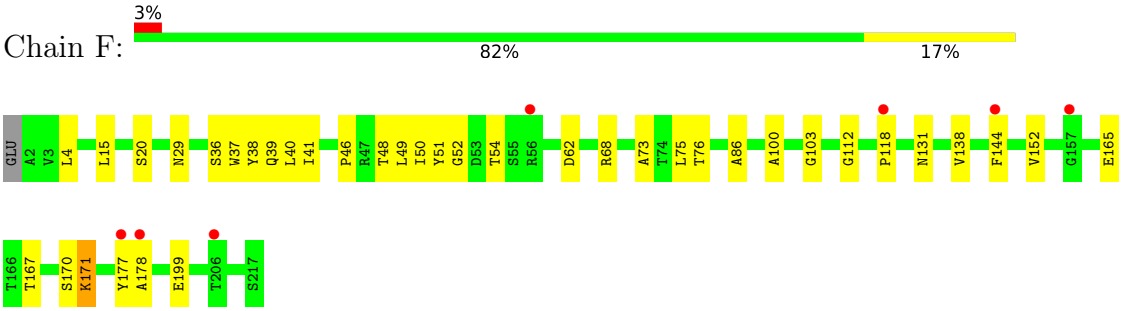
• Molecule 1: Bovine ultralong antibody BOV-1 Heavy chain



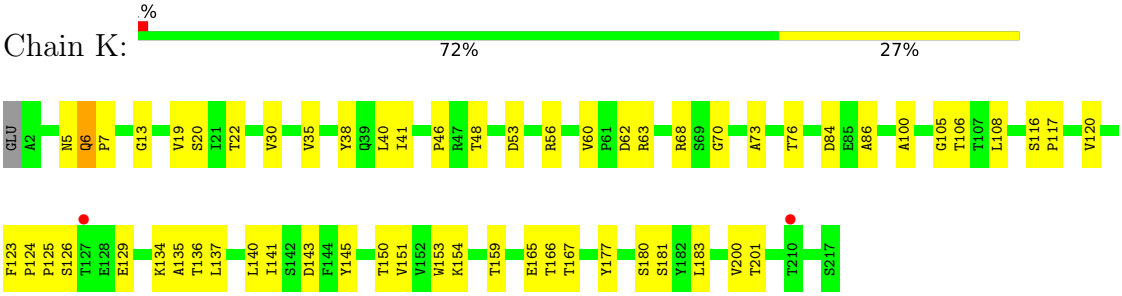
• Molecule 2: Bovine ultralong antibody BOV-1 light chain



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

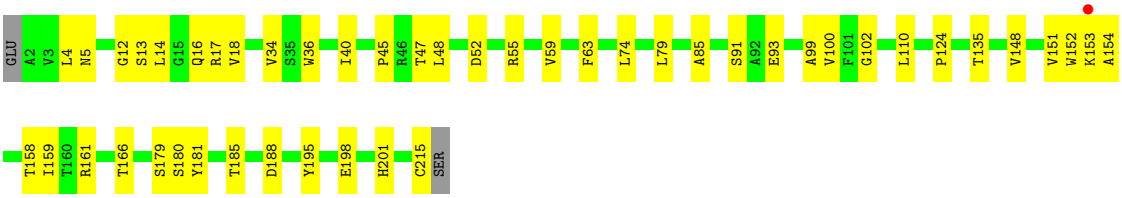


• Molecule 2: Bovine ultralong antibody BOV-1 light chain



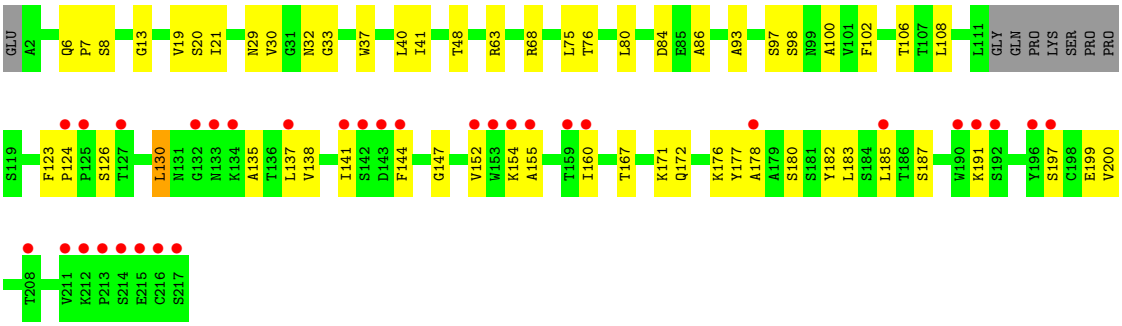
• Molecule 2: Bovine ultralong antibody BOV-1 light chain

Chain L:



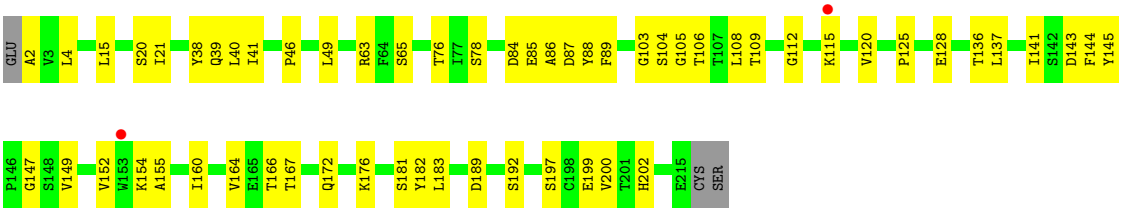
• Molecule 2: Bovine ultralong antibody BOV-1 light chain

Chain P:



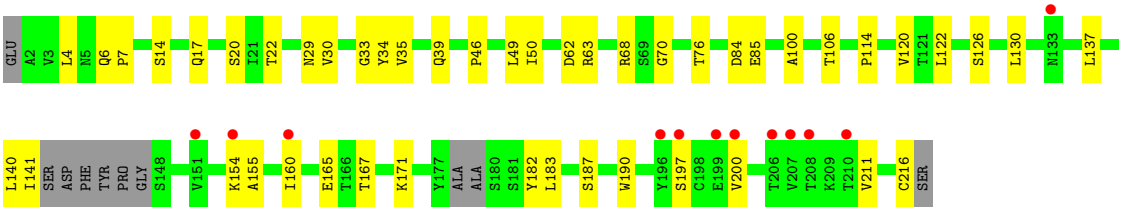
• Molecule 2: Bovine ultralong antibody BOV-1 light chain

Chain V:



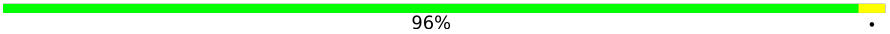
• Molecule 2: Bovine ultralong antibody BOV-1 light chain

Chain Z:



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

Chain d:



GLU
A2
S36
S92
S104
P114
P117
L130
P146
S217

4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 42 21 2	Depositor
Cell constants a, b, c, α, β, γ	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
$< I/\sigma(I) >$ [1]	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^2)	92.8	Xtriage
Anisotropy	0.925	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.30 , 84.1	EDS
L-test for twinning[2]	$< \|L\| > = 0.46$, $< L^2 > = 0.29$	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^2)	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.*

[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 (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.

