



# Full wwPDB NMR Structure Validation Report ⓘ

May 29, 2020 – 07:49 am BST

PDB ID : 5MS9  
Title : Solution structure of Human Fibrillin-1 EGF2-EGF3-Hybrid1-cbEGF1 four domain fragment  
Authors : Robertson, I.B.; Redfield, C.; Handford, P.A.  
Deposited on : 2017-01-01

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

<https://www.wwpdb.org/validation/2017/NMRValidationReportHelp>

with specific help available everywhere you see the ⓘ symbol.

---

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  
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 : 2.11  
Ideal geometry (proteins) : Engh & Huber (2001)  
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)  
Validation Pipeline (wwPDB-VP) : 2.11

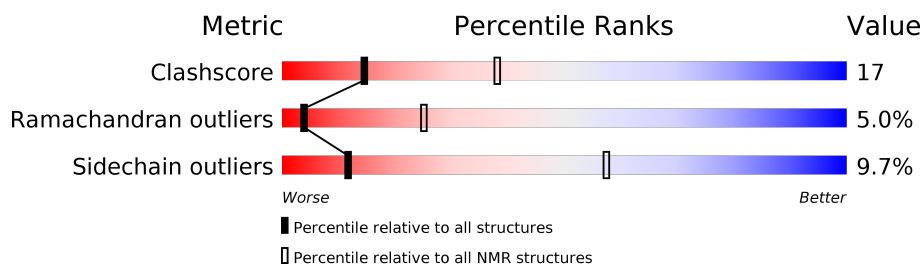
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*SOLUTION NMR*

The overall completeness of chemical shifts assignment is 79%.

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  $\geq 3$ , 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	177	

## 2 Ensemble composition and analysis

This entry contains 20 models. Model 1 is the overall representative, medoid model (most similar to other models).

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:140-A:287 (148)	1.12	1

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 4 clusters. No single-model clusters were found.

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

### 3 Entry composition

There are 2 unique types of molecules in this entry. The entry contains 2498 atoms, of which 1202 are hydrogens and 0 are deuteriums.

- Molecule 1 is a protein called Fibrillin-1.

Mol	Chain	Residues	Atoms						Trace
1	A	177	Total	C	H	N	O	S	0
			2497	773	1202	246	247	29	

There are 3 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	111	SER	-	expression tag	UNP P35555
A	112	ALA	-	expression tag	UNP P35555
A	204	SER	CYS	conflict	UNP P35555

- Molecule 2 is CALCIUM ION (three-letter code: CA) (formula: Ca).

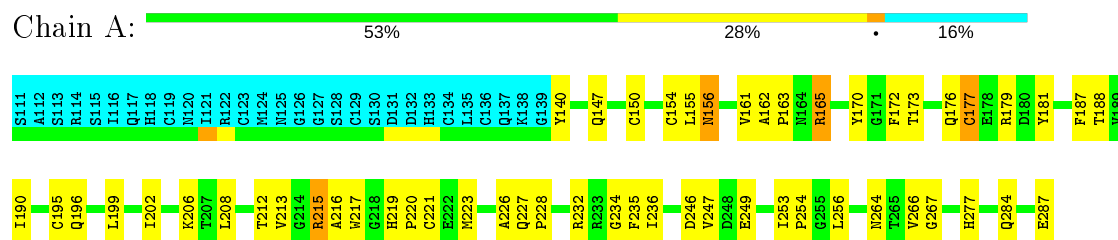
Mol	Chain	Residues	Atoms	
2	A	1	Total	Ca
			1	1

## 4 Residue-property plots

### 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: Fibrillin-1

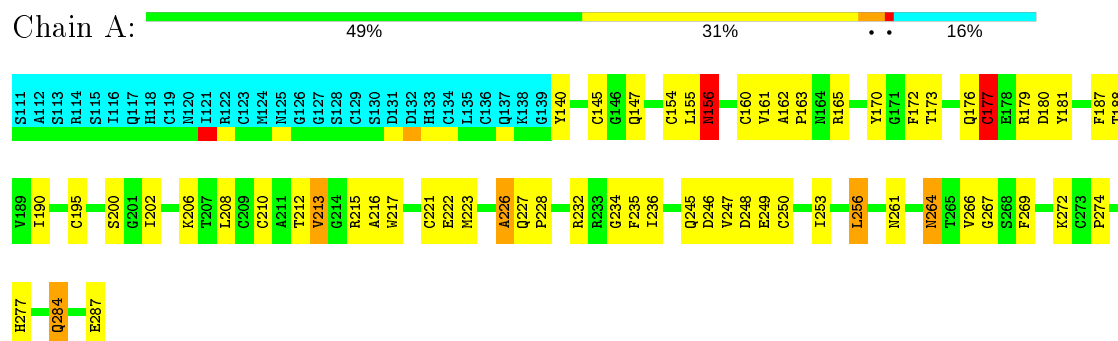


### 4.2 Scores per residue for each member of the ensemble

Colouring as in section 4.1 above.

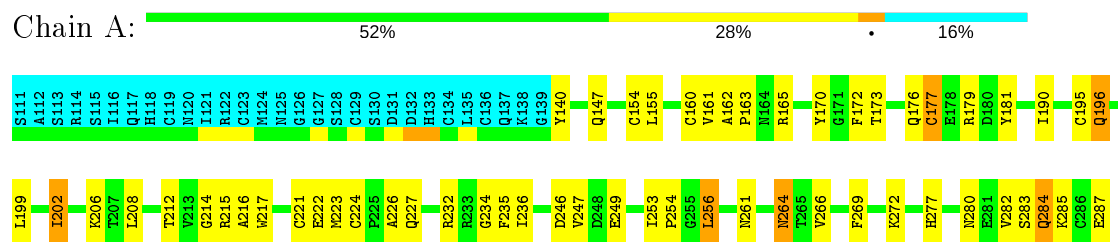
#### 4.2.1 Score per residue for model 1 (medoid)

- Molecule 1: Fibrillin-1



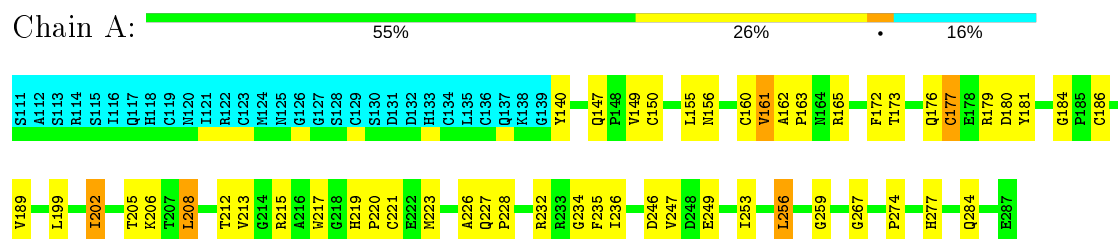
#### 4.2.2 Score per residue for model 2

