



Full wwPDB NMR Structure Validation Report ⓘ

May 28, 2020 – 11:00 pm BST

PDB ID : 2LCW
Title : solution structure of FUS/TLS RRM domain
Authors : Liu, X.; Ren, J.; Niu, C.; Gong, W.; Feng, W.
Deposited on : 2011-05-10

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 ⓘ 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

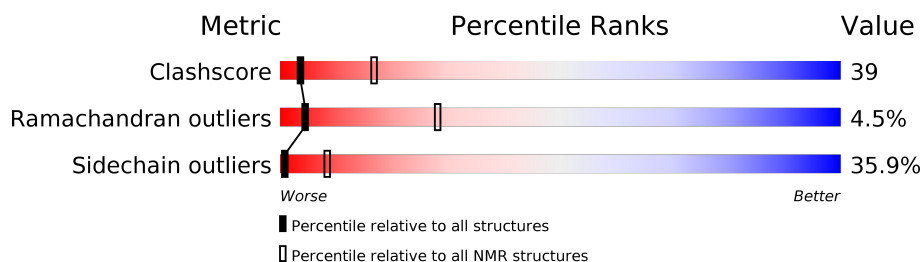
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

SOLUTION NMR

The overall completeness of chemical shifts assignment is 95%.

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 $\leq 5\%$

Mol	Chain	Length	Quality of chain
1	A	116	<div> <div></div> <div>20%</div> <div></div> <div>34%</div> <div></div> <div>12%</div> <div></div> <div>28%</div> <div></div> <div>7%</div> </div>

2 Ensemble composition and analysis

This entry contains 20 models. Model 17 is the overall representative, medoid model (most similar to other models). The authors have identified model 1 as representative, based on the following criterion: *closest to the average*.

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:284-A:325, A:335-A:368 (76)	0.33	17

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

3 Entry composition

There is only 1 type of molecule in this entry. The entry contains 1626 atoms, of which 799 are hydrogens and 0 are deuteriums.

- Molecule 1 is a protein called RNA-binding protein FUS.

Mol	Chain	Residues	Atoms						Trace
1	A	108	Total	C	H	N	O	S	0
			1626	513	799	146	167	1	

There are 8 discrepancies between the modelled and reference sequences:

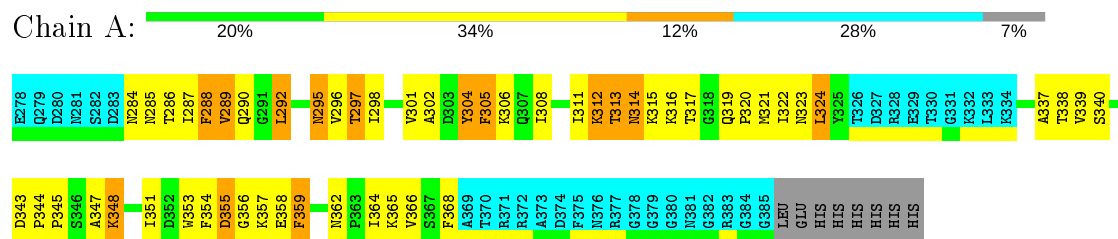
Chain	Residue	Modelled	Actual	Comment	Reference
A	386	LEU	-	EXPRESSION TAG	UNP P35637
A	387	GLU	-	EXPRESSION TAG	UNP P35637
A	388	HIS	-	EXPRESSION TAG	UNP P35637
A	389	HIS	-	EXPRESSION TAG	UNP P35637
A	390	HIS	-	EXPRESSION TAG	UNP P35637
A	391	HIS	-	EXPRESSION TAG	UNP P35637
A	392	HIS	-	EXPRESSION TAG	UNP P35637
A	393	HIS	-	EXPRESSION TAG	UNP P35637

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: RNA-binding protein FUS

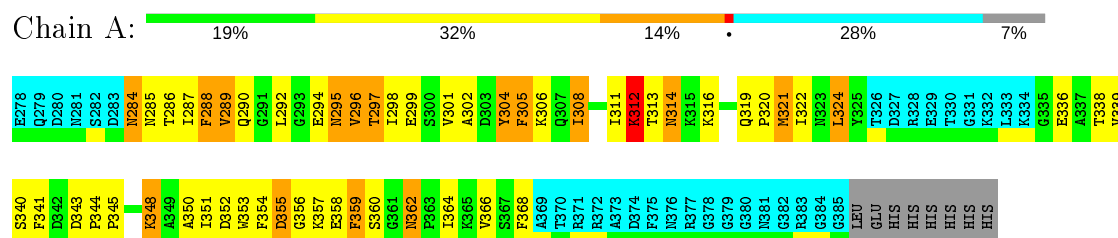


4.2 Scores per residue for each member of the ensemble

Colouring as in section 4.1 above.

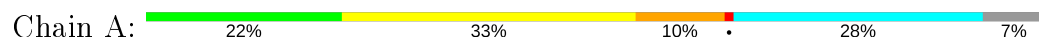
4.2.1 Score per residue for model 1

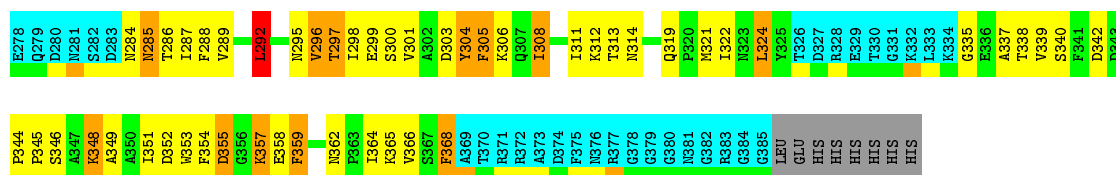
- Molecule 1: RNA-binding protein FUS



4.2.2 Score per residue for model 2

- Molecule 1: RNA-binding protein FUS

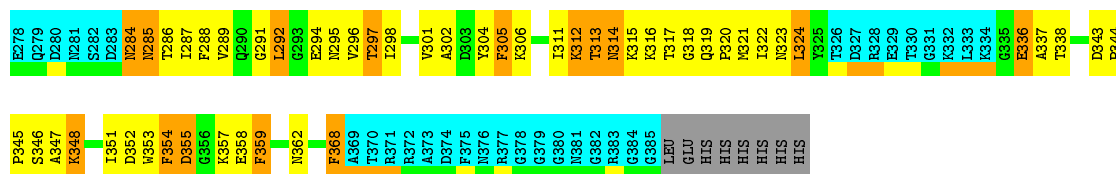




4.2.3 Score per residue for model 3

- Molecule 1: RNA-binding protein FUS

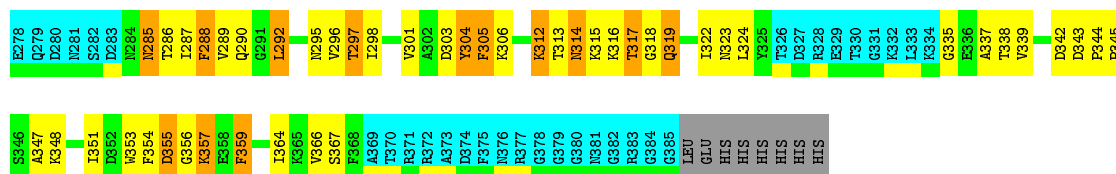
Chain A: 22% 31% 13% 28% 7%



4.2.4 Score per residue for model 4

- Molecule 1: RNA-binding protein FUS

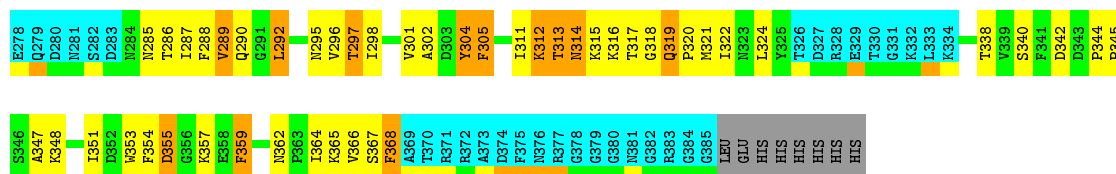
Chain A: 25% 29% 11% 28% 7%



4.2.5 Score per residue for model 5

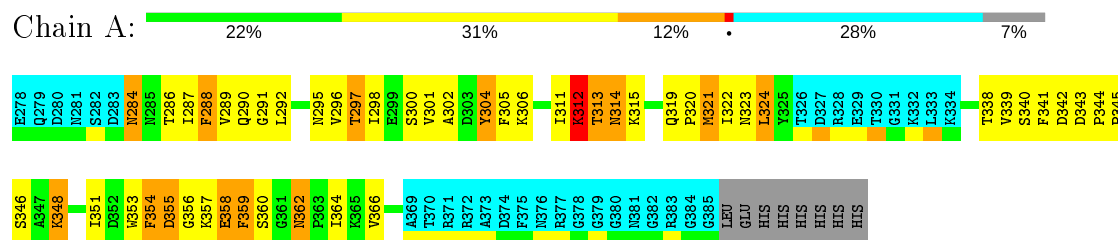
- Molecule 1: RNA-binding protein FUS

Chain A: 25% 30% 10% 28% 7%



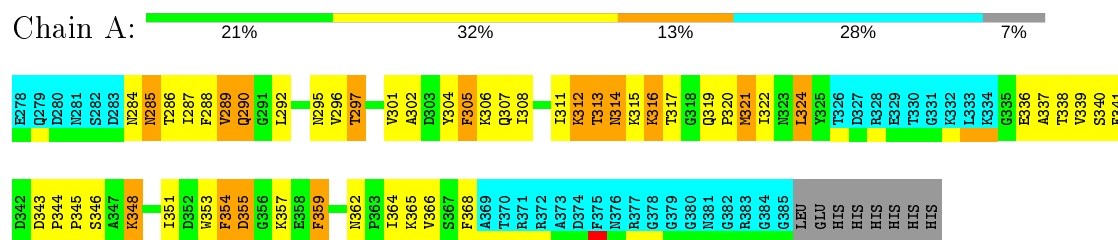
4.2.6 Score per residue for model 6

- Molecule 1: RNA-binding protein FUS



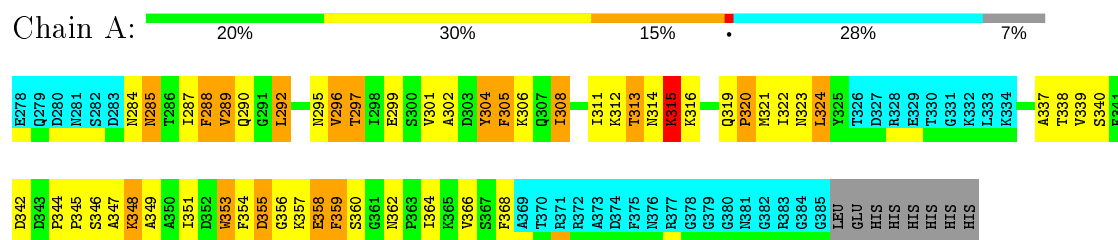
4.2.7 Score per residue for model 7

- Molecule 1: RNA-binding protein FUS



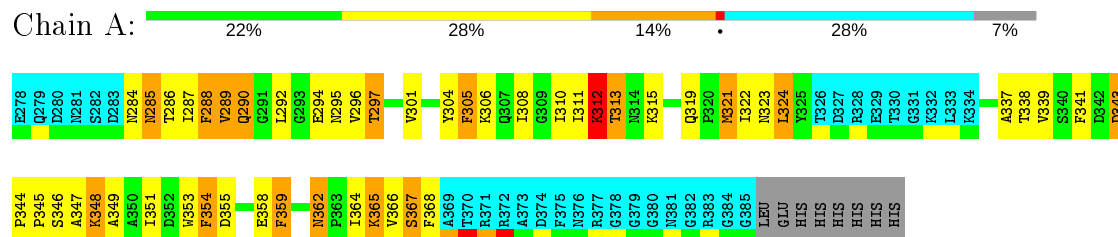
4.2.8 Score per residue for model 8

- Molecule 1: RNA-binding protein FUS



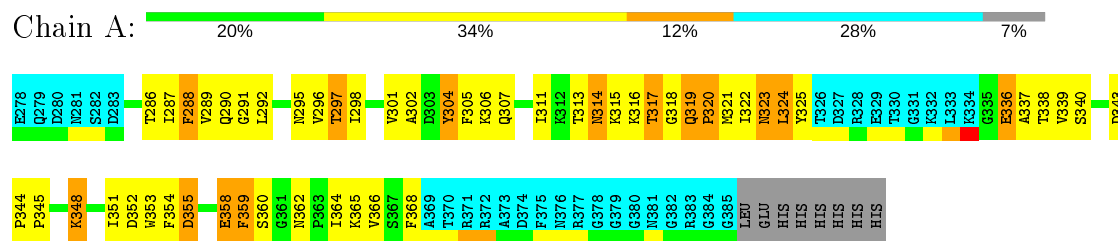
4.2.9 Score per residue for model 9

- Molecule 1: RNA-binding protein FUS



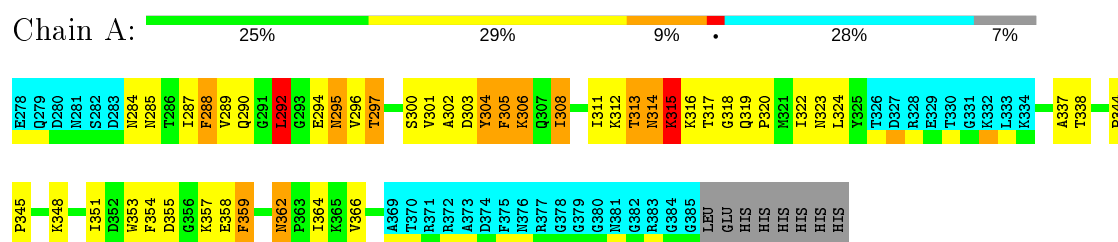
4.2.10 Score per residue for model 10

- Molecule 1: RNA-binding protein FUS



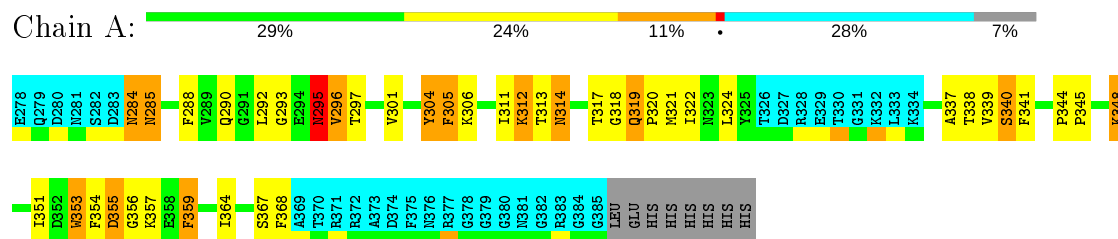
4.2.11 Score per residue for model 11

- Molecule 1: RNA-binding protein FUS



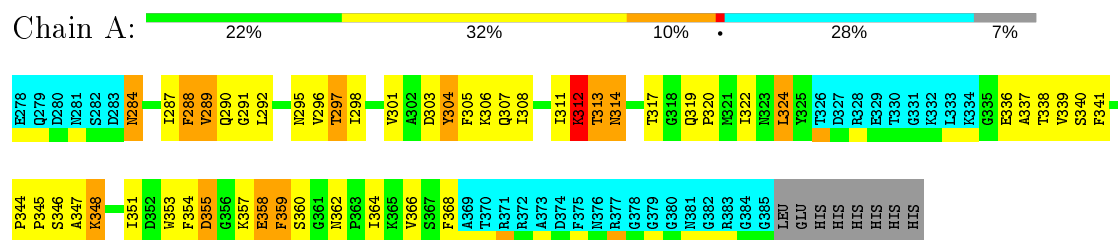
4.2.12 Score per residue for model 12

- Molecule 1: RNA-binding protein FUS



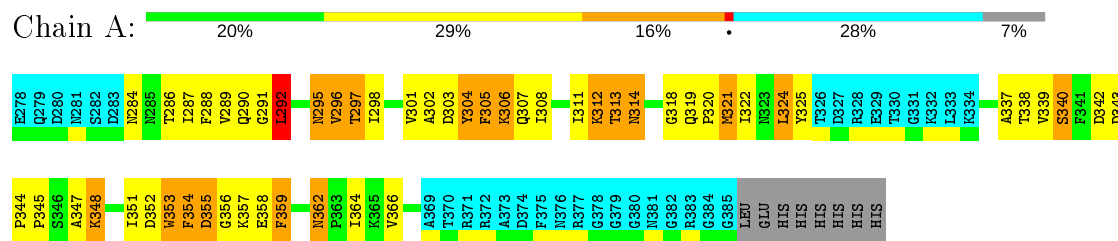
4.2.13 Score per residue for model 13

- Molecule 1: RNA-binding protein FUS



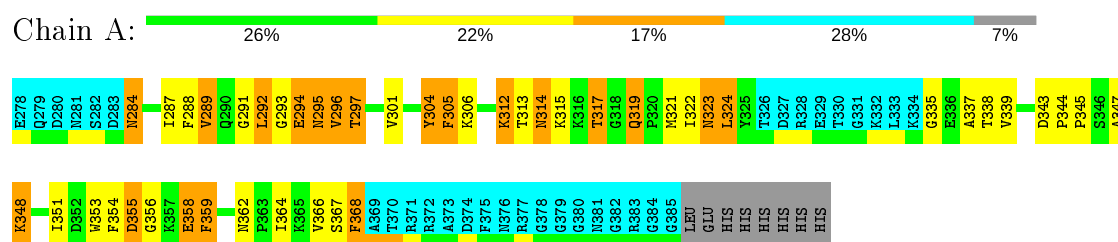
