Full wwPDB NMR Structure Validation Report (i)

Apr 20, 2024 – 04:41 PM EDT

PDB ID	:	2K9U
Title	:	Solution NMR structure of the Filamin-migfilin complex
Authors	:	Ithychanda, S.N.; Qin, J.
Deposited on	:	2008-10-24

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 types of validation reports are described at
http://www.wwpdb.org/validation/2017/FAQs#types.

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

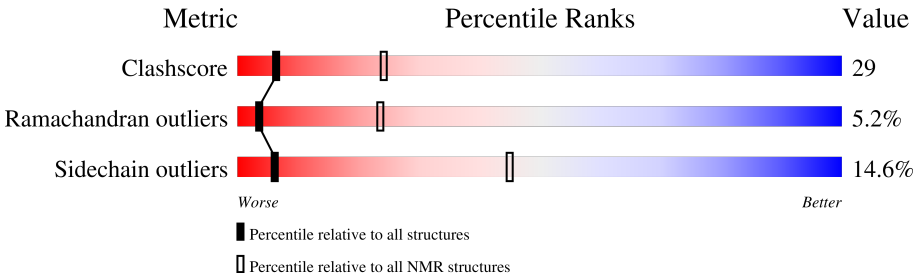
MolProbity	:	4.02b-467
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
wwPDB-RCI	:	v_1n_11_5_13_A (Berjanski et al., 2005)
PANAV	:	Wang et al. (2010)
wwPDB-ShiftChecker	:	v1.2
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.36.2

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	119	45% 24% 7% 24%
2	B	24	21% 21% 58%

2 Ensemble composition and analysis (i)

This entry contains 20 models. Model 20 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:16-A:66, A:72-A:110, B:8-B:17 (100)	0.54	20

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 5 single-model clusters were found.

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

3 Entry composition (i)

There are 2 unique types of molecules in this entry. The entry contains 2109 atoms, of which 1045 are hydrogens and 0 are deuteriums.

- Molecule 1 is a protein called Gamma filamin.

Mol	Chain	Residues	Atoms						Trace
			Total	C	H	N	O	S	
1	A	119	1721	552	843	149	176	1	0

There are 5 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	1	GLY	-	expression tag	UNP Q59H94
A	2	ILE	-	expression tag	UNP Q59H94
A	3	PRO	-	expression tag	UNP Q59H94
A	4	GLU	-	expression tag	UNP Q59H94
A	5	PHE	-	expression tag	UNP Q59H94

- Molecule 2 is a protein called Filamin-binding LIM protein 1.

Mol	Chain	Residues	Atoms						Trace
			Total	C	H	N	O	S	
2	B	24	388	117	202	35	33	1	0

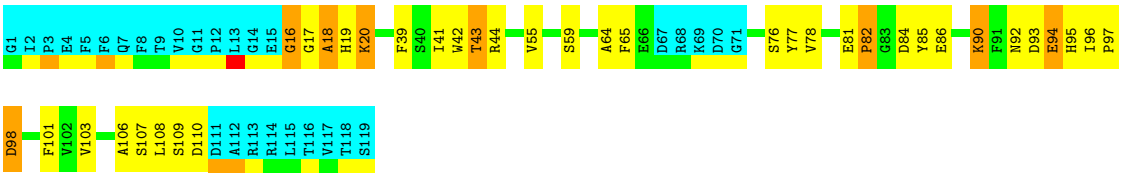
4 Residue-property plots (i)

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.

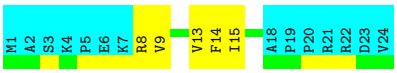
• Molecule 1: Gamma filamin

Chain A: 45% 24% 7% 24%



• Molecule 2: Filamin-binding LIM protein 1

Chain B: 21% 21% 58%



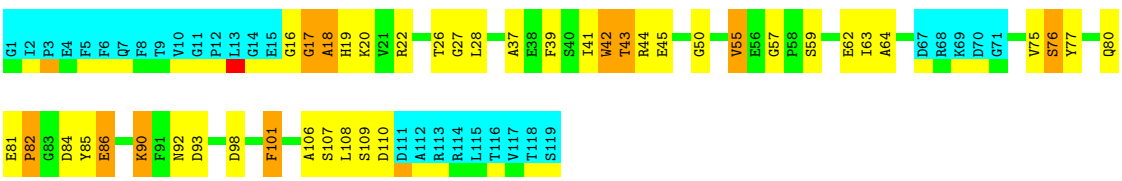
4.2 Scores per residue for each member of the ensemble

Colouring as in section 4.1 above.

4.2.1 Score per residue for model 1

• Molecule 1: Gamma filamin

Chain A: 40% 27% 8% 24%



• Molecule 2: Filamin-binding LIM protein 1

Chain B: 12% 25% • 58%

M1 A2 S3 K4 P5 E6 K7 R8 V9 A10 S11 S12 V13 F14 I15 T16 L17 A18 P19 P20 R21 R22 D23 V24

4.2.2 Score per residue for model 2

- Molecule 1: Gamma filamin

Chain A: 41% 24% 10% • 24%

G1 I2 P3 E4 F5 F6 Q7 F8 T9 V10 G11 P12 L13 G14 E15 G16 G17 A18 H19 F39 S40 I41 W42 T43 R44 V55 E56 G57 P58 S59 K60 A61 E62 I63 A64 F65 E66 D67 R68 K69 D70 G71 S72 C73 S76 Y77 E81 P82 G83 D84 Y85 E86 V87 K90 F91

N92 D93 E94 H95 I96 P97 D98 F101 V102 V103 A106 S107 L108 S109 D110 D111 A112 R113 R114 L115 T116 V117 T118 S119

- Molecule 2: Filamin-binding LIM protein 1

Chain B: 25% 17% 58%

M1 A2 S3 K4 P5 E6 K7 R8 V9 V13 F14 A18 P19 P20 R21 R22 D23 V24

4.2.3 Score per residue for model 3

- Molecule 1: Gamma filamin

Chain A: 45% 23% 8% 24%

G1 I2 P3 E4 F5 F6 Q7 F8 T9 V10 G11 P12 L13 G14 E15 G16 G17 A18 H19 K20 V21 L28 F39 S40 I41 W42 T43 R44 G50 V55 E56 G57 P58 S59 E62 I63 A64 D67 R68 K69 D70 G71 S72 C73 S76 Y77 E81 P82 Y85 E86