- Molecule 1: Fibrillin-1



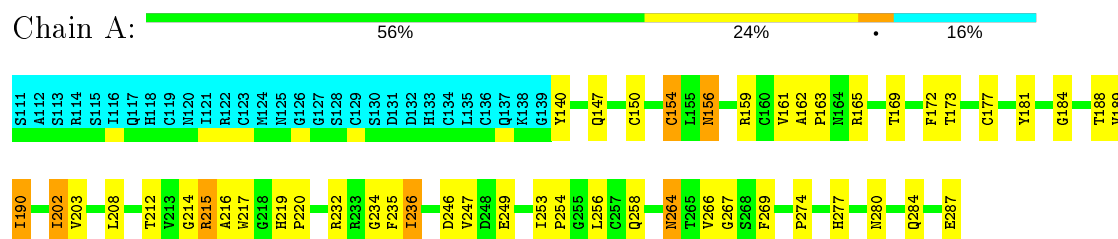
### 4.2.3 Score per residue for model 3

- Molecule 1: Fibrillin-1



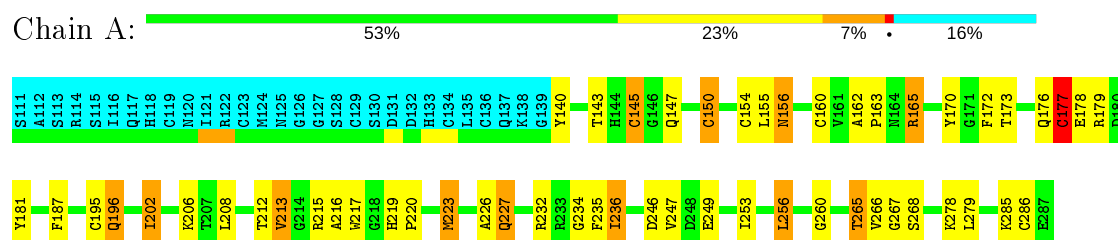
### 4.2.4 Score per residue for model 4

- Molecule 1: Fibrillin-1



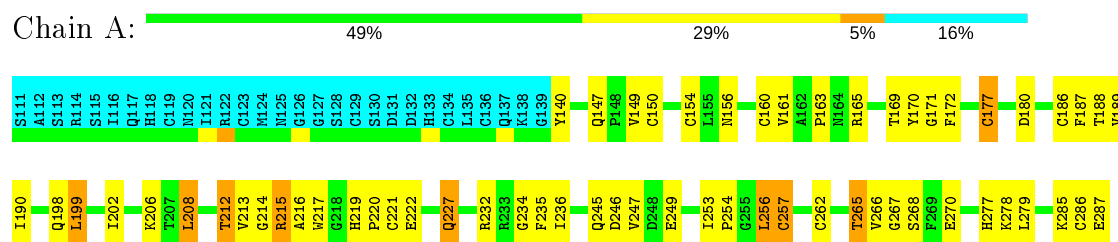
### 4.2.5 Score per residue for model 5

- Molecule 1: Fibrillin-1



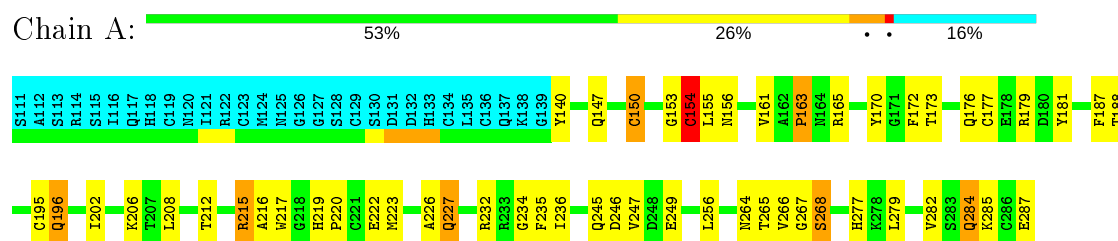
### 4.2.6 Score per residue for model 6

- Molecule 1: Fibrillin-1



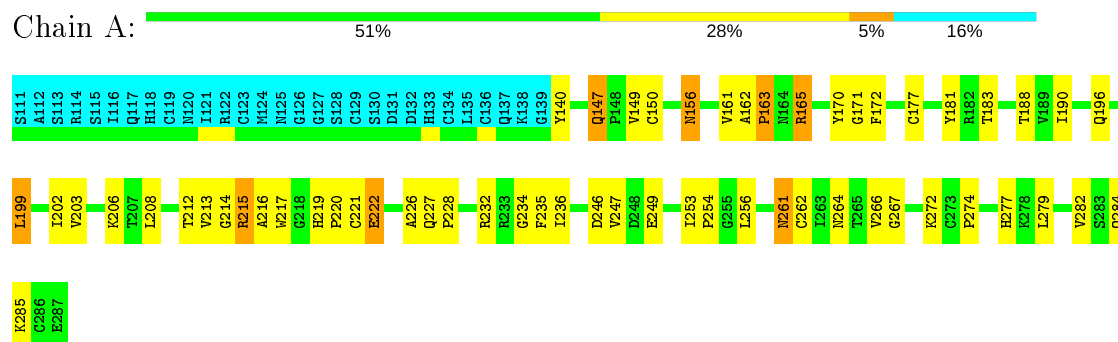
### 4.2.7 Score per residue for model 7

- Molecule 1: Fibrillin-1



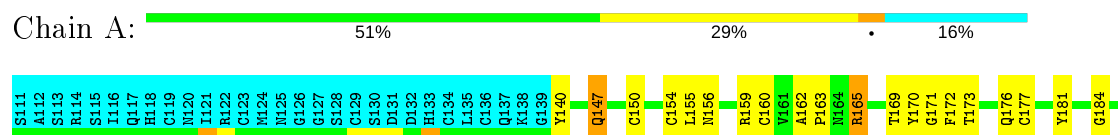
### 4.2.8 Score per residue for model 8

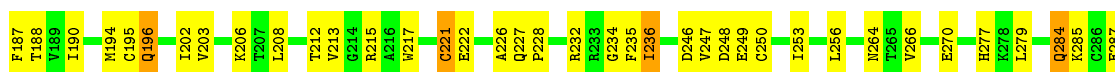
