Full wwPDB NMR Structure Validation Report (i)

Feb 28, 2022 – 12:19 AM EST

PDB ID	:	2DB8
Title	:	Solution structures of the fn3 domain of human Tripartite motif protein 9
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Deposited on	:	2005-12-15

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:

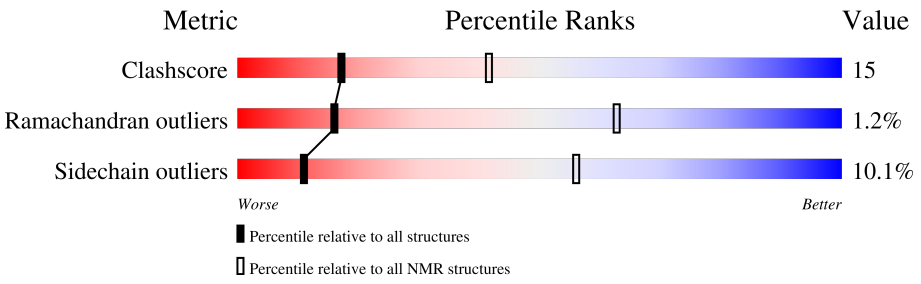
MolProbity	:	4.02b-467
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
RCI	:	v_1n_11_5_13_A (Berjanski et al., 2005)
PANAV	:	Wang et al. (2010)
ShiftChecker	:	2.27
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
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	110	57% 23% 20%

2 Ensemble composition and analysis (i)

This entry contains 20 models. Model 7 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:18, A:26-A:102 (88)	0.32	7

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 5 clusters and 2 single-model clusters were found.

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

3 Entry composition (i)

There is only 1 type of molecule in this entry. The entry contains 1586 atoms, of which 777 are hydrogens and 0 are deuteriums.

- Molecule 1 is a protein called Tripartite motif protein 9, isoform 2.

Mol	Chain	Residues	Atoms						Trace
			Total	C	H	N	O	S	
1	A	110	1586	501	777	136	168	4	0

There are 13 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	1	GLY	-	cloning artifact	UNP Q9C026
A	2	SER	-	cloning artifact	UNP Q9C026
A	3	SER	-	cloning artifact	UNP Q9C026
A	4	GLY	-	cloning artifact	UNP Q9C026
A	5	SER	-	cloning artifact	UNP Q9C026
A	6	SER	-	cloning artifact	UNP Q9C026
A	7	GLY	-	cloning artifact	UNP Q9C026
A	105	SER	-	cloning artifact	UNP Q9C026
A	106	GLY	-	cloning artifact	UNP Q9C026
A	107	PRO	-	cloning artifact	UNP Q9C026
A	108	SER	-	cloning artifact	UNP Q9C026
A	109	SER	-	cloning artifact	UNP Q9C026
A	110	GLY	-	cloning artifact	UNP Q9C026

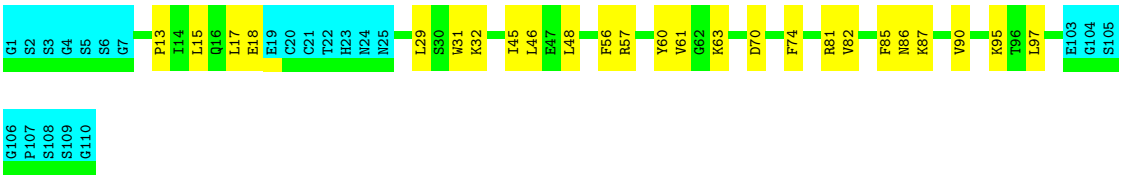
4 Residue-property plots (i)

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: Tripartite motif protein 9, isoform 2

Chain A: 57% 23% 20%



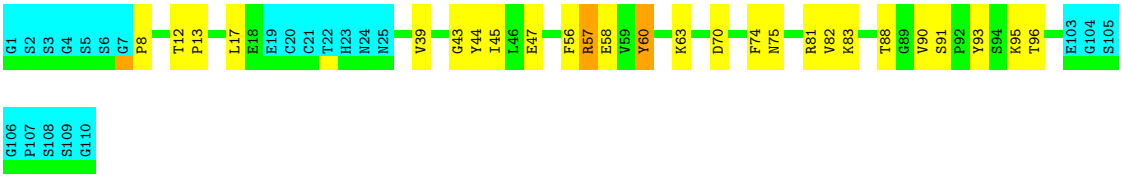
4.2 Scores per residue for each member of the ensemble

Colouring as in section 4.1 above.

