



# Full wwPDB NMR Structure Validation Report ⓘ

Apr 26, 2016 – 07:55 PM BST

PDB ID : 2DMB  
Title : Solution structure of the 15th Filamin domain from human Filamin-B  
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Deposited on : 2006-04-20

This is a Full wwPDB NMR Structure Validation Report for a publicly released PDB entry.  
We welcome your comments at [validation@mail.wwpdb.org](mailto:validation@mail.wwpdb.org)  
A user guide is available at  
<http://wwpdb.org/validation/2016/NMRValidationReportHelp>  
with specific help available everywhere you see the ⓘ symbol.

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The following versions of software and data (see [references ⓘ](#)) were used in the production of this report:

Cyrange : Kirchner and Güntert (2011)  
NmrClust : Kelley et al. (1996)  
MolProbity : 4.02b-467  
Mogul : unknown  
Percentile statistics : 20151230.v01 (using entries in the PDB archive December 30th 2015)  
RCI : v\_1n\_11\_5\_13\_A (Berjanski et al., 2005)  
PANAV : Wang et al. (2010)  
ShiftChecker : rb-20027457  
Ideal geometry (proteins) : Engh & Huber (2001)  
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)  
Validation Pipeline (wwPDB-VP) : rb-20027457

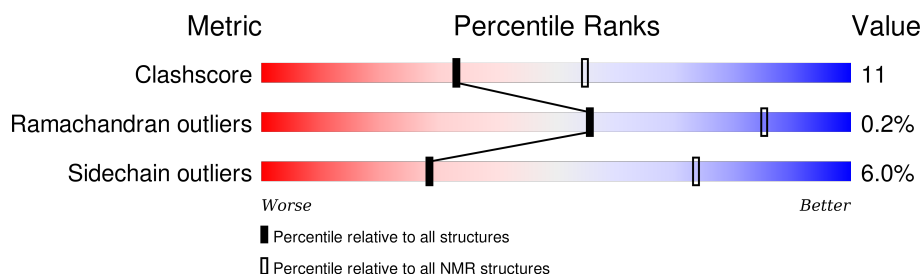
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*SOLUTION NMR*

The overall completeness of chemical shifts assignment is 94%.

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	114402	11133
Ramachandran outliers	111179	9975
Sidechain outliers	111093	9958

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  $\geq 3$ , 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  $\leq 5\%$

Mol	Chain	Length	Quality of chain
1	A	124	

## 2 Ensemble composition and analysis ⓘ

This entry contains 20 models. Model 3 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:10-A:102 (93)	0.23	3

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 2 clusters. No single-model clusters were found.

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

### 3 Entry composition

There is only 1 type of molecule in this entry. The entry contains 1688 atoms, of which 824 are hydrogens and 0 are deuteriums.

- Molecule 1 is a protein called Filamin-B.

Mol	Chain	Residues	Atoms						Trace
1	A	124	Total	C	H	N	O	S	0
			1688	534	824	136	190	4	

There are 13 discrepancies between the modelled and reference sequences:

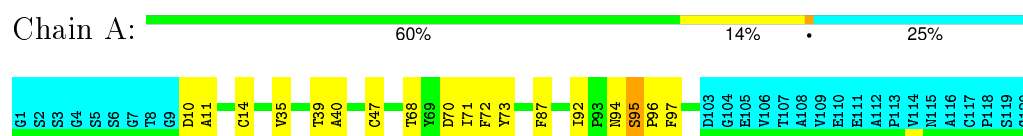
Chain	Residue	Modelled	Actual	Comment	Reference
A	1	GLY	-	CLONING ARTIFACT	UNP O75369
A	2	SER	-	CLONING ARTIFACT	UNP O75369
A	3	SER	-	CLONING ARTIFACT	UNP O75369
A	4	GLY	-	CLONING ARTIFACT	UNP O75369
A	5	SER	-	CLONING ARTIFACT	UNP O75369
A	6	SER	-	CLONING ARTIFACT	UNP O75369
A	7	GLY	-	CLONING ARTIFACT	UNP O75369
A	119	SER	-	CLONING ARTIFACT	UNP O75369
A	120	GLY	-	CLONING ARTIFACT	UNP O75369
A	121	PRO	-	CLONING ARTIFACT	UNP O75369
A	122	SER	-	CLONING ARTIFACT	UNP O75369
A	123	SER	-	CLONING ARTIFACT	UNP O75369
A	124	GLY	-	CLONING ARTIFACT	UNP O75369