I89 K90 F91 N92 D93 E94 H95 S99 V103 A106 S107 L108 S109 D110 D111 A112 R113 R114 L115 T116 V117 T118 S119

- Molecule 2: Filamin-binding LIM protein 1

Chain B: 17% 17% 8% 58%

M1 A2 S3 K4 P5 E6 K7 R8 V9 V13 F14 I15 T16 L17 A18 P19 P20 R21 R22 D23 V24

4.2.4 Score per residue for model 4

- Molecule 1: Gamma filamin

Chain A: 48% 21% 7% 24%

G1 I2 P3 E4 F5 F6 Q7 F8 T9 V10 G11 P12 L13 G14 E15 G16 G17 A18 H19 K20 V21 L28 F39 W42 T43 R44 E45 V55 F65 E66 D67 R68 K69 D70 G71 V75 E81 P82 G83 D84 Y85 E86 K90 F91 N92 D93 E94 H95 I96 P97 D98

V103 A106 S107 L108 S109 D110 D111 A112 R113 R114 L115 T116 V117 T118 S119

- Molecule 2: Filamin-binding LIM protein 1

Chain B: 29% 12% 58%

M1 A2 S3 K4 P5 E6 K7 R8 V13 F14 A18 P19 P20 R21 R22 D23 V24

4.2.5 Score per residue for model 5

- Molecule 1: Gamma filamin

Chain A: 41% 27% 8% 24%

G1 I2 P3 E4 F5 F6 Q7 F8 T9 V10 G11 P12 L13 G14 E15 G16 G17 A18 H19 K20 R30 F39 W42 T43 R44 E45 V55 E56 G57 P58 S59 E62 I63 E66 D67 R68 K69 D70 G71 G74 V75 S76 Y77 V78 V79 Q80 E81 P82 Y85 E86 V87 S88

I89 K90 F91 N92 D93 E94 H95 I96 P97 D98 V103 A106 S107 L108 S109 D110 D111 A112 R113 R114 L115 T116 V117 T118 S119

- Molecule 2: Filamin-binding LIM protein 1

Chain B: 17% 17% • • 58%

M1 A2 S3 K4 P5 E6 K7 R8 V9 V13 F14 I15 T16 L17 A18 P19 P20 R21 R22 D23 V24

4.2.6 Score per residue for model 6

- Molecule 1: Gamma filamin

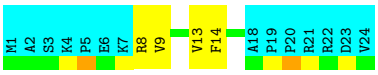
Chain A: 43% 25% 8% 24%

G1 I2 P3 E4 F5 F6 Q7 F8 T9 V10 G11 P12 L13 G14 E15 G16 G17 A18 H19 K20 V21 A33 F39 S40 I41 W42 T43 R44 E56 S59 A64 F65 E66 D67 R68 K69 D70 G71 S72 C73 S76 V79 Q80 E81 P82 G83 D84 Y85 E86 V87 K90 F91

N92 D93 E94 H95 I96 P97 D98 F101 V105 A106 S107 L108 S109 D110 D111 A112 R113 R114 L115 T116 V117 T118 S119

- Molecule 2: Filamin-binding LIM protein 1

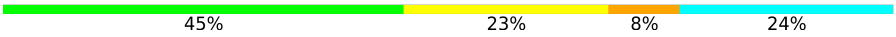
Chain B: 25% 17% 58%

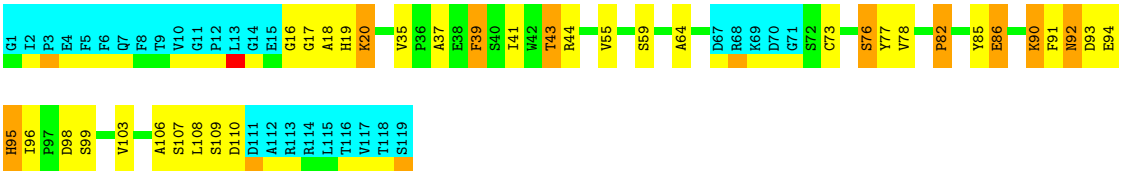


4.2.7 Score per residue for model 7

- Molecule 1: Gamma filamin

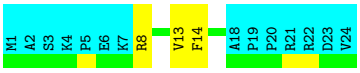
Chain A:





- Molecule 2: Filamin-binding LIM protein 1

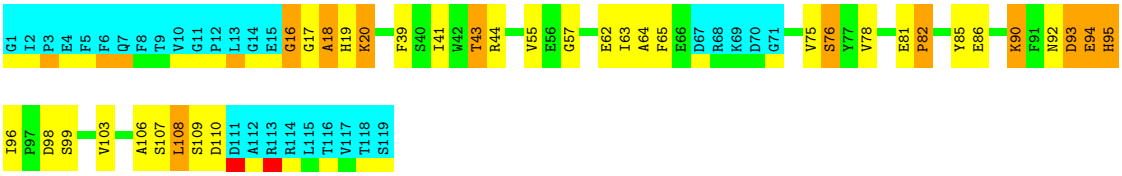
Chain B:



4.2.8 Score per residue for model 8

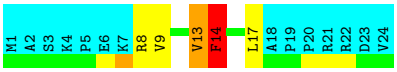
- Molecule 1: Gamma filamin

Chain A:



- Molecule 2: Filamin-binding LIM protein 1

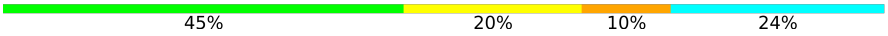
Chain B:



4.2.9 Score per residue for model 9

- Molecule 1: Gamma filamin

Chain A:



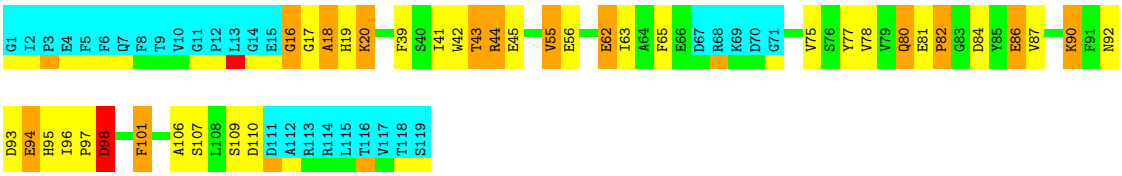
• Molecule 2: Filamin-binding LIM protein 1

Chain B: 12% 29% 58%

4.2.10 Score per residue for model 10

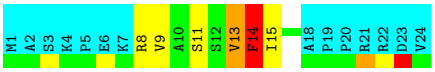
• Molecule 1: Gamma filamin

Chain A: 44% 20% 11% • 24%



• Molecule 2: Filamin-binding LIM protein 1

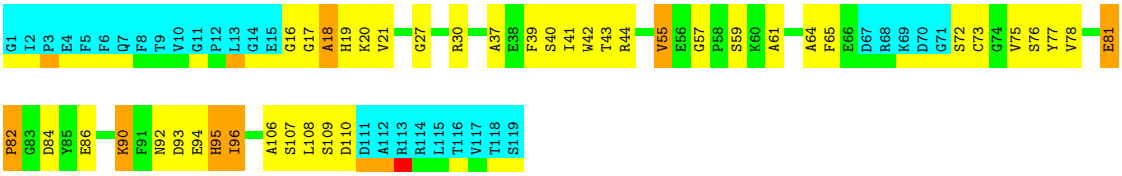
Chain B: 17% 17% • • 58%



4.2.11 Score per residue for model 11

• Molecule 1: Gamma filamin

Chain A: 40% 29% 6% 24%



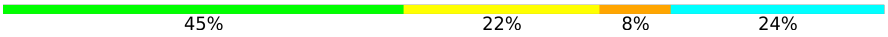
• Molecule 2: Filamin-binding LIM protein 1

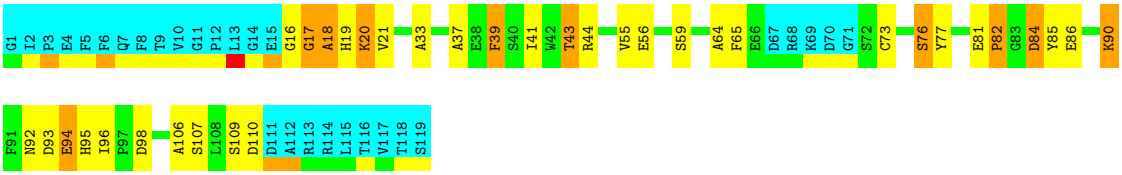
Chain B: 21% 21% 58%

4.2.12 Score per residue for model 12

- Molecule 1: Gamma filamin

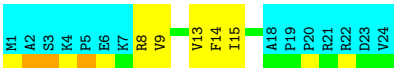
Chain A:





- Molecule 2: Filamin-binding LIM protein 1

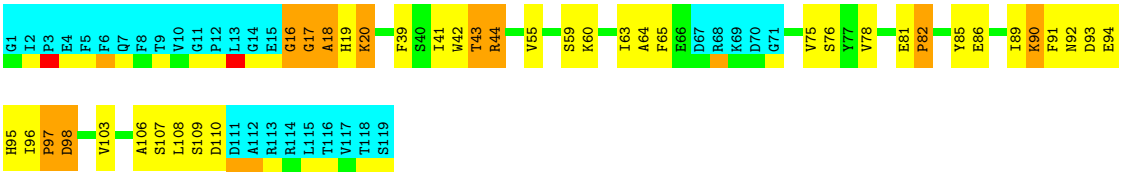
Chain B:



4.2.13 Score per residue for model 13

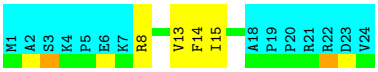
- Molecule 1: Gamma filamin

Chain A:



- Molecule 2: Filamin-binding LIM protein 1

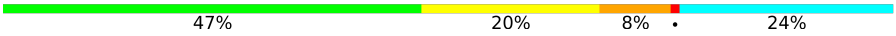
Chain B:

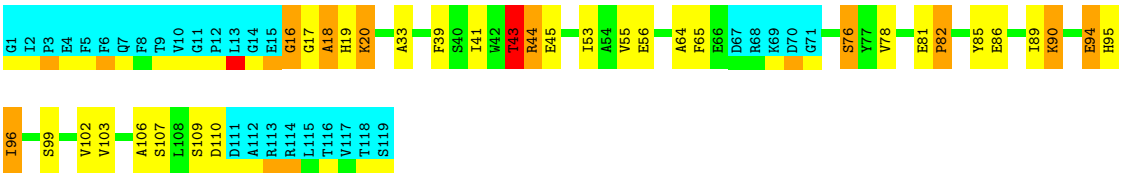


4.2.14 Score per residue for model 14

- Molecule 1: Gamma filamin

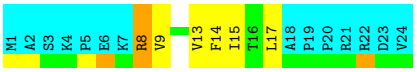
Chain A:





• Molecule 2: Filamin-binding LIM protein 1

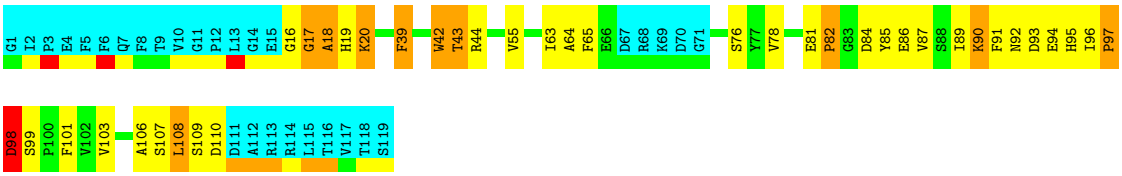
Chain B: 17% 21% • 58%



4.2.15 Score per residue for model 15

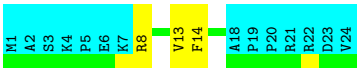
• Molecule 1: Gamma filamin

Chain A: 43% 24% 8% • 24%



• Molecule 2: Filamin-binding LIM protein 1

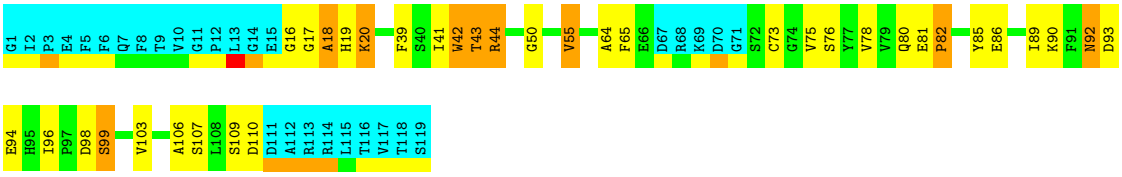
Chain B: 29% 12% 58%



4.2.16 Score per residue for model 16

• Molecule 1: Gamma filamin

Chain A: 45% 23% 8% 24%

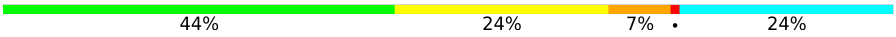


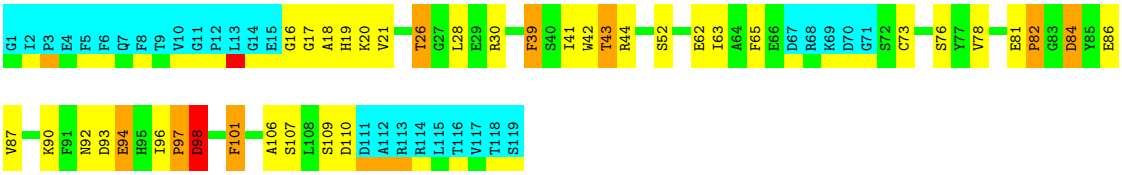
• Molecule 2: Filamin-binding LIM protein 1

Chain B: 17% 25% 58%

4.2.17 Score per residue for model 17

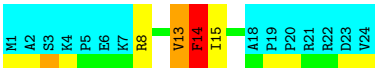
- Molecule 1: Gamma filamin

Chain A: 



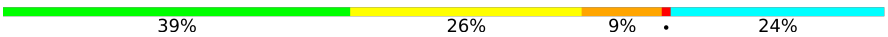
- Molecule 2: Filamin-binding LIM protein 1

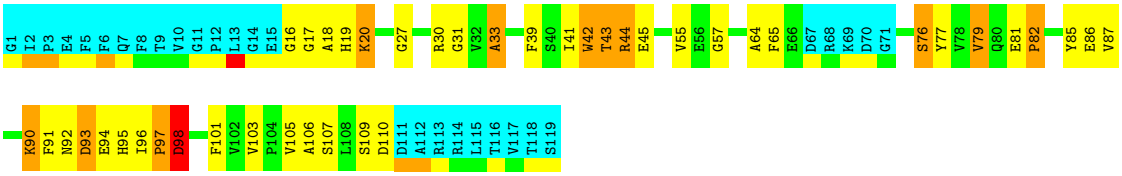
Chain B:



4.2.18 Score per residue for model 18

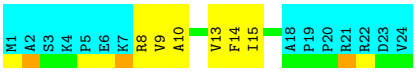
- Molecule 1: Gamma filamin

Chain A: 



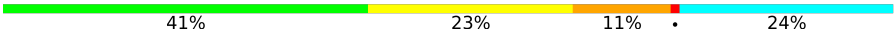
- Molecule 2: Filamin-binding LIM protein 1

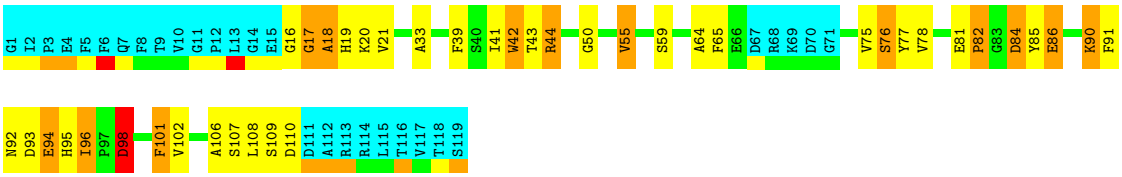
Chain B:



4.2.19 Score per residue for model 19

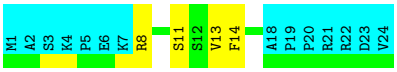
- Molecule 1: Gamma filamin

Chain A: 



• Molecule 2: Filamin-binding LIM protein 1

Chain B: 25% 17% 58%



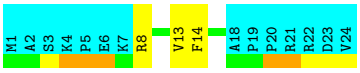
4.2.20 Score per residue for model 20 (medoid)

• Molecule 1: Gamma filamin

Chain A: 44% 24% 8% 24%

• Molecule 2: Filamin-binding LIM protein 1

Chain B: 29% 12% 58%



5 Refinement protocol and experimental data overview (i)

The models were refined using the following method: *simulated annealing*.

Of the 30 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
X-PLOR	structure solution	
X-PLOR	refinement	

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	651	622	622	37±6
2	B	76	84	84	7±2
All	All	14540	14120	14120	817

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 29.