- Molecule 1: Fibrillin-1



### 4.2.9 Score per residue for model 9

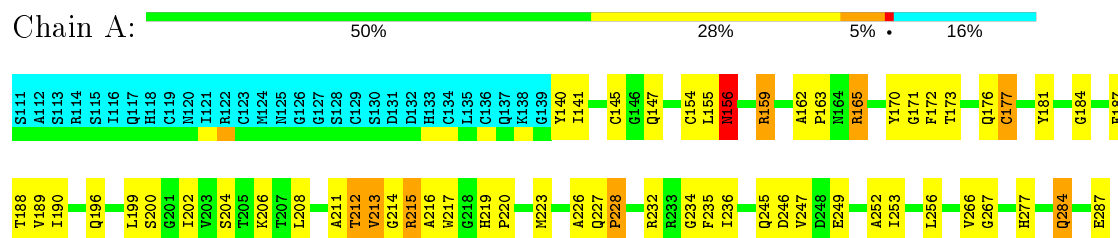
- Molecule 1: Fibrillin-1





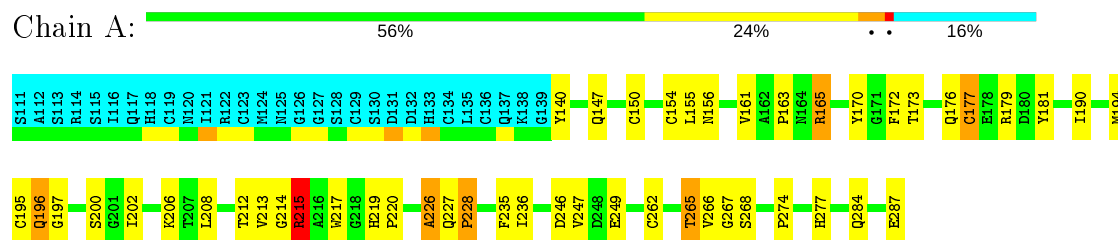
#### 4.2.10 Score per residue for model 10

- Molecule 1: Fibrillin-1



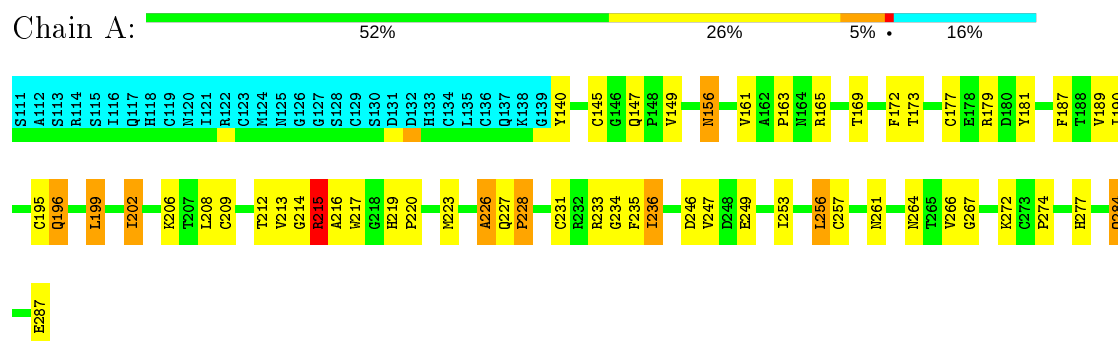
#### 4.2.11 Score per residue for model 11

- Molecule 1: Fibrillin-1



#### 4.2.12 Score per residue for model 12

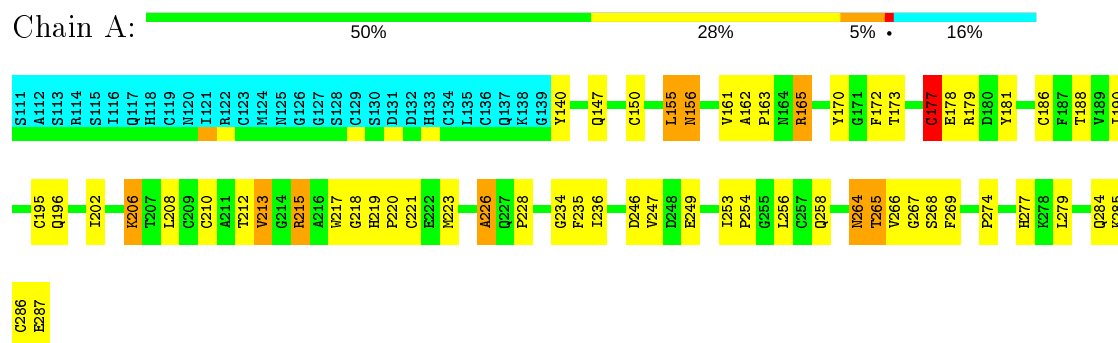
- Molecule 1: Fibrillin-1



#### 4.2.13 Score per residue for model 13

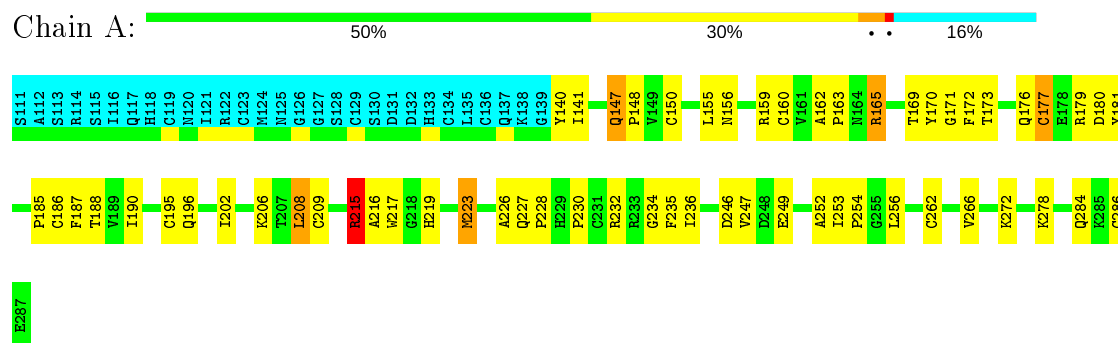
- Molecule 1: Fibrillin-1





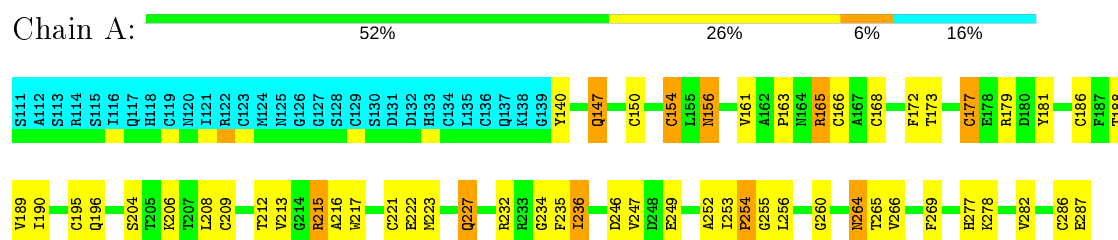
#### 4.2.14 Score per residue for model 14