All (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
1:A:132:CYS:SG	1:A:133:PRO:HD2	2.26	0.75
1:H:60:VAL:HG11	1:H:104:VAL:HG21	1.68	0.75
2:Z:154:LYS:HB2	2:Z:197:SER:HB2	1.69	0.74
1:A:92:ARG:NH1	1:A:115:ASP:OD2	2.20	0.74
1:A:39:LYS:HE2	1:A:42:GLN:HG3	1.68	0.74
1:J:219:THR:HG22	1:J:265:THR:HG23	1.70	0.73
2:Z:6:GLN:HE21	2:Z:106:THR:HG23	1.54	0.73
2:B:154:LYS:HB2	2:B:197:SER:HB2	1.70	0.73
1:Y:37:LEU:HD13	1:Y:229:PRO:HB3	1.70	0.73
1:Y:251:VAL:HG12	2:Z:167:THR:HB	1.71	0.72
1:H:92:ARG:NH1	1:H:115:ASP:OD2	2.23	0.71
1:O:71:LEU:HD21	2:P:40:LEU:HD11	1.72	0.71
2:B:155:ALA:HB2	2:B:160:ILE:HD11	1.72	0.71

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:6:GLN:HE21	2:B:105:THR:HG23	1.56	0.70
2:Z:130:LEU:HD23	2:Z:187:SER:HB2	1.74	0.70
2:B:26:SER:HA	2:B:30:GLY:HA3	1.74	0.69
1:E:251:VAL:HG12	2:F:167:THR:HB	1.75	0.68
2:F:41:ILE:HG12	2:F:86:ALA:HB2	1.73	0.68
1:H:220:LEU:HD21	1:H:294:PRO:HG3	1.76	0.68
2:K:6:GLN:HE22	2:K:105:GLY:C	1.98	0.68
2:V:4:LEU:HB2	2:V:103:GLY:HA2	1.76	0.67
2:V:125:PRO:HB3	2:V:136:THR:H	1.58	0.67
1:Y:278:ASN:ND2	1:Y:289:ASP:OD1	2.28	0.67
2:Z:63:ARG:NH2	2:Z:84:ASP:OD2	2.27	0.67
2:P:6:GLN:HE21	2:P:106:THR:HG23	1.59	0.66
1:Y:130:LYS:HA	1:Y:176:SER:HA	1.78	0.66
2:Z:165:GLU:HB3	2:Z:182:TYR:HB2	1.77	0.66
2:Z:120:VAL:HG22	2:Z:141:ILE:HG22	1.77	0.66
1:A:66:ALA:HB3	1:A:69:LYS:HB2	1.77	0.65
1:H:205:PRO:HB3	1:H:292:VAL:HG22	1.78	0.65
1:H:180:LEU:HD23	2:L:99:ALA:HB2	1.79	0.65
2:K:41:ILE:HG12	2:K:86:ALA:HB2	1.78	0.64
2:F:171:LYS:HA	2:F:177:TYR:HA	1.78	0.64
1:O:205:PRO:HG3	1:O:290:LYS:HG2	1.79	0.64
1:O:30:LEU:HD11	1:O:123:THR:HG23	1.81	0.63
1:O:206:LEU:HD11	1:O:223:LEU:HB2	1.81	0.63
2:B:120:VAL:HB	2:B:141:ILE:HG23	1.81	0.62
2:F:118:PRO:HB3	2:F:144:PHE:HB3	1.81	0.62
2:P:20:SER:HB3	2:P:76:THR:HG22	1.81	0.62
1:E:228:MET:HG2	1:E:229:PRO:HA	1.80	0.62
2:K:120:VAL:HG22	2:K:141:ILE:HG22	1.81	0.61
1:A:122:THR:HG22	1:A:185:TRP:HA	1.83	0.61
2:P:154:LYS:HB2	2:P:197:SER:HB2	1.82	0.61
1:A:39:LYS:H	1:A:39:LYS:HD3	1.65	0.61
2:Z:20:SER:HB3	2:Z:76:THR:HG22	1.83	0.61
2:F:152:VAL:HG13	2:F:199:GLU:HB2	1.83	0.61
2:P:130:LEU:HD23	2:P:187:SER:HB2	1.83	0.60
1:Y:38:VAL:HG23	1:Y:193:VAL:HG23	1.83	0.60
2:Z:137:LEU:HD12	2:Z:183:LEU:HD23	1.83	0.60
2:P:13:GLY:HA3	2:P:19:VAL:HG11	1.84	0.60
2:P:29:ASN:OD1	2:P:30:VAL:N	2.33	0.60
1:H:241:LEU:HD21	1:H:264:VAL:HG21	1.83	0.60
1:U:122:THR:HB	1:U:182:VAL:HG13	1.84	0.60
1:E:241:LEU:HD21	1:E:264:VAL:HG21	1.83	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:P:93:ALA:HA	2:P:100:ALA:HA	1.83	0.59
1:A:64:ARG:HB3	1:A:74:LEU:HD11	1.83	0.59
1:A:206:LEU:HD11	1:A:223:LEU:HB2	1.83	0.59
1:U:290:LYS:NZ	2:V:128:GLU:OE1	2.35	0.59
2:K:19:VAL:HG21	2:K:108:LEU:HD21	1.85	0.59
2:V:120:VAL:HG21	2:V:200:VAL:HG11	1.85	0.59
1:A:206:LEU:HB2	1:A:221:GLY:HA3	1.84	0.59
1:H:65:GLN:HB2	1:H:71:LEU:HD23	1.85	0.59
2:B:12:GLY:HA3	2:B:18:VAL:HG11	1.85	0.59
1:O:251:VAL:HG12	2:P:167:THR:HB	1.85	0.59
2:B:84:GLU:HG3	2:B:109:VAL:HG23	1.84	0.58
2:K:20:SER:HB3	2:K:76:THR:HG22	1.85	0.58
1:U:185:TRP:CD2	2:V:46:PRO:HG2	2.39	0.58
2:K:125:PRO:HG3	2:K:135:ALA:HB1	1.84	0.58
2:B:19:SER:HB3	2:B:75:THR:HG22	1.85	0.58
1:H:64:ARG:HD3	1:H:74:LEU:HD21	1.86	0.58
2:K:35:VAL:HG12	2:K:53:ASP:HA	1.86	0.58
1:U:66:ALA:HB3	1:U:69:LYS:HE2	1.86	0.57
2:V:155:ALA:HB2	2:V:160:ILE:HD11	1.87	0.57
1:Y:180:LEU:HD22	2:Z:100:ALA:HB2	1.86	0.57
1:O:38:VAL:HG23	1:O:193:VAL:HG22	1.84	0.57
2:L:151:VAL:HG13	2:L:198:GLU:HB2	1.87	0.56
2:K:63:ARG:NH2	2:K:84:ASP:OD1	2.39	0.56
1:O:180:LEU:HD22	2:P:100:ALA:HB2	1.88	0.56
2:V:125:PRO:HD3	2:V:137:LEU:HD23	1.87	0.56
2:V:166:THR:HG23	2:V:181:SER:HB2	1.87	0.56
2:L:152:TRP:HB3	2:L:159:ILE:HD12	1.87	0.56
2:K:137:LEU:HD12	2:K:183:LEU:HD23	1.88	0.56
1:J:38:VAL:HG23	1:J:193:VAL:HG23	1.88	0.56
2:F:29:ASN:OD1	2:K:5:ASN:ND2	2.34	0.56
1:J:30:LEU:HD11	1:J:123:THR:HG23	1.88	0.55
2:F:15:LEU:HD23	2:F:112:GLY:HA3	1.86	0.55
1:U:251:VAL:HG12	2:V:167:THR:HB	1.88	0.55
1:A:116:SER:HB3	1:A:193:VAL:HG12	1.89	0.55
1:E:253:GLN:HA	2:F:165:GLU:OE2	2.06	0.55
1:O:209:CYS:HB2	2:P:124:PRO:HG3	1.88	0.55
1:J:201:PRO:HD3	1:J:281:HIS:ND1	2.21	0.55
2:Z:29:ASN:OD1	2:Z:30:VAL:N	2.31	0.55
1:E:142:CYS:HA	1:E:162:CYS:SG	2.47	0.55
2:L:12:GLY:HA3	2:L:18:VAL:HG11	1.88	0.55
1:O:84:GLY:HA3	2:P:98:SER:HB2	1.89	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:U:205:PRO:HB3	1:U:292:VAL:HG22	1.88	0.55