## 4 Residue-property plots [i](#)

### 4.1 Average score per residue in the NMR ensemble

These plots are provided for all protein, RNA and DNA 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: Filamin-B

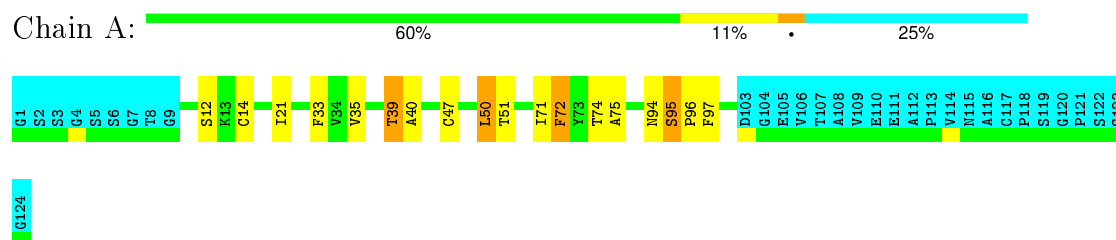


### 4.2 Scores per residue for each member of the ensemble

Colouring as in section 4.1 above.

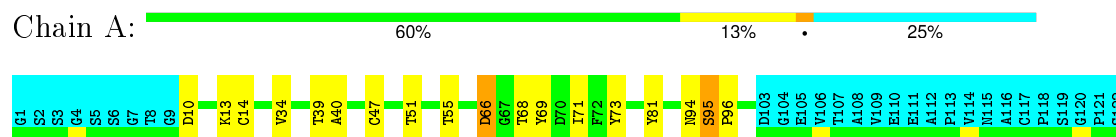
#### 4.2.1 Score per residue for model 1

- Molecule 1: Filamin-B



#### 4.2.2 Score per residue for model 2

- Molecule 1: Filamin-B

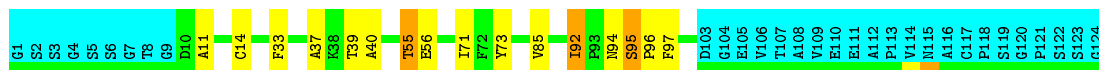


S123  
G124

### 4.2.3 Score per residue for model 3 (medoid)

- Molecule 1: Filamin-B

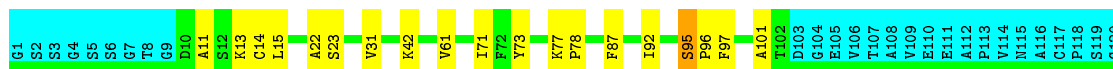
Chain A: 



### 4.2.4 Score per residue for model 4

- Molecule 1: Filamin-B

Chain A: 

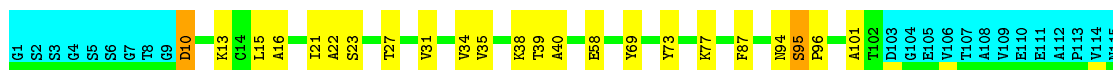


P121  
S122  
S123  
G124

### 4.2.5 Score per residue for model 5

- Molecule 1: Filamin-B

Chain A: 

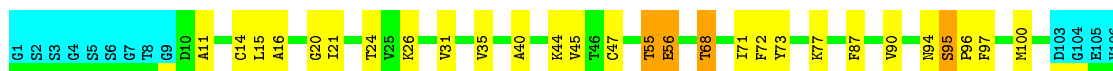


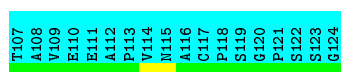
A116  
C117  
P118  
S119  
G120  
P121  
S122  
S123  
G124

### 4.2.6 Score per residue for model 6

- Molecule 1: Filamin-B

Chain A: 





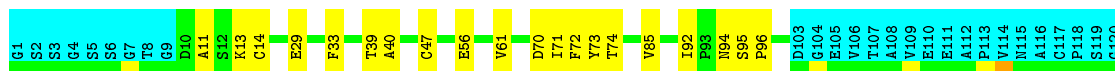
#### 4.2.7 Score per residue for model 7