4.2.1 Score per residue for model 1

• Molecule 1: Tripartite motif protein 9, isoform 2

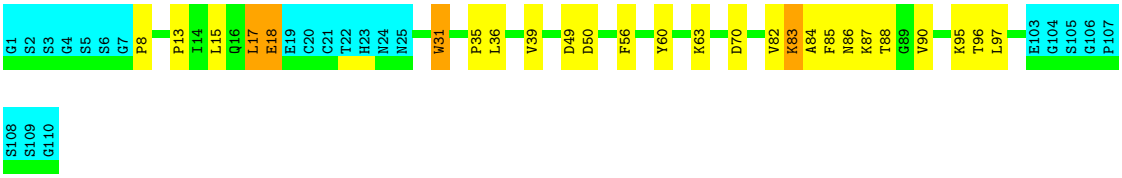
Chain A: 56% 22% • 20%



4.2.2 Score per residue for model 2

• Molecule 1: Tripartite motif protein 9, isoform 2

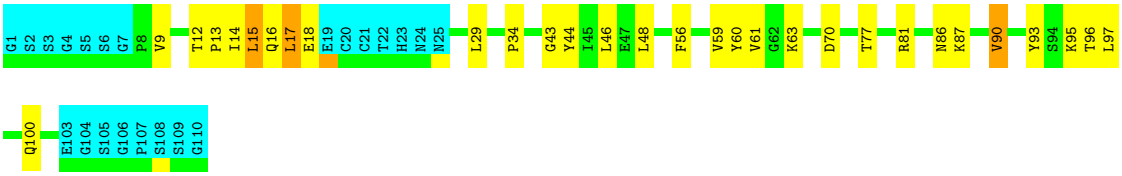
Chain A: 56% 20% • 20%



4.2.3 Score per residue for model 3

- Molecule 1: Tripartite motif protein 9, isoform 2

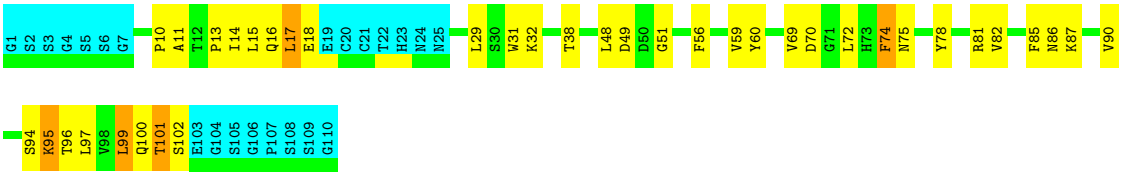
Chain A:



4.2.4 Score per residue for model 4

- Molecule 1: Tripartite motif protein 9, isoform 2

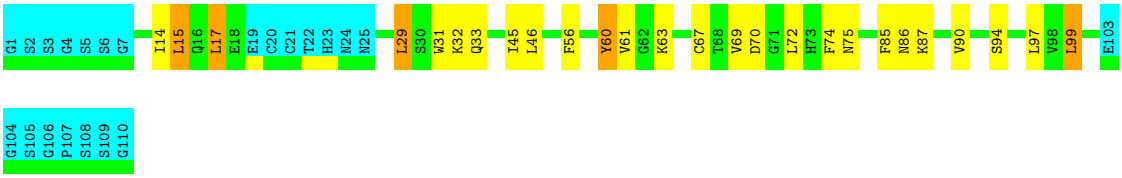
Chain A:



4.2.5 Score per residue for model 5

- Molecule 1: Tripartite motif protein 9, isoform 2

Chain A:



4.2.6 Score per residue for model 6

- Molecule 1: Tripartite motif protein 9, isoform 2

Chain A: 50% 28% • 20%

G1 S2 S3 G4 S5 S6 G7 P8 T12 P13 I14 L15 Q16 L17 E18 E19 C20 C21 T22 H23 N24 N25 K32 V39 G43 Y44 E47 L48 D49 D50 Q55 F56 R57 E58 V59 Y60 V61 G62 K63 V69 D70 G71 L72 N79 A80 R81 V82 T88 G89 V90 S91

P92 Y93 L99 E103 G104 S105 G106 P107 S108 S109 G110

4.2.7 Score per residue for model 7 (medoid)

- Molecule 1: Tripartite motif protein 9, isoform 2

Chain A: 46% 32% • 20%

G1 S2 S3 G4 S5 S6 G7 P8 P13 I14 L15 Q16 L17 E18 E19 C20 C21 T22 H23 N24 N25 T28 W31 K32 V39 G43 Y44 I45 L48 D49 D50 F56 Y60 K63 T68 V69 L72 Y78 N79 A80 R81 V82 K83 A84 F85 N86 K87 T88

G89 V90 Y93 S94 K95 T96 L97 V98 L99 E103 G104 S105 G106 P107 S108 S109 G110

4.2.8 Score per residue for model 8

- Molecule 1: Tripartite motif protein 9, isoform 2

Chain A: 46% 31% • 20%

G1 S2 S3 G4 S5 S6 G7 P8 P13 I14 L15 Q16 L17 E18 E19 C20 C21 T22 H23 N24 N25 S26 A27 T28 L29 L36 S37 T38 V39 D42 I45 L46 E47 L48 F56 R57 E58 V59 Y60 V61 G62 K63 M66 C67 T68 V69 D70 N75 Y78 R81 V82

K83 N86 K87 T88 G89 V90 Y93 S94 K95 T96 E103 G104 S105 G106 P107 S108 S109 G110

4.2.9 Score per residue for model 9

- Molecule 1: Tripartite motif protein 9, isoform 2

Chain A: 46% 29% 5% 20%

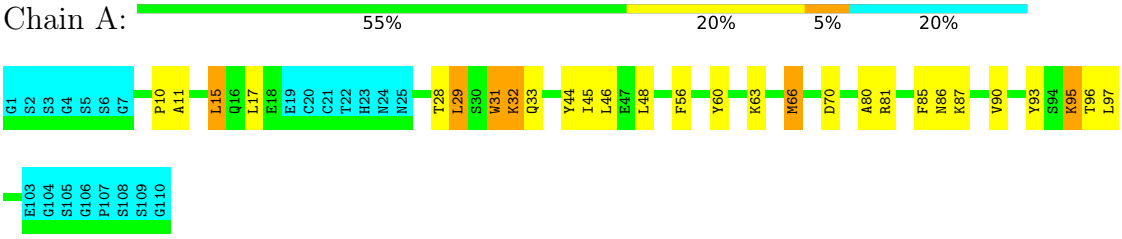
G1 S2 S3 G4 S5 S6 G7 P8 A11 T12 P13 I14 L15 Q16 L17 E18 E19 C20 C21 T22 H23 N24 N25 T28 L29 S30 W31 S37 T38 V39 G43 Y44 I45 L46 E47 L48 D49 D50 G51 F56 Y60 V61 G62 K63 E64 T65 T68 H73 F74 N75 Y78

N79 V82 N86 K87 V90 L97 V98 L99 Q100 T101 S102 E103 G104 S105 G106 P107 S108 S109 G110

4.2.10 Score per residue for model 10

- Molecule 1: Tripartite motif protein 9, isoform 2

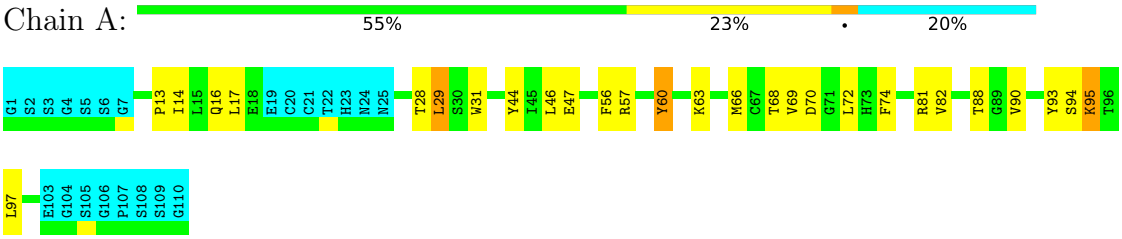
Chain A:



4.2.11 Score per residue for model 11

- Molecule 1: Tripartite motif protein 9, isoform 2

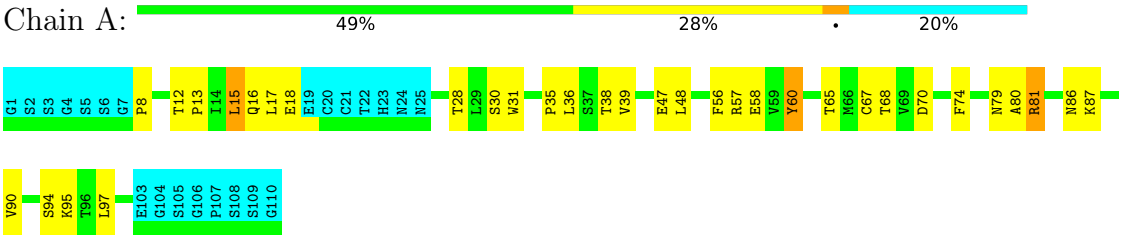
Chain A:



4.2.12 Score per residue for model 12

- Molecule 1: Tripartite motif protein 9, isoform 2

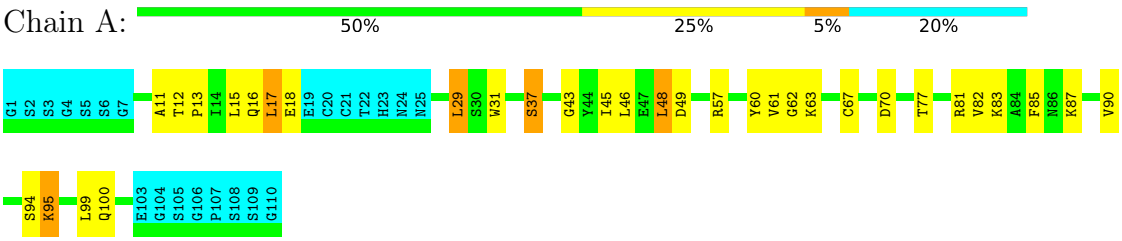
Chain A:



4.2.13 Score per residue for model 13

- Molecule 1: Tripartite motif protein 9, isoform 2

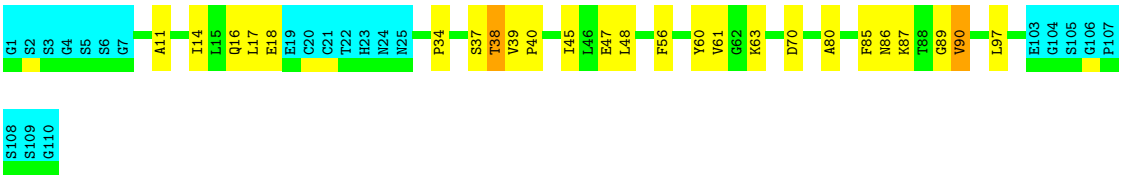
Chain A:



4.2.14 Score per residue for model 14

- Molecule 1: Tripartite motif protein 9, isoform 2

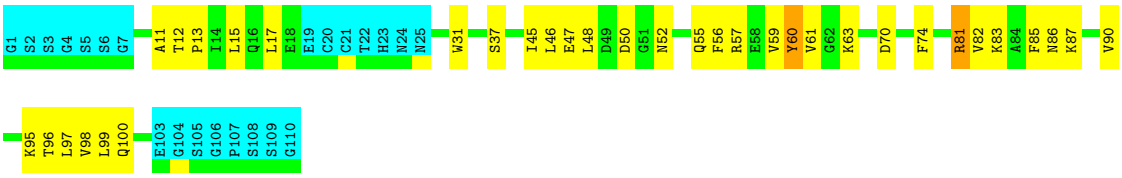
Chain A: 57% 21% • 20%



4.2.15 Score per residue for model 15

- Molecule 1: Tripartite motif protein 9, isoform 2

Chain A: 48% 30% • 20%



4.2.16 Score per residue for model 16

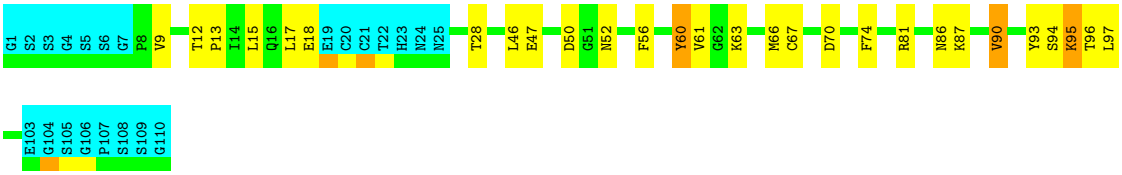
- Molecule 1: Tripartite motif protein 9, isoform 2

Chain A: 48% 27% 5% 20%

4.2.17 Score per residue for model 17

- Molecule 1: Tripartite motif protein 9, isoform 2

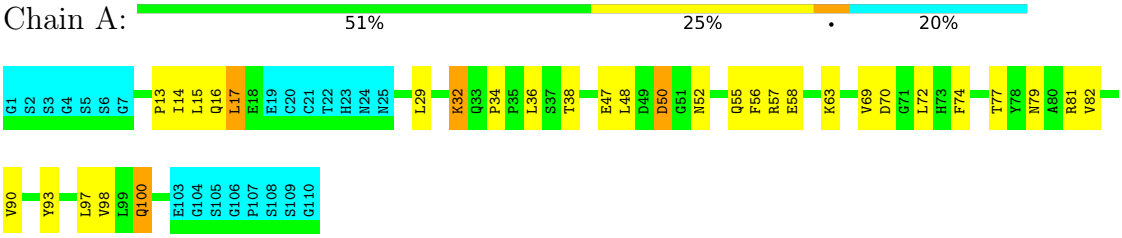
Chain A: 55% 23% • 20%



4.2.18 Score per residue for model 18

- Molecule 1: Tripartite motif protein 9, isoform 2

Chain A:



4.2.19 Score per residue for model 19

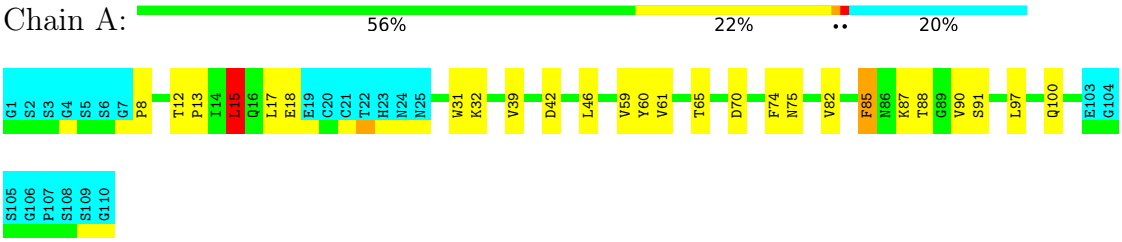
- Molecule 1: Tripartite motif protein 9, isoform 2

Chain A:

4.2.20 Score per residue for model 20

- Molecule 1: Tripartite motif protein 9, isoform 2

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	673	668	667	21±4
All	All	13460	13360	13340	411

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 15.

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:LEU:HD21	1:A:97:LEU:HD22	0.92	1.38	17	2
1:A:15:LEU:HD11	1:A:97:LEU:HD22	0.91	1.42	20	5
1:A:17:LEU:HD12	1:A:97:LEU:HD21	0.84	1.49	17	3
1:A:13:PRO:C	1:A:14:ILE:HD13	0.81	1.95	6	1
1:A:14:ILE:HD12	1:A:32:LYS:O	0.80	1.76	7	2
1:A:45:ILE:HG22	1:A:47:GLU:OE2	0.79	1.77	14	5
1:A:45:ILE:HD12	1:A:83:LYS:NZ	0.78	1.92	16	5
1:A:77:THR:HG23	1:A:100:GLN:NE2	0.74	1.96	13	3
1:A:13:PRO:HG2	1:A:82:VAL:HG13	0.72	1.62	11	12
1:A:8:PRO:O	1:A:39:VAL:HG11	0.71	1.86	12	5
1:A:14:ILE:HG22	1:A:16:GLN:HG3	0.71	1.61	11	1
1:A:45:ILE:HD12	1:A:83:LYS:HZ1	0.71	1.44	16	3
1:A:15:LEU:HD13	1:A:16:GLN:N	0.68	2.03	12	1
1:A:69:VAL:HG11	1:A:72:LEU:HD21	0.67	1.67	11	2

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:28:THR:HG22	1:A:66:MET:SD	0.67	2.30	10	1
1:A:11:ALA:HB2	1:A:37:SER:OG	0.67	1.89	13	2
1:A:17:LEU:HD23	1:A:18:GLU:N	0.66	2.05	9	3
1:A:14:ILE:HD13	1:A:32:LYS:HD2	0.66	1.67	18	2
1:A:17:LEU:CD1	1:A:97:LEU:HD21	0.66	2.19	17	1
1:A:45:ILE:HG23	1:A:61:VAL:HG22	0.64	1.67	9	3
1:A:45:ILE:HG12	1:A:61:VAL:HG13	0.64	1.69	9	1
1:A:8:PRO:C	1:A:88:THR:HG21	0.64	2.13	7	5
1:A:15:LEU:HD11	1:A:97:LEU:HB2	0.63	1.69	2	1
1:A:43:GLY:C	1:A:44:TYR:CD1	0.62	2.72	19	7
1:A:31:TRP:HB3	1:A:82:VAL:HG11	0.62	1.70	20	2
1:A:14:ILE:HD13	1:A:32:LYS:CD	0.61	2.24	18	3
1:A:48:LEU:HD22	1:A:49:ASP:N	0.61	2.10	4	1
1:A:17:LEU:HB2	1:A:97:LEU:HD21	0.61	1.72	11	1
1:A:81:ARG:CZ	1:A:93:TYR:CD2	0.60	2.84	1	2
1:A:49:ASP:OD1	1:A:56:PHE:CD2	0.60	2.54	9	1
1:A:48:LEU:HD12	1:A:79:ASN:O	0.60	1.97	18	5
1:A:48:LEU:HD13	1:A:80:ALA:HB2	0.60	1.74	10	3
1:A:14:ILE:HG22	1:A:16:GLN:CG	0.60	2.26	11	2
1:A:60:TYR:CD2	1:A:67:CYS:SG	0.60	2.95	12	1
1:A:49:ASP:OD1	1:A:56:PHE:CE2	0.59	2.55	9	1
1:A:17:LEU:HD12	1:A:18:GLU:N	0.59	2.13	8	3
1:A:29:LEU:CD1	1:A:46:LEU:HD21	0.58	2.27	9	1
1:A:31:TRP:CZ3	1:A:46:LEU:HD11	0.58	2.33	13	7
1:A:17:LEU:HD12	1:A:29:LEU:HB3	0.58	1.74	10	1
1:A:14:ILE:HD13	1:A:32:LYS:NZ	0.58	2.13	7	1
1:A:15:LEU:CD1	1:A:97:LEU:HD22	0.58	2.26	20	1
1:A:45:ILE:HD12	1:A:83:LYS:HE3	0.57	1.76	1	1
1:A:14:ILE:HG22	1:A:16:GLN:HG2	0.57	1.74	3	1
1:A:47:GLU:CD	1:A:93:TYR:CZ	0.57	2.78	11	1
1:A:77:THR:HG23	1:A:100:GLN:HE22	0.57	1.59	13	1
1:A:8:PRO:HG2	1:A:39:VAL:HG21	0.57	1.76	1	7
1:A:81:ARG:NH2	1:A:93:TYR:CE2	0.56	2.72	1	1
1:A:73:HIS:O	1:A:101:THR:HG21	0.56	2.01	9	1
1:A:69:VAL:HG13	1:A:72:LEU:HD11	0.56	1.75	4	3
1:A:31:TRP:CB	1:A:82:VAL:HG11	0.56	2.29	20	3
1:A:99:LEU:HD22	1:A:99:LEU:N	0.56	2.16	9	2
1:A:15:LEU:HD12	1:A:95:LYS:O	0.56	2.01	7	1
1:A:17:LEU:HD13	1:A:18:GLU:N	0.56	2.14	4	5
1:A:44:TYR:CD1	1:A:44:TYR:N	0.55	2.74	9	5
1:A:49:ASP:OD1	1:A:56:PHE:CG	0.55	2.59	9	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:49:ASP:OD1	1:A:56:PHE:CZ	0.55	2.60	9	1
1:A:60:TYR:CD1	1:A:67:CYS:SG	0.55	2.98	13	1
1:A:13:PRO:O	1:A:14:ILE:HD13	0.55	2.02	6	1
1:A:17:LEU:HD11	1:A:97:LEU:HD21	0.54	1.80	7	1
1:A:28:THR:HG23	1:A:66:MET:SD	0.54	2.43	17	1
1:A:99:LEU:HD12	1:A:99:LEU:N	0.54	2.17	5	2
1:A:69:VAL:CG1	1:A:72:LEU:HD11	0.53	2.34	7	3
1:A:38:THR:HG22	1:A:38:THR:O	0.53	2.04	12	2
1:A:49:ASP:OD1	1:A:56:PHE:CD1	0.53	2.62	9	1
1:A:28:THR:HG23	1:A:68:THR:OG1	0.52	2.04	12	2
1:A:15:LEU:HD13	1:A:97:LEU:HB2	0.52	1.81	18	2
1:A:45:ILE:HD12	1:A:83:LYS:HZ2	0.52	1.64	8	3
1:A:98:VAL:HG12	1:A:100:GLN:NE2	0.52	2.20	15	1
1:A:56:PHE:CD1	1:A:56:PHE:N	0.51	2.78	8	13
1:A:49:ASP:OD1	1:A:56:PHE:CE1	0.51	2.63	9	1
1:A:51:GLY:N	1:A:78:TYR:CE1	0.51	2.79	9	1
1:A:49:ASP:OD1	1:A:49:ASP:N	0.51	2.44	9	1
1:A:14:ILE:HD13	1:A:14:ILE:N	0.51	2.20	6	1
1:A:81:ARG:NE	1:A:93:TYR:CD2	0.51	2.79	1	2
1:A:13:PRO:CG	1:A:82:VAL:HG13	0.50	2.37	19	4
1:A:12:THR:HG23	1:A:13:PRO:HD2	0.50	1.84	20	8
1:A:9:VAL:HG11	1:A:90:VAL:O	0.50	2.07	3	2
1:A:47:GLU:OE1	1:A:93:TYR:CZ	0.50	2.65	11	2
1:A:31:TRP:CE2	1:A:82:VAL:HG21	0.50	2.41	4	1
1:A:47:GLU:OE1	1:A:57:ARG:N	0.50	2.45	12	3
1:A:35:PRO:HG2	1:A:36:LEU:HD12	0.50	1.83	12	2
1:A:16:GLN:O	1:A:18:GLU:N	0.49	2.45	16	1
1:A:47:GLU:OE1	1:A:47:GLU:N	0.49	2.46	8	1
1:A:47:GLU:OE2	1:A:58:GLU:N	0.49	2.45	18	3
1:A:28:THR:CG2	1:A:66:MET:SD	0.49	3.01	10	2
1:A:46:LEU:C	1:A:47:GLU:CD	0.49	2.71	8	3
1:A:65:THR:O	1:A:65:THR:CG2	0.49	2.60	12	2
1:A:60:TYR:CG	1:A:61:VAL:N	0.49	2.81	3	7
1:A:46:LEU:HD12	1:A:60:TYR:CD1	0.49	2.41	15	2
1:A:46:LEU:CD1	1:A:67:CYS:SG	0.48	3.01	17	1
1:A:85:PHE:CD1	1:A:85:PHE:C	0.48	2.87	20	4
1:A:60:TYR:O	1:A:61:VAL:CG2	0.48	2.61	14	4
1:A:100:GLN:HE21	1:A:100:GLN:N	0.48	2.06	18	1
1:A:74:PHE:CD1	1:A:74:PHE:N	0.48	2.80	4	3
1:A:60:TYR:C	1:A:60:TYR:CD1	0.48	2.86	11	1
1:A:28:THR:OG1	1:A:68:THR:HG23	0.48	2.09	9	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:98:VAL:HG12	1:A:100:GLN:HE21	0.48	1.68	15	1
1:A:36:LEU:O	1:A:38:THR:HG23	0.48	2.09	8	1
1:A:56:PHE:CD1	1:A:81:ARG:NH2	0.47	2.82	4	1
1:A:45:ILE:CG2	1:A:47:GLU:OE2	0.47	2.60	8	2
1:A:60:TYR:CD1	1:A:60:TYR:C	0.47	2.88	19	2
1:A:17:LEU:C	1:A:17:LEU:HD13	0.47	2.29	20	1
1:A:48:LEU:HD11	1:A:78:TYR:CD1	0.47	2.45	7	1
1:A:29:LEU:HD12	1:A:31:TRP:CZ3	0.47	2.45	5	4
1:A:31:TRP:CH2	1:A:46:LEU:HD11	0.47	2.45	11	2
1:A:69:VAL:HB	1:A:72:LEU:HD11	0.47	1.86	11	2
1:A:81:ARG:HD3	1:A:93:TYR:CD1	0.47	2.45	3	2
1:A:29:LEU:HD11	1:A:46:LEU:CD2	0.47	2.40	9	1
1:A:81:ARG:CZ	1:A:93:TYR:CE2	0.47	2.98	1	1
1:A:56:PHE:CE2	1:A:81:ARG:NH1	0.47	2.83	12	1
1:A:43:GLY:CA	1:A:62:GLY:O	0.46	2.63	16	2
1:A:15:LEU:HD11	1:A:81:ARG:HA	0.46	1.86	4	2
1:A:32:LYS:CD	1:A:33:GLN:O	0.46	2.64	16	2
1:A:45:ILE:HG13	1:A:85:PHE:CE1	0.46	2.45	10	3
1:A:37:SER:O	1:A:39:VAL:N	0.46	2.49	14	1
1:A:29:LEU:O	1:A:31:TRP:CZ3	0.46	2.69	13	1
1:A:48:LEU:HB3	1:A:59:VAL:HG11	0.46	1.88	3	3
1:A:77:THR:CG2	1:A:98:VAL:HG13	0.46	2.40	19	1
1:A:56:PHE:CZ	1:A:81:ARG:NH1	0.46	2.84	3	1
1:A:51:GLY:HA3	1:A:78:TYR:CE1	0.45	2.46	4	1
1:A:100:GLN:N	1:A:100:GLN:NE2	0.45	2.63	18	1
1:A:95:LYS:O	1:A:96:THR:C	0.45	2.55	10	8
1:A:81:ARG:HG3	1:A:93:TYR:CD1	0.45	2.47	10	5
1:A:16:GLN:O	1:A:17:LEU:C	0.45	2.55	18	3
1:A:86:ASN:O	1:A:87:LYS:C	0.45	2.55	4	14
1:A:47:GLU:OE1	1:A:81:ARG:NH2	0.45	2.50	11	1
1:A:94:SER:OG	1:A:95:LYS:N	0.45	2.50	13	3
1:A:14:ILE:HD11	1:A:34:PRO:CA	0.45	2.42	19	2
1:A:85:PHE:C	1:A:85:PHE:CD1	0.45	2.90	2	1
1:A:49:ASP:OD2	1:A:56:PHE:CE2	0.45	2.70	6	1
1:A:69:VAL:HG11	1:A:72:LEU:CD2	0.45	2.41	11	1
1:A:48:LEU:HD22	1:A:49:ASP:H	0.44	1.71	4	1
1:A:47:GLU:OE1	1:A:81:ARG:NE	0.44	2.49	11	1
1:A:39:VAL:HG13	1:A:40:PRO:HD2	0.44	1.89	14	1
1:A:50:ASP:O	1:A:50:ASP:CG	0.44	2.56	17	1
1:A:60:TYR:O	1:A:61:VAL:HG23	0.44	2.12	14	1
1:A:57:ARG:CD	1:A:58:GLU:O	0.44	2.66	1	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:15:LEU:HD23	1:A:94:SER:OG	0.44	2.13	16	1
1:A:31:TRP:CH2	1:A:60:TYR:CE1	0.44	3.05	19	1
1:A:47:GLU:OE1	1:A:93:TYR:CE2	0.44	2.71	11	1
1:A:81:ARG:HD3	1:A:93:TYR:CG	0.44	2.48	19	1
1:A:74:PHE:O	1:A:75:ASN:C	0.44	2.55	1	5
1:A:14:ILE:HD11	1:A:34:PRO:HB3	0.44	1.89	14	2
1:A:43:GLY:O	1:A:85:PHE:CD1	0.44	2.70	13	1
1:A:14:ILE:HD12	1:A:14:ILE:H	0.44	1.73	4	2
1:A:30:SER:O	1:A:31:TRP:C	0.44	2.56	12	1
1:A:17:LEU:HD23	1:A:97:LEU:HD21	0.44	1.90	19	1
1:A:48:LEU:HD11	1:A:78:TYR:HD1	0.44	1.72	7	1
1:A:94:SER:O	1:A:95:LYS:C	0.43	2.57	4	2
1:A:47:GLU:OE1	1:A:56:PHE:C	0.43	2.57	6	2
1:A:99:LEU:N	1:A:99:LEU:CD2	0.43	2.82	7	2
1:A:27:ALA:O	1:A:68:THR:HG23	0.43	2.14	8	1
1:A:37:SER:O	1:A:38:THR:C	0.43	2.56	14	1
1:A:11:ALA:CB	1:A:37:SER:OG	0.43	2.67	9	1
1:A:9:VAL:N	1:A:88:THR:HG21	0.43	2.28	19	1
1:A:47:GLU:N	1:A:47:GLU:OE1	0.43	2.52	19	1
1:A:29:LEU:HD12	1:A:31:TRP:CE3	0.42	2.49	10	2
1:A:31:TRP:CD2	1:A:82:VAL:HG21	0.42	2.49	20	2
1:A:56:PHE:CE1	1:A:81:ARG:NH1	0.42	2.87	11	1
1:A:45:ILE:HG12	1:A:61:VAL:CG2	0.42	2.44	19	2
1:A:61:VAL:O	1:A:61:VAL:HG13	0.42	2.14	19	2
1:A:48:LEU:HD11	1:A:78:TYR:HD2	0.42	1.75	8	1
1:A:60:TYR:CB	1:A:67:CYS:SG	0.42	3.07	5	1
1:A:46:LEU:HB3	1:A:59:VAL:CG2	0.42	2.44	15	4
1:A:32:LYS:CE	1:A:33:GLN:O	0.42	2.68	5	1
1:A:49:ASP:CG	1:A:50:ASP:N	0.42	2.73	7	2
1:A:10:PRO:HB2	1:A:41:ALA:HB2	0.42	1.92	16	1
1:A:56:PHE:CD1	1:A:81:ARG:NH1	0.41	2.88	11	1
1:A:47:GLU:OE2	1:A:58:GLU:CD	0.41	2.58	12	1
1:A:14:ILE:O	1:A:31:TRP:CB	0.41	2.68	5	1
1:A:10:PRO:O	1:A:11:ALA:C	0.41	2.57	4	2
1:A:47:GLU:OE1	1:A:57:ARG:C	0.41	2.58	6	1
1:A:47:GLU:OE1	1:A:57:ARG:CA	0.41	2.68	6	2
1:A:50:ASP:OD2	1:A:52:ASN:ND2	0.41	2.53	15	1
1:A:15:LEU:HD11	1:A:97:LEU:CB	0.41	2.42	2	1
1:A:89:GLY:O	1:A:90:VAL:HG13	0.41	2.15	14	1
1:A:97:LEU:CD2	1:A:99:LEU:HD21	0.41	2.45	4	1
1:A:15:LEU:C	1:A:15:LEU:HD13	0.41	2.36	9	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:48:LEU:CD2	1:A:49:ASP:O	0.41	2.68	13	1
1:A:81:ARG:HD3	1:A:93:TYR:CD2	0.41	2.50	19	1
1:A:45:ILE:CD1	1:A:85:PHE:CD2	0.41	3.04	5	1
1:A:32:LYS:CD	1:A:33:GLN:N	0.41	2.83	10	1
1:A:14:ILE:CD1	1:A:32:LYS:CD	0.41	2.98	18	1
1:A:77:THR:HG23	1:A:98:VAL:CG1	0.41	2.46	19	1
1:A:31:TRP:CE2	1:A:65:THR:HA	0.41	2.50	20	1
1:A:28:THR:HG23	1:A:68:THR:HB	0.41	1.93	11	1
1:A:14:ILE:CD1	1:A:32:LYS:HD2	0.41	2.42	18	1
1:A:17:LEU:HD11	1:A:29:LEU:HD22	0.41	1.93	18	1
1:A:77:THR:CG2	1:A:98:VAL:CG1	0.41	2.99	18	1
1:A:49:ASP:OD1	1:A:55:GLN:C	0.40	2.60	6	1
1:A:11:ALA:HB2	1:A:37:SER:CB	0.40	2.46	14	1
1:A:81:ARG:CZ	1:A:81:ARG:HB3	0.40	2.46	19	1
1:A:86:ASN:C	1:A:86:ASN:OD1	0.40	2.60	19	1
1:A:83:LYS:NZ	1:A:84:ALA:O	0.40	2.55	2	1
1:A:100:GLN:O	1:A:101:THR:C	0.40	2.59	4	1
1:A:11:ALA:HB2	1:A:37:SER:HB3	0.40	1.93	14	1
1:A:15:LEU:HD23	1:A:95:LYS:O	0.40	2.16	15	1
1:A:50:ASP:OD1	1:A:52:ASN:CB	0.40	2.70	18	1
1:A:99:LEU:HD12	1:A:99:LEU:H	0.40	1.74	5	1
1:A:81:ARG:CG	1:A:81:ARG:O	0.40	2.68	6	1
1:A:47:GLU:OE1	1:A:81:ARG:O	0.40	2.40	15	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	88/110 (80%)	73±2 (83±2%)	14±1 (15±2%)	1±1 (1±1%)	16	63
All	All	1760/2200 (80%)	1466 (83%)	272 (15%)	22 (1%)	16	63

All 10 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	TRP	4
1	A	17	LEU	4
1	A	15	LEU	3
1	A	88	THR	3
1	A	95	LYS	2
1	A	94	SER	2
1	A	101	THR	1
1	A	37	SER	1
1	A	38	THR	1
1	A	100	GLN	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	76/92 (83%)	68±2 (90±3%)	8±2 (10±3%)	11 56
All	All	1520/1840 (83%)	1367 (90%)	153 (10%)	11 56

All 35 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	VAL	20
1	A	70	ASP	18
1	A	63	LYS	15
1	A	60	TYR	13
1	A	17	LEU	8
1	A	29	LEU	8
1	A	57	ARG	7
1	A	32	LYS	6
1	A	74	PHE	5
1	A	15	LEU	5
1	A	81	ARG	5
1	A	99	LEU	4
1	A	95	LYS	4
1	A	91	SER	3
1	A	16	GLN	3
1	A	50	ASP	3

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Mol	Chain	Res	Type	Models (Total)
1	A	36	LEU	3
1	A	42	ASP	2
1	A	66	MET	2
1	A	48	LEU	2
1	A	87	LYS	2
1	A	55	GLN	2
1	A	18	GLU	1
1	A	83	LYS	1
1	A	102	SER	1
1	A	75	ASN	1
1	A	44	TYR	1
1	A	49	ASP	1
1	A	37	SER	1
1	A	14	ILE	1
1	A	98	VAL	1
1	A	52	ASN	1
1	A	38	THR	1
1	A	100	GLN	1
1	A	85	PHE	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