- Molecule 1: Fibrillin-1



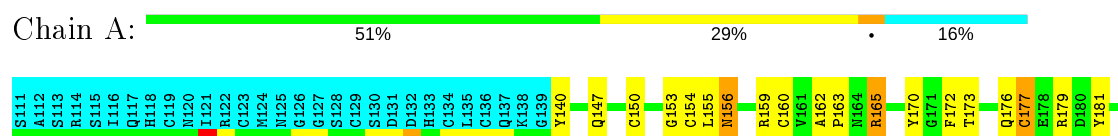
#### 4.2.15 Score per residue for model 15

- Molecule 1: Fibrillin-1



#### 4.2.16 Score per residue for model 16

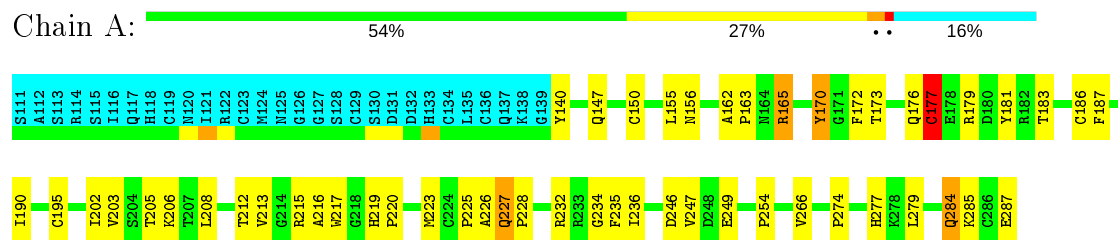
- Molecule 1: Fibrillin-1





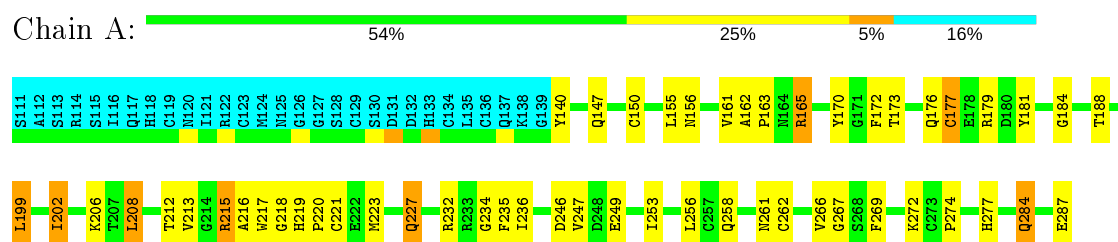
#### 4.2.17 Score per residue for model 17

- Molecule 1: Fibrillin-1



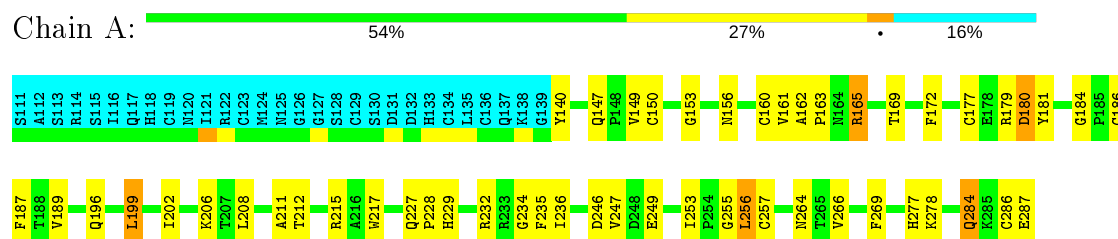
#### 4.2.18 Score per residue for model 18

- Molecule 1: Fibrillin-1



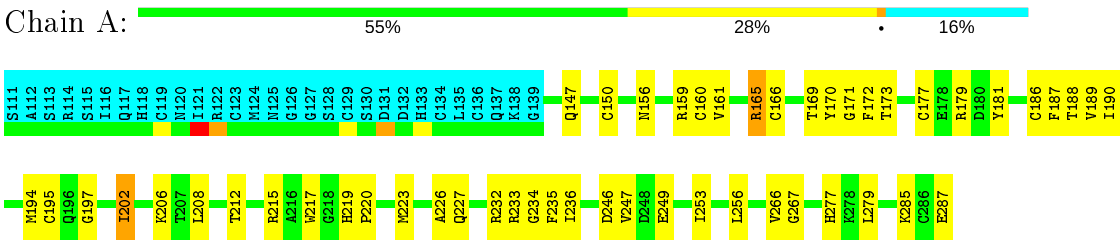
#### 4.2.19 Score per residue for model 19

- Molecule 1: Fibrillin-1



#### 4.2.20 Score per residue for model 20

- Molecule 1: Fibrillin-1



## 5 Refinement protocol and experimental data overview

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

Of the 40 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
Xplor-NIH	structure calculation	
ARIA	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)	input_cs.cif
Number of chemical shift lists	1
Total number of shifts	1759
Number of shifts mapped to atoms	1759
Number of unparsed shifts	0
Number of shifts with mapping errors	0
Number of shifts with mapping warnings	0
Assignment completeness (well-defined parts)	79%

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

## 6 Model quality

### 6.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section:  
CA

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

Chiral center outliers are detected by calculating the chiral volume of a chiral center and verifying if the center is modelled as a planar moiety or with the opposite hand. A planarity outlier is detected by checking planarity of atoms in a peptide group, atoms in a mainchain group or atoms of a sidechain that are expected to be planar.

Mol	Chain	Chirality	Planarity
1	A	0.0±0.0	0.1±0.2
All	All	0	1

There are no bond-length outliers.

There are no bond-angle outliers.

There are no chirality outliers.

All unique planar outliers are listed below.

Mol	Chain	Res	Type	Group	Models (Total)
1	A	190	ILE	Peptide	1

### 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	1085	1013	1013	36±4
All	All	21720	20260	20260	717

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 17.