- Molecule 1: Filamin-B



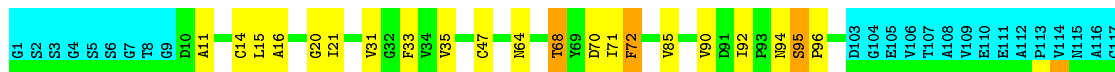
#### 4.2.8 Score per residue for model 8

- Molecule 1: Filamin-B



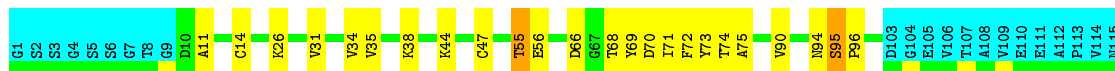
#### 4.2.9 Score per residue for model 9

- Molecule 1: Filamin-B



#### 4.2.10 Score per residue for model 10

- Molecule 1: Filamin-B



A116  
G117  
P118  
S119  
G120  
P121  
S122  
S123  
G124

#### 4.2.11 Score per residue for model 11

- Molecule 1: Filamin-B

Chain A: 52% 21% 25%

G1 S2 S3 S4 S5 S6 G7 T8 G9 D10 A11 C14 L15 A16 I21 A22 S23 T24 T27 F33 T39 A40 G41 K44 V45 T46 D70 I71 F72 Y73 K77 V85 R86 F87 I92 P93 N94 S95 P96 F97 T102 D103 G104 E105 V106 T107 A108 V109 E110

E111 A112 P113 V114 M115 A116 G117 P118 S119 P121 S122 S123 G124

#### 4.2.12 Score per residue for model 12

- Molecule 1: Filamin-B

Chain A: 58% 15% 25%

G1 S2 S3 S4 S5 S6 G7 T8 G9 D10 A11 S12 K13 C14 L15 A22 S23 F33 V34 V35 D36 K42 G43 K44 C47 E56 T68 I71 F72 K77 F87 N94 S95 P96 D103 G104 E105 V106 T107 A108 V109 E110 E111 A112 P113 V114 M115 C117

P118 S119 G120 P121 S122 S123 G124

#### 4.2.13 Score per residue for model 13

- Molecule 1: Filamin-B

Chain A: 53% 21% 25%

G1 S2 S3 S4 S5 S6 G7 T8 G9 D10 A11 S12 K13 C14 L15 E30 V31 G32 F33 V34 V35 A40 V45 T46 C47 T68 Y69 D70 I71 F72 Y73 T74 A75 A76 K77 F87 I92 P93 N94 S95 P96 F97 D103 G104 E105 V106 T107 A108 V109 E110 E111 A112 P113

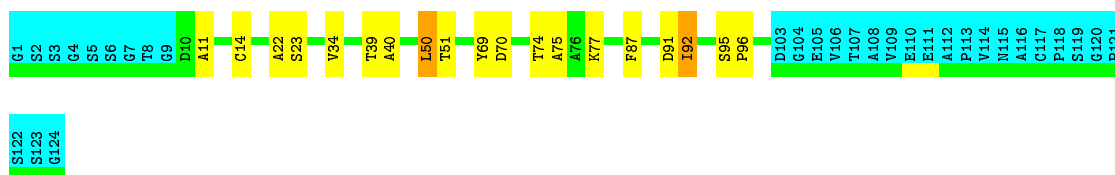
V114 M115 A116 G117 P118 S119 G120 P121 S122 S123 G124

