Full wwPDB NMR Structure Validation Report (i)

Feb 27, 2022 – 11:07 AM EST

PDB ID	:	2CTQ
Title	:	Solution structure of J-domain from human DnaJ subfamily C menber 12
Authors	:	Kobayashi, N.; Tochio, N.; Koshiba, S.; Inoue, M.; Kigawa, T.; Yokoyama, S.; RIKEN Structural Genomics/Proteomics Initiative (RSGI)
Deposited on	:	2005-05-24

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:

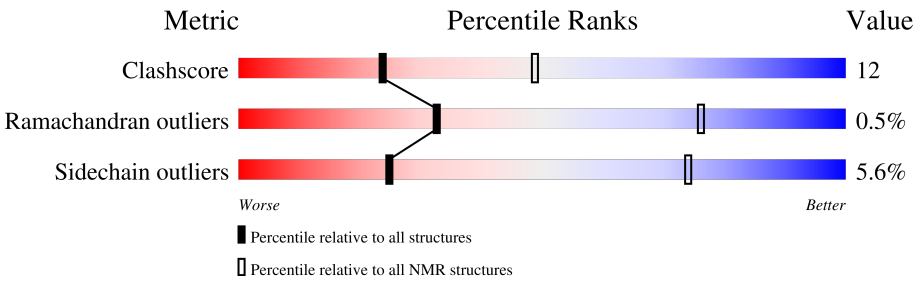
MolProbity	:	4.02b-467
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
RCI	:	v_1n_11_5_13_A (Berjanski et al., 2005)
PANAV	:	Wang et al. (2010)
ShiftChecker	:	2.27
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
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	112	56% 13% 30%

2 Ensemble composition and analysis (i)

This entry contains 20 models. Model 6 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:21-A:98 (78)	0.38	6

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 4 clusters and 1 single-model cluster was found.

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

3 Entry composition (i)

There is only 1 type of molecule in this entry. The entry contains 1734 atoms, of which 843 are hydrogens and 0 are deuteriums.

- Molecule 1 is a protein called DnaJ homolog subfamily C member 12.

Mol	Chain	Residues	Atoms						Trace
			Total	C	H	N	O	S	
1	A	112	1734	548	843	155	183	5	0

There are 13 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	1	GLY	-	cloning artifact	UNP Q9UKB3
A	2	SER	-	cloning artifact	UNP Q9UKB3
A	3	SER	-	cloning artifact	UNP Q9UKB3
A	4	GLY	-	cloning artifact	UNP Q9UKB3
A	5	SER	-	cloning artifact	UNP Q9UKB3
A	6	SER	-	cloning artifact	UNP Q9UKB3
A	7	GLY	-	cloning artifact	UNP Q9UKB3
A	107	SER	-	cloning artifact	UNP Q9UKB3
A	108	GLY	-	cloning artifact	UNP Q9UKB3
A	109	PRO	-	cloning artifact	UNP Q9UKB3
A	110	SER	-	cloning artifact	UNP Q9UKB3
A	111	SER	-	cloning artifact	UNP Q9UKB3
A	112	GLY	-	cloning artifact	UNP Q9UKB3

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: DnaJ homolog subfamily C member 12

Chain A: 56% 13% 30%

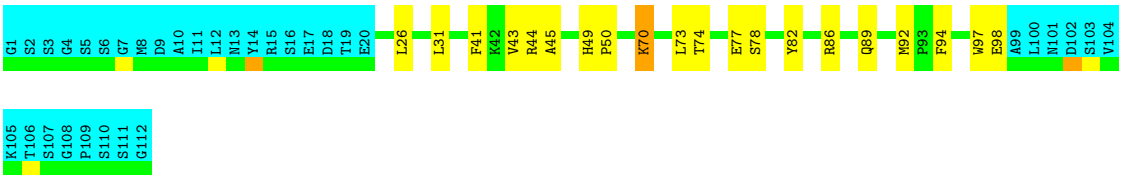
4.2 Scores per residue for each member of the ensemble

Colouring as in section 4.1 above.

4.2.1 Score per residue for model 1

• Molecule 1: DnaJ homolog subfamily C member 12

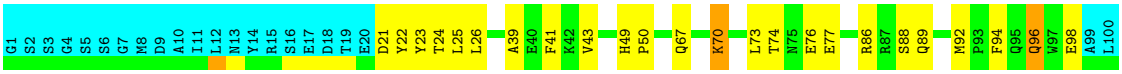
Chain A: 52% 17% • 30%



4.2.2 Score per residue for model 2

• Molecule 1: DnaJ homolog subfamily C member 12

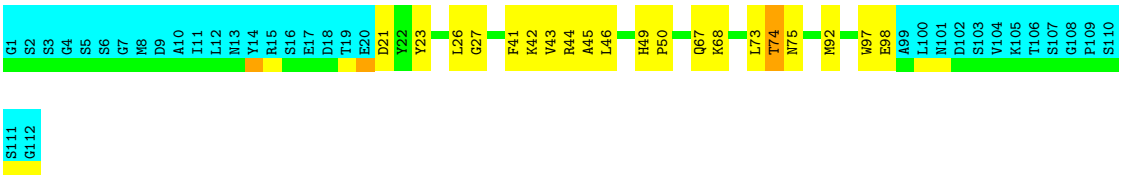
Chain A: 48% 20% • 30%



4.2.3 Score per residue for model 3

• Molecule 1: DnaJ homolog subfamily C member 12

Chain A:



4.2.4 Score per residue for model 4

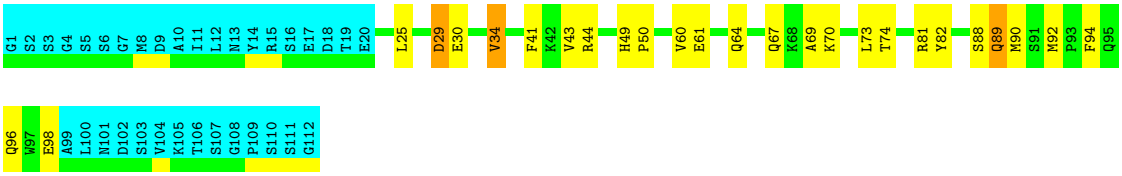
• Molecule 1: DnaJ homolog subfamily C member 12

Chain A:

4.2.5 Score per residue for model 5

• Molecule 1: DnaJ homolog subfamily C member 12

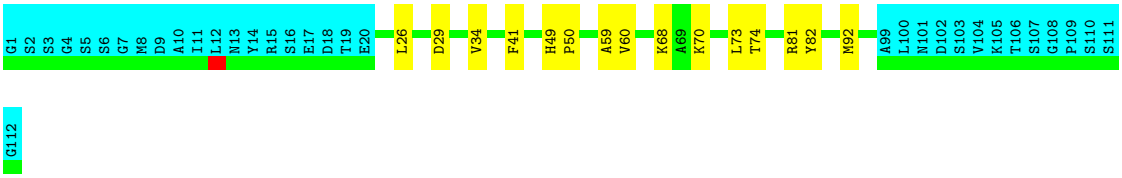
Chain A:



4.2.6 Score per residue for model 6 (medoid)

• Molecule 1: DnaJ homolog subfamily C member 12

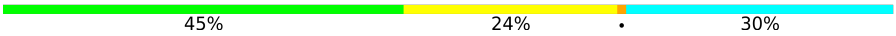
Chain A:

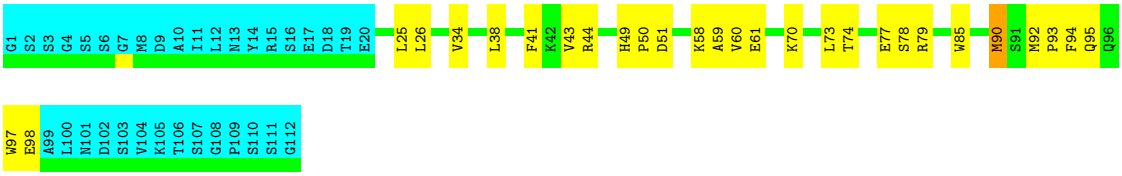


4.2.7 Score per residue for model 7

- Molecule 1: DnaJ homolog subfamily C member 12

Chain A:





4.2.8 Score per residue for model 8

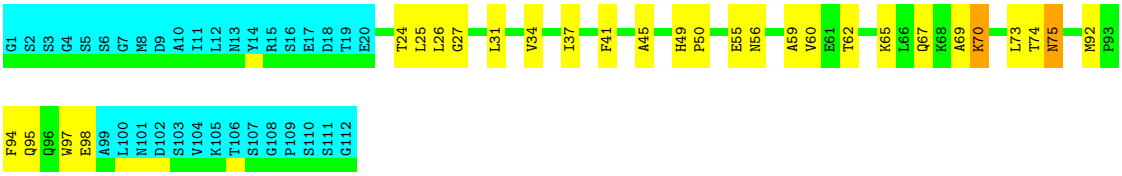
- Molecule 1: DnaJ homolog subfamily C member 12

Chain A:

4.2.9 Score per residue for model 9

- Molecule 1: DnaJ homolog subfamily C member 12

Chain A:



4.2.10 Score per residue for model 10

- Molecule 1: DnaJ homolog subfamily C member 12

Chain A: 52% 17% • 30%

G1 S2 S3 G4 S5 S6 G7 M8 D9 A10 I11 L12 N13 Y14 R15 S16 E17 D18 T19 E20 L26 V34 F41 K42 V43 R44 H49 P50 D51 N56 V60 F63 Q64 K65 K68 E71 I72 L73 T74 N75 M92 P93 F94 W97 E98 A99 L100 N101 D102

S103 V104 K105 T106 S107 G108 P109 S110 S111 G112

4.2.11 Score per residue for model 11

- Molecule 1: DnaJ homolog subfamily C member 12

Chain A: 50% 20% 30%

G1 S2 S3 G4 S5 S6 G7 M8 D9 A10 I11 L12 N13 Y14 R15 S16 E17 D18 T19 E20 L26 D29 L38 A39 E40 F41 K42 V43 R44 C48 H49 P50 A59 V60 E61 T62 L66 Q67 K70 L73 T74 D83 N92 W97 E98 A99 L100 N101 D102

S103 V104 K105 T106 S107 G108 P109 S110 S111 G112

4.2.12 Score per residue for model 12

- Molecule 1: DnaJ homolog subfamily C member 12

Chain A: 44% 24% • 30%

G1 S2 S3 G4 S5 S6 G7 M8 D9 A10 I11 L12 N13 Y14 R15 S16 E17 D18 T19 E20 Y23 T24 L25 L26 D29 V34 E35 Q36 I37 L38 F41 K42 V43 R44 A45 H49 P50 D51 K52 K58 A59 K65 L66 A69 K70 L73 T74 N75 E76 Y82

D83 H84 W85 M92 W97 E98 A99 L100 N101 D102 S103 V104 K105 T106 S107 G108 P109 S110 S111 G112

4.2.13 Score per residue for model 13

- Molecule 1: DnaJ homolog subfamily C member 12

Chain A: 54% 15% 30%

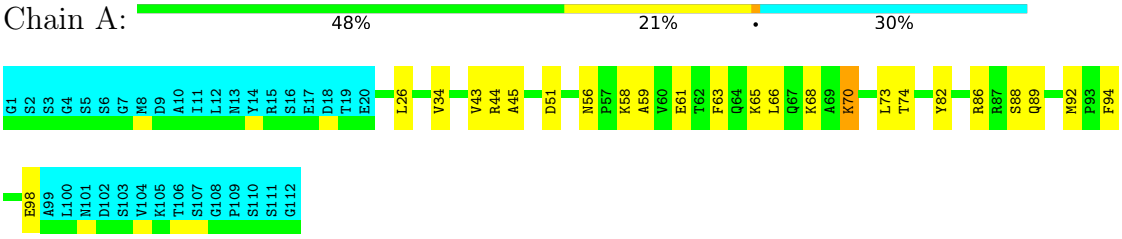
G1 S2 S3 G4 S5 S6 G7 M8 D9 A10 I11 L12 N13 Y14 R15 S16 E17 D18 T19 E20 L25 L26 L31 F41 H49 P50 K58 A69 K70 L73 T74 D83 H84 W85 R86 M92 P93 F94 E98 A99 L100 N101 D102 S103 V104 K105 T106 S107 G108 P109

S110 S111 G112

4.2.14 Score per residue for model 14

• Molecule 1: DnaJ homolog subfamily C member 12

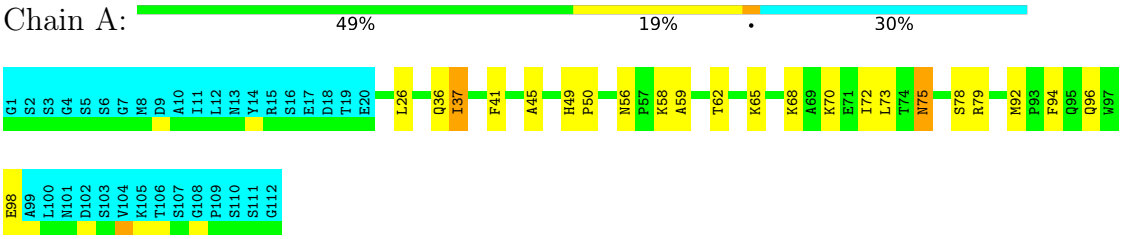
Chain A:



4.2.15 Score per residue for model 15

• Molecule 1: DnaJ homolog subfamily C member 12

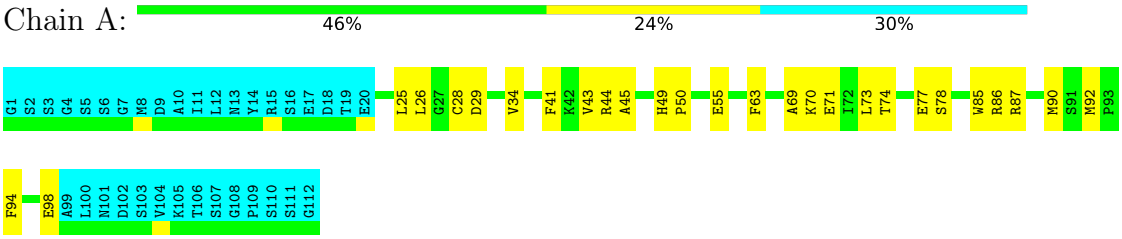
Chain A:



4.2.16 Score per residue for model 16

• Molecule 1: DnaJ homolog subfamily C member 12

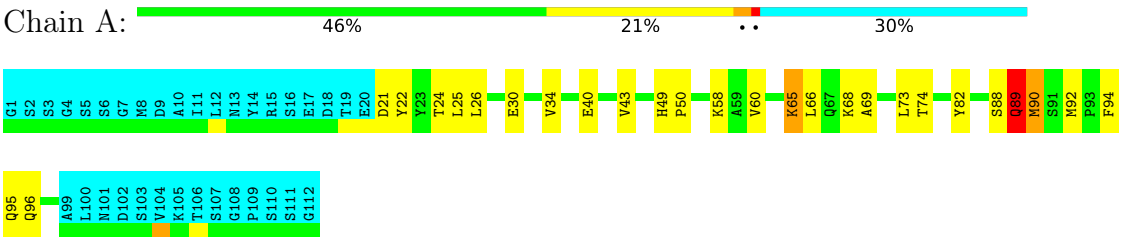
Chain A:



4.2.17 Score per residue for model 17

• Molecule 1: DnaJ homolog subfamily C member 12

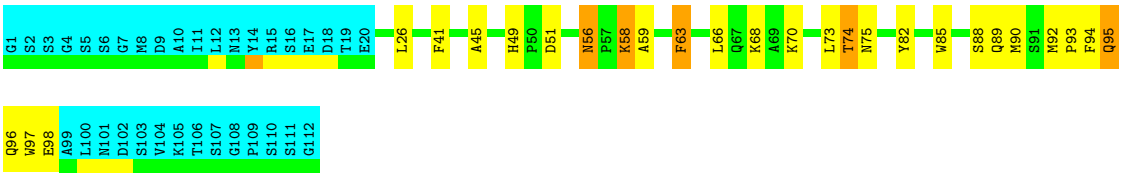
Chain A:



4.2.18 Score per residue for model 18

- Molecule 1: DnaJ homolog subfamily C member 12

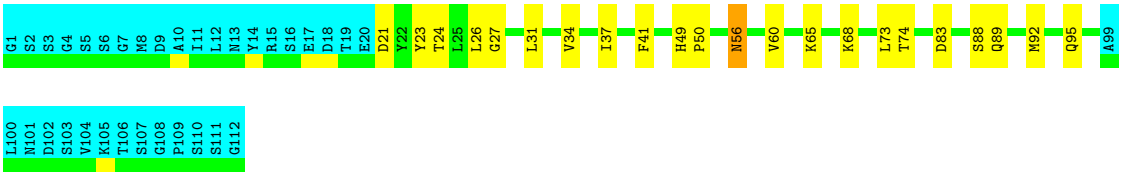
Chain A: 46% 20% • 30%



4.2.19 Score per residue for model 19

- Molecule 1: DnaJ homolog subfamily C member 12

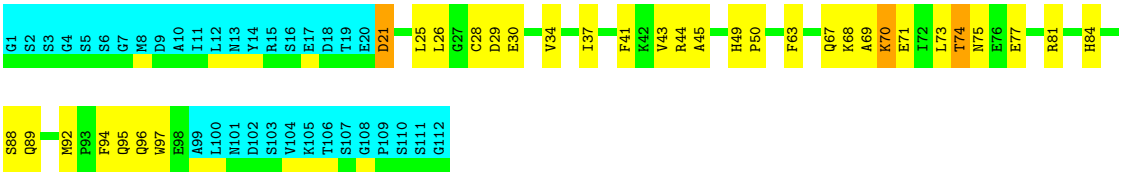
Chain A: 50% 19% • 30%



4.2.20 Score per residue for model 20

- Molecule 1: DnaJ homolog subfamily C member 12

Chain A: 40% 27% • 30%



5 Refinement protocol and experimental data overview (i)

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

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

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	657	630	630	16±4
All	All	13140	12600	12600	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 12.

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

Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:45:ALA:HB1	1:A:63:PHE:CE2	0.77	2.15	14	1
1:A:26:LEU:HD12	1:A:73:LEU:HD12	0.77	1.55	19	16
1:A:25:LEU:HD13	1:A:65:LYS:HG3	0.76	1.58	12	1
1:A:39:ALA:O	1:A:43:VAL:HG22	0.76	1.80	8	2
1:A:34:VAL:HG23	1:A:74:THR:HG22	0.73	1.59	10	9
1:A:56:ASN:ND2	1:A:59:ALA:HB2	0.69	2.03	9	2
1:A:26:LEU:HD22	1:A:41:PHE:HB2	0.69	1.63	13	6
1:A:34:VAL:HG13	1:A:35:GLU:OE1	0.67	1.89	12	1
1:A:70:LYS:O	1:A:74:THR:HG23	0.67	1.90	12	9
1:A:45:ALA:HB1	1:A:63:PHE:CE1	0.66	2.25	20	2
1:A:25:LEU:HD12	1:A:69:ALA:HB2	0.66	1.66	13	7
1:A:42:LYS:O	1:A:46:LEU:HD23	0.66	1.90	3	1
1:A:50:PRO:HB3	1:A:60:VAL:HG22	0.65	1.66	9	6
1:A:94:PHE:CE2	1:A:98:GLU:CD	0.65	2.70	14	3

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:25:LEU:HD22	1:A:65:LYS:CD	0.62	2.24	12	2
1:A:26:LEU:HD13	1:A:37:ILE:CG2	0.60	2.26	19	3
1:A:26:LEU:HD23	1:A:66:LEU:HD23	0.60	1.72	12	3
1:A:85:TRP:CD1	1:A:90:MET:SD	0.60	2.95	7	3
1:A:94:PHE:CE1	1:A:98:GLU:OE1	0.60	2.55	18	1
1:A:34:VAL:HG13	1:A:74:THR:HG22	0.59	1.74	20	1
1:A:45:ALA:HB1	1:A:63:PHE:CZ	0.59	2.32	14	2
1:A:25:LEU:HD22	1:A:65:LYS:HD3	0.57	1.76	12	1
1:A:45:ALA:HB1	1:A:63:PHE:HE1	0.56	1.60	20	1
1:A:26:LEU:CD2	1:A:66:LEU:HD23	0.55	2.31	12	1
1:A:26:LEU:HD11	1:A:70:LYS:CA	0.55	2.31	20	2
1:A:56:ASN:ND2	1:A:59:ALA:CB	0.55	2.69	9	1
1:A:26:LEU:HD11	1:A:70:LYS:HA	0.55	1.79	20	3
1:A:43:VAL:HG23	1:A:44:ARG:N	0.54	2.18	16	11
1:A:26:LEU:HD12	1:A:73:LEU:CD1	0.52	2.33	19	4
1:A:96:GLN:NE2	1:A:96:GLN:C	0.52	2.62	2	1
1:A:94:PHE:CZ	1:A:98:GLU:CD	0.52	2.83	2	1
1:A:85:TRP:CE3	1:A:86:ARG:N	0.52	2.77	16	1
1:A:49:HIS:CE1	1:A:51:ASP:HB3	0.52	2.40	18	1
1:A:41:PHE:CD2	1:A:70:LYS:HD3	0.52	2.39	7	1
1:A:38:LEU:HD23	1:A:70:LYS:HD2	0.51	1.82	7	1
1:A:31:LEU:HD12	1:A:31:LEU:H	0.50	1.66	13	4
1:A:26:LEU:CD1	1:A:73:LEU:HD12	0.50	2.35	19	3
1:A:41:PHE:CE1	1:A:67:GLN:HA	0.50	2.42	5	6
1:A:62:THR:HG23	1:A:65:LYS:HZ2	0.50	1.67	9	1
1:A:75:ASN:OD1	1:A:78:SER:CB	0.49	2.60	15	1
1:A:45:ALA:HB1	1:A:63:PHE:CD1	0.49	2.42	16	1
1:A:21:ASP:O	1:A:24:THR:N	0.49	2.46	2	1
1:A:94:PHE:CZ	1:A:98:GLU:OE1	0.49	2.65	2	2
1:A:60:VAL:HG12	1:A:64:GLN:NE2	0.49	2.23	5	1
1:A:41:PHE:O	1:A:45:ALA:CB	0.49	2.60	1	3
1:A:95:GLN:OE1	1:A:96:GLN:N	0.49	2.45	18	1
1:A:23:TYR:CE2	1:A:86:ARG:NH1	0.49	2.81	2	1
1:A:89:GLN:NE2	1:A:89:GLN:O	0.49	2.46	17	1
1:A:29:ASP:OD1	1:A:29:ASP:N	0.48	2.45	5	2
1:A:34:VAL:HG23	1:A:74:THR:HA	0.48	1.86	9	3
1:A:38:LEU:O	1:A:41:PHE:N	0.48	2.47	4	3
1:A:62:THR:HG22	1:A:66:LEU:HD12	0.48	1.86	11	1
1:A:50:PRO:CB	1:A:60:VAL:HG22	0.48	2.38	9	2
1:A:94:PHE:CE2	1:A:98:GLU:HG3	0.48	2.43	4	1
1:A:26:LEU:HD23	1:A:66:LEU:CD2	0.48	2.39	18	2

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:94:PHE:CE1	1:A:98:GLU:CD	0.48	2.86	13	2
1:A:73:LEU:O	1:A:75:ASN:N	0.47	2.47	18	4
1:A:56:ASN:N	1:A:56:ASN:OD1	0.47	2.47	18	1
1:A:62:THR:HG23	1:A:65:LYS:NZ	0.47	2.24	9	1
1:A:82:TYR:CE2	1:A:86:ARG:HD2	0.47	2.45	14	1
1:A:86:ARG:O	1:A:89:GLN:NE2	0.47	2.47	1	1
1:A:49:HIS:CE1	1:A:51:ASP:HB2	0.47	2.44	10	2
1:A:70:LYS:O	1:A:74:THR:CG2	0.47	2.60	2	1
1:A:41:PHE:CD2	1:A:70:LYS:HD2	0.47	2.45	4	2
1:A:21:ASP:OD1	1:A:21:ASP:N	0.46	2.48	20	1
1:A:81:ARG:O	1:A:84:HIS:N	0.46	2.48	20	1
1:A:49:HIS:CD2	1:A:63:PHE:CE1	0.46	3.04	20	1
1:A:41:PHE:CE2	1:A:70:LYS:HD2	0.46	2.46	16	3
1:A:96:GLN:C	1:A:96:GLN:CD	0.46	2.74	2	1
1:A:22:TYR:HB2	1:A:82:TYR:CE2	0.46	2.45	17	2
1:A:83:ASP:O	1:A:86:ARG:N	0.46	2.48	13	1
1:A:63:PHE:O	1:A:66:LEU:N	0.46	2.49	8	1
1:A:75:ASN:O	1:A:79:ARG:CB	0.46	2.64	15	1
1:A:93:PRO:CG	1:A:95:GLN:NE2	0.45	2.79	18	1
1:A:45:ALA:O	1:A:49:HIS:N	0.45	2.49	15	2
1:A:23:TYR:O	1:A:27:GLY:N	0.45	2.49	19	2
1:A:73:LEU:O	1:A:74:THR:C	0.45	2.55	18	15
1:A:96:GLN:NE2	1:A:96:GLN:O	0.45	2.50	2	1
1:A:58:LYS:O	1:A:61:GLU:N	0.45	2.49	7	1
1:A:26:LEU:HD11	1:A:70:LYS:N	0.45	2.26	20	1
1:A:82:TYR:CD1	1:A:82:TYR:C	0.45	2.90	17	1
1:A:65:LYS:O	1:A:68:LYS:N	0.45	2.50	17	2
1:A:93:PRO:HG2	1:A:95:GLN:NE2	0.45	2.27	18	1
1:A:82:TYR:HA	1:A:94:PHE:CE1	0.45	2.47	1	1
1:A:97:TRP:O	1:A:98:GLU:C	0.45	2.55	18	7
1:A:88:SER:O	1:A:89:GLN:C	0.45	2.56	4	8
1:A:25:LEU:O	1:A:44:ARG:CZ	0.45	2.65	7	1
1:A:82:TYR:O	1:A:85:TRP:N	0.45	2.50	12	1
1:A:21:ASP:O	1:A:22:TYR:C	0.44	2.56	2	1
1:A:48:CYS:O	1:A:59:ALA:HB1	0.44	2.13	11	1
1:A:38:LEU:HD21	1:A:70:LYS:CE	0.44	2.42	12	2
1:A:82:TYR:C	1:A:82:TYR:CD1	0.44	2.91	18	1
1:A:94:PHE:CE2	1:A:98:GLU:OE1	0.44	2.71	5	2
1:A:25:LEU:O	1:A:44:ARG:NH1	0.44	2.50	7	1
1:A:61:GLU:O	1:A:64:GLN:N	0.44	2.51	5	1
1:A:43:VAL:HG23	1:A:44:ARG:H	0.44	1.71	10	2

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:85:TRP:CE3	1:A:85:TRP:C	0.44	2.91	13	1
1:A:49:HIS:CG	1:A:50:PRO:HD2	0.44	2.48	6	16
1:A:94:PHE:O	1:A:97:TRP:N	0.43	2.50	18	2
1:A:77:GLU:CG	1:A:78:SER:N	0.43	2.81	1	2
1:A:70:LYS:HD3	1:A:71:GLU:N	0.43	2.28	8	2
1:A:55:GLU:CD	1:A:55:GLU:O	0.43	2.57	9	1
1:A:88:SER:O	1:A:90:MET:N	0.43	2.52	17	1
1:A:72:ILE:O	1:A:75:ASN:ND2	0.43	2.51	15	1
1:A:70:LYS:C	1:A:70:LYS:CD	0.42	2.88	1	1
1:A:76:GLU:O	1:A:77:GLU:C	0.42	2.57	2	1
1:A:62:THR:HG22	1:A:66:LEU:CD1	0.42	2.44	11	1
1:A:86:ARG:HG3	1:A:87:ARG:N	0.42	2.29	16	1
1:A:33:SER:O	1:A:34:VAL:C	0.42	2.57	8	1
1:A:28:CYS:O	1:A:29:ASP:CG	0.42	2.57	20	1
1:A:77:GLU:HG3	1:A:78:SER:N	0.42	2.29	1	2
1:A:41:PHE:CD2	1:A:70:LYS:HG3	0.42	2.49	6	1
1:A:94:PHE:O	1:A:95:GLN:C	0.42	2.57	7	6
1:A:70:LYS:HE2	1:A:74:THR:HG21	0.42	1.90	12	1
1:A:81:ARG:O	1:A:82:TYR:C	0.42	2.58	5	3
1:A:23:TYR:CD1	1:A:29:ASP:HA	0.42	2.50	12	1
1:A:24:THR:O	1:A:27:GLY:N	0.42	2.52	9	2
1:A:62:THR:HG23	1:A:65:LYS:HE2	0.42	1.90	15	1
1:A:58:LYS:HD3	1:A:59:ALA:N	0.42	2.30	12	1
1:A:94:PHE:O	1:A:96:GLN:N	0.41	2.53	15	1
1:A:89:GLN:O	1:A:90:MET:C	0.41	2.59	17	1
1:A:58:LYS:O	1:A:59:ALA:C	0.41	2.59	7	3
1:A:93:PRO:O	1:A:94:PHE:C	0.41	2.58	7	1
1:A:75:ASN:ND2	1:A:75:ASN:C	0.41	2.71	15	1
1:A:82:TYR:O	1:A:83:ASP:C	0.41	2.58	12	1
1:A:96:GLN:CD	1:A:96:GLN:O	0.41	2.59	2	1
1:A:56:ASN:HD22	1:A:59:ALA:HB2	0.41	1.72	9	1
1:A:59:ALA:O	1:A:60:VAL:C	0.41	2.57	6	1
1:A:40:GLU:O	1:A:43:VAL:CG2	0.41	2.68	17	1
1:A:38:LEU:O	1:A:39:ALA:C	0.41	2.59	4	2
1:A:73:LEU:HD23	1:A:79:ARG:HD2	0.41	1.92	7	1
1:A:56:ASN:OD1	1:A:56:ASN:N	0.41	2.54	19	1
1:A:31:LEU:H	1:A:31:LEU:HD12	0.41	1.76	9	1
1:A:41:PHE:CD1	1:A:66:LEU:O	0.41	2.74	11	1
1:A:28:CYS:C	1:A:29:ASP:OD1	0.41	2.59	16	1
1:A:95:GLN:CG	1:A:96:GLN:N	0.41	2.84	17	1
1:A:70:LYS:CD	1:A:71:GLU:N	0.41	2.84	8	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:71:GLU:OE2	1:A:75:ASN:ND2	0.41	2.54	10	1
1:A:41:PHE:CG	1:A:70:LYS:HD3	0.40	2.51	7	1
1:A:36:GLN:O	1:A:37:ILE:C	0.40	2.60	15	1
1:A:95:GLN:C	1:A:95:GLN:CD	0.40	2.80	8	1
1:A:25:LEU:HD13	1:A:65:LYS:CG	0.40	2.40	12	1
1:A:38:LEU:HD21	1:A:70:LYS:HE2	0.40	1.93	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	78/112 (70%)	67±2 (85±3%)	11±2 (14±3%)	0±1 (1±1%)	32	76
All	All	1560/2240 (70%)	1332 (85%)	220 (14%)	8 (1%)	32	76

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	74	THR	3
1	A	89	GLN	2
1	A	90	MET	2
1	A	37	ILE	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	72/99 (73%)	68±2 (94±2%)	4±2 (6±2%)	25	74
All	All	1440/1980 (73%)	1359 (94%)	81 (6%)	25	74

All 28 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	92	MET	20
1	A	68	LYS	8
1	A	70	LYS	7
1	A	58	LYS	5
1	A	56	ASN	4
1	A	30	GLU	3
1	A	63	PHE	3
1	A	65	LYS	3
1	A	96	GLN	2
1	A	52	LYS	2
1	A	29	ASP	2
1	A	51	ASP	2
1	A	75	ASN	2
1	A	83	ASP	2
1	A	95	GLN	2
1	A	21	ASP	2
1	A	34	VAL	1
1	A	90	MET	1
1	A	42	LYS	1
1	A	97	TRP	1
1	A	35	GLU	1
1	A	36	GLN	1
1	A	76	GLU	1
1	A	61	GLU	1
1	A	55	GLU	1
1	A	71	GLU	1
1	A	89	GLN	1
1	A	77	GLU	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