



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 1, 2026 – 04:37 PM UTC

PDB ID : 6QN8 / pdb_00006qn8
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

A user guide is available at

<https://www.wwpdb.org/validation/2017/XrayValidationReportHelp>

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

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

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

MolProbity	:	4-5-2 with Phenix2.0
Xtriage (Phenix)	:	2.0
EDS	:	3.0
Percentile statistics	:	20250101.v01 (using entries in the PDB archive January 1st 2025)
CCP4	:	9.0.010 (Gargrove)
Density-Fitness	:	1.0.12
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.49

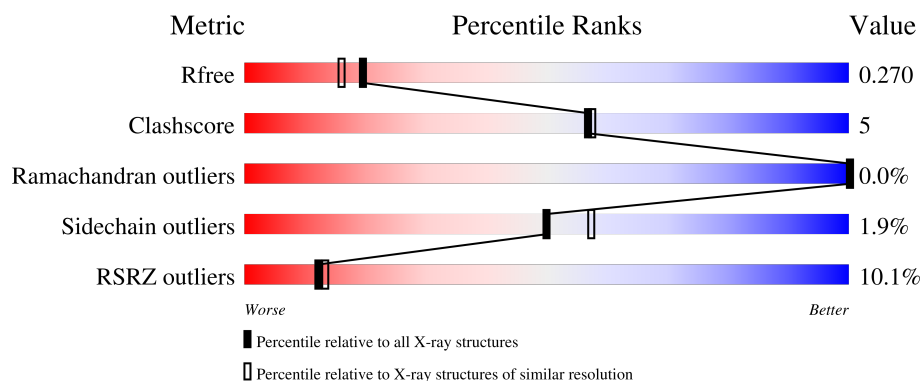
1 Overall quality at a glance

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}	180053	8290 (2.14-2.10)
Clashscore	190562	8817 (2.14-2.10)
Ramachandran outliers	187476	8738 (2.14-2.10)
Sidechain outliers	187428	8739 (2.14-2.10)
RSRZ outliers	180081	8294 (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 ≥ 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	8% 90% 7%
1	C	243	16% 80% 12% 7%
1	E	243	6% 85% 8% 7%
1	G	243	14% 84% 9% 8%
1	H	243	15% 85% 7% 7%

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Mol	Chain	Length	Quality of chain
1	J	243	
2	B	216	
2	D	216	
2	F	216	
2	I	216	
2	K	216	
2	L	216	

2 Entry composition [i](#)

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 (CCD ID: 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

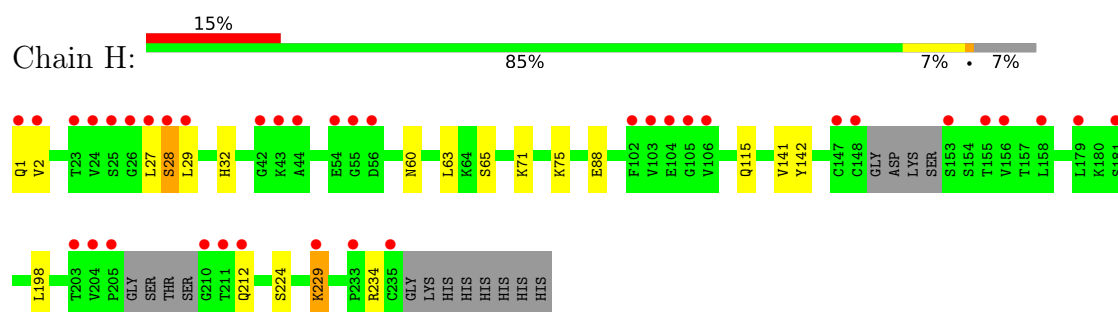
- Molecule 4 is water.