#### 4.2.14 Score per residue for model 14

- Molecule 1: Filamin-B

Chain A: 60% 14% 25%

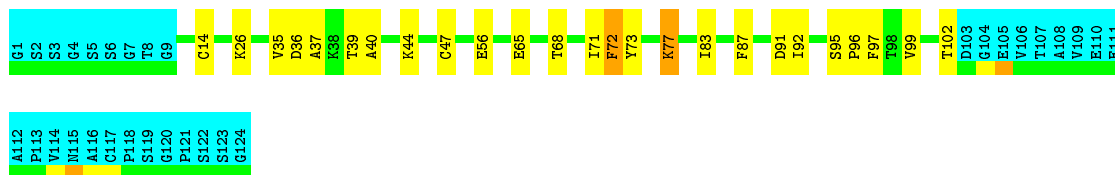




#### 4.2.15 Score per residue for model 15

- Molecule 1: Filamin-B

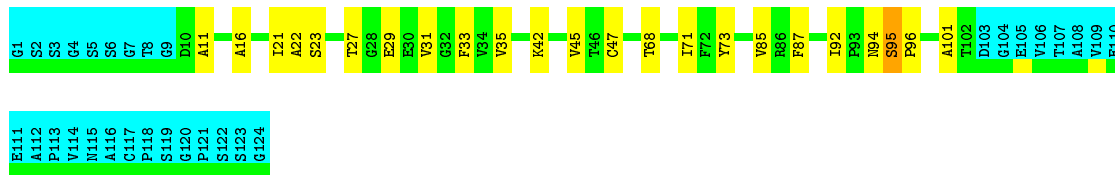
Chain A: 55% 19% 25%



#### 4.2.16 Score per residue for model 16

- Molecule 1: Filamin-B

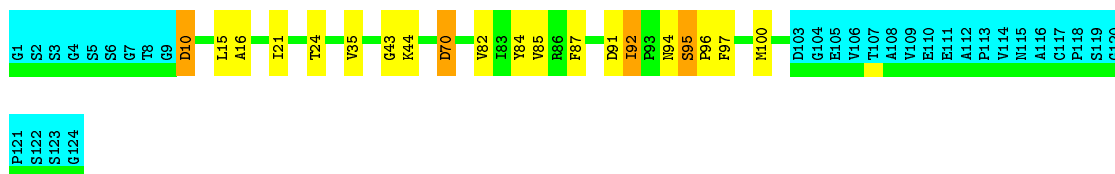
Chain A: 56% 18% 25%



#### 4.2.17 Score per residue for model 17

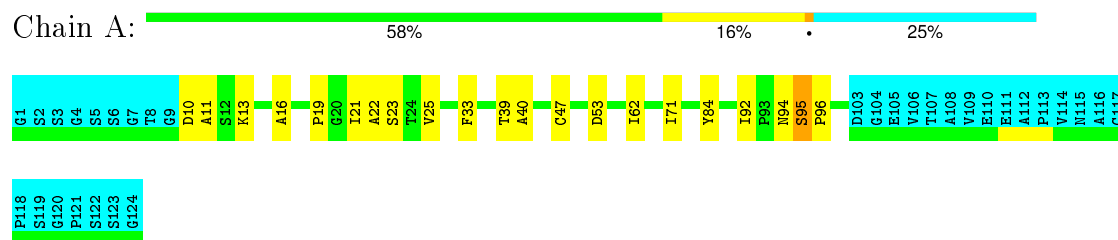
- Molecule 1: Filamin-B

Chain A: 59% 13% 25%



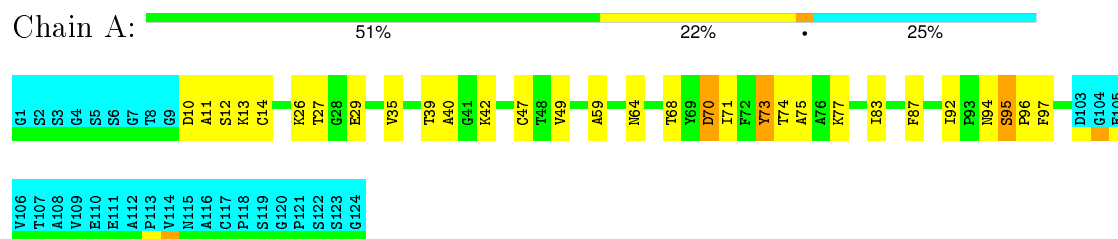
#### 4.2.18 Score per residue for model 18

- Molecule 1: Filamin-B



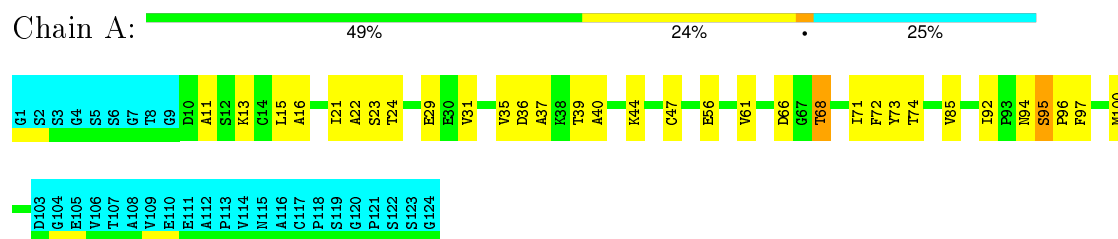
#### 4.2.19 Score per residue for model 19

- Molecule 1: Filamin-B



#### 4.2.20 Score per residue for model 20

- Molecule 1: Filamin-B



## 5 Refinement protocol and experimental data overview

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

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

The following table shows chemical shift validation statistics as aggregates over all chemical shift files. Detailed validation can be found in section 7 of this report.

