Full wwPDB NMR Structure Validation Report (i)

Apr 21, 2024 – 02:20 PM EDT

PDB ID	:	2M0M
BMRB ID	:	18811
Title	:	Structural Characterization of Minor Ampullate Spidroin Domains and their Distinct Roles in Fibroin Solubility and Fiber Formation
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Deposited on	:	2012-10-30

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 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:

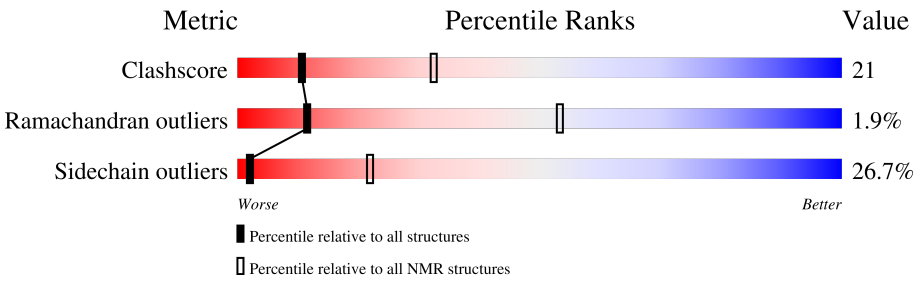
MolProbity	:	4.02b-467
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
wwPDB-RCI	:	v_1n_11_5_13_A (Berjanski et al., 2005)
PANAV	:	Wang et al. (2010)
wwPDB-ShiftChecker	:	v1.2
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson 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 is 43%.

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	107	51% 40% 6% •
1	B	107	52% 43% 5%

2 Ensemble composition and analysis (i)

This entry contains 10 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:17-A:45, A:49-A:123, B:17-B:123 (211)	0.41	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 1 clusters and 3 single-model clusters were found.

Cluster number	Models
1	1, 2, 3, 4, 5, 6, 7
Single-model clusters	8; 9; 10

3 Entry composition (i)

There is only 1 type of molecule in this entry. The entry contains 2962 atoms, of which 1494 are hydrogens and 0 are deuteriums.

- Molecule 1 is a protein called Minor ampullate fibroin 1.

Mol	Chain	Residues	Atoms						Trace
			Total	C	H	N	O	S	
1	A	107	1481	453	747	121	158	2	0
1	B	107	1481	453	747	121	158	2	0

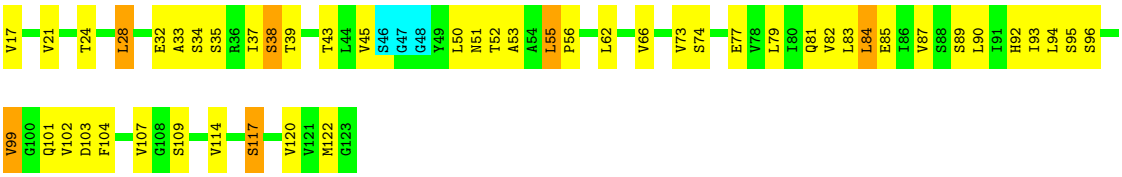
4 Residue-property plots (i)

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.

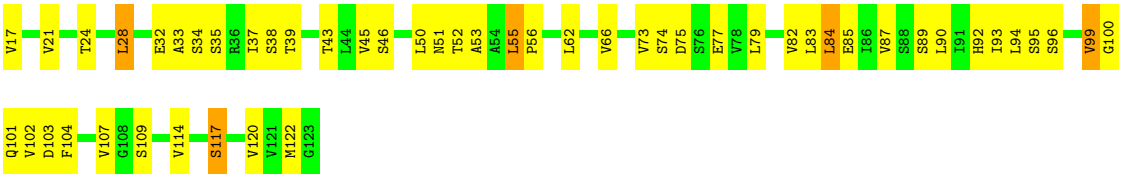
• Molecule 1: Minor ampullate fibroin 1

Chain A: 51% 40% 6% •



• Molecule 1: Minor ampullate fibroin 1

Chain B: 52% 43% 5%



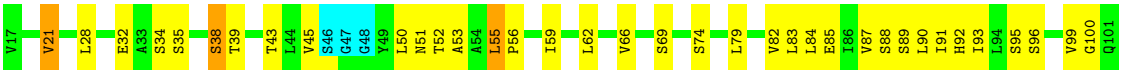
4.2 Scores per residue for each member of the ensemble

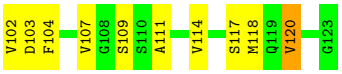
Colouring as in section 4.1 above.

4.2.1 Score per residue for model 1

• Molecule 1: Minor ampullate fibroin 1

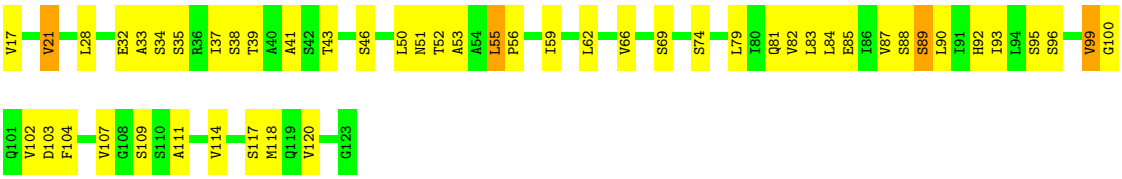
Chain A: 54% 39% • •





• Molecule 1: Minor ampullate fibroin 1

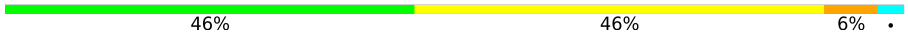
Chain B:

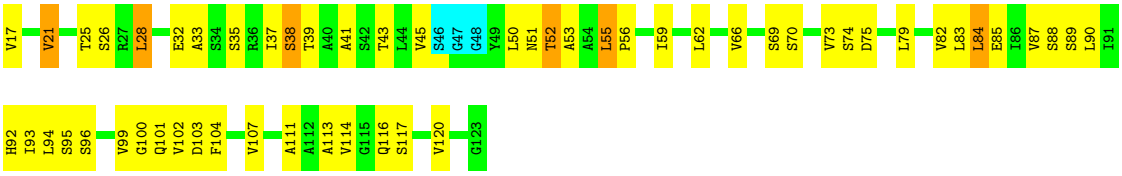


4.2.2 Score per residue for model 2

• Molecule 1: Minor ampullate fibroin 1

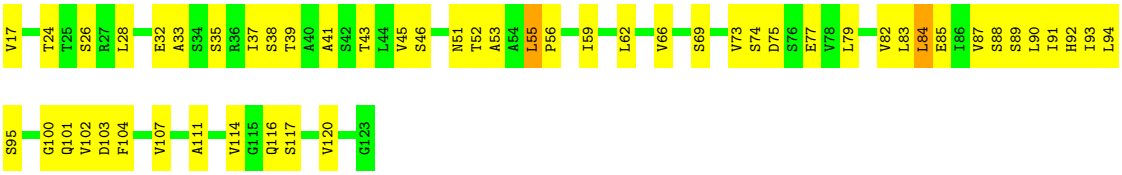
Chain A:





• Molecule 1: Minor ampullate fibroin 1

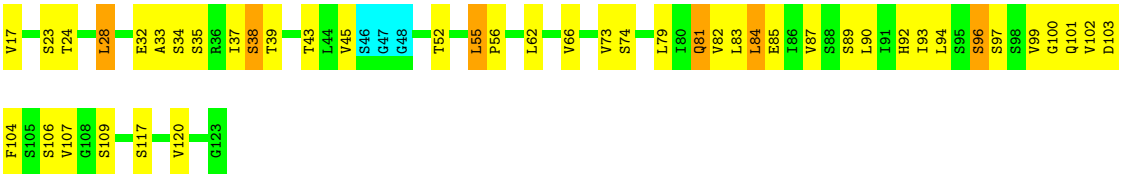
Chain B:



4.2.3 Score per residue for model 3 (medoid)

• Molecule 1: Minor ampullate fibroin 1

Chain A:



• Molecule 1: Minor ampullate fibroin 1

Chain B: 55% 39% 6%

V17 V21 A22 S23 T24 L28 E32 A33 S34 S35 R36 I37 S38 T39 T43 T52 L55 P56 L62 V66 V73 S74 D75 S76 E77 V78 L79 V82 L83 L84 E85 I86 V87 S88 S89 L90 I91 H92 I93 L94 S95 S96 S97 S98 V99 G100 Q101 V102 D103 F104

S105 S106 V107 G108 S109 V114 S117 M118 Q119 V120 G123

4.2.4 Score per residue for model 4

- Molecule 1: Minor ampullate fibroin 1

Chain A: 57% 34% 7% •

V17 R27 L28 E32 A33 S34 S35 S38 T39 T43 L44 V45 S46 G47 G48 N51 T52 A53 A54 L55 P56 L62 V66 S74 D75 L79 V82 L83 L84 V87 S88 S89 L90 I91 H92 I93 L94 S95 S96 V99 G100 Q101 V102 D103 F104 V107 G108

S109 S110 A111 Q116 S117 V120 V121 M122 G123

- Molecule 1: Minor ampullate fibroin 1

Chain B: 55% 40% 5%

V17 R27 L28 E32 A33 S34 S35 R36 I37 S38 T39 A40 A41 S42 T43 L44 V45 S46 L50 N51 T52 A53 A54 L55 P56 L62 V66 V73 S74 L79 V82 L83 L84 E85 I86 V87 S88 S89 L90 I91 H92 I93 L94 S95 S96 S97 S98 V99 G100 Q101 V102 D103

F104 V107 G108 S109 Q116 S117 V120 V121 M122 G123

4.2.5 Score per residue for model 5

- Molecule 1: Minor ampullate fibroin 1

Chain A: 52% 39% 6% •

V17 T20 V21 T24 L28 E32 A33 S34 S35 R36 I37 S38 T39 L44 V45 S46 G47 G48 Y49 L50 N51 T52 L55 P56 L62 V66 V73 S74 E77 V78 L79 I80 Q81 V82 L83 L84 E85 I86 V87 S88 S89 L90 I91 H92 I93 L94 S95 S96 S97 S98

V99 G100 Q101 V102 D103 F104 V107 G108 S109 V114 S117 V120 V121 M122 G123

- Molecule 1: Minor ampullate fibroin 1

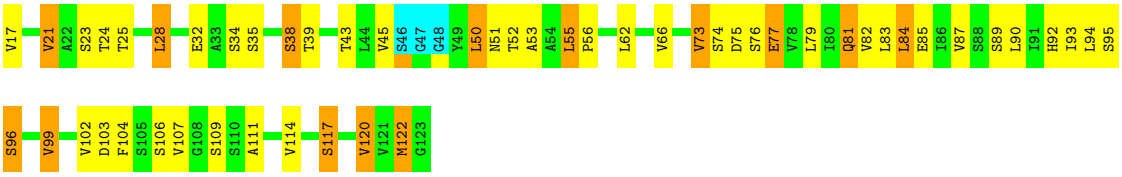
Chain B: 58% 36% 7%

V17 V21 L28 E32 A33 S34 I37 S38 T39 T43 L44 V45 L50 N51 T52 L55 P56 L62 V66 V73 S74 D75 L79 V82 L83 L84 E85 I86 V87 S88 S89 L90 I91 H92 I93 L94 S95 S96 S97 S98 V99 G100 Q101 V102 D103 F104 S109

4.2.6 Score per residue for model 6

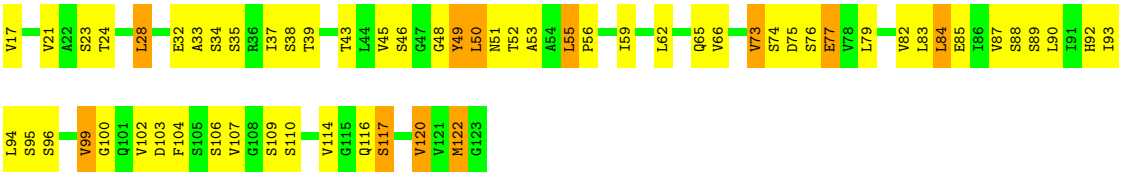
- Molecule 1: Minor ampullate fibroin 1

Chain A:



- Molecule 1: Minor ampullate fibroin 1

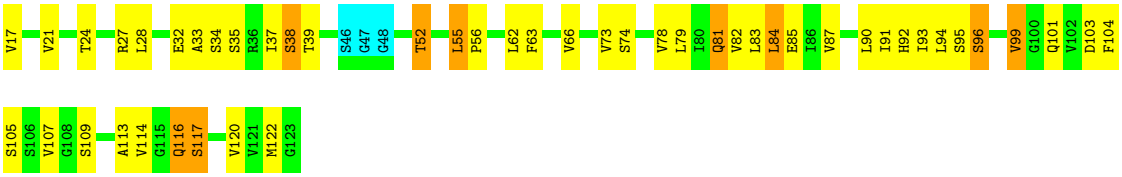
Chain B:



4.2.7 Score per residue for model 7

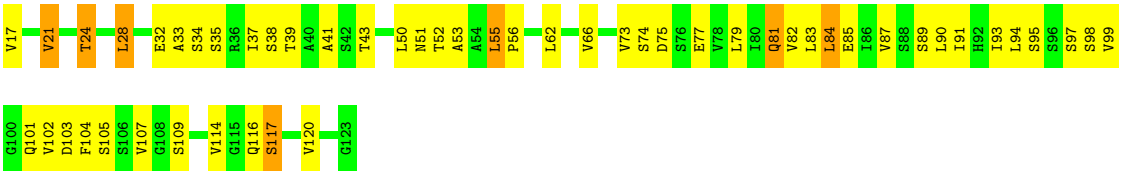
- Molecule 1: Minor ampullate fibroin 1

Chain A:



- Molecule 1: Minor ampullate fibroin 1

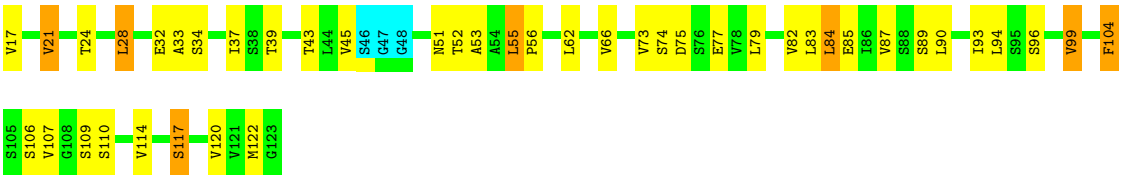
Chain B:



4.2.8 Score per residue for model 8

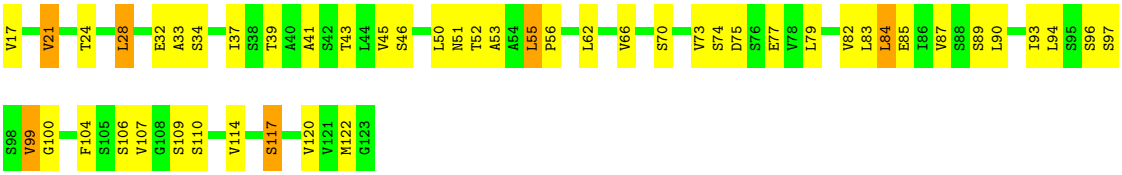
- Molecule 1: Minor ampullate fibroin 1

Chain A: 57% 34% 7%



- Molecule 1: Minor ampullate fibroin 1

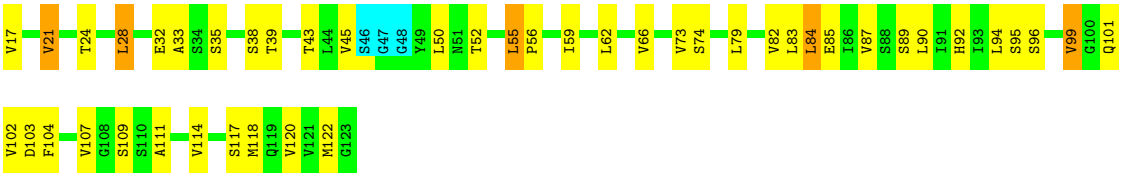
Chain B: 54% 40% 6%



4.2.9 Score per residue for model 9

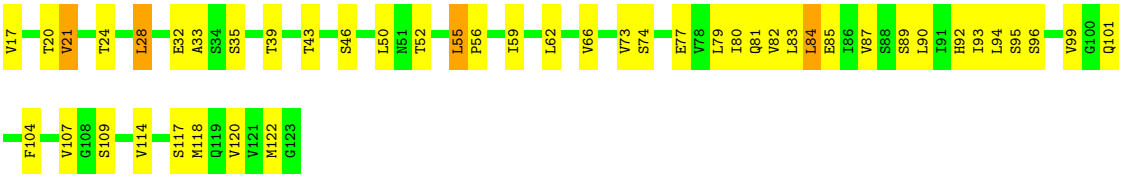
- Molecule 1: Minor ampullate fibroin 1

Chain A: 55% 37% 5%



- Molecule 1: Minor ampullate fibroin 1

Chain B: 57% 39%



4.2.10 Score per residue for model 10

- Molecule 1: Minor ampullate fibroin 1

Chain A: 50% 39% 7% •

V17 T20 V21 A22 S23 T24 L28 E32 A33 S34 I37 S38 T39 T43 L44 V45 S46 G47 G48 Y49 L50 N51 T52 A53 A54 L55 P56 L62 V66 S74 D75 S76 E77 V78 L79 I80 Q81 V82 L83 L84 E85 I86 V87 L90 I91 H92 I93 L94 S95 S96

V99 G100 Q101 V102 D103 F104 V107 G108 S109 S110 V114 G115 Q116 S117 V120 V121 M122 G123

- Molecule 1: Minor ampullate fibroin 1

Chain B: 53% 40% 7%

V17 V21 A22 S23 T24 L28 E32 A33 S34 I37 S38 T39 T43 L44 V45 G48 Y49 L50 N51 T52 A53 A54 L55 P56 L62 F63 V66 S74 D75 S76 E77 V78 L79 I80 Q81 V82 L83 L84 E85 I86 V87 L90 I91 H92 I93 L94 S95 S96 V99

G100 Q101 F104 V107 G108 S109 S110 V114 G115 Q116 S117 V120 G123

5 Refinement protocol and experimental data overview (i)

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

Of the 100 calculated structures, 10 were deposited, based on the following criterion: *structures with the lowest energy*.