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

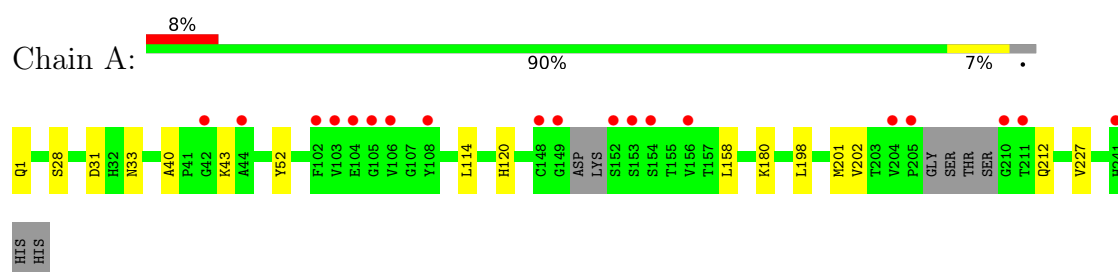
3 Residue-property plots [i](#)

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.

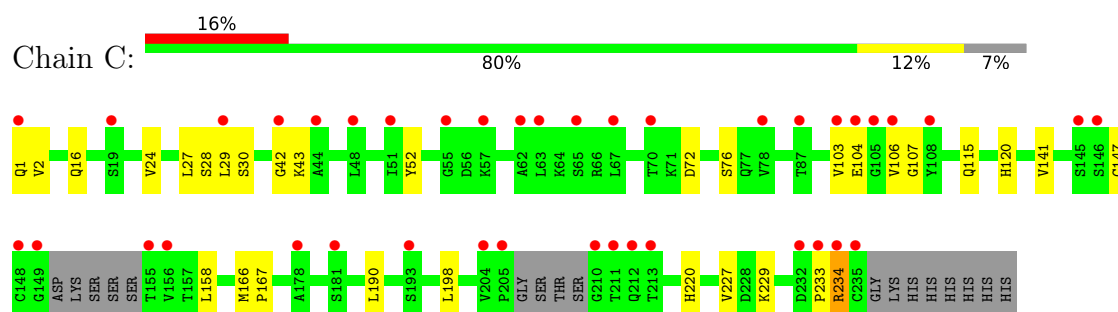
- Molecule 1: Heavy chain of bovine anti-RSV B13 Fab



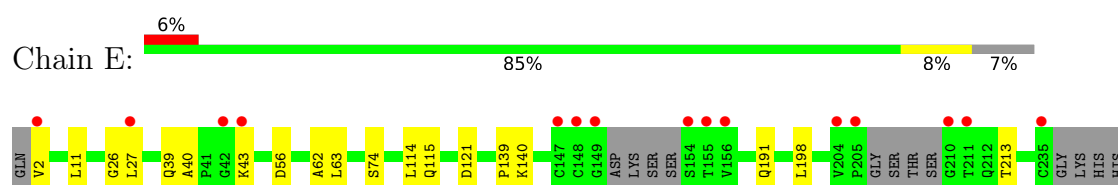
- Molecule 1: Heavy chain of bovine anti-RSV B13 Fab