Chemical shift file(s)	BMRB entry 10325
Number of chemical shift lists	1
Total number of shifts	1144
Number of shifts mapped to atoms	1144
Number of unparsed shifts	0
Number of shifts with mapping errors	0
Number of shifts with mapping warnings	0
Assignment completeness (well-defined parts)	94%

No validations of the models with respect to experimental NMR restraints is performed at this time.

## 6 Model quality ⓘ

### 6.1 Standard geometry ⓘ

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 ⓘ

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	674	658	658	15±3
All	All	13480	13160	13160	294

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 11.

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

Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:73:TYR:OH	1:A:99:VAL:HG11	0.73	1.83	15	1
1:A:31:VAL:HG22	1:A:73:TYR:O	0.73	1.84	16	4
1:A:29:GLU:O	1:A:74:THR:HG23	0.71	1.84	20	4
1:A:47:CYS:HB2	1:A:71:ILE:HD13	0.71	1.60	8	12
1:A:35:VAL:O	1:A:68:THR:HG22	0.68	1.89	9	6
1:A:37:ALA:HB1	1:A:40:ALA:HB3	0.66	1.68	3	3
1:A:13:LYS:O	1:A:15:LEU:HD22	0.63	1.92	4	1
1:A:44:LYS:HE2	1:A:46:THR:HG22	0.63	1.70	11	1
1:A:36:ASP:HA	1:A:68:THR:HG22	0.61	1.72	12	3
1:A:11:ALA:HB1	1:A:92:ILE:CG2	0.60	2.25	3	5
1:A:61:VAL:HG22	1:A:71:ILE:HG12	0.60	1.72	8	4
1:A:92:ILE:HD11	1:A:97:PHE:CE1	0.59	2.32	15	2
1:A:11:ALA:HB1	1:A:92:ILE:HG23	0.59	1.74	19	3
1:A:40:ALA:O	1:A:87:PHE:CE2	0.58	2.56	13	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:33:PHE:CE2	1:A:71:ILE:HD12	0.58	2.33	9	3
1:A:77:LYS:N	1:A:77:LYS:CD	0.58	2.67	15	2
1:A:10:ASP:O	1:A:87:PHE:CD2	0.58	2.57	19	5
1:A:10:ASP:O	1:A:40:ALA:HB1	0.58	1.98	2	2
1:A:15:LEU:O	1:A:35:VAL:HG13	0.58	1.99	17	3
1:A:47:CYS:CB	1:A:71:ILE:HD13	0.58	2.29	19	7
1:A:40:ALA:O	1:A:87:PHE:CZ	0.57	2.57	13	1
1:A:14:CYS:SG	1:A:87:PHE:CD2	0.57	2.98	14	3
1:A:72:PHE:N	1:A:72:PHE:CD1	0.56	2.73	15	4
1:A:85:VAL:HB	1:A:92:ILE:HD11	0.55	1.78	3	7
1:A:34:VAL:HG23	1:A:69:TYR:O	0.55	2.02	2	4
1:A:50:LEU:HD13	1:A:51:THR:N	0.55	2.17	1	2
1:A:66:ASP:OD1	1:A:68:THR:HG23	0.55	2.01	10	2
1:A:73:TYR:CD1	1:A:73:TYR:C	0.55	2.79	19	7
1:A:72:PHE:CD1	1:A:72:PHE:N	0.54	2.74	9	7
1:A:47:CYS:SG	1:A:71:ILE:HG21	0.54	2.43	10	3
1:A:27:THR:CG2	1:A:101:ALA:HB1	0.54	2.33	5	2
1:A:14:CYS:SG	1:A:87:PHE:CG	0.53	3.02	14	2
1:A:27:THR:HG22	1:A:101:ALA:HB1	0.53	1.81	5	2
1:A:94:ASN:HB3	1:A:97:PHE:CZ	0.53	2.38	17	7
1:A:13:LYS:HB2	1:A:40:ALA:HB2	0.52	1.79	2	1
1:A:31:VAL:HG21	1:A:73:TYR:CZ	0.52	2.39	10	1
1:A:94:ASN:CB	1:A:97:PHE:CZ	0.52	2.93	17	4
1:A:73:TYR:C	1:A:73:TYR:CD1	0.51	2.83	15	5
1:A:35:VAL:HG21	1:A:45:VAL:HG11	0.51	1.83	13	3
1:A:13:LYS:O	1:A:15:LEU:HD12	0.51	2.05	20	2
1:A:94:ASN:HB2	1:A:97:PHE:CZ	0.51	2.41	20	2
1:A:31:VAL:HG21	1:A:73:TYR:CE1	0.51	2.40	5	1
1:A:92:ILE:HD11	1:A:97:PHE:HE1	0.50	1.66	15	1
1:A:11:ALA:HB1	1:A:92:ILE:HG22	0.50	1.82	13	1
1:A:70:ASP:N	1:A:70:ASP:OD1	0.50	2.44	17	2
1:A:14:CYS:SG	1:A:35:VAL:CG1	0.50	3.00	13	5
1:A:24:THR:HG22	1:A:100:MET:HB3	0.50	1.82	17	2
1:A:73:TYR:CE2	1:A:83:ILE:HD11	0.50	2.42	15	2
1:A:91:ASP:OD1	1:A:95:SER:CB	0.50	2.60	14	2
1:A:16:ALA:O	1:A:21:ILE:CD1	0.49	2.60	18	9
1:A:51:THR:HG22	1:A:81:TYR:CE2	0.49	2.41	2	1
1:A:10:ASP:OD1	1:A:13:LYS:CG	0.49	2.60	18	1
1:A:11:ALA:HB2	1:A:87:PHE:HB3	0.49	1.82	19	1
1:A:74:THR:HG22	1:A:75:ALA:N	0.49	2.23	10	4
1:A:11:ALA:HB2	1:A:90:VAL:HB	0.48	1.85	10	3