1:J:41:SER:HA	1:J:110:SER:HA	1.88	0.55
1:E:223:LEU:HD22	2:F:138:VAL:HG21	1.88	0.54
2:K:151:VAL:HG21	2:K:166:THR:HG21	1.90	0.54
1:Y:201:PRO:HB3	1:Y:227:TYR:HB3	1.90	0.54
1:J:64:ARG:HD3	1:J:74:LEU:HD21	1.90	0.54
1:A:34:GLY:HA3	1:A:46:LEU:HD23	1.88	0.54
2:L:154:ALA:HB2	2:L:159:ILE:HD11	1.89	0.54
2:V:63:ARG:NH2	2:V:84:ASP:OD2	2.40	0.54
1:E:38:VAL:HG23	1:E:193:VAL:HG22	1.89	0.54
1:E:93:LEU:HD22	1:E:106:LEU:HD11	1.89	0.54
2:F:40:LEU:HG	2:F:46:PRO:HB3	1.89	0.54
1:J:185:TRP:CD2	2:K:46:PRO:HB2	2.43	0.54
2:L:55:ARG:NH1	2:L:63:PHE:O	2.41	0.54
2:B:180:SER:HB2	2:B:182:TYR:HE1	1.73	0.53
1:H:77:ILE:HD13	1:H:97:LYS:HB3	1.89	0.53
1:U:138:TYR:CZ	1:U:147:GLY:HA3	2.43	0.53
2:Z:68:ARG:NH1	2:Z:70:GLY:O	2.42	0.53
2:B:55:ARG:HD3	2:B:61:ASP:HA	1.91	0.53
2:K:125:PRO:HB3	2:K:136:THR:H	1.73	0.53
1:O:92:ARG:NH1	1:O:115:ASP:OD2	2.42	0.53
1:J:71:LEU:HD21	2:K:40:LEU:HD21	1.91	0.53
1:H:206:LEU:HD11	1:H:223:LEU:HB2	1.90	0.53
1:A:179:GLU:HG3	2:B:33:TYR:HB3	1.91	0.52
1:U:134:ASP:OD1	1:U:134:ASP:N	2.41	0.52
1:Y:248:PHE:CZ	2:Z:140:LEU:HB3	2.44	0.52
2:F:20:SER:HB3	2:F:76:THR:HG22	1.92	0.52
1:U:201:PRO:HB3	1:U:227:TYR:HB3	1.92	0.52
1:Y:204:TYR:HB3	2:Z:126:SER:OG	2.10	0.52
2:L:4:LEU:HB2	2:L:102:GLY:HA2	1.91	0.52
2:L:185:THR:HG23	2:L:188:ASP:H	1.75	0.52
1:A:263:MET:HE1	2:B:121:THR:HB	1.90	0.52
2:K:166:THR:HG23	2:K:181:SER:HB2	1.91	0.52
2:L:153:LYS:HG2	2:L:158:THR:HG22	1.92	0.51
1:U:241:LEU:HD21	1:U:264:VAL:HG21	1.92	0.51
1:J:253:GLN:NE2	2:K:165:GLU:OE1	2.44	0.51
1:Y:78:ASP:OD1	1:Y:80:GLY:N	2.43	0.51
2:Z:39:GLN:HB2	2:Z:49:LEU:HD11	1.92	0.51
1:A:274:THR:O	1:A:274:THR:OG1	2.28	0.51
1:Y:96:THR:HG1	1:Y:105:SER:HG	1.51	0.51
2:F:38:TYR:CE1	2:F:48:THR:HG22	2.46	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:281:HIS:CE1	1:A:283:ALA:HB3	2.45	0.51
1:J:28:VAL:HG13	1:J:53:PHE:CD1	2.45	0.51
2:P:63:ARG:NH2	2:P:84:ASP:OD1	2.44	0.51
1:U:219:THR:HG22	1:U:265:THR:HG23	1.92	0.51
2:P:32:ASN:OD1	2:P:33:GLY:N	2.45	0.51
1:J:248:PHE:CZ	2:K:140:LEU:HB3	2.46	0.50
1:Y:253:GLN:HA	2:Z:165:GLU:OE2	2.11	0.50
2:V:108:LEU:HD22	2:V:109:THR:H	1.76	0.50
1:Y:205:PRO:O	2:Z:126:SER:HB3	2.10	0.50
1:J:205:PRO:O	2:K:126:SER:HB3	2.10	0.50
1:E:126:GLN:HB3	1:E:180:LEU:HD13	1.94	0.50
1:J:206:LEU:HD11	1:J:223:LEU:HB2	1.93	0.50
2:K:30:VAL:O	2:K:68:ARG:NH1	2.45	0.50
2:L:36:TRP:CD2	2:L:74:LEU:HB2	2.47	0.50
2:V:137:LEU:HB2	2:V:183:LEU:HB3	1.94	0.50
1:Y:219:THR:HG22	1:Y:265:THR:HG23	1.94	0.50
2:F:37:TRP:N	2:F:50:ILE:O	2.44	0.50
2:Z:7:PRO:HD3	2:Z:22:THR:HG23	1.94	0.50
1:A:180:LEU:HD12	2:B:96:SER:O	2.11	0.49
1:J:60:VAL:HG11	1:J:104:VAL:HG21	1.94	0.49
2:B:40:ILE:HG12	2:B:85:ALA:HB2	1.94	0.49
2:B:62:ARG:NH2	2:B:78:SER:O	2.45	0.49
1:Y:179:GLU:HG3	2:Z:34:TYR:HB3	1.94	0.49
1:E:122:THR:HB	1:E:182:VAL:HG13	1.94	0.49
2:L:12:GLY:HA3	2:L:18:VAL:CG1	2.42	0.49
1:H:64:ARG:HB3	1:H:74:LEU:HD11	1.94	0.49
1:E:278:ASN:ND2	1:E:289:ASP:OD2	2.45	0.49
2:P:13:GLY:HA3	2:P:19:VAL:CG1	2.43	0.49
1:O:75:GLY:HA2	1:O:85:TYR:HA	1.95	0.49
1:O:206:LEU:HB2	1:O:221:GLY:HA3	1.95	0.49
1:Y:206:LEU:HB2	1:Y:221:GLY:HA3	1.95	0.49
2:P:137:LEU:HB2	2:P:183:LEU:HB3	1.94	0.49
1:J:73:TRP:CZ2	1:J:76:SER:HB3	2.47	0.49
1:U:247:THR:HA	1:U:262:SER:HA	1.95	0.49
1:A:182:VAL:HG11	1:A:185:TRP:CE2	2.48	0.48
1:E:180:LEU:HD23	2:F:100:ALA:HB2	1.95	0.48
1:E:185:TRP:CG	2:F:46:PRO:HG2	2.48	0.48
2:Z:155:ALA:HB2	2:Z:160:ILE:HD11	1.94	0.48
2:F:4:LEU:HB2	2:F:103:GLY:HA2	1.95	0.48
1:H:185:TRP:CD2	2:L:45:PRO:HG2	2.48	0.48
1:U:38:VAL:HG23	1:U:193:VAL:HG22	1.94	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:39:LEU:HG	2:B:45:PRO:HB3	1.94	0.48
1:E:142:CYS:SG	1:E:160:ARG:NH1	2.86	0.48
2:V:20:SER:HB3	2:V:76:THR:HG22	1.94	0.48
2:B:7:PRO:O	2:B:9:SER:N	2.43	0.48
2:V:41:ILE:HG12	2:V:86:ALA:HB2	1.95	0.48
1:A:71:LEU:HD21	2:B:39:LEU:HD21	1.95	0.48
1:A:113:THR:HA	1:A:193:VAL:HG11	1.96	0.48
1:O:201:PRO:HB3	1:O:227:TYR:HB3	1.96	0.48
2:V:38:TYR:HB2	2:V:89:PHE:HB2	1.95	0.48
1:Y:112:THR:O	1:Y:193:VAL:HG11	2.14	0.48
1:U:224:VAL:HB	1:U:260:LEU:HD23	1.95	0.47
2:K:167:THR:HG22	2:K:180:SER:H	1.78	0.47
2:L:148:VAL:HG12	2:L:201:HIS:HB2	1.95	0.47
1:E:165:GLY:O	1:E:169:CYS:HB3	2.14	0.47
1:J:209:CYS:SG	2:K:124:PRO:HG3	2.54	0.47
2:V:63:ARG:HB3	2:V:78:SER:O	2.15	0.47
2:V:149:VAL:HG12	2:V:202:HIS:HB2	1.95	0.47
1:A:69:LYS:HG2	1:H:69:LYS:HE3	1.96	0.47
2:P:123:PHE:HB2	2:P:138:VAL:HB	1.96	0.47