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

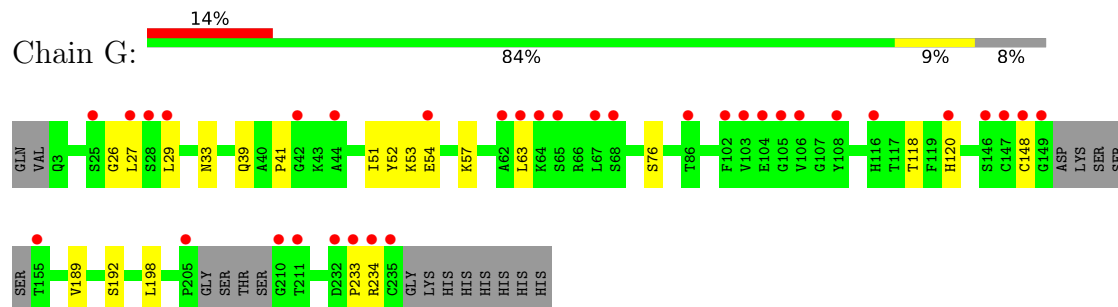


- Molecule 1: Heavy chain of bovine anti-RSV B13 Fab

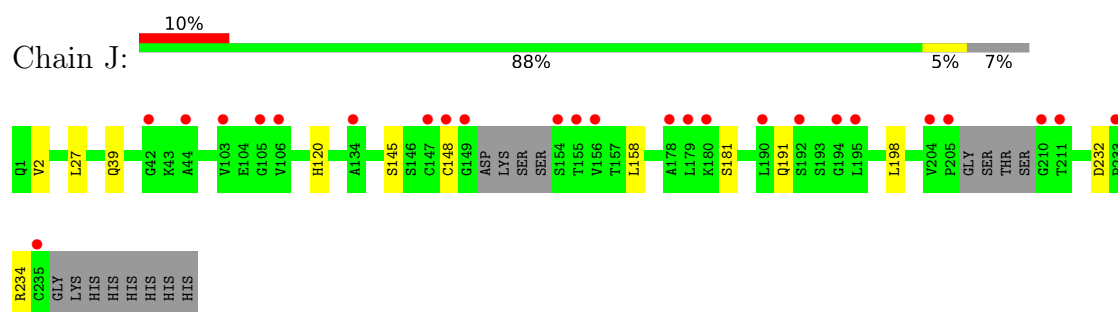


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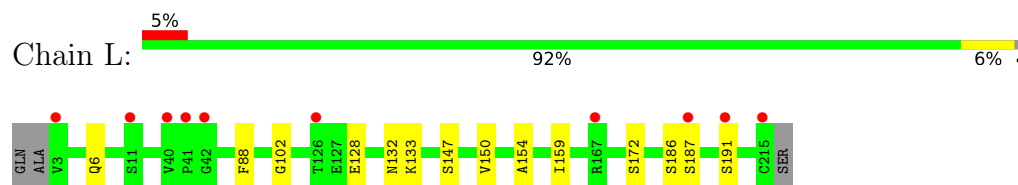
- Molecule 1: Heavy chain of bovine anti-RSV B13 Fab



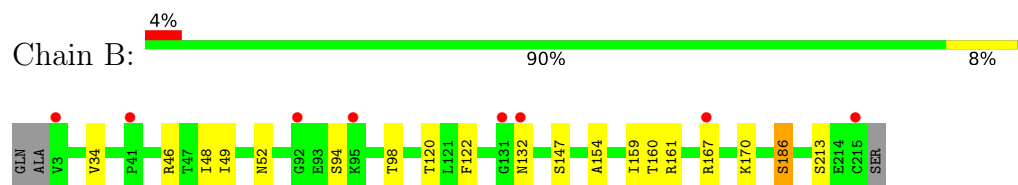
- Molecule 1: Heavy chain of bovine anti-RSV B13 Fab



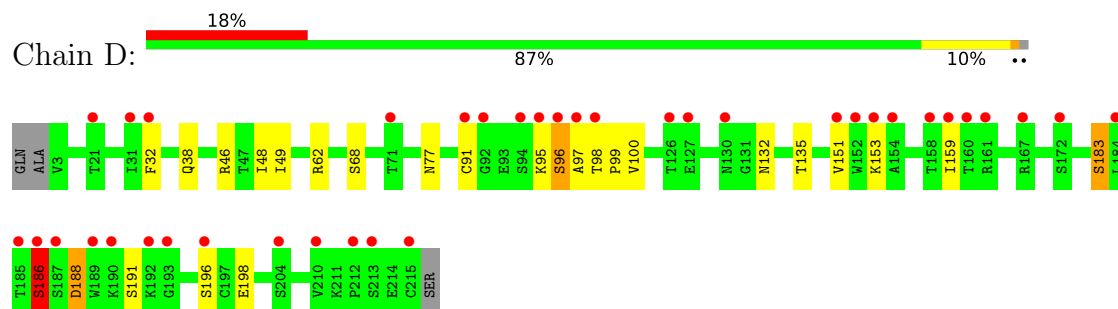
- Molecule 2: Light chain of bovine anti-RSV Fab B13



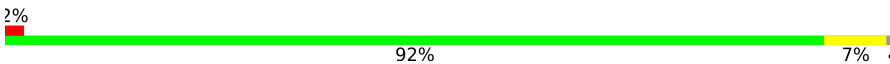
- Molecule 2: Light chain of bovine anti-RSV Fab B13