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:33:PHE:CZ	1:A:71:ILE:HB	0.48	2.43	3	4
1:A:95:SER:HA	1:A:96:PRO:C	0.48	2.29	11	20
1:A:68:THR:C	1:A:69:TYR:CD1	0.48	2.87	13	1
1:A:94:ASN:HB2	1:A:97:PHE:CE1	0.48	2.44	20	1
1:A:52:PRO:HD3	1:A:81:TYR:CE1	0.47	2.44	7	1
1:A:33:PHE:CE1	1:A:71:ILE:HD12	0.47	2.44	8	3
1:A:14:CYS:N	1:A:40:ALA:HB2	0.47	2.24	2	1
1:A:14:CYS:O	1:A:15:LEU:HD22	0.46	2.10	9	1
1:A:11:ALA:O	1:A:92:ILE:HG22	0.46	2.11	20	3
1:A:82:VAL:CG1	1:A:84:TYR:CE1	0.46	2.98	17	1
1:A:22:ALA:O	1:A:24:THR:N	0.46	2.48	20	2
1:A:27:THR:HG23	1:A:102:THR:O	0.46	2.11	11	1
1:A:34:VAL:HG23	1:A:69:TYR:C	0.46	2.30	5	2
1:A:64:ASN:ND2	1:A:70:ASP:OD1	0.46	2.48	9	2
1:A:14:CYS:SG	1:A:37:ALA:HB2	0.46	2.51	3	1
1:A:77:LYS:HD2	1:A:77:LYS:N	0.45	2.26	15	2
1:A:39:THR:O	1:A:41:GLY:N	0.45	2.50	11	1
1:A:77:LYS:N	1:A:77:LYS:HD2	0.45	2.26	11	1
1:A:55:THR:OG1	1:A:56:GLU:N	0.45	2.50	3	3
1:A:78:PRO:HA	1:A:101:ALA:HB3	0.45	1.89	4	1
1:A:10:ASP:OD2	1:A:13:LYS:CG	0.45	2.65	5	1
1:A:11:ALA:O	1:A:14:CYS:N	0.44	2.49	11	4
1:A:22:ALA:O	1:A:23:SER:C	0.44	2.56	18	7
1:A:20:GLY:CA	1:A:31:VAL:CG1	0.44	2.95	9	1
1:A:84:TYR:CE1	1:A:96:PRO:HB3	0.44	2.48	18	1
1:A:21:ILE:HG23	1:A:33:PHE:CD2	0.44	2.47	1	1
1:A:39:THR:O	1:A:40:ALA:C	0.44	2.56	19	9
1:A:14:CYS:SG	1:A:87:PHE:CD1	0.44	3.11	6	1
1:A:33:PHE:HE2	1:A:71:ILE:HD12	0.44	1.73	9	1
1:A:49:VAL:HG23	1:A:59:ALA:HB2	0.43	1.90	19	1
1:A:21:ILE:HG23	1:A:33:PHE:CG	0.43	2.48	1	1
1:A:31:VAL:HG21	1:A:73:TYR:CE2	0.43	2.48	6	2
1:A:71:ILE:C	1:A:72:PHE:CD1	0.43	2.92	1	2
1:A:66:ASP:OD1	1:A:66:ASP:C	0.43	2.57	2	1
1:A:30:GLU:CD	1:A:30:GLU:O	0.43	2.56	13	1
1:A:56:GLU:OE1	1:A:56:GLU:N	0.43	2.52	20	1
1:A:19:PRO:O	1:A:25:VAL:HG12	0.42	2.14	18	1
1:A:42:LYS:O	1:A:87:PHE:CZ	0.42	2.73	12	1
1:A:94:ASN:O	1:A:96:PRO:O	0.42	2.38	8	13
1:A:52:PRO:HD3	1:A:81:TYR:CD1	0.42	2.49	7	1
1:A:87:PHE:CD1	1:A:87:PHE:C	0.42	2.93	16	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:43:GLY:HA3	1:A:87:PHE:CZ	0.41	2.51	17	1
1:A:62:ILE:N	1:A:62:ILE:HD12	0.41	2.30	18	1
1:A:91:ASP:O	1:A:92:ILE:C	0.41	2.58	17	1
1:A:22:ALA:C	1:A:24:THR:N	0.41	2.74	20	1
1:A:14:CYS:C	1:A:15:LEU:HD22	0.41	2.36	13	1
1:A:27:THR:HG22	1:A:75:ALA:O	0.41	2.15	19	1
1:A:20:GLY:HA2	1:A:31:VAL:HG21	0.41	1.93	6	1
1:A:27:THR:C	1:A:29:GLU:OE1	0.41	2.59	19	1
1:A:33:PHE:CE1	1:A:71:ILE:HB	0.41	2.51	1	1
1:A:31:VAL:CG2	1:A:73:TYR:CE1	0.41	3.04	5	1
1:A:20:GLY:CA	1:A:31:VAL:HG11	0.40	2.45	9	1
1:A:91:ASP:O	1:A:92:ILE:O	0.40	2.40	17	1