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

Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
2:B:15:ILE:HD13	2:B:15:ILE:N	0.80	1.92	3	1
1:A:96:ILE:HD13	1:A:96:ILE:O	0.80	1.77	19	1
2:B:14:PHE:O	2:B:15:ILE:HD13	0.78	1.78	13	2
1:A:18:ALA:HB2	1:A:94:GLU:OE1	0.78	1.79	8	9
1:A:96:ILE:H	1:A:96:ILE:HD13	0.77	1.40	9	4
1:A:62:GLU:C	1:A:63:ILE:HD12	0.74	2.03	8	3
1:A:41:ILE:HD12	1:A:75:VAL:HG21	0.73	1.61	1	6
1:A:20:LYS:HZ2	1:A:44:ARG:N	0.71	1.81	18	1
1:A:84:ASP:H	2:B:8:ARG:HH12	0.71	1.29	20	6
1:A:33:ALA:HB2	1:A:107:SER:OG	0.70	1.87	20	1
1:A:84:ASP:N	2:B:8:ARG:HH12	0.68	1.87	19	4
1:A:84:ASP:H	2:B:8:ARG:NH1	0.65	1.90	20	6
1:A:96:ILE:O	1:A:98:ASP:N	0.64	2.30	5	10

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:106:ALA:HB1	1:A:110:ASP:N	0.64	2.06	8	20
2:B:13:VAL:HG22	2:B:14:PHE:N	0.63	2.09	10	20
1:A:94:GLU:OE2	1:A:96:ILE:HD13	0.62	1.95	6	1
2:B:15:ILE:N	2:B:15:ILE:CD1	0.61	2.63	3	1
1:A:101:PHE:N	1:A:101:PHE:CD1	0.61	2.69	6	3
2:B:13:VAL:HG22	2:B:14:PHE:H	0.61	1.55	10	3
1:A:79:VAL:CG1	1:A:85:TYR:CE2	0.59	2.85	18	1
1:A:18:ALA:HB2	1:A:94:GLU:CD	0.59	2.17	6	3
1:A:20:LYS:NZ	1:A:44:ARG:N	0.59	2.50	18	1
1:A:17:GLY:O	1:A:19:HIS:N	0.59	2.35	20	20
1:A:39:PHE:CE2	1:A:41:ILE:HD11	0.59	2.32	20	10
1:A:78:VAL:O	1:A:78:VAL:HG13	0.58	1.98	20	12
1:A:82:PRO:HG3	1:A:107:SER:N	0.58	2.14	4	20
1:A:39:PHE:N	1:A:39:PHE:CD1	0.58	2.71	2	16
1:A:84:ASP:N	2:B:8:ARG:NH1	0.58	2.51	19	3
1:A:41:ILE:HD12	1:A:75:VAL:CG2	0.57	2.29	1	4
1:A:96:ILE:H	1:A:96:ILE:CD1	0.57	2.04	9	4
1:A:62:GLU:O	1:A:63:ILE:HD13	0.57	1.98	17	1
1:A:21:VAL:O	1:A:21:VAL:HG13	0.57	1.99	6	6
1:A:95:HIS:H	1:A:95:HIS:CD2	0.57	2.16	2	4
1:A:98:ASP:CB	1:A:101:PHE:CE2	0.56	2.88	1	1
1:A:64:ALA:N	1:A:76:SER:O	0.56	2.39	14	15
1:A:96:ILE:HD13	1:A:96:ILE:N	0.56	2.15	11	4
1:A:63:ILE:HD12	1:A:63:ILE:N	0.56	2.16	15	6
1:A:91:PHE:O	1:A:92:ASN:ND2	0.56	2.37	19	1
1:A:43:THR:OG1	1:A:44:ARG:N	0.56	2.38	1	6
1:A:87:VAL:CG1	1:A:101:PHE:CE2	0.56	2.88	6	5
2:B:17:LEU:N	2:B:17:LEU:HD22	0.55	2.16	8	1
1:A:20:LYS:NZ	1:A:43:THR:OG1	0.55	2.39	13	11
1:A:84:ASP:O	2:B:8:ARG:NH1	0.55	2.39	6	1
1:A:16:GLY:O	1:A:18:ALA:N	0.55	2.39	13	8
1:A:95:HIS:CD2	1:A:95:HIS:O	0.55	2.60	11	2
1:A:50:GLY:O	1:A:92:ASN:N	0.54	2.40	3	4
1:A:95:HIS:CD2	1:A:95:HIS:N	0.54	2.73	2	2
1:A:41:ILE:O	1:A:73:CYS:N	0.54	2.40	12	8
2:B:8:ARG:HH11	2:B:8:ARG:CG	0.54	2.16	14	4
1:A:42:TRP:CD2	1:A:42:TRP:O	0.53	2.62	17	2
1:A:57:GLY:O	2:B:9:VAL:N	0.53	2.41	3	3
1:A:80:GLN:NE2	1:A:80:GLN:O	0.53	2.41	10	1
1:A:39:PHE:CD1	1:A:75:VAL:O	0.53	2.61	11	1
1:A:42:TRP:CD1	1:A:43:THR:N	0.53	2.77	10	3

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:61:ALA:O	1:A:63:ILE:HD12	0.53	2.03	2	1
1:A:65:PHE:CD2	1:A:65:PHE:O	0.53	2.62	8	14
1:A:84:ASP:OD2	2:B:8:ARG:NE	0.53	2.41	2	2
1:A:84:ASP:OD2	2:B:8:ARG:NH2	0.53	2.41	2	4
1:A:30:ARG:NH1	1:A:110:ASP:OD1	0.53	2.41	18	3
1:A:84:ASP:OD1	2:B:8:ARG:NH2	0.53	2.42	17	1
1:A:108:LEU:HD12	1:A:108:LEU:N	0.53	2.19	4	4
1:A:94:GLU:O	1:A:94:GLU:CG	0.53	2.57	3	16
1:A:42:TRP:CG	1:A:43:THR:N	0.53	2.76	9	1
1:A:84:ASP:OD1	2:B:8:ARG:NE	0.53	2.42	15	1
1:A:37:ALA:HB3	1:A:77:TYR:CZ	0.52	2.39	7	3
1:A:18:ALA:N	1:A:94:GLU:CD	0.52	2.63	17	8
1:A:84:ASP:OD1	1:A:84:ASP:N	0.52	2.42	15	2
2:B:8:ARG:CG	2:B:8:ARG:NH1	0.52	2.72	14	4
1:A:44:ARG:HH11	1:A:44:ARG:CG	0.52	2.17	13	1
1:A:30:ARG:NH1	1:A:30:ARG:CG	0.52	2.71	17	1
1:A:30:ARG:CG	1:A:30:ARG:HH11	0.52	2.17	17	1
1:A:44:ARG:CG	1:A:44:ARG:NH1	0.52	2.71	13	1
2:B:17:LEU:N	2:B:17:LEU:CD2	0.52	2.71	8	1
1:A:44:ARG:NH1	1:A:44:ARG:CG	0.51	2.72	6	4
1:A:95:HIS:ND1	1:A:95:HIS:O	0.51	2.42	7	1
1:A:18:ALA:N	1:A:94:GLU:OE2	0.51	2.43	20	5
2:B:15:ILE:HD13	2:B:15:ILE:H	0.51	1.60	3	1
1:A:77:TYR:O	1:A:77:TYR:CD1	0.51	2.63	20	1
2:B:8:ARG:NH1	2:B:8:ARG:CG	0.51	2.73	15	4
1:A:18:ALA:N	1:A:94:GLU:OE1	0.51	2.42	11	2
1:A:95:HIS:O	1:A:95:HIS:CG	0.51	2.63	3	6
1:A:44:ARG:CG	1:A:44:ARG:HH11	0.51	2.18	6	3
1:A:85:TYR:O	1:A:103:VAL:N	0.51	2.42	8	11
1:A:107:SER:O	1:A:108:LEU:CB	0.51	2.58	6	6
1:A:92:ASN:OD1	1:A:92:ASN:O	0.51	2.28	19	1
1:A:84:ASP:N	1:A:84:ASP:OD1	0.51	2.43	12	3
1:A:98:ASP:CG	1:A:101:PHE:CE2	0.51	2.85	19	1
1:A:17:GLY:C	1:A:19:HIS:N	0.51	2.64	20	20
1:A:98:ASP:OD1	1:A:98:ASP:N	0.51	2.44	16	3
1:A:82:PRO:CD	1:A:107:SER:OG	0.51	2.58	20	2
1:A:42:TRP:C	1:A:42:TRP:CD1	0.50	2.85	16	2
1:A:96:ILE:HD13	1:A:96:ILE:C	0.50	2.27	19	1
2:B:13:VAL:CG2	2:B:14:PHE:N	0.50	2.75	12	20
1:A:84:ASP:CA	2:B:8:ARG:HH12	0.50	2.20	12	2
1:A:108:LEU:N	1:A:108:LEU:CD1	0.50	2.74	4	3

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:82:PRO:CG	1:A:107:SER:OG	0.50	2.59	11	3
2:B:13:VAL:C	2:B:14:PHE:CG	0.50	2.85	10	3
1:A:59:SER:OG	1:A:60:LYS:N	0.50	2.45	13	1
1:A:98:ASP:OD2	1:A:101:PHE:CD1	0.49	2.66	10	1
1:A:65:PHE:O	1:A:65:PHE:CG	0.49	2.65	13	5
1:A:94:GLU:O	1:A:94:GLU:OE1	0.49	2.31	5	2
1:A:61:ALA:O	1:A:63:ILE:N	0.49	2.45	2	1
1:A:77:TYR:CD1	1:A:77:TYR:N	0.49	2.79	11	5
1:A:107:SER:C	1:A:109:SER:H	0.49	2.11	2	16
1:A:42:TRP:O	1:A:43:THR:CB	0.49	2.60	6	1
1:A:98:ASP:CG	1:A:101:PHE:CZ	0.49	2.86	19	1
1:A:42:TRP:CD2	1:A:43:THR:OG1	0.49	2.62	6	1
1:A:20:LYS:CE	1:A:43:THR:OG1	0.49	2.61	16	2
1:A:17:GLY:CA	1:A:94:GLU:OE2	0.49	2.60	18	3
1:A:86:GLU:OE2	2:B:8:ARG:NH1	0.49	2.45	6	1
1:A:66:GLU:N	1:A:74:GLY:O	0.49	2.46	5	1
1:A:92:ASN:O	1:A:93:ASP:CB	0.49	2.61	6	19
1:A:27:GLY:N	1:A:38:GLU:O	0.48	2.45	20	1
1:A:107:SER:C	1:A:109:SER:N	0.48	2.67	5	13
2:B:14:PHE:N	2:B:14:PHE:CD1	0.48	2.78	17	3
1:A:62:GLU:N	1:A:62:GLU:CD	0.48	2.67	9	2
1:A:78:VAL:O	1:A:78:VAL:CG1	0.48	2.62	10	12
1:A:18:ALA:CB	1:A:94:GLU:OE1	0.48	2.62	12	4
1:A:84:ASP:CG	2:B:8:ARG:HE	0.48	2.10	15	1
1:A:21:VAL:O	1:A:21:VAL:CG1	0.48	2.61	6	6
1:A:96:ILE:C	1:A:98:ASP:N	0.48	2.66	8	3
1:A:110:ASP:N	1:A:110:ASP:OD1	0.48	2.47	4	2
1:A:84:ASP:CB	2:B:8:ARG:HH12	0.48	2.21	19	3
1:A:33:ALA:HB2	1:A:82:PRO:HD3	0.48	1.85	6	2
1:A:28:LEU:HD21	1:A:39:PHE:CD2	0.47	2.44	4	1
2:B:8:ARG:CG	2:B:8:ARG:HH11	0.47	2.21	18	4
1:A:16:GLY:O	1:A:94:GLU:CB	0.47	2.62	14	3
1:A:84:ASP:CG	2:B:8:ARG:NH2	0.47	2.67	17	1
1:A:62:GLU:OE1	1:A:78:VAL:CG1	0.47	2.63	9	1
1:A:90:LYS:O	1:A:90:LYS:CG	0.47	2.62	18	16
1:A:17:GLY:N	1:A:94:GLU:OE2	0.47	2.48	16	1
1:A:64:ALA:HB3	1:A:76:SER:OG	0.47	2.10	19	2
2:B:8:ARG:H	2:B:8:ARG:CD	0.47	2.23	1	1
1:A:20:LYS:HZ2	1:A:21:VAL:HG23	0.46	1.71	17	1
1:A:42:TRP:CD1	1:A:42:TRP:C	0.46	2.87	5	5
1:A:94:GLU:OE1	1:A:94:GLU:O	0.46	2.34	8	6

