Full wwPDB NMR Structure Validation Report (i)

Feb 28, 2022 – 06:12 PM EST

PDB ID	:	2EQO
Title	:	Solution structure of the stn_TRAF3IP1_nd domain of interleukin 13 receptor alpha 1-binding protein-1 [Homo sapiens]
Authors	:	Dang, W.; Muto, Y.; Inoue, M.; Kigawa, T.; Shirouzu, M.; Terada, T.; Yokoyama, S.; RIKEN Structural Genomics/Proteomics Initiative (RSGI)
Deposited on	:	2007-03-30

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:

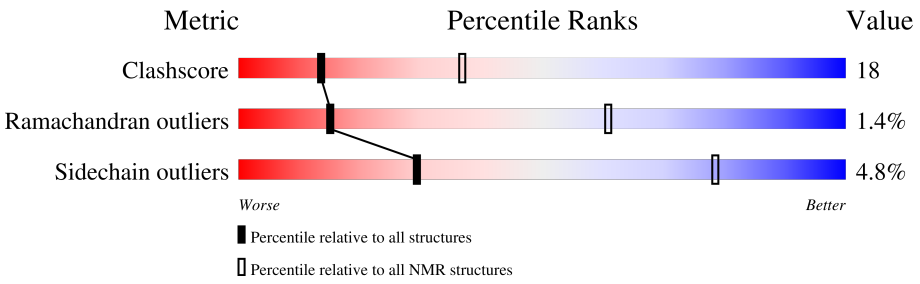
MolProbity	:	4.02b-467
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
RCI	:	v_1n_11_5_13_A (Berjanski et al., 2005)
PANAV	:	Wang et al. (2010)
ShiftChecker	:	2.27
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
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	140	62% 30% 8%

2 Ensemble composition and analysis (i)

This entry contains 20 models. Model 15 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:9-A:137 (129)	0.21	15

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

3 Entry composition (i)

There is only 1 type of molecule in this entry. The entry contains 2208 atoms, of which 1134 are hydrogens and 0 are deuteriums.

- Molecule 1 is a protein called TNF receptor-associated factor 3-interacting protein 1.

Mol	Chain	Residues	Atoms						Trace
			Total	C	H	N	O	S	
1	A	140	2208	674	1134	194	199	7	0

There are 7 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	1	GLY	-	expression tag	UNP Q8TDR0
A	2	SER	-	expression tag	UNP Q8TDR0
A	3	SER	-	expression tag	UNP Q8TDR0
A	4	GLY	-	expression tag	UNP Q8TDR0
A	5	SER	-	expression tag	UNP Q8TDR0
A	6	SER	-	expression tag	UNP Q8TDR0
A	7	GLY	-	expression tag	UNP Q8TDR0

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: TNF receptor-associated factor 3-interacting protein 1

Chain A: 62% 30% 8%

G1 S2 S3 G4 S5 S6 G7 M8 N9 A10 A11 V12 V13 L20 I24 R25 R26 P27 T30 E31 K32 L33 L34 S35 K36 P37 P38 F39 I45 L59 Y60 T61 D62 S67 D68 K73 D74 A75 K76 F79 K82 V86 V87 V88 M89 L96 A97 E107

P108 E109 R110 T111 N112 L115 K120 V132 V135 G138 E139 K140

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: TNF receptor-associated factor 3-interacting protein 1

Chain A: 58% 32% •• 8%

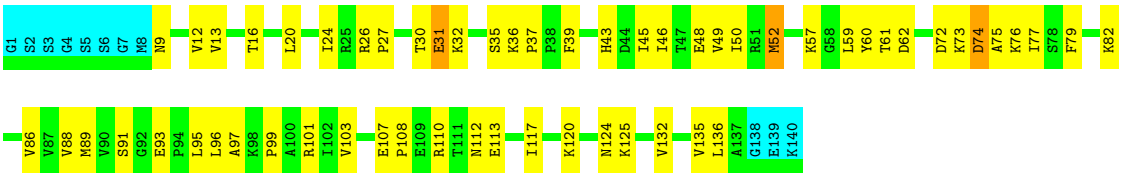
G1 S2 S3 G4 S5 S6 G7 M8 V12 V13 Q17 L20 I24 R25 R26 P27 P28 L29 L34 S35 K36 P37 P38 F39 I45 E48 R51 M52 T53 G54 F55 M56 L59 Y60 T61 D62 S67 D68 N69 V70 K73 D74 A75 K76 I77 S78 F79 K82