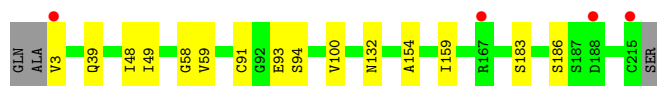


- Molecule 2: Light chain of bovine anti-RSV Fab B13



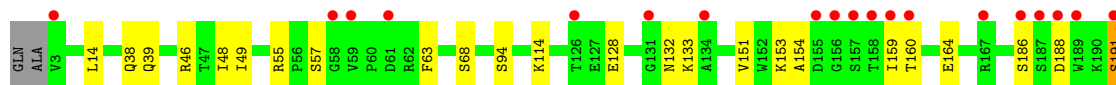
- Molecule 2: Light chain of bovine anti-RSV Fab B13

Chain F:  2% 92% 7%

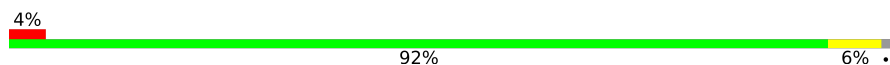


- Molecule 2: Light chain of bovine anti-RSV Fab B13

Chain I:  13% 86% 12%



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

Chain K:  4% 92% 6%



4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α , β , γ	87.91Å 132.46Å 118.18Å 90.00° 102.93° 90.00°	Depositor
Resolution (Å)	87.07 – 2.12 87.07 – 2.12	Depositor EDS
% Data completeness (in resolution range)	99.0 (87.07-2.12) 99.0 (87.07-2.12)	Depositor EDS
R_{merge}	0.13	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	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	7341 reflections (4.95%)	wwPDB-VP
Wilson B-factor (Å ²)	28.5	Xtriage
Anisotropy	0.251	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.27 , 35.1	EDS
L-test for twinning ²	$\langle L \rangle = 0.48$, $\langle L^2 \rangle = 0.31$	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 ²)	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.*

¹Intensities estimated from amplitudes.

²Theoretical values of $\langle |L| \rangle$, $\langle L^2 \rangle$ for acentric reflections are 0.5, 0.333 respectively for untwinned datasets, and 0.375, 0.2 for perfectly twinned datasets.

5 Model quality ⓘ

5.1 Standard geometry ⓘ

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	1.06	0/1790	1.13	0/2442
1	C	1.01	0/1715	1.12	1/2342 (0.0%)
1	E	1.03	0/1712	1.11	0/2338
1	G	1.02	0/1699	1.11	0/2320
1	H	1.05	0/1723	1.12	0/2353
1	J	1.04	1/1721 (0.1%)	1.09	0/2350
2	B	1.08	0/1599	1.11	1/2178 (0.0%)
2	D	1.05	0/1599	1.17	2/2178 (0.1%)
2	F	1.05	1/1599 (0.1%)	1.13	0/2178
2	I	1.03	0/1599	1.14	0/2178
2	K	1.04	0/1599	1.11	0/2178
2	L	1.03	0/1599	1.10	0/2178
All	All	1.04	2/19954 (0.0%)	1.12	4/27213 (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 (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	F	59	VAL	N-CA	5.42	1.50	1.46
1	J	120	HIS	CE1-NE2	5.02	1.37	1.32

All (4) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	D	186	SER	CA-C-N	5.33	127.43	120.28
2	D	186	SER	C-N-CA	5.33	127.43	120.28
1	C	234	ARG	CB-CA-C	5.24	120.18	109.76
2	B	186	SER	CA-C-O	-5.20	115.02	120.63

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	17	0
1	C	1679	0	1645	29	0
1	E	1676	0	1639	15	0
1	G	1663	0	1625	23	0
1	H	1687	0	1652	25	0
1	J	1685	0	1650	8	0
2	B	1567	0	1533	11	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	1	0
4	H	120	0	0	3	0
4	I	86	0	0	2	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
4	J	119	0	0	3	0
4	K	114	0	0	2	0
4	L	114	0	0	0	0
All	All	20946	0	19113	176	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 5.

All (176) 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:H:141:VAL:C	1:H:229:LYS:HZ1	1.95	0.69
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:H:1:GLN:CD	1:H:1:GLN:O	2.38	0.66

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:2:VAL:HG13	1:E:115:GLN:OE1	1.96	0.65
1:C:1:GLN:H2	1:C:115:GLN:HE22	1.43	0.64
1:H:2:VAL:HG13	1:H:27:LEU:CD1	2.27	0.64
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
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: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:C:141:VAL:C	1:C:229:LYS:HE3	2.32	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:H:141:VAL:C	1:H:229:LYS:NZ	2.60	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:98:THR:HG21	4:B:546:HOH:O	2.09	0.53
1:A:201:MET:HE1	2:B:120:THR:HG21	1.92	0.52
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: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:C:141:VAL:CG2	1:C:227:VAL:HG11	2.42	0.49
1:H:142:TYR:CA	1:H:229:LYS:HZ2	2.26	0.49
2:B:160:THR:O	4:B:402:HOH:O	2.20	0.49
1:A:1:GLN:H3	1:A:1:GLN:CD	2.10	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:E:62:ALA:C	1:E:63:LEU:HD23	2.40	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:G:26:GLY:C	1:G:27:LEU:HD12	2.40	0.46
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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
1:A:201:MET:HE3	2:B:122:PHE:CE2	2.51	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
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:C:1:GLN:H2	1:C:115:GLN:NE2	2.14	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:E:198:LEU:C	1:E:198:LEU:HD12	2.44	0.42
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
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
1:C:1:GLN:CD	1:C:1:GLN:H3	2.11	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:198:LEU:HD12	1:A:198:LEU:C	2.45	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:J:198:LEU:HD12	1:J:198:LEU:C	2.44	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
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
2:L:133:LYS:HB2	2:L:133:LYS:HE3	1.81	0.41
1:H:198:LEU:HD12	1:H:198:LEU:C	2.46	0.41
2:I:132:ASN:HA	2:I:186:SER:OG	2.21	0.41
1:G:198:LEU:HD12	1:G:198:LEU:C	2.46	0.41
1:H:142:TYR:HA	1:H:229:LYS:HZ2	1.86	0.41
1:A:40:ALA:HB3	1:A:43:LYS:CD	2.51	0.41
1:C:198:LEU:C	1:C:198:LEU:HD12	2.46	0.41
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 ⓘ

5.3.1 Protein backbone ⓘ

In the following table, the Percentiles column shows the percent Ramachandran outliers of the chain as a percentile score with respect to all X-ray entries followed by that with respect to entries of similar resolution.

The Analysed column shows the number of residues for which the backbone conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	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
2	D	211/216 (98%)	202 (96%)	8 (4%)	1 (0%)	24	22
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%)	81	87
1	C	195/210 (93%)	189 (97%)	6 (3%)	35	38
1	E	195/210 (93%)	193 (99%)	2 (1%)	68	76
1	G	193/210 (92%)	192 (100%)	1 (0%)	81	87
1	H	197/210 (94%)	191 (97%)	6 (3%)	36	40
1	J	196/210 (93%)	194 (99%)	2 (1%)	68	76
2	B	182/184 (99%)	178 (98%)	4 (2%)	45	52

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
2	D	182/184 (99%)	175 (96%)	7 (4%)	29	30
2	F	182/184 (99%)	181 (100%)	1 (0%)	81	87
2	I	182/184 (99%)	177 (97%)	5 (3%)	39	44
2	K	182/184 (99%)	178 (98%)	4 (2%)	45	52
2	L	182/184 (99%)	178 (98%)	4 (2%)	45	52
All	All	2271/2364 (96%)	2228 (98%)	43 (2%)	50	57

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	88	GLU
1	H	224	SER
1	H	229	LYS
1	H	234	ARG
2	L	147	SER
2	L	150	VAL
2	L	172	SER
2	L	191	SER
1	A	114	LEU
2	B	46	ARG
2	B	94	SER
2	B	147	SER
2	B	213	SER
1	C	28	SER
1	C	30	SER
1	C	104	GLU
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	159	ILE
2	D	183	SER
2	D	186	SER
2	D	188	ASP
1	E	74	SER
1	E	114	LEU

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Mol	Chain	Res	Type
2	F	94	SER
1	G	148	CYS
2	I	14	LEU
2	I	68	SER
2	I	94	SER
2	I	191	SER
2	I	215	CYS
1	J	145	SER
1	J	158	LEU
2	K	23	SER
2	K	133	LYS
2	K	167	ARG
2	K	190	LYS