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:93:ASP:OD1	1:A:93:ASP:N	0.46	2.47	9	1
1:A:17:GLY:N	1:A:94:GLU:CD	0.46	2.69	11	1
1:A:96:ILE:CD1	1:A:96:ILE:N	0.46	2.79	4	2
1:A:17:GLY:C	1:A:19:HIS:H	0.46	2.13	14	15
1:A:20:LYS:HZ2	1:A:21:VAL:CG2	0.46	2.24	17	1
1:A:84:ASP:CG	2:B:8:ARG:NE	0.45	2.70	15	1
1:A:94:GLU:CD	1:A:94:GLU:O	0.45	2.55	17	4
1:A:65:PHE:O	1:A:65:PHE:CD2	0.45	2.69	15	1
1:A:42:TRP:HE1	1:A:44:ARG:CG	0.45	2.25	3	1
1:A:94:GLU:O	1:A:94:GLU:CD	0.45	2.55	3	3
1:A:27:GLY:O	1:A:77:TYR:OH	0.45	2.35	11	1
1:A:61:ALA:HB1	1:A:77:TYR:HB2	0.45	1.86	11	1
1:A:90:LYS:NZ	1:A:95:HIS:CD2	0.45	2.84	12	2
1:A:35:VAL:O	1:A:35:VAL:CG1	0.45	2.65	7	1
1:A:63:ILE:N	1:A:63:ILE:CD1	0.45	2.80	13	3
1:A:17:GLY:C	1:A:94:GLU:OE2	0.45	2.55	20	3
1:A:89:ILE:N	1:A:99:SER:OG	0.45	2.39	14	2
1:A:87:VAL:CG1	1:A:101:PHE:CZ	0.45	3.00	2	1
1:A:17:GLY:CA	1:A:94:GLU:OE1	0.45	2.65	11	1
1:A:26:THR:C	1:A:28:LEU:N	0.45	2.70	1	2
1:A:95:HIS:O	1:A:96:ILE:C	0.45	2.55	6	1
1:A:16:GLY:C	1:A:18:ALA:N	0.44	2.70	1	4
1:A:95:HIS:O	1:A:95:HIS:CD2	0.44	2.71	19	1
1:A:19:HIS:O	1:A:19:HIS:CG	0.44	2.70	10	4
1:A:42:TRP:CE3	1:A:43:THR:N	0.44	2.86	6	1
1:A:84:ASP:O	1:A:86:GLU:OE2	0.44	2.36	20	2
1:A:65:PHE:CD1	1:A:65:PHE:N	0.44	2.84	11	1
1:A:55:VAL:O	2:B:11:SER:O	0.44	2.35	1	6
1:A:97:PRO:O	1:A:98:ASP:CB	0.44	2.66	18	2
1:A:19:HIS:CG	1:A:19:HIS:O	0.44	2.70	17	1
1:A:84:ASP:OD2	2:B:8:ARG:CZ	0.44	2.65	17	1
1:A:106:ALA:HB1	1:A:110:ASP:H	0.44	1.72	15	6
1:A:31:GLY:C	1:A:105:VAL:HG13	0.44	2.33	18	1
1:A:110:ASP:OD1	1:A:110:ASP:O	0.44	2.36	18	1
1:A:60:LYS:O	1:A:62:GLU:OE2	0.44	2.36	9	1
1:A:44:ARG:CD	1:A:44:ARG:C	0.44	2.86	19	1
1:A:59:SER:O	1:A:85:TYR:OH	0.43	2.36	19	7
1:A:94:GLU:CD	1:A:94:GLU:C	0.43	2.77	6	2
1:A:91:PHE:O	1:A:92:ASN:CG	0.43	2.57	19	1
1:A:94:GLU:O	1:A:94:GLU:HG3	0.43	2.13	6	2
1:A:21:VAL:HG11	1:A:96:ILE:CG2	0.43	2.44	19	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:56:GLU:OE2	2:B:9:VAL:O	0.43	2.36	12	4
1:A:95:HIS:N	1:A:95:HIS:ND1	0.43	2.65	12	1
1:A:57:GLY:O	2:B:9:VAL:O	0.43	2.36	1	5
1:A:81:GLU:O	1:A:82:PRO:O	0.43	2.37	2	6
1:A:59:SER:OG	1:A:85:TYR:OH	0.43	2.34	1	1
1:A:28:LEU:HD21	1:A:39:PHE:CG	0.43	2.49	3	1
1:A:26:THR:C	1:A:28:LEU:H	0.43	2.17	17	1
1:A:80:GLN:O	1:A:81:GLU:OE2	0.43	2.37	1	3
1:A:26:THR:HG23	1:A:27:GLY:N	0.43	2.29	1	1
1:A:27:GLY:CA	1:A:77:TYR:OH	0.43	2.67	18	1
1:A:107:SER:O	1:A:107:SER:OG	0.43	2.36	18	1
1:A:77:TYR:O	1:A:77:TYR:CG	0.43	2.71	2	2
1:A:62:GLU:OE2	1:A:63:ILE:O	0.43	2.37	10	1
1:A:40:SER:OG	1:A:72:SER:OG	0.43	2.36	11	1
1:A:96:ILE:O	1:A:99:SER:O	0.43	2.37	16	1
1:A:59:SER:CB	1:A:85:TYR:OH	0.42	2.67	2	1
1:A:39:PHE:CE1	1:A:75:VAL:O	0.42	2.72	11	1
1:A:16:GLY:O	1:A:94:GLU:OE1	0.42	2.37	20	1
1:A:84:ASP:O	1:A:86:GLU:OE1	0.42	2.38	1	3
2:B:13:VAL:O	2:B:14:PHE:CB	0.42	2.66	17	3
1:A:91:PHE:O	1:A:92:ASN:CB	0.42	2.66	4	5
1:A:96:ILE:C	1:A:98:ASP:H	0.42	2.18	6	1
1:A:95:HIS:ND1	1:A:95:HIS:N	0.42	2.65	7	1
1:A:63:ILE:HD12	1:A:63:ILE:H	0.42	1.74	15	1
1:A:44:ARG:CD	1:A:44:ARG:N	0.42	2.82	16	1
2:B:16:THR:HG22	2:B:17:LEU:N	0.42	2.29	3	1
1:A:102:VAL:HG22	1:A:103:VAL:N	0.42	2.29	14	1
1:A:92:ASN:O	1:A:93:ASP:OD2	0.42	2.37	16	1
1:A:102:VAL:O	1:A:102:VAL:HG13	0.42	2.13	19	1
1:A:37:ALA:HB3	1:A:77:TYR:CE1	0.41	2.50	1	1
1:A:18:ALA:CA	1:A:94:GLU:OE1	0.41	2.68	12	2
1:A:97:PRO:O	1:A:98:ASP:CG	0.41	2.59	2	5
1:A:91:PHE:O	1:A:94:GLU:OE1	0.41	2.38	7	4
1:A:53:ILE:O	2:B:13:VAL:O	0.41	2.38	14	1
1:A:17:GLY:O	1:A:18:ALA:C	0.41	2.58	16	1
1:A:18:ALA:CB	1:A:94:GLU:CD	0.41	2.88	6	1
1:A:109:SER:O	1:A:110:ASP:CG	0.41	2.59	3	2
1:A:107:SER:O	1:A:109:SER:N	0.41	2.54	4	4
2:B:8:ARG:H	2:B:8:ARG:NE	0.41	2.13	1	1
1:A:61:ALA:O	1:A:63:ILE:CD1	0.41	2.69	2	1
1:A:86:GLU:OE2	2:B:8:ARG:NH2	0.41	2.53	7	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:98:ASP:HB3	1:A:101:PHE:CE2	0.41	2.49	1	1
2:B:9:VAL:CG1	2:B:10:ALA:N	0.41	2.84	9	3
1:A:96:ILE:CD1	1:A:98:ASP:OD1	0.41	2.68	12	1
1:A:33:ALA:HB2	1:A:107:SER:HB3	0.41	1.91	19	1
1:A:88:SER:O	1:A:88:SER:OG	0.41	2.38	5	1
2:B:13:VAL:CG2	2:B:14:PHE:H	0.41	2.27	10	1
1:A:39:PHE:CD1	1:A:39:PHE:N	0.41	2.88	20	1
1:A:79:VAL:HG11	1:A:105:VAL:HG21	0.40	1.92	6	1
1:A:33:ALA:HB2	1:A:107:SER:HB2	0.40	1.91	12	2
1:A:91:PHE:O	1:A:94:GLU:CD	0.40	2.59	4	1
1:A:84:ASP:O	1:A:86:GLU:CD	0.40	2.60	6	1
1:A:20:LYS:HG2	1:A:46:ALA:HB2	0.40	1.92	9	1
1:A:101:PHE:CD1	1:A:101:PHE:N	0.40	2.88	15	1
1:A:77:TYR:N	1:A:77:TYR:CD1	0.40	2.90	10	1
1:A:39:PHE:CZ	1:A:41:ILE:HD11	0.40	2.51	14	1
1:A:20:LYS:NZ	1:A:21:VAL:CG2	0.40	2.84	17	1
1:A:28:LEU:HD21	1:A:39:PHE:CE2	0.40	2.52	4	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	90/119 (76%)	74±2 (82±2%)	11±2 (12±2%)	5±2 (5±2%)	3 23
2	B	10/24 (42%)	7±1 (66±6%)	3±1 (30±10%)	0±1 (4±7%)	5 31
All	All	2000/2860 (70%)	1612 (81%)	283 (14%)	105 (5%)	3 23

All 16 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	82	PRO	20
1	A	18	ALA	19
1	A	44	ARG	11
1	A	16	GLY	10

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Mol	Chain	Res	Type	Models (Total)
1	A	98	ASP	9
1	A	97	PRO	8
1	A	17	GLY	6
1	A	45	GLU	6
1	A	43	THR	5
2	B	13	VAL	3
2	B	14	PHE	3
2	B	15	ILE	1
1	A	62	GLU	1
1	A	110	ASP	1
2	B	9	VAL	1
1	A	33	ALA	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	67/91 (74%)	57±2 (85±2%)	10±2 (15±2%)	6 44
2	B	9/21 (43%)	8±1 (89±11%)	1±1 (11±11%)	10 55
All	All	1520/2240 (68%)	1298 (85%)	222 (15%)	6 45

All 40 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	86	GLU	20
1	A	90	LYS	20
1	A	20	LYS	18
1	A	55	VAL	18
1	A	43	THR	14
1	A	76	SER	12
1	A	94	GLU	11
1	A	81	GLU	10
1	A	39	PHE	9
1	A	42	TRP	8
2	B	15	ILE	7
1	A	96	ILE	6

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Mol	Chain	Res	Type	Models (Total)
1	A	98	ASP	6
1	A	101	PHE	5
1	A	93	ASP	5
1	A	95	HIS	5
1	A	89	ILE	4
1	A	99	SER	4
1	A	84	ASP	4
2	B	8	ARG	3
1	A	44	ARG	3
1	A	108	LEU	3
2	B	14	PHE	3
2	B	16	THR	2
1	A	59	SER	2
1	A	97	PRO	2
2	B	9	VAL	2
1	A	75	VAL	2
1	A	92	ASN	2
2	B	17	LEU	2
1	A	22	ARG	1
1	A	58	PRO	1
1	A	30	ARG	1
1	A	62	GLU	1
1	A	80	GLN	1
1	A	78	VAL	1
1	A	26	THR	1
1	A	52	SER	1
1	A	45	GLU	1
1	A	79	VAL	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