



# Full wwPDB X-ray Structure Validation Report ⓘ

Jun 24, 2024 – 07:43 PM EDT

PDB ID : 6QN8  
Title : Structure of bovine anti-RSV Fab B13  
Authors : Ren, J.; Nettleship, J.E.; Harris, G.; Mwangi, W.; Rhaman, N.; Grant, C.; Kotecha, A.; Fry, E.; Charleston, B.; Stuart, D.I.; Hammond, J.; Owens, R.J.  
Deposited on : 2019-02-10  
Resolution : 2.12 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](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.

The types of validation reports are described at

<http://www.wwpdb.org/validation/2017/FAQs#types>.

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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	:	2.37.1
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

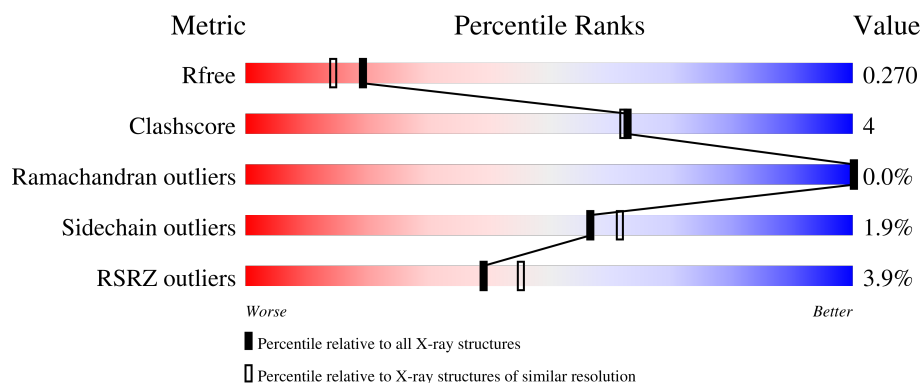
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

The reported resolution of this entry is 2.12 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	6241 (2.14-2.10)
Clashscore	141614	6778 (2.14-2.10)
Ramachandran outliers	138981	6705 (2.14-2.10)
Sidechain outliers	138945	6706 (2.14-2.10)
RSRZ outliers	127900	6112 (2.14-2.10)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments of the lower bar indicate the fraction of residues that contain outliers for  $\geq 3$ , 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  $\leq 5\%$ . 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	243	<div> <div>2%</div> <div> <div></div> <div>91%</div> <div>6%</div> <div></div> </div> </div>
1	C	243	<div> <div>6%</div> <div> <div></div> <div>80%</div> <div>13%</div> <div>7%</div> </div> </div>
1	E	243	<div> <div>2%</div> <div> <div></div> <div>86%</div> <div>7%</div> <div>7%</div> </div> </div>
1	G	243	<div> <div>7%</div> <div> <div></div> <div>84%</div> <div>9%</div> <div>8%</div> </div> </div>
1	H	243	<div> <div>8%</div> <div> <div></div> <div>86%</div> <div>7%</div> <div>7%</div> </div> </div>

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Mol	Chain	Length	Quality of chain
1	J	243	<div><div></div><div>3%</div><div>89%</div><div>5%</div><div>7%</div></div>
2	B	216	<div><div></div><div>%</div><div>90%</div><div>8%</div><div>.</div></div>
2	D	216	<div><div></div><div>4%</div><div>87%</div><div>10%</div><div>..</div></div>
2	F	216	<div><div></div><div>2%</div><div>91%</div><div>7%</div><div>.</div></div>
2	I	216	<div><div></div><div>4%</div><div>85%</div><div>12%</div><div>..</div></div>
2	K	216	<div><div></div><div>%</div><div>93%</div><div>6%</div><div>.</div></div>
2	L	216	<div><div></div><div>2%</div><div>93%</div><div>6%</div><div>.</div></div>

## 2 Entry composition

There are 4 unique types of molecules in this entry. The entry contains 20946 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 Heavy chain of bovine anti-RSV B13 Fab.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	H	227	Total	C	N	O	S	0	0	0
			1687	1060	276	340	11			
1	A	235	Total	C	N	O	S	0	0	0
			1750	1097	293	349	11			
1	C	226	Total	C	N	O	S	0	0	0
			1679	1056	275	337	11			
1	E	226	Total	C	N	O	S	0	0	0
			1676	1054	274	337	11			
1	G	224	Total	C	N	O	S	0	0	0
			1663	1046	272	334	11			
1	J	227	Total	C	N	O	S	0	0	0
			1685	1059	276	339	11			

- Molecule 2 is a protein called Light chain of bovine anti-RSV Fab B13.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	L	213	Total	C	N	O	S	0	0	0
			1567	973	263	325	6			
2	B	213	Total	C	N	O	S	0	0	0
			1567	973	263	325	6			
2	D	213	Total	C	N	O	S	0	0	0
			1567	973	263	325	6			
2	F	213	Total	C	N	O	S	0	0	0
			1567	973	263	325	6			
2	I	213	Total	C	N	O	S	0	0	0
			1567	973	263	325	6			
2	K	213	Total	C	N	O	S	0	0	0
			1567	973	263	325	6			

- Molecule 3 is CHLORIDE ION (three-letter code: CL) (formula: Cl).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	B	1	Total 1	Cl 1	0	0
3	J	1	Total 1	Cl 1	0	0

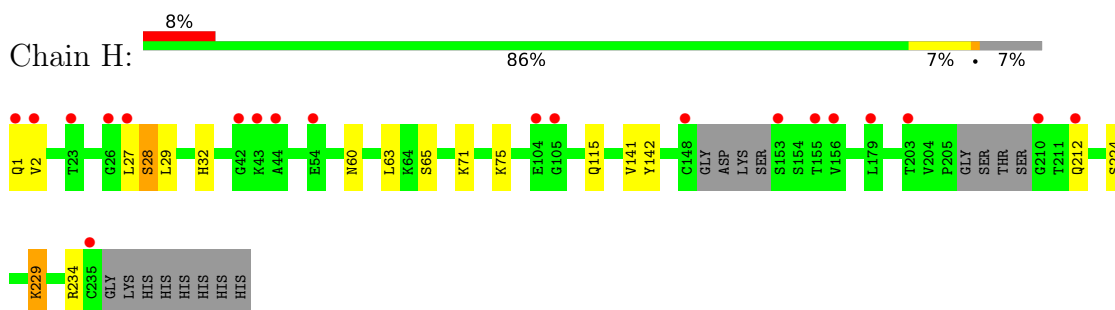
- Molecule 4 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	H	120	Total 120	O 120	0	0
4	L	114	Total 114	O 114	0	0
4	A	136	Total 136	O 136	0	0
4	B	163	Total 163	O 163	0	0
4	C	83	Total 83	O 83	0	0
4	D	85	Total 85	O 85	0	0
4	E	160	Total 160	O 160	0	0
4	F	156	Total 156	O 156	0	0
4	G	66	Total 66	O 66	0	0
4	I	86	Total 86	O 86	0	0
4	J	119	Total 119	O 119	0	0
4	K	114	Total 114	O 114	0	0

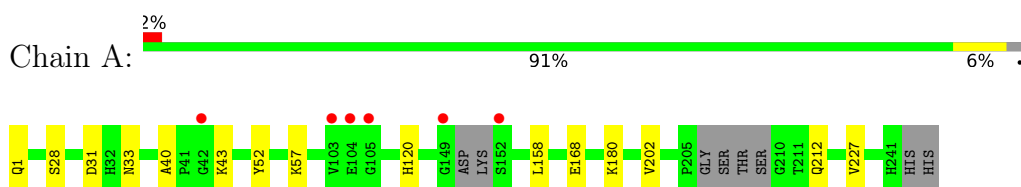
### 3 Residue-property plots [i](#)

These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. Residues are color-coded according to the number of geometric quality criteria for which they contain at least one outlier: green = 0, yellow = 1, orange = 2 and red = 3 or more. A red dot above a residue indicates a poor fit to the electron density ( $RSRZ > 2$ ). Stretches of 2 or more consecutive residues without any outlier are shown as a green connector. Residues present in the sample, but not in the model, are shown in grey.

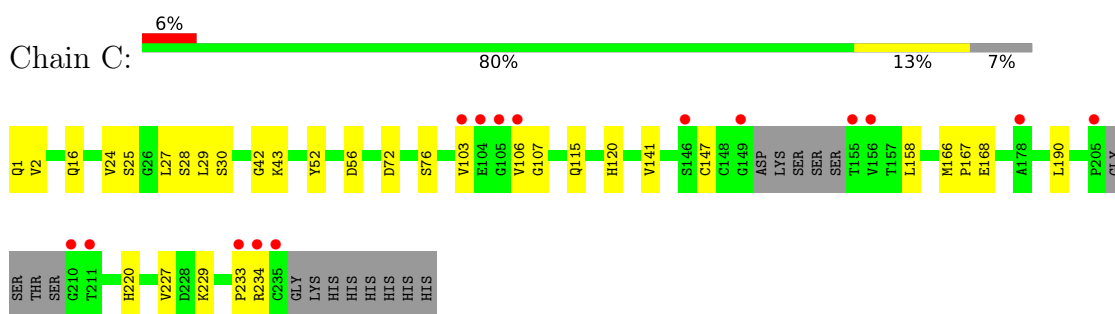
- Molecule 1: Heavy chain of bovine anti-RSV B13 Fab



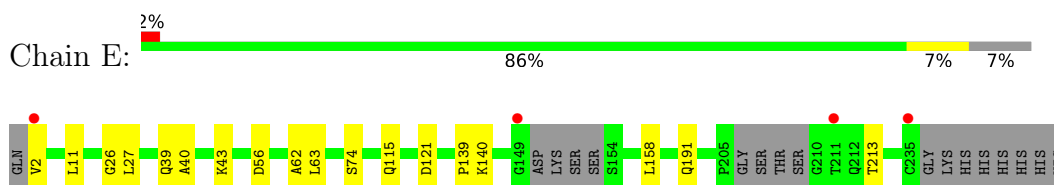
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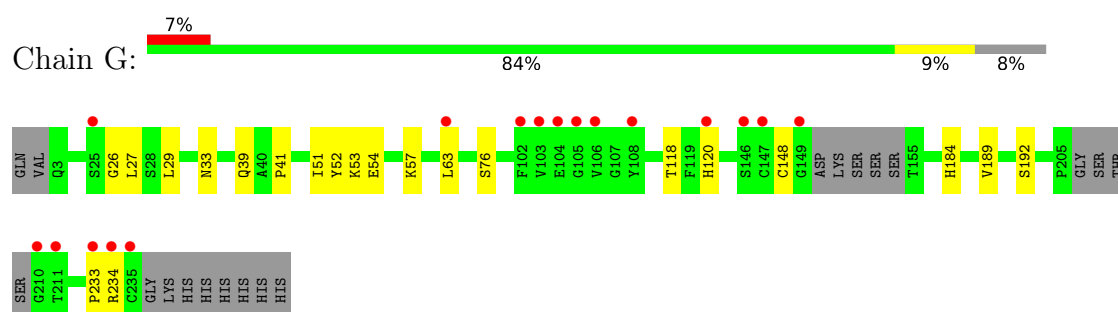
- Molecule 1: Heavy chain of bovine anti-RSV B13 Fab



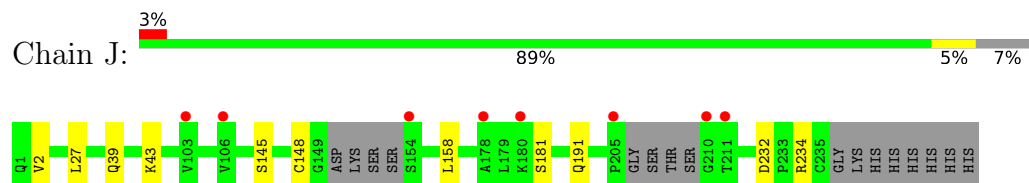
- Molecule 1: Heavy chain of bovine anti-RSV B13 Fab



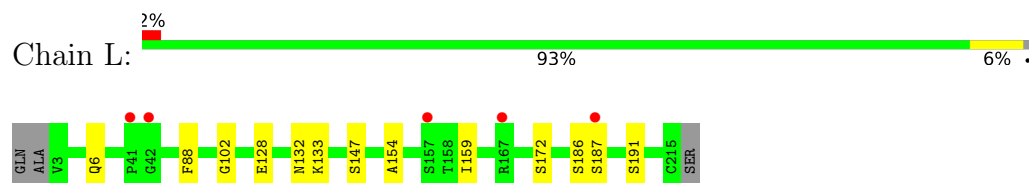
- Molecule 1: Heavy chain of bovine anti-RSV B13 Fab



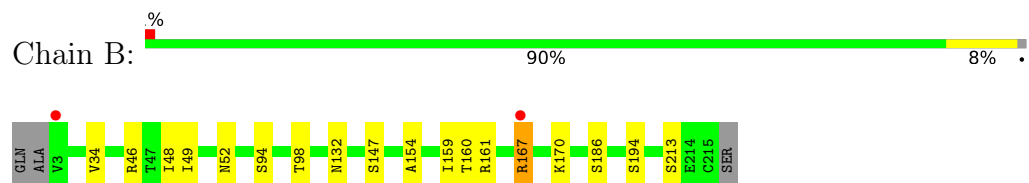
- Molecule 1: Heavy chain of bovine anti-RSV B13 Fab



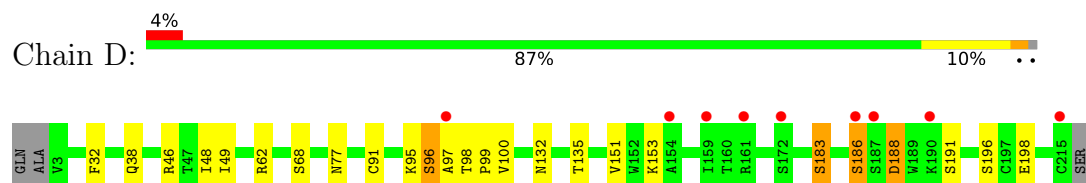
- Molecule 2: Light chain of bovine anti-RSV Fab B13



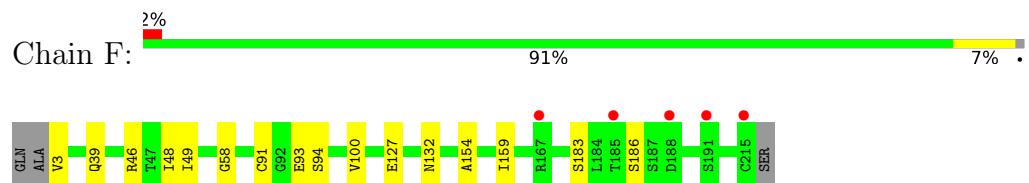
- Molecule 2: Light chain of bovine anti-RSV Fab B13



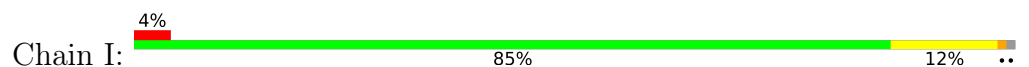
- Molecule 2: Light chain of bovine anti-RSV Fab B13

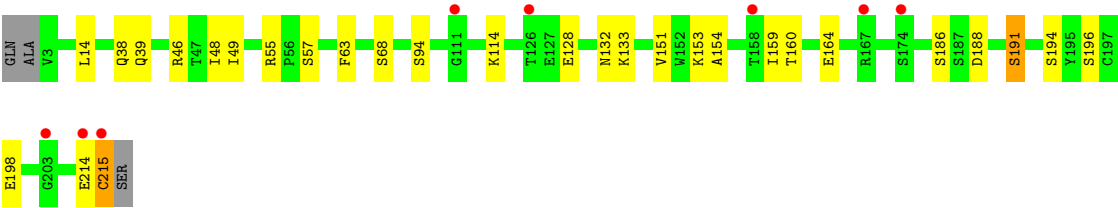


- Molecule 2: Light chain of bovine anti-RSV Fab B13

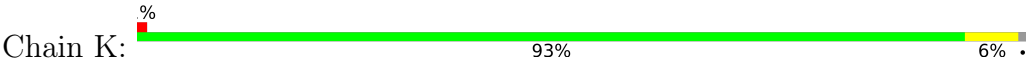


- Molecule 2: Light chain of bovine anti-RSV Fab B13





● Molecule 2: Light chain of bovine anti-RSV Fab B13





## 4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	87.91Å 132.46Å 118.18Å 90.00° 102.93° 90.00°	Depositor
Resolution (Å)	87.07 – 2.12 86.92 – 2.12	Depositor EDS
% Data completeness (in resolution range)	99.0 (87.07-2.12) 99.0 (86.92-2.12)	Depositor EDS
$R_{merge}$	0.13	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	2.06 (at 2.12Å)	Xtriage
Refinement program	REFMAC 5.8.0238	Depositor
R, $R_{free}$	0.235 , 0.267 0.240 , 0.270	Depositor DCC
$R_{free}$ test set	7327 reflections (4.96%)	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	28.5	Xtriage
Anisotropy	0.251	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.29 , 41.3	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.48$ , $\langle L^2 \rangle = 0.31$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
$F_o, F_c$ correlation	0.93	EDS
Total number of atoms	20946	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	41.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The analyses of the Patterson function reveals a significant off-origin peak that is 32.14 % of the origin peak, indicating pseudo-translational symmetry. The chance of finding a peak of this or larger height randomly in a structure without pseudo-translational symmetry is equal to 9.8613e-04. The detected translational NCS is most likely also responsible for the elevated intensity ratio.*

<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](#)

Bond lengths and bond angles in the following residue types are not validated in this section: CL

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	0.74	1/1790 (0.1%)	0.81	0/2442
1	C	0.70	1/1715 (0.1%)	0.79	0/2342
1	E	0.70	0/1712	0.77	0/2338
1	G	0.69	0/1699	0.78	0/2320
1	H	0.72	0/1723	0.80	0/2353
1	J	0.70	0/1721	0.77	0/2350
2	B	0.74	0/1599	0.76	1/2178 (0.0%)
2	D	0.70	0/1599	0.80	0/2178
2	F	0.75	1/1599 (0.1%)	0.76	0/2178
2	I	0.70	0/1599	0.77	0/2178
2	K	0.72	0/1599	0.76	0/2178
2	L	0.70	0/1599	0.74	0/2178
All	All	0.71	3/19954 (0.0%)	0.78	1/27213 (0.0%)

Chiral center outliers are detected by calculating the chiral volume of a chiral center and verifying if the center is modelled as a planar moiety or with the opposite hand. A planarity outlier is detected by checking planarity of atoms in a peptide group, atoms in a mainchain group or atoms of a sidechain that are expected to be planar.

Mol	Chain	#Chirality outliers	#Planarity outliers
1	G	0	1

All (3) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	C	168	GLU	CD-OE1	6.27	1.32	1.25
1	A	168	GLU	CD-OE1	5.62	1.31	1.25
2	F	127	GLU	CD-OE2	5.48	1.31	1.25

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	167	ARG	CB-CA-C	-5.51	99.38	110.40

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	G	63	LEU	Peptide

## 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	1750	0	1704	13	0
1	C	1679	0	1645	27	0
1	E	1676	0	1639	14	0
1	G	1663	0	1625	23	0
1	H	1687	0	1652	24	0
1	J	1685	0	1650	7	0
2	B	1567	0	1533	9	0
2	D	1567	0	1533	14	0
2	F	1567	0	1533	9	0
2	I	1567	0	1533	22	0
2	K	1567	0	1533	12	0
2	L	1567	0	1533	9	0
3	B	1	0	0	0	0
3	J	1	0	0	0	0
4	A	136	0	0	4	0
4	B	163	0	0	5	1
4	C	83	0	0	2	0
4	D	85	0	0	3	0
4	E	160	0	0	2	0
4	F	156	0	0	2	1
4	G	66	0	0	2	0
4	H	120	0	0	3	0
4	I	86	0	0	2	0
4	J	119	0	0	3	0
4	K	114	0	0	2	0
4	L	114	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
All	All	20946	0	19113	167	1

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 4.

All (167) 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:A:28:SER:OG	4:A:301:HOH:O	1.70	1.08
1:E:2:VAL:N	1:G:192:SER:O	1.93	1.01
1:H:141:VAL:O	1:H:229:LYS:NZ	1.97	0.97
1:G:41:PRO:O	4:G:301:HOH:O	1.87	0.92
1:H:2:VAL:HG13	1:H:27:LEU:HD11	1.50	0.91
1:H:27:LEU:HD23	1:H:32:HIS:NE2	1.84	0.91
1:C:42:GLY:O	1:C:43:LYS:HG2	1.70	0.91
1:C:141:VAL:O	1:C:229:LYS:HE3	1.73	0.89
1:C:103:VAL:HG23	1:C:106:VAL:HB	1.55	0.89
1:E:43:LYS:O	4:E:301:HOH:O	1.92	0.87
2:L:6:GLN:HE21	2:L:102:GLY:HA3	1.39	0.87
1:E:2:VAL:HG12	1:E:27:LEU:HD21	1.60	0.84
2:D:151:VAL:HG23	2:D:198:GLU:HB2	1.60	0.83
1:E:39:GLN:HE22	2:F:39:GLN:HE22	1.30	0.79
1:H:27:LEU:HD23	1:H:32:HIS:CE1	2.17	0.79
2:B:161:ARG:NH1	4:B:401:HOH:O	2.15	0.79
1:G:120:HIS:CE1	2:K:164:GLU:OE2	2.38	0.77
1:H:2:VAL:CG1	1:H:27:LEU:HD11	2.17	0.74
1:G:29:LEU:CD1	1:G:76:SER:HA	2.19	0.72
2:B:34:VAL:H	2:B:52:ASN:ND2	1.87	0.72
1:G:33:ASN:HD22	1:G:52:TYR:HA	1.53	0.72
1:J:39:GLN:HE22	2:K:39:GLN:HE22	1.36	0.72
1:C:16:GLN:NE2	4:C:301:HOH:O	2.12	0.71
2:B:132:ASN:HA	2:B:186:SER:OG	1.90	0.71
1:A:31:ASP:OD1	4:A:302:HOH:O	2.08	0.70
1:A:227:VAL:HG22	2:K:204:SER:HB3	1.76	0.67
2:D:97:ALA:O	2:D:99:PRO:HD3	1.94	0.67
1:G:39:GLN:HE22	2:I:39:GLN:HE22	1.42	0.67
1:E:2:VAL:HG13	1:E:115:GLN:OE1	1.96	0.65
1:H:2:VAL:HG13	1:H:27:LEU:CD1	2.27	0.64
1:H:141:VAL:C	1:H:229:LYS:HZ1	1.97	0.63
1:C:29:LEU:H	1:C:29:LEU:HD12	1.64	0.63
2:I:214:GLU:O	2:I:215:CYS:HB3	1.99	0.63

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1:GLN:HG3	1:A:120:HIS:CE1	2.34	0.62
1:A:33:ASN:HD22	1:A:52:TYR:HA	1.63	0.62
1:C:141:VAL:HG21	1:C:227:VAL:HG11	1.80	0.62
1:H:1:GLN:CD	1:H:1:GLN:O	2.38	0.61
1:A:43:LYS:O	4:A:303:HOH:O	2.16	0.61
1:H:28:SER:HB3	4:H:314:HOH:O	2.01	0.61
1:G:29:LEU:HD12	1:G:76:SER:HA	1.82	0.61
1:C:141:VAL:O	1:C:229:LYS:CE	2.45	0.61
1:G:51:ILE:HD12	1:G:57:LYS:HG3	1.82	0.60
1:A:40:ALA:HB3	1:A:43:LYS:HD2	1.82	0.60
2:D:62:ARG:HD2	2:D:77:ASN:O	2.03	0.59
1:G:189:VAL:HG21	2:I:164:GLU:HB3	1.83	0.59
1:G:120:HIS:CE1	2:I:57:SER:OG	2.56	0.59
2:L:128:GLU:HG2	2:L:133:LYS:HG3	1.85	0.58
2:L:132:ASN:HA	2:L:186:SER:OG	2.03	0.58
2:F:93:GLU:HG3	4:F:331:HOH:O	2.05	0.57
1:G:233:PRO:HG2	1:G:234:ARG:HG3	1.86	0.57
2:B:167:ARG:HG2	4:B:509:HOH:O	2.05	0.56
2:B:170:LYS:HE2	4:B:406:HOH:O	2.05	0.56
1:E:191:GLN:NE2	2:F:183:SER:OG	2.38	0.56
2:I:151:VAL:HG13	2:I:198:GLU:HB2	1.86	0.56
1:H:27:LEU:CD2	1:H:32:HIS:CE1	2.88	0.56
2:K:17:ARG:HD3	4:K:304:HOH:O	2.06	0.56
1:J:181:SER:HB3	4:J:436:HOH:O	2.05	0.56
2:D:38:GLN:HE22	2:D:46:ARG:HH21	1.54	0.55
2:I:128:GLU:HG2	2:I:133:LYS:HB3	1.89	0.55
1:G:120:HIS:ND1	2:I:57:SER:HB2	2.21	0.55
2:L:187:SER:HB3	1:A:180:LYS:HE2	1.89	0.55
1:G:189:VAL:CG2	2:I:164:GLU:HB3	2.36	0.55
1:H:2:VAL:HG21	1:H:27:LEU:HD21	1.88	0.54
1:E:2:VAL:HG21	1:E:121:ASP:O	2.07	0.54
1:G:51:ILE:HD12	1:G:57:LYS:CG	2.37	0.54
1:G:118:THR:HB	1:G:120:HIS:CD2	2.43	0.54
2:D:188:ASP:HA	2:D:191:SER:OG	2.08	0.53
1:C:158:LEU:CD2	1:C:233:PRO:HB3	2.38	0.53
2:B:98:THR:HG21	4:B:546:HOH:O	2.09	0.53
2:K:11:SER:HB2	2:K:110:LEU:CD1	2.39	0.52
1:H:2:VAL:HG22	1:H:27:LEU:HD11	1.90	0.52
1:C:1:GLN:N	1:C:115:GLN:HE22	2.08	0.52
1:H:29:LEU:HD23	1:H:71:LYS:HG3	1.92	0.51
1:C:1:GLN:H2	1:C:115:GLN:HE22	1.59	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:42:GLY:O	1:C:43:LYS:CG	2.52	0.51
2:F:91:CYS:O	2:F:100:VAL:HG12	2.10	0.51
1:C:167:PRO:O	1:C:220:HIS:HE1	1.94	0.51
1:C:103:VAL:HG22	1:C:107:GLY:O	2.11	0.51
2:D:135:THR:OG1	4:D:301:HOH:O	2.20	0.50
2:D:91:CYS:O	2:D:100:VAL:HG12	2.11	0.50
2:K:17:ARG:NH1	4:K:304:HOH:O	2.43	0.50
1:C:29:LEU:CD1	1:C:76:SER:HA	2.42	0.50
1:H:1:GLN:O	1:H:1:GLN:NE2	2.45	0.50
1:A:158:LEU:HD23	1:A:202:VAL:HB	1.94	0.50
1:H:142:TYR:CA	1:H:229:LYS:HZ2	2.25	0.49
1:H:141:VAL:C	1:H:229:LYS:NZ	2.60	0.49
1:C:141:VAL:CG2	1:C:227:VAL:HG11	2.42	0.49
2:B:160:THR:O	4:B:402:HOH:O	2.20	0.49
2:I:151:VAL:CG1	2:I:198:GLU:HB2	2.42	0.48
2:K:132:ASN:HA	2:K:186:SER:OG	2.13	0.48
1:G:29:LEU:HD11	1:G:76:SER:HA	1.95	0.48
2:F:58:GLY:O	2:I:160:THR:HB	2.13	0.48
1:H:2:VAL:CG2	1:H:27:LEU:HD11	2.44	0.48
1:J:148:CYS:HB2	2:K:123:PRO:HG3	1.96	0.48
1:C:141:VAL:HG21	1:C:227:VAL:CG1	2.43	0.48
1:J:191:GLN:O	4:J:401:HOH:O	2.20	0.48
2:I:153:LYS:HE3	2:I:198:GLU:OE1	2.13	0.48
2:D:32:PHE:CE1	2:D:95:LYS:O	2.67	0.47
1:C:141:VAL:C	1:C:229:LYS:HE3	2.32	0.47
2:D:183:SER:OG	4:D:302:HOH:O	2.20	0.47
2:I:214:GLU:O	2:I:215:CYS:CB	2.63	0.47
1:H:27:LEU:CD2	1:H:32:HIS:NE2	2.70	0.46
2:L:128:GLU:OE1	2:L:133:LYS:HE2	2.16	0.46
1:C:158:LEU:HD23	1:C:233:PRO:HB3	1.97	0.46
1:C:52:TYR:OH	2:D:95:LYS:HE2	2.14	0.46
2:I:38:GLN:HE22	2:I:46:ARG:HH21	1.62	0.46
1:H:212:GLN:NE2	4:H:303:HOH:O	2.35	0.46
1:E:26:GLY:O	1:E:27:LEU:HD13	2.16	0.46
2:D:183:SER:HB3	4:D:301:HOH:O	2.17	0.45
2:F:132:ASN:HA	2:F:186:SER:OG	2.17	0.45
2:K:154:ALA:HB2	2:K:159:ILE:HD11	1.98	0.45
2:I:39:GLN:NE2	4:I:301:HOH:O	2.48	0.45
1:H:60:ASN:HB3	1:H:63:LEU:HD12	1.98	0.45
2:L:6:GLN:HE22	2:L:88:PHE:HA	1.82	0.45
2:L:154:ALA:HB2	2:L:159:ILE:HD11	1.99	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:24:VAL:HG11	1:C:27:LEU:HD11	1.98	0.45
1:G:53:LYS:HE2	1:G:54:GLU:OE1	2.17	0.45
1:C:29:LEU:HD12	1:C:29:LEU:N	2.32	0.45
1:G:120:HIS:CE1	2:I:57:SER:CB	2.99	0.44
2:K:11:SER:HB2	2:K:110:LEU:HD13	1.99	0.44
2:K:11:SER:HB2	2:K:110:LEU:HD11	1.99	0.44
1:G:51:ILE:CD1	1:G:57:LYS:HG3	2.47	0.44
1:A:212:GLN:HG3	4:A:329:HOH:O	2.16	0.44
2:D:132:ASN:HA	2:D:186:SER:OG	2.18	0.44
2:F:48:ILE:HG22	2:F:49:ILE:HG12	1.99	0.44
2:I:153:LYS:HB2	2:I:196:SER:OG	2.18	0.44
2:I:114:LYS:NZ	4:I:304:HOH:O	2.51	0.43
2:B:154:ALA:HB2	2:B:159:ILE:HD11	2.00	0.43
1:J:2:VAL:HG11	1:J:27:LEU:HD23	2.00	0.43
2:F:154:ALA:HB2	2:F:159:ILE:HD11	2.01	0.43
1:E:40:ALA:HB3	1:E:43:LYS:CG	2.48	0.43
1:E:139:PRO:O	1:E:140:LYS:HE2	2.19	0.43
1:C:72:ASP:OD2	4:C:302:HOH:O	2.21	0.43
2:D:48:ILE:HG22	2:D:49:ILE:HG12	2.00	0.43
1:G:33:ASN:HD22	1:G:52:TYR:CA	2.29	0.43
1:G:51:ILE:CD1	1:G:57:LYS:CG	2.96	0.42
1:E:11:LEU:HD12	1:E:11:LEU:HA	1.92	0.42
1:E:62:ALA:C	1:E:63:LEU:HD23	2.40	0.42
2:K:190:LYS:HB2	2:K:190:LYS:HE2	1.77	0.42
1:H:2:VAL:HG23	1:H:115:GLN:NE2	2.34	0.42
1:J:39:GLN:NE2	4:J:411:HOH:O	2.51	0.42
1:J:232:ASP:OD1	1:J:234:ARG:HD3	2.19	0.42
2:B:48:ILE:HG22	2:B:49:ILE:HG12	2.01	0.42
2:L:6:GLN:NE2	2:L:102:GLY:HA3	2.20	0.42
1:C:29:LEU:HD11	1:C:76:SER:HA	2.01	0.42
2:I:154:ALA:HB2	2:I:159:ILE:HD11	2.02	0.42
1:C:1:GLN:HG3	1:C:120:HIS:CD2	2.54	0.42
2:I:188:ASP:HA	2:I:191:SER:HB3	2.02	0.42
1:H:142:TYR:HA	1:H:229:LYS:NZ	2.35	0.42
2:D:153:LYS:HB2	2:D:196:SER:OG	2.20	0.42
1:E:213:THR:HG22	4:E:316:HOH:O	2.19	0.42
1:A:43:LYS:HE2	1:A:43:LYS:HB3	1.76	0.41
1:G:26:GLY:C	1:G:27:LEU:HD12	2.40	0.41
2:I:55:ARG:HD3	2:I:63:PHE:O	2.20	0.41
2:F:3:VAL:HG23	4:F:354:HOH:O	2.21	0.41
1:E:56:ASP:OD2	1:E:56:ASP:N	2.52	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:1:GLN:N	1:C:1:GLN:OE1	2.36	0.41
2:L:133:LYS:HB2	2:L:133:LYS:HE3	1.81	0.41
2:I:132:ASN:HA	2:I:186:SER:OG	2.21	0.41
1:A:40:ALA:HB3	1:A:43:LYS:CD	2.51	0.41
1:G:53:LYS:NZ	4:G:317:HOH:O	2.53	0.40
1:H:142:TYR:HA	1:H:229:LYS:HZ2	1.86	0.40
1:A:158:LEU:CD2	1:A:202:VAL:HB	2.51	0.40
1:C:2:VAL:HG11	1:C:27:LEU:HD23	2.02	0.40
2:I:48:ILE:HG22	2:I:49:ILE:HG12	2.03	0.40
1:H:65:SER:HA	4:H:396:HOH:O	2.20	0.40
1:C:166:MET:HA	1:C:167:PRO:HA	1.91	0.40

All (1) symmetry-related close contacts are listed below. The label for Atom-2 includes the symmetry operator and encoded unit-cell translations to be applied.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:B:434:HOH:O	4:F:426:HOH:O[2_454]	2.00	0.20

## 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	229/243 (94%)	219 (96%)	10 (4%)	0	100	100
1	C	220/243 (90%)	212 (96%)	8 (4%)	0	100	100
1	E	220/243 (90%)	214 (97%)	6 (3%)	0	100	100
1	G	218/243 (90%)	209 (96%)	9 (4%)	0	100	100
1	H	221/243 (91%)	215 (97%)	6 (3%)	0	100	100
1	J	221/243 (91%)	214 (97%)	7 (3%)	0	100	100
2	B	211/216 (98%)	207 (98%)	4 (2%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
2	D	211/216 (98%)	202 (96%)	8 (4%)	1 (0%)	29	25
2	F	211/216 (98%)	208 (99%)	3 (1%)	0	100	100
2	I	211/216 (98%)	207 (98%)	4 (2%)	0	100	100
2	K	211/216 (98%)	207 (98%)	4 (2%)	0	100	100
2	L	211/216 (98%)	207 (98%)	4 (2%)	0	100	100
All	All	2595/2754 (94%)	2521 (97%)	73 (3%)	1 (0%)	100	100

All (1) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
2	D	96	SER

### 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	203/210 (97%)	202 (100%)	1 (0%)	88	92
1	C	195/210 (93%)	188 (96%)	7 (4%)	35	35
1	E	195/210 (93%)	193 (99%)	2 (1%)	76	81
1	G	193/210 (92%)	191 (99%)	2 (1%)	76	81
1	H	197/210 (94%)	192 (98%)	5 (2%)	47	50
1	J	196/210 (93%)	193 (98%)	3 (2%)	65	70
2	B	182/184 (99%)	177 (97%)	5 (3%)	44	47
2	D	182/184 (99%)	176 (97%)	6 (3%)	38	39
2	F	182/184 (99%)	180 (99%)	2 (1%)	73	79
2	I	182/184 (99%)	176 (97%)	6 (3%)	38	39
2	K	182/184 (99%)	181 (100%)	1 (0%)	88	92
2	L	182/184 (99%)	179 (98%)	3 (2%)	62	68
All	All	2271/2364 (96%)	2228 (98%)	43 (2%)	57	61

All (43) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	H	28	SER
1	H	75	LYS
1	H	224	SER
1	H	229	LYS
1	H	234	ARG
2	L	147	SER
2	L	172	SER
2	L	191	SER
1	A	57	LYS
2	B	46	ARG
2	B	94	SER
2	B	147	SER
2	B	194	SER
2	B	213	SER
1	C	25	SER
1	C	28	SER
1	C	30	SER
1	C	56	ASP
1	C	147	CYS
1	C	190	LEU
1	C	234	ARG
2	D	68	SER
2	D	96	SER
2	D	98	THR
2	D	183	SER
2	D	186	SER
2	D	188	ASP
1	E	74	SER
1	E	158	LEU
2	F	46	ARG
2	F	94	SER
1	G	148	CYS
1	G	184	HIS
2	I	14	LEU
2	I	68	SER
2	I	94	SER
2	I	191	SER
2	I	194	SER
2	I	215	CYS
1	J	43	LYS
1	J	145	SER
1	J	158	LEU

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Mol	Chain	Res	Type
2	K	167	ARG

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (28) such sidechains are listed below:

Mol	Chain	Res	Type
1	H	16	GLN
1	H	115	GLN
2	L	6	GLN
2	L	201	HIS
1	A	33	ASN
2	B	52	ASN
1	C	16	GLN
1	C	115	GLN
1	C	220	HIS
2	D	38	GLN
2	D	162	ASN
1	E	39	GLN
1	E	191	GLN
2	F	70	ASN
2	F	80	GLN
2	F	201	HIS
1	G	33	ASN
1	G	77	GLN
1	G	120	HIS
1	G	191	GLN
2	I	16	GLN
2	I	38	GLN
2	I	39	GLN
2	I	80	GLN
1	J	39	GLN
1	J	191	GLN
2	K	80	GLN
2	K	162	ASN

### 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 monosaccharides in this entry.

## 5.6 Ligand geometry [i](#)

Of 2 ligands modelled in this entry, 2 are monoatomic - leaving 0 for Mogul analysis.

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

No monomer is involved in short contacts.

## 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	235/243 (96%)	-0.02	6 (2%) 56 61	20, 33, 73, 108	0
1	C	226/243 (93%)	0.42	15 (6%) 18 22	27, 49, 92, 123	0
1	E	226/243 (93%)	-0.04	4 (1%) 68 72	18, 31, 67, 91	0
1	G	224/243 (92%)	0.35	17 (7%) 13 17	26, 46, 91, 122	0
1	H	227/243 (93%)	0.30	20 (8%) 10 12	22, 37, 80, 100	0
1	J	227/243 (93%)	0.07	8 (3%) 44 50	19, 34, 78, 105	0
2	B	213/216 (98%)	-0.05	2 (0%) 84 86	20, 31, 53, 72	0
2	D	213/216 (98%)	0.38	9 (4%) 36 42	25, 46, 88, 124	0
2	F	213/216 (98%)	-0.12	5 (2%) 60 65	19, 31, 53, 82	0
2	I	213/216 (98%)	0.30	8 (3%) 40 46	26, 48, 77, 120	0
2	K	213/216 (98%)	0.02	3 (1%) 75 78	20, 37, 61, 92	0
2	L	213/216 (98%)	0.09	5 (2%) 60 65	21, 36, 60, 77	0
All	All	2643/2754 (95%)	0.14	102 (3%) 39 45	18, 37, 78, 124	0

All (102) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
2	D	190	LYS	7.1
1	A	149	GLY	7.1
2	D	215	CYS	5.6
1	G	104	GLU	5.5
1	J	154	SER	5.5
1	G	234	ARG	5.0
1	C	146	SER	4.9
1	C	234	ARG	4.8
1	H	26	GLY	4.7
1	G	211	THR	4.4
1	H	43	LYS	4.3

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Mol	Chain	Res	Type	RSRZ
1	H	148	CYS	4.3
1	A	105	GLY	4.2
1	C	178	ALA	4.1
2	I	203	GLY	4.0
1	J	211	THR	3.9
1	G	235	CYS	3.8
2	I	215	CYS	3.8
1	C	233	PRO	3.8
2	L	42	GLY	3.7
1	G	103	VAL	3.7
2	D	187	SER	3.6
2	I	214	GLU	3.6
2	B	167	ARG	3.5
1	E	211	THR	3.4
2	L	167	ARG	3.4
1	H	27	LEU	3.3
1	G	147	CYS	3.3
1	C	210	GLY	3.3
2	K	95	LYS	3.3
1	A	152	SER	3.2
1	J	106	VAL	3.2
1	J	210	GLY	3.1
1	J	103	VAL	3.1
1	H	179	LEU	3.0
2	I	167	ARG	3.0
1	G	102	PHE	3.0
1	G	210	GLY	3.0
1	H	23	THR	3.0
2	D	172	SER	2.9
1	H	104	GLU	2.9
2	F	215	CYS	2.8
1	E	2	VAL	2.7
1	A	104	GLU	2.7
1	H	42	GLY	2.7
1	H	210	GLY	2.7
1	H	235	CYS	2.7
2	B	3	VAL	2.6
2	K	41	PRO	2.6
1	C	155	THR	2.6
2	F	191	SER	2.6
2	I	126	THR	2.6
2	F	167	ARG	2.6

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Mol	Chain	Res	Type	RSRZ
1	H	2	VAL	2.6
1	C	104	GLU	2.6
1	C	149	GLY	2.6
1	A	42	GLY	2.6
1	G	120	HIS	2.5
2	L	41	PRO	2.5
1	C	235	CYS	2.5
1	E	235	CYS	2.5
1	G	108	TYR	2.5
1	G	149	GLY	2.5
1	H	203	THR	2.5
1	A	103	VAL	2.4
1	G	63	LEU	2.4
2	D	154	ALA	2.4
1	C	103	VAL	2.4
1	H	1	GLN	2.4
1	G	146	SER	2.4
2	D	97	ALA	2.4
1	H	155	THR	2.3
1	C	211	THR	2.3
1	J	205	PRO	2.3
1	H	153	SER	2.3
1	G	105	GLY	2.3
2	L	187	SER	2.3
1	C	205	PRO	2.3
2	I	111	GLY	2.3
1	H	44	ALA	2.2
2	K	167	ARG	2.2
1	C	105	GLY	2.2
2	L	157	SER	2.2
1	H	156	VAL	2.2
1	C	156	VAL	2.2
1	E	149	GLY	2.2
1	J	178	ALA	2.2
2	D	186	SER	2.2
1	H	212	GLN	2.1
1	C	106	VAL	2.1
2	D	159	ILE	2.1
2	I	174	SER	2.1
2	I	158	THR	2.1
1	G	233	PRO	2.1
1	G	106	VAL	2.1

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Mol	Chain	Res	Type	RSRZ
2	F	188	ASP	2.1
1	J	180	LYS	2.0
1	H	105	GLY	2.0
1	G	25	SER	2.0
1	H	54	GLU	2.0
2	F	185	THR	2.0
2	D	161	ARG	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](#)

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95<sup>th</sup> percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
3	CL	J	301	1/1	0.88	0.15	56,56,56,56	0
3	CL	B	301	1/1	0.89	0.07	57,57,57,57	0

## 6.5 Other polymers [i](#)

There are no such residues in this entry.