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

Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:206:LYS:HB3	1:A:217:TRP:CE3	0.83	2.07	12	3
1:A:173:THR:HG23	1:A:181:TYR:CE2	0.77	2.14	11	6
1:A:209:CYS:HA	1:A:215:ARG:CZ	0.75	2.11	14	1
1:A:187:PHE:O	1:A:215:ARG:HB2	0.74	1.83	14	5
1:A:173:THR:HG23	1:A:181:TYR:CE1	0.72	2.20	13	1
1:A:217:TRP:O	1:A:222:GLU:HB2	0.72	1.85	9	6
1:A:212:THR:HG22	1:A:234:GLY:HA2	0.70	1.63	7	13
1:A:247:VAL:HG23	1:A:249:GLU:HG3	0.70	1.63	13	20
1:A:235:PHE:CE2	1:A:267:GLY:HA2	0.70	2.22	20	4
1:A:156:ASN:OD1	1:A:169:THR:HB	0.70	1.87	20	6
1:A:206:LYS:HB2	1:A:217:TRP:CE3	0.70	2.22	14	16
1:A:156:ASN:HB2	1:A:172:PHE:CZ	0.67	2.24	8	9
1:A:246:ASP:CG	1:A:266:VAL:HA	0.67	2.10	13	18
1:A:195:CYS:O	1:A:196:GLN:HB2	0.67	1.89	5	6
1:A:232:ARG:HB2	1:A:235:PHE:CD2	0.67	2.24	6	8
1:A:235:PHE:CE1	1:A:266:VAL:HG12	0.66	2.26	20	1
1:A:156:ASN:HB3	1:A:172:PHE:CZ	0.66	2.24	7	6
1:A:253:ILE:HG22	1:A:256:LEU:HB3	0.66	1.67	18	11
1:A:187:PHE:O	1:A:215:ARG:HB3	0.65	1.90	10	3
1:A:264:ASN:ND2	1:A:269:PHE:HB3	0.64	2.07	4	5
1:A:190:ILE:HD11	1:A:216:ALA:HB2	0.64	1.70	8	3
1:A:161:VAL:HG22	1:A:165:ARG:HG2	0.64	1.69	1	2
1:A:156:ASN:ND2	1:A:177:CYS:HB2	0.64	2.07	11	1
1:A:208:LEU:HD11	1:A:247:VAL:HG11	0.63	1.70	10	6
1:A:155:LEU:HD12	1:A:176:GLN:O	0.63	1.94	14	12
1:A:253:ILE:O	1:A:256:LEU:HB2	0.63	1.94	3	1
1:A:186:CYS:SG	1:A:217:TRP:HD1	0.63	2.16	16	7
1:A:219:HIS:HA	1:A:220:PRO:C	0.63	2.13	6	14
1:A:162:ALA:HB3	1:A:165:ARG:HB2	0.61	1.72	14	11
1:A:150:CYS:HB3	1:A:154:CYS:SG	0.61	2.34	15	2
1:A:190:ILE:CG1	1:A:195:CYS:HA	0.61	2.26	1	2
1:A:277:HIS:HA	1:A:287:GLU:O	0.60	1.96	20	8
1:A:156:ASN:ND2	1:A:169:THR:H	0.60	1.94	12	2
1:A:156:ASN:HB2	1:A:172:PHE:CE2	0.60	2.31	3	4
1:A:186:CYS:SG	1:A:215:ARG:HD2	0.60	2.37	17	1
1:A:140:TYR:CE1	1:A:163:PRO:HD3	0.60	2.31	9	5
1:A:202:ILE:HD12	1:A:253:ILE:HA	0.59	1.73	2	1
1:A:253:ILE:O	1:A:256:LEU:HG	0.59	1.96	19	1
1:A:190:ILE:HD11	1:A:216:ALA:CB	0.59	2.27	4	7
1:A:235:PHE:HE1	1:A:267:GLY:N	0.59	1.95	11	3
1:A:172:PHE:CB	1:A:177:CYS:HA	0.59	2.28	3	3
1:A:172:PHE:HA	1:A:179:ARG:O	0.58	1.98	16	10

Continued on next page...

*Continued from previous page...*

Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:235:PHE:HE2	1:A:267:GLY:N	0.58	1.96	18	5
1:A:253:ILE:O	1:A:256:LEU:HB3	0.58	1.97	9	1
1:A:162:ALA:HB3	1:A:165:ARG:CB	0.58	2.29	14	9
1:A:140:TYR:CE2	1:A:163:PRO:HD3	0.58	2.33	2	2
1:A:140:TYR:CZ	1:A:163:PRO:HD3	0.58	2.34	13	11
1:A:199:LEU:HD13	1:A:199:LEU:H	0.58	1.58	18	1
1:A:212:THR:CG2	1:A:234:GLY:HA2	0.58	2.29	16	3
1:A:259:GLY:HA3	1:A:286:CYS:SG	0.58	2.39	16	1
1:A:187:PHE:HB2	1:A:216:ALA:HB3	0.58	1.76	12	2
1:A:172:PHE:CD1	1:A:172:PHE:N	0.57	2.73	20	2
1:A:154:CYS:O	1:A:155:LEU:HD23	0.57	1.99	1	6
1:A:173:THR:N	1:A:181:TYR:HE2	0.57	1.98	2	6
1:A:253:ILE:HB	1:A:256:LEU:CD2	0.57	2.30	6	1
1:A:256:LEU:HA	1:A:284:GLN:OE1	0.57	1.99	14	1
1:A:232:ARG:HB2	1:A:235:PHE:CD1	0.56	2.35	10	5
1:A:265:THR:HG23	1:A:268:SER:O	0.56	2.00	5	4
1:A:286:CYS:O	1:A:287:GLU:HB2	0.56	1.99	16	1
1:A:214:GLY:O	1:A:215:ARG:HD2	0.56	2.01	2	2
1:A:172:PHE:N	1:A:172:PHE:CD2	0.56	2.74	10	3
1:A:172:PHE:CE1	1:A:180:ASP:HA	0.56	2.36	3	1
1:A:181:TYR:HA	1:A:205:THR:HG21	0.56	1.78	17	2
1:A:278:LYS:O	1:A:286:CYS:HA	0.55	2.01	15	6
1:A:184:GLY:HA3	1:A:217:TRP:CZ2	0.55	2.36	19	6
1:A:212:THR:HG21	1:A:247:VAL:CG2	0.55	2.31	9	8
1:A:188:THR:HA	1:A:215:ARG:HB3	0.55	1.78	9	3
1:A:190:ILE:HG13	1:A:195:CYS:SG	0.55	2.42	13	1
1:A:173:THR:OG1	1:A:179:ARG:HG3	0.55	2.02	5	3
1:A:190:ILE:HG12	1:A:195:CYS:HA	0.55	1.79	1	7
1:A:150:CYS:HB3	1:A:153:GLY:O	0.55	2.01	7	1
1:A:181:TYR:CD1	1:A:181:TYR:O	0.55	2.60	11	9
1:A:218:GLY:O	1:A:221:CYS:HA	0.55	2.01	18	3
1:A:172:PHE:N	1:A:172:PHE:CD1	0.54	2.75	19	6
1:A:172:PHE:CD2	1:A:172:PHE:N	0.54	2.75	6	7
1:A:173:THR:N	1:A:181:TYR:HE1	0.54	2.01	7	2
1:A:187:PHE:CD2	1:A:195:CYS:HB2	0.54	2.38	9	1
1:A:188:THR:O	1:A:215:ARG:HB3	0.54	2.02	9	2
1:A:188:THR:HA	1:A:215:ARG:CB	0.52	2.35	7	6
1:A:176:GLN:O	1:A:176:GLN:HG2	0.52	2.04	3	2
1:A:232:ARG:HG3	1:A:235:PHE:CD1	0.52	2.40	15	1
1:A:172:PHE:HB3	1:A:177:CYS:HA	0.52	1.81	3	10
1:A:279:LEU:HA	1:A:285:LYS:O	0.52	2.05	20	6

