



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 5, 2026 – 11:59 AM UTC

PDB ID : 1TQC / pdb_00001tqc
Title : Ovine recombinant PrP(114-234), ARR variant in complex with the VRQ14 Fab fragment (IgG2a)
Authors : Eghiaian, F.; Grosclaude, J.; Lesceu, S.; Debey, P.; Doublet, B.; Treguer, E.; Rezaei, H.; Knossow, M.
Deposited on : 2004-06-17
Resolution : 2.80 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) : **NOT EXECUTED**
EDS : **NOT EXECUTED**
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.49

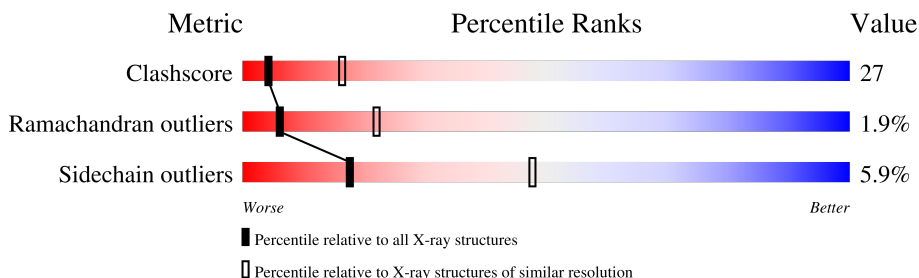
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.80 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))
Clashscore	190562	4276 (2.80-2.80)
Ramachandran outliers	187476	4196 (2.80-2.80)
Sidechain outliers	187428	4198 (2.80-2.80)

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 $\leq 5\%$.

Note EDS was not executed.

Mol	Chain	Length	Quality of chain
1	A	102	
2	B	212	
3	C	219	

2 Entry composition

There are 4 unique types of molecules in this entry. The entry contains 4181 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 prion protein.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	102	Total	C	N	O	S	0	0	0
			855	532	150	166	7			

- Molecule 2 is a protein called VRQ14 Fab Heavy chain.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B	212	Total	C	N	O	S	0	0	0
			1607	1023	256	322	6			

- Molecule 3 is a protein called VRQ14 Fab light chain.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	C	219	Total	C	N	O	S	0	0	0
			1697	1059	288	343	7			

- Molecule 4 is water.

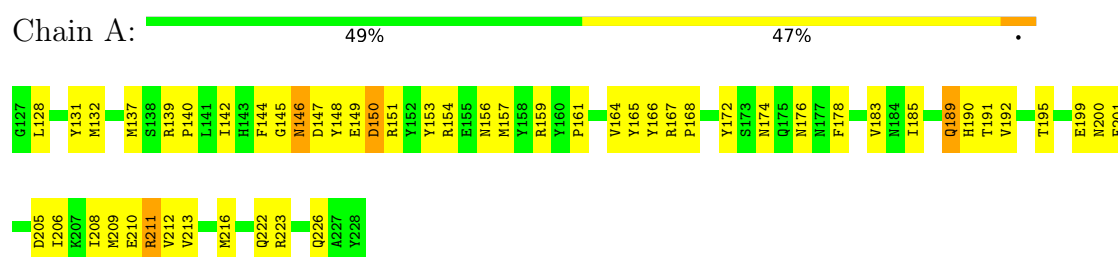
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	2	Total	O	0	0
			2	2		
4	B	7	Total	O	0	0
			7	7		
4	C	13	Total	O	0	0
			13	13		

