Full wwPDB NMR Structure Validation Report (i)

Feb 28, 2022 – 02:24 PM EST

PDB ID	:	2EQY
Title	:	Solution structure of the ARID domain of Jarid1b protein
Authors	:	Tanabe, W.; Suzuki, S.; Muto, Y.; Inoue, M.; Kigawa, T.; Terada, T.; Shirouzu, M.; Yokoyama, S.; RIKEN Structural Genomics/Proteomics Initiative (RSGI)
Deposited on	:	2007-03-30

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:

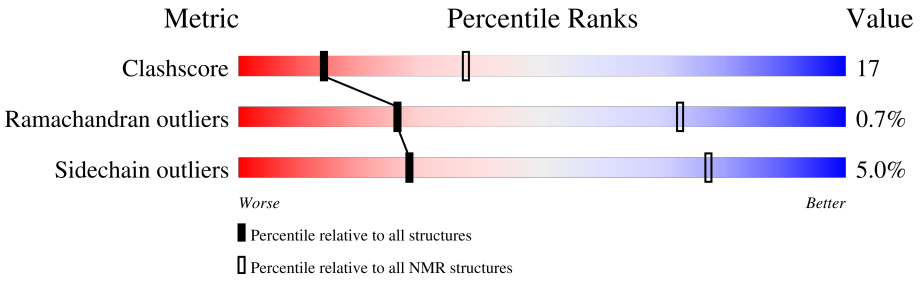
MolProbity	:	4.02b-467
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
RCI	:	v_1n_11_5_13_A (Berjanski et al., 2005)
PANAV	:	Wang et al. (2010)
ShiftChecker	:	2.27
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.27

1 Overall quality at a glance (i)

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	122	57% 16% • 25%

2 Ensemble composition and analysis (i)

This entry contains 20 models. Model 20 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:97-A:187 (91)	0.35	20

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 3 clusters. No single-model clusters were found.

Cluster number	Models
1	2, 4, 5, 6, 7, 9, 10, 13, 14, 15, 16, 17, 19, 20
2	1, 3, 8, 12
3	11, 18

3 Entry composition (i)

There is only 1 type of molecule in this entry. The entry contains 1946 atoms, of which 981 are hydrogens and 0 are deuteriums.

- Molecule 1 is a protein called Jumonji, AT rich interactive domain 1B.

Mol	Chain	Residues	Atoms						Trace
			Total	C	H	N	O	S	
1	A	122	1946	614	981	171	177	3	0

There are 7 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	87	GLY	-	expression tag	UNP Q80Y84
A	88	SER	-	expression tag	UNP Q80Y84
A	89	SER	-	expression tag	UNP Q80Y84
A	90	GLY	-	expression tag	UNP Q80Y84
A	91	SER	-	expression tag	UNP Q80Y84
A	92	SER	-	expression tag	UNP Q80Y84
A	93	GLY	-	expression tag	UNP Q80Y84

4 Residue-property plots (i)

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: Jumonji, AT rich interactive domain 1B

Chain A: 57% 16% • 25%

G87 S88 S89 G90 S91 S92 G93 E94 A95 Q96 K100 F103 I107 A108 K109 Y110 W111 L118 L128 F131 Q132 L133 G142 V145 V146 R150 K151 W152 I155 V167 I171 Y175 L179 N180 P181 G188 D189 S190 L191 R192 C193 L194 Q195 K196 P197

N198 L199 T200 S201 D202 T203 K204 D205 K206 E207 Y208

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: Jumonji, AT rich interactive domain 1B

Chain A: 47% 24% • 25%

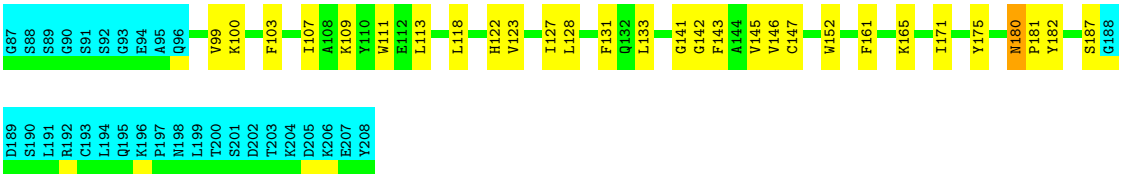
G87 S88 S89 G90 S91 S92 G93 E94 A95 Q96 F103 L104 D105 K109 Y110 W111 E112 L113 Q114 I120 P121 H122 V123 I127 L128 D129 L130 F131 Q132 L133 G142 V145 V146 D149 R150 K151 W152 I155 A156 F161 V167 I171 H174 Y175 L179 N180 P181

G188 D189 S190 L191 R192 C193 L194 Q195 K196 P197 N198 L199 T200 S201 D202 T203 K204 D205 K206 E207 Y208

4.2.2 Score per residue for model 2

• Molecule 1: Jumonji, AT rich interactive domain 1B

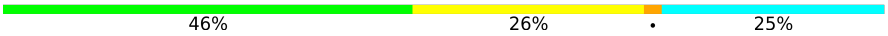
Chain A: 51% 23% • 25%

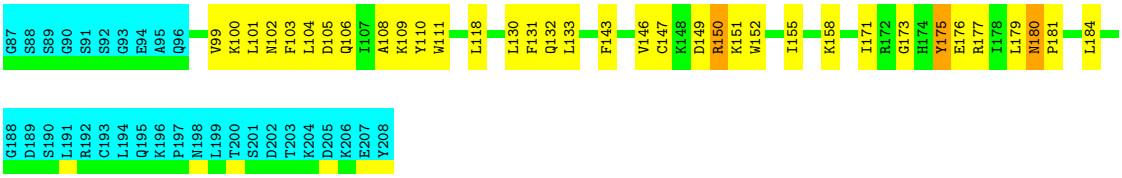


4.2.3 Score per residue for model 3

- Molecule 1: Jumonji, AT rich interactive domain 1B

Chain A:

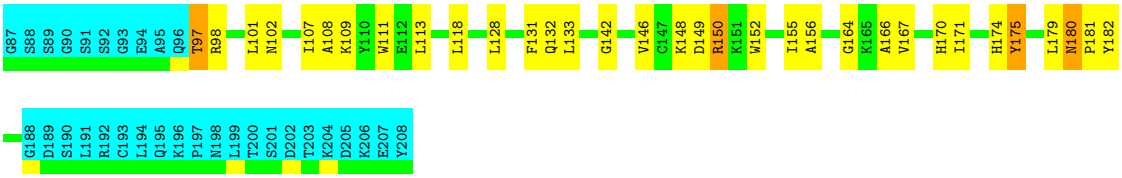




4.2.4 Score per residue for model 4

- Molecule 1: Jumonji, AT rich interactive domain 1B

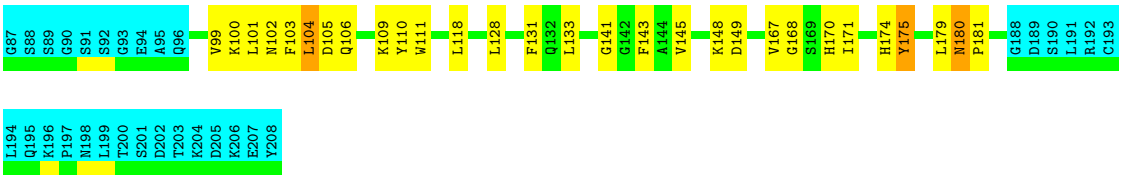
Chain A:



4.2.5 Score per residue for model 5

- Molecule 1: Jumonji, AT rich interactive domain 1B

Chain A:



4.2.6 Score per residue for model 6

- Molecule 1: Jumonji, AT rich interactive domain 1B

Chain A: 53% 17% • 25%

G87 S88 S89 G90 S91 S92 G93 E94 A95 Q96 K100 F103 I107 A108 L118 K119 I120 P121 H122 V123 I127 L128 F131 Q132 L133 V137 G142 V145 V146 R150 I155 H170 I171 Y175 N180 P181 Y182 N183 G188 D189 S190 L191 R192 C193 L194

Q195 K196 P197 N198 L199 T200 S201 D202 T203 K204 D205 K206 E207 Y208

4.2.7 Score per residue for model 7

- Molecule 1: Jumonji, AT rich interactive domain 1B

Chain A: 51% 21% • 25%

G87 S88 S89 G90 S91 S92 G93 E94 A95 Q96 K100 F103 I107 W111 L118 K119 V123 E124 R125 K126 I127 L128 F131 Q132 L133 N134 F143 D149 R150 K151 W152 K158 F161 A166 V167 H170 I171 R172 Y175 N180 P181 Y182 G188 D189

S190 L191 R192 C193 L194 Q195 K196 P197 N198 L199 T200 S201 D202 T203 K204 D205 K206 E207 Y208

4.2.8 Score per residue for model 8

- Molecule 1: Jumonji, AT rich interactive domain 1B

Chain A: 50% 21% • 25%

G87 S88 S89 G90 S91 S92 G93 E94 A95 Q96 V99 K100 I107 A108 W111 L118 F131 Q132 L133 N134 K135 E140 G141 G142 F143 A144 V145 V146 R150 K151 W152 T153 K154 I155 A166 V167 G168 S169 H170 I171 Y175 L179 N180 P181 Y182 F185 G188 D189