A83 I84 V88 M89 V90 L96 A97 K98 P99 E107 P108 E109 R110 T111 L115 Q116 R133 G138 E139 K140

4.2.2 Score per residue for model 2

• Molecule 1: TNF receptor-associated factor 3-interacting protein 1

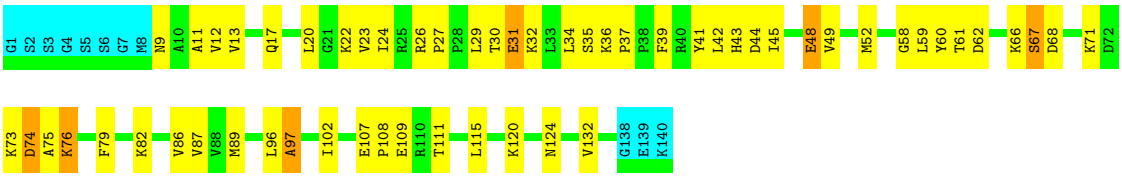
Chain A: 51% 39% • 8%



4.2.3 Score per residue for model 3

- Molecule 1: TNF receptor-associated factor 3-interacting protein 1

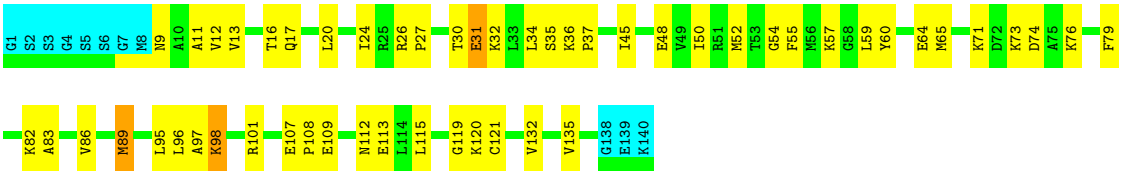
Chain A:



4.2.4 Score per residue for model 4

- Molecule 1: TNF receptor-associated factor 3-interacting protein 1

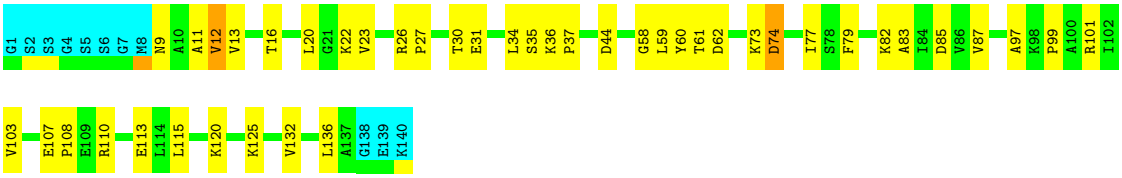
Chain A:



4.2.5 Score per residue for model 5

- Molecule 1: TNF receptor-associated factor 3-interacting protein 1

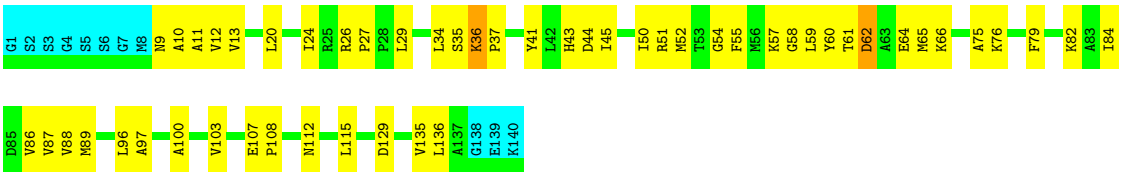
Chain A:



4.2.6 Score per residue for model 6

- Molecule 1: TNF receptor-associated factor 3-interacting protein 1

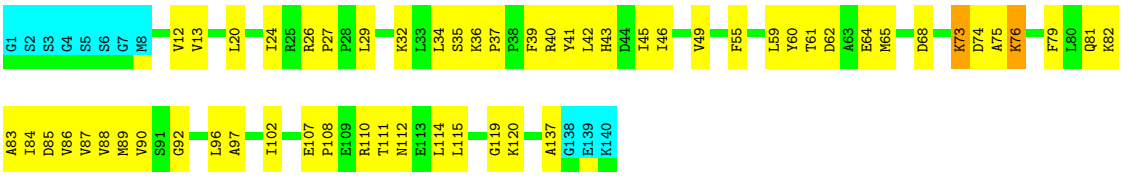
Chain A: 55% 36% • 8%



4.2.7 Score per residue for model 7

- Molecule 1: TNF receptor-associated factor 3-interacting protein 1

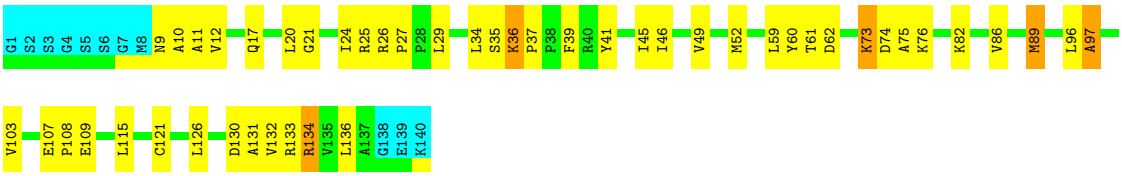
Chain A: 51% 39% • 8%



4.2.8 Score per residue for model 8

- Molecule 1: TNF receptor-associated factor 3-interacting protein 1

Chain A: 58% 31% • 8%



4.2.9 Score per residue for model 9

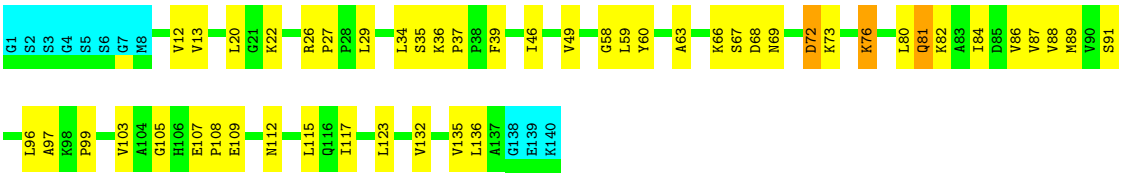
- Molecule 1: TNF receptor-associated factor 3-interacting protein 1

