



Full wwPDB X-ray Structure Validation Report ⓘ

Feb 20, 2018 – 01:45 am GMT

PDB ID : 1TQB
Title : Ovine recombinant PrP(114-234), VRQ variant in complex with the Fab of the VRQ14 antibody
Authors : Eghiaian, F.; Grosclaude, J.; Debey, P.; Doublet, B.; Treguer, E.; Rezaei, H.; Knossow, M.
Deposited on : 2004-06-17
Resolution : 2.55 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 following versions of software and data (see [references ⓘ](#)) were used in the production of this report:

MolProbity : 4.02b-467
Xtriage (Phenix) : **NOT EXECUTED**
EDS : **NOT EXECUTED**
Percentile statistics : 20171227.v01 (using entries in the PDB archive December 27th 2017)
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : trunk30686

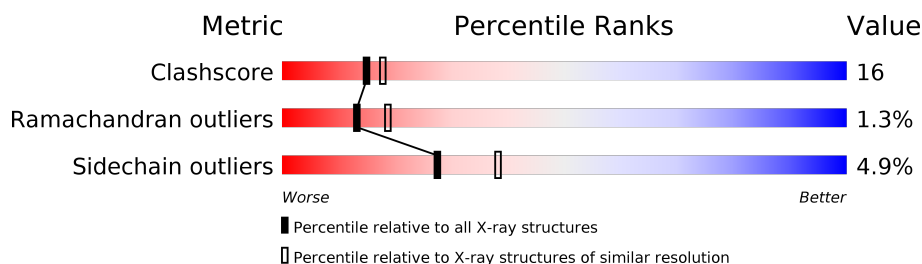
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.55 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	122078	1097 (2.56-2.52)
Ramachandran outliers	120005	1087 (2.56-2.52)
Sidechain outliers	119972	1087 (2.56-2.52)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments on the lower bar indicate the fraction of residues that contain outliers for ≥ 3 , 2, 1 and 0 types of geometric quality criteria. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions $\leq 5\%$. The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density. The numeric value is given above the bar.

Note EDS was not executed.

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

2 Entry composition [i](#)

There are 4 unique types of molecules in this entry. The entry contains 4216 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	533	148	167	7			

There are 2 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	136	VAL	ALA	SEE REMARK 999	UNP P23907
A	171	GLN	ARG	SEE REMARK 999	UNP P23907

- 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	13	Total	O	0	0
			13	13		
4	B	19	Total	O	0	0
			19	19		
4	C	25	Total	O	0	0
			25	25		

3 Residue-property plots

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

Note EDS was not executed.

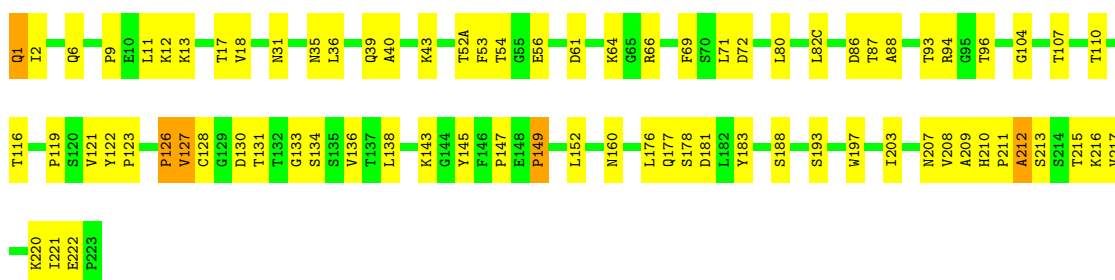
- Molecule 1: prion protein

Chain A: 



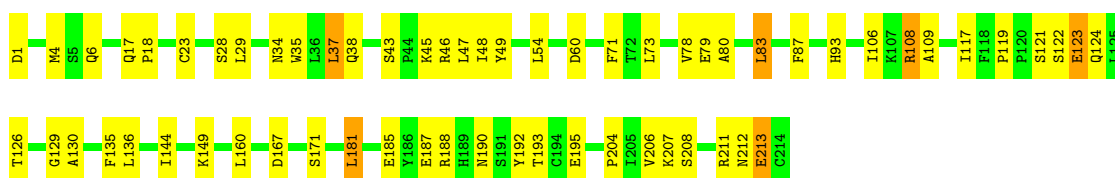
- Molecule 2: VRQ14 Fab Heavy chain

Chain B: 



- Molecule 3: VRQ14 Fab light chain

Chain C: 



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	92.05Å 145.68Å 43.20Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	14.99 – 2.55	Depositor
% Data completeness (in resolution range)	99.8 (14.99-2.55)	Depositor
R_{merge}	0.05	Depositor
R_{sym}	(Not available)	Depositor
Refinement program	CNS 1.1	Depositor
R, R_{free}	0.214 , 0.268	Depositor
Estimated twinning fraction	No twinning to report.	Xtriage
Total number of atoms	4216	wwPDB-VP
Average B, all atoms (Å ²)	44.0	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	0.38	0/874	0.59	0/1181
2	B	0.39	0/1650	0.65	1/2254 (0.0%)
3	C	0.37	0/1734	0.63	0/2351
All	All	0.38	0/4258	0.63	1/5786 (0.0%)

There are no bond length outliers.

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	72	ASP	N-CA-C	-5.02	97.44	111.00

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	799	37	0
2	B	1607	0	1562	62	0
3	C	1697	0	1647	48	0
4	A	13	0	0	0	0
4	B	19	0	0	0	0
4	C	25	0	0	1	0
All	All	4216	0	4008	132	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 16.

All (132) 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:B:96:THR:HG22	3:C:46:ARG:HD3	1.38	1.02
2:B:11:LEU:HD13	2:B:147:PRO:HG3	1.59	0.84
3:C:181:LEU:HD12	3:C:185:GLU:HG2	1.62	0.82
2:B:12:LYS:HE3	2:B:18:VAL:HG12	1.62	0.81
1:A:139:ARG:HG3	1:A:139:ARG:HH11	1.48	0.78
2:B:12:LYS:HG3	2:B:18:VAL:CG1	2.16	0.76
2:B:6:GLN:HE21	2:B:104:GLY:HA3	1.50	0.75
1:A:150:ASP:O	1:A:154:ARG:HD3	1.86	0.74
3:C:211:ARG:HB3	3:C:211:ARG:HH11	1.54	0.73
1:A:146:ASN:N	1:A:146:ASN:HD22	1.86	0.71
2:B:36:LEU:HD23	2:B:80:LEU:HD22	1.71	0.71
3:C:195:GLU:HG2	3:C:206:VAL:HG22	1.72	0.71
3:C:83:LEU:HB3	3:C:106:ILE:HG12	1.72	0.71
2:B:131:THR:HG23	2:B:134:SER:HA	1.72	0.71
2:B:54:THR:HG22	2:B:56:GLU:H	1.59	0.67
3:C:28:SER:O	3:C:93:HIS:HE1	1.81	0.64
3:C:108:ARG:HD3	3:C:109:ALA:O	1.98	0.63
2:B:127:VAL:HG11	3:C:119:PRO:HD3	1.81	0.63
1:A:139:ARG:HB2	1:A:157:MET:HE3	1.81	0.62
1:A:188:LYS:O	1:A:192:VAL:HG13	2.00	0.62
2:B:126:PRO:HD3	2:B:138:LEU:HD22	1.82	0.61
1:A:199:GLU:HG2	1:A:201:PHE:CZ	2.34	0.61
3:C:130:ALA:O	3:C:181:LEU:HD23	2.01	0.60
1:A:139:ARG:HG3	1:A:139:ARG:NH1	2.17	0.60
3:C:48:ILE:HG12	3:C:54:LEU:HD23	1.84	0.60
2:B:87:THR:HG23	2:B:110:THR:HA	1.84	0.59
2:B:52(A):THR:HA	2:B:71:LEU:HD11	1.84	0.59
2:B:40:ALA:HB3	2:B:43:LYS:HE2	1.85	0.59
3:C:192:TYR:O	3:C:208:SER:HB2	2.04	0.58
2:B:96:THR:HG21	3:C:34:ASN:CG	2.24	0.58
1:A:146:ASN:ND2	1:A:146:ASN:H	2.00	0.57
1:A:155:GLU:C	1:A:156:ASN:HD22	2.07	0.57
1:A:174:ASN:ND2	1:A:177:ASN:H	2.01	0.57
2:B:17:THR:HG22	2:B:18:VAL:N	2.19	0.57
2:B:119:PRO:HG3	2:B:145:TYR:CB	2.35	0.57
1:A:146:ASN:N	1:A:146:ASN:ND2	2.51	0.56
1:A:146:ASN:H	1:A:146:ASN:HD22	1.53	0.56
1:A:146:ASN:O	1:A:148:TYR:N	2.36	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:147:PRO:HD2	2:B:212:ALA:CB	2.37	0.55
2:B:96:THR:HG22	3:C:46:ARG:CD	2.25	0.55
2:B:116:THR:OG1	2:B:213:SER:HB3	2.07	0.54
2:B:176:LEU:HG	2:B:183:TYR:CE1	2.42	0.54
2:B:61:ASP:O	2:B:64:LYS:HG2	2.07	0.54
2:B:9:PRO:HB3	2:B:149:PRO:HD2	1.90	0.54
2:B:119:PRO:HG3	2:B:145:TYR:HB3	1.89	0.54
3:C:136:LEU:HD23	3:C:144:ILE:HD11	1.89	0.54
2:B:220:LYS:NZ	2:B:222:GLU:HG2	2.22	0.54
1:A:202:THR:O	1:A:206:ILE:HG12	2.09	0.53
1:A:199:GLU:HG3	1:A:200:ASN:N	2.23	0.53
1:A:174:ASN:HD22	1:A:176:ASN:N	2.07	0.52
2:B:96:THR:CG2	3:C:46:ARG:HD3	2.26	0.52
3:C:190:ASN:HD21	3:C:212:ASN:H	1.57	0.52
2:B:152:LEU:HD23	2:B:152:LEU:C	2.30	0.52
1:A:199:GLU:HG2	1:A:201:PHE:CE2	2.45	0.52
1:A:188:LYS:HD3	2:B:53:PHE:CD2	2.45	0.51
3:C:124:GLN:HG2	3:C:129:GLY:O	2.10	0.51
1:A:139:ARG:CZ	1:A:162:ASN:HB3	2.41	0.50
2:B:18:VAL:HG13	2:B:82(C):LEU:HD11	1.92	0.50
1:A:188:LYS:NZ	2:B:31:ASN:ND2	2.59	0.50
3:C:83:LEU:C	3:C:83:LEU:HD12	2.32	0.50
1:A:142:ILE:HD13	1:A:211:ARG:HG2	1.94	0.50
2:B:119:PRO:CB	2:B:145:TYR:HB3	2.43	0.49
1:A:144:PHE:CB	1:A:146:ASN:HD21	2.25	0.49
3:C:6:GLN:OE1	3:C:87:PHE:HA	2.12	0.49
1:A:174:ASN:HD21	1:A:177:ASN:H	1.61	0.49
3:C:78:VAL:CG1	3:C:79:GLU:N	2.76	0.49
1:A:144:PHE:HB3	1:A:146:ASN:HD21	1.78	0.48
3:C:35:TRP:CE2	3:C:73:LEU:HB2	2.48	0.48
2:B:87:THR:O	2:B:88:ALA:HB2	2.14	0.48
2:B:12:LYS:HG3	2:B:18:VAL:HG13	1.95	0.48
3:C:167:ASP:O	3:C:171:SER:HA	2.14	0.47
2:B:209:ALA:HB2	2:B:216:LYS:HG3	1.96	0.47
2:B:138:LEU:HD13	2:B:221:ILE:HG21	1.96	0.47
2:B:40:ALA:CB	2:B:43:LYS:HE2	2.45	0.47
2:B:39:GLN:O	2:B:88:ALA:HB1	2.14	0.47
2:B:35:ASN:HB2	2:B:93:THR:OG1	2.15	0.47
2:B:121:VAL:HG21	2:B:217:VAL:CG2	2.45	0.46
2:B:36:LEU:HD22	2:B:69:PHE:CE1	2.49	0.46
3:C:187:GLU:HA	3:C:211:ARG:NE	2.30	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:C:17:GLN:HB3	3:C:18:PRO:HD2	1.98	0.46
2:B:188:SER:HB3	3:C:135:PHE:CE2	2.51	0.46
3:C:123:GLU:HG2	3:C:123:GLU:H	1.33	0.46
3:C:211:ARG:HB3	3:C:211:ARG:NH1	2.24	0.46
3:C:206:VAL:HG12	3:C:207:LYS:N	2.30	0.46
2:B:128:CYS:SG	3:C:117:ILE:HG22	2.56	0.45
2:B:40:ALA:HB3	2:B:43:LYS:HB2	1.98	0.45
3:C:37:LEU:HD22	3:C:38:GLN:N	2.31	0.45
2:B:96:THR:HG21	3:C:34:ASN:OD1	2.16	0.45
2:B:220:LYS:HZ3	2:B:222:GLU:HG2	1.80	0.45
1:A:220:GLN:O	1:A:224:GLU:HG2	2.16	0.45
3:C:211:ARG:C	3:C:213:GLU:H	2.20	0.44
1:A:212:VAL:HG12	1:A:216:MET:HE2	1.98	0.44
2:B:66:ARG:NH2	2:B:86:ASP:OD1	2.50	0.44
1:A:139:ARG:NH2	1:A:162:ASN:HB3	2.33	0.44
1:A:212:VAL:HG12	1:A:216:MET:CE	2.47	0.44
2:B:152:LEU:HA	2:B:207:ASN:O	2.18	0.44
2:B:193:SER:O	2:B:197:TRP:O	2.35	0.43
1:A:199:GLU:HG3	1:A:200:ASN:H	1.82	0.43
1:A:142:ILE:HD12	1:A:212:VAL:HG22	2.00	0.43
2:B:208:VAL:HG12	2:B:209:ALA:N	2.33	0.43
2:B:177:GLN:NE2	3:C:160:LEU:HD11	2.33	0.43
2:B:1:GLN:NE2	2:B:1:GLN:N	2.67	0.43
2:B:119:PRO:CG	2:B:145:TYR:HB3	2.49	0.43
3:C:35:TRP:CD2	3:C:73:LEU:HB2	2.54	0.43
1:A:200:ASN:HB3	3:C:49:TYR:CZ	2.54	0.43
2:B:178:SER:OG	2:B:181:ASP:N	2.52	0.43
3:C:181:LEU:HD23	3:C:181:LEU:H	1.84	0.43
2:B:119:PRO:HB3	2:B:145:TYR:HB3	1.99	0.42
3:C:45:LYS:NZ	3:C:47:LEU:HD23	2.34	0.42
2:B:160:ASN:HD21	2:B:203:ILE:HA	1.85	0.42
2:B:17:THR:CG2	2:B:18:VAL:N	2.82	0.42
3:C:122:SER:O	3:C:126:THR:HG23	2.19	0.42
3:C:204:PRO:HG2	4:C:229:HOH:O	2.19	0.42
1:A:139:ARG:HA	1:A:140:PRO:HD3	1.93	0.42
3:C:4:MET:HE3	3:C:23:CYS:SG	2.60	0.42
2:B:2:ILE:HD13	2:B:94:ARG:NH1	2.35	0.42
3:C:78:VAL:CG1	3:C:106:ILE:HD12	2.50	0.42
3:C:149:LYS:HB2	3:C:193:THR:HB	2.02	0.42
2:B:123:PRO:HD2	3:C:123:GLU:HG3	2.00	0.41
3:C:29:LEU:HD12	3:C:71:PHE:CE1	2.55	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:146:ASN:HD21	1:A:149:GLU:HB2	1.86	0.41
1:A:128:LEU:HD11	1:A:189:GLN:CG	2.51	0.41
2:B:121:VAL:HG21	2:B:217:VAL:HG21	2.02	0.41
3:C:78:VAL:HG12	3:C:79:GLU:N	2.35	0.41
1:A:139:ARG:CG	1:A:139:ARG:NH1	2.80	0.41
2:B:96:THR:CG2	2:B:96:THR:O	2.67	0.41
2:B:210:HIS:HB3	2:B:215:THR:HB	2.02	0.40
3:C:206:VAL:CG1	3:C:207:LYS:N	2.83	0.40
1:A:165:TYR:HB2	1:A:185:ILE:HG22	2.04	0.40
2:B:122:TYR:HB3	3:C:121:SER:OG	2.21	0.40
1:A:167:ARG:NH2	1:A:171:GLN:HE22	2.19	0.40
2:B:177:GLN:NE2	3:C:160:LEU:CD1	2.85	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%)	96 (96%)	3 (3%)	1 (1%)	17	26
2	B	210/212 (99%)	185 (88%)	20 (10%)	5 (2%)	6	6
3	C	217/219 (99%)	207 (95%)	9 (4%)	1 (0%)	31	44
All	All	527/533 (99%)	488 (93%)	32 (6%)	7 (1%)	13	19

All (7) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
2	B	127	VAL
3	C	80	ALA
1	A	147	ASP
2	B	212	ALA
2	B	126	PRO

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Mol	Chain	Res	Type
2	B	133	GLY
2	B	211	PRO

5.3.2 Protein sidechains ⓘ

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	95/95 (100%)	89 (94%)	6 (6%)	20	26
2	B	182/182 (100%)	175 (96%)	7 (4%)	36	50
3	C	196/196 (100%)	186 (95%)	10 (5%)	26	36
All	All	473/473 (100%)	450 (95%)	23 (5%)	27	38

All (23) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	132	MET
1	A	146	ASN
1	A	156	ASN
1	A	162	ASN
1	A	174	ASN
1	A	189	GLN
2	B	1	GLN
2	B	13	LYS
2	B	107	THR
2	B	130	ASP
2	B	136	VAL
2	B	143	LYS
2	B	149	PRO
3	C	1	ASP
3	C	37	LEU
3	C	43	SER
3	C	60	ASP
3	C	83	LEU
3	C	108	ARG
3	C	123	GLU

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Mol	Chain	Res	Type
3	C	181	LEU
3	C	188	ARG
3	C	213	GLU

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (15) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	146	ASN
1	A	171	GLN
1	A	174	ASN
1	A	177	ASN
1	A	200	ASN
2	B	1	GLN
2	B	31	ASN
2	B	170	HIS
2	B	177	GLN
2	B	201	GLN
3	C	93	HIS
3	C	157	ASN
3	C	190	ASN
3	C	210	ASN
3	C	212	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 carbohydrates in this entry.

5.6 Ligand geometry ⓘ

There are no ligands in this entry.

5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

6 Fit of model and data

6.1 Protein, DNA and RNA chains

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.