S190 L191 R192 C193 L194 Q195 K196 P197 N198 L199 T200 S201 D202 T203 K204 D205 K206 E207 Y208

4.2.9 Score per residue for model 9

- Molecule 1: Jumonji, AT rich interactive domain 1B

Chain A: 55% 16% • 25%

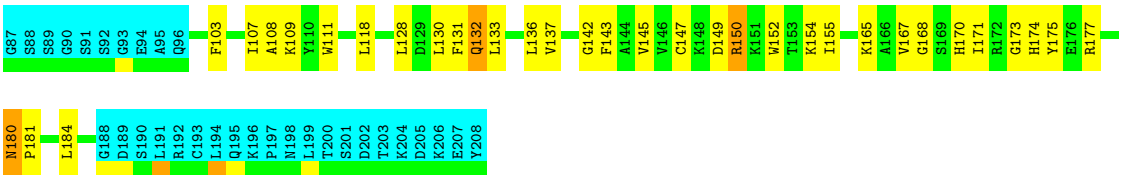
G87 S88 S89 G90 S91 S92 G93 E94 A95 Q96 V99 K100 F103 L104 L118 V123 L128 D129 L130 F131 Q132 L133 E140 V146 R150 K151 W152 I155 A156 F161 H170 I171 Y175 N180 P181 G188 D189 S190 L191 R192 C193 L194 Q195 K196 P197 N198

L199 T200 S201 D202 T203 K204 D205 K206 E207 Y208

4.2.10 Score per residue for model 10

- Molecule 1: Jumonji, AT rich interactive domain 1B

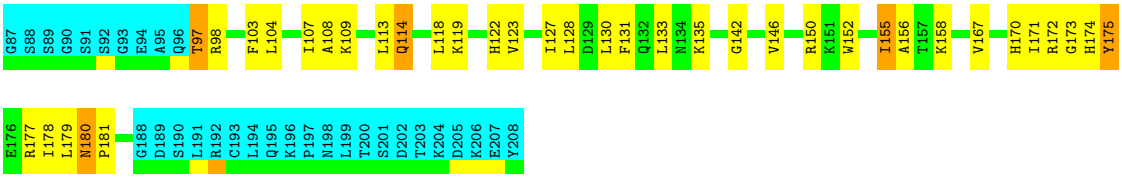
Chain A: 47% 25% • 25%



4.2.11 Score per residue for model 11

- Molecule 1: Jumonji, AT rich interactive domain 1B

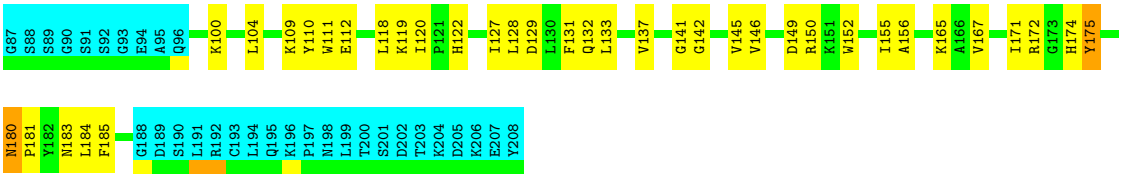
Chain A: 43% 27% • 25%



4.2.12 Score per residue for model 12

- Molecule 1: Jumonji, AT rich interactive domain 1B

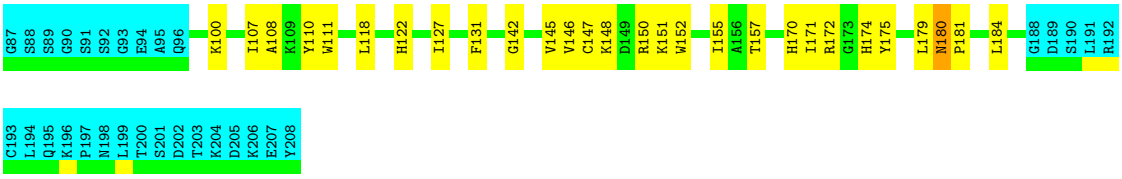
Chain A: 44% 29% • 25%



4.2.13 Score per residue for model 13

- Molecule 1: Jumonji, AT rich interactive domain 1B

Chain A: 52% 22% • 25%



4.2.14 Score per residue for model 14

• Molecule 1: Jumonji, AT rich interactive domain 1B

Chain A: 57% 16% • 25%

G87 S88 S89 G90 S91 S92 G93 E94 A95 Q96 T97 R98 N102 I107 L118 R125 Q132 L133 M134 K135 E139 G142 V146 I155 A156 F161 V167 I171 Y175 L179 N180 P181 Y182 G188 D189 S190 L191 R192 C193 L194 Q195 K196 P197 N198 L199

T200 S201 D202 T203 K204 D205 K206 E207 Y208

4.2.15 Score per residue for model 15

• Molecule 1: Jumonji, AT rich interactive domain 1B

Chain A: 51% 22% • 25%

G87 S88 S89 G90 S91 S92 G93 E94 A95 Q96 T97 R98 V99 K100 F103 L104 D105 Q106 I107 W111 L118 K119 L128 L133 N134 K135 L136 V137 G142 V146 D149 R150 K151 W152 I155 K165 I171 Y175 L179 N180 P181 Y182 L186 S187 G188 D189

S190 L191 R192 C193 L194 Q195 K196 P197 N198 L199 T200 S201 D202 T203 K204 D205 K206 E207 Y208

4.2.16 Score per residue for model 16

• Molecule 1: Jumonji, AT rich interactive domain 1B

Chain A: 47% 26% • 25%

G87 S88 S89 G90 S91 S92 G93 E94 A95 Q96 I107 A108 K109 Y110 W111 E112 L113 T117 L118 K119 H122 K126 I127 L128 F131 Q132 L133 G141 G142 V145 V146 K151 W152 I155 A156 G164 V167 I171 H174 Y175 E176 R177 I178 L179 N180 P181 Y182

N183 L184 G188 D189 S190 L191 R192 C193 L194 Q195 K196 P197 N198 L199 T200 S201 D202 T203 K204 D205 K206 E207 Y208

4.2.17 Score per residue for model 17

• Molecule 1: Jumonji, AT rich interactive domain 1B

Chain A: 47% 27% • 25%

G87 S88 S89 G90 S91 S92 G93 E94 A95 Q96 T97 K100 L101 N102 F103 I107 W111 E112 L118 P121 H122 V123 L128 D129 L130 F131 V137 G141 G142 F143 A144 V145 V146 C147 K148 D149 R150 K151 W152 T153 K154 I155 A156 T157 K158 F161 I171 Y175

L179 N180 P181 Y182 G188 D189 S190 L191 R192 C193 L194 Q195 K196 P197 N198 L199 T200 S201 D202 T203 K204 D205 K206 E207 Y208

4.2.18 Score per residue for model 18

- Molecule 1: Jumonji, AT rich interactive domain 1B

Chain A: 52% 20% • 25%

G87 S88 S89 G90 S91 S92 G93 E94 A95 Q96 V99 F103 L104 I107 L118 K119 I120 P121 H122 V123 L128 F131 Q132 L133 L136 V137 G141 G142 V145 V146 W152 T153 K154 I155 I171 H174 Y175 N180 P181 Y182 N183 L184 G188 D189 S190 L191

R192 C193 L194 Q195 K196 P197 N198 L199 T200 S201 D202 T203 K204 D205 K206 E207 Y208

4.2.19 Score per residue for model 19

- Molecule 1: Jumonji, AT rich interactive domain 1B

Chain A: 53% 20% • 25%

G87 S88 S89 G90 S91 S92 G93 E94 A95 Q96 V99 K100 W111 L118 H122 R125 K126 L130 F131 Q132 L133 N134 K135 L136 V137 G142 V146 D149 R150 K151 W152 I155 A156 T157 K158 I171 Y175 N180 P181 G188 D189 S190 L191 R192 C193 L194

Q195 K196 P197 N198 L199 T200 S201 D202 T203 K204 D205 K206 E207 Y208

4.2.20 Score per residue for model 20 (medoid)

- Molecule 1: Jumonji, AT rich interactive domain 1B

Chain A: 55% 17% • 25%

G87 S88 S89 G90 S91 S92 G93 E94 A95 Q96 T97 R98 F103 I107 A108 K109 Y110 W111 L118 L130 F131 Q132 L133 G142 V146 R150 K151 I155 A156 G164 V167 I171 R172 Y175 E176 N180 P181 G188 D189 S190 L191 R192 C193 L194 Q195 K196

P197 N198 L199 T200 S201 D202 T203 K204 D205 K206 E207 Y208

5 Refinement protocol and experimental data overview (i)

The models were refined using the following method: *torsion angle dyanamics, simulated annealing.*

Of the 100 calculated structures, 20 were deposited, based on the following criterion: *structures with the least restraint violations, structures with the lowest energy, target function.*

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

Software name	Classification	Version
CYANA	structure solution	2.0.17
CYANA	refinement	2.0.17

No chemical shift data was provided.

6 Model quality (i)

6.1 Standard geometry (i)

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 (i)

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	739	768	768	26±4
All	All	14780	15360	15360	526

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 17.

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

Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:118:LEU:HD13	1:A:119:LYS:N	0.85	1.86	12	2
1:A:128:LEU:HD11	1:A:133:LEU:HD22	0.85	1.47	9	7
1:A:133:LEU:HD11	1:A:171:ILE:CG2	0.84	2.03	7	13
1:A:133:LEU:HD11	1:A:171:ILE:HG23	0.83	1.49	1	13
1:A:111:TRP:CD1	1:A:118:LEU:HD12	0.82	2.10	2	7
1:A:152:TRP:CZ3	1:A:171:ILE:HG21	0.79	2.13	1	15
1:A:143:PHE:CZ	1:A:175:TYR:CD1	0.79	2.70	7	1
1:A:118:LEU:HD13	1:A:118:LEU:C	0.75	2.01	6	1
1:A:118:LEU:HD22	1:A:119:LYS:H	0.71	1.46	6	1
1:A:133:LEU:HD21	1:A:171:ILE:HG23	0.70	1.64	6	4
1:A:132:GLN:NE2	1:A:136:LEU:HD12	0.70	2.01	10	1
1:A:118:LEU:HD23	1:A:119:LYS:N	0.69	2.02	15	5
1:A:152:TRP:CZ3	1:A:171:ILE:CG2	0.68	2.75	7	14
1:A:104:LEU:HD22	1:A:120:ILE:HD11	0.68	1.65	12	1

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:184:LEU:HD12	1:A:184:LEU:C	0.67	2.09	18	1
1:A:143:PHE:CE2	1:A:175:TYR:CD1	0.66	2.83	5	1
1:A:137:VAL:HG22	1:A:155:ILE:HD13	0.66	1.67	18	7
1:A:111:TRP:HD1	1:A:118:LEU:HD12	0.65	1.51	4	10
1:A:175:TYR:C	1:A:175:TYR:CD1	0.64	2.72	12	8
1:A:128:LEU:HD21	1:A:133:LEU:HD22	0.62	1.71	15	1
1:A:118:LEU:HD22	1:A:119:LYS:N	0.62	2.10	6	1
1:A:99:VAL:HG22	1:A:131:PHE:CE1	0.62	2.30	9	1
1:A:184:LEU:HD12	1:A:184:LEU:O	0.61	1.95	18	1
1:A:103:PHE:O	1:A:107:ILE:HG22	0.61	1.94	20	6
1:A:107:ILE:HD12	1:A:182:TYR:CG	0.61	2.31	14	5
1:A:107:ILE:HD12	1:A:182:TYR:CD1	0.60	2.31	14	6
1:A:120:ILE:HG21	1:A:128:LEU:O	0.60	1.97	6	2
1:A:142:GLY:O	1:A:146:VAL:HG23	0.59	1.98	4	12
1:A:152:TRP:CE3	1:A:171:ILE:HG21	0.59	2.33	13	5
1:A:109:LYS:O	1:A:113:LEU:HD12	0.58	1.98	4	2
1:A:118:LEU:C	1:A:118:LEU:HD23	0.58	2.19	7	5
1:A:107:ILE:CD1	1:A:182:TYR:CG	0.57	2.87	4	4
1:A:152:TRP:CD1	1:A:172:ARG:NH2	0.57	2.72	13	1
1:A:118:LEU:C	1:A:118:LEU:CD1	0.55	2.74	6	1
1:A:180:ASN:ND2	1:A:180:ASN:C	0.55	2.61	11	6
1:A:128:LEU:CD2	1:A:174:HIS:CD2	0.54	2.90	16	3
1:A:122:HIS:CE1	1:A:127:ILE:CD1	0.54	2.91	16	4
1:A:166:ALA:O	1:A:170:HIS:CG	0.54	2.60	7	2
1:A:121:PRO:HG2	1:A:128:LEU:HD23	0.54	1.79	18	2
1:A:164:GLY:O	1:A:167:VAL:HG12	0.54	2.03	20	2
1:A:175:TYR:CD2	1:A:179:LEU:HB2	0.54	2.38	13	5
1:A:118:LEU:HD23	1:A:118:LEU:C	0.53	2.24	11	3
1:A:141:GLY:HA3	1:A:145:VAL:HG11	0.53	1.81	16	4
1:A:170:HIS:O	1:A:174:HIS:CD2	0.53	2.62	10	5
1:A:143:PHE:CE2	1:A:175:TYR:CE1	0.53	2.97	7	1
1:A:175:TYR:CE2	1:A:183:ASN:OD1	0.53	2.61	6	1
1:A:156:ALA:HB1	1:A:167:VAL:CG2	0.52	2.34	16	5
1:A:122:HIS:NE2	1:A:127:ILE:HD11	0.52	2.19	1	1
1:A:145:VAL:HG13	1:A:146:VAL:N	0.52	2.18	12	5
1:A:180:ASN:CB	1:A:181:PRO:CD	0.52	2.88	9	20
1:A:155:ILE:HD12	1:A:155:ILE:H	0.52	1.63	3	2
1:A:141:GLY:C	1:A:145:VAL:CG1	0.51	2.78	12	3
1:A:109:LYS:O	1:A:111:TRP:N	0.51	2.44	12	2
1:A:121:PRO:HB2	1:A:174:HIS:CE1	0.51	2.41	18	1
1:A:175:TYR:CD1	1:A:175:TYR:C	0.51	2.84	7	2

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:133:LEU:HD11	1:A:171:ILE:HG21	0.51	1.82	10	2
1:A:175:TYR:CD2	1:A:179:LEU:CB	0.50	2.94	13	2
1:A:99:VAL:HG22	1:A:131:PHE:CZ	0.50	2.41	5	2
1:A:180:ASN:OD1	1:A:181:PRO:N	0.50	2.44	5	2
1:A:181:PRO:HA	1:A:184:LEU:HD12	0.50	1.82	10	1
1:A:128:LEU:HD21	1:A:133:LEU:CD2	0.50	2.36	15	1
1:A:141:GLY:CA	1:A:145:VAL:HG11	0.50	2.37	12	3
1:A:180:ASN:O	1:A:184:LEU:CB	0.50	2.60	16	3
1:A:142:GLY:O	1:A:146:VAL:CG2	0.50	2.60	1	10
1:A:118:LEU:C	1:A:118:LEU:CD2	0.50	2.80	11	5
1:A:133:LEU:CD1	1:A:171:ILE:HG23	0.50	2.36	10	2
1:A:131:PHE:CE1	1:A:135:LYS:HG3	0.50	2.41	8	1
1:A:146:VAL:O	1:A:150:ARG:N	0.49	2.45	11	8
1:A:123:VAL:HB	1:A:161:PHE:CZ	0.49	2.43	9	3
1:A:151:LYS:O	1:A:155:ILE:CD1	0.49	2.60	3	3
1:A:111:TRP:CZ2	1:A:181:PRO:HG3	0.49	2.43	12	2
1:A:118:LEU:HD13	1:A:119:LYS:H	0.49	1.62	12	1
1:A:147:CYS:SG	1:A:148:LYS:N	0.49	2.85	13	1
1:A:120:ILE:HG23	1:A:121:PRO:HD2	0.49	1.83	1	1
1:A:125:ARG:O	1:A:126:LYS:CG	0.49	2.61	19	1
1:A:122:HIS:CE1	1:A:127:ILE:HD11	0.49	2.43	6	2
1:A:104:LEU:O	1:A:108:ALA:HB2	0.49	2.08	11	1
1:A:141:GLY:C	1:A:145:VAL:HG11	0.48	2.28	8	2
1:A:143:PHE:C	1:A:143:PHE:CD1	0.48	2.85	8	2
1:A:108:ALA:HA	1:A:118:LEU:HD12	0.48	1.85	3	1
1:A:103:PHE:O	1:A:106:GLN:N	0.48	2.47	5	3
1:A:103:PHE:O	1:A:105:ASP:N	0.48	2.47	3	3
1:A:133:LEU:CD1	1:A:171:ILE:HD12	0.48	2.38	1	1
1:A:123:VAL:CG2	1:A:128:LEU:HD22	0.48	2.39	18	2
1:A:100:LYS:HG2	1:A:131:PHE:CD1	0.48	2.44	5	6
1:A:149:ASP:O	1:A:150:ARG:C	0.47	2.51	4	8
1:A:155:ILE:O	1:A:158:LYS:N	0.47	2.47	19	2
1:A:123:VAL:O	1:A:126:LYS:N	0.47	2.47	7	1
1:A:140:GLU:N	1:A:140:GLU:OE1	0.47	2.47	8	1
1:A:183:ASN:O	1:A:185:PHE:N	0.47	2.48	12	1
1:A:99:VAL:HG13	1:A:100:LYS:N	0.47	2.24	3	1
1:A:107:ILE:HG23	1:A:108:ALA:N	0.47	2.24	6	5
1:A:132:GLN:HE22	1:A:136:LEU:HD12	0.47	1.67	10	1
1:A:122:HIS:CE1	1:A:127:ILE:HD13	0.47	2.44	11	1
1:A:110:TYR:C	1:A:110:TYR:CD1	0.47	2.87	13	1
1:A:134:ASN:O	1:A:137:VAL:N	0.47	2.48	15	1

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:99:VAL:HG22	1:A:131:PHE:CE2	0.47	2.45	2	2
1:A:107:ILE:HA	1:A:182:TYR:CE1	0.46	2.45	16	3
1:A:109:LYS:O	1:A:113:LEU:CD1	0.46	2.62	4	2
1:A:123:VAL:HG23	1:A:128:LEU:HD22	0.46	1.88	18	1
1:A:109:LYS:CG	1:A:110:TYR:N	0.46	2.79	5	2
1:A:131:PHE:CD1	1:A:131:PHE:C	0.46	2.89	16	1
1:A:180:ASN:N	1:A:181:PRO:HD2	0.46	2.25	12	16
1:A:107:ILE:HD13	1:A:182:TYR:CD2	0.46	2.46	4	1
1:A:161:PHE:CB	1:A:167:VAL:HG21	0.46	2.40	14	2
1:A:155:ILE:HD13	1:A:155:ILE:N	0.46	2.24	8	1
1:A:111:TRP:CH2	1:A:181:PRO:HG3	0.46	2.45	20	6
1:A:123:VAL:HG12	1:A:161:PHE:CE1	0.46	2.46	1	1
1:A:145:VAL:HG13	1:A:146:VAL:H	0.46	1.71	12	3
1:A:131:PHE:CD2	1:A:132:GLN:N	0.46	2.84	9	3
1:A:100:LYS:HA	1:A:131:PHE:CD2	0.46	2.46	13	2
1:A:132:GLN:O	1:A:136:LEU:CG	0.46	2.64	18	1
1:A:143:PHE:CE1	1:A:175:TYR:CD1	0.46	3.03	7	1
1:A:148:LYS:CG	1:A:149:ASP:N	0.45	2.79	4	2
1:A:103:PHE:CD1	1:A:104:LEU:N	0.45	2.84	9	1
1:A:134:ASN:OD1	1:A:134:ASN:C	0.45	2.55	7	1
1:A:103:PHE:C	1:A:103:PHE:CD1	0.45	2.90	17	1
1:A:142:GLY:N	1:A:145:VAL:CG1	0.45	2.78	6	3
1:A:175:TYR:CD1	1:A:175:TYR:O	0.45	2.70	6	2
1:A:175:TYR:O	1:A:179:LEU:C	0.45	2.55	15	9
1:A:132:GLN:O	1:A:133:LEU:C	0.45	2.55	1	7
1:A:109:LYS:C	1:A:111:TRP:N	0.45	2.70	16	2
1:A:133:LEU:CD2	1:A:171:ILE:HG23	0.44	2.41	6	1
1:A:152:TRP:CZ2	1:A:172:ARG:HG2	0.44	2.46	11	1
1:A:114:GLN:OE1	1:A:114:GLN:C	0.44	2.55	1	2
1:A:99:VAL:HG13	1:A:100:LYS:HD2	0.44	1.89	8	1
1:A:107:ILE:HD11	1:A:179:LEU:CD1	0.44	2.42	11	1
1:A:128:LEU:HD22	1:A:174:HIS:CD2	0.44	2.48	12	2
1:A:130:LEU:O	1:A:131:PHE:C	0.44	2.55	20	7
1:A:99:VAL:CG1	1:A:100:LYS:N	0.44	2.81	3	1
1:A:135:LYS:O	1:A:139:GLU:CD	0.44	2.56	14	1
1:A:155:ILE:O	1:A:156:ALA:C	0.44	2.55	4	8
1:A:156:ALA:HB1	1:A:167:VAL:HG22	0.44	1.89	16	2
1:A:123:VAL:HG21	1:A:128:LEU:HD22	0.44	1.88	6	1
1:A:167:VAL:HG13	1:A:168:GLY:N	0.43	2.28	5	3
1:A:100:LYS:HA	1:A:131:PHE:CE2	0.43	2.48	17	2
1:A:152:TRP:CE3	1:A:171:ILE:CG2	0.43	3.00	13	1

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:134:ASN:O	1:A:135:LYS:C	0.43	2.57	15	1
1:A:184:LEU:C	1:A:184:LEU:CD1	0.43	2.81	18	1
1:A:143:PHE:O	1:A:147:CYS:CB	0.43	2.66	2	4
1:A:103:PHE:C	1:A:105:ASP:N	0.43	2.72	3	1
1:A:173:GLY:O	1:A:177:ARG:N	0.43	2.52	10	2
1:A:142:GLY:H	1:A:146:VAL:HG23	0.43	1.74	12	2
1:A:175:TYR:O	1:A:180:ASN:N	0.43	2.52	4	3
1:A:146:VAL:O	1:A:150:ARG:CA	0.43	2.67	11	1
1:A:178:ILE:HG22	1:A:179:LEU:HD13	0.43	1.91	11	1
1:A:180:ASN:OD1	1:A:180:ASN:C	0.42	2.56	6	3
1:A:137:VAL:HG13	1:A:146:VAL:HG21	0.42	1.90	19	1
1:A:123:VAL:CG1	1:A:161:PHE:CZ	0.42	3.02	1	1
1:A:143:PHE:CZ	1:A:172:ARG:NE	0.42	2.87	7	1
1:A:100:LYS:HG2	1:A:131:PHE:CD2	0.42	2.50	9	1
1:A:183:ASN:C	1:A:185:PHE:N	0.42	2.72	12	1
1:A:123:VAL:CG1	1:A:161:PHE:CE1	0.42	3.02	1	1
1:A:146:VAL:HG22	1:A:151:LYS:HB2	0.42	1.89	8	1
1:A:122:HIS:NE2	1:A:127:ILE:CD1	0.42	2.82	13	2
1:A:175:TYR:HA	1:A:179:LEU:HD12	0.42	1.90	3	1
1:A:129:ASP:OD1	1:A:129:ASP:C	0.42	2.57	17	1
1:A:151:LYS:O	1:A:155:ILE:HD12	0.42	2.14	16	1
1:A:103:PHE:O	1:A:104:LEU:C	0.41	2.58	5	3
1:A:97:THR:HG22	1:A:101:LEU:HD11	0.41	1.91	17	1
1:A:109:LYS:HG3	1:A:110:TYR:N	0.41	2.30	3	1
1:A:180:ASN:CB	1:A:181:PRO:HD3	0.41	2.46	18	2
1:A:109:LYS:O	1:A:113:LEU:HD13	0.41	2.15	11	1
1:A:112:GLU:HG3	1:A:113:LEU:HD22	0.41	1.91	16	1
1:A:101:LEU:O	1:A:102:ASN:C	0.41	2.58	5	3
1:A:132:GLN:NE2	1:A:132:GLN:C	0.41	2.74	10	1
1:A:143:PHE:CD1	1:A:143:PHE:C	0.41	2.93	10	1
1:A:111:TRP:O	1:A:113:LEU:N	0.41	2.53	1	1
1:A:105:ASP:O	1:A:109:LYS:CD	0.41	2.69	1	1
1:A:173:GLY:O	1:A:176:GLU:N	0.41	2.54	3	1
1:A:120:ILE:CG2	1:A:128:LEU:O	0.41	2.67	6	1
1:A:132:GLN:O	1:A:136:LEU:HD12	0.41	2.16	18	1
1:A:109:LYS:O	1:A:112:GLU:N	0.41	2.53	12	1
1:A:172:ARG:C	1:A:176:GLU:OE1	0.41	2.59	20	1
1:A:97:THR:HG22	1:A:101:LEU:CD1	0.41	2.46	17	1
1:A:152:TRP:O	1:A:153:THR:C	0.41	2.59	17	1
1:A:125:ARG:NH1	1:A:125:ARG:CB	0.41	2.85	14	1
1:A:182:TYR:CE2	1:A:186:LEU:HD11	0.41	2.51	15	1

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:177:ARG:NH1	1:A:177:ARG:CB	0.41	2.84	16	1
1:A:181:PRO:O	1:A:182:TYR:C	0.41	2.59	18	1
1:A:111:TRP:C	1:A:113:LEU:N	0.40	2.75	1	1
1:A:170:HIS:O	1:A:171:ILE:C	0.40	2.60	9	2
1:A:177:ARG:N	1:A:177:ARG:HD2	0.40	2.31	3	1
1:A:175:TYR:OH	1:A:183:ASN:CG	0.40	2.60	6	1
1:A:131:PHE:CD1	1:A:132:GLN:N	0.40	2.90	7	1
1:A:140:GLU:N	1:A:140:GLU:CD	0.40	2.74	9	1
1:A:98:ARG:O	1:A:102:ASN:CG	0.40	2.60	14	1
1:A:122:HIS:N	1:A:122:HIS:CD2	0.40	2.88	19	1
1:A:164:GLY:C	1:A:166:ALA:N	0.40	2.75	4	1
1:A:123:VAL:O	1:A:124:GLU:C	0.40	2.59	7	1
1:A:128:LEU:CD2	1:A:133:LEU:HD22	0.40	2.43	15	1
1:A:104:LEU:O	1:A:107:ILE:CG2	0.40	2.69	18	1
1:A:149:ASP:O	1:A:151:LYS:N	0.40	2.55	19	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	91/122 (75%)	72±3 (79±4%)	18±3 (20±3%)	1±1 (1±1%)	26	73
All	All	1820/2440 (75%)	1446 (79%)	361 (20%)	13 (1%)	26	73

All 8 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	155	ILE	2
1	A	104	LEU	2
1	A	97	THR	2
1	A	150	ARG	2
1	A	110	TYR	2
1	A	171	ILE	1
1	A	129	ASP	1

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Models (Total)
1	A	184	LEU	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	78/104 (75%)	74±1 (95±2%)	4±1 (5±2%)	28 77
All	All	1560/2080 (75%)	1482 (95%)	78 (5%)	28 77

All 23 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	180	ASN	20
1	A	175	TYR	16
1	A	150	ARG	6
1	A	165	LYS	4
1	A	109	LYS	3
1	A	158	LYS	3
1	A	135	LYS	3
1	A	154	LYS	3
1	A	112	GLU	2
1	A	114	GLN	2
1	A	119	LYS	2
1	A	140	GLU	2
1	A	151	LYS	2
1	A	149	ASP	1
1	A	118	LEU	1
1	A	132	GLN	1
1	A	172	ARG	1
1	A	157	THR	1
1	A	100	LYS	1
1	A	117	THR	1
1	A	126	LYS	1
1	A	184	LEU	1
1	A	98	ARG	1

6.3.3 RNA (i)

There are no RNA molecules in this entry.

6.4 Non-standard residues in protein, DNA, RNA chains (i)

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

6.5 Carbohydrates (i)

There are no monosaccharides in this entry.

6.6 Ligand geometry (i)

There are no ligands in this entry.

6.7 Other polymers (i)

There are no such molecules in this entry.

6.8 Polymer linkage issues (i)

There are no chain breaks in this entry.

7 Chemical shift validation (i)

No chemical shift data were provided