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (47) such sidechains are listed below:

Mol	Chain	Res	Type
1	H	115	GLN
1	H	116	HIS
1	H	212	GLN
2	L	6	GLN
2	L	16	GLN
2	L	38	GLN
2	L	162	ASN
2	L	201	HIS
1	A	16	GLN
1	A	33	ASN
1	A	39	GLN
1	A	125	GLN
1	A	239	HIS
2	B	39	GLN
2	B	52	ASN
2	B	201	HIS
1	C	16	GLN
1	C	115	GLN
1	C	120	HIS
1	C	125	GLN
1	C	220	HIS
2	D	16	GLN
2	D	38	GLN
2	D	80	GLN
2	D	162	ASN

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Mol	Chain	Res	Type
1	E	39	GLN
1	E	191	GLN
2	F	16	GLN
2	F	70	ASN
2	F	77	ASN
2	F	162	ASN
1	G	33	ASN
1	G	77	GLN
1	G	116	HIS
1	G	120	HIS
1	G	191	GLN
2	I	38	GLN
2	I	39	GLN
2	I	70	ASN
2	I	80	GLN
2	I	201	HIS
1	J	39	GLN
2	K	16	GLN
2	K	70	ASN
2	K	77	ASN
2	K	162	ASN
2	K	201	HIS

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates ⓘ

There are no oligosaccharides in this entry.

5.6 Ligand geometry ⓘ

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, 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	235/243 (96%)	0.40	19 (8%) 18 19	20, 33, 73, 108	0
1	C	226/243 (93%)	1.18	40 (17%) 4 4	27, 49, 92, 123	0
1	E	226/243 (93%)	0.35	15 (6%) 24 26	18, 31, 67, 91	0
1	G	224/243 (92%)	0.97	34 (15%) 5 5	26, 46, 91, 122	0
1	H	227/243 (93%)	0.82	37 (16%) 4 5	22, 37, 80, 100	0
1	J	227/243 (93%)	0.50	25 (11%) 10 11	19, 34, 78, 105	0
2	B	213/216 (98%)	0.26	8 (3%) 44 47	20, 31, 53, 72	0
2	D	213/216 (98%)	1.07	38 (17%) 4 4	25, 46, 88, 124	0
2	F	213/216 (98%)	0.17	4 (1%) 66 69	19, 31, 53, 82	0
2	I	213/216 (98%)	0.97	28 (13%) 7 8	26, 48, 78, 120	0
2	K	213/216 (98%)	0.43	8 (3%) 44 47	20, 37, 61, 92	0
2	L	213/216 (98%)	0.44	10 (4%) 36 39	21, 36, 60, 77	0
All	All	2643/2754 (95%)	0.63	266 (10%) 12 13	18, 37, 78, 124	0

All (266) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	C	149	GLY	6.8
1	H	204	VAL	6.3
1	A	149	GLY	6.0
2	D	97	ALA	5.6
1	A	105	GLY	5.4
1	C	205	PRO	5.4
1	H	205	PRO	5.2
1	C	210	GLY	5.1
1	J	210	GLY	5.0
1	C	155	THR	4.8
2	D	96	SER	4.7

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Mol	Chain	Res	Type	RSRZ
1	J	106	VAL	4.6
2	D	95	LYS	4.6
1	G	103	VAL	4.5
1	J	205	PRO	4.4
1	G	104	GLU	4.4
1	E	205	PRO	4.4
2	I	203	GLY	4.3
1	G	106	VAL	4.3
1	J	154	SER	4.3
1	C	156	VAL	4.2
1	C	233	PRO	4.2
1	H	2	VAL	4.2
1	H	43	LYS	4.2
2	D	159	ILE	4.1
2	K	41	PRO	4.1
1	E	2	VAL	4.1
2	I	215	CYS	4.0
1	H	26	GLY	4.0
1	A	42	GLY	4.0
1	H	29	LEU	4.0
2	D	98	THR	4.0
1	E	149	GLY	4.0
1	G	210	GLY	4.0
1	J	105	GLY	3.9
1	G	102	PHE	3.9
2	I	159	ILE	3.9
1	G	63	LEU	3.9
1	E	211	THR	3.9
1	J	155	THR	3.9
1	E	210	GLY	3.8
1	G	149	GLY	3.8
1	J	149	GLY	3.8
1	C	178	ALA	3.8
1	E	156	VAL	3.8
1	C	106	VAL	3.8
1	C	204	VAL	3.8
1	E	235	CYS	3.7
1	G	235	CYS	3.7
1	H	1	GLN	3.7
1	H	104	GLU	3.6
2	B	167	ARG	3.6
1	H	203	THR	3.6

