Full wwPDB NMR Structure Validation Report (i)

Feb 28, 2022 – 01:27 AM EST

PDB ID	:	2E7G
Title	:	Solution structure of putative ribosome-binding factor A (RbfA) from human mutochondrial precursor
Authors	:	Furue, M.; Suzuki, S.; Muto, Y.; Inoue, M.; Kigawa, T.; Terada, T.; Shirouzu, M.; Yokoyama, S.; RIKEN Structural Genomics/Proteomics Initiative (RSGI)
Deposited on	:	2007-01-09

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:

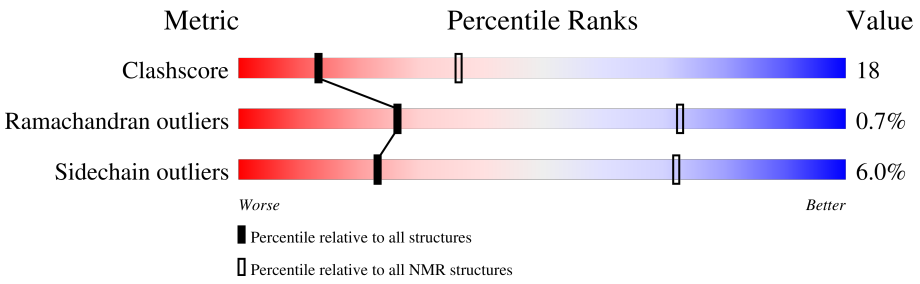
MolProbity	:	4.02b-467
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
RCI	:	v_1n_11_5_13_A (Berjanski et al., 2005)
PANAV	:	Wang et al. (2010)
ShiftChecker	:	2.27
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
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	129	46% 29% 25%

2 Ensemble composition and analysis (i)

This entry contains 20 models. Model 10 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:88-A:184 (97)	0.19	10

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 and 1 single-model cluster was found.

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

3 Entry composition (i)

There is only 1 type of molecule in this entry. The entry contains 1958 atoms, of which 978 are hydrogens and 0 are deuteriums.

- Molecule 1 is a protein called Putative ribosome-binding factor A.

Mol	Chain	Residues	Atoms						Trace
			Total	C	H	N	O	S	
1	A	129	1958	607	978	176	192	5	0

There are 14 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	79	GLY	-	cloning artifact	UNP Q8N0V3
A	80	SER	-	cloning artifact	UNP Q8N0V3
A	81	SER	-	cloning artifact	UNP Q8N0V3
A	82	GLY	-	cloning artifact	UNP Q8N0V3
A	83	SER	-	cloning artifact	UNP Q8N0V3
A	84	SER	-	cloning artifact	UNP Q8N0V3
A	85	GLY	-	cloning artifact	UNP Q8N0V3
A	122	VAL	MET	SEE REMARK 999	UNP Q8N0V3
A	202	SER	-	cloning artifact	UNP Q8N0V3
A	203	GLY	-	cloning artifact	UNP Q8N0V3
A	204	PRO	-	cloning artifact	UNP Q8N0V3
A	205	SER	-	cloning artifact	UNP Q8N0V3
A	206	SER	-	cloning artifact	UNP Q8N0V3
A	207	GLY	-	cloning artifact	UNP Q8N0V3

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: Putative ribosome-binding factor A

Chain A: 46% 29% 25%

G79 S80 S81 G82 S83 S84 G85 R86 K87 E88 D89 H90 A91 A95 L96 L99 L100 Y101 K102 A103 L104 T105 T110 P111 E112 V113 S114 Y118 D119 L120 L129 F133 S134 R137 W140 K141 T142 Q148 H151 M152 E153 A154 V155 L156 L166 L167 M168 S169 Q170

Q171 T172 L173 P177 P178 I179 V180 F181 K185 G186 N187 A188 A189 L190 A191 E192 L193 D194 Q195 L196 L197 A198 V199 A200 D201 S202 G203 P204 S205 S206 G207

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: Putative ribosome-binding factor A

Chain A: 47% 28% • 25%

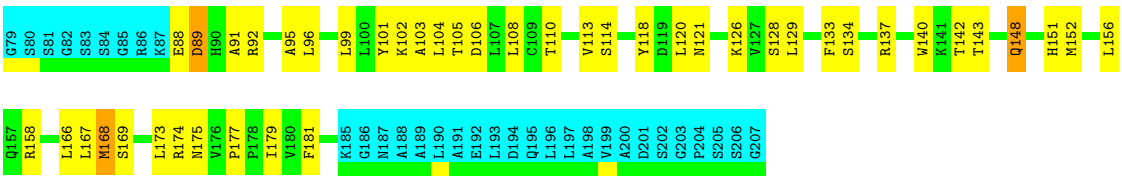
G79 S80 S81 G82 S83 S84 G85 R86 K87 E88 D89 H90 A91 R92 L93 R94 A95 L96 L99 L100 Y101 K102 A103 L104 T105 V113 S114 L117 Y118 D119 L120 N121 F133 S134 W140 K141 T142 T143 L144 Q148 V155 L156 L166 L167 M168 S169 Q170 Q171 T172 L173 R174 N175

V176 P177 P178 I179 V180 F181 K185 G186 N187 A188 A189 L190 A191 E192 L193 D194 Q195 L196 L197 A198 V199 A200 D201 S202 G203 P204 S205 S206 G207

4.2.2 Score per residue for model 2

• Molecule 1: Putative ribosome-binding factor A

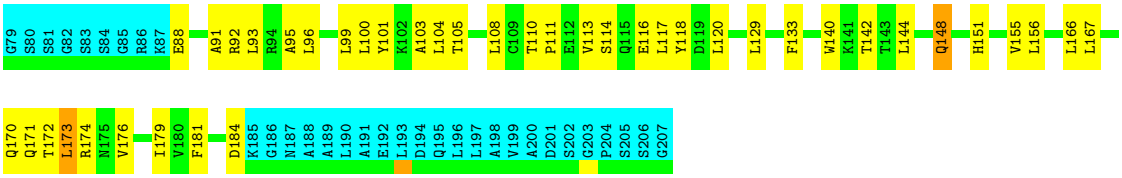
Chain A: 41% 32% • 25%



4.2.3 Score per residue for model 3

- Molecule 1: Putative ribosome-binding factor A

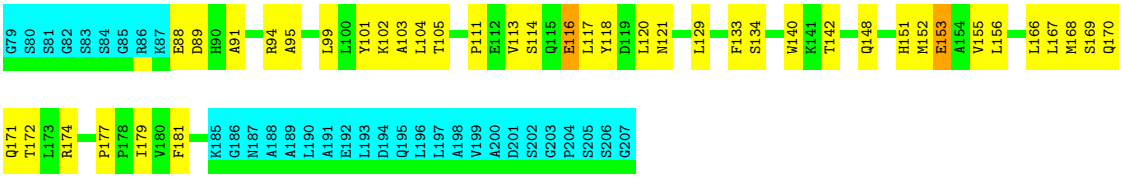
Chain A: 43% 30% • 25%



4.2.4 Score per residue for model 4

- Molecule 1: Putative ribosome-binding factor A

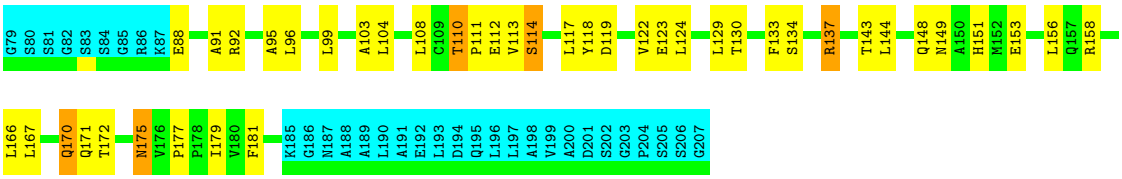
Chain A: 43% 30% • 25%



4.2.5 Score per residue for model 5

- Molecule 1: Putative ribosome-binding factor A

Chain A: 43% 29% • 25%



4.2.6 Score per residue for model 6

- Molecule 1: Putative ribosome-binding factor A

Chain A: 48% 26% • 25%

G79 S80 S81 G82 S83 S84 G85 R86 K87 E88 A91 R92 A95 L96 L99 L100 Y101 K102 A103 L104 T105 P111 E112 V113 S114 Y118 N121 L129 F133 S134 R137 Q148 H151 L156 L166 L167 Q171 T172 L173 R174 N175 V176 I179 V180 F181

V182 Q183 D184 K185 G186 N187 A188 A189 L190 A191 E192 L193 D194 Q195 L196 L197 A198 V199 A200 D201 S202 G203 P204 S205 S206 G207

4.2.7 Score per residue for model 7

- Molecule 1: Putative ribosome-binding factor A

Chain A: 55% 19% • 25%

G79 S80 S81 G82 S83 S84 G85 R86 K87 L96 Y101 K102 A103 L104 T105 T110 V113 S114 Y118 D119 L120 N121 F133 R137 W140 K141 T142 Q148 M152 V155 L156 L166 L167 L173 R174 N175 V176 I179 V180 F181 K185 G186 N187 A188 A189

L190 A191 E192 L193 D194 Q195 L196 L197 A198 V199 A200 D201 S202 G203 P204 S205 S206 G207

4.2.8 Score per residue for model 8

- Molecule 1: Putative ribosome-binding factor A

Chain A: 50% 24% • 25%

G79 S80 S81 G82 S83 S84 G85 R86 K87 E88 D89 H90 A91 R92 L96 Y101 K102 A103 L104 T105 D106 T110 P111 E112 V113 S114 L120 F133 R137 W140 K141 T142 T143 L144 S145 N149 E153 A154 V155 L156 L166 L167 Q171 T172 I179 V180 F181

K185 G186 N187 A188 A189 L190 A191 E192 L193 D194 Q195 L196 L197 A198 V199 A200 D201 S202 G203 P204 S205 S206 G207

4.2.9 Score per residue for model 9

- Molecule 1: Putative ribosome-binding factor A

Chain A: 50% 24% • 25%

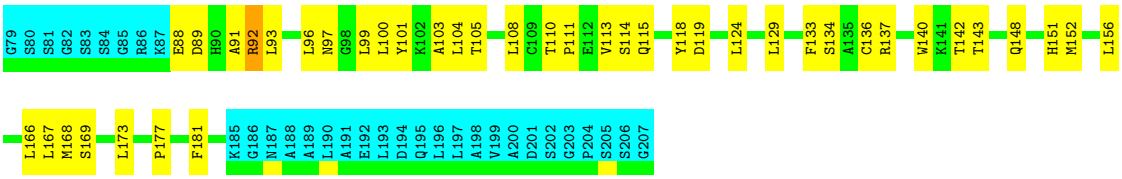
G79 S80 S81 G82 S83 S84 G85 R86 K87 A95 L96 L99 L100 Y101 K102 A103 L104 T105 V113 S114 Y118 N121 K126 V127 S128 L129 C136 R137 W140 K141 T142 T143 Q148 L156 Q157 R158 L166 L167 M168 S169 Q170 Q171 T172 L173 I179 V180 F181

K185 G186 N187 A188 A189 L190 A191 E192 L193 D194 Q195 L196 L197 A198 V199 A200 D201 S202 G203 P204 S205 S206 G207

4.2.10 Score per residue for model 10 (medoid)

- Molecule 1: Putative ribosome-binding factor A

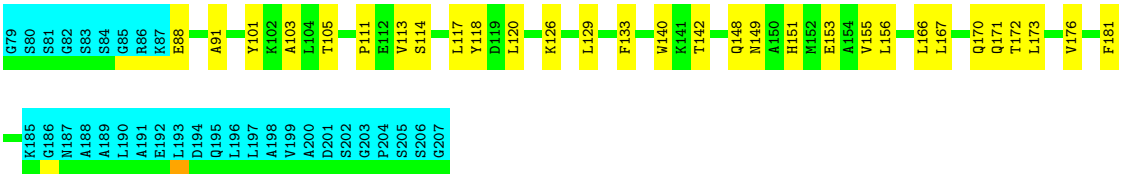
Chain A: 43% 31% • 25%



4.2.11 Score per residue for model 11

- Molecule 1: Putative ribosome-binding factor A

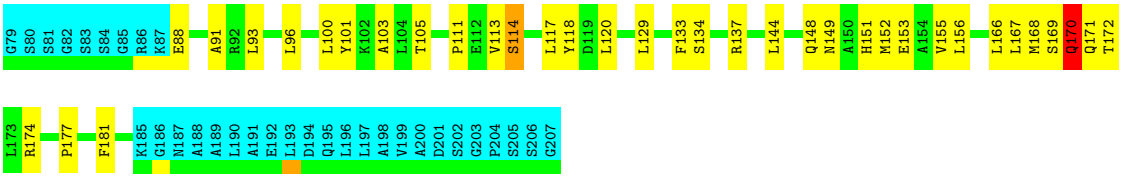
Chain A: 52% 23% 25%



4.2.12 Score per residue for model 12

- Molecule 1: Putative ribosome-binding factor A

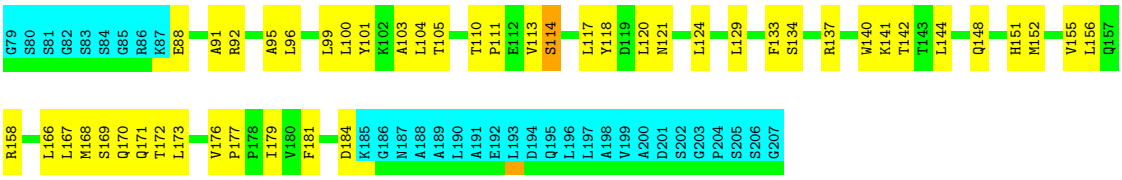
Chain A: 47% 26% •• 25%



4.2.13 Score per residue for model 13

- Molecule 1: Putative ribosome-binding factor A

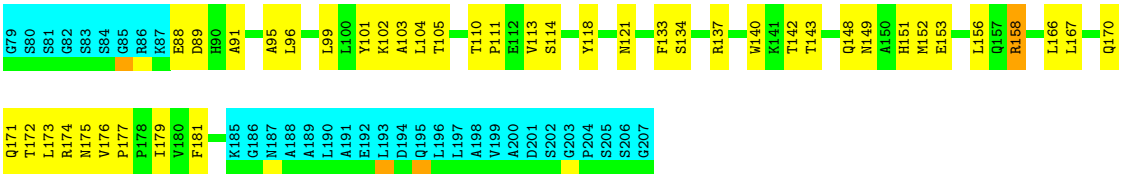
Chain A: 39% 36% • 25%



4.2.14 Score per residue for model 14

- Molecule 1: Putative ribosome-binding factor A

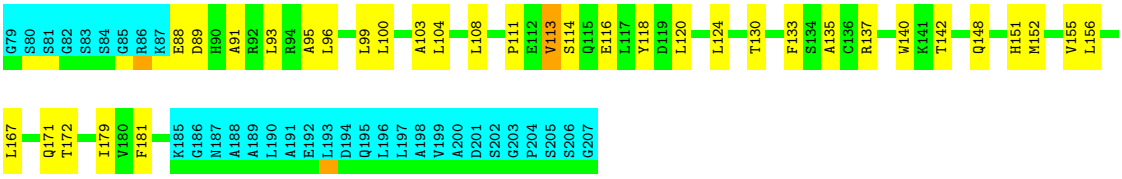
Chain A: 43% 32% • 25%



4.2.15 Score per residue for model 15

- Molecule 1: Putative ribosome-binding factor A

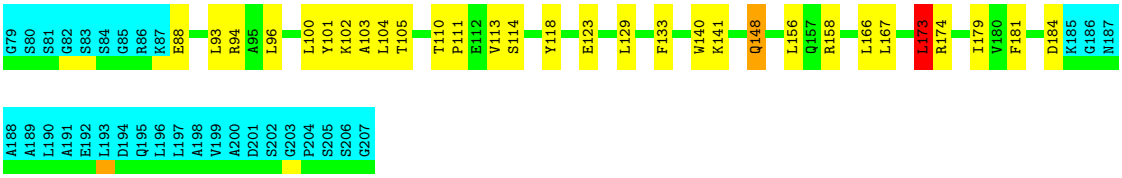
Chain A: 49% 26% • 25%



4.2.16 Score per residue for model 16

- Molecule 1: Putative ribosome-binding factor A

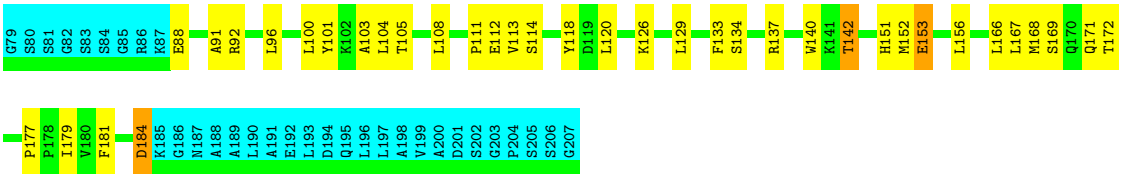
Chain A: 52% 22% •• 25%



4.2.17 Score per residue for model 17

- Molecule 1: Putative ribosome-binding factor A

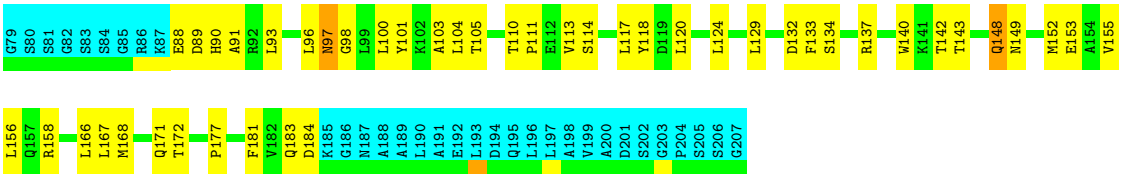
Chain A: 47% 26% • 25%



4.2.18 Score per residue for model 18

- Molecule 1: Putative ribosome-binding factor A

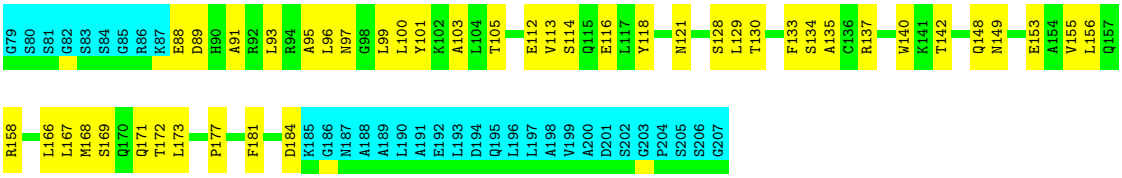
Chain A: 40% 33% • 25%



4.2.19 Score per residue for model 19

- Molecule 1: Putative ribosome-binding factor A

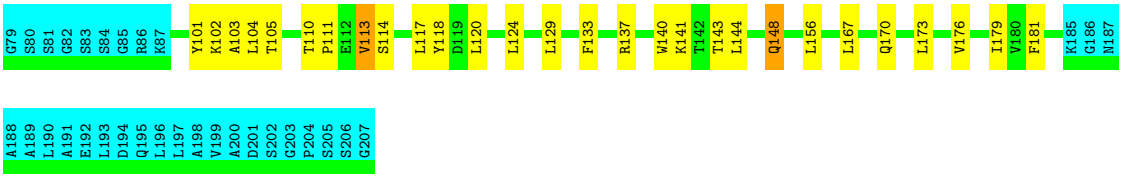
Chain A: 42% 33% 25%



4.2.20 Score per residue for model 20

- Molecule 1: Putative ribosome-binding factor A

Chain A: 53% 20% • 25%



5 Refinement protocol and experimental data overview (i)

The models were refined using the following method: *torsion angle dyanamics, restrainted molecular dynamics.*

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	772	773	773	28±5
All	All	15440	15460	15460	567

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 18.

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

Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:113:VAL:HG21	1:A:166:LEU:HD11	0.99	1.29	4	18
1:A:173:LEU:HD23	1:A:176:VAL:HG22	0.95	1.32	13	1
1:A:173:LEU:HD11	1:A:176:VAL:HG22	0.93	1.36	3	3
1:A:103:ALA:HB1	1:A:167:LEU:HD22	0.92	1.35	7	20
1:A:113:VAL:HG21	1:A:166:LEU:CD1	0.80	2.05	8	16
1:A:151:HIS:O	1:A:155:VAL:HG12	0.80	1.77	13	1
1:A:173:LEU:CD2	1:A:176:VAL:HG22	0.79	2.08	13	1
1:A:104:LEU:HD21	1:A:179:ILE:HD13	0.79	1.54	8	15
1:A:173:LEU:HD23	1:A:176:VAL:CG2	0.77	2.10	13	1
1:A:101:TYR:O	1:A:105:THR:HG22	0.76	1.79	16	18
1:A:173:LEU:C	1:A:173:LEU:HD22	0.70	2.07	16	2
1:A:103:ALA:CB	1:A:167:LEU:HD22	0.68	2.15	7	3
1:A:140:TRP:CZ3	1:A:142:THR:HG22	0.68	2.23	19	9
1:A:103:ALA:HB1	1:A:167:LEU:CD2	0.68	2.19	17	10

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:173:LEU:HD11	1:A:176:VAL:CG2	0.67	2.18	3	4
1:A:144:LEU:HD23	1:A:144:LEU:O	0.63	1.94	12	4
1:A:140:TRP:O	1:A:142:THR:HG23	0.63	1.93	11	4
1:A:113:VAL:HG13	1:A:114:SER:N	0.62	2.10	16	18
1:A:120:LEU:HD13	1:A:152:MET:HG2	0.62	1.71	17	6
1:A:173:LEU:HD21	1:A:175:ASN:O	0.61	1.95	14	1
1:A:104:LEU:HB3	1:A:124:LEU:HD11	0.61	1.73	5	5
1:A:96:LEU:CD2	1:A:100:LEU:HD12	0.60	2.26	9	10
1:A:96:LEU:HD22	1:A:129:LEU:HD22	0.59	1.74	9	3
1:A:120:LEU:HD11	1:A:155:VAL:HG11	0.58	1.74	8	7
1:A:97:ASN:OD1	1:A:97:ASN:C	0.58	2.42	18	1
1:A:113:VAL:HG13	1:A:114:SER:H	0.58	1.59	11	20
1:A:140:TRP:CH2	1:A:142:THR:CG2	0.57	2.87	17	1
1:A:172:THR:HG23	1:A:173:LEU:HD12	0.57	1.75	19	1
1:A:129:LEU:HD21	1:A:133:PHE:CD1	0.56	2.35	5	11
1:A:173:LEU:HD22	1:A:174:ARG:N	0.56	2.15	16	1
1:A:99:LEU:HD13	1:A:173:LEU:CB	0.56	2.30	6	1
1:A:117:LEU:HD11	1:A:156:LEU:HD13	0.56	1.77	11	5
1:A:140:TRP:CE3	1:A:141:LYS:O	0.55	2.59	16	3
1:A:140:TRP:CZ3	1:A:142:THR:CG2	0.55	2.89	17	1
1:A:96:LEU:HD23	1:A:96:LEU:O	0.55	2.01	15	10
1:A:110:THR:HG21	1:A:112:GLU:OE1	0.54	2.02	5	1
1:A:104:LEU:O	1:A:108:LEU:HD13	0.54	2.01	17	6
1:A:140:TRP:CH2	1:A:142:THR:HG22	0.53	2.39	17	12
1:A:143:THR:HG23	1:A:148:GLN:OE1	0.52	2.05	18	1
1:A:173:LEU:CD1	1:A:176:VAL:HG22	0.52	2.23	3	3
1:A:173:LEU:HD23	1:A:174:ARG:N	0.52	2.19	14	1
1:A:151:HIS:CD2	1:A:151:HIS:C	0.52	2.82	6	11
1:A:143:THR:HG23	1:A:148:GLN:NE2	0.52	2.20	10	3
1:A:99:LEU:HD13	1:A:173:LEU:CD1	0.51	2.36	19	1
1:A:96:LEU:HD21	1:A:100:LEU:CD1	0.51	2.36	18	2
1:A:158:ARG:O	1:A:158:ARG:NE	0.51	2.44	14	1
1:A:93:LEU:HD23	1:A:133:PHE:CE1	0.50	2.41	15	4
1:A:96:LEU:HD13	1:A:133:PHE:CD1	0.50	2.41	5	5
1:A:97:ASN:OD1	1:A:98:GLY:N	0.50	2.45	18	1
1:A:149:ASN:O	1:A:153:GLU:CB	0.50	2.60	18	6
1:A:148:GLN:CD	1:A:148:GLN:C	0.50	2.71	19	4
1:A:156:LEU:HD21	1:A:181:PHE:CD1	0.50	2.41	6	2
1:A:88:GLU:O	1:A:91:ALA:N	0.49	2.45	18	16
1:A:117:LEU:HD11	1:A:122:VAL:HG11	0.49	1.82	5	1
1:A:148:GLN:O	1:A:148:GLN:NE2	0.49	2.45	3	4

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:96:LEU:HD13	1:A:133:PHE:CE1	0.49	2.42	5	1
1:A:93:LEU:HG	1:A:133:PHE:CZ	0.49	2.42	18	2
1:A:100:LEU:HD13	1:A:136:CYS:SG	0.49	2.48	9	2
1:A:129:LEU:HD21	1:A:133:PHE:CE1	0.49	2.43	12	9
1:A:148:GLN:NE2	1:A:152:MET:SD	0.48	2.86	12	4
1:A:167:LEU:O	1:A:169:SER:N	0.48	2.47	2	1
1:A:113:VAL:CG1	1:A:114:SER:N	0.48	2.77	17	18
1:A:175:ASN:N	1:A:175:ASN:OD1	0.48	2.47	5	1
1:A:173:LEU:HD13	1:A:176:VAL:HG22	0.48	1.86	14	1
1:A:173:LEU:HD12	1:A:174:ARG:N	0.48	2.24	2	1
1:A:118:TYR:O	1:A:121:ASN:N	0.48	2.47	2	9
1:A:156:LEU:HG	1:A:181:PHE:CE2	0.47	2.44	15	19
1:A:156:LEU:HG	1:A:181:PHE:CD2	0.47	2.45	15	14
1:A:99:LEU:HD13	1:A:173:LEU:HB3	0.47	1.85	6	1
1:A:96:LEU:HD23	1:A:96:LEU:C	0.47	2.29	12	3
1:A:173:LEU:HD12	1:A:174:ARG:C	0.47	2.30	2	1
1:A:93:LEU:HD23	1:A:133:PHE:CZ	0.46	2.45	1	1
1:A:96:LEU:HD13	1:A:129:LEU:HD21	0.46	1.88	10	3
1:A:143:THR:OG1	1:A:144:LEU:N	0.46	2.48	20	3
1:A:88:GLU:CG	1:A:89:ASP:N	0.46	2.78	15	1
1:A:96:LEU:CD2	1:A:100:LEU:CD1	0.46	2.94	17	8
1:A:92:ARG:HD2	1:A:133:PHE:CZ	0.46	2.45	10	1
1:A:116:GLU:CD	1:A:116:GLU:C	0.46	2.75	19	1
1:A:134:SER:O	1:A:177:PRO:CB	0.46	2.64	19	11
1:A:170:GLN:N	1:A:170:GLN:CD	0.46	2.69	12	2
1:A:173:LEU:N	1:A:173:LEU:CD1	0.46	2.79	9	2
1:A:148:GLN:CD	1:A:148:GLN:O	0.46	2.54	16	1
1:A:116:GLU:OE1	1:A:155:VAL:HG21	0.45	2.11	19	1
1:A:88:GLU:O	1:A:89:ASP:C	0.45	2.55	18	7
1:A:122:VAL:HG22	1:A:123:GLU:N	0.45	2.27	5	1
1:A:99:LEU:HD13	1:A:173:LEU:CD2	0.45	2.42	1	1
1:A:171:GLN:O	1:A:172:THR:C	0.45	2.55	9	15
1:A:93:LEU:O	1:A:97:ASN:ND2	0.45	2.49	19	1
1:A:173:LEU:CD2	1:A:174:ARG:N	0.45	2.80	16	1
1:A:143:THR:CG2	1:A:148:GLN:OE1	0.45	2.65	18	1
1:A:153:GLU:OE1	1:A:153:GLU:C	0.45	2.55	4	1
1:A:130:THR:HG23	1:A:135:ALA:O	0.44	2.12	19	2
1:A:116:GLU:C	1:A:116:GLU:OE1	0.44	2.55	19	1
1:A:112:GLU:CG	1:A:113:VAL:N	0.44	2.79	19	1
1:A:95:ALA:O	1:A:99:LEU:CG	0.44	2.66	3	11
1:A:117:LEU:CD1	1:A:156:LEU:HD13	0.44	2.42	3	2

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:173:LEU:HD13	1:A:175:ASN:O	0.44	2.12	2	1
1:A:105:THR:HB	1:A:124:LEU:HD12	0.44	1.90	13	1
1:A:90:HIS:CD2	1:A:90:HIS:C	0.44	2.91	18	1
1:A:174:ARG:O	1:A:175:ASN:C	0.44	2.55	6	1
1:A:89:ASP:OD2	1:A:93:LEU:HD11	0.44	2.13	10	1
1:A:148:GLN:NE2	1:A:148:GLN:C	0.44	2.71	3	2
1:A:184:ASP:O	1:A:184:ASP:CG	0.43	2.55	17	2
1:A:114:SER:OG	1:A:117:LEU:CB	0.43	2.66	5	3
1:A:173:LEU:CD1	1:A:176:VAL:CG2	0.43	2.96	6	1
1:A:148:GLN:NE2	1:A:149:ASN:OD1	0.43	2.51	5	1
1:A:152:MET:O	1:A:155:VAL:CG1	0.43	2.66	7	3
1:A:130:THR:CG2	1:A:137:ARG:NH1	0.43	2.82	5	1
1:A:183:GLN:O	1:A:184:ASP:C	0.43	2.57	6	2
1:A:148:GLN:OE1	1:A:148:GLN:C	0.43	2.57	9	3
1:A:111:PRO:HB3	1:A:118:TYR:CG	0.43	2.49	12	14
1:A:173:LEU:C	1:A:173:LEU:CD2	0.43	2.79	16	1
1:A:96:LEU:HD23	1:A:100:LEU:HD12	0.43	1.90	1	1
1:A:116:GLU:HG3	1:A:155:VAL:CG2	0.43	2.44	4	1
1:A:140:TRP:CE3	1:A:142:THR:HG22	0.43	2.48	19	1
1:A:112:GLU:HG3	1:A:113:VAL:N	0.42	2.28	19	1
1:A:143:THR:HG23	1:A:148:GLN:HE22	0.42	1.73	2	1
1:A:130:THR:HG23	1:A:137:ARG:NH1	0.42	2.28	5	1
1:A:173:LEU:HD11	1:A:176:VAL:HG23	0.42	1.89	20	1
1:A:99:LEU:HD13	1:A:173:LEU:HG	0.42	1.91	10	1
1:A:111:PRO:HB3	1:A:118:TYR:CD2	0.42	2.49	15	2
1:A:168:MET:O	1:A:169:SER:C	0.42	2.58	1	8
1:A:167:LEU:O	1:A:170:GLN:CD	0.42	2.58	5	1
1:A:148:GLN:C	1:A:148:GLN:OE1	0.42	2.58	7	1
1:A:152:MET:HA	1:A:155:VAL:CG1	0.42	2.45	13	1
1:A:116:GLU:CD	1:A:116:GLU:O	0.42	2.57	19	1
1:A:95:ALA:O	1:A:99:LEU:HD12	0.41	2.15	2	1
1:A:140:TRP:O	1:A:141:LYS:C	0.41	2.58	20	1
1:A:174:ARG:HG3	1:A:175:ASN:N	0.41	2.30	14	1
1:A:173:LEU:HD13	1:A:173:LEU:N	0.41	2.30	16	1
1:A:128:SER:O	1:A:137:ARG:O	0.41	2.39	19	3
1:A:167:LEU:C	1:A:169:SER:N	0.41	2.73	2	1
1:A:92:ARG:CZ	1:A:92:ARG:HB2	0.41	2.46	6	1
1:A:113:VAL:CG2	1:A:166:LEU:HD11	0.41	2.23	8	1
1:A:152:MET:O	1:A:156:LEU:CB	0.41	2.69	13	1
1:A:111:PRO:O	1:A:112:GLU:C	0.41	2.59	17	1
1:A:153:GLU:OE2	1:A:153:GLU:C	0.41	2.59	17	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:143:THR:CG2	1:A:148:GLN:HG2	0.41	2.46	20	1
1:A:167:LEU:O	1:A:168:MET:C	0.41	2.59	2	1
1:A:117:LEU:HA	1:A:120:LEU:HD12	0.41	1.93	20	1
1:A:100:LEU:O	1:A:104:LEU:CG	0.40	2.69	17	1
1:A:110:THR:CG2	1:A:112:GLU:OE1	0.40	2.70	5	1
1:A:173:LEU:CD2	1:A:175:ASN:O	0.40	2.69	14	1
1:A:116:GLU:HG2	1:A:117:LEU:N	0.40	2.32	4	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	97/129 (75%)	87±1 (90±1%)	9±2 (10±2%)	1±1 (1±1%)	26	73
All	All	1940/2580 (75%)	1740 (90%)	187 (10%)	13 (1%)	26	73

All 4 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	170	GLN	8
1	A	173	LEU	3
1	A	168	MET	1
1	A	184	ASP	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	86/107 (80%)	81±2 (94±2%)	5±2 (6±2%)	23	72

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
All	All	1720/2140 (80%)	1617 (94%)	103 (6%)	23 72

All 31 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	137	ARG	12
1	A	110	THR	11
1	A	148	GLN	9
1	A	158	ARG	8
1	A	92	ARG	7
1	A	102	LYS	5
1	A	126	LYS	4
1	A	184	ASP	4
1	A	175	ASN	3
1	A	89	ASP	3
1	A	116	GLU	3
1	A	174	ARG	3
1	A	153	GLU	3
1	A	114	SER	3
1	A	106	ASP	2
1	A	94	ARG	2
1	A	119	ASP	2
1	A	141	LYS	2
1	A	170	GLN	2
1	A	173	LEU	2
1	A	97	ASN	2
1	A	113	VAL	2
1	A	144	LEU	1
1	A	134	SER	1
1	A	112	GLU	1
1	A	145	SER	1
1	A	115	GLN	1
1	A	123	GLU	1
1	A	142	THR	1
1	A	132	ASP	1
1	A	168	MET	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