## 6.3 Torsion angles ⓘ

### 6.3.1 Protein backbone ⓘ

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	93/124 (75%)	86±2 (93±2%)	7±1 (7±2%)	0±0 (0±0%)	56	85
All	All	1860/2480 (75%)	1724 (93%)	132 (7%)	4 (0%)	56	85

All 4 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	14	CYS	1
1	A	92	ILE	1
1	A	40	ALA	1
1	A	23	SER	1

### 6.3.2 Protein sidechains ⓘ

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	72/93 (77%)	68±2 (94±2%)	4±2 (6±2%)	28	74
All	All	1440/1860 (77%)	1353 (94%)	87 (6%)	28	74

All 26 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	95	SER	17
1	A	77	LYS	7
1	A	70	ASP	7
1	A	44	LYS	6
1	A	56	GLU	4
1	A	55	THR	4
1	A	39	THR	4
1	A	42	LYS	4
1	A	26	LYS	4
1	A	68	THR	4
1	A	72	PHE	3
1	A	13	LYS	3
1	A	50	LEU	2
1	A	92	ILE	2
1	A	12	SER	2
1	A	66	ASP	2
1	A	10	ASP	2
1	A	38	LYS	2
1	A	65	GLU	1
1	A	29	GLU	1
1	A	86	ARG	1
1	A	73	TYR	1
1	A	102	THR	1
1	A	53	ASP	1
1	A	100	MET	1
1	A	58	GLU	1

### 6.3.3 RNA ⓘ

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 carbohydrates 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

The completeness of assignment taking into account all chemical shift lists is 94% for the well-defined parts and 78% for the entire structure.

### 7.1 Chemical shift list 1

File name: BMRB entry 10325

Chemical shift list name: *assigned\_chem\_shift\_list\_1*

#### 7.1.1 Bookkeeping

The following table shows the results of parsing the chemical shift list and reports the number of nuclei with statistically unusual chemical shifts.

Total number of shifts	1144
Number of shifts mapped to atoms	1144
Number of unparsed shifts	0
Number of shifts with mapping errors	0
Number of shifts with mapping warnings	0
Number of shift outliers (ShiftChecker)	4

#### 7.1.2 Chemical shift referencing

The following table shows the suggested chemical shift referencing corrections.

Nucleus	# values	Correction $\pm$ precision, ppm	Suggested action
$^{13}\text{C}_\alpha$	98	$-0.08 \pm 0.11$	None needed ( $< 0.5$ ppm)
$^{13}\text{C}_\beta$	85	$-0.01 \pm 0.14$	None needed ( $< 0.5$ ppm)
$^{13}\text{C}'$	99	$0.13 \pm 0.14$	None needed ( $< 0.5$ ppm)
$^{15}\text{N}$	93	$0.04 \pm 0.41$	None needed ( $< 0.5$ ppm)

#### 7.1.3 Completeness of resonance assignments

The following table shows the completeness of the chemical shift assignments for the well-defined regions of the structure. The overall completeness is 94%, i.e. 940 atoms were assigned a chemical shift out of a possible 996. 0 out of 13 assigned methyl groups (LEU and VAL) were assigned stereospecifically.

	Total	$^1\text{H}$	$^{13}\text{C}$	$^{15}\text{N}$
Backbone	455/455 (100%)	181/181 (100%)	186/186 (100%)	88/88 (100%)
Sidechain	417/473 (88%)	252/270 (93%)	163/192 (85%)	2/11 (18%)

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	<b>Total</b>	<b><sup>1</sup>H</b>	<b><sup>13</sup>C</b>	<b><sup>15</sup>N</b>
Aromatic	68/68 (100%)	36/36 (100%)	32/32 (100%)	0/0 (—%)
Overall	940/996 (94%)	469/487 (96%)	381/410 (93%)	90/99 (91%)

The following table shows the completeness of the chemical shift assignments for the full structure. The overall completeness is 78%, i.e. 977 atoms were assigned a chemical shift out of a possible 1260. 0 out of 16 assigned methyl groups (LEU and VAL) were assigned stereospecifically.

	<b>Total</b>	<b><sup>1</sup>H</b>	<b><sup>13</sup>C</b>	<b><sup>15</sup>N</b>
Backbone	481/604 (80%)	191/240 (80%)	197/248 (79%)	93/116 (80%)
Sidechain	428/588 (73%)	259/338 (77%)	167/238 (70%)	2/12 (17%)
Aromatic	68/68 (100%)	36/36 (100%)	32/32 (100%)	0/0 (—%)
Overall	977/1260 (78%)	486/614 (79%)	396/518 (76%)	95/128 (74%)

#### 7.1.4 Statistically unusual chemical shifts ⓘ

The following table lists the statistically unusual chemical shifts. These are statistical measures, and large deviations from the mean do not necessarily imply incorrect assignments. Molecules containing paramagnetic centres or hemes are expected to give rise to anomalous chemical shifts.

Mol	Chain	Res	Type	Atom	Shift, ppm	Expected range, ppm	Z-score
1	A	21	ILE	HG21	-1.11	2.13 – -0.57	-7.0
1	A	21	ILE	HG22	-1.11	2.13 – -0.57	-7.0
1	A	21	ILE	HG23	-1.11	2.13 – -0.57	-7.0
1	A	71	ILE	HB	-0.20	3.24 – 0.34	-6.9

#### 7.1.5 Random Coil Index (RCI) plots ⓘ

The image below reports *random coil index* values for the protein chains in the structure. The height of each bar gives a probability of a given residue to be disordered, as predicted from the available chemical shifts and the amino acid sequence. A value above 0.2 is an indication of significant predicted disorder. The colour of the bar shows whether the residue is in the well-defined core (black) or in the ill-defined residue ranges (cyan), as described in section 2 on ensemble composition.

Random coil index (RCI) for chain A:

