Full wwPDB NMR Structure Validation Report (i)

Nov 1, 2021 – 02:47 PM EDT

PDB ID	:	2KTM
Title	:	Solution NMR structure of H2H3 domain of ovine prion protein (residues 167-234)
Authors	:	Pastore, A.; Adrover, M.; Pauwels, K.; de Chiara, C.; Prigent, S.; Rezeai, H.
Deposited on	:	2010-02-04

This is a Full wwPDB NMR 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/NMRValidationReportHelp
with specific help available everywhere you see the (i) symbol.

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

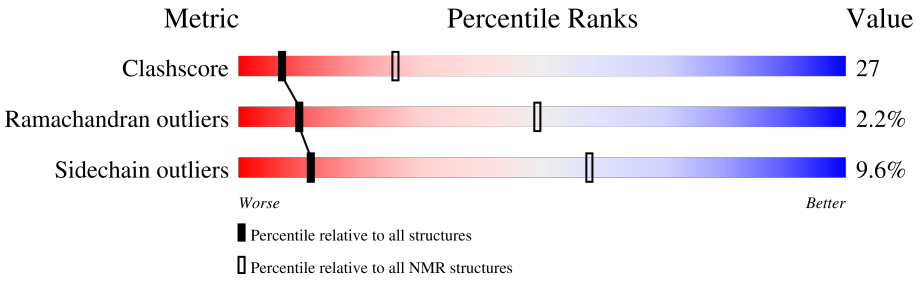
MolProbity	:	4.02b-467
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
RCI	:	v_1n_11_5_13_A (Berjanski et al., 2005)
PANAV	:	Wang et al. (2010)
ShiftChecker	:	2.23.2
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.23.2

1 Overall quality at a glance

The following experimental techniques were used to determine the structure:
SOLUTION NMR

The overall completeness of chemical shifts assignment was not calculated.

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)	NMR archive (#Entries)
Clashscore	158937	12864
Ramachandran outliers	154571	11451
Sidechain outliers	154315	11428

The table below summarises the geometric issues observed across the polymeric chains and their fit to the experimental data. The red, orange, yellow and green segments indicate the fraction of residues that contain outliers for >=3, 2, 1 and 0 types of geometric quality criteria. A cyan segment indicates the fraction of residues that are not part of the well-defined cores, and a grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions <=5%

Mol	Chain	Length	Quality of chain
1	A	89	34% 34% • 8% 24%

2 Ensemble composition and analysis

This entry contains 12 models. Model 3 is the overall representative, medoid model (most similar to other models). The authors have identified model 1 as representative, based on the following criterion: *lowest energy*.

The following residues are included in the computation of the global validation metrics.

Well-defined (core) protein residues			
Well-defined core	**Residue range (total)**	**Backbone RMSD (Å)**	**Medoid model**
1	A:169-A:229 (61)	0.34	3

Ill-defined regions of proteins are excluded from the global statistics.

Ligands and non-protein polymers are included in the analysis.

The models can be grouped into 2 clusters and 1 single-model cluster was found.

Cluster number	Models
1	1, 2, 3, 5, 6, 8, 9, 10, 11
2	4, 12
Single-model clusters	7

3 Entry composition (i)

There is only 1 type of molecule in this entry. The entry contains 1076 atoms, of which 521 are hydrogens and 0 are deuteriums.

- Molecule 1 is a protein called Major prion protein.

Mol	Chain	Residues	Atoms						Trace
			Total	C	H	N	O	S	
1	A	68	1076	337	521	100	114	4	0