4.2.14 Score per residue for model 14

- Molecule 1: RNA-binding protein FUS



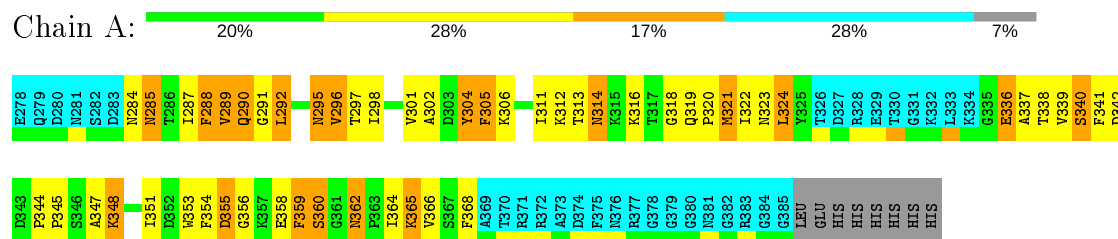
4.2.15 Score per residue for model 15

- Molecule 1: RNA-binding protein FUS



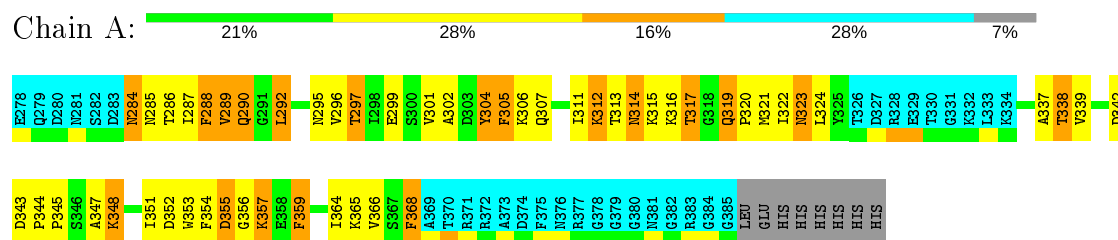
4.2.16 Score per residue for model 16

- Molecule 1: RNA-binding protein FUS



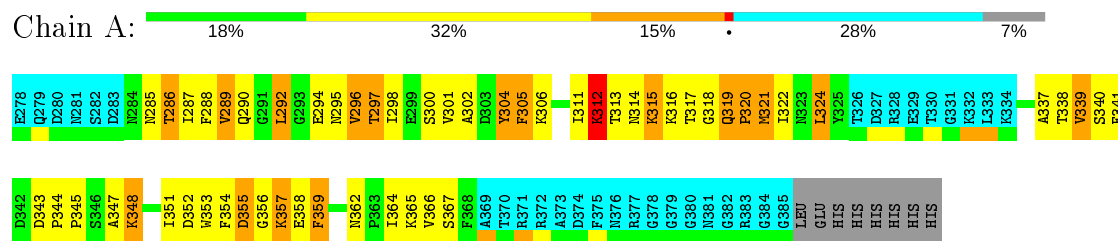
4.2.17 Score per residue for model 17 (medoid)

- Molecule 1: RNA-binding protein FUS



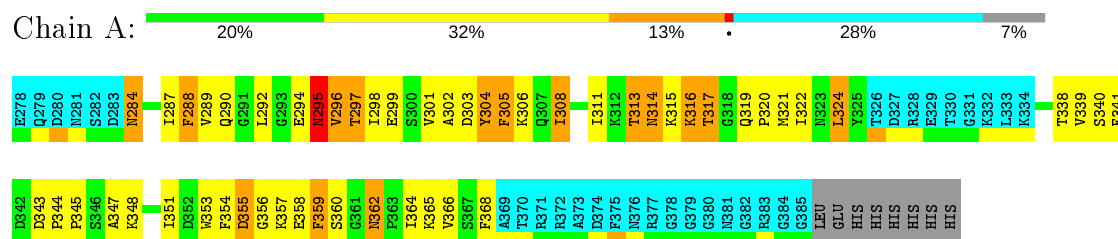
4.2.18 Score per residue for model 18

- Molecule 1: RNA-binding protein FUS