1:U:252:LEU:HD23	1:U:258:TYR:CE2	2.50	0.47
1:E:124:VAL:HG12	1:E:182:VAL:HG22	1.96	0.47
1:O:116:SER:HB3	1:O:193:VAL:H	1.79	0.47
2:B:141:ILE:HD13	2:B:200:VAL:HG21	1.96	0.47
1:J:185:TRP:HE1	2:K:48:THR:HG22	1.80	0.47
1:J:293:GLU:HG3	1:J:294:PRO:HD2	1.97	0.47
2:P:21:ILE:HG23	2:P:106:THR:HG21	1.96	0.47
1:U:167:GLY:O	1:U:169:CYS:N	2.47	0.47
1:O:116:SER:HB2	1:O:192:THR:HA	1.97	0.47
1:O:205:PRO:HB3	1:O:292:VAL:HG22	1.97	0.47
2:K:150:THR:HB	2:K:201:THR:OG1	2.15	0.47
2:Z:85:GLU:OE1	2:Z:171:LYS:NZ	2.48	0.47
1:J:122:THR:HB	1:J:182:VAL:HG13	1.97	0.47
1:A:71:LEU:HB2	2:B:101:PHE:CD2	2.50	0.46
1:Y:261:SER:HB2	2:Z:140:LEU:HD21	1.96	0.46
1:H:230:GLU:N	1:H:231:PRO:HD2	2.29	0.46
1:O:205:PRO:O	2:P:126:SER:HB3	2.14	0.46
2:P:141:ILE:HD13	2:P:200:VAL:HG21	1.96	0.46
2:L:34:VAL:HG12	2:L:52:ASP:HA	1.97	0.46
2:Z:49:LEU:C	2:Z:50:ILE:HD12	2.36	0.46
1:E:64:ARG:HB3	1:E:74:LEU:HD11	1.96	0.46
1:E:78:ASP:OD1	1:E:81:GLY:N	2.49	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:Y:185:TRP:CD2	2:Z:46:PRO:HB2	2.51	0.46
2:F:39:GLN:HB2	2:F:49:LEU:HD11	1.98	0.46
1:H:185:TRP:HE1	2:L:47:THR:HG22	1.81	0.46
1:Y:61:GLY:HA2	1:Y:76:SER:HA	1.98	0.46
1:Y:78:ASP:OD2	1:Y:82:SER:HB2	2.16	0.46
2:V:85:GLU:OE2	2:V:145:TYR:OH	2.24	0.46
1:E:234:VAL:HG22	1:E:279:VAL:HG22	1.98	0.46
2:P:144:PHE:CE2	2:P:147:GLY:HA2	2.50	0.46
2:P:187:SER:O	2:P:191:LYS:HD3	2.15	0.46
2:V:144:PHE:HE2	2:V:147:GLY:HA2	1.80	0.46
1:E:41:SER:OG	2:K:165:GLU:HG2	2.16	0.46
1:J:66:ALA:HB3	1:J:69:LYS:HB2	1.98	0.46
2:L:93:GLU:HB2	2:L:100:VAL:HG13	1.97	0.46
2:K:154:LYS:HE2	2:K:159:THR:HG22	1.98	0.45
2:K:167:THR:CG2	2:K:180:SER:H	2.29	0.45
1:O:121:CYS:O	1:O:186:GLY:N	2.49	0.45
2:V:21:ILE:HG23	2:V:106:THR:HG21	1.98	0.45
1:A:38:VAL:HG23	1:A:193:VAL:HG23	1.98	0.45
1:O:64:ARG:HB3	1:O:74:LEU:HD11	1.97	0.45
2:V:15:LEU:HB2	2:V:112:GLY:HA3	1.98	0.45
2:V:108:LEU:HD22	2:V:109:THR:N	2.31	0.45
2:V:143:ASP:OD1	2:V:172:GLN:NE2	2.31	0.45
2:F:36:SER:HA	2:F:51:TYR:HA	1.97	0.45
2:K:68:ARG:HA	2:K:73:ALA:HA	1.97	0.45
2:B:4:LEU:HD23	2:L:5:ASN:HD22	1.81	0.45
2:K:6:GLN:HE21	2:K:106:THR:HG23	1.81	0.45
2:P:144:PHE:HE2	2:P:147:GLY:HA2	1.82	0.45
1:A:93:LEU:HD22	1:A:106:LEU:HD11	1.98	0.45
1:H:65:GLN:HB2	1:H:71:LEU:CD2	2.46	0.45
1:J:180:LEU:HD22	2:K:100:ALA:HB2	1.99	0.45
2:L:124:PRO:HB3	2:L:135:THR:H	1.81	0.45
2:P:155:ALA:HB2	2:P:160:ILE:HD11	1.98	0.45
2:V:87:ASP:HA	2:V:106:THR:O	2.17	0.45
1:A:205:PRO:O	2:B:126:SER:HB3	2.16	0.45
2:P:19:VAL:HG21	2:P:108:LEU:HD21	1.99	0.45
2:B:7:PRO:C	2:B:9:SER:H	2.21	0.45
2:K:13:GLY:HA3	2:K:19:VAL:HG11	1.98	0.45
1:A:201:PRO:HB3	1:A:227:TYR:HB3	1.99	0.44
2:B:4:LEU:HB2	2:B:102:GLY:HA2	1.99	0.44
1:H:133:PRO:HG3	1:H:172:PHE:HZ	1.83	0.44
1:J:230:GLU:N	1:J:231:PRO:HD2	2.32	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:J:251:VAL:O	1:J:258:TYR:HA	2.17	0.44
2:P:40:LEU:HD23	2:P:40:LEU:HA	1.87	0.44
1:U:232:VAL:HG12	1:U:281:HIS:HD2	1.82	0.44
2:B:37:TYR:CE2	2:B:47:THR:HG22	2.52	0.44
2:B:48:LEU:HB3	2:B:49:ILE:HD12	2.00	0.44
1:J:182:VAL:HG11	1:J:185:TRP:CE2	2.52	0.44
2:B:6:GLN:HB3	2:B:105:THR:CG2	2.47	0.44
1:U:70:ALA:HB2	2:V:104:SER:HA	2.00	0.44
1:H:36:SER:HB2	1:H:231:PRO:HG3	2.00	0.44
1:O:182:VAL:HG11	1:O:185:TRP:CE2	2.52	0.44
1:H:116:SER:HB3	1:H:193:VAL:H	1.83	0.44
2:P:37:TRP:CE2	2:P:75:LEU:HB2	2.52	0.44
1:U:36:SER:HB2	1:U:231:PRO:HG3	2.00	0.44
1:J:77:ILE:HD13	1:J:97:LYS:HG2	1.99	0.44
2:K:6:GLN:HG2	2:K:7:PRO:HD2	1.99	0.44
2:L:36:TRP:CE2	2:L:74:LEU:HB2	2.52	0.44
2:V:141:ILE:HD13	2:V:200:VAL:HG21	2.00	0.44
1:A:113:THR:HA	1:A:193:VAL:CG1	2.48	0.43
2:B:129:GLU:HG2	2:B:134:LYS:O	2.17	0.43
1:E:73:TRP:CZ2	1:E:76:SER:HB3	2.53	0.43
2:K:125:PRO:HD3	2:K:137:LEU:HD23	2.00	0.43
1:O:131:ARG:O	1:O:133:PRO:HD3	2.18	0.43
1:U:263:MET:HB2	1:U:263:MET:HE3	1.88	0.43
2:B:180:SER:HB2	2:B:182:TYR:CE1	2.54	0.43
1:H:201:PRO:HB3	1:H:227:TYR:HB3	1.99	0.43
1:J:182:VAL:HB	2:K:38:TYR:CE2	2.53	0.43
2:B:166:THR:HA	2:B:181:SER:HA	2.01	0.43
2:P:80:LEU:HD23	2:P:80:LEU:HA	1.83	0.43
1:A:130:LYS:HA	1:A:130:LYS:HD2	1.83	0.43
2:B:61:ASP:OD1	2:B:61:ASP:N	2.50	0.43
1:E:37:LEU:HD11	1:E:194:SER:HB3	1.99	0.43
1:Y:73:TRP:CZ2	1:Y:76:SER:HB3	2.54	0.43
1:Y:116:SER:OG	1:Y:193:VAL:HG12	2.18	0.43
1:Y:227:TYR:O	1:Y:258:TYR:N	2.46	0.43
1:U:198:THR:OG1	1:U:284:SER:HB3	2.18	0.43
1:Y:64:ARG:HB3	1:Y:74:LEU:HD11	2.01	0.43
1:E:205:PRO:HD3	1:E:290:LYS:HE3	2.01	0.43