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:181:TYR:CG	1:A:181:TYR:O	0.52	2.63	18	7
1:A:262:CYS:SG	1:A:269:PHE:HB2	0.52	2.45	18	1
1:A:186:CYS:SG	1:A:215:ARG:NE	0.51	2.80	14	1
1:A:277:HIS:HA	1:A:287:GLU:OXT	0.51	2.05	12	6
1:A:172:PHE:CE2	1:A:180:ASP:HA	0.51	2.41	1	1
1:A:234:GLY:O	1:A:246:ASP:HA	0.51	2.06	6	16
1:A:149:VAL:O	1:A:163:PRO:HA	0.51	2.05	12	1
1:A:232:ARG:HB3	1:A:235:PHE:CD2	0.50	2.41	9	3
1:A:283:SER:O	1:A:285:LYS:HG3	0.50	2.07	2	1
1:A:256:LEU:O	1:A:284:GLN:HB3	0.50	2.06	18	1
1:A:162:ALA:HB3	1:A:165:ARG:HB3	0.50	1.82	1	2
1:A:187:PHE:HB3	1:A:195:CYS:O	0.50	2.07	5	3
1:A:181:TYR:O	1:A:181:TYR:CG	0.50	2.65	14	5
1:A:161:VAL:HG22	1:A:165:ARG:O	0.50	2.07	8	12
1:A:149:VAL:HG13	1:A:149:VAL:O	0.50	2.07	12	2
1:A:267:GLY:O	1:A:268:SER:HB2	0.49	2.07	7	1
1:A:173:THR:O	1:A:179:ARG:HG3	0.49	2.07	14	1
1:A:215:ARG:NH2	1:A:253:ILE:HG13	0.49	2.22	14	1
1:A:274:PRO:O	1:A:277:HIS:HB2	0.49	2.07	18	9
1:A:253:ILE:CG2	1:A:256:LEU:HB3	0.49	2.38	13	8
1:A:280:ASN:OD1	1:A:282:VAL:HB	0.49	2.08	2	1
1:A:257:CYS:HA	1:A:284:GLN:O	0.49	2.08	19	1
1:A:235:PHE:CE1	1:A:267:GLY:N	0.49	2.81	11	3
1:A:172:PHE:HB2	1:A:177:CYS:HB3	0.49	1.82	11	2
1:A:246:ASP:CB	1:A:266:VAL:HA	0.49	2.38	4	3
1:A:188:THR:C	1:A:215:ARG:HG2	0.49	2.28	15	1
1:A:156:ASN:ND2	1:A:168:CYS:HA	0.49	2.22	15	1
1:A:223:MET:O	1:A:225:PRO:HD3	0.48	2.08	17	1
1:A:211:ALA:HB2	1:A:229:HIS:CE1	0.48	2.43	19	1
1:A:256:LEU:O	1:A:284:GLN:HB2	0.48	2.08	2	1
1:A:246:ASP:HB3	1:A:266:VAL:HG13	0.48	1.84	20	1
1:A:156:ASN:HB2	1:A:172:PHE:CE1	0.48	2.44	19	3
1:A:277:HIS:ND1	1:A:287:GLU:HA	0.48	2.23	18	3
1:A:170:TYR:CG	1:A:171:GLY:N	0.48	2.81	6	2
1:A:155:LEU:C	1:A:156:ASN:HD22	0.48	2.12	1	1
1:A:173:THR:O	1:A:179:ARG:HD2	0.48	2.08	2	1
1:A:208:LEU:CD1	1:A:247:VAL:HG11	0.48	2.39	6	4
1:A:140:TYR:CE2	1:A:148:PRO:HB3	0.48	2.43	14	1
1:A:188:THR:HA	1:A:215:ARG:HB2	0.48	1.85	14	1
1:A:210:CYS:O	1:A:226:ALA:HA	0.48	2.07	1	2
1:A:187:PHE:CD1	1:A:195:CYS:HB2	0.48	2.43	12	1

*Continued on next page...*



*Continued from previous page...*

Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:232:ARG:HB2	1:A:235:PHE:CE2	0.48	2.43	20	1
1:A:202:ILE:HD11	1:A:253:ILE:HG23	0.48	1.85	18	7
1:A:178:GLU:O	1:A:179:ARG:HD3	0.48	2.09	5	2
1:A:257:CYS:HA	1:A:284:GLN:HB3	0.47	1.85	12	1
1:A:155:LEU:HB2	1:A:177:CYS:O	0.47	2.09	13	1
1:A:181:TYR:O	1:A:181:TYR:CD1	0.47	2.67	8	4
1:A:199:LEU:HD13	1:A:199:LEU:N	0.47	2.23	16	2
1:A:190:ILE:HD12	1:A:216:ALA:CB	0.47	2.39	1	1
1:A:140:TYR:HB2	1:A:145:CYS:SG	0.47	2.49	5	1
1:A:172:PHE:CB	1:A:177:CYS:HB3	0.47	2.40	11	4
1:A:140:TYR:HA	1:A:147:GLN:O	0.47	2.10	8	1
1:A:235:PHE:HA	1:A:245:GLN:O	0.47	2.10	7	4
1:A:188:THR:O	1:A:215:ARG:HG2	0.47	2.10	4	2
1:A:204:SER:OG	1:A:208:LEU:HD23	0.47	2.10	10	1
1:A:261:ASN:HB3	1:A:272:LYS:CG	0.47	2.40	18	1
1:A:188:THR:O	1:A:215:ARG:HD2	0.46	2.10	1	2
1:A:247:VAL:CG2	1:A:249:GLU:HG3	0.46	2.38	13	2
1:A:232:ARG:HG3	1:A:235:PHE:CE1	0.46	2.45	15	1
1:A:202:ILE:CD1	1:A:253:ILE:HA	0.46	2.40	2	2
1:A:155:LEU:HD13	1:A:178:GLU:HB3	0.46	1.86	13	1
1:A:214:GLY:O	1:A:215:ARG:HD3	0.46	2.11	11	3
1:A:209:CYS:HA	1:A:215:ARG:NH1	0.46	2.26	14	1
1:A:156:ASN:HD21	1:A:168:CYS:HA	0.46	1.69	15	1
1:A:216:ALA:CB	1:A:223:MET:HA	0.46	2.41	5	7
1:A:194:MET:SD	1:A:197:GLY:HA2	0.46	2.51	11	2
1:A:226:ALA:O	1:A:228:PRO:HD3	0.46	2.10	12	2
1:A:257:CYS:SG	1:A:262:CYS:HB3	0.46	2.51	6	1
1:A:212:THR:HG21	1:A:247:VAL:HG21	0.46	1.88	7	2
1:A:181:TYR:O	1:A:181:TYR:CD2	0.46	2.69	19	3
1:A:235:PHE:CE1	1:A:246:ASP:HB2	0.46	2.45	10	2
1:A:181:TYR:HA	1:A:205:THR:CG2	0.45	2.41	3	1
1:A:208:LEU:HD21	1:A:252:ALA:HB1	0.45	1.88	15	2
1:A:202:ILE:HG13	1:A:254:PRO:HD2	0.45	1.88	2	1
1:A:156:ASN:CB	1:A:172:PHE:CE2	0.45	3.00	3	1
1:A:247:VAL:HG23	1:A:249:GLU:CG	0.45	2.40	13	9
1:A:141:ILE:O	1:A:145:CYS:HA	0.45	2.11	10	1
1:A:149:VAL:O	1:A:149:VAL:HG13	0.45	2.12	6	3
1:A:199:LEU:N	1:A:199:LEU:HD13	0.45	2.27	19	2
1:A:159:ARG:O	1:A:166:CYS:HA	0.45	2.12	20	1
1:A:253:ILE:O	1:A:255:GLY:N	0.45	2.50	15	1
1:A:235:PHE:C	1:A:236:ILE:HD13	0.45	2.32	5	3

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:212:THR:O	1:A:214:GLY:N	0.44	2.51	6	4
1:A:188:THR:HA	1:A:215:ARG:CG	0.44	2.42	10	1
1:A:156:ASN:HD21	1:A:169:THR:H	0.44	1.54	12	1
1:A:204:SER:HB3	1:A:209:CYS:SG	0.44	2.53	15	1
1:A:156:ASN:HB3	1:A:172:PHE:CE2	0.44	2.46	4	1
1:A:170:TYR:CD2	1:A:171:GLY:N	0.44	2.86	8	2
1:A:214:GLY:O	1:A:215:ARG:HB2	0.44	2.12	4	2
1:A:235:PHE:CE2	1:A:246:ASP:HB2	0.44	2.48	5	3
1:A:211:ALA:HA	1:A:228:PRO:CD	0.44	2.43	10	1
1:A:156:ASN:ND2	1:A:177:CYS:CB	0.44	2.80	11	1
1:A:279:LEU:HD12	1:A:285:LYS:O	0.44	2.13	5	3
1:A:280:ASN:O	1:A:284:GLN:N	0.44	2.50	4	1
1:A:156:ASN:C	1:A:156:ASN:HD22	0.44	2.15	5	1
1:A:162:ALA:HB1	1:A:163:PRO:HD2	0.44	1.90	8	1
1:A:181:TYR:CD2	1:A:181:TYR:O	0.44	2.71	10	1
1:A:190:ILE:HD11	1:A:216:ALA:HB3	0.44	1.88	14	3
1:A:261:ASN:HB2	1:A:272:LYS:HB3	0.43	1.88	12	2
1:A:235:PHE:O	1:A:236:ILE:HD13	0.43	2.13	12	2
1:A:249:GLU:O	1:A:256:LEU:HG	0.43	2.13	6	1
1:A:235:PHE:CZ	1:A:266:VAL:HB	0.43	2.48	1	1
1:A:147:GLN:C	1:A:147:GLN:HE21	0.43	2.17	9	2
1:A:235:PHE:CE2	1:A:267:GLY:N	0.43	2.87	1	4
1:A:190:ILE:HD13	1:A:221:CYS:SG	0.43	2.54	6	1
1:A:183:THR:HB	1:A:203:VAL:HG13	0.43	1.90	8	1
1:A:170:TYR:HE2	1:A:183:THR:HG1	0.43	1.56	17	1
1:A:216:ALA:HA	1:A:222:GLU:O	0.43	2.12	8	1
1:A:213:VAL:HG21	1:A:256:LEU:CD1	0.43	2.44	5	1
1:A:235:PHE:HE2	1:A:267:GLY:CA	0.43	2.27	16	1
1:A:235:PHE:CE2	1:A:267:GLY:CA	0.42	3.03	8	1
1:A:259:GLY:O	1:A:274:PRO:HD3	0.42	2.14	3	1
1:A:261:ASN:OD1	1:A:272:LYS:HE2	0.42	2.14	2	1
1:A:170:TYR:CD1	1:A:171:GLY:N	0.42	2.87	14	3
1:A:256:LEU:HD13	1:A:269:PHE:CZ	0.42	2.49	19	1
1:A:249:GLU:HB2	1:A:264:ASN:HD21	0.42	1.74	13	1
1:A:189:VAL:O	1:A:195:CYS:HA	0.42	2.15	12	1
1:A:253:ILE:HG21	1:A:256:LEU:HD13	0.42	1.92	14	1
1:A:202:ILE:O	1:A:202:ILE:HG23	0.42	2.15	19	1
1:A:184:GLY:CA	1:A:217:TRP:CZ2	0.42	3.03	19	1
1:A:253:ILE:C	1:A:255:GLY:H	0.42	2.18	19	1
1:A:190:ILE:CG1	1:A:221:CYS:SG	0.42	3.08	9	1
1:A:156:ASN:ND2	1:A:177:CYS:SG	0.42	2.93	13	1

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:186:CYS:SG	1:A:217:TRP:CD1	0.42	3.10	15	1
1:A:173:THR:CG2	1:A:181:TYR:CE2	0.42	3.03	5	4
1:A:261:ASN:HD22	1:A:262:CYS:N	0.42	2.13	8	1
1:A:179:ARG:O	1:A:180:ASP:HB3	0.42	2.15	19	1
1:A:248:ASP:OD1	1:A:250:CYS:HB2	0.42	2.15	9	1
1:A:225:PRO:O	1:A:227:GLN:N	0.41	2.52	17	1
1:A:233:ARG:HG3	1:A:234:GLY:N	0.41	2.30	20	1
1:A:265:THR:CG2	1:A:270:GLU:HG3	0.41	2.45	6	1
1:A:213:VAL:HG11	1:A:284:GLN:HE21	0.41	1.74	10	1
1:A:185:PRO:HG2	1:A:219:HIS:CE1	0.41	2.50	14	1
1:A:212:THR:HG22	1:A:233:ARG:O	0.41	2.15	12	1
1:A:248:ASP:OD2	1:A:250:CYS:HB2	0.41	2.15	1	1
1:A:154:CYS:SG	1:A:160:CYS:SG	0.41	3.18	6	2
1:A:159:ARG:HG2	1:A:159:ARG:O	0.41	2.15	10	1
1:A:173:THR:O	1:A:179:ARG:HG2	0.41	2.16	20	3
1:A:252:ALA:C	1:A:253:ILE:HD12	0.41	2.36	14	1
1:A:188:THR:HB	1:A:282:VAL:O	0.41	2.16	8	1
1:A:141:ILE:HG12	1:A:147:GLN:O	0.41	2.15	14	1
1:A:188:THR:HG23	1:A:215:ARG:HE	0.41	1.74	6	1
1:A:253:ILE:HG22	1:A:256:LEU:HB2	0.41	1.93	9	1
1:A:258:GLN:O	1:A:286:CYS:HB3	0.41	2.16	13	1
1:A:173:THR:HG22	1:A:181:TYR:CE2	0.40	2.51	2	1
1:A:198:GLN:O	1:A:199:LEU:HB2	0.40	2.17	6	1
1:A:215:ARG:NH1	1:A:282:VAL:HA	0.40	2.31	7	1
1:A:170:TYR:HD2	1:A:171:GLY:N	0.40	2.14	9	1
1:A:215:ARG:NH2	1:A:282:VAL:HA	0.40	2.31	15	1
1:A:216:ALA:HB2	1:A:223:MET:HA	0.40	1.93	14	1
1:A:235:PHE:CZ	1:A:246:ASP:HB2	0.40	2.51	11	1
1:A:261:ASN:HB3	1:A:272:LYS:HG3	0.40	1.94	18	1
1:A:176:GLN:HG2	1:A:176:GLN:O	0.40	2.16	9	1
1:A:194:MET:HG3	1:A:196:GLN:H	0.40	1.76	9	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	147/177 (83%)	117±2 (80±2%)	22±3 (15±2%)	7±2 (5±1%)	4	25
All	All	2940/3540 (83%)	2346 (80%)	448 (15%)	146 (5%)	4	25

All 30 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	226	ALA	14
1	A	196	GLN	13
1	A	213	VAL	12
1	A	228	PRO	12
1	A	284	GLN	12
1	A	170	TYR	9
1	A	215	ARG	8
1	A	254	PRO	8
1	A	189	VAL	7
1	A	227	GLN	6
1	A	221	CYS	6
1	A	177	CYS	5
1	A	199	LEU	3
1	A	200	SER	3
1	A	180	ASP	3
1	A	163	PRO	3
1	A	154	CYS	3
1	A	156	ASN	2
1	A	260	GLY	2
1	A	212	THR	2
1	A	256	LEU	2
1	A	258	GLN	2
1	A	153	GLY	2
1	A	202	ILE	1
1	A	230	PRO	1
1	A	268	SER	1
1	A	222	GLU	1
1	A	155	LEU	1
1	A	257	CYS	1
1	A	231	CYS	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	121/146 (83%)	109±2 (90±2%)	12±2 (10±2%)	12	57
All	All	2420/2920 (83%)	2186 (90%)	234 (10%)	12	57

All 32 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	236	ILE	20
1	A	147	GLN	20
1	A	177	CYS	19
1	A	202	ILE	17
1	A	227	GLN	17
1	A	208	LEU	16
1	A	150	CYS	15
1	A	165	ARG	13
1	A	264	ASN	11
1	A	156	ASN	9
1	A	223	MET	9
1	A	160	CYS	8
1	A	215	ARG	7
1	A	256	LEU	7
1	A	199	LEU	6
1	A	265	THR	6
1	A	159	ARG	5
1	A	284	GLN	5
1	A	213	VAL	3
1	A	203	VAL	3
1	A	262	CYS	3
1	A	154	CYS	3
1	A	145	CYS	2
1	A	272	LYS	2
1	A	209	CYS	1
1	A	224	CYS	1
1	A	261	ASN	1
1	A	166	CYS	1
1	A	254	PRO	1
1	A	270	GLU	1
1	A	161	VAL	1
1	A	206	LYS	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 carbohydrates in this entry.

## 6.6 Ligand geometry [i](#)

Of 1 ligands modelled in this entry, 1 is monoatomic - leaving 0 for Mogul analysis.

## 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 79% for the well-defined parts and 80% for the entire structure.

### 7.1 Chemical shift list 1

File name: input\_cs.cif

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	1759
Number of shifts mapped to atoms	1759
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

The following table shows the suggested chemical shift referencing corrections.

Nucleus	# values	Correction $\pm$ precision, ppm	Suggested action
$^{13}\text{C}_\alpha$	168	$0.26 \pm 0.12$	None needed ( $< 0.5$ ppm)
$^{13}\text{C}_\beta$	145	$0.10 \pm 0.09$	None needed ( $< 0.5$ ppm)
$^{13}\text{C}'$	164	$0.10 \pm 0.15$	None needed ( $< 0.5$ ppm)
$^{15}\text{N}$	154	$0.11 \pm 0.37$	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 79%, i.e. 1324 atoms were assigned a chemical shift out of a possible 1668. 0 out of 13 assigned methyl groups (LEU and VAL) were assigned stereospecifically.

	Total	$^1\text{H}$	$^{13}\text{C}$	$^{15}\text{N}$
Backbone	663/718 (92%)	263/285 (92%)	274/296 (93%)	126/137 (92%)
Sidechain	600/850 (71%)	369/508 (73%)	219/297 (74%)	12/45 (27%)

*Continued on next page...*

*Continued from previous page...*

	<b>Total</b>	<b><sup>1</sup>H</b>	<b><sup>13</sup>C</b>	<b><sup>15</sup>N</b>
Aromatic	61/100 (61%)	41/54 (76%)	19/41 (46%)	1/5 (20%)
Overall	1324/1668 (79%)	673/847 (79%)	512/634 (81%)	139/187 (74%)

The following table shows the completeness of the chemical shift assignments for the full structure. The overall completeness is 80%, i.e. 1585 atoms were assigned a chemical shift out of a possible 1991. 0 out of 14 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	805/863 (93%)	319/343 (93%)	332/354 (94%)	154/166 (93%)
Sidechain	718/1014 (71%)	441/607 (73%)	262/351 (75%)	15/56 (27%)
Aromatic	62/114 (54%)	42/62 (68%)	19/45 (42%)	1/7 (14%)
Overall	1585/1991 (80%)	802/1012 (79%)	613/750 (82%)	170/229 (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	206	LYS	HB3	-0.90	3.10 – 0.40	-9.8
1	A	206	LYS	HA	1.98	6.46 – 2.06	-5.2

#### 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:



