Full wwPDB NMR Structure Validation Report (i)

Feb 27, 2022 – 05:11 PM EST

PDB ID	:	2DJT
Title	:	Solution structures of the PDZ domain of human unnamed protein product
Authors	:	Sato, M.; Koshiba, S.; Inoue, M.; Kigawa, T.; Yokoyama, S.; RIKEN Structural Genomics/Proteomics Initiative (RSGI)
Deposited on	:	2006-04-05

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:

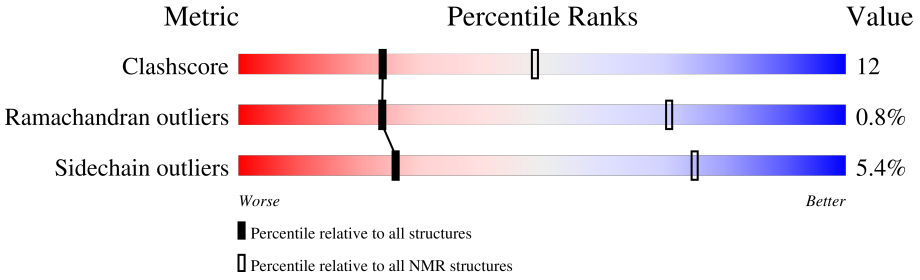
MolProbity	:	4.02b-467
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
RCI	:	v_1n_11_5_13_A (Berjanski et al., 2005)
PANAV	:	Wang et al. (2010)
ShiftChecker	:	2.27
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
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	104	70% 12% • 17%

2 Ensemble composition and analysis (i)

This entry contains 20 models. Model 12 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:12-A:97 (86)	0.33	12

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 6 single-model clusters were found.

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

3 Entry composition (i)

There is only 1 type of molecule in this entry. The entry contains 1484 atoms, of which 744 are hydrogens and 0 are deuteriums.

- Molecule 1 is a protein called unnamed protein product.

Mol	Chain	Residues	Atoms						Trace
			Total	C	H	N	O	S	
1	A	104	1484	452	744	146	141	1	0

There are 13 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	1	GLY	-	cloning artifact	UNP Q9H6Y5
A	2	SER	-	cloning artifact	UNP Q9H6Y5
A	3	SER	-	cloning artifact	UNP Q9H6Y5
A	4	GLY	-	cloning artifact	UNP Q9H6Y5
A	5	SER	-	cloning artifact	UNP Q9H6Y5
A	6	SER	-	cloning artifact	UNP Q9H6Y5
A	7	GLY	-	cloning artifact	UNP Q9H6Y5
A	99	SER	-	cloning artifact	UNP Q9H6Y5
A	100	GLY	-	cloning artifact	UNP Q9H6Y5
A	101	PRO	-	cloning artifact	UNP Q9H6Y5
A	102	SER	-	cloning artifact	UNP Q9H6Y5
A	103	SER	-	cloning artifact	UNP Q9H6Y5
A	104	GLY	-	cloning artifact	UNP Q9H6Y5

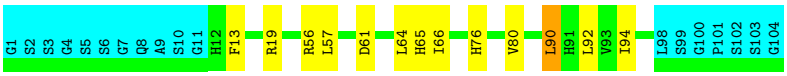
4 Residue-property plots (i)

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: unnamed protein product

Chain A: 70% 12% • 17%



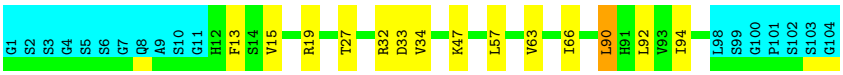
4.2 Scores per residue for each member of the ensemble

Colouring as in section 4.1 above.

4.2.1 Score per residue for model 1

• Molecule 1: unnamed protein product

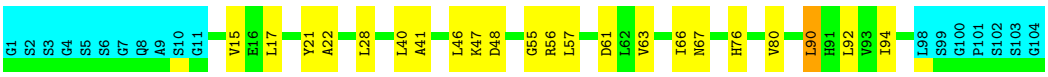
Chain A: 69% 12% • 17%



4.2.2 Score per residue for model 2

• Molecule 1: unnamed protein product

Chain A: 62% 20% • 17%



4.2.3 Score per residue for model 3

- Molecule 1: unnamed protein product

Chain A: 75% 7% • 17%

G1 S2 S3 G4 S5 S6 G7 Q8 A9 S10 G11 D37 L64 H65 I66 H76 V80 L90 H91 L92 L98 S99 G100 P101 S102 S103 G104

4.2.4 Score per residue for model 4

- Molecule 1: unnamed protein product

Chain A: 55% 27% • 17%

G1 S2 S3 G4 S5 S6 G7 Q8 A9 S10 G11 H12 F13 S14 V15 R19 G20 Y21 F24 T27 L28 G29 R32 D33 L40 R43 L57 E58 L64 H65 I66 E69 S70 T71 L74 T75 H76 V80 L90 H91 L92 V93 I94 R95 R96 P97 L98 S99

G100 P101 S102 S103 G104

4.2.5 Score per residue for model 5

- Molecule 1: unnamed protein product

Chain A: 58% 24% • 17%

G1 S2 S3 G4 S5 S6 G7 Q8 A9 S10 G11 H12 V15 E16 L17 F24 D37 T38 V42 C54 G55 R56 L57 D61 L62 V63 L64 H65 I66 N67 G68 E69 A77 Q78 R82 L90 H91 L92 V93 I94 R95 L98 S99 G100 P101 S102 S103 G104

4.2.6 Score per residue for model 6

- Molecule 1: unnamed protein product

Chain A: 70% 12% • 17%

G1 S2 S3 G4 S5 S6 G7 Q8 A9 S10 G11 R19 F24 R43 L46 K47 I66 N67 H76 A79 V80 I83 L90 H91 L92 L98 S99 G100 P101 S102 S103 G104

4.2.7 Score per residue for model 7

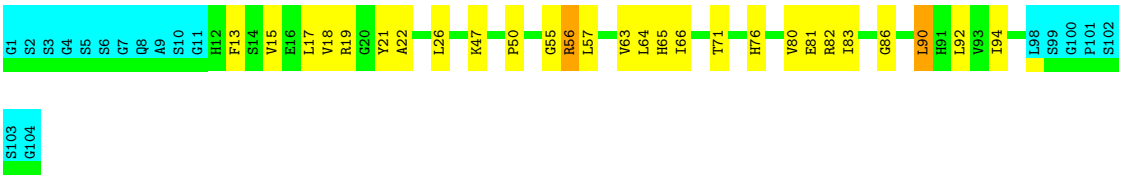
- Molecule 1: unnamed protein product

Chain A: 61% 21% • 17%

4.2.8 Score per residue for model 8

- Molecule 1: unnamed protein product

Chain A: 57% 24% • 17%



4.2.9 Score per residue for model 9

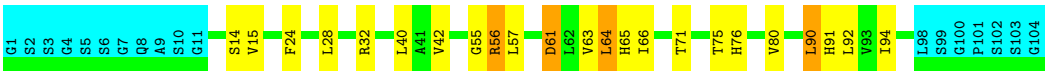
- Molecule 1: unnamed protein product

Chain A: 68% 12% • 17%

4.2.10 Score per residue for model 10

- Molecule 1: unnamed protein product

Chain A: 61% 18% • 17%



4.2.11 Score per residue for model 11

- Molecule 1: unnamed protein product

Chain A: 64% 18% 17%

4.2.12 Score per residue for model 12 (medoid)

- Molecule 1: unnamed protein product

Chain A: 60% 19% • 17%

G1 S2 S3 G4 S5 S6 G7 Q8 A9 S10 G11 H12 F13 S14 V15 V18 R19 T27 L28 D33 A41 V42 R43 K47 D48 G55 R56 L57 D61 L64 H65 T71 H76 V80 L90 H91 L92 V93 I94 L98 S99 G100 P101 S102 S103 G104

4.2.13 Score per residue for model 13

- Molecule 1: unnamed protein product

Chain A: 60% 22% • 17%

G1 S2 S3 G4 S5 S6 G7 Q8 A9 S10 G11 H12 F13 L17 V18 R19 L26 R32 R43 L46 K47 L57 E58 V59 V63 L64 H65 I66 N67 T71 L74 T75 H76 V80 R84 A85 L90 I94 L98 S99 G100 P101 S102 S103 G104

4.2.14 Score per residue for model 14

- Molecule 1: unnamed protein product

Chain A: 68% 14% 17%

G1 S2 S3 G4 S5 S6 G7 Q8 A9 S10 G11 L26 T27 L28 A41 L46 L57 D61 L64 H65 I66 N67 H76 V80 R84 A85 L90 H91 L92 L98 S99 G100 P101 S102 S103 G104

4.2.15 Score per residue for model 15

- Molecule 1: unnamed protein product

Chain A: 58% 22% • 17%

G1 S2 S3 G4 S5 S6 G7 Q8 A9 S10 G11 H12 F13 S14 V15 E16 L17 V18 R19 G20 Y21 F24 K47 G55 R56 L57 D61 L64 H65 I66 E69 S70 T71 H76 V80 E81 L90 H91 L92 R95 L98 S99 G100 P101 S102 S103 G104

4.2.16 Score per residue for model 16

- Molecule 1: unnamed protein product

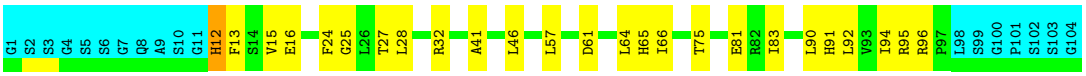
Chain A: 55% 27% • 17%

G1 S2 S3 G4 S5 S6 G7 Q8 A9 S10 G11 H12 F13 L17 V18 R19 F24 G25 L26 T27 L28 G31 T38 P39 L40 A41 V42 R43 K47 D48 C54 L57 V63 L64 H65 I66 T71 H76 A79 V80 I83 L90 H91 L92 V93 I94

4.2.17 Score per residue for model 17

- Molecule 1: unnamed protein product

Chain A:



4.2.18 Score per residue for model 18

- Molecule 1: unnamed protein product

Chain A:

4.2.19 Score per residue for model 19

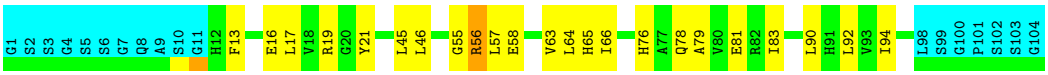
- Molecule 1: unnamed protein product

Chain A:

4.2.20 Score per residue for model 20

- Molecule 1: unnamed protein product

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: *target function, 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	639	655	651	16±5
All	All	12780	13100	13020	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:15:VAL:HG21	1:A:57:LEU:HD21	0.87	1.44	2	6
1:A:91:HIS:O	1:A:92:LEU:HD23	0.82	1.75	17	4
1:A:66:ILE:HG22	1:A:67:ASN:ND2	0.79	1.92	18	2
1:A:76:HIS:O	1:A:80:VAL:HG23	0.77	1.79	4	14
1:A:66:ILE:HG21	1:A:83:ILE:CD1	0.77	2.10	16	2
1:A:64:LEU:O	1:A:71:THR:HG22	0.76	1.79	4	9
1:A:90:LEU:C	1:A:90:LEU:HD23	0.74	2.03	12	4
1:A:15:VAL:HG21	1:A:57:LEU:HD11	0.71	1.60	17	2
1:A:90:LEU:HD23	1:A:90:LEU:O	0.70	1.87	12	7
1:A:90:LEU:HD11	1:A:92:LEU:HD11	0.69	1.62	8	5
1:A:63:VAL:HG22	1:A:94:ILE:CD1	0.68	2.19	1	9
1:A:63:VAL:HG22	1:A:94:ILE:HD11	0.67	1.67	16	5
1:A:32:ARG:HB3	1:A:75:THR:HG22	0.66	1.68	19	2
1:A:66:ILE:HG23	1:A:92:LEU:CD2	0.65	2.22	1	7

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:66:ILE:HG22	1:A:67:ASN:OD1	0.65	1.92	6	3
1:A:66:ILE:HG23	1:A:92:LEU:HD23	0.65	1.67	2	9
1:A:64:LEU:HD22	1:A:64:LEU:N	0.62	2.10	4	5
1:A:32:ARG:CB	1:A:75:THR:HG22	0.62	2.25	19	2
1:A:64:LEU:N	1:A:64:LEU:CD2	0.59	2.65	10	5
1:A:17:LEU:CG	1:A:90:LEU:HD22	0.59	2.26	13	2
1:A:64:LEU:HD11	1:A:95:ARG:HB3	0.59	1.74	18	1
1:A:63:VAL:HA	1:A:94:ILE:HD13	0.58	1.76	16	2
1:A:42:VAL:HG23	1:A:61:ASP:OD1	0.57	1.99	10	1
1:A:13:PHE:CE1	1:A:94:ILE:O	0.57	2.57	1	2
1:A:17:LEU:HD12	1:A:90:LEU:HD22	0.57	1.76	7	3
1:A:37:ASP:O	1:A:38:THR:HG23	0.56	2.00	5	2
1:A:13:PHE:CD1	1:A:94:ILE:O	0.56	2.59	1	1
1:A:26:LEU:HD22	1:A:57:LEU:HD13	0.56	1.77	8	2
1:A:90:LEU:O	1:A:90:LEU:HD23	0.56	2.01	18	4
1:A:15:VAL:HG23	1:A:92:LEU:O	0.55	2.01	12	1
1:A:69:GLU:OE1	1:A:74:LEU:HD11	0.55	2.01	11	2
1:A:26:LEU:CD2	1:A:57:LEU:HD13	0.54	2.32	14	4
1:A:41:ALA:HB1	1:A:61:ASP:O	0.54	2.02	2	3
1:A:24:PHE:CZ	1:A:90:LEU:CB	0.53	2.91	5	1
1:A:64:LEU:CD2	1:A:64:LEU:N	0.53	2.71	12	2
1:A:45:LEU:HD11	1:A:58:GLU:HA	0.52	1.80	7	2
1:A:64:LEU:N	1:A:64:LEU:HD22	0.52	2.19	12	1
1:A:17:LEU:HD21	1:A:54:CYS:SG	0.52	2.44	16	1
1:A:15:VAL:O	1:A:90:LEU:HD23	0.52	2.05	1	2
1:A:66:ILE:HG21	1:A:83:ILE:HD13	0.51	1.81	16	1
1:A:17:LEU:HG	1:A:90:LEU:HD22	0.51	1.82	13	1
1:A:24:PHE:CZ	1:A:90:LEU:HB2	0.51	2.40	5	8
1:A:66:ILE:HG22	1:A:67:ASN:HD22	0.50	1.66	5	3
1:A:90:LEU:C	1:A:90:LEU:CD2	0.50	2.75	12	1
1:A:14:SER:CB	1:A:91:HIS:CE1	0.50	2.95	15	1
1:A:28:LEU:HD23	1:A:41:ALA:C	0.50	2.27	14	1
1:A:17:LEU:HD22	1:A:50:PRO:O	0.49	2.07	8	1
1:A:66:ILE:CD1	1:A:79:ALA:HB1	0.49	2.36	16	2
1:A:54:CYS:O	1:A:56:ARG:CZ	0.49	2.60	7	2
1:A:14:SER:HB3	1:A:91:HIS:CE1	0.49	2.42	15	2
1:A:21:TYR:CG	1:A:22:ALA:N	0.49	2.80	2	1
1:A:41:ALA:CB	1:A:61:ASP:O	0.49	2.61	2	4
1:A:43:ARG:O	1:A:59:VAL:HG22	0.49	2.07	13	1
1:A:69:GLU:CD	1:A:82:ARG:CZ	0.49	2.81	5	1
1:A:24:PHE:CE2	1:A:90:LEU:HB2	0.49	2.43	6	2

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:17:LEU:HB2	1:A:90:LEU:HD22	0.49	1.84	15	2
1:A:66:ILE:HG23	1:A:92:LEU:HD22	0.49	1.84	3	1
1:A:83:ILE:HG12	1:A:92:LEU:HD21	0.48	1.84	11	5
1:A:55:GLY:O	1:A:57:LEU:N	0.48	2.45	10	5
1:A:66:ILE:O	1:A:69:GLU:N	0.48	2.46	18	2
1:A:42:VAL:HG23	1:A:61:ASP:OD2	0.48	2.07	5	1
1:A:12:HIS:CD2	1:A:95:ARG:HD2	0.48	2.44	4	3
1:A:90:LEU:HD21	1:A:92:LEU:HG	0.47	1.85	17	2
1:A:27:THR:HG22	1:A:28:LEU:N	0.47	2.24	4	3
1:A:13:PHE:CZ	1:A:94:ILE:HB	0.47	2.45	7	7
1:A:65:HIS:HB2	1:A:93:VAL:HG21	0.47	1.85	5	3
1:A:16:GLU:O	1:A:17:LEU:HD23	0.46	2.10	20	2
1:A:12:HIS:CD2	1:A:12:HIS:N	0.46	2.82	17	1
1:A:90:LEU:HD23	1:A:90:LEU:C	0.46	2.30	4	2
1:A:64:LEU:O	1:A:65:HIS:CG	0.46	2.69	18	1
1:A:64:LEU:HD12	1:A:64:LEU:N	0.46	2.25	20	1
1:A:28:LEU:HB3	1:A:40:LEU:HD22	0.45	1.88	4	1
1:A:19:ARG:HG3	1:A:24:PHE:CZ	0.45	2.46	16	1
1:A:18:VAL:O	1:A:19:ARG:C	0.45	2.55	16	7
1:A:15:VAL:HG11	1:A:57:LEU:CD1	0.45	2.40	5	1
1:A:17:LEU:CB	1:A:90:LEU:HD22	0.45	2.42	13	2
1:A:55:GLY:O	1:A:56:ARG:C	0.45	2.55	10	10
1:A:64:LEU:O	1:A:65:HIS:ND1	0.45	2.50	10	10
1:A:66:ILE:HD12	1:A:79:ALA:HB1	0.45	1.88	20	2
1:A:61:ASP:OD1	1:A:61:ASP:C	0.45	2.55	9	1
1:A:61:ASP:C	1:A:61:ASP:OD1	0.45	2.55	5	1
1:A:64:LEU:C	1:A:65:HIS:CG	0.45	2.91	18	1
1:A:13:PHE:CD2	1:A:94:ILE:O	0.45	2.70	4	1
1:A:75:THR:O	1:A:76:HIS:C	0.44	2.55	9	1
1:A:13:PHE:CE1	1:A:94:ILE:HB	0.44	2.47	11	4
1:A:19:ARG:N	1:A:24:PHE:CE1	0.44	2.86	4	1
1:A:71:THR:HA	1:A:74:LEU:HD12	0.44	1.89	18	2
1:A:66:ILE:HD13	1:A:83:ILE:HD11	0.44	1.89	8	1
1:A:47:LYS:O	1:A:48:ASP:CG	0.44	2.56	12	3
1:A:57:LEU:C	1:A:58:GLU:OE2	0.43	2.56	4	1
1:A:42:VAL:HG23	1:A:61:ASP:CG	0.43	2.33	5	1
1:A:17:LEU:HD11	1:A:57:LEU:HD12	0.43	1.90	11	1
1:A:78:GLN:O	1:A:81:GLU:N	0.43	2.51	20	1
1:A:84:ARG:CG	1:A:85:ALA:N	0.43	2.82	13	2
1:A:13:PHE:CE2	1:A:94:ILE:HB	0.43	2.48	17	1
1:A:28:LEU:HD13	1:A:40:LEU:HD22	0.43	1.89	16	3

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:41:ALA:O	1:A:42:VAL:C	0.43	2.57	16	1
1:A:12:HIS:CD2	1:A:12:HIS:H	0.43	2.31	17	1
1:A:64:LEU:N	1:A:64:LEU:CD1	0.43	2.81	20	1
1:A:80:VAL:HA	1:A:83:ILE:HD12	0.42	1.91	18	1
1:A:77:ALA:O	1:A:78:GLN:C	0.42	2.58	5	1
1:A:83:ILE:N	1:A:83:ILE:HD13	0.42	2.30	8	1
1:A:69:GLU:OE1	1:A:82:ARG:NE	0.42	2.53	5	1
1:A:69:GLU:HG3	1:A:74:LEU:HD11	0.42	1.91	18	1
1:A:32:ARG:O	1:A:75:THR:HG22	0.42	2.14	10	1
1:A:17:LEU:CD2	1:A:54:CYS:SG	0.42	3.08	5	1
1:A:57:LEU:HD21	1:A:94:ILE:HG13	0.42	1.92	20	2
1:A:75:THR:OG1	1:A:76:HIS:N	0.42	2.52	9	1
1:A:82:ARG:O	1:A:86:GLY:N	0.41	2.53	8	1
1:A:69:GLU:CD	1:A:74:LEU:CD1	0.41	2.89	4	1
1:A:37:ASP:O	1:A:38:THR:CG2	0.41	2.69	5	1
1:A:66:ILE:O	1:A:67:ASN:C	0.41	2.57	18	1
1:A:14:SER:OG	1:A:91:HIS:CE1	0.41	2.74	15	1
1:A:66:ILE:HG21	1:A:83:ILE:HD11	0.41	1.89	8	1
1:A:25:GLY:HA3	1:A:46:LEU:CB	0.41	2.46	17	1
1:A:66:ILE:HG22	1:A:67:ASN:CG	0.41	2.35	6	1
1:A:33:ASP:N	1:A:33:ASP:OD1	0.41	2.53	12	1
1:A:66:ILE:CG2	1:A:83:ILE:CD1	0.41	2.94	16	1
1:A:95:ARG:NH1	1:A:96:ARG:O	0.41	2.54	17	1
1:A:29:GLY:N	1:A:43:ARG:HB2	0.41	2.31	4	1
1:A:65:HIS:O	1:A:66:ILE:CG1	0.41	2.69	4	1
1:A:21:TYR:O	1:A:22:ALA:C	0.41	2.58	8	1
1:A:26:LEU:HD21	1:A:57:LEU:HD13	0.41	1.93	16	1
1:A:21:TYR:O	1:A:21:TYR:CG	0.41	2.74	20	1
1:A:83:ILE:HD13	1:A:83:ILE:N	0.40	2.31	16	1
1:A:17:LEU:HD11	1:A:57:LEU:CD1	0.40	2.46	11	1
1:A:80:VAL:O	1:A:81:GLU:C	0.40	2.60	15	1
1:A:90:LEU:HD23	1:A:91:HIS:N	0.40	2.31	17	1
1:A:32:ARG:CB	1:A:32:ARG:NH1	0.40	2.84	10	1
1:A:31:GLY:CA	1:A:38:THR:O	0.40	2.70	16	1
1:A:24:PHE:CE1	1:A:90:LEU:HB3	0.40	2.52	18	1
1:A:64:LEU:HD11	1:A:95:ARG:CZ	0.40	2.46	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	86/104 (83%)	76±3 (89±3%)	9±3 (10±3%)	1±1 (1±1%)	24	71
All	All	1720/2080 (83%)	1527 (89%)	180 (10%)	13 (1%)	24	71

All 3 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	19	ARG	6
1	A	56	ARG	5
1	A	20	GLY	2

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	64/75 (85%)	61±1 (95±2%)	3±1 (5±2%)	26	75
All	All	1280/1500 (85%)	1211 (95%)	69 (5%)	26	75

All 19 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	90	LEU	17
1	A	47	LYS	7
1	A	46	LEU	7
1	A	43	ARG	6
1	A	61	ASP	5
1	A	33	ASP	4
1	A	32	ARG	3

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Models (Total)
1	A	37	ASP	3
1	A	64	LEU	3
1	A	81	GLU	3
1	A	21	TYR	2
1	A	56	ARG	2
1	A	27	THR	1
1	A	34	VAL	1
1	A	75	THR	1
1	A	12	HIS	1
1	A	16	GLU	1
1	A	38	THR	1
1	A	76	HIS	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