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

Software name	Classification	Version
CYANA	structure solution	
CYANA	refinement	

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)	working_cs.cif
Number of chemical shift lists	1
Total number of shifts	1103
Number of shifts mapped to atoms	1103
Number of unparsed shifts	0
Number of shifts with mapping errors	0
Number of shifts with mapping warnings	0
Assignment completeness (well-defined parts)	43%

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	720	736	735	40±5
1	B	734	747	746	39±5
All	All	14540	14830	14810	613

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 21.

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

Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:114:VAL:HG21	1:B:87:VAL:HG11	0.92	1.41	5	6
1:A:83:LEU:HD22	1:B:83:LEU:HD22	0.91	1.40	4	1
1:A:87:VAL:HG11	1:B:114:VAL:HG21	0.89	1.41	5	8
1:A:45:VAL:HG11	1:B:99:VAL:HG21	0.82	1.49	6	2
1:A:28:LEU:HD12	1:A:33:ALA:HB1	0.79	1.54	4	1
1:B:28:LEU:HD13	1:B:84:LEU:HD12	0.77	1.57	9	5
1:A:17:VAL:HG21	1:B:79:LEU:HD22	0.76	1.56	6	2
1:A:111:ALA:HB1	1:B:28:LEU:HD11	0.73	1.58	4	1
1:A:104:PHE:CZ	1:B:41:ALA:HB3	0.72	2.19	8	1
1:A:21:VAL:HG21	1:B:122:MET:HE1	0.72	1.62	5	4
1:A:45:VAL:HG21	1:B:99:VAL:HG11	0.71	1.60	6	3
1:A:90:LEU:HD13	1:B:90:LEU:HD13	0.70	1.62	9	8
1:A:90:LEU:HA	1:A:93:ILE:HD12	0.70	1.63	4	9

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:B:90:LEU:HA	1:B:93:ILE:HD12	0.68	1.64	8	10
1:B:62:LEU:O	1:B:66:VAL:HG12	0.67	1.90	10	5
1:A:24:THR:HG23	1:A:77:GLU:OE2	0.67	1.89	10	1
1:A:114:VAL:HG21	1:B:87:VAL:CG1	0.66	2.20	8	5
1:A:62:LEU:O	1:A:66:VAL:HG12	0.65	1.91	1	4
1:A:62:LEU:O	1:A:66:VAL:HG22	0.64	1.91	5	6
1:A:87:VAL:CG1	1:B:114:VAL:HG21	0.64	2.23	10	6
1:A:94:LEU:HD21	1:B:94:LEU:HD21	0.64	1.69	2	8
1:A:28:LEU:HD13	1:A:84:LEU:HD12	0.63	1.69	5	3
1:A:45:VAL:CG2	1:B:99:VAL:HG11	0.63	2.23	6	3
1:B:62:LEU:HD13	1:B:85:GLU:HB2	0.62	1.72	7	10
1:A:33:ALA:O	1:A:37:ILE:HD12	0.62	1.94	5	6
1:A:94:LEU:CD2	1:B:94:LEU:HD11	0.61	2.25	4	1
1:A:96:SER:HB3	1:B:102:VAL:HG12	0.61	1.73	7	3
1:A:62:LEU:HD13	1:A:85:GLU:HB2	0.61	1.72	7	9
1:B:83:LEU:O	1:B:87:VAL:HG12	0.61	1.95	1	10
1:A:104:PHE:CE1	1:A:107:VAL:HG11	0.60	2.31	10	9
1:A:25:THR:HA	1:A:28:LEU:HD23	0.60	1.72	2	1
1:A:28:LEU:HD12	1:A:33:ALA:CB	0.60	2.25	4	1
1:A:62:LEU:HD22	1:A:85:GLU:OE1	0.60	1.96	6	2
1:B:28:LEU:HD22	1:B:33:ALA:HB1	0.60	1.74	4	1
1:A:117:SER:O	1:A:120:VAL:HG22	0.59	1.97	8	10
1:A:122:MET:CE	1:B:21:VAL:HG21	0.59	2.27	5	4
1:B:62:LEU:HD22	1:B:85:GLU:OE1	0.59	1.97	6	1
1:B:117:SER:O	1:B:120:VAL:HG22	0.59	1.98	3	10
1:A:83:LEU:HD12	1:A:84:LEU:N	0.59	2.13	2	10
1:A:28:LEU:HD22	1:A:84:LEU:HD23	0.58	1.72	1	1
1:A:45:VAL:CB	1:B:99:VAL:HG11	0.58	2.29	4	3
1:A:28:LEU:HD12	1:A:28:LEU:O	0.58	1.97	2	1
1:A:102:VAL:HG11	1:B:93:ILE:HG23	0.58	1.73	1	4
1:A:99:VAL:HG21	1:B:45:VAL:CG1	0.58	2.29	4	2
1:B:28:LEU:CD1	1:B:84:LEU:HD12	0.58	2.27	9	7
1:A:28:LEU:CD1	1:A:84:LEU:HD12	0.58	2.29	9	5
1:B:104:PHE:O	1:B:107:VAL:HG22	0.57	1.99	2	6
1:A:28:LEU:HD22	1:A:84:LEU:CD2	0.57	2.30	1	1
1:A:45:VAL:CG1	1:B:99:VAL:HG21	0.56	2.30	8	5
1:A:21:VAL:HG21	1:B:122:MET:CE	0.56	2.30	5	3
1:A:93:ILE:HG23	1:B:102:VAL:HG11	0.56	1.77	4	3
1:B:83:LEU:HD12	1:B:84:LEU:N	0.56	2.15	1	10
1:A:79:LEU:HD22	1:B:17:VAL:HG21	0.56	1.78	6	7
1:B:24:THR:HG21	1:B:80:ILE:HB	0.56	1.76	9	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:B:56:PRO:O	1:B:120:VAL:HG21	0.56	2.01	10	10
1:A:83:LEU:O	1:A:87:VAL:HG12	0.56	2.00	8	10
1:A:66:VAL:HG11	1:A:81:GLN:HG2	0.56	1.77	10	2
1:A:56:PRO:O	1:A:120:VAL:HG21	0.56	2.01	10	9
1:A:79:LEU:CD2	1:B:17:VAL:HG21	0.55	2.30	8	7
1:A:104:PHE:O	1:A:107:VAL:HG22	0.55	2.01	1	5
1:A:24:THR:HG22	1:A:81:GLN:HG3	0.55	1.78	3	3
1:B:55:LEU:N	1:B:56:PRO:HD2	0.55	2.17	6	10
1:B:62:LEU:O	1:B:66:VAL:HG22	0.55	2.01	4	5
1:A:55:LEU:N	1:A:56:PRO:HD2	0.55	2.17	6	10
1:B:28:LEU:C	1:B:28:LEU:HD13	0.54	2.23	4	1
1:A:75:ASP:CB	1:B:17:VAL:HG13	0.54	2.33	2	1
1:B:33:ALA:O	1:B:37:ILE:HD12	0.53	2.03	10	9
1:A:33:ALA:HB1	1:A:85:GLU:OE2	0.53	2.03	3	3
1:A:93:ILE:HA	1:B:102:VAL:HG21	0.53	1.79	5	1
1:A:28:LEU:CD2	1:A:84:LEU:HD12	0.53	2.33	4	1
1:A:17:VAL:HG11	1:B:79:LEU:CD2	0.53	2.34	5	1
1:A:114:VAL:HG11	1:B:87:VAL:HG22	0.53	1.81	10	2
1:B:28:LEU:HD13	1:B:28:LEU:O	0.53	2.04	4	1
1:A:21:VAL:HG21	1:B:118:MET:HB3	0.52	1.82	1	1
1:B:33:ALA:HB1	1:B:85:GLU:OE2	0.52	2.04	5	3
1:A:99:VAL:HG13	1:B:93:ILE:HG23	0.52	1.79	7	2
1:A:63:PHE:CE1	1:A:78:VAL:HG22	0.52	2.39	7	1
1:A:56:PRO:CB	1:A:120:VAL:HG11	0.52	2.35	4	5
1:B:51:ASN:HD21	1:B:53:ALA:HB3	0.52	1.65	1	6
1:A:50:LEU:HD11	1:A:55:LEU:HD23	0.52	1.82	1	4
1:B:50:LEU:HD11	1:B:55:LEU:HD23	0.52	1.80	1	3
1:A:51:ASN:HD21	1:A:53:ALA:HB3	0.52	1.64	10	6
1:A:41:ALA:O	1:A:45:VAL:HG22	0.52	2.05	2	1
1:B:28:LEU:HD12	1:B:81:GLN:NE2	0.52	2.20	7	1
1:A:104:PHE:CD1	1:A:107:VAL:HG12	0.52	2.40	8	1
1:A:118:MET:HB3	1:B:21:VAL:HG21	0.51	1.80	1	1
1:A:38:SER:CB	1:B:104:PHE:CE1	0.51	2.93	6	7
1:A:51:ASN:ND2	1:A:53:ALA:HB3	0.51	2.20	10	5
1:B:28:LEU:HD22	1:B:84:LEU:CD2	0.51	2.35	1	1
1:A:122:MET:HE1	1:B:21:VAL:HG21	0.51	1.82	6	1
1:A:94:LEU:CD2	1:B:94:LEU:HD21	0.51	2.35	10	1
1:B:83:LEU:HD12	1:B:83:LEU:C	0.51	2.26	7	9
1:B:41:ALA:O	1:B:45:VAL:HG22	0.51	2.05	2	1
1:B:28:LEU:HD22	1:B:84:LEU:HD23	0.51	1.82	1	1
1:A:17:VAL:HG21	1:B:79:LEU:CD2	0.51	2.31	6	2

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:94:LEU:HD21	1:B:94:LEU:CD2	0.51	2.36	5	1
1:A:28:LEU:HD22	1:A:84:LEU:CG	0.50	2.36	1	1
1:A:28:LEU:HD11	1:B:111:ALA:HB1	0.50	1.82	2	1
1:A:28:LEU:HD22	1:A:84:LEU:HB3	0.50	1.83	4	1
1:A:83:LEU:HD12	1:A:83:LEU:C	0.50	2.27	7	8
1:B:56:PRO:CB	1:B:120:VAL:HG11	0.50	2.36	4	5
1:B:104:PHE:CE1	1:B:107:VAL:HG11	0.50	2.42	10	9
1:A:56:PRO:HB2	1:A:120:VAL:HG11	0.50	1.84	10	8
1:B:56:PRO:HB2	1:B:120:VAL:HG11	0.49	1.83	10	7
1:B:51:ASN:ND2	1:B:53:ALA:HB3	0.49	2.22	1	3
1:A:83:LEU:HD22	1:B:83:LEU:CD2	0.49	2.28	4	1
1:B:66:VAL:HG21	1:B:81:GLN:HG2	0.49	1.84	1	1
1:A:59:ILE:HD12	1:A:117:SER:HB3	0.49	1.85	9	2
1:A:122:MET:HG2	1:B:17:VAL:HG13	0.49	1.83	8	2
1:A:88:SER:OG	1:B:111:ALA:HB2	0.49	2.08	2	2
1:A:45:VAL:HB	1:B:99:VAL:HG11	0.49	1.83	4	2
1:A:27:ARG:NH1	1:A:66:VAL:HG23	0.49	2.23	4	1
1:B:28:LEU:HD22	1:B:33:ALA:CB	0.48	2.37	4	1
1:A:87:VAL:HG22	1:B:114:VAL:HG11	0.48	1.85	7	1
1:A:99:VAL:HG21	1:B:45:VAL:HB	0.48	1.85	2	4
1:A:99:VAL:HG11	1:B:45:VAL:CB	0.48	2.39	4	1
1:A:111:ALA:HB2	1:B:88:SER:OG	0.47	2.09	1	3
1:A:59:ILE:HD12	1:A:117:SER:HB2	0.47	1.86	2	1
1:A:91:ILE:HG23	1:B:50:LEU:HD21	0.47	1.85	10	2
1:A:96:SER:CB	1:B:102:VAL:HG12	0.47	2.38	7	1
1:B:28:LEU:HD13	1:B:84:LEU:CD1	0.47	2.37	9	1
1:A:17:VAL:HG13	1:B:75:ASP:CB	0.47	2.39	2	3
1:B:45:VAL:HG12	1:B:49:TYR:C	0.47	2.30	6	1
1:B:45:VAL:HG23	1:B:45:VAL:O	0.46	2.10	10	1
1:A:75:ASP:HB3	1:B:17:VAL:HG13	0.46	1.88	2	1
1:A:99:VAL:HG11	1:B:45:VAL:HG21	0.46	1.87	4	1
1:A:90:LEU:HD22	1:B:90:LEU:CD1	0.46	2.40	8	3
1:A:50:LEU:HD21	1:B:91:ILE:HG23	0.46	1.87	10	2
1:B:98:SER:O	1:B:99:VAL:HB	0.46	2.10	7	1
1:A:93:ILE:CG2	1:B:99:VAL:HG22	0.46	2.40	10	1
1:B:20:THR:HG23	1:B:77:GLU:OE1	0.46	2.10	9	1
1:A:102:VAL:HG22	1:B:92:HIS:CE1	0.46	2.45	5	1
1:B:90:LEU:C	1:B:90:LEU:HD12	0.46	2.32	2	4
1:A:99:VAL:HG11	1:B:45:VAL:CG2	0.45	2.40	4	1
1:B:90:LEU:HD12	1:B:91:ILE:N	0.45	2.26	7	2
1:A:17:VAL:HG23	1:B:122:MET:SD	0.45	2.52	8	2

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:B:41:ALA:HB2	1:B:89:SER:CB	0.45	2.41	4	2
1:A:102:VAL:HG21	1:B:93:ILE:HA	0.45	1.87	5	1
1:B:24:THR:HG23	1:B:77:GLU:HG3	0.45	1.85	8	2
1:A:90:LEU:HD12	1:A:90:LEU:C	0.45	2.31	4	3
1:B:41:ALA:HB2	1:B:89:SER:HB3	0.45	1.88	7	1
1:B:63:PHE:CE1	1:B:78:VAL:HG22	0.45	2.47	10	1
1:B:55:LEU:N	1:B:56:PRO:CD	0.45	2.80	6	10
1:B:79:LEU:O	1:B:79:LEU:HD12	0.45	2.11	1	7
1:B:24:THR:HG22	1:B:81:GLN:HG2	0.45	1.87	9	1
1:A:102:VAL:HG12	1:B:96:SER:HB3	0.44	1.89	3	1
1:A:44:LEU:HD21	1:A:55:LEU:HD22	0.44	1.89	5	1
1:B:28:LEU:HA	1:B:33:ALA:HB2	0.44	1.89	9	1
1:B:59:ILE:HD12	1:B:117:SER:HB2	0.44	1.89	2	1
1:A:79:LEU:HD23	1:B:17:VAL:HG21	0.44	1.89	8	2
1:A:17:VAL:HG23	1:B:122:MET:HG2	0.44	1.89	8	1
1:A:55:LEU:N	1:A:56:PRO:CD	0.44	2.81	2	10
1:B:28:LEU:HD22	1:B:84:LEU:CG	0.43	2.43	1	1
1:B:28:LEU:CD2	1:B:33:ALA:HB1	0.43	2.41	4	1
1:A:92:HIS:CE1	1:B:102:VAL:HG22	0.43	2.48	5	1
1:A:50:LEU:CD1	1:A:55:LEU:HD23	0.43	2.43	6	1
1:A:28:LEU:HD12	1:A:85:GLU:OE2	0.43	2.13	9	1
1:A:45:VAL:CG2	1:B:99:VAL:HG22	0.43	2.43	9	1
1:A:24:THR:HG21	1:A:80:ILE:HB	0.43	1.89	10	1
1:A:79:LEU:HD12	1:A:79:LEU:O	0.43	2.13	2	7
1:A:24:THR:HG23	1:A:77:GLU:HG3	0.43	1.90	8	1
1:B:28:LEU:HD22	1:B:28:LEU:O	0.43	2.13	4	1
1:A:93:ILE:HG23	1:B:99:VAL:HG13	0.43	1.88	7	1
1:A:24:THR:HG23	1:A:77:GLU:CD	0.43	2.34	10	1
1:B:73:VAL:HG22	1:B:77:GLU:HB3	0.43	1.90	3	1
1:A:24:THR:HG22	1:A:81:GLN:CG	0.43	2.44	6	1
1:A:28:LEU:O	1:A:33:ALA:HB3	0.43	2.14	8	3
1:A:33:ALA:HB1	1:A:85:GLU:OE1	0.43	2.13	9	1
1:B:28:LEU:HD12	1:B:85:GLU:OE2	0.43	2.14	9	1
1:A:90:LEU:CD1	1:B:90:LEU:HD22	0.43	2.44	10	1
1:A:104:PHE:CD1	1:A:107:VAL:HG11	0.42	2.48	6	4
1:B:50:LEU:CD1	1:B:55:LEU:HD23	0.42	2.44	6	2
1:A:111:ALA:HB1	1:B:28:LEU:HD21	0.42	1.91	9	1
1:A:52:THR:CG2	1:A:113:ALA:HB1	0.42	2.45	7	2
1:A:99:VAL:HG11	1:B:45:VAL:HB	0.42	1.91	4	1
1:A:122:MET:CG	1:B:17:VAL:HG13	0.42	2.43	8	2
1:A:116:GLN:HG3	1:A:117:SER:N	0.42	2.30	7	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:122:MET:HE3	1:B:21:VAL:HG21	0.42	1.92	10	3
1:B:51:ASN:OD1	1:B:53:ALA:HB3	0.41	2.15	7	1
1:A:28:LEU:HD13	1:A:84:LEU:CD1	0.41	2.42	9	1
1:A:45:VAL:CB	1:B:99:VAL:HG21	0.41	2.45	10	1
1:A:90:LEU:HD12	1:A:91:ILE:N	0.41	2.31	1	3
1:B:28:LEU:HD22	1:B:84:LEU:HG	0.41	1.93	1	1
1:A:21:VAL:O	1:A:25:THR:HG23	0.41	2.16	2	2
1:B:24:THR:HG21	1:B:77:GLU:O	0.41	2.16	2	1
1:A:99:VAL:O	1:A:102:VAL:HG12	0.41	2.15	9	1
1:A:36:ARG:NH1	1:A:66:VAL:HG13	0.41	2.30	5	1
1:A:102:VAL:HG13	1:A:102:VAL:O	0.41	2.15	9	1
1:B:55:LEU:CD1	1:B:59:ILE:HD11	0.41	2.46	6	1
1:A:93:ILE:HG21	1:B:99:VAL:HG22	0.41	1.92	10	1
1:B:45:VAL:CG1	1:B:93:ILE:HD13	0.41	2.46	4	1
1:A:28:LEU:HD22	1:A:84:LEU:HG	0.41	1.92	1	1
1:B:59:ILE:HD12	1:B:117:SER:HB3	0.41	1.92	1	2
1:A:24:THR:HG21	1:A:77:GLU:O	0.41	2.16	5	1
1:A:73:VAL:HG21	1:A:77:GLU:CD	0.41	2.36	6	1
1:A:82:VAL:CG1	1:A:83:LEU:N	0.41	2.84	4	1
1:A:90:LEU:HD22	1:B:90:LEU:HD13	0.40	1.93	8	1
1:A:17:VAL:HG11	1:B:79:LEU:HD22	0.40	1.92	5	1
1:A:99:VAL:HG21	1:B:45:VAL:CB	0.40	2.47	5	1
1:A:50:LEU:HD12	1:A:51:ASN:N	0.40	2.31	6	1
1:B:73:VAL:HG21	1:B:77:GLU:CD	0.40	2.37	6	1
1:A:91:ILE:HG23	1:B:50:LEU:CD2	0.40	2.46	1	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	102/107 (95%)	96±2 (94±2%)	4±2 (4±2%)	2±0 (1±0%)	14	59
1	B	105/107 (98%)	97±2 (92±2%)	6±2 (5±2%)	2±1 (2±1%)	9	46
All	All	2070/2140 (97%)	1930 (93%)	100 (5%)	40 (2%)	11	53

All 11 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	99	VAL	8
1	B	100	GLY	8
1	B	99	VAL	7
1	A	100	GLY	5
1	B	97	SER	5
1	B	48	GLY	2
1	A	106	SER	1
1	B	106	SER	1
1	A	45	VAL	1
1	B	45	VAL	1
1	B	49	TYR	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	84/85 (99%)	62±3 (73±4%)	22±3 (27±4%)	2 21
1	B	85/85 (100%)	62±4 (73±5%)	23±4 (27±5%)	2 22
All	All	1690/1700 (99%)	1239 (73%)	451 (27%)	2 22

All 87 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	32	GLU	10
1	A	39	THR	10
1	A	52	THR	10
1	A	55	LEU	10
1	A	74	SER	10
1	A	82	VAL	10
1	B	32	GLU	10
1	B	39	THR	10
1	B	43	THR	10
1	B	52	THR	10
1	B	55	LEU	10

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Mol	Chain	Res	Type	Models (Total)
1	B	74	SER	10
1	B	82	VAL	10
1	A	96	SER	9
1	A	103	ASP	9
1	A	109	SER	9
1	B	109	SER	9
1	A	84	LEU	9
1	B	84	LEU	9
1	A	38	SER	8
1	A	43	THR	8
1	A	89	SER	8
1	A	92	HIS	8
1	B	89	SER	8
1	B	73	VAL	8
1	A	21	VAL	7
1	A	34	SER	7
1	A	35	SER	7
1	B	21	VAL	7
1	B	34	SER	7
1	B	35	SER	7
1	B	38	SER	7
1	B	92	HIS	7
1	B	96	SER	7
1	B	103	ASP	7
1	A	28	LEU	7
1	A	73	VAL	7
1	B	101	GLN	7
1	A	95	SER	6
1	B	46	SER	6
1	B	95	SER	6
1	A	101	GLN	6
1	B	28	LEU	6
1	B	116	GLN	5
1	A	117	SER	5
1	B	117	SER	5
1	A	116	GLN	4
1	A	81	GLN	4
1	B	24	THR	4
1	A	75	ASP	4
1	B	75	ASP	4
1	A	120	VAL	3
1	A	23	SER	3

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Mol	Chain	Res	Type	Models (Total)
1	B	23	SER	3
1	B	110	SER	3
1	A	69	SER	2
1	B	69	SER	2
1	A	97	SER	2
1	A	106	SER	2
1	B	106	SER	2
1	B	118	MET	2
1	A	27	ARG	2
1	A	122	MET	2
1	B	122	MET	2
1	A	20	THR	2
1	B	120	VAL	2
1	A	76	SER	2
1	A	77	GLU	2
1	B	49	TYR	2
1	B	50	LEU	2
1	B	76	SER	2
1	B	81	GLN	2
1	A	110	SER	2
1	A	24	THR	2
1	A	26	SER	1
1	A	70	SER	1
1	B	26	SER	1
1	B	27	ARG	1
1	A	50	LEU	1
1	B	65	GLN	1
1	B	77	GLU	1
1	A	105	SER	1
1	B	105	SER	1
1	A	104	PHE	1
1	B	70	SER	1
1	A	118	MET	1
1	A	99	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)

The completeness of assignment taking into account all chemical shift lists is 43% for the well-defined parts and 43% for the entire structure.

7.1 Chemical shift list 1

File name: working_cs.cif

Chemical shift list name: *assigned_chem_shift_list_1*

7.1.1 Bookkeeping (i)

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	1103
Number of shifts mapped to atoms	1103
Number of unparsed shifts	0
Number of shifts with mapping errors	0
Number of shifts with mapping warnings	0
Number of shift outliers (ShiftChecker)	2

7.1.2 Chemical shift referencing (i)

The following table shows the suggested chemical shift referencing corrections.

Nucleus	# values	Correction ± precision, *ppm*	Suggested action
$^{13}C_{\alpha}$	107	-0.82 ± 0.18	Should be checked
$^{13}C_{\beta}$	95	0.29 ± 0.11	None needed (< 0.5 ppm)
$^{13}C'$	0	—	None (insufficient data)
^{15}N	105	0.14 ± 0.33	None needed (< 0.5 ppm)

7.1.3 Completeness of resonance assignments (i)

The following table shows the completeness of the chemical shift assignments for the well-defined regions of the structure. The overall completeness is 43%, i.e. 1085 atoms were assigned a chemical shift out of a possible 2544. 0 out of 50 assigned methyl groups (LEU and VAL) were assigned stereospecifically.

	Total	^{1}H	^{13}C	^{15}N
Backbone	417/1063 (39%)	211/434 (49%)	104/422 (25%)	102/207 (49%)
Sidechain	652/1409 (46%)	448/950 (47%)	197/435 (45%)	7/24 (29%)

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	Total	^{1}H	^{13}C	^{15}N
Aromatic	16/72 (22%)	8/36 (22%)	8/34 (24%)	0/2 (0%)
Overall	1085/2544 (43%)	667/1420 (47%)	309/891 (35%)	109/233 (47%)

The following table shows the completeness of the chemical shift assignments for the full structure. The overall completeness is 43%, i.e. 1102 atoms were assigned a chemical shift out of a possible 2564. 0 out of 50 assigned methyl groups (LEU and VAL) were assigned stereospecifically.

	Total	^{1}H	^{13}C	^{15}N
Backbone	431/1080 (40%)	219/442 (50%)	107/428 (25%)	105/210 (50%)
Sidechain	655/1412 (46%)	450/952 (47%)	198/436 (45%)	7/24 (29%)
Aromatic	16/72 (22%)	8/36 (22%)	8/34 (24%)	0/2 (0%)
Overall	1102/2564 (43%)	677/1430 (47%)	313/898 (35%)	112/236 (47%)

7.1.4 Statistically unusual chemical shifts (i)

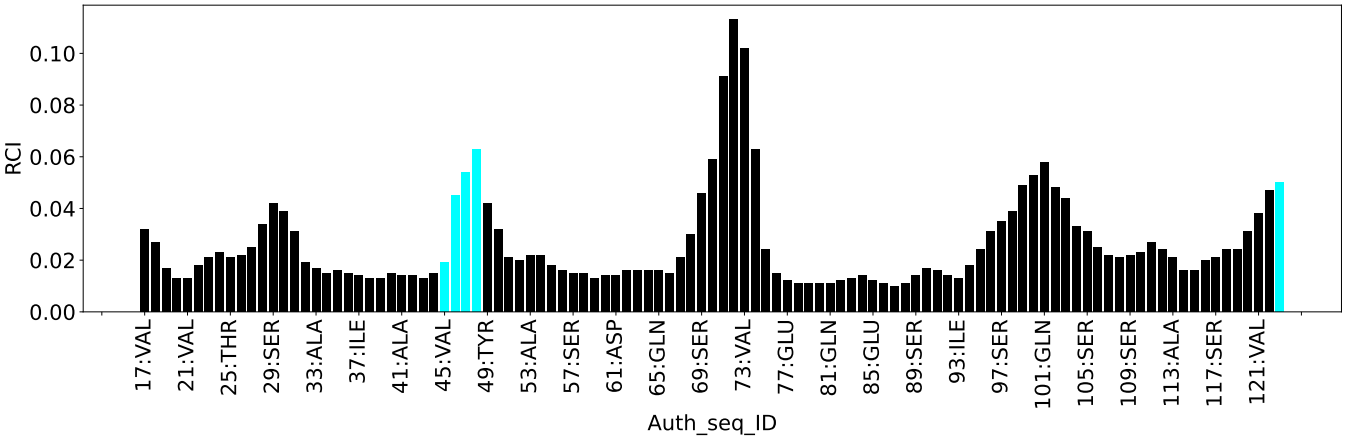
The following table lists the statistically unusual chemical shifts. These are statistical measures, and large deviations from the mean do not necessarily imply incorrect assignments. Molecules containing paramagnetic centres or hemes are expected to give rise to anomalous chemical shifts.

List Id	Chain	Res	Type	Atom	Shift, *ppm*	Expected range, *ppm*	Z-score
1	A	36	ARG	HE	11.67	4.52 – 10.19	7.6
1	A	81	GLN	HE21	9.71	5.02 – 9.43	5.6

7.1.5 Random Coil Index (RCI) plots (i)

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.If well-defined core and ill-defined regions are not identified then it is shown as gray bars.

Random coil index (RCI) for chain A:


RCI
0.00
0.02
0.04
0.06
0.08
0.10
17:VAL
21:VAL
25:THR
29:SER
33:ALA
37:ILE
41:ALA
45:VAL
49:TYR
53:ALA
57:SER
61:ASP
65:GLN
69:SER
73:VAL
77:GLU
81:GLN
85:GLU
89:SER
93:ILE
97:SER
101:GLN
105:SER
109:SER
113:ALA
117:SER
121:VAL
Auth_seq_ID