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Mol	Chain	Res	Type	RSRZ
2	D	215	CYS	3.6
1	H	148	CYS	3.6
1	G	105	GLY	3.5
2	D	31	ILE	3.4
1	A	210	GLY	3.4
2	L	42	GLY	3.4
1	C	211	THR	3.4
2	I	167	ARG	3.4
1	G	155	THR	3.4
1	C	105	GLY	3.4
1	C	181	SER	3.4
1	G	146	SER	3.4
1	G	62	ALA	3.4
1	H	27	LEU	3.4
2	D	189	TRP	3.3
1	G	205	PRO	3.3
1	C	44	ALA	3.3
1	E	154	SER	3.3
2	D	186	SER	3.3
1	A	106	VAL	3.3
1	J	103	VAL	3.3
1	H	210	GLY	3.2
1	C	42	GLY	3.2
1	C	63	LEU	3.2
1	H	55	GLY	3.2
2	F	188	ASP	3.2
1	A	152	SER	3.2
1	H	42	GLY	3.2
1	H	179	LEU	3.2
2	I	126	THR	3.2
2	D	190	LYS	3.2
1	A	241	HIS	3.1
2	D	160	THR	3.1
1	H	156	VAL	3.1
1	C	234	ARG	3.1
1	G	234	ARG	3.1
1	A	154	SER	3.1
1	A	103	VAL	3.1
1	E	42	GLY	3.1
1	E	148	CYS	3.0
1	G	29	LEU	3.0
1	G	148	CYS	3.0

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Mol	Chain	Res	Type	RSRZ
2	D	94	SER	3.0
1	H	102	PHE	3.0
1	H	235	CYS	3.0
2	D	185	THR	3.0
1	C	108	TYR	3.0
2	I	189	TRP	3.0
1	C	193	SER	2.9
1	C	235	CYS	2.9
1	G	147	CYS	2.9
1	C	103	VAL	2.9
1	E	155	THR	2.9
2	I	160	THR	2.9
1	J	233	PRO	2.9
2	L	3	VAL	2.9
2	D	158	THR	2.9
1	G	233	PRO	2.9
2	I	213	SER	2.9
1	J	44	ALA	2.9
1	C	148	CYS	2.8
1	C	104	GLU	2.8
2	I	194	SER	2.8
1	G	44	ALA	2.8
2	L	40	VAL	2.8
2	B	3	VAL	2.8
2	I	191	SER	2.8
2	F	167	ARG	2.8
1	A	108	TYR	2.8
2	F	215	CYS	2.8
1	J	192	SER	2.8
2	I	131	GLY	2.7
1	C	67	LEU	2.7
1	E	27	LEU	2.7
1	E	204	VAL	2.7
1	C	65	SER	2.7
1	C	146	SER	2.7
2	D	187	SER	2.7
2	I	187	SER	2.7
1	G	27	LEU	2.7
1	G	108	TYR	2.7
1	C	55	GLY	2.7
1	H	103	VAL	2.7
1	A	156	VAL	2.7

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Mol	Chain	Res	Type	RSRZ
2	I	3	VAL	2.7
1	E	147	CYS	2.7
2	D	193	GLY	2.7
1	H	23	THR	2.6
1	G	211	THR	2.6
2	L	11	SER	2.6
1	J	180	LYS	2.6
1	J	211	THR	2.6
2	L	187	SER	2.6
1	H	24	VAL	2.6
2	F	3	VAL	2.6
1	H	147	CYS	2.6
2	K	42	GLY	2.6
1	A	104	GLU	2.6
1	A	211	THR	2.6
1	J	178	ALA	2.6
1	G	232	ASP	2.6
1	J	179	LEU	2.6
1	A	148	CYS	2.6
2	D	192	LYS	2.6
2	K	161	ARG	2.6
1	G	28	SER	2.5
1	H	229	LYS	2.5
2	K	167	ARG	2.5
1	H	211	THR	2.5
1	H	25	SER	2.5
2	B	41	PRO	2.5
2	D	204	SER	2.5
1	G	42	GLY	2.5
2	I	192	LYS	2.5
2	L	167	ARG	2.5
1	G	67	LEU	2.5
2	K	95	LYS	2.5
2	D	92	GLY	2.5
2	B	132	ASN	2.5
2	K	27	ASP	2.4
1	J	148	CYS	2.4
1	J	235	CYS	2.4
1	C	70	THR	2.4
2	D	161	ARG	2.4
2	B	131	GLY	2.4
1	H	233	PRO	2.4

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Mol	Chain	Res	Type	RSRZ
1	G	120	HIS	2.4
1	J	194	GLY	2.4
1	C	212	GLN	2.4
1	G	54	GLU	2.4
1	H	56	ASP	2.4
2	I	157	SER	2.4
2	B	215	CYS	2.4
1	C	213	THR	2.4
2	I	58	GLY	2.4
2	I	155	ASP	2.4
2	D	210	VAL	2.4
1	G	25	SER	2.4
2	I	134	ALA	2.3
1	H	153	SER	2.3
1	C	78	VAL	2.3
1	H	54	GLU	2.3
1	A	44	ALA	2.3
1	E	43	LYS	2.3
2	D	153	LYS	2.3
1	G	68	SER	2.3
2	D	196	SER	2.3
1	J	156	VAL	2.3
1	H	155	THR	2.3
1	G	86	THR	2.3
1	J	134	ALA	2.3
2	D	154	ALA	2.3
1	C	29	LEU	2.3
1	C	57	LYS	2.3
2	I	211	LYS	2.3
1	G	65	SER	2.3
1	J	204	VAL	2.3
2	D	167	ARG	2.3
1	C	62	ALA	2.3
1	C	232	ASP	2.3
1	J	195	LEU	2.3
1	C	51	ILE	2.2
2	L	41	PRO	2.2
2	D	21	THR	2.2
2	I	188	ASP	2.2
1	J	42	GLY	2.2
2	I	186	SER	2.2
1	A	204	VAL	2.2

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Mol	Chain	Res	Type	RSRZ
1	G	64	LYS	2.2
2	D	126	THR	2.2
1	J	190	LEU	2.2
2	K	94	SER	2.2
1	A	102	PHE	2.2
1	C	87	THR	2.2
2	L	126	THR	2.2
2	I	59	VAL	2.2
2	D	127	GLU	2.2
1	C	145	SER	2.2
2	L	191	SER	2.2
1	H	105	GLY	2.1
2	D	184	LEU	2.1
1	A	153	SER	2.1
2	D	213	SER	2.1
2	D	212	PRO	2.1
1	C	1	GLN	2.1
2	D	172	SER	2.1
2	K	174	SER	2.1
2	D	151	VAL	2.1
2	I	210	VAL	2.1
2	D	91	CYS	2.1
1	A	205	PRO	2.1
2	D	71	THR	2.1
2	B	92	GLY	2.1
2	D	32	PHE	2.1
1	H	28	SER	2.1
1	C	48	LEU	2.0
2	D	130	ASN	2.0
1	H	212	GLN	2.0
1	J	147	CYS	2.0
2	I	61	ASP	2.0
2	I	158	THR	2.0
2	I	212	PRO	2.0
1	H	106	VAL	2.0
1	H	181	SER	2.0
1	C	19	SER	2.0
1	H	44	ALA	2.0
2	D	152	TRP	2.0
1	H	158	LEU	2.0
2	L	215	CYS	2.0
1	G	116	HIS	2.0

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Mol	Chain	Res	Type	RSRZ
2	B	95	LYS	2.0
2	I	205	THR	2.0
2	I	156	GLY	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 oligosaccharides 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, 95th 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(Å ²)	Q<0.9
3	CL	B	301	1/1	0.90	0.10	57,57,57,57	0
3	CL	J	301	1/1	0.96	0.10	56,56,56,56	0

6.5 Other polymers [i](#)

There are no such residues in this entry.