Full wwPDB NMR Structure Validation Report (i)

Feb 23, 2022 – 02:55 PM EST

PDB ID	:	1XS3
Title	:	Solution Structure Analysis of the XC975 protein
Authors	:	Chin, K.-H.; Lin, F.-Y.; Hu, Y.-C.; Sze, K.-H.; Lyu, P.-C.; Chou, S.-H.
Deposited on	:	2004-10-18

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:

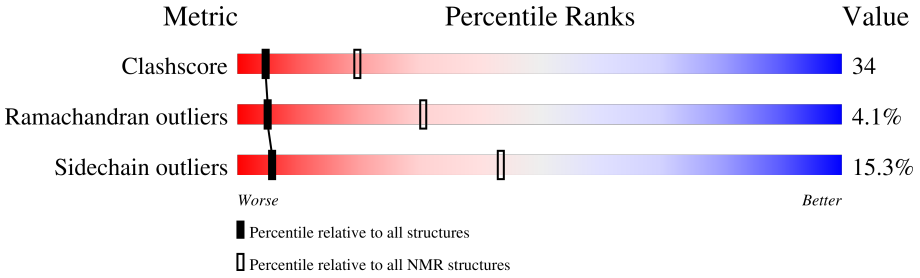
MolProbity	:	4.02b-467
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
RCI	:	v_1n_11_5_13_A (Berjanski et al., 2005)
PANAV	:	Wang et al. (2010)
ShiftChecker	:	2.26
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
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	80	39% 46% • 12%

2 Ensemble composition and analysis (i)

This entry contains 20 models. Model 5 is the overall representative, medoid model (most similar to other models). The authors have identified model 6 as representative, based on the following criterion: *fewest violations*.

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:17-A:74, A:78-A:89 (70)	0.26	5

Ill-defined regions of proteins are excluded from the global statistics.

Ligands and non-protein polymers are included in the analysis.

The models can be grouped into 3 clusters. No single-model clusters were found.

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

3 Entry composition (i)

There is only 1 type of molecule in this entry. The entry contains 1136 atoms, of which 528 are hydrogens and 0 are deuteriums.

- Molecule 1 is a protein called hypothetical protein XC975.

Mol	Chain	Residues	Atoms						Trace
			Total	C	H	N	O	S	
1	A	80	1136	383	528	110	112	3	0

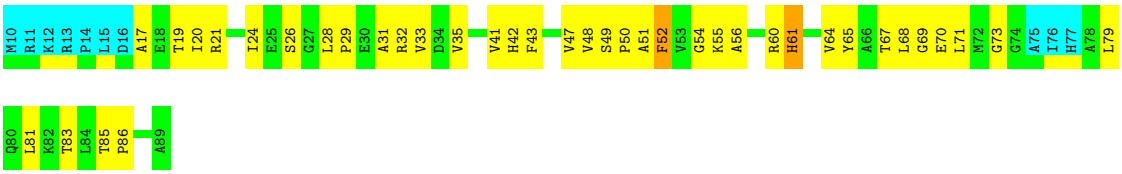
4 Residue-property plots (i)

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: hypothetical protein XC975

Chain A:

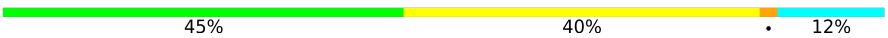


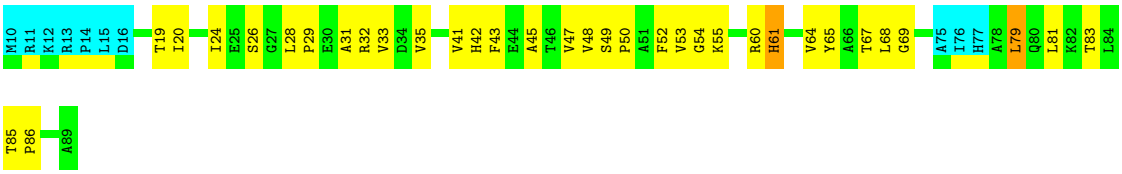
4.2 Scores per residue for each member of the ensemble

Colouring as in section 4.1 above.

4.2.1 Score per residue for model 1

• Molecule 1: hypothetical protein XC975

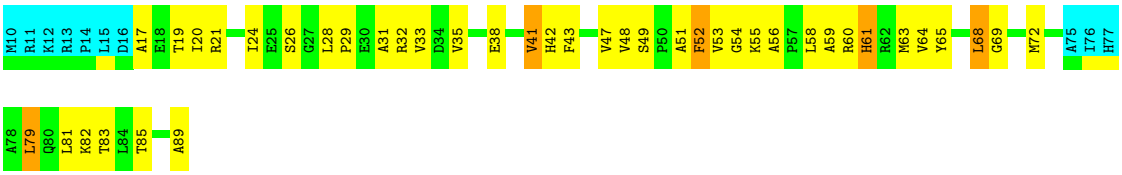
Chain A: 



4.2.2 Score per residue for model 2

• Molecule 1: hypothetical protein XC975

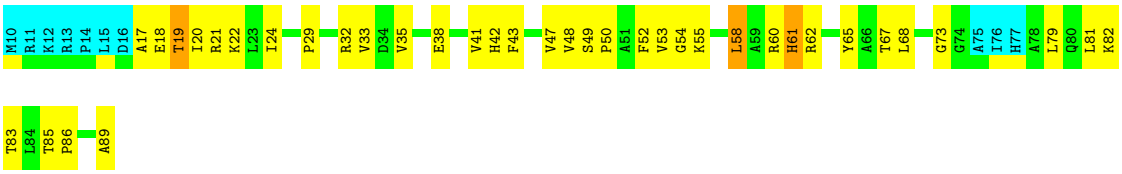
Chain A:



4.2.3 Score per residue for model 3

- Molecule 1: hypothetical protein XC975

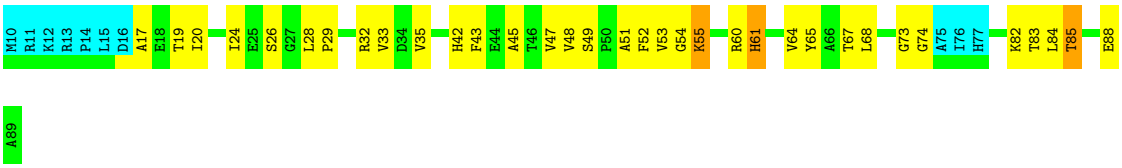
Chain A: 40% 44% • 12%



4.2.4 Score per residue for model 4

- Molecule 1: hypothetical protein XC975

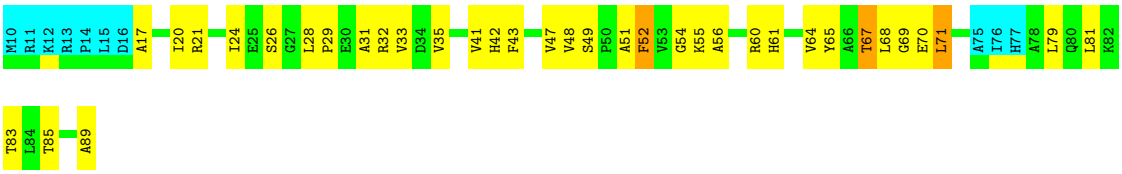
Chain A: 45% 39% • 12%



4.2.5 Score per residue for model 5 (medoid)

- Molecule 1: hypothetical protein XC975

Chain A: 42% 41% • 12%



4.2.6 Score per residue for model 6

- Molecule 1: hypothetical protein XC975

Chain A: 36% 46% 5% 12%

M10 R11 K12 R13 P14 L15 D16 A17 I20 R21 I24 E25 S26 G27 L28 P29 E30 A31 R32 V33 D34 V35 E38 V41 H42 F43 E44 A45 T46 V47 V48 S49 P50 A51 F52 V53 G54 K55 R60 H61 V64 Y65 A66 T67 L68 G69 G73 G74 A75 I76 H77 A78 L79

Q80 L81 K82 T83 L84 T85 P86 A89

4.2.7 Score per residue for model 7

- Molecule 1: hypothetical protein XC975

Chain A: 46% 38% • 12%

M10 R11 K12 R13 P14 L15 D16 T19 I20 R21 K22 L23 I24 E25 S26 P29 R32 V33 H42 F43 V47 V48 S49 P50 A51 F52 K55 A56 R60 H61 V64 Y65 A66 T67 L68 G69 E70 L71 A75 I76 H77 A78 L79 Q80 L81 K82 T83 L84 T85 P86

A89

4.2.8 Score per residue for model 8

- Molecule 1: hypothetical protein XC975

Chain A: 44% 40% • 12%

M10 R11 K12 R13 P14 L15 D16 A17 E18 T19 I20 R21 I24 E25 S26 P29 R32 V33 D34 V35 H42 F43 V47 V48 S49 P50 A51 F52 A56 R60 H61 V64 Y65 A66 T67 L68 G69 E70 L71 G74 A75 I76 H77 A78 L79 Q80 L81 K82 T83 L84 T85

P86 A89

4.2.9 Score per residue for model 9

- Molecule 1: hypothetical protein XC975

Chain A: 39% 41% 8% 12%

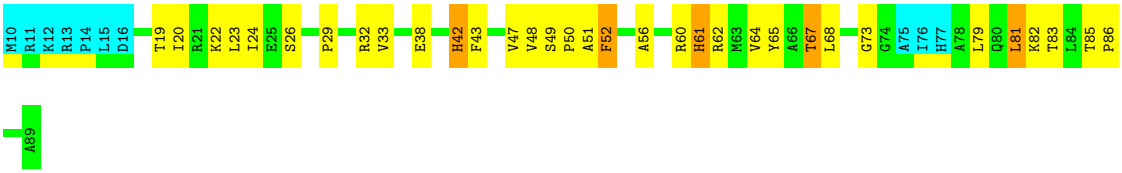
M10 R11 K12 R13 P14 L15 D16 A17 E18 T19 I20 R21 K22 L23 I24 E25 S26 V33 D34 V35 G40 V41 H42 F43 V47 V48 S49 P50 A51 F52 V53 G54 K55 A56 A59 R60 H61 R62 M63 V64 Y65 A66 T67 L68 G69 E70 L71 M72 G73 G74 A75 I76 H77 A78 L79 Q80

L81 K82 T83 L84 T85 P86 A89

4.2.10 Score per residue for model 10

- Molecule 1: hypothetical protein XC975

Chain A: 46% 35% 6% 12%



4.2.11 Score per residue for model 11

- Molecule 1: hypothetical protein XC975

Chain A: 36% 41% 10% 12%

4.2.12 Score per residue for model 12

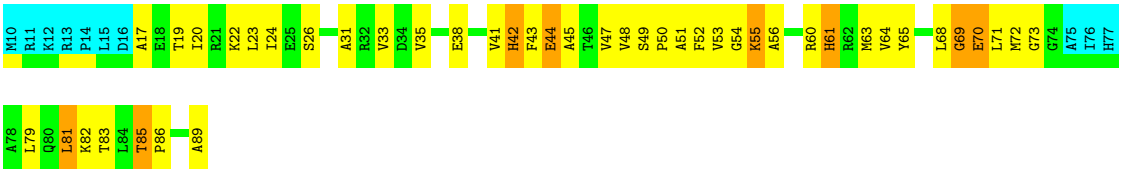
- Molecule 1: hypothetical protein XC975

Chain A: 45% 38% 5% 12%

4.2.13 Score per residue for model 13

- Molecule 1: hypothetical protein XC975

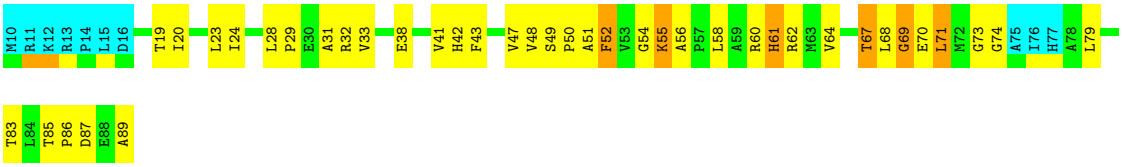
Chain A: 32% 45% 10% 12%



4.2.14 Score per residue for model 14

- Molecule 1: hypothetical protein XC975

Chain A: 38% 42% 8% 12%



4.2.15 Score per residue for model 15

- Molecule 1: hypothetical protein XC975

Chain A: 49% 32% 6% 12%

4.2.16 Score per residue for model 16

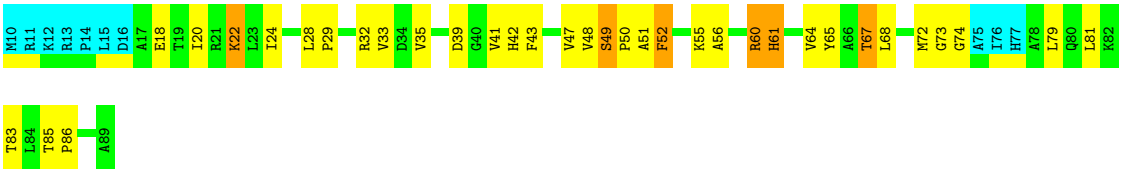
- Molecule 1: hypothetical protein XC975

Chain A: 34% 48% 6% 12%

4.2.17 Score per residue for model 17

- Molecule 1: hypothetical protein XC975

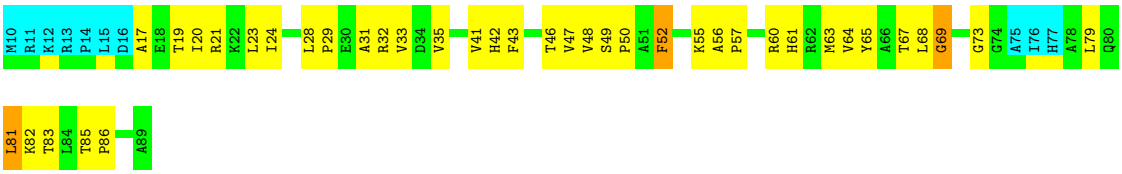
Chain A: 44% 36% 8% 12%



4.2.18 Score per residue for model 18

- Molecule 1: hypothetical protein XC975

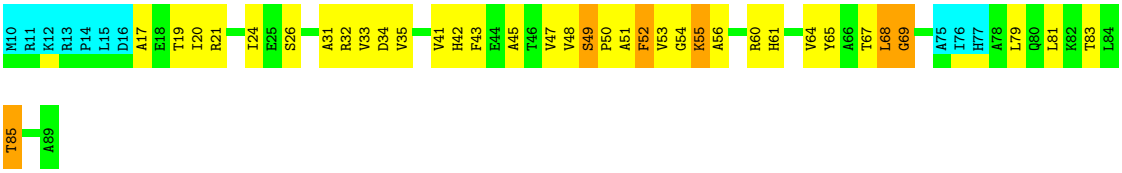
Chain A: 39% 45% • 12%



4.2.19 Score per residue for model 19

- Molecule 1: hypothetical protein XC975

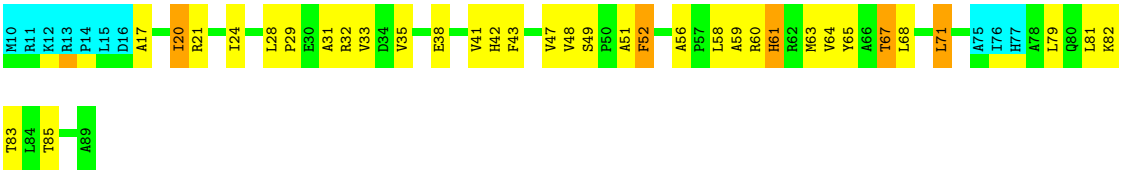
Chain A: 42% 38% 8% 12%



4.2.20 Score per residue for model 20

- Molecule 1: hypothetical protein XC975

Chain A: 44% 38% 6% 12%



5 Refinement protocol and experimental data overview (i)

The models were refined using the following method: *distance geometry simulated annealing molecular dynamics.*

Of the 100 calculated structures, 20 were deposited, based on the following criterion: *structures with the lowest energy.*

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

Software name	Classification	Version
CYANA	structure solution	2.0
CYANA	refinement	2.0

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	523	454	532	36±6
All	All	10460	9080	10640	720

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 34.

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

Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:20:ILE:HD11	1:A:35:VAL:HG11	1.04	1.29	8	9
1:A:33:VAL:HG13	1:A:47:VAL:HG22	1.04	1.29	1	16
1:A:17:ALA:HB1	1:A:35:VAL:HG13	1.02	1.25	13	10
1:A:68:LEU:HD22	1:A:68:LEU:O	0.95	1.61	19	1
1:A:65:TYR:CE1	1:A:81:LEU:HD22	0.94	1.96	9	3
1:A:65:TYR:CE1	1:A:81:LEU:HD13	0.94	1.97	8	9
1:A:20:ILE:HD11	1:A:35:VAL:CG1	0.91	1.96	2	4
1:A:68:LEU:HD13	1:A:69:GLY:N	0.91	1.80	19	1
1:A:33:VAL:HG22	1:A:47:VAL:HG13	0.89	1.42	3	10
1:A:48:VAL:HG21	1:A:89:ALA:HB2	0.88	1.42	2	7
1:A:20:ILE:HD12	1:A:21:ARG:N	0.85	1.86	16	4
1:A:43:PHE:CE2	1:A:79:LEU:HD11	0.85	2.06	19	13
1:A:20:ILE:HD12	1:A:68:LEU:HD22	0.84	1.47	18	1
1:A:19:THR:O	1:A:23:LEU:HD23	0.83	1.74	15	4

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:43:PHE:CE1	1:A:79:LEU:HD11	0.82	2.10	2	7
1:A:17:ALA:HB1	1:A:35:VAL:CG1	0.80	2.04	16	4
1:A:43:PHE:CZ	1:A:79:LEU:HD21	0.78	2.12	11	4
1:A:68:LEU:HD13	1:A:68:LEU:C	0.78	1.99	19	1
1:A:43:PHE:CZ	1:A:79:LEU:HD11	0.76	2.16	13	15
1:A:65:TYR:CZ	1:A:81:LEU:HD22	0.75	2.16	11	4
1:A:20:ILE:CD1	1:A:35:VAL:HG11	0.75	2.11	2	1
1:A:63:MET:O	1:A:67:THR:HG23	0.73	1.83	18	1
1:A:28:LEU:HD23	1:A:31:ALA:CB	0.72	2.15	18	3
1:A:51:ALA:HB1	1:A:60:ARG:HD2	0.72	1.62	12	12
1:A:24:ILE:CG2	1:A:33:VAL:HG21	0.71	2.15	7	19
1:A:64:VAL:O	1:A:68:LEU:HD13	0.70	1.87	11	2
1:A:17:ALA:HA	1:A:20:ILE:HD11	0.69	1.63	20	1
1:A:43:PHE:CZ	1:A:79:LEU:CD1	0.69	2.76	6	7
1:A:84:LEU:HD22	1:A:88:GLU:OE1	0.69	1.88	4	1
1:A:20:ILE:HD12	1:A:68:LEU:HG	0.68	1.65	10	1
1:A:35:VAL:HG13	1:A:45:ALA:HB2	0.68	1.64	4	2
1:A:70:GLU:HG3	1:A:71:LEU:HD23	0.68	1.66	11	1
1:A:24:ILE:HG21	1:A:33:VAL:HG21	0.67	1.65	17	17
1:A:33:VAL:HG13	1:A:47:VAL:CG1	0.67	2.19	13	2
1:A:20:ILE:H	1:A:20:ILE:HD13	0.67	1.50	20	2
1:A:24:ILE:HG22	1:A:28:LEU:HD12	0.67	1.65	1	2
1:A:24:ILE:CD1	1:A:33:VAL:HG11	0.67	2.20	17	7
1:A:33:VAL:HG13	1:A:47:VAL:CG2	0.66	2.20	7	5
1:A:20:ILE:HD13	1:A:68:LEU:HD23	0.66	1.67	8	1
1:A:84:LEU:HD22	1:A:88:GLU:CD	0.66	2.11	4	1
1:A:20:ILE:HD13	1:A:68:LEU:HB2	0.66	1.67	19	1
1:A:71:LEU:O	1:A:71:LEU:HD13	0.65	1.91	16	3
1:A:43:PHE:CE2	1:A:79:LEU:HD21	0.65	2.26	11	3
1:A:28:LEU:CB	1:A:31:ALA:HB3	0.65	2.22	14	4
1:A:51:ALA:HB1	1:A:60:ARG:CD	0.64	2.23	13	9
1:A:33:VAL:HG13	1:A:47:VAL:HG12	0.64	1.67	13	2
1:A:52:PHE:HB3	1:A:56:ALA:HB2	0.62	1.71	12	15
1:A:24:ILE:HD13	1:A:33:VAL:HG11	0.62	1.71	17	5
1:A:24:ILE:HD11	1:A:67:THR:OG1	0.61	1.95	14	2
1:A:24:ILE:CG2	1:A:28:LEU:HD12	0.61	2.25	1	2
1:A:20:ILE:HD13	1:A:68:LEU:HG	0.61	1.72	13	2
1:A:20:ILE:HD12	1:A:20:ILE:C	0.61	2.16	16	3
1:A:42:HIS:CD2	1:A:78:ALA:O	0.61	2.54	6	1
1:A:43:PHE:CE1	1:A:79:LEU:CD1	0.60	2.84	14	6
1:A:20:ILE:CD1	1:A:21:ARG:N	0.60	2.63	16	2

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:68:LEU:C	1:A:68:LEU:HD12	0.60	2.17	16	4
1:A:42:HIS:CD2	1:A:42:HIS:O	0.60	2.54	10	4
1:A:17:ALA:CB	1:A:35:VAL:HG13	0.60	2.10	16	3
1:A:51:ALA:HB1	1:A:60:ARG:HD3	0.59	1.73	9	1
1:A:68:LEU:C	1:A:68:LEU:CD1	0.59	2.71	19	2
1:A:51:ALA:HB1	1:A:60:ARG:NE	0.58	2.14	17	5
1:A:24:ILE:HD11	1:A:67:THR:CG2	0.58	2.29	12	1
1:A:43:PHE:CE2	1:A:79:LEU:CD1	0.58	2.84	19	1
1:A:19:THR:CG2	1:A:20:ILE:N	0.58	2.67	3	2
1:A:32:ARG:HB3	1:A:48:VAL:HG12	0.57	1.74	20	13
1:A:20:ILE:HD12	1:A:68:LEU:HD23	0.57	1.76	4	2
1:A:43:PHE:HE1	1:A:45:ALA:HB2	0.57	1.60	19	1
1:A:23:LEU:O	1:A:23:LEU:HD13	0.56	2.00	9	1
1:A:70:GLU:HG3	1:A:71:LEU:HD22	0.56	1.75	9	1
1:A:61:HIS:CE1	1:A:65:TYR:OH	0.56	2.59	9	9
1:A:38:GLU:O	1:A:41:VAL:HG12	0.56	2.01	20	4
1:A:18:GLU:CD	1:A:19:THR:N	0.56	2.60	12	1
1:A:71:LEU:C	1:A:71:LEU:CD2	0.56	2.74	8	1
1:A:35:VAL:HG22	1:A:45:ALA:HB1	0.56	1.77	1	1
1:A:64:VAL:O	1:A:67:THR:HG22	0.55	2.02	5	7
1:A:42:HIS:CD2	1:A:42:HIS:C	0.55	2.81	6	1
1:A:48:VAL:O	1:A:48:VAL:HG13	0.55	2.02	16	13
1:A:49:SER:OG	1:A:52:PHE:CE2	0.55	2.60	1	4
1:A:43:PHE:CD1	1:A:79:LEU:HD11	0.54	2.37	12	4
1:A:68:LEU:HD11	1:A:70:GLU:HG2	0.54	1.79	16	2
1:A:64:VAL:HG21	1:A:81:LEU:HD21	0.54	1.80	9	2
1:A:33:VAL:HG12	1:A:47:VAL:HG22	0.54	1.80	11	1
1:A:52:PHE:CE1	1:A:60:ARG:HB3	0.54	2.38	13	5
1:A:41:VAL:HG22	1:A:42:HIS:N	0.54	2.18	20	2
1:A:33:VAL:CG1	1:A:47:VAL:HG22	0.53	2.28	14	2
1:A:46:THR:HG23	1:A:82:LYS:HB2	0.53	1.79	11	2
1:A:51:ALA:HB1	1:A:60:ARG:HE	0.53	1.62	17	2
1:A:52:PHE:CE2	1:A:60:ARG:HB3	0.53	2.39	20	14
1:A:68:LEU:HD11	1:A:70:GLU:CG	0.53	2.33	16	1
1:A:42:HIS:CG	1:A:42:HIS:O	0.53	2.62	3	8
1:A:53:VAL:HA	1:A:85:THR:HG23	0.53	1.80	6	4
1:A:81:LEU:C	1:A:81:LEU:HD13	0.52	2.25	2	1
1:A:41:VAL:HG12	1:A:42:HIS:N	0.52	2.19	1	6
1:A:17:ALA:HB1	1:A:35:VAL:O	0.52	2.04	9	2
1:A:45:ALA:CB	1:A:68:LEU:HD21	0.52	2.34	6	1
1:A:61:HIS:CD2	1:A:81:LEU:CD2	0.51	2.92	17	1

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:24:ILE:HD11	1:A:68:LEU:CD1	0.51	2.35	1	1
1:A:61:HIS:O	1:A:64:VAL:CG2	0.51	2.58	20	14
1:A:24:ILE:CG2	1:A:28:LEU:HD13	0.51	2.35	4	2
1:A:63:MET:O	1:A:67:THR:HG22	0.51	2.05	9	1
1:A:67:THR:HG23	1:A:68:LEU:HD12	0.51	1.83	15	5
1:A:64:VAL:O	1:A:68:LEU:CD1	0.51	2.58	11	3
1:A:65:TYR:CE1	1:A:81:LEU:HG	0.51	2.41	12	5
1:A:43:PHE:CD2	1:A:79:LEU:HD11	0.51	2.39	9	2
1:A:68:LEU:HD22	1:A:68:LEU:C	0.51	2.22	19	1
1:A:53:VAL:O	1:A:55:LYS:N	0.51	2.43	4	10
1:A:33:VAL:HG22	1:A:47:VAL:HG22	0.51	1.81	7	1
1:A:48:VAL:O	1:A:48:VAL:CG1	0.51	2.59	1	12
1:A:20:ILE:CG2	1:A:67:THR:O	0.51	2.59	8	1
1:A:61:HIS:O	1:A:64:VAL:HG22	0.51	2.05	10	15
1:A:61:HIS:CD2	1:A:65:TYR:HH	0.51	2.24	20	1
1:A:33:VAL:HG22	1:A:47:VAL:HG12	0.50	1.83	19	2
1:A:68:LEU:HD12	1:A:69:GLY:N	0.50	2.21	16	2
1:A:71:LEU:O	1:A:71:LEU:CD1	0.50	2.60	20	3
1:A:24:ILE:HD11	1:A:68:LEU:HD12	0.50	1.82	1	1
1:A:18:GLU:OE1	1:A:21:ARG:NE	0.50	2.45	9	1
1:A:20:ILE:HG12	1:A:21:ARG:N	0.50	2.21	9	2
1:A:52:PHE:CD2	1:A:60:ARG:HB3	0.50	2.42	2	2
1:A:20:ILE:HD11	1:A:35:VAL:HG21	0.50	1.83	5	2
1:A:43:PHE:CD1	1:A:43:PHE:C	0.50	2.85	13	11
1:A:21:ARG:NE	1:A:33:VAL:O	0.50	2.45	8	1
1:A:68:LEU:CD1	1:A:70:GLU:CB	0.49	2.90	7	1
1:A:65:TYR:O	1:A:68:LEU:CD1	0.49	2.60	19	1
1:A:61:HIS:O	1:A:65:TYR:CD2	0.49	2.66	17	1
1:A:52:PHE:CD2	1:A:83:THR:HB	0.49	2.43	6	5
1:A:20:ILE:HD11	1:A:35:VAL:CG2	0.49	2.38	6	1
1:A:68:LEU:O	1:A:69:GLY:C	0.49	2.51	19	7
1:A:20:ILE:HD12	1:A:21:ARG:CA	0.49	2.38	16	1
1:A:20:ILE:HG21	1:A:68:LEU:HA	0.49	1.84	19	1
1:A:58:LEU:CD2	1:A:62:ARG:CD	0.48	2.92	3	2
1:A:84:LEU:N	1:A:84:LEU:HD23	0.48	2.24	11	1
1:A:20:ILE:CD1	1:A:35:VAL:HG21	0.47	2.39	17	3
1:A:40:GLY:CA	1:A:73:GLY:O	0.47	2.62	9	1
1:A:20:ILE:HD13	1:A:68:LEU:CG	0.47	2.39	13	1
1:A:20:ILE:O	1:A:24:ILE:HD12	0.47	2.09	19	1
1:A:67:THR:HG23	1:A:68:LEU:HD13	0.47	1.86	9	1
1:A:23:LEU:C	1:A:23:LEU:CD1	0.47	2.83	9	1

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:65:TYR:HE1	1:A:81:LEU:HD13	0.47	1.63	11	1
1:A:50:PRO:N	1:A:86:PRO:HD3	0.47	2.24	12	14
1:A:70:GLU:HG3	1:A:71:LEU:HD13	0.47	1.85	8	1
1:A:17:ALA:O	1:A:21:ARG:CB	0.47	2.63	6	3
1:A:70:GLU:CG	1:A:71:LEU:HD22	0.47	2.40	9	1
1:A:70:GLU:OE1	1:A:70:GLU:C	0.47	2.54	11	1
1:A:20:ILE:HD13	1:A:68:LEU:CD1	0.47	2.40	13	1
1:A:38:GLU:O	1:A:41:VAL:CG2	0.47	2.63	6	1
1:A:28:LEU:CD2	1:A:31:ALA:CB	0.46	2.92	5	1
1:A:63:MET:SD	1:A:63:MET:C	0.46	2.94	11	1
1:A:81:LEU:HD13	1:A:82:LYS:N	0.46	2.25	2	1
1:A:59:ALA:O	1:A:63:MET:CG	0.46	2.63	2	2
1:A:68:LEU:CD1	1:A:70:GLU:HB2	0.46	2.41	7	1
1:A:19:THR:HG23	1:A:20:ILE:N	0.46	2.25	12	6
1:A:20:ILE:HG13	1:A:21:ARG:N	0.46	2.25	19	5
1:A:32:ARG:HB2	1:A:48:VAL:HG13	0.46	1.88	19	2
1:A:23:LEU:HD13	1:A:23:LEU:C	0.46	2.30	9	1
1:A:24:ILE:HG21	1:A:33:VAL:HG11	0.46	1.87	11	1
1:A:67:THR:CG2	1:A:68:LEU:N	0.46	2.79	19	1
1:A:22:LYS:CG	1:A:23:LEU:N	0.46	2.79	10	2
1:A:64:VAL:HG23	1:A:65:TYR:N	0.45	2.26	18	3
1:A:39:ASP:OD2	1:A:72:MET:C	0.45	2.54	17	1
1:A:24:ILE:HG12	1:A:67:THR:HG21	0.45	1.88	11	2
1:A:24:ILE:HD12	1:A:33:VAL:HG11	0.45	1.87	18	2
1:A:61:HIS:CE1	1:A:81:LEU:HD23	0.45	2.46	11	1
1:A:52:PHE:CD1	1:A:60:ARG:HB3	0.45	2.47	15	2
1:A:24:ILE:HB	1:A:33:VAL:HG21	0.45	1.89	11	1
1:A:71:LEU:HD13	1:A:71:LEU:H	0.45	1.72	8	1
1:A:52:PHE:CG	1:A:83:THR:HB	0.44	2.47	13	20
1:A:21:ARG:O	1:A:25:GLU:CG	0.44	2.65	9	1
1:A:65:TYR:CE1	1:A:81:LEU:CD1	0.44	3.00	6	2
1:A:45:ALA:HB1	1:A:68:LEU:HD21	0.44	1.89	11	2
1:A:61:HIS:CE1	1:A:65:TYR:HH	0.44	2.28	17	2
1:A:20:ILE:CG1	1:A:21:ARG:N	0.44	2.81	5	2
1:A:52:PHE:HB3	1:A:56:ALA:CB	0.44	2.43	10	3
1:A:65:TYR:CZ	1:A:81:LEU:HG	0.44	2.48	18	1
1:A:24:ILE:HD11	1:A:67:THR:CB	0.44	2.43	8	1
1:A:22:LYS:CD	1:A:22:LYS:C	0.44	2.86	17	1
1:A:43:PHE:CZ	1:A:68:LEU:HD13	0.44	2.47	17	1
1:A:56:ALA:CB	1:A:83:THR:OG1	0.44	2.66	10	1
1:A:35:VAL:HG23	1:A:43:PHE:CD1	0.44	2.48	19	1

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:79:LEU:HD13	1:A:80:GLN:N	0.43	2.28	11	1
1:A:17:ALA:HA	1:A:20:ILE:CD1	0.43	2.44	9	1
1:A:71:LEU:C	1:A:71:LEU:HD23	0.43	2.34	14	1
1:A:20:ILE:O	1:A:24:ILE:CD1	0.43	2.67	19	1
1:A:24:ILE:HD11	1:A:67:THR:HG23	0.43	1.89	12	2
1:A:32:ARG:HB2	1:A:48:VAL:CG1	0.43	2.44	15	5
1:A:46:THR:HG23	1:A:82:LYS:CB	0.43	2.43	11	1
1:A:31:ALA:CB	1:A:49:SER:CB	0.43	2.97	19	1
1:A:65:TYR:CD1	1:A:81:LEU:HD13	0.43	2.43	8	1
1:A:32:ARG:CB	1:A:48:VAL:HG12	0.42	2.44	20	2
1:A:60:ARG:HD2	1:A:60:ARG:N	0.42	2.29	16	1
1:A:49:SER:CB	1:A:50:PRO:HD2	0.42	2.44	17	2
1:A:28:LEU:HD13	1:A:31:ALA:CB	0.42	2.44	1	2
1:A:28:LEU:N	1:A:28:LEU:HD22	0.42	2.30	16	1
1:A:31:ALA:CB	1:A:49:SER:HB3	0.42	2.44	13	1
1:A:70:GLU:HG2	1:A:71:LEU:HD22	0.42	1.90	13	1
1:A:55:LYS:CD	1:A:55:LYS:C	0.42	2.88	14	1
1:A:32:ARG:HB3	1:A:48:VAL:CG1	0.42	2.45	16	7
1:A:58:LEU:HD21	1:A:62:ARG:NE	0.42	2.30	14	2
1:A:44:GLU:OE2	1:A:45:ALA:C	0.42	2.57	13	1
1:A:24:ILE:HD11	1:A:67:THR:HG21	0.42	1.92	16	1
1:A:65:TYR:HA	1:A:68:LEU:HD12	0.42	1.91	19	1
1:A:81:LEU:C	1:A:81:LEU:CD1	0.42	2.87	2	1
1:A:65:TYR:HA	1:A:68:LEU:HD21	0.42	1.92	7	2
1:A:50:PRO:CA	1:A:86:PRO:HD3	0.41	2.45	12	3
1:A:58:LEU:CD2	1:A:62:ARG:HD2	0.41	2.45	3	2
1:A:35:VAL:HG22	1:A:45:ALA:CB	0.41	2.45	1	1
1:A:60:ARG:N	1:A:60:ARG:HD3	0.41	2.30	3	1
1:A:24:ILE:CG2	1:A:28:LEU:HD23	0.41	2.46	6	1
1:A:67:THR:CG2	1:A:68:LEU:HD12	0.41	2.46	14	1
1:A:38:GLU:OE2	1:A:39:ASP:CG	0.41	2.58	16	1
1:A:70:GLU:HG3	1:A:71:LEU:N	0.41	2.31	8	1
1:A:64:VAL:HA	1:A:67:THR:HG22	0.41	1.92	9	1
1:A:44:GLU:OE2	1:A:45:ALA:N	0.41	2.54	13	1
1:A:17:ALA:HB1	1:A:35:VAL:HB	0.41	1.92	4	1
1:A:58:LEU:HD21	1:A:62:ARG:CD	0.41	2.46	16	1
1:A:42:HIS:HB3	1:A:78:ALA:HB3	0.41	1.92	7	1
1:A:68:LEU:HD11	1:A:70:GLU:CB	0.41	2.46	7	1
1:A:59:ALA:O	1:A:63:MET:SD	0.41	2.79	9	1
1:A:81:LEU:CD1	1:A:83:THR:CG2	0.41	2.99	12	1
1:A:81:LEU:HD12	1:A:83:THR:HG23	0.41	1.93	12	1

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:55:LYS:O	1:A:57:PRO:HD3	0.41	2.15	18	1
1:A:20:ILE:HG21	1:A:68:LEU:O	0.41	2.16	20	1
1:A:58:LEU:CD2	1:A:62:ARG:HG3	0.41	2.46	16	1
1:A:20:ILE:C	1:A:20:ILE:CD1	0.40	2.86	16	1
1:A:24:ILE:CD1	1:A:67:THR:HG21	0.40	2.47	12	1
1:A:81:LEU:CD1	1:A:83:THR:HG23	0.40	2.47	12	1
1:A:47:VAL:O	1:A:82:LYS:O	0.40	2.40	20	1
1:A:42:HIS:O	1:A:42:HIS:CG	0.40	2.74	2	1
1:A:28:LEU:N	1:A:28:LEU:HD12	0.40	2.31	5	1
1:A:83:THR:C	1:A:84:LEU:HD22	0.40	2.36	15	1
1:A:49:SER:HB2	1:A:50:PRO:HD2	0.40	1.92	13	1
1:A:41:VAL:CG2	1:A:42:HIS:N	0.40	2.84	20	1
1:A:24:ILE:HG12	1:A:67:THR:CG2	0.40	2.47	3	1
1:A:21:ARG:CG	1:A:33:VAL:O	0.40	2.69	16	1
1:A:42:HIS:O	1:A:42:HIS:ND1	0.40	2.54	20	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	69/80 (86%)	62±1 (89±1%)	5±1 (7±2%)	3±1 (4±2%)	5 31
All	All	1380/1600 (86%)	1231 (89%)	92 (7%)	57 (4%)	5 31

All 5 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	29	PRO	17
1	A	54	GLY	14
1	A	73	GLY	11
1	A	69	GLY	9
1	A	74	GLY	6

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	54/63 (86%)	46±2 (85±4%)	8±2 (15±4%)	6 43
All	All	1080/1260 (86%)	915 (85%)	165 (15%)	6 43

All 32 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	85	THR	20
1	A	61	HIS	18
1	A	49	SER	15
1	A	52	PHE	14
1	A	26	SER	12
1	A	55	LYS	10
1	A	67	THR	8
1	A	82	LYS	6
1	A	71	LEU	6
1	A	23	LEU	5
1	A	81	LEU	5
1	A	20	ILE	4
1	A	70	GLU	4
1	A	79	LEU	3
1	A	58	LEU	3
1	A	68	LEU	3
1	A	22	LYS	3
1	A	38	GLU	3
1	A	34	ASP	3
1	A	63	MET	3
1	A	72	MET	2
1	A	18	GLU	2
1	A	60	ARG	2
1	A	42	HIS	2
1	A	87	ASP	2
1	A	41	VAL	1
1	A	19	THR	1
1	A	62	ARG	1
1	A	33	VAL	1

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Models (Total)
1	A	84	LEU	1
1	A	44	GLU	1
1	A	36	GLN	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