3 Residue-property plots

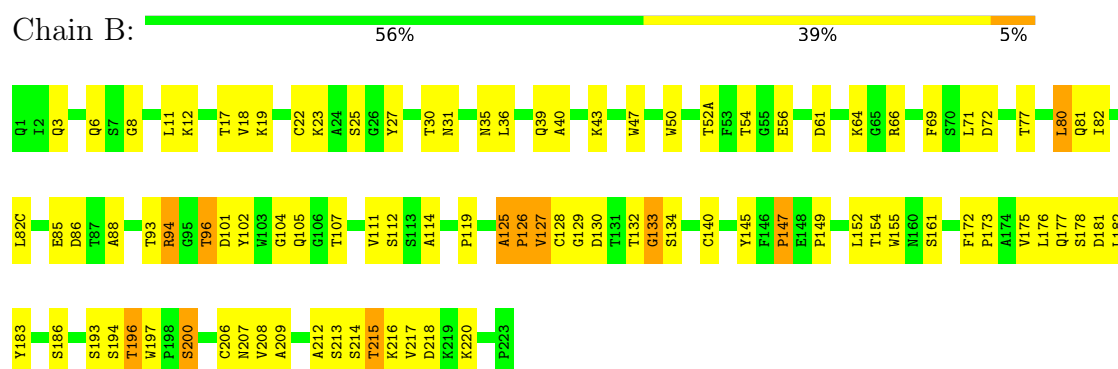
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry. Residues are color-coded 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. 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.

Note EDS was not executed.

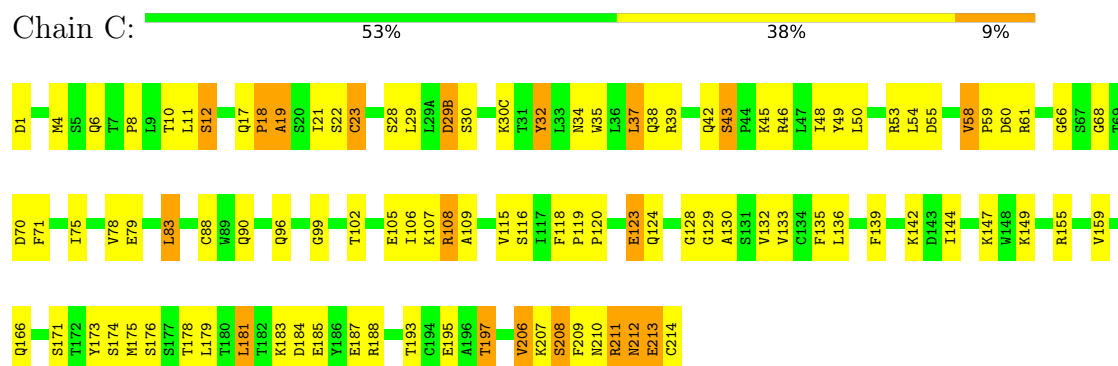
• Molecule 1: prion protein



• Molecule 2: VRQ14 Fab Heavy chain



• Molecule 3: VRQ14 Fab light chain



4 Data and refinement statistics

Xtriage (Phenix) and EDS were not executed - this section is therefore incomplete.

Property	Value	Source
Space group	P 21 21 2	Depositor
Cell constants a, b, c, α , β , γ	91.66 Å 145.45 Å 43.60 Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	14.95 – 2.80	Depositor
% Data completeness (in resolution range)	99.4 (14.95-2.80)	Depositor
R_{merge}	0.09	Depositor
R_{sym}	(Not available)	Depositor
Refinement program	CNS 1.1	Depositor
R, R_{free}	0.222 , 0.288	Depositor
Estimated twinning fraction	No twinning to report.	Xtriage
Total number of atoms	4181	wwPDB-VP
Average B, all atoms (Å ²)	45.0	wwPDB-VP

5 Model quality

5.1 Standard geometry

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	0.45	0/874	0.91	2/1180 (0.2%)
2	B	0.45	0/1650	1.01	7/2254 (0.3%)
3	C	0.46	0/1734	0.96	7/2351 (0.3%)
All	All	0.45	0/4258	0.97	16/5785 (0.3%)

There are no bond length outliers.

All (16) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	8	GLY	CA-C-N	11.23	131.35	119.78
2	B	8	GLY	C-N-CA	11.23	131.35	119.78
3	C	58	VAL	CA-C-N	7.25	127.01	119.76
3	C	58	VAL	C-N-CA	7.25	127.01	119.76
2	B	94	ARG	N-CA-C	-6.84	98.09	108.96
1	A	164	VAL	N-CA-C	6.42	119.32	108.86
2	B	72	ASP	N-CA-C	-6.30	97.38	110.80
3	C	206	VAL	N-CA-C	6.18	118.04	109.45
2	B	125	ALA	CA-C-N	5.67	126.93	119.84
2	B	125	ALA	C-N-CA	5.67	126.93	119.84
3	C	99	GLY	N-CA-C	-5.57	104.16	113.02
2	B	132	THR	N-CA-C	-5.52	106.22	113.17
3	C	213	GLU	N-CA-C	-5.42	104.75	111.90
3	C	43	SER	N-CA-C	-5.24	102.91	110.40
1	A	150	ASP	N-CA-C	-5.22	105.27	111.69
3	C	32	TYR	N-CA-C	5.13	117.55	109.39

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts ⓘ

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	855	0	800	58	0
2	B	1607	0	1562	82	0
3	C	1697	0	1647	93	0
4	A	2	0	0	0	0
4	B	7	0	0	0	0
4	C	13	0	0	0	0
All	All	4181	0	4009	221	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 27.

All (221) 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:199:GLU:HG3	1:A:200:ASN:H	1.12	1.12
2:B:96:THR:HG22	3:C:46:ARG:HH11	1.12	1.06
2:B:119:PRO:HB3	2:B:145:TYR:HB3	1.39	1.04
2:B:161:SER:H	2:B:207:ASN:ND2	1.55	1.04
3:C:211:ARG:HH11	3:C:211:ARG:HB3	1.20	1.03
2:B:161:SER:H	2:B:207:ASN:HD21	0.96	0.93
3:C:211:ARG:HB3	3:C:211:ARG:NH1	1.89	0.88
1:A:146:ASN:HD21	1:A:149:GLU:HB3	1.41	0.84
3:C:184:ASP:HB3	3:C:188:ARG:NH1	1.93	0.83
2:B:161:SER:N	2:B:207:ASN:HD21	1.76	0.82
2:B:6:GLN:HE21	2:B:104:GLY:HA3	1.43	0.81
1:A:174:ASN:HD22	1:A:176:ASN:H	1.24	0.81
3:C:211:ARG:HH11	3:C:211:ARG:CB	1.92	0.81
2:B:96:THR:HG22	3:C:46:ARG:NH1	1.95	0.79
1:A:199:GLU:HG3	1:A:200:ASN:N	1.92	0.79
1:A:174:ASN:ND2	1:A:176:ASN:HB2	1.99	0.78
1:A:174:ASN:HD21	1:A:176:ASN:HB2	1.47	0.77
3:C:193:THR:HA	3:C:208:SER:HB3	1.66	0.76
1:A:199:GLU:HG2	1:A:201:PHE:CE2	2.22	0.75
2:B:161:SER:N	2:B:207:ASN:ND2	2.34	0.74
2:B:12:LYS:HG3	2:B:18:VAL:CG1	2.17	0.74

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:183:VAL:HG22	1:A:213:VAL:HG12	1.71	0.73
1:A:199:GLU:HG2	1:A:201:PHE:CZ	2.23	0.73
2:B:119:PRO:CB	2:B:145:TYR:HB3	2.18	0.72
2:B:209:ALA:HB2	2:B:216:LYS:HG3	1.74	0.69
2:B:119:PRO:HB3	2:B:145:TYR:CB	2.19	0.69
2:B:40:ALA:HB3	2:B:43:LYS:HD2	1.74	0.68
2:B:66:ARG:NH2	2:B:86:ASP:OD1	2.27	0.68
2:B:11:LEU:HD13	2:B:147:PRO:HG3	1.75	0.66
3:C:211:ARG:C	3:C:213:GLU:H	2.03	0.66
3:C:184:ASP:HB3	3:C:188:ARG:HH12	1.59	0.66
2:B:102:TYR:CZ	3:C:45:LYS:HE2	2.30	0.66
3:C:83:LEU:C	3:C:83:LEU:HD12	2.20	0.66
1:A:131:TYR:CE2	1:A:185:ILE:HG12	2.33	0.63
2:B:17:THR:HG22	2:B:18:VAL:N	2.13	0.63
1:A:208:ILE:O	1:A:212:VAL:HG23	1.97	0.63
2:B:105:GLN:OE1	2:B:105:GLN:N	2.32	0.63
3:C:28:SER:HA	3:C:68:GLY:O	1.99	0.63
1:A:167:ARG:HB2	1:A:172:TYR:CE2	2.34	0.62
3:C:210:ASN:HB2	3:C:214:CYS:OXT	1.99	0.62
3:C:108:ARG:HD3	3:C:109:ALA:O	2.00	0.61
2:B:18:VAL:HG13	2:B:82(C):LEU:HD11	1.83	0.61
1:A:151:ARG:HA	1:A:154:ARG:NH1	2.15	0.61
1:A:167:ARG:HB2	1:A:172:TYR:HE2	1.66	0.60
1:A:206:ILE:O	1:A:210:GLU:HG2	2.02	0.60
1:A:128:LEU:HD11	1:A:189:GLN:NE2	2.17	0.60
3:C:18:PRO:O	3:C:19:ALA:HB2	2.02	0.59
2:B:36:LEU:HD22	2:B:69:PHE:CE1	2.37	0.59
1:A:165:TYR:HB2	1:A:185:ILE:HG22	1.85	0.59
1:A:146:ASN:N	1:A:146:ASN:HD22	2.01	0.59
3:C:6:GLN:HE21	3:C:21:ILE:HG21	1.66	0.58
3:C:133:VAL:HG22	3:C:178:THR:HG23	1.86	0.58
2:B:11:LEU:HD22	2:B:147:PRO:HD3	1.86	0.58
2:B:61:ASP:HA	2:B:64:LYS:HE3	1.86	0.58
2:B:196:THR:C	2:B:200:SER:HB3	2.29	0.57
1:A:144:PHE:O	1:A:146:ASN:ND2	2.38	0.57
1:A:146:ASN:ND2	1:A:149:GLU:HB3	2.15	0.57
1:A:174:ASN:HD22	1:A:176:ASN:N	1.98	0.56
1:A:222:GLN:O	1:A:226:GLN:HB2	2.05	0.56
2:B:35:ASN:C	2:B:36:LEU:HD12	2.30	0.55
2:B:206:CYS:O	2:B:218:ASP:HA	2.05	0.55
3:C:181:LEU:N	3:C:181:LEU:HD23	2.22	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:C:124:GLN:HG2	3:C:129:GLY:O	2.07	0.55
2:B:69:PHE:HE1	2:B:80:LEU:HD13	1.72	0.55
1:A:191:THR:O	1:A:195:THR:HG23	2.06	0.55
3:C:105:GLU:HG3	3:C:166:GLN:NE2	2.21	0.55
1:A:147:ASP:O	1:A:151:ARG:HB2	2.07	0.55
2:B:52(A):THR:HA	2:B:71:LEU:HD11	1.89	0.54
2:B:66:ARG:HH22	2:B:86:ASP:CG	2.15	0.54
2:B:152:LEU:HD23	2:B:152:LEU:C	2.33	0.54
1:A:151:ARG:HA	1:A:154:ARG:CZ	2.38	0.54
2:B:177:GLN:O	2:B:178:SER:C	2.49	0.54
3:C:10:THR:HG22	3:C:11:LEU:N	2.23	0.53
3:C:6:GLN:HA	3:C:22:SER:O	2.08	0.53
3:C:206:VAL:HG12	3:C:207:LYS:N	2.23	0.53
1:A:161:PRO:HG3	1:A:190:HIS:CG	2.43	0.53
2:B:47:TRP:CE2	3:C:96:GLN:HG3	2.44	0.53
3:C:181:LEU:HD23	3:C:181:LEU:H	1.71	0.53
2:B:17:THR:HG23	2:B:82:ILE:O	2.09	0.53
3:C:211:ARG:C	3:C:213:GLU:N	2.67	0.53
1:A:139:ARG:HD2	1:A:157:MET:HE3	1.89	0.52
3:C:108:ARG:HD3	3:C:108:ARG:C	2.34	0.52
3:C:128:GLY:HA2	3:C:183:LYS:HB2	1.91	0.52
3:C:135:PHE:C	3:C:136:LEU:HD12	2.34	0.52
1:A:156:ASN:OD1	3:C:53:ARG:NH2	2.43	0.52
3:C:119:PRO:HG3	3:C:209:PHE:CD2	2.45	0.52
1:A:140:PRO:HB2	1:A:142:ILE:CD1	2.40	0.52
3:C:66:GLY:HA3	3:C:70:ASP:O	2.09	0.52
1:A:132:MET:O	1:A:165:TYR:HA	2.10	0.52
3:C:39:ARG:HB2	3:C:42:GLN:HG3	1.92	0.51
3:C:211:ARG:O	3:C:213:GLU:N	2.43	0.51
1:A:148:TYR:O	1:A:151:ARG:N	2.44	0.51
1:A:174:ASN:ND2	1:A:176:ASN:H	2.00	0.51
2:B:140:CYS:HB2	2:B:155:TRP:CH2	2.46	0.51
3:C:8:PRO:O	3:C:102:THR:HG23	2.11	0.51
3:C:139:PHE:CE1	3:C:174:SER:HA	2.45	0.50
3:C:193:THR:CA	3:C:208:SER:HB3	2.39	0.50
2:B:181:ASP:O	2:B:182:LEU:HD23	2.11	0.50
3:C:105:GLU:HG3	3:C:166:GLN:HE22	1.76	0.50
2:B:69:PHE:CE1	2:B:80:LEU:HD13	2.46	0.49
3:C:136:LEU:HD12	3:C:136:LEU:N	2.28	0.49
1:A:174:ASN:ND2	1:A:176:ASN:N	2.60	0.49
3:C:130:ALA:O	3:C:181:LEU:HD23	2.11	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:C:108:ARG:HG2	3:C:171:SER:HB2	1.95	0.49
1:A:205:ASP:O	1:A:209:MET:HG3	2.13	0.49
2:B:36:LEU:HD12	2:B:36:LEU:N	2.27	0.49
3:C:29:LEU:HD12	3:C:71:PHE:CE1	2.48	0.49
2:B:54:THR:HG22	2:B:56:GLU:H	1.77	0.49
2:B:154:THR:OG1	2:B:207:ASN:HB2	2.14	0.48
1:A:128:LEU:O	1:A:131:TYR:HB2	2.13	0.48
2:B:39:GLN:O	2:B:88:ALA:HB1	2.13	0.48
1:A:140:PRO:HB2	1:A:142:ILE:HD11	1.95	0.48
1:A:137:MET:HE2	1:A:223:ARG:NH1	2.29	0.48
2:B:85:GLU:OE2	2:B:85:GLU:HA	2.13	0.48
2:B:194:SER:C	2:B:197:TRP:H	2.22	0.48
3:C:209:PHE:C	3:C:209:PHE:CD1	2.91	0.48
2:B:12:LYS:HG3	2:B:18:VAL:HG13	1.92	0.48
1:A:144:PHE:O	1:A:146:ASN:N	2.46	0.48
1:A:172:TYR:CE1	1:A:178:PHE:HA	2.49	0.48
2:B:61:ASP:O	2:B:64:LYS:HG2	2.14	0.48
3:C:78:VAL:CG1	3:C:79:GLU:N	2.77	0.48
2:B:36:LEU:HD23	2:B:80:LEU:HD22	1.96	0.47
2:B:147:PRO:HD2	2:B:212:ALA:CB	2.44	0.47
2:B:96:THR:HG23	2:B:96:THR:O	2.13	0.47
2:B:197:TRP:HA	2:B:200:SER:N	2.30	0.47
3:C:4:MET:HE2	3:C:88:CYS:SG	2.55	0.47
3:C:12:SER:HB3	3:C:107:LYS:NZ	2.30	0.47
1:A:139:ARG:NH1	1:A:139:ARG:HG3	2.30	0.47
1:A:167:ARG:O	1:A:168:PRO:C	2.56	0.47
2:B:17:THR:CG2	2:B:18:VAL:N	2.78	0.47
3:C:181:LEU:N	3:C:181:LEU:CD2	2.78	0.47
3:C:49:TYR:OH	3:C:53:ARG:HD3	2.15	0.46
3:C:136:LEU:HD23	3:C:144:ILE:HD11	1.98	0.46
2:B:133:GLY:O	2:B:134:SER:HB3	2.15	0.46
3:C:147:LYS:HD2	3:C:149:LYS:HE3	1.97	0.46
2:B:96:THR:HG21	3:C:34:ASN:CG	2.40	0.46
3:C:23:CYS:HB2	3:C:35:TRP:CH2	2.51	0.46
1:A:139:ARG:HG3	1:A:139:ARG:HH11	1.80	0.46
2:B:96:THR:HG23	3:C:46:ARG:HD3	1.97	0.46
3:C:78:VAL:CG1	3:C:106:ILE:HD12	2.46	0.46
3:C:12:SER:HB3	3:C:107:LYS:HZ3	1.79	0.46
3:C:48:ILE:HG12	3:C:54:LEU:HD23	1.96	0.46
2:B:152:LEU:HA	2:B:207:ASN:O	2.16	0.46
1:A:142:ILE:HG23	1:A:211:ARG:HH21	1.81	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:161:PRO:HG3	1:A:190:HIS:ND1	2.31	0.45
2:B:22:CYS:O	2:B:77:THR:HG23	2.17	0.45
2:B:213:SER:OG	2:B:215:THR:HB	2.16	0.45
2:B:17:THR:HG22	2:B:18:VAL:H	1.80	0.45
3:C:50:LEU:HD23	3:C:50:LEU:HA	1.82	0.45
3:C:83:LEU:HB3	3:C:106:ILE:HG12	1.99	0.45
3:C:123:GLU:CD	3:C:123:GLU:H	2.25	0.45
2:B:19:LYS:HG3	2:B:81:GLN:HB2	1.99	0.45
2:B:35:ASN:OD1	2:B:50:TRP:HB3	2.17	0.45
3:C:10:THR:CG2	3:C:11:LEU:N	2.80	0.45
3:C:18:PRO:HA	3:C:75:ILE:O	2.17	0.45
3:C:206:VAL:CG1	3:C:207:LYS:N	2.79	0.45
1:A:199:GLU:CG	1:A:200:ASN:H	1.99	0.45
1:A:172:TYR:CD1	1:A:178:PHE:HA	2.52	0.44
3:C:55:ASP:O	3:C:58:VAL:HG23	2.17	0.44
3:C:59:PRO:C	3:C:61:ARG:N	2.71	0.44
1:A:159:ARG:HA	3:C:30(C):LYS:HE3	1.99	0.44
2:B:12:LYS:HG3	2:B:18:VAL:HG12	1.98	0.44
2:B:175:VAL:O	2:B:183:TYR:HA	2.17	0.44
3:C:149:LYS:HD2	3:C:195:GLU:OE1	2.18	0.44
3:C:193:THR:CG2	3:C:206:VAL:HG13	2.48	0.44
2:B:40:ALA:HA	2:B:88:ALA:HB2	1.99	0.44
2:B:194:SER:O	2:B:197:TRP:N	2.51	0.44
3:C:37:LEU:HD23	3:C:38:GLN:N	2.33	0.44
3:C:212:ASN:C	3:C:214:CYS:N	2.74	0.43
1:A:192:VAL:HG12	2:B:31:ASN:C	2.43	0.43
1:A:209:MET:O	1:A:210:GLU:C	2.61	0.43
2:B:12:LYS:O	2:B:111:VAL:HA	2.18	0.43
2:B:213:SER:C	2:B:215:THR:N	2.76	0.43
1:A:185:ILE:O	1:A:189:GLN:HB2	2.18	0.43
3:C:18:PRO:O	3:C:19:ALA:CB	2.66	0.43
3:C:90:GLN:O	3:C:96:GLN:HB3	2.19	0.43
3:C:142:LYS:HB3	3:C:173:TYR:CE2	2.54	0.43
1:A:213:VAL:HA	1:A:216:MET:CE	2.49	0.43
3:C:116:SER:HG	3:C:118:PHE:HE1	1.66	0.43
3:C:212:ASN:O	3:C:213:GLU:C	2.61	0.43
3:C:120:PRO:HD3	3:C:132:VAL:HG22	2.01	0.43
3:C:175:MET:HG2	3:C:176:SER:N	2.34	0.43
3:C:115:VAL:HG22	3:C:136:LEU:HG	2.00	0.42
3:C:159:VAL:HG22	3:C:179:LEU:HD13	2.00	0.42
2:B:127:VAL:HG13	2:B:128:CYS:N	2.35	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:152:LEU:HD12	2:B:208:VAL:HG22	2.01	0.42
3:C:197:THR:O	3:C:197:THR:HG22	2.19	0.42
2:B:128:CYS:O	2:B:129:GLY:C	2.63	0.42
3:C:34:ASN:O	3:C:88:CYS:HA	2.19	0.42
3:C:35:TRP:CZ3	3:C:88:CYS:HB3	2.53	0.42
2:B:101:ASP:HB3	3:C:46:ARG:CZ	2.50	0.42
2:B:215:THR:CG2	2:B:216:LYS:N	2.83	0.42
1:A:132:MET:HB3	1:A:166:TYR:CE2	2.54	0.42
2:B:134:SER:O	2:B:193:SER:HB2	2.20	0.41
1:A:131:TYR:HA	1:A:166:TYR:O	2.19	0.41
2:B:126:PRO:O	2:B:127:VAL:HB	2.20	0.41
3:C:155:ARG:HH22	3:C:185:GLU:CD	2.29	0.41
3:C:187:GLU:HA	3:C:211:ARG:NE	2.35	0.41
1:A:153:TYR:O	1:A:157:MET:HG2	2.20	0.41
2:B:47:TRP:CD2	3:C:96:GLN:HG3	2.55	0.41
2:B:197:TRP:CA	2:B:200:SER:H	2.33	0.41
2:B:30:THR:HG22	2:B:52(A):THR:O	2.21	0.41
2:B:213:SER:O	2:B:214:SER:C	2.61	0.41
3:C:30(C):LYS:HB2	3:C:32:TYR:CE1	2.56	0.41
1:A:167:ARG:HB2	1:A:172:TYR:OH	2.21	0.41
2:B:27:TYR:CE1	2:B:94:ARG:HD3	2.56	0.41
3:C:59:PRO:O	3:C:61:ARG:N	2.54	0.41
3:C:184:ASP:O	3:C:188:ARG:HD3	2.21	0.41
1:A:142:ILE:HG23	1:A:211:ARG:NH2	2.36	0.41
1:A:159:ARG:HA	3:C:30(C):LYS:CE	2.51	0.41
1:A:139:ARG:HD2	1:A:157:MET:HB2	2.03	0.41
2:B:3:GLN:HG3	2:B:25:SER:OG	2.21	0.41
2:B:93:THR:HA	2:B:102:TYR:O	2.20	0.41
2:B:172:PHE:HA	2:B:173:PRO:HD3	1.88	0.41
3:C:17:GLN:HB3	3:C:18:PRO:HD2	2.02	0.40
2:B:112:SER:C	2:B:114:ALA:H	2.29	0.40
2:B:125:ALA:HA	2:B:126:PRO:HD3	1.89	0.40
2:B:11:LEU:HD22	2:B:147:PRO:CD	2.49	0.40
3:C:29(B):ASP:CG	3:C:30:SER:N	2.79	0.40
3:C:60:ASP:O	3:C:61:ARG:C	2.64	0.40
3:C:119:PRO:O	3:C:120:PRO:C	2.65	0.40

There are no symmetry-related clashes.

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	100/102 (98%)	87 (87%)	12 (12%)	1 (1%)	12	38
2	B	210/212 (99%)	179 (85%)	26 (12%)	5 (2%)	4	17
3	C	217/219 (99%)	193 (89%)	20 (9%)	4 (2%)	6	23
All	All	527/533 (99%)	459 (87%)	58 (11%)	10 (2%)	6	22

All (10) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	145	GLY
2	B	126	PRO
2	B	127	VAL
2	B	196	THR
3	C	19	ALA
3	C	212	ASN
2	B	200	SER
3	C	18	PRO
3	C	29(B)	ASP
2	B	133	GLY

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	94/94 (100%)	90 (96%)	4 (4%)	26	60
2	B	182/182 (100%)	170 (93%)	12 (7%)	15	43

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
3	C	196/196 (100%)	184 (94%)	12 (6%)	17	46
All	All	472/472 (100%)	444 (94%)	28 (6%)	18	48

All (28) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	146	ASN
1	A	150	ASP
1	A	189	GLN
1	A	211	ARG
2	B	23	LYS
2	B	80	LEU
2	B	96	THR
2	B	107	THR
2	B	130	ASP
2	B	147	PRO
2	B	149	PRO
2	B	176	LEU
2	B	186	SER
2	B	215	THR
2	B	217	VAL
2	B	220	LYS
3	C	1	ASP
3	C	12	SER
3	C	23	CYS
3	C	37	LEU
3	C	43	SER
3	C	83	LEU
3	C	108	ARG
3	C	123	GLU
3	C	181	LEU
3	C	197	THR
3	C	208	SER
3	C	211	ARG

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (22) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	146	ASN
1	A	163	GLN
1	A	174	ASN

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Mol	Chain	Res	Type
1	A	177	ASN
1	A	200	ASN
1	A	220	GLN
1	A	222	GLN
2	B	3	GLN
2	B	6	GLN
2	B	31	ASN
2	B	39	GLN
2	B	81	GLN
2	B	84	ASN
2	B	170	HIS
2	B	207	ASN
3	C	6	GLN
3	C	17	GLN
3	C	27	GLN
3	C	96	GLN
3	C	124	GLN
3	C	156	GLN
3	C	157	ASN

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 ⓘ

There are no ligands in this entry.

5.7 Other polymers ⓘ

There are no such residues in this entry.

5.8 Polymer linkage issues ⓘ

There are no chain breaks in this entry.

6 Fit of model and data

6.1 Protein, DNA and RNA chains

EDS was not executed - this section is therefore empty.

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

EDS was not executed - this section is therefore empty.

6.3 Carbohydrates

EDS was not executed - this section is therefore empty.

6.4 Ligands

EDS was not executed - this section is therefore empty.

6.5 Other polymers

EDS was not executed - this section is therefore empty.