2:K:6:GLN:HE22	2:K:106:THR:N	2.17	0.43
1:O:207:SER:HB2	1:O:294:PRO:HA	2.00	0.43
2:P:152:VAL:HG13	2:P:199:GLU:HB2	2.01	0.43
1:O:69:LYS:HE3	1:O:69:LYS:HB3	1.87	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:V:40:LEU:HD22	2:V:89:PHE:HZ	1.84	0.43
2:B:112:GLN:HA	2:B:113:PRO:HD3	1.86	0.43
2:P:6:GLN:NE2	2:P:106:THR:HG23	2.30	0.42
2:V:88:TYR:O	2:V:105:GLY:HA2	2.19	0.42
2:F:62:ASP:OD1	2:F:62:ASP:N	2.51	0.42
2:L:16:GLN:HB3	2:L:17:ARG:H	1.63	0.42
2:V:40:LEU:HD22	2:V:89:PHE:CZ	2.54	0.42
1:J:205:PRO:HB3	1:J:292:VAL:HG22	2.01	0.42
2:L:40:ILE:HG12	2:L:85:ALA:HB2	2.01	0.42
1:E:153:ASN:ND2	1:E:153:ASN:H	2.17	0.42
2:F:68:ARG:HA	2:F:73:ALA:HA	2.00	0.42
1:J:280:ALA:HA	1:J:287:LYS:HG3	2.02	0.42
1:O:180:LEU:HD12	2:P:97:SER:O	2.19	0.42
1:A:132:CYS:HG	1:A:133:PRO:HD2	1.82	0.42
2:K:56:ARG:HB3	2:K:60:VAL:HB	2.00	0.42
1:U:85:TYR:HE1	1:U:95:ILE:HB	1.83	0.42
1:E:78:ASP:OD1	1:E:82:SER:N	2.52	0.42
1:O:182:VAL:O	2:P:48:THR:HG21	2.19	0.42
2:P:180:SER:HB2	2:P:182:TYR:HE1	1.85	0.42
2:P:183:LEU:HG	2:P:185:LEU:HG	2.01	0.42
1:U:227:TYR:OH	1:U:260:LEU:HD22	2.20	0.42
1:E:156:TYR:HB2	1:E:163:TYR:CE2	2.55	0.42
1:H:43:THR:HA	1:H:109:SER:HA	2.02	0.42
2:P:172:GLN:OE1	2:P:178:ALA:HB2	2.20	0.42
2:V:164:VAL:HG22	2:V:183:LEU:HD13	2.02	0.42
2:K:7:PRO:HD3	2:K:22:THR:HG23	2.01	0.42
1:Y:251:VAL:O	1:Y:258:TYR:HA	2.20	0.42
1:A:93:LEU:HD21	1:A:108:VAL:HG22	2.02	0.41
1:J:73:TRP:CH2	1:J:76:SER:HB3	2.55	0.41
1:J:250:ALA:HB1	1:J:258:TYR:HB3	2.02	0.41
2:L:48:LEU:O	2:L:59:VAL:HG21	2.20	0.41
2:B:36:TRP:CE2	2:B:74:LEU:HB2	2.54	0.41
2:B:126:SER:O	2:B:130:LEU:HD12	2.20	0.41
1:U:125:HIS:NE2	2:Z:62:ASP:HB3	2.35	0.41
1:A:30:LEU:HD21	1:A:123:THR:HG23	2.01	0.41
1:J:48:CYS:O	1:J:103:GLN:HA	2.21	0.41
2:K:6:GLN:NE2	2:K:106:THR:N	2.68	0.41
2:K:116:SER:H	2:K:145:TYR:HB3	1.85	0.41
1:U:182:VAL:HG11	1:U:185:TRP:CE2	2.55	0.41
2:Z:33:GLY:O	2:Z:35:VAL:N	2.51	0.41
2:B:38:GLN:HB2	2:B:48:LEU:HD11	2.02	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:K:143:ASP:N	2:K:177:TYR:O	2.51	0.41
2:V:39:GLN:HB2	2:V:49:LEU:HD11	2.03	0.41
1:Y:48:CYS:O	1:Y:103:GLN:HA	2.20	0.41
2:V:172:GLN:N	2:V:176:LYS:O	2.30	0.41
2:V:181:SER:C	2:V:182:TYR:HD1	2.23	0.41
1:A:64:ARG:NH2	1:A:72:GLU:OE1	2.46	0.41
1:E:63:VAL:HG11	1:E:71:LEU:HD23	2.03	0.41
1:U:165:GLY:O	1:U:169:CYS:HB3	2.20	0.41
1:U:293:GLU:HA	1:U:294:PRO:HD3	1.92	0.41
1:H:106:LEU:HD12	1:H:107:SER:H	1.86	0.41
2:K:129:GLU:HG2	2:K:134:LYS:O	2.20	0.41
1:O:64:ARG:HD3	1:O:74:LEU:HD21	2.03	0.41
2:B:8:SER:H	2:B:105:THR:HG22	1.84	0.41
2:K:6:GLN:NE2	2:K:106:THR:HG23	2.36	0.41
2:L:166:THR:HG22	2:L:179:SER:O	2.21	0.41
1:O:71:LEU:HB2	2:P:102:PHE:CD2	2.56	0.41
2:V:154:LYS:HB2	2:V:197:SER:HB2	2.03	0.41
1:A:62:TRP:HD1	1:A:95:ILE:HD13	1.86	0.41
1:H:234:VAL:HG22	1:H:279:VAL:HG22	2.03	0.41
1:J:206:LEU:HD22	2:K:123:PHE:HB3	2.02	0.41
2:K:120:VAL:HG21	2:K:200:VAL:HG11	2.02	0.41
2:P:135:ALA:O	2:P:185:LEU:N	2.50	0.41
1:U:140:TYR:CE1	2:Z:17:GLN:HB3	2.56	0.41
2:V:65:SER:HB3	2:V:76:THR:OG1	2.21	0.41
2:V:152:VAL:HG13	2:V:199:GLU:HB2	2.02	0.41
1:Y:85:TYR:CD2	1:Y:90:LYS:HG3	2.56	0.41
2:Z:130:LEU:HD21	2:Z:190:TRP:CD1	2.55	0.41
1:J:113:THR:HA	1:J:193:VAL:HG11	2.02	0.41
2:K:116:SER:HA	2:K:117:PRO:HD3	1.93	0.41
2:L:188:ASP:O	2:L:195:TYR:OH	2.35	0.41
2:P:7:PRO:O	2:P:106:THR:HG22	2.21	0.41
2:P:137:LEU:HD12	2:P:183:LEU:HD23	2.03	0.41
2:V:189:ASP:O	2:V:192:SER:OG	2.34	0.41
2:Z:122:LEU:HD11	2:Z:211:VAL:HG22	2.02	0.41
2:Z:165:GLU:N	2:Z:182:TYR:O	2.54	0.41
2:B:7:PRO:HD2	2:B:105:THR:HG21	2.03	0.40
1:E:185:TRP:CD2	2:F:46:PRO:HG2	2.56	0.40
2:P:41:ILE:HG12	2:P:86:ALA:HB2	2.03	0.40
2:P:180:SER:HB2	2:P:182:TYR:CE1	2.55	0.40
1:Y:62:TRP:HD1	1:Y:95:ILE:HD13	1.84	0.40
2:F:37:TRP:CE2	2:F:75:LEU:HB2	2.56	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:H:122:THR:HB	1:H:182:VAL:HG13	2.03	0.40
2:L:14:LEU:HB2	2:L:110:LEU:O	2.21	0.40
2:Z:4:LEU:HD23	2:Z:4:LEU:HA	1.91	0.40
2:F:38:TYR:HE1	2:F:48:THR:HG22	1.86	0.40
2:F:52:GLY:O	2:F:54:THR:N	2.51	0.40
2:F:170:SER:O	2:F:178:ALA:N	2.52	0.40
2:L:13:SER:O	2:L:79:LEU:HD12	2.20	0.40
2:P:33:GLY:HA3	2:P:68:ARG:CZ	2.51	0.40
2:L:180:SER:C	2:L:181:TYR:HD1	2.25	0.40
2:P:172:GLN:N	2:P:176:LYS:O	2.34	0.40
1:U:69:LYS:NZ	1:U:72:GLU:OE1	2.54	0.40
1:E:252:LEU:HD12	1:E:252:LEU:HA	1.86	0.40
2:K:153:TRP:HE1	2:K:181:SER:HG	1.69	0.40
1:O:40:PRO:HB2	1:U:252:LEU:CD1	2.52	0.40

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%)	29 66
1	E	249/274 (91%)	240 (96%)	9 (4%)	0	100 100
1	H	249/274 (91%)	234 (94%)	13 (5%)	2 (1%)	19 57
1	J	202/274 (74%)	191 (95%)	9 (4%)	2 (1%)	15 52
1	O	201/274 (73%)	188 (94%)	12 (6%)	1 (0%)	29 66
1	U	249/274 (91%)	236 (95%)	12 (5%)	1 (0%)	34 70
1	Y	203/274 (74%)	195 (96%)	7 (3%)	1 (0%)	29 66
1	c	248/274 (90%)	237 (96%)	11 (4%)	0	100 100
2	B	207/216 (96%)	190 (92%)	17 (8%)	0	100 100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
2	F	213/216 (99%)	202 (95%)	11 (5%)	0	100	100
2	K	213/216 (99%)	193 (91%)	19 (9%)	1 (0%)	29	66
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%)	29	66
2	d	213/216 (99%)	193 (91%)	17 (8%)	3 (1%)	11	46
All	All	3478/3920 (89%)	3256 (94%)	209 (6%)	13 (0%)	34	70

All (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
2	d	114	PRO
1	A	226	SER
1	H	167	GLY
1	J	78	ASP
1	Y	130	LYS
2	K	70	GLY
1	U	168	GLY
2	d	146	PRO

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	A	180/229 (79%)	174 (97%)	6 (3%)	38	65
1	E	204/229 (89%)	199 (98%)	5 (2%)	47	70

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	H	212/229 (93%)	209 (99%)	3 (1%)	67	81
1	J	166/229 (72%)	163 (98%)	3 (2%)	59	77
1	O	173/229 (76%)	172 (99%)	1 (1%)	86	92
1	U	206/229 (90%)	202 (98%)	4 (2%)	57	76
1	Y	171/229 (75%)	169 (99%)	2 (1%)	71	84
1	c	205/229 (90%)	201 (98%)	4 (2%)	55	75
2	B	165/184 (90%)	165 (100%)	0	100	100
2	F	176/184 (96%)	174 (99%)	2 (1%)	73	85
2	K	163/184 (89%)	161 (99%)	2 (1%)	71	84
2	L	179/184 (97%)	176 (98%)	3 (2%)	60	78
2	P	173/184 (94%)	172 (99%)	1 (1%)	86	92
2	V	164/184 (89%)	163 (99%)	1 (1%)	86	92
2	Z	166/184 (90%)	165 (99%)	1 (1%)	86	92
2	d	168/184 (91%)	164 (98%)	4 (2%)	49	71
All	All	2871/3304 (87%)	2829 (98%)	42 (2%)	65	81

All (42) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	39	LYS
1	A	130	LYS
1	A	131	ARG
1	A	132	CYS
1	A	136	TYR
1	A	190	LEU
1	E	107	SER
1	E	142	CYS
1	E	144	TYR
1	E	222	CYS
1	E	289	ASP
2	F	131	ASN
2	F	171	LYS
1	H	138	TYR
1	H	166	TYR
1	H	169	CYS
1	J	127	TYR
1	J	246	HIS

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Mol	Chain	Res	Type
1	J	277	CYS
2	K	6	GLN
2	K	62	ASP
2	L	91	SER
2	L	161	ARG
2	L	215	CYS
1	O	290	LYS
2	P	130	LEU
1	U	142	CYS
1	U	166	TYR
1	U	179	GLU
1	U	220	LEU
2	V	115	LYS
1	Y	31	ARG
1	Y	127	TYR
2	Z	216	CYS
1	c	157	TYR
1	c	166	TYR
1	c	190	LEU
1	c	220	LEU
2	d	36	SER
2	d	92	SER
2	d	104	SER
2	d	130	LEU

Sometimes 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 (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 monosaccharides 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, 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	214/274 (78%)	0.78	27 (12%)	3	4	76, 132, 199, 289	0
1	E	255/274 (93%)	0.06	4 (1%)	72	64	74, 101, 150, 191	0
1	H	255/274 (93%)	0.01	4 (1%)	72	64	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	64	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	40	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	38	70, 112, 175, 279	0
2	K	215/216 (99%)	-0.06	2 (0%)	84	79	69, 99, 150, 179	0
2	L	214/216 (99%)	0.01	1 (0%)	91	87	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	79	69, 105, 150, 180	0
2	Z	206/216 (95%)	0.25	12 (5%)	23	18	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	18	67, 105, 187, 330	0

All (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

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Mol	Chain	Res	Type	RSRZ
1	O	171	SER	5.9
1	Y	219	THR	5.1
1	A	261	SER	5.1
2	P	197	SER	5.1
1	Y	55	LEU	5.0
2	B	206	THR	5.0
1	A	134	ASP	4.9
2	P	142	SER	4.9
1	A	210	CYS	4.9
2	B	190	TRP	4.9
1	O	209	CYS	4.7
2	P	196	TYR	4.6
2	B	197	SER	4.6
1	J	291	ALA	4.6
1	A	207	SER	4.6
1	J	292	VAL	4.5
1	A	51	SER	4.5
1	A	208	SER	4.5
2	P	153	TRP	4.4
2	Z	196	TYR	4.3
2	B	186	THR	4.3
2	B	154	LYS	4.1
1	Y	245	VAL	4.0
2	F	144	PHE	3.9
2	B	201	THR	3.9
2	B	133	ASN	3.8
2	P	190	TRP	3.8
1	Y	56	SER	3.8
1	Y	220	LEU	3.8
2	P	208	THR	3.8
1	J	293	GLU	3.8
2	P	133	ASN	3.7
2	P	143	ASP	3.7
1	Y	294	PRO	3.7
1	Y	207	SER	3.7
1	O	50	ALA	3.7
1	c	145	GLY	3.7
2	P	213	PRO	3.6
2	P	154	LYS	3.6
1	A	278	ASN	3.6
2	Z	199	GLU	3.4
1	J	286	THR	3.4

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Mol	Chain	Res	Type	RSRZ
1	Y	203	VAL	3.4
1	Y	58	LYS	3.3
2	F	157	GLY	3.3
2	P	127	THR	3.3
1	Y	99	ASN	3.3
1	Y	222	CYS	3.3
1	A	276	THR	3.3
2	P	152	VAL	3.3
1	E	144	TYR	3.3
2	B	160	ILE	3.3
1	Y	265	THR	3.2
1	Y	266	VAL	3.2
2	P	212	LYS	3.2
2	P	124	PRO	3.2
2	P	141	ILE	3.2
2	P	215	GLU	3.2
1	A	274	THR	3.1
1	A	50	ALA	3.1
1	A	205	PRO	3.1
2	B	214	SER	3.1
2	P	211	VAL	3.1
1	O	204	TYR	3.1
1	O	99	ASN	3.1
2	B	178	ALA	3.1
2	F	118	PRO	3.1
2	B	211	VAL	3.0
1	O	102	SER	3.0
2	P	159	THR	3.0
1	O	173	SER	3.0
2	P	125	PRO	3.0
2	Z	210	THR	3.0
1	J	290	LYS	2.9
2	Z	200	VAL	2.9
1	J	58	LYS	2.9
2	B	216	CYS	2.9
1	Y	278	ASN	2.9
2	B	127	THR	2.8
2	B	138	VAL	2.8
2	B	123	PHE	2.8
1	Y	280	ALA	2.8
1	Y	290	LYS	2.8
2	P	160	ILE	2.8

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Mol	Chain	Res	Type	RSRZ
1	H	55	LEU	2.8
2	B	119	SER	2.8
1	A	133	PRO	2.8
2	B	196	TYR	2.8
2	P	214	SER	2.7
1	J	288	VAL	2.7
1	Y	210	CYS	2.7
1	J	279	VAL	2.7
1	Y	205	PRO	2.7
2	P	216	CYS	2.7
1	O	277	CYS	2.7
1	A	219	THR	2.7
2	P	155	ALA	2.7
1	Y	204	TYR	2.7
1	A	291	ALA	2.7
2	Z	206	THR	2.6
1	A	275	PHE	2.6
1	Y	262	SER	2.6
1	O	55	LEU	2.6
1	Y	28	VAL	2.6
2	B	208	THR	2.6
2	B	153	TRP	2.6
1	Y	289	ASP	2.6
1	O	97	LYS	2.6
2	Z	154	LYS	2.6
1	A	55	LEU	2.6
1	Y	243	SER	2.6
1	J	280	ALA	2.5
2	B	137	LEU	2.5
1	A	288	VAL	2.5
1	A	290	LYS	2.5
1	O	207	SER	2.5
1	U	144	TYR	2.5
2	P	137	LEU	2.5
1	J	275	PHE	2.5
2	K	210	THR	2.5
1	Y	292	VAL	2.5
2	B	141	ILE	2.4
1	c	53	PHE	2.4
2	P	178	ALA	2.4
1	J	220	LEU	2.4
1	Y	241	LEU	2.4

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Mol	Chain	Res	Type	RSRZ
1	Y	276	THR	2.4
1	A	206	LEU	2.4
2	B	215	GLU	2.4
1	Y	53	PHE	2.4
2	B	126	SER	2.4
2	B	217	SER	2.4
2	L	153	LYS	2.4
2	B	131	ASN	2.4
1	O	279	VAL	2.4
2	Z	207	VAL	2.4
2	F	177	TYR	2.4
1	A	97	LYS	2.3
1	A	220	LEU	2.3
1	c	170	SER	2.3
1	J	55	LEU	2.3
1	Y	293	GLU	2.3
1	Y	244	GLY	2.3
2	P	134	LYS	2.3
1	J	53	PHE	2.3
2	F	56	ARG	2.3
2	B	212	LYS	2.3
1	J	103	GLN	2.3
1	A	204	TYR	2.3
2	V	115	LYS	2.3
2	K	127	THR	2.3
1	c	146	THR	2.3
2	P	185	LEU	2.3
2	B	125	PRO	2.2
2	B	184	SER	2.2
1	J	97	LYS	2.2
1	U	292	VAL	2.2
2	B	205	SER	2.2
2	P	217	SER	2.2
1	Y	103	GLN	2.2
1	A	99	ASN	2.2
2	F	178	ALA	2.2
1	Y	238	SER	2.2
1	c	144	TYR	2.2
2	B	213	PRO	2.2
1	O	172	PHE	2.2
2	P	191	LYS	2.2
1	A	289	ASP	2.2

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Mol	Chain	Res	Type	RSRZ
1	J	289	ASP	2.2
2	Z	160	ILE	2.2
1	U	141	TRP	2.2
1	E	58	LYS	2.2
1	A	135	GLY	2.2
1	A	235	THR	2.2
2	Z	208	THR	2.2
1	O	103	GLN	2.2
2	V	153	TRP	2.2
1	J	174	ALA	2.1
1	J	81	GLY	2.1
1	J	133	PRO	2.1
2	Z	197	SER	2.1
2	F	206	THR	2.1
2	P	132	GLY	2.1
1	Y	223	LEU	2.1
1	Y	279	VAL	2.1
2	Z	133	ASN	2.1
1	c	280	ALA	2.1
2	B	189	ASP	2.1
1	E	53	PHE	2.1
1	J	210	CYS	2.1
1	U	55	LEU	2.1
1	c	58	LYS	2.1
1	H	220	LEU	2.1
2	P	192	SER	2.1
1	c	143	GLY	2.1
1	H	171	SER	2.0
1	Y	97	LYS	2.0
1	Y	59	ALA	2.0
1	Y	54	SER	2.0
1	Y	246	HIS	2.0
2	P	144	PHE	2.0
1	E	264	VAL	2.0
2	Z	151	VAL	2.0
1	H	153	ASN	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.