Chain A: 59% 31% • 8%

4.2.10 Score per residue for model 10

• Molecule 1: TNF receptor-associated factor 3-interacting protein 1

Chain A: 57% 33% • 8%



4.2.11 Score per residue for model 11

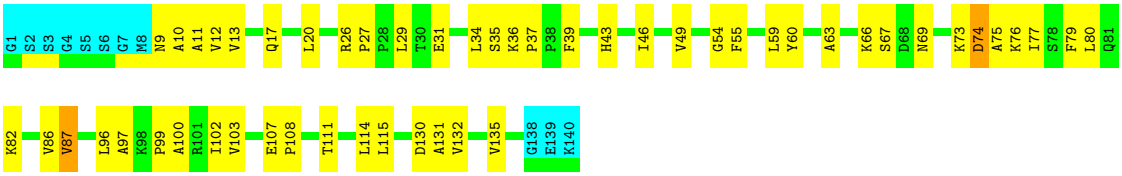
• Molecule 1: TNF receptor-associated factor 3-interacting protein 1

Chain A: 55% 33% • 8%

4.2.12 Score per residue for model 12

• Molecule 1: TNF receptor-associated factor 3-interacting protein 1

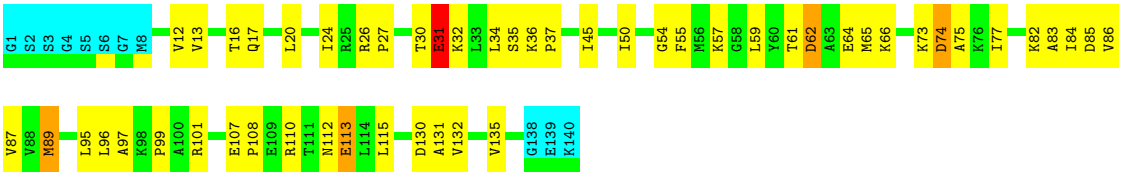
Chain A: 55% 36% • 8%



4.2.13 Score per residue for model 13

• Molecule 1: TNF receptor-associated factor 3-interacting protein 1

Chain A: 55% 34% • • 8%



4.2.14 Score per residue for model 14

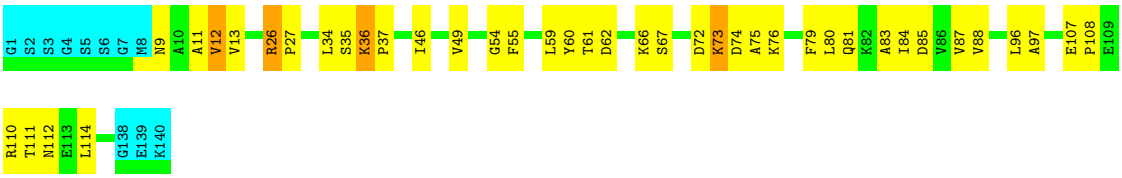
• Molecule 1: TNF receptor-associated factor 3-interacting protein 1

Chain A: 60% 29% • 8%

4.2.15 Score per residue for model 15 (medoid)

• Molecule 1: TNF receptor-associated factor 3-interacting protein 1

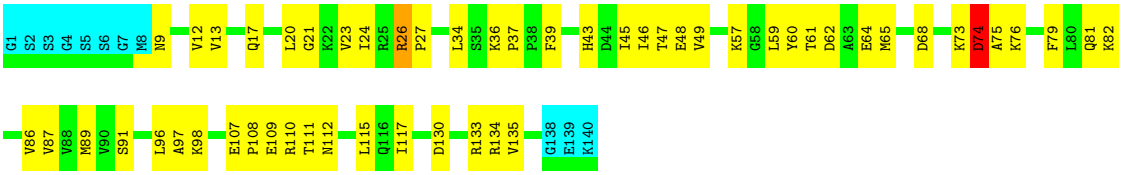
Chain A: 63% 26% • 8%



4.2.16 Score per residue for model 16

• Molecule 1: TNF receptor-associated factor 3-interacting protein 1

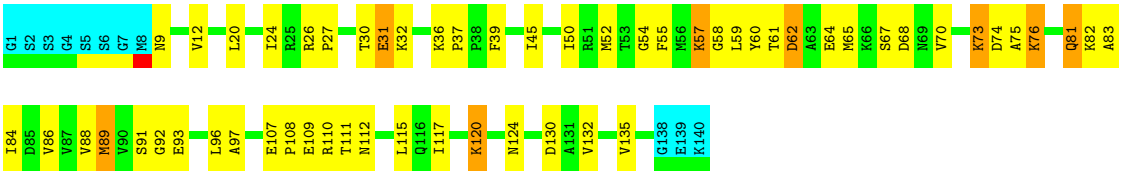
Chain A: 54% 37% •• 8%



4.2.17 Score per residue for model 17

• Molecule 1: TNF receptor-associated factor 3-interacting protein 1

Chain A: 51% 35% 6% 8%



4.2.18 Score per residue for model 18

- Molecule 1: TNF receptor-associated factor 3-interacting protein 1

Chain A: 59% 29% • 8%

G1 S2 S3 G4 S5 S6 G7 M8 N9 A10 A11 V12 V13 Q17 L20 G21 I24 R25 R26 P27 P28 L29 T30 E31 K32 L33 L34 S35 K36 P37 Y41 L42 H43 D44 I45 M52 Y60 K66 S67 D68 K73 D74 A75 K76 I77 S78 F79 L80 V86 V87 V88

M89 P99 V103 E107 P108 E109 R110 T111 N112 E113 L114 L115 G138 E139 K140

4.2.19 Score per residue for model 19

- Molecule 1: TNF receptor-associated factor 3-interacting protein 1

Chain A: 59% 31% • 8%

G1 S2 S3 G4 S5 S6 G7 M8 N9 A10 A11 V12 V13 T16 L20 R26 P27 T30 E31 K32 L33 L34 S35 K36 P37 Y41 L42 H43 D44 L59 Y60 E64 M65 K66 S67 K73 I77 I84 D85 V86 V87 V88 M89 L96 A97 K98 P99 E107

P108 E109 R110 E113 L114 L115 Q116 I117 I118 G119 K120 V135 G138 E139 K140

4.2.20 Score per residue for model 20

- Molecule 1: TNF receptor-associated factor 3-interacting protein 1

Chain A: 55% 36% • 8%

G1 S2 S3 G4 S5 S6 G7 M8 A11 V12 V13 L20 C21 K22 V23 I24 R25 R26 P27 P28 L29 T30 E31 K32 L33 L34 S35 K36 P37 P38 F39 D44 V49 M52 L59 Y60 T61 D62 A63 E64 M65 A75 K76 I77 S78 F79 K82 A83 V87 V88 M89

L96 A97 K98 P99 A100 R101 E107 P108 E109 R110 L115 Q116 C122 D130 A131 V132 R133 R134 V135 G138 E139 K140

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, structures with the lowest energy, target function*.

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

Software name	Classification	Version
CYANA	structure solution	2.0.17
CYANA	refinement	2.0.17

No chemical shift data was provided.

6 Model quality (i)

6.1 Standard geometry (i)

There are no covalent bond-length or bond-angle outliers.

There are no bond-length outliers.

There are no bond-angle outliers.

There are no chirality outliers.

There are no planarity outliers.

6.2 Too-close contacts (i)

In the following table, the Non-H and H(model) columns list the number of non-hydrogen atoms and hydrogen atoms in each chain respectively. The H(added) column lists the number of hydrogen atoms added and optimized by MolProbity. The Clashes column lists the number of clashes averaged over the ensemble.

Mol	Chain	Non-H	H(model)	H(added)	Clashes
1	A	1008	1074	1074	37±5
All	All	20160	21480	21480	745

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 18.

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

Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:12:VAL:HG11	1:A:109:GLU:OE1	0.86	1.69	9	5
1:A:58:GLY:O	1:A:136:LEU:HD11	0.85	1.72	5	3
1:A:9:ASN:O	1:A:12:VAL:HG12	0.85	1.71	17	9
1:A:13:VAL:HG13	1:A:34:LEU:HD13	0.79	1.54	3	12
1:A:97:ALA:HB2	1:A:110:ARG:HB3	0.78	1.55	19	10
1:A:42:LEU:CD2	1:A:115:LEU:HD11	0.73	2.14	3	1
1:A:59:LEU:HD12	1:A:60:TYR:CZ	0.71	2.20	4	10
1:A:13:VAL:HG13	1:A:34:LEU:CD1	0.70	2.15	9	11
1:A:20:LEU:HD11	1:A:115:LEU:HB3	0.70	1.61	13	18
1:A:59:LEU:HD11	1:A:82:LYS:CB	0.69	2.17	5	1
1:A:59:LEU:HD12	1:A:60:TYR:CE2	0.69	2.23	20	12
1:A:59:LEU:HD13	1:A:59:LEU:C	0.68	2.09	19	10
1:A:59:LEU:HD11	1:A:82:LYS:HB3	0.67	1.67	8	12
1:A:24:ILE:HG22	1:A:52:MET:SD	0.66	2.29	20	3

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:96:LEU:HD12	1:A:110:ARG:CZ	0.65	2.21	19	1
1:A:20:LEU:HB2	1:A:29:LEU:HD11	0.65	1.67	10	4
1:A:43:HIS:NE2	1:A:79:PHE:CE2	0.64	2.65	2	6
1:A:96:LEU:HD12	1:A:110:ARG:NH2	0.64	2.07	19	1
1:A:131:ALA:O	1:A:135:VAL:HG12	0.63	1.94	12	2
1:A:36:LYS:N	1:A:37:PRO:CD	0.63	2.60	14	20
1:A:97:ALA:HB2	1:A:110:ARG:CB	0.63	2.24	11	8
1:A:42:LEU:HD22	1:A:115:LEU:HD21	0.63	1.70	19	2
1:A:121:CYS:HA	1:A:126:LEU:HD12	0.62	1.71	9	2
1:A:20:LEU:HD13	1:A:45:ILE:HG21	0.62	1.69	2	3
1:A:60:TYR:OH	1:A:83:ALA:HB2	0.62	1.94	5	4
1:A:59:LEU:HD13	1:A:59:LEU:O	0.61	1.95	13	8
1:A:24:ILE:HG22	1:A:52:MET:HG3	0.60	1.73	4	4
1:A:77:ILE:HG23	1:A:99:PRO:HG2	0.60	1.73	18	8
1:A:55:PHE:CE1	1:A:90:VAL:HG21	0.60	2.32	14	1
1:A:84:ILE:O	1:A:88:VAL:HG23	0.59	1.98	1	6
1:A:59:LEU:CD1	1:A:60:TYR:CE1	0.58	2.87	1	10
1:A:29:LEU:HD23	1:A:41:TYR:OH	0.58	1.98	7	4
1:A:24:ILE:HD12	1:A:26:ARG:O	0.57	2.00	3	2
1:A:83:ALA:O	1:A:87:VAL:HG23	0.57	1.98	7	4
1:A:81:GLN:HA	1:A:84:ILE:HD12	0.57	1.75	7	3
1:A:77:ILE:HG23	1:A:99:PRO:CG	0.56	2.31	13	2
1:A:82:LYS:HA	1:A:135:VAL:HG21	0.55	1.76	20	6
1:A:24:ILE:CD1	1:A:45:ILE:HG23	0.55	2.31	6	3
1:A:46:ILE:O	1:A:49:VAL:HG12	0.55	2.02	10	8
1:A:59:LEU:HA	1:A:132:VAL:HG13	0.55	1.77	13	4
1:A:59:LEU:CD1	1:A:60:TYR:CZ	0.55	2.90	20	4
1:A:60:TYR:CE1	1:A:79:PHE:CD2	0.54	2.96	14	1
1:A:43:HIS:CE1	1:A:79:PHE:CZ	0.54	2.95	12	1
1:A:39:PHE:CE2	1:A:76:LYS:CG	0.54	2.91	14	2
1:A:59:LEU:HD11	1:A:82:LYS:HB2	0.53	1.78	5	1
1:A:59:LEU:HD12	1:A:60:TYR:CD1	0.53	2.39	16	1
1:A:29:LEU:HD22	1:A:34:LEU:HD21	0.53	1.80	8	2
1:A:22:LYS:HE2	1:A:123:LEU:HD21	0.52	1.80	10	1
1:A:9:ASN:ND2	1:A:11:ALA:H	0.52	2.02	12	1
1:A:59:LEU:C	1:A:59:LEU:CD1	0.52	2.78	19	4
1:A:79:PHE:C	1:A:79:PHE:CD1	0.52	2.84	2	7
1:A:59:LEU:HD12	1:A:60:TYR:CD2	0.52	2.39	17	3
1:A:9:ASN:CG	1:A:10:ALA:N	0.51	2.64	12	1
1:A:24:ILE:HD13	1:A:45:ILE:HG23	0.51	1.83	13	7
1:A:132:VAL:HG12	1:A:136:LEU:HD12	0.51	1.82	8	3

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:50:ILE:HG23	1:A:57:LYS:HA	0.51	1.80	17	5
1:A:35:SER:C	1:A:37:PRO:CD	0.51	2.79	2	17
1:A:79:PHE:CD1	1:A:80:LEU:N	0.51	2.79	18	2
1:A:30:THR:O	1:A:33:LEU:N	0.51	2.44	18	1
1:A:132:VAL:HG12	1:A:136:LEU:CD1	0.51	2.36	8	2
1:A:30:THR:O	1:A:32:LYS:N	0.51	2.45	2	10
1:A:39:PHE:CZ	1:A:76:LYS:HG3	0.50	2.41	10	7
1:A:39:PHE:CE2	1:A:76:LYS:HG3	0.50	2.41	14	1
1:A:99:PRO:O	1:A:103:VAL:CG1	0.50	2.60	2	4
1:A:98:LYS:CE	1:A:101:ARG:NH2	0.50	2.75	4	1
1:A:11:ALA:O	1:A:13:VAL:N	0.50	2.45	20	5
1:A:9:ASN:O	1:A:11:ALA:N	0.50	2.44	11	3
1:A:59:LEU:HD12	1:A:60:TYR:CE1	0.50	2.41	6	5
1:A:60:TYR:CE1	1:A:79:PHE:CE2	0.50	3.00	14	2
1:A:39:PHE:CE2	1:A:76:LYS:HG2	0.50	2.42	1	2
1:A:73:LYS:O	1:A:75:ALA:N	0.50	2.45	13	9
1:A:86:VAL:O	1:A:89:MET:N	0.50	2.45	14	15
1:A:12:VAL:HG22	1:A:112:ASN:CB	0.50	2.37	14	9
1:A:120:LYS:O	1:A:124:ASN:ND2	0.50	2.45	11	3
1:A:34:LEU:O	1:A:112:ASN:ND2	0.50	2.45	6	1
1:A:108:PRO:O	1:A:111:THR:N	0.49	2.45	9	2
1:A:75:ALA:O	1:A:78:SER:N	0.49	2.45	11	2
1:A:60:TYR:CZ	1:A:79:PHE:CE1	0.49	3.00	2	2
1:A:107:GLU:N	1:A:108:PRO:CD	0.49	2.75	12	20
1:A:58:GLY:O	1:A:132:VAL:CG1	0.49	2.60	17	3
1:A:91:SER:CB	1:A:117:ILE:CG2	0.49	2.90	2	2
1:A:99:PRO:O	1:A:103:VAL:HG12	0.49	2.07	2	2
1:A:131:ALA:O	1:A:134:ARG:N	0.49	2.45	20	1
1:A:58:GLY:O	1:A:132:VAL:HG11	0.49	2.08	3	1
1:A:72:ASP:N	1:A:72:ASP:OD1	0.49	2.45	11	1
1:A:88:VAL:O	1:A:92:GLY:N	0.49	2.45	17	2
1:A:12:VAL:O	1:A:116:GLN:NE2	0.49	2.45	20	2
1:A:9:ASN:N	1:A:9:ASN:OD1	0.48	2.46	16	1
1:A:130:ASP:CG	1:A:131:ALA:N	0.48	2.66	20	1
1:A:90:VAL:HG21	1:A:128:SER:OG	0.48	2.07	9	1
1:A:39:PHE:CZ	1:A:76:LYS:HG2	0.48	2.43	12	3
1:A:43:HIS:NE2	1:A:79:PHE:CZ	0.48	2.82	11	4
1:A:55:PHE:CD2	1:A:56:MET:HG3	0.48	2.44	1	2
1:A:130:ASP:O	1:A:133:ARG:N	0.48	2.47	8	2
1:A:96:LEU:O	1:A:97:ALA:C	0.48	2.52	4	17
1:A:17:GLN:HG2	1:A:34:LEU:HD11	0.47	1.85	8	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:26:ARG:HA	1:A:27:PRO:C	0.47	2.30	4	20
1:A:86:VAL:HG23	1:A:135:VAL:HG11	0.47	1.86	14	3
1:A:39:PHE:CE2	1:A:76:LYS:HB3	0.47	2.44	2	1
1:A:20:LEU:HD13	1:A:45:ILE:HD13	0.47	1.85	4	3
1:A:60:TYR:CZ	1:A:79:PHE:CZ	0.47	3.03	2	1
1:A:88:VAL:HG13	1:A:93:GLU:O	0.47	2.09	2	1
1:A:39:PHE:CE2	1:A:76:LYS:CB	0.47	2.97	2	1
1:A:13:VAL:HG12	1:A:17:GLN:HG3	0.46	1.88	3	1
1:A:93:GLU:OE2	1:A:117:ILE:CD1	0.46	2.62	17	1
1:A:73:LYS:O	1:A:76:LYS:N	0.46	2.48	16	2
1:A:100:ALA:O	1:A:103:VAL:HG12	0.46	2.10	6	2
1:A:23:VAL:HG21	1:A:122:CYS:SG	0.46	2.50	9	1
1:A:36:LYS:N	1:A:37:PRO:HD3	0.46	2.25	2	20
1:A:66:LYS:O	1:A:68:ASP:N	0.46	2.48	10	2
1:A:35:SER:O	1:A:108:PRO:CB	0.46	2.64	4	3
1:A:111:THR:O	1:A:114:LEU:N	0.46	2.49	7	3
1:A:70:VAL:HG12	1:A:76:LYS:HD2	0.46	1.86	11	1
1:A:64:GLU:O	1:A:66:LYS:N	0.46	2.49	13	2
1:A:30:THR:O	1:A:31:GLU:C	0.46	2.54	5	10
1:A:31:GLU:OE1	1:A:31:GLU:C	0.46	2.55	13	1
1:A:42:LEU:HD22	1:A:115:LEU:HD11	0.45	1.83	3	1
1:A:75:ALA:O	1:A:76:LYS:C	0.45	2.55	11	9
1:A:58:GLY:C	1:A:132:VAL:HG11	0.45	2.31	5	2
1:A:86:VAL:O	1:A:87:VAL:C	0.45	2.55	7	11
1:A:61:THR:O	1:A:62:ASP:C	0.45	2.55	5	12
1:A:23:VAL:HG11	1:A:49:VAL:HG23	0.45	1.87	16	2
1:A:47:THR:HG21	1:A:65:MET:O	0.45	2.10	16	1
1:A:66:LYS:O	1:A:67:SER:C	0.45	2.55	14	6
1:A:96:LEU:CD1	1:A:110:ARG:NH2	0.45	2.80	19	1
1:A:17:GLN:O	1:A:21:GLY:N	0.45	2.50	16	3
1:A:73:LYS:O	1:A:74:ASP:C	0.45	2.55	11	9
1:A:44:ASP:O	1:A:48:GLU:CD	0.45	2.55	3	1
1:A:119:GLY:O	1:A:120:LYS:C	0.44	2.56	14	3
1:A:17:GLN:HA	1:A:29:LEU:HD13	0.44	1.89	12	2
1:A:54:GLY:O	1:A:55:PHE:C	0.44	2.55	1	8
1:A:110:ARG:O	1:A:113:GLU:N	0.44	2.50	11	2
1:A:23:VAL:HG13	1:A:53:THR:CG2	0.44	2.42	9	1
1:A:72:ASP:O	1:A:76:LYS:CD	0.44	2.65	10	1
1:A:67:SER:O	1:A:70:VAL:N	0.44	2.51	17	2
1:A:24:ILE:HD11	1:A:45:ILE:HG23	0.44	1.89	2	1
1:A:22:LYS:O	1:A:23:VAL:C	0.44	2.56	20	3

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:97:ALA:HB2	1:A:110:ARG:HB2	0.44	1.89	11	1
1:A:83:ALA:O	1:A:84:ILE:C	0.44	2.55	17	2
1:A:23:VAL:HG12	1:A:24:ILE:HG23	0.44	1.90	16	2
1:A:39:PHE:CE1	1:A:76:LYS:HG2	0.44	2.47	16	2
1:A:106:HIS:O	1:A:107:GLU:C	0.44	2.56	14	1
1:A:63:ALA:HB1	1:A:69:ASN:OD1	0.44	2.13	10	1
1:A:111:THR:O	1:A:112:ASN:C	0.44	2.55	18	5
1:A:48:GLU:O	1:A:52:MET:N	0.43	2.51	1	1
1:A:72:ASP:O	1:A:75:ALA:HB3	0.43	2.13	15	3
1:A:130:ASP:O	1:A:131:ALA:C	0.43	2.55	8	2
1:A:64:GLU:O	1:A:65:MET:C	0.43	2.57	7	8
1:A:55:PHE:CZ	1:A:90:VAL:HG21	0.43	2.48	1	2
1:A:59:LEU:CD1	1:A:60:TYR:CD1	0.43	3.02	9	2
1:A:117:ILE:O	1:A:118:ILE:C	0.43	2.55	19	1
1:A:39:PHE:CD1	1:A:76:LYS:HG2	0.43	2.48	20	1
1:A:39:PHE:CD1	1:A:39:PHE:C	0.43	2.91	8	2
1:A:73:LYS:C	1:A:75:ALA:N	0.43	2.72	2	3
1:A:11:ALA:C	1:A:13:VAL:N	0.43	2.72	19	4
1:A:81:GLN:OE1	1:A:85:ASP:CG	0.43	2.56	7	1
1:A:113:GLU:OE1	1:A:113:GLU:C	0.43	2.57	9	1
1:A:102:ILE:CG1	1:A:111:THR:OG1	0.43	2.66	7	4
1:A:58:GLY:C	1:A:132:VAL:CG1	0.43	2.87	5	1
1:A:13:VAL:O	1:A:16:THR:N	0.43	2.52	2	2
1:A:80:LEU:O	1:A:81:GLN:C	0.43	2.57	10	2
1:A:60:TYR:CZ	1:A:79:PHE:CE2	0.43	3.06	18	1
1:A:109:GLU:OE1	1:A:110:ARG:NH1	0.42	2.52	16	1
1:A:79:PHE:CD1	1:A:79:PHE:C	0.42	2.93	16	5
1:A:66:LYS:C	1:A:68:ASP:N	0.42	2.72	10	1
1:A:63:ALA:O	1:A:69:ASN:ND2	0.42	2.52	12	1
1:A:119:GLY:O	1:A:121:CYS:N	0.42	2.52	14	2
1:A:9:ASN:C	1:A:11:ALA:N	0.42	2.73	6	3
1:A:31:GLU:CD	1:A:31:GLU:C	0.42	2.78	12	1
1:A:67:SER:O	1:A:68:ASP:C	0.42	2.57	1	5
1:A:77:ILE:HD11	1:A:100:ALA:HA	0.42	1.90	9	1
1:A:42:LEU:CD2	1:A:115:LEU:HD21	0.42	2.44	18	1
1:A:113:GLU:O	1:A:114:LEU:C	0.42	2.58	19	1
1:A:117:ILE:HG23	1:A:120:LYS:HE3	0.42	1.90	19	1
1:A:131:ALA:O	1:A:132:VAL:C	0.42	2.58	20	1
1:A:39:PHE:CE1	1:A:76:LYS:HG3	0.42	2.50	3	1
1:A:26:ARG:CZ	1:A:26:ARG:HB3	0.42	2.45	18	1
1:A:130:ASP:O	1:A:134:ARG:NE	0.42	2.52	8	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:20:LEU:HD11	1:A:115:LEU:HD13	0.42	1.90	12	1
1:A:30:THR:C	1:A:32:LYS:N	0.41	2.73	3	3
1:A:81:GLN:O	1:A:82:LYS:C	0.41	2.59	17	2
1:A:54:GLY:O	1:A:57:LYS:N	0.41	2.53	17	1
1:A:41:TYR:CZ	1:A:45:ILE:HD11	0.41	2.50	6	1
1:A:117:ILE:O	1:A:119:GLY:N	0.41	2.52	19	1
1:A:110:ARG:O	1:A:111:THR:C	0.41	2.58	11	3
1:A:16:THR:O	1:A:17:GLN:C	0.41	2.58	11	3
1:A:20:LEU:O	1:A:22:LYS:N	0.41	2.53	9	1
1:A:108:PRO:O	1:A:109:GLU:C	0.41	2.58	9	2
1:A:49:VAL:CG1	1:A:122:CYS:SG	0.41	3.08	20	1
1:A:48:GLU:O	1:A:52:MET:SD	0.41	2.79	2	1
1:A:59:LEU:HD12	1:A:60:TYR:CG	0.41	2.49	16	1
1:A:52:MET:SD	1:A:52:MET:N	0.41	2.94	2	1
1:A:124:ASN:O	1:A:125:LYS:C	0.41	2.58	2	1
1:A:9:ASN:O	1:A:10:ALA:C	0.41	2.59	11	1
1:A:110:ARG:NE	1:A:110:ARG:HA	0.41	2.31	15	3
1:A:85:ASP:HB2	1:A:135:VAL:HG21	0.41	1.91	19	1
1:A:42:LEU:CD1	1:A:102:ILE:HG21	0.41	2.45	7	1
1:A:76:LYS:HB3	1:A:103:VAL:HG21	0.41	1.92	18	1
1:A:39:PHE:HB2	1:A:103:VAL:HG23	0.41	1.92	8	1
1:A:12:VAL:CG2	1:A:112:ASN:HB2	0.41	2.46	13	1
1:A:91:SER:HB3	1:A:117:ILE:CG2	0.41	2.45	10	1
1:A:64:GLU:C	1:A:66:LYS:N	0.41	2.74	13	1
1:A:95:LEU:HD21	1:A:113:GLU:OE1	0.41	2.16	13	1
1:A:86:VAL:CG2	1:A:135:VAL:HG11	0.41	2.46	14	1
1:A:95:LEU:HD23	1:A:113:GLU:OE2	0.41	2.15	4	1
1:A:11:ALA:O	1:A:12:VAL:C	0.41	2.58	20	2
1:A:41:TYR:O	1:A:44:ASP:CG	0.41	2.59	19	1
1:A:9:ASN:OD1	1:A:11:ALA:N	0.40	2.53	18	1
1:A:13:VAL:HG13	1:A:34:LEU:HD12	0.40	1.93	18	1
1:A:50:ILE:CG2	1:A:57:LYS:HD2	0.40	2.47	2	1
1:A:88:VAL:CG2	1:A:95:LEU:HD12	0.40	2.46	2	1
1:A:39:PHE:CD2	1:A:76:LYS:HB3	0.40	2.51	2	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	129/140 (92%)	101±3 (78±3%)	26±3 (20±2%)	2±1 (1±1%)	15	61
All	All	2580/2800 (92%)	2018 (78%)	525 (20%)	37 (1%)	15	61

All 12 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	31	GLU	10
1	A	74	ASP	7
1	A	12	VAL	5
1	A	10	ALA	3
1	A	67	SER	2
1	A	97	ALA	2
1	A	65	MET	2
1	A	87	VAL	2
1	A	105	GLY	1
1	A	120	LYS	1
1	A	86	VAL	1
1	A	118	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	112/119 (94%)	107±2 (95±2%)	5±2 (5±2%)	29	78
All	All	2240/2380 (94%)	2132 (95%)	108 (5%)	29	78

All 36 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	89	MET	9
1	A	74	ASP	8
1	A	98	LYS	7
1	A	73	LYS	7

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Mol	Chain	Res	Type	Models (Total)
1	A	36	LYS	6
1	A	68	ASP	5
1	A	101	ARG	5
1	A	44	ASP	5
1	A	62	ASP	4
1	A	120	LYS	4
1	A	76	LYS	4
1	A	48	GLU	3
1	A	85	ASP	3
1	A	113	GLU	3
1	A	57	LYS	3
1	A	81	GLN	3
1	A	51	ARG	2
1	A	133	ARG	2
1	A	71	LYS	2
1	A	129	ASP	2
1	A	32	LYS	2
1	A	134	ARG	2
1	A	72	ASP	2
1	A	130	ASP	2
1	A	26	ARG	2
1	A	79	PHE	1
1	A	52	MET	1
1	A	125	LYS	1
1	A	40	ARG	1
1	A	25	ARG	1
1	A	122	CYS	1
1	A	22	LYS	1
1	A	31	GLU	1
1	A	91	SER	1
1	A	9	ASN	1
1	A	16	THR	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