Full wwPDB NMR Structure Validation Report (i)

Feb 22, 2022 – 02:08 PM EST

PDB ID	:	1WJN
Title	:	Solution structure of the C-terminal ubiquitin-like domain of mouse tubulin-specific chaperone e
Authors	:	Sato, M.; Tochio, N.; Koshiba, S.; Inoue, M.; Kigawa, T.; Yokoyama, S.; RIKEN Structural Genomics/Proteomics Initiative (RSGI)
Deposited on	:	2004-05-29

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:

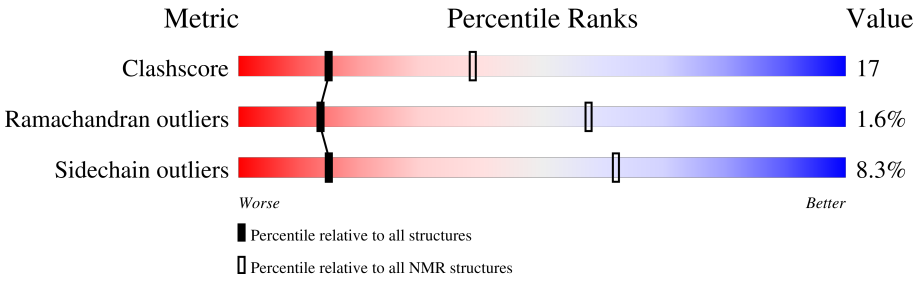
MolProbity	:	4.02b-467
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
RCI	:	v_1n_11_5_13_A (Berjanski et al., 2005)
PANAV	:	Wang et al. (2010)
ShiftChecker	:	2.26
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.26

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	97	60% 19% • 21%

2 Ensemble composition and analysis (i)

This entry contains 20 models. Model 13 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:8-A:16, A:24-A:91 (77)	0.23	13

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 8 single-model clusters were found.

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

3 Entry composition (i)

There is only 1 type of molecule in this entry. The entry contains 1518 atoms, of which 771 are hydrogens and 0 are deuteriums.

- Molecule 1 is a protein called Tubulin-folding protein TBCE.

Mol	Chain	Residues	Atoms						Trace
			Total	C	H	N	O	S	
1	A	97	1518	468	771	127	148	4	0

There are 13 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	1	GLY	-	cloning artifact	UNP Q8CIV8
A	2	SER	-	cloning artifact	UNP Q8CIV8
A	3	SER	-	cloning artifact	UNP Q8CIV8
A	4	GLY	-	cloning artifact	UNP Q8CIV8
A	5	SER	-	cloning artifact	UNP Q8CIV8
A	6	SER	-	cloning artifact	UNP Q8CIV8
A	7	GLY	-	cloning artifact	UNP Q8CIV8
A	92	SER	-	cloning artifact	UNP Q8CIV8
A	93	GLY	-	cloning artifact	UNP Q8CIV8
A	94	PRO	-	cloning artifact	UNP Q8CIV8
A	95	SER	-	cloning artifact	UNP Q8CIV8
A	96	SER	-	cloning artifact	UNP Q8CIV8
A	97	GLY	-	cloning artifact	UNP Q8CIV8

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: Tubulin-folding protein TBCE

Chain A: 60% 19% • 21%

G1 S2 S3 G4 S5 S6 G7 L10 S17 N18 Q19 P20 E21 R22 Q23 I24 L25 Q28 L29 P30 D31 S32 M33 K39 L42 L45 L46 K47 V48 P49 E66 L69 D72 L76 Y79 D85 S92 G93 P94 S95 S96 G97

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: Tubulin-folding protein TBCE

Chain A: 46% 26% 7% 21%

G1 S2 S3 G4 S5 S6 G7 L10 T11 L12 C16 S17 N18 Q19 P20 E21 R22 Q23 I24 L25 Q28 L29 M33 T34 V35 Q36 K37 V38 K39 G40 L41 L42 L45 L46 K47 V48 P49 V50 S51 E52 L53 L54 L55 E66 L69 D72 L76 Y79 N83

G84 D85 R90 W91 S92 G93 P94 S95 S96 G97

4.2.2 Score per residue for model 2

• Molecule 1: Tubulin-folding protein TBCE

Chain A: 57% 19% • 21%

G1 S2 S3 G4 S5 S6 G7 L10 S17 N18 Q19 P20 E21 R22 Q23 K27 Q28 L29 M33 K39 L46 K47 V48 P49 L55 S56 Y57 K61 I67 E68 L69 E70 N71 Q74 P75 L76 Y79 N83 G84 D85 C86 S92 G93 P94 S95 S96 G97

4.2.3 Score per residue for model 3

- Molecule 1: Tubulin-folding protein TBCE

Chain A: 55% 21% • 21%

G1 S2 S3 G4 S5 S6 G7 Q8 L9 L10 K13 S17 N18 Q19 P20 E21 R22 Q23 I24 L25 E26 K27 Q28 L29 P30 D31 S32 M33 K37 V38 K39 V48 P49 L55 S56 Y57 M62 I67 N71 D72 L73 Q74 P75 L76 S92 G93 P94 S95 S96 G97

4.2.4 Score per residue for model 4

- Molecule 1: Tubulin-folding protein TBCE

Chain A: 63% 13% • 21%

G1 S2 S3 G4 S5 S6 G7 L10 S17 N18 Q19 P20 E21 R22 Q23 I24 L25 Q28 L29 M33 L42 S43 R44 L45 V48 P49 Y57 E66 I67 D72 L76 N83 S92 G93 P94 S95 S96 G97

4.2.5 Score per residue for model 5

- Molecule 1: Tubulin-folding protein TBCE

Chain A: 45% 29% 5% 21%

G1 S2 S3 G4 S5 S6 G7 Q8 L9 I14 K15 C16 S17 N18 Q19 P20 E21 R22 Q23 I24 L25 E26 K27 Q28 L29 P30 D31 S32 M33 K39 L42 S43 R44 L45 L46 K47 V48 P49 L54 L55 R65 E66 I67 E68 L69 D72 Y79 D85 V89 R90 W91

S92 G93 P94 S95 S96 G97

4.2.6 Score per residue for model 6

- Molecule 1: Tubulin-folding protein TBCE

Chain A: 52% 26% • 21%

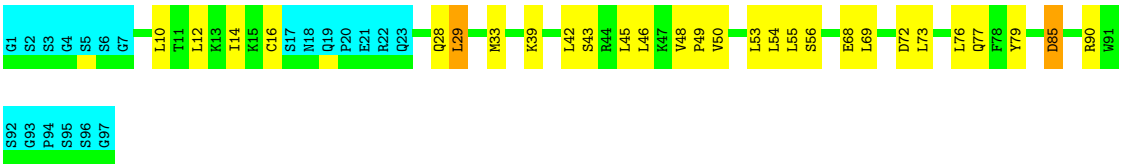
G1 S2 S3 G4 S5 S6 G7 L10 I14 K15 C16 S17 N18 Q19 P20 E21 R22 Q23 I24 L25 E26 K27 Q28 L29 M33 L42 L45 L46 K47 V48 P49 V50 S51 E52 Y57 E66 L69 D72 L76 Y79 S80 V81 E82 N83 G84 D85 W91 S92

G93 P94 S95 S96 G97

4.2.7 Score per residue for model 7

- Molecule 1: Tubulin-folding protein TBCE

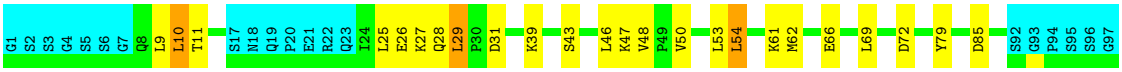
Chain A: 51% 27% • 21%



4.2.8 Score per residue for model 8

- Molecule 1: Tubulin-folding protein TBCE

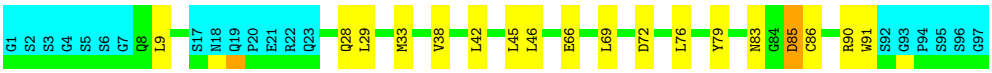
Chain A: 55% 22% • 21%



4.2.9 Score per residue for model 9

- Molecule 1: Tubulin-folding protein TBCE

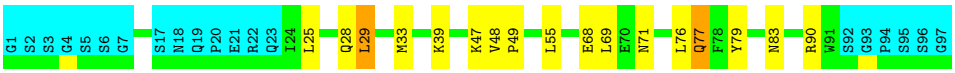
Chain A: 61% 18% • 21%



4.2.10 Score per residue for model 10

- Molecule 1: Tubulin-folding protein TBCE

Chain A: 62% 15% • 21%



4.2.11 Score per residue for model 11

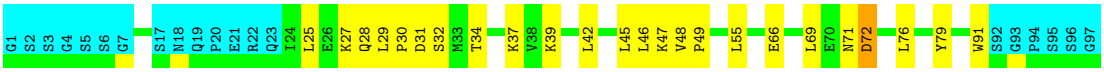
- Molecule 1: Tubulin-folding protein TBCE

Chain A: 60% 19% • 21%

4.2.12 Score per residue for model 12

- Molecule 1: Tubulin-folding protein TBCE

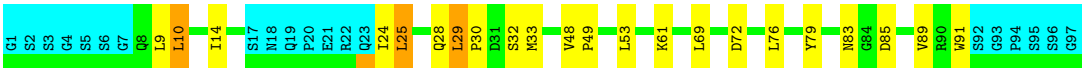
Chain A: 55% 24% • 21%



4.2.13 Score per residue for model 13 (medoid)

- Molecule 1: Tubulin-folding protein TBCE

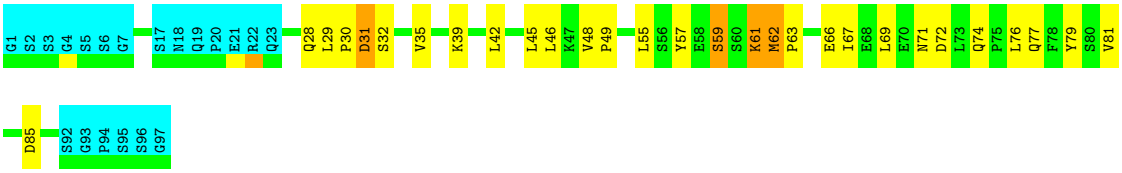
Chain A: 57% 20% • 21%



4.2.14 Score per residue for model 14

- Molecule 1: Tubulin-folding protein TBCE

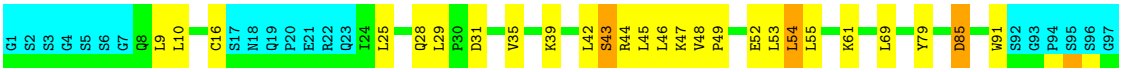
Chain A: 49% 26% • 21%



4.2.15 Score per residue for model 15

- Molecule 1: Tubulin-folding protein TBCE

Chain A: 53% 24% • 21%



4.2.16 Score per residue for model 16

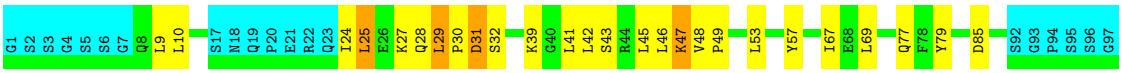
- Molecule 1: Tubulin-folding protein TBCE

Chain A: 62% 13% • 21%

4.2.17 Score per residue for model 17

- Molecule 1: Tubulin-folding protein TBCE

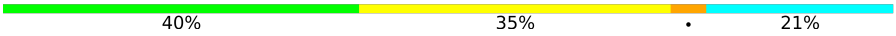
Chain A:

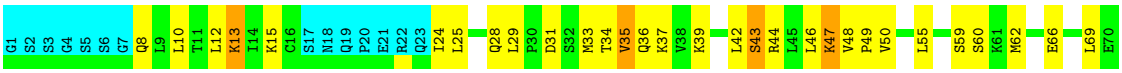


4.2.18 Score per residue for model 18

- Molecule 1: Tubulin-folding protein TBCE

Chain A:

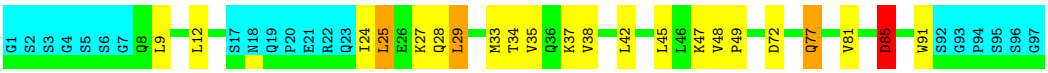




4.2.19 Score per residue for model 19

- Molecule 1: Tubulin-folding protein TBCE

Chain A:



4.2.20 Score per residue for model 20

- Molecule 1: Tubulin-folding protein TBCE

Chain A:

5 Refinement protocol and experimental data overview (i)

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

Of the 100 calculated structures, 20 were deposited, based on the following criterion: *structures with the least restraint violations, 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	619	661	661	22±6
All	All	12380	13220	13220	432

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:46:LEU:O	1:A:48:VAL:HG23	0.94	1.63	17	9
1:A:28:GLN:C	1:A:29:LEU:HD22	0.83	1.94	15	20
1:A:62:MET:HE1	1:A:67:ILE:HD11	0.80	1.52	20	1
1:A:73:LEU:N	1:A:73:LEU:HD13	0.79	1.93	16	1
1:A:29:LEU:HD22	1:A:29:LEU:N	0.78	1.94	20	19
1:A:25:LEU:N	1:A:25:LEU:HD22	0.78	1.94	13	2
1:A:12:LEU:HD22	1:A:85:ASP:OD1	0.77	1.79	18	1
1:A:25:LEU:HD22	1:A:25:LEU:N	0.76	1.95	1	3
1:A:69:LEU:HD22	1:A:79:TYR:CD2	0.74	2.17	15	11
1:A:25:LEU:HD13	1:A:25:LEU:N	0.74	1.97	19	3
1:A:24:ILE:C	1:A:25:LEU:HD13	0.74	2.03	19	6
1:A:55:LEU:HB3	1:A:69:LEU:HD12	0.73	1.59	7	5
1:A:54:LEU:HD22	1:A:54:LEU:N	0.73	1.98	1	3
1:A:62:MET:CE	1:A:67:ILE:HD11	0.73	2.13	20	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:46:LEU:HD22	1:A:91:TRP:CH2	0.72	2.20	20	1
1:A:39:LYS:CG	1:A:55:LEU:HD23	0.72	2.15	12	6
1:A:39:LYS:HG2	1:A:55:LEU:HD23	0.71	1.62	1	8
1:A:42:LEU:HD23	1:A:45:LEU:HD12	0.67	1.66	9	3
1:A:39:LYS:HG3	1:A:55:LEU:HD23	0.67	1.67	5	1
1:A:9:LEU:HD13	1:A:29:LEU:C	0.66	2.10	8	1
1:A:28:GLN:O	1:A:29:LEU:HD13	0.66	1.91	13	12
1:A:39:LYS:HB3	1:A:50:VAL:HG22	0.66	1.68	18	1
1:A:9:LEU:HD12	1:A:28:GLN:C	0.65	2.12	19	4
1:A:35:VAL:HG23	1:A:74:GLN:O	0.64	1.93	20	3
1:A:81:VAL:HG13	1:A:85:ASP:OD2	0.64	1.93	19	2
1:A:69:LEU:HD22	1:A:79:TYR:CG	0.63	2.28	12	10
1:A:69:LEU:CD2	1:A:79:TYR:CG	0.63	2.81	15	13
1:A:25:LEU:HD22	1:A:25:LEU:H	0.62	1.55	16	6
1:A:54:LEU:HD22	1:A:54:LEU:H	0.62	1.53	8	3
1:A:42:LEU:HD23	1:A:45:LEU:HD22	0.61	1.72	11	2
1:A:42:LEU:HD13	1:A:89:VAL:HG21	0.60	1.74	5	1
1:A:10:LEU:HD11	1:A:31:ASP:HB3	0.59	1.74	15	2
1:A:16:CYS:SG	1:A:91:TRP:CZ3	0.59	2.95	1	4
1:A:69:LEU:HD22	1:A:79:TYR:CD1	0.59	2.33	17	3
1:A:14:ILE:O	1:A:24:ILE:HG23	0.58	1.99	5	1
1:A:29:LEU:N	1:A:29:LEU:CD2	0.57	2.66	20	15
1:A:9:LEU:HD12	1:A:29:LEU:N	0.57	2.15	9	4
1:A:46:LEU:HD13	1:A:91:TRP:CZ3	0.57	2.34	9	5
1:A:69:LEU:HD23	1:A:79:TYR:CE1	0.57	2.34	8	1
1:A:10:LEU:N	1:A:10:LEU:HD23	0.56	2.15	13	3
1:A:57:TYR:CD2	1:A:81:VAL:HG22	0.56	2.35	14	2
1:A:69:LEU:CD2	1:A:79:TYR:CD1	0.56	2.89	16	4
1:A:12:LEU:HD22	1:A:85:ASP:HB3	0.56	1.77	1	1
1:A:69:LEU:HD23	1:A:79:TYR:CD1	0.56	2.36	16	5
1:A:65:ARG:HH21	1:A:67:ILE:HD11	0.55	1.61	5	1
1:A:54:LEU:N	1:A:54:LEU:CD2	0.55	2.69	1	2
1:A:16:CYS:SG	1:A:91:TRP:CH2	0.54	3.01	1	1
1:A:65:ARG:NH2	1:A:67:ILE:HD11	0.53	2.19	5	1
1:A:69:LEU:CD2	1:A:79:TYR:CD2	0.53	2.91	7	4
1:A:25:LEU:N	1:A:25:LEU:CD2	0.53	2.67	13	3
1:A:27:LYS:HD2	1:A:29:LEU:HD21	0.53	1.79	12	1
1:A:48:VAL:HG13	1:A:49:PRO:HD2	0.53	1.81	17	16
1:A:12:LEU:HD22	1:A:85:ASP:CG	0.52	2.24	19	2
1:A:9:LEU:CD1	1:A:29:LEU:CA	0.52	2.87	8	2
1:A:85:ASP:CG	1:A:86:CYS:N	0.52	2.63	2	2

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:12:LEU:CD2	1:A:85:ASP:CG	0.51	2.79	18	1
1:A:9:LEU:CD1	1:A:29:LEU:C	0.51	2.78	8	1
1:A:15:LYS:HB2	1:A:24:ILE:HD12	0.51	1.81	18	1
1:A:9:LEU:HD23	1:A:28:GLN:HB3	0.50	1.83	5	2
1:A:33:MET:O	1:A:76:LEU:CD2	0.50	2.60	2	11
1:A:42:LEU:HA	1:A:45:LEU:HD12	0.50	1.81	1	2
1:A:73:LEU:HD13	1:A:73:LEU:H	0.50	1.63	16	1
1:A:8:GLN:N	1:A:31:ASP:OD1	0.50	2.45	18	1
1:A:42:LEU:O	1:A:44:ARG:N	0.50	2.45	15	2
1:A:42:LEU:O	1:A:45:LEU:N	0.50	2.45	17	9
1:A:54:LEU:N	1:A:90:ARG:O	0.50	2.45	5	2
1:A:52:GLU:O	1:A:91:TRP:CB	0.50	2.60	15	3
1:A:34:THR:O	1:A:37:LYS:N	0.50	2.44	18	2
1:A:31:ASP:OD1	1:A:77:GLN:N	0.50	2.45	17	1
1:A:62:MET:CG	1:A:62:MET:O	0.49	2.59	20	1
1:A:66:GLU:CD	1:A:66:GLU:C	0.49	2.70	8	3
1:A:72:ASP:N	1:A:72:ASP:OD1	0.49	2.46	1	2
1:A:57:TYR:CE1	1:A:67:ILE:HB	0.49	2.43	2	4
1:A:77:GLN:O	1:A:77:GLN:NE2	0.49	2.45	7	2
1:A:61:LYS:CG	1:A:62:MET:SD	0.49	3.01	14	1
1:A:57:TYR:CE1	1:A:67:ILE:HD13	0.49	2.43	14	2
1:A:73:LEU:H	1:A:73:LEU:HD22	0.49	1.67	16	1
1:A:77:GLN:CD	1:A:77:GLN:C	0.48	2.71	10	2
1:A:69:LEU:HD23	1:A:79:TYR:CD2	0.48	2.42	2	3
1:A:73:LEU:N	1:A:73:LEU:CD1	0.48	2.66	16	1
1:A:12:LEU:CD2	1:A:85:ASP:OD2	0.48	2.61	18	1
1:A:31:ASP:OD1	1:A:32:SER:N	0.48	2.47	14	2
1:A:27:LYS:CG	1:A:29:LEU:HD21	0.48	2.39	5	2
1:A:14:ILE:HG23	1:A:89:VAL:CG2	0.48	2.39	13	2
1:A:73:LEU:HD12	1:A:73:LEU:N	0.47	2.23	7	1
1:A:57:TYR:CZ	1:A:67:ILE:HD13	0.47	2.45	4	4
1:A:9:LEU:C	1:A:10:LEU:HD23	0.47	2.29	13	3
1:A:30:PRO:O	1:A:32:SER:N	0.47	2.48	3	6
1:A:76:LEU:HD22	1:A:76:LEU:N	0.47	2.24	18	7
1:A:48:VAL:HG21	1:A:91:TRP:CD2	0.47	2.45	20	1
1:A:68:GLU:N	1:A:68:GLU:CD	0.47	2.67	7	1
1:A:73:LEU:HD12	1:A:73:LEU:H	0.47	1.68	7	1
1:A:42:LEU:HD23	1:A:45:LEU:CD1	0.46	2.40	9	2
1:A:69:LEU:HD22	1:A:79:TYR:CE2	0.46	2.45	15	1
1:A:46:LEU:O	1:A:47:LYS:C	0.46	2.53	17	1
1:A:71:ASN:ND2	1:A:74:GLN:CG	0.46	2.78	18	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:48:VAL:HG12	1:A:53:LEU:HG	0.46	1.88	15	1
1:A:66:GLU:N	1:A:66:GLU:OE1	0.45	2.49	1	1
1:A:14:ILE:HD12	1:A:14:ILE:N	0.45	2.25	6	2
1:A:42:LEU:O	1:A:43:SER:C	0.45	2.54	15	5
1:A:34:THR:O	1:A:36:GLN:N	0.45	2.49	18	2
1:A:59:SER:CB	1:A:62:MET:SD	0.45	3.05	14	1
1:A:27:LYS:HE2	1:A:41:LEU:HD21	0.44	1.89	17	1
1:A:49:PRO:O	1:A:51:SER:N	0.44	2.51	6	1
1:A:67:ILE:N	1:A:67:ILE:HD12	0.44	2.28	3	2
1:A:71:ASN:ND2	1:A:74:GLN:HG3	0.44	2.27	18	2
1:A:71:ASN:CG	1:A:74:GLN:CG	0.43	2.86	16	1
1:A:11:THR:OG1	1:A:28:GLN:NE2	0.43	2.51	8	1
1:A:39:LYS:CE	1:A:53:LEU:O	0.43	2.65	15	2
1:A:83:ASN:OD1	1:A:83:ASN:C	0.43	2.55	20	1
1:A:83:ASN:OD1	1:A:83:ASN:N	0.43	2.51	10	2
1:A:57:TYR:CG	1:A:81:VAL:HG22	0.43	2.49	14	1
1:A:27:LYS:HB3	1:A:29:LEU:HD21	0.43	1.90	19	1
1:A:85:ASP:C	1:A:85:ASP:OD1	0.43	2.56	19	1
1:A:34:THR:O	1:A:35:VAL:C	0.43	2.57	19	4
1:A:27:LYS:HD2	1:A:29:LEU:HD11	0.43	1.91	12	1
1:A:30:PRO:C	1:A:32:SER:N	0.43	2.72	17	5
1:A:10:LEU:HD11	1:A:31:ASP:CB	0.43	2.43	8	1
1:A:59:SER:O	1:A:60:SER:C	0.43	2.56	18	1
1:A:25:LEU:HD12	1:A:25:LEU:N	0.42	2.29	11	1
1:A:72:ASP:OD1	1:A:72:ASP:N	0.42	2.51	12	1
1:A:9:LEU:HD12	1:A:29:LEU:CA	0.42	2.44	19	2
1:A:68:GLU:CD	1:A:68:GLU:O	0.42	2.57	11	1
1:A:61:LYS:O	1:A:63:PRO:CD	0.42	2.67	14	1
1:A:33:MET:SD	1:A:38:VAL:HG22	0.42	2.55	16	3
1:A:43:SER:CB	1:A:48:VAL:O	0.42	2.68	17	2
1:A:66:GLU:CD	1:A:66:GLU:N	0.42	2.72	12	1
1:A:12:LEU:HD22	1:A:85:ASP:HB2	0.42	1.89	7	1
1:A:43:SER:O	1:A:47:LYS:N	0.42	2.53	20	1
1:A:61:LYS:HG3	1:A:62:MET:N	0.42	2.30	20	1
1:A:25:LEU:N	1:A:25:LEU:HD13	0.42	2.30	17	1
1:A:39:LYS:NZ	1:A:53:LEU:O	0.42	2.50	15	1
1:A:25:LEU:N	1:A:25:LEU:CD1	0.42	2.70	19	1
1:A:49:PRO:O	1:A:52:GLU:N	0.42	2.53	6	1
1:A:47:LYS:N	1:A:47:LYS:HD2	0.42	2.30	18	1
1:A:13:LYS:HD2	1:A:24:ILE:HG21	0.42	1.92	3	1
1:A:33:MET:CE	1:A:38:VAL:HG22	0.42	2.44	9	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:76:LEU:N	1:A:76:LEU:CD2	0.42	2.83	14	1
1:A:55:LEU:HD11	1:A:89:VAL:HG22	0.42	1.92	18	1
1:A:76:LEU:CD2	1:A:76:LEU:N	0.42	2.83	18	1
1:A:10:LEU:HD11	1:A:31:ASP:CG	0.41	2.35	17	1
1:A:49:PRO:C	1:A:51:SER:N	0.41	2.74	6	1
1:A:71:ASN:ND2	1:A:74:GLN:HG2	0.41	2.31	3	2
1:A:13:LYS:NZ	1:A:24:ILE:HG22	0.41	2.30	18	1
1:A:48:VAL:HG11	1:A:91:TRP:CB	0.41	2.45	13	1
1:A:43:SER:HA	1:A:53:LEU:HD11	0.41	1.91	8	1
1:A:44:ARG:N	1:A:44:ARG:CD	0.41	2.84	4	1
1:A:50:VAL:HA	1:A:53:LEU:HD12	0.41	1.92	7	1
1:A:39:LYS:C	1:A:50:VAL:HG22	0.41	2.37	8	1
1:A:71:ASN:CG	1:A:74:GLN:HG3	0.41	2.37	16	1
1:A:43:SER:O	1:A:47:LYS:CA	0.41	2.69	5	1
1:A:76:LEU:N	1:A:76:LEU:HD22	0.41	2.31	12	1
1:A:10:LEU:HD23	1:A:10:LEU:N	0.40	2.30	3	1
1:A:30:PRO:O	1:A:33:MET:N	0.40	2.53	5	1
1:A:66:GLU:CD	1:A:66:GLU:O	0.40	2.60	8	1
1:A:42:LEU:C	1:A:44:ARG:N	0.40	2.74	18	2
1:A:90:ARG:HG2	1:A:91:TRP:N	0.40	2.31	11	1
1:A:27:LYS:HE3	1:A:29:LEU:HD11	0.40	1.93	12	1
1:A:35:VAL:HG22	1:A:69:LEU:HD13	0.40	1.93	15	1
1:A:27:LYS:HD2	1:A:29:LEU:CD2	0.40	2.45	12	1
1:A:40:GLY:HA2	1:A:50:VAL:CG2	0.40	2.46	1	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	77/97 (79%)	70±2 (91±2%)	6±2 (8±2%)	1±1 (2±1%)	13	57
All	All	1540/1940 (79%)	1398 (91%)	118 (8%)	24 (2%)	13	57

All 6 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	85	ASP	12
1	A	31	ASP	5
1	A	35	VAL	2
1	A	53	LEU	2
1	A	43	SER	2
1	A	50	VAL	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	74/89 (83%)	68±2 (92±3%)	6±2 (8±3%)	15	62
All	All	1480/1780 (83%)	1357 (92%)	123 (8%)	15	62

All 25 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	72	ASP	16
1	A	25	LEU	15
1	A	29	LEU	13
1	A	47	LYS	12
1	A	10	LEU	10
1	A	61	LYS	6
1	A	66	GLU	6
1	A	83	ASN	5
1	A	71	ASN	5
1	A	85	ASP	5
1	A	90	ARG	4
1	A	27	LYS	4
1	A	62	MET	4
1	A	54	LEU	3
1	A	37	LYS	2
1	A	68	GLU	2
1	A	26	GLU	2
1	A	77	GLN	2
1	A	44	ARG	1
1	A	31	ASP	1

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Mol	Chain	Res	Type	Models (Total)
1	A	56	SER	1
1	A	59	SER	1
1	A	73	LEU	1
1	A	13	LYS	1
1	A	39	LYS	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