There are 22 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	146	MET	-	expression tag	UNP Q072G4
A	147	GLY	-	expression tag	UNP Q072G4
A	148	SER	-	expression tag	UNP Q072G4
A	149	SER	-	expression tag	UNP Q072G4
A	150	HIS	-	expression tag	UNP Q072G4
A	151	HIS	-	expression tag	UNP Q072G4
A	152	HIS	-	expression tag	UNP Q072G4
A	153	HIS	-	expression tag	UNP Q072G4
A	154	HIS	-	expression tag	UNP Q072G4
A	155	HIS	-	expression tag	UNP Q072G4
A	156	SER	-	expression tag	UNP Q072G4
A	157	SER	-	expression tag	UNP Q072G4
A	158	GLY	-	expression tag	UNP Q072G4
A	159	LEU	-	expression tag	UNP Q072G4
A	160	VAL	-	expression tag	UNP Q072G4
A	161	PRO	-	expression tag	UNP Q072G4
A	162	ARG	-	expression tag	UNP Q072G4
A	163	GLY	-	expression tag	UNP Q072G4
A	164	SER	-	expression tag	UNP Q072G4
A	165	HIS	-	expression tag	UNP Q072G4
A	166	MET	-	expression tag	UNP Q072G4
A	208	ALA	ILE	engineered mutation	UNP Q072G4

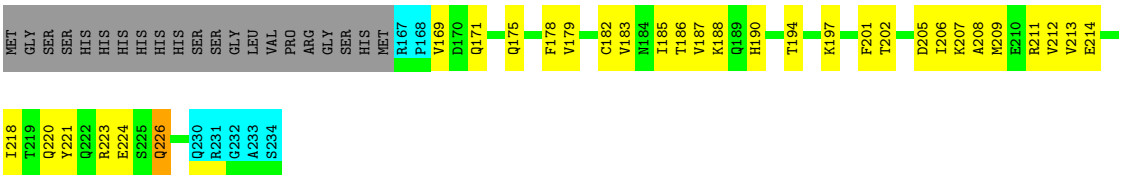
4 Residue-property plots

4.1 Average score per residue in the NMR ensemble

These plots are provided for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic is the same as shown in the summary in section 1 of this report. The second graphic shows the sequence where residues are colour-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 outliers are shown as green connectors. Residues which are classified as ill-defined in the NMR ensemble, are shown in cyan with an underline colour-coded according to the previous scheme. Residues which were present in the experimental sample, but not modelled in the final structure are shown in grey.

• Molecule 1: Major prion protein

Chain A:



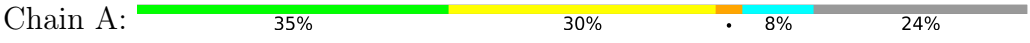
4.2 Scores per residue for each member of the ensemble

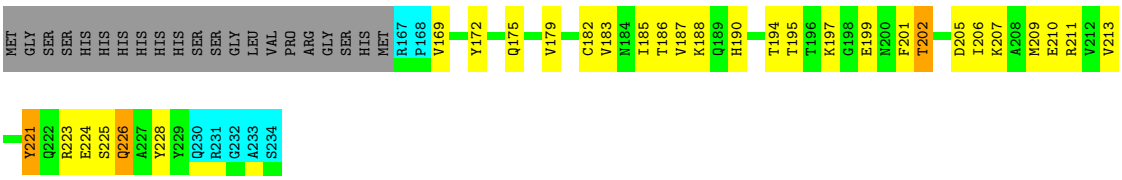
Colouring as in section 4.1 above.

4.2.1 Score per residue for model 1

• Molecule 1: Major prion protein

Chain A:

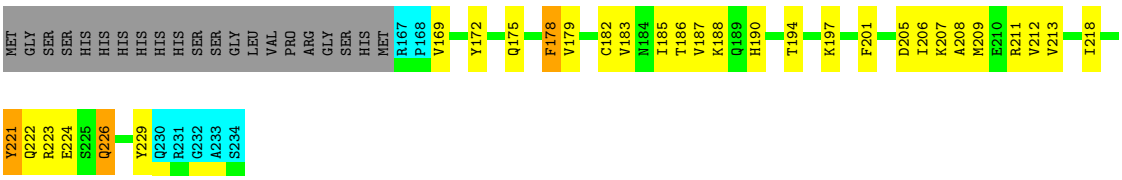




4.2.2 Score per residue for model 2

• Molecule 1: Major prion protein

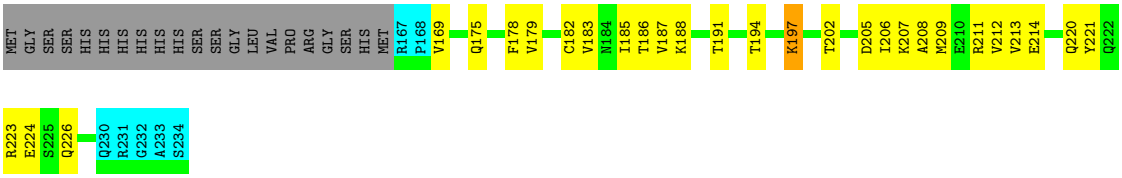
Chain A:



4.2.3 Score per residue for model 3 (medoid)

• Molecule 1: Major prion protein

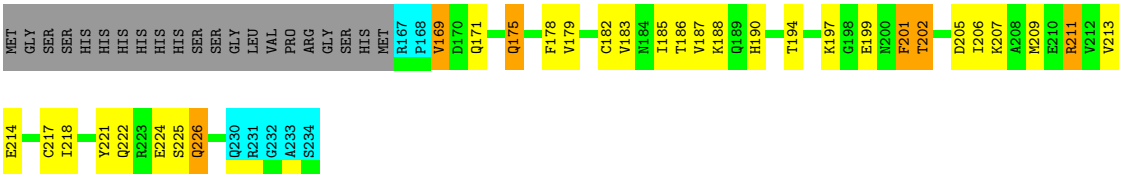
Chain A: 37% 30% • 8% 24%



4.2.4 Score per residue for model 4

• Molecule 1: Major prion protein

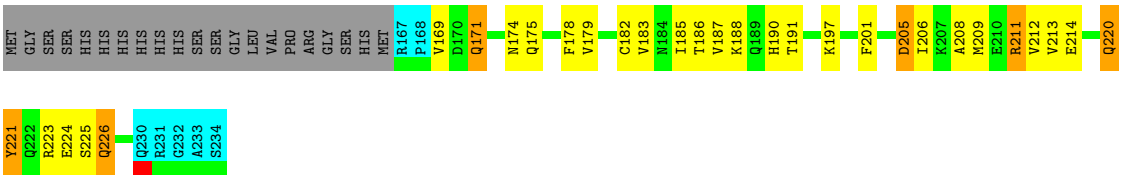
Chain A: 34% 28% 7% 8% 24%



4.2.5 Score per residue for model 5

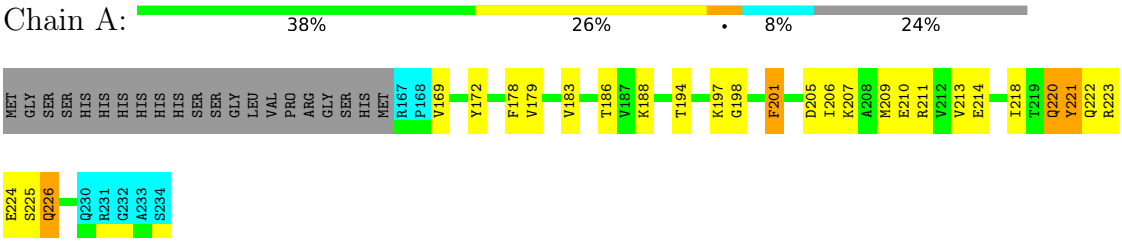
• Molecule 1: Major prion protein

Chain A: 35% 27% 7% 8% 24%



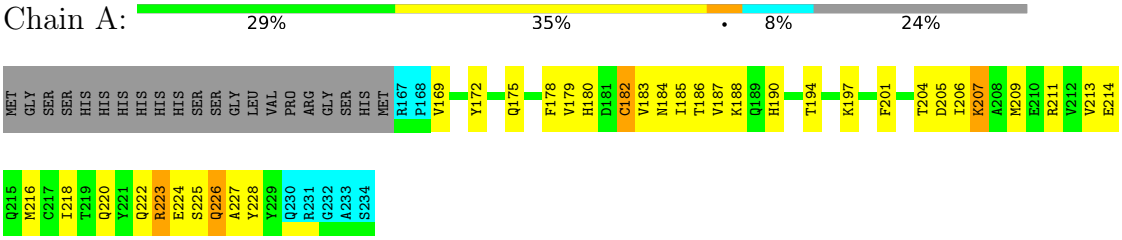
4.2.6 Score per residue for model 6

• Molecule 1: Major prion protein



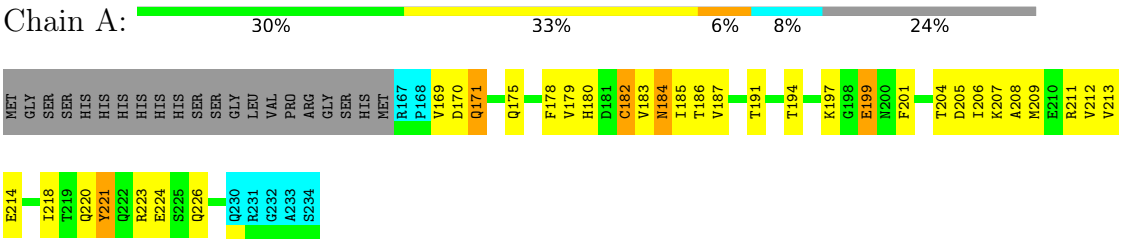
4.2.7 Score per residue for model 7

• Molecule 1: Major prion protein



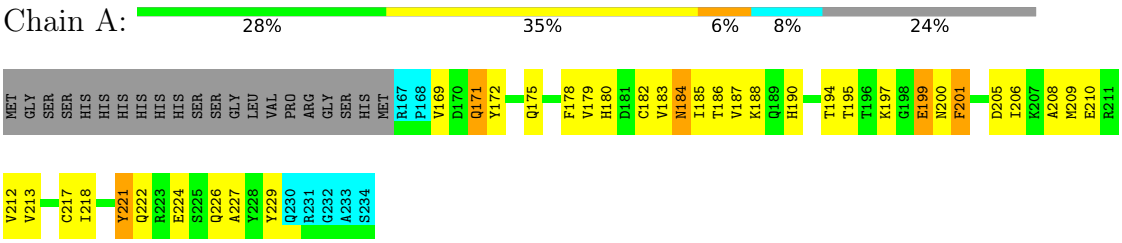
4.2.8 Score per residue for model 8

• Molecule 1: Major prion protein



4.2.9 Score per residue for model 9

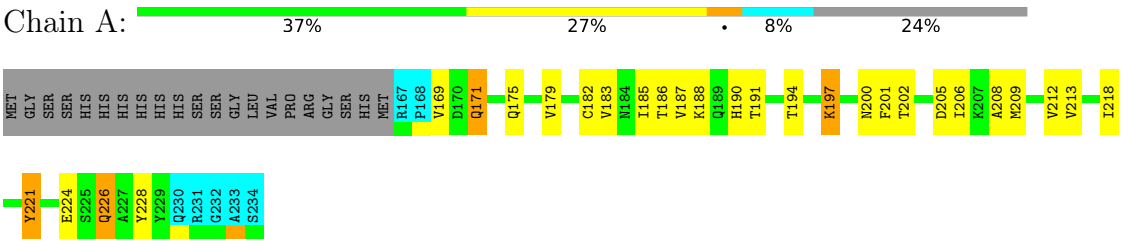
• Molecule 1: Major prion protein



4.2.10 Score per residue for model 10

• Molecule 1: Major prion protein

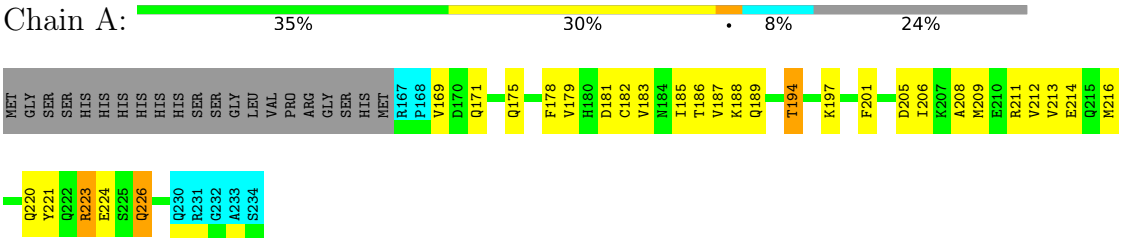
Chain A:



4.2.11 Score per residue for model 11

• Molecule 1: Major prion protein

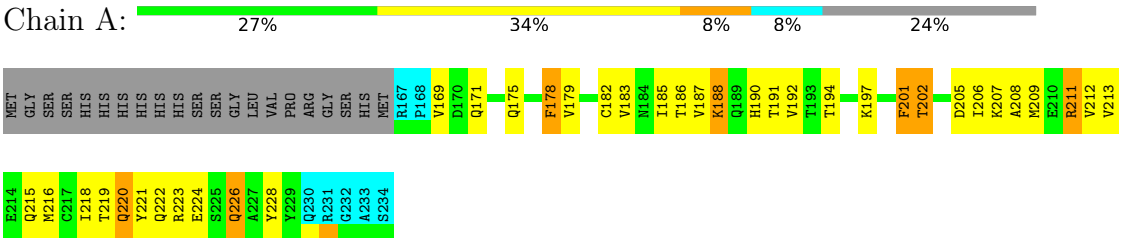
Chain A:



4.2.12 Score per residue for model 12

• Molecule 1: Major prion protein

Chain A:



5 Refinement protocol and experimental data overview

The models were refined using the following method: *molecular dynamics*.

Of the 50 calculated structures, 12 were deposited, based on the following criterion: *structures with the lowest energy*.

The following table shows the software used for structure solution, optimisation and refinement.

Software name	Classification	Version
ARIA	structure solution	v2.2
ARIA	geometry optimization	v2.2
ARIA	refinement	v2.2

No chemical shift data was provided.

6 Model quality

6.1 Standard geometry

There are no covalent bond-length or bond-angle outliers.

There are no bond-length outliers.

There are no bond-angle outliers.

There are no chirality outliers.

There are no planarity outliers.

6.2 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 each 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 averaged over the ensemble.

Mol	Chain	Non-H	H(model)	H(added)	Clashes
1	A	501	467	469	26±7
All	All	6012	5604	5628	311

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 unique clashes are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:206:ILE:HG13	1:A:209:MET:HE3	0.89	1.41	4	2
1:A:206:ILE:HG12	1:A:209:MET:HE3	0.85	1.48	5	5
1:A:220:GLN:HE21	1:A:220:GLN:HA	0.82	1.33	12	3
1:A:194:THR:HG23	1:A:197:LYS:HE2	0.80	1.52	7	5
1:A:175:GLN:HA	1:A:178:PHE:CE2	0.78	2.14	7	3
1:A:194:THR:HG21	1:A:201:PHE:HB3	0.77	1.55	7	3
1:A:171:GLN:HG3	1:A:221:TYR:HA	0.73	1.60	10	2
1:A:206:ILE:CG1	1:A:209:MET:HE3	0.72	2.15	5	4
1:A:194:THR:O	1:A:197:LYS:HG2	0.70	1.86	11	8
1:A:194:THR:HG23	1:A:197:LYS:HE3	0.69	1.63	2	2
1:A:211:ARG:O	1:A:214:GLU:HG2	0.67	1.90	11	6
1:A:202:THR:O	1:A:206:ILE:HD12	0.67	1.89	10	2
1:A:169:VAL:HG11	1:A:228:TYR:HB2	0.65	1.69	10	1
1:A:201:PHE:CD1	1:A:206:ILE:HD11	0.65	2.26	6	6

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:205:ASP:O	1:A:209:MET:HG3	0.64	1.92	11	12
1:A:197:LYS:HE3	1:A:200:ASN:HB3	0.64	1.69	10	2
1:A:171:GLN:HG3	1:A:178:PHE:CE1	0.63	2.28	5	3
1:A:194:THR:HG21	1:A:209:MET:HE2	0.62	1.69	8	2
1:A:206:ILE:HG13	1:A:209:MET:CE	0.62	2.24	4	2
1:A:171:GLN:NE2	1:A:221:TYR:HD1	0.61	1.92	10	2
1:A:171:GLN:HE21	1:A:221:TYR:HD1	0.60	1.37	8	2
1:A:178:PHE:CE2	1:A:221:TYR:HB2	0.60	2.30	3	4
1:A:194:THR:O	1:A:197:LYS:HG3	0.60	1.95	3	1
1:A:184:ASN:O	1:A:188:LYS:HD2	0.60	1.97	7	1
1:A:175:GLN:O	1:A:179:VAL:HG23	0.59	1.97	7	11
1:A:218:ILE:O	1:A:222:GLN:HG3	0.59	1.97	6	5
1:A:191:THR:HA	1:A:209:MET:SD	0.59	2.37	10	5
1:A:195:THR:HA	1:A:199:GLU:HA	0.58	1.76	9	1
1:A:171:GLN:HB3	1:A:221:TYR:CD1	0.57	2.34	12	1
1:A:218:ILE:HG23	1:A:221:TYR:CD2	0.57	2.34	8	2
1:A:179:VAL:O	1:A:183:VAL:HB	0.57	2.00	12	4
1:A:182:CYS:O	1:A:185:ILE:HG13	0.56	2.00	5	11
1:A:171:GLN:HB3	1:A:221:TYR:HD1	0.56	1.59	12	1
1:A:172:TYR:HD1	1:A:221:TYR:HE1	0.56	1.44	2	2
1:A:180:HIS:O	1:A:184:ASN:HB2	0.55	2.01	7	3
1:A:169:VAL:HG11	1:A:228:TYR:HB3	0.55	1.76	12	1
1:A:223:ARG:O	1:A:226:GLN:HG3	0.55	2.01	2	7
1:A:169:VAL:HB	1:A:224:GLU:HG2	0.54	1.79	3	1
1:A:194:THR:HG21	1:A:209:MET:CE	0.54	2.33	3	2
1:A:220:GLN:O	1:A:223:ARG:HB3	0.54	2.02	7	4
1:A:194:THR:HG22	1:A:197:LYS:HE2	0.54	1.81	9	1
1:A:169:VAL:HA	1:A:224:GLU:CG	0.53	2.34	6	8
1:A:206:ILE:HA	1:A:209:MET:HE3	0.53	1.81	8	2
1:A:186:THR:HB	1:A:213:VAL:HG13	0.53	1.81	7	10
1:A:194:THR:CG2	1:A:201:PHE:HB3	0.53	2.33	11	2
1:A:215:GLN:O	1:A:219:THR:HB	0.52	2.04	12	1
1:A:187:VAL:HG23	1:A:213:VAL:HG11	0.52	1.79	9	4
1:A:206:ILE:O	1:A:210:GLU:HG3	0.51	2.05	9	1
1:A:194:THR:HG23	1:A:197:LYS:CE	0.51	2.34	8	6
1:A:201:PHE:HD1	1:A:206:ILE:HD11	0.51	1.62	6	3
1:A:208:ALA:O	1:A:212:VAL:HG23	0.51	2.05	5	8
1:A:172:TYR:HA	1:A:221:TYR:CE1	0.51	2.39	9	1
1:A:178:PHE:O	1:A:182:CYS:HB3	0.51	2.05	12	2
1:A:184:ASN:O	1:A:188:LYS:HD3	0.51	2.05	9	1
1:A:183:VAL:HA	1:A:186:THR:OG1	0.50	2.05	7	4

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:171:GLN:HE21	1:A:171:GLN:CA	0.50	2.19	9	1
1:A:179:VAL:O	1:A:183:VAL:HG23	0.50	2.06	6	1
1:A:206:ILE:CA	1:A:209:MET:HE3	0.50	2.36	8	2
1:A:220:GLN:HA	1:A:220:GLN:NE2	0.50	2.15	12	2
1:A:204:THR:O	1:A:207:LYS:HG2	0.50	2.06	7	2
1:A:224:GLU:O	1:A:227:ALA:HB3	0.50	2.07	9	2
1:A:183:VAL:HG13	1:A:213:VAL:HG12	0.50	1.83	7	2
1:A:218:ILE:HG23	1:A:221:TYR:HD2	0.50	1.66	8	1
1:A:172:TYR:HA	1:A:221:TYR:HE1	0.50	1.67	9	1
1:A:183:VAL:O	1:A:187:VAL:HG23	0.50	2.07	1	10
1:A:194:THR:HA	1:A:197:LYS:HG2	0.50	1.83	9	2
1:A:178:PHE:CE1	1:A:221:TYR:HB2	0.50	2.42	8	1
1:A:201:PHE:HD2	1:A:206:ILE:HD11	0.49	1.68	7	1
1:A:178:PHE:CZ	1:A:221:TYR:HB2	0.49	2.43	4	1
1:A:169:VAL:HG12	1:A:224:GLU:HG3	0.48	1.86	4	2
1:A:194:THR:CG2	1:A:197:LYS:HE2	0.48	2.31	7	1
1:A:186:THR:CB	1:A:213:VAL:HG13	0.47	2.40	11	9
1:A:218:ILE:HG23	1:A:221:TYR:CE2	0.47	2.44	10	1
1:A:220:GLN:HE21	1:A:220:GLN:CA	0.47	2.16	12	1
1:A:169:VAL:CG1	1:A:228:TYR:HB3	0.47	2.40	12	1
1:A:194:THR:HG21	1:A:209:MET:HE1	0.47	1.85	11	1
1:A:194:THR:HA	1:A:197:LYS:HD3	0.47	1.85	2	3
1:A:172:TYR:CD1	1:A:221:TYR:HE1	0.47	2.27	6	1
1:A:210:GLU:O	1:A:214:GLU:HG3	0.46	2.10	6	1
1:A:171:GLN:HB3	1:A:221:TYR:CD2	0.46	2.45	4	1
1:A:175:GLN:HA	1:A:178:PHE:CD2	0.46	2.45	12	2
1:A:169:VAL:HA	1:A:224:GLU:HG2	0.46	1.87	10	2
1:A:178:PHE:CZ	1:A:221:TYR:HB3	0.46	2.46	2	1
1:A:172:TYR:HD1	1:A:221:TYR:CE1	0.46	2.28	6	2
1:A:216:MET:O	1:A:220:GLN:HG2	0.46	2.10	12	3
1:A:195:THR:O	1:A:199:GLU:HG3	0.46	2.11	1	1
1:A:171:GLN:HG3	1:A:178:PHE:CD1	0.45	2.46	9	1
1:A:169:VAL:CB	1:A:224:GLU:HG2	0.45	2.41	3	1
1:A:201:PHE:HD1	1:A:202:THR:H	0.45	1.54	12	1
1:A:207:LYS:O	1:A:211:ARG:HD2	0.45	2.12	6	4
1:A:187:VAL:CG2	1:A:213:VAL:HG11	0.45	2.41	9	1
1:A:201:PHE:O	1:A:202:THR:CB	0.44	2.65	12	3
1:A:210:GLU:HA	1:A:213:VAL:HB	0.44	1.89	1	1
1:A:201:PHE:CD2	1:A:206:ILE:HD11	0.44	2.48	7	1
1:A:182:CYS:SG	1:A:221:TYR:HE2	0.44	2.36	12	1
1:A:206:ILE:HA	1:A:209:MET:HG3	0.43	1.89	4	2

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:178:PHE:CZ	1:A:217:CYS:SG	0.43	3.11	9	1
1:A:205:ASP:HB3	1:A:209:MET:HE2	0.43	1.89	10	1
1:A:169:VAL:HG11	1:A:228:TYR:CB	0.43	2.43	1	1
1:A:194:THR:HG22	1:A:197:LYS:CE	0.43	2.43	9	1
1:A:207:LYS:O	1:A:211:ARG:HG2	0.43	2.12	1	2
1:A:171:GLN:HB2	1:A:224:GLU:HG2	0.42	1.91	4	3
1:A:218:ILE:O	1:A:222:GLN:HG2	0.42	2.14	4	1
1:A:206:ILE:HG12	1:A:209:MET:CE	0.42	2.35	12	1
1:A:201:PHE:O	1:A:202:THR:HB	0.42	2.15	12	1
1:A:169:VAL:HB	1:A:224:GLU:OE2	0.42	2.15	3	1
1:A:169:VAL:CG1	1:A:228:TYR:HB2	0.42	2.44	10	1
1:A:169:VAL:C	1:A:171:GLN:H	0.42	2.18	8	1
1:A:171:GLN:NE2	1:A:221:TYR:CD1	0.41	2.85	8	1
1:A:194:THR:HA	1:A:197:LYS:HG3	0.41	1.90	10	1
1:A:201:PHE:HB2	1:A:206:ILE:CG1	0.41	2.46	2	1
1:A:178:PHE:HD1	1:A:182:CYS:SG	0.41	2.38	7	1
1:A:171:GLN:HE21	1:A:171:GLN:N	0.41	2.14	9	1
1:A:204:THR:HA	1:A:207:LYS:HD3	0.41	1.91	8	2
1:A:208:ALA:HA	1:A:211:ARG:HG2	0.41	1.92	8	1
1:A:178:PHE:HE2	1:A:221:TYR:HB2	0.41	1.73	6	1
1:A:202:THR:O	1:A:205:ASP:N	0.41	2.54	4	1
1:A:194:THR:HA	1:A:197:LYS:CG	0.41	2.45	7	1
1:A:178:PHE:CE1	1:A:218:ILE:HA	0.41	2.50	4	1
1:A:194:THR:HG22	1:A:201:PHE:HB3	0.41	1.93	4	1
1:A:172:TYR:CD2	1:A:221:TYR:CE1	0.40	3.09	1	1
1:A:217:CYS:O	1:A:221:TYR:HD1	0.40	1.99	4	1
1:A:209:MET:O	1:A:213:VAL:HG23	0.40	2.17	3	1
1:A:178:PHE:CD1	1:A:178:PHE:C	0.40	2.94	12	1
1:A:199:GLU:H	1:A:199:GLU:CD	0.40	2.19	8	1
1:A:188:LYS:O	1:A:192:VAL:HG23	0.40	2.17	12	1
1:A:169:VAL:O	1:A:172:TYR:HD1	0.40	2.00	7	1

6.3 Torsion angles (i)

6.3.1 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 PDB entries followed by that with respect to all NMR entries. 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	61/89 (69%)	55±2 (90±3%)	5±1 (8±2%)	1±1 (2±2%)	10 49
All	All	732/1068 (69%)	659 (90%)	57 (8%)	16 (2%)	10 49

All 7 unique Ramachandran outliers are listed below. They are sorted by the frequency of occurrence in the ensemble.

Mol	Chain	Res	Type	Models (Total)
1	A	201	PHE	7
1	A	202	THR	3
1	A	199	GLU	2
1	A	169	VAL	1
1	A	198	GLY	1
1	A	170	ASP	1
1	A	229	TYR	1

6.3.2 Protein sidechains (i)

In the following table, the Percentiles column shows the percent sidechain outliers of the chain as a percentile score with respect to all PDB entries followed by that with respect to all NMR entries. 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	58/81 (72%)	52±2 (90±3%)	6±2 (10±3%)	12 58
All	All	696/972 (72%)	629 (90%)	67 (10%)	12 58

All 21 unique residues with a non-rotameric sidechain are listed below. They are sorted by the frequency of occurrence in the ensemble.

Mol	Chain	Res	Type	Models (Total)
1	A	226	GLN	12
1	A	188	LYS	9
1	A	190	HIS	8
1	A	221	TYR	8
1	A	171	GLN	4
1	A	197	LYS	3
1	A	211	ARG	3
1	A	220	GLN	3
1	A	178	PHE	2
1	A	182	CYS	2
1	A	223	ARG	2

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Mol	Chain	Res	Type	Models (Total)
1	A	184	ASN	2
1	A	202	THR	1
1	A	175	GLN	1
1	A	174	ASN	1
1	A	205	ASP	1
1	A	207	LYS	1
1	A	199	GLU	1
1	A	181	ASP	1
1	A	189	GLN	1
1	A	194	THR	1

6.3.3 RNA

There are no RNA molecules in this entry.

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

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

6.5 Carbohydrates

There are no monosaccharides in this entry.

6.6 Ligand geometry

There are no ligands in this entry.

6.7 Other polymers

There are no such molecules in this entry.

6.8 Polymer linkage issues

There are no chain breaks in this entry.

7 Chemical shift validation (i)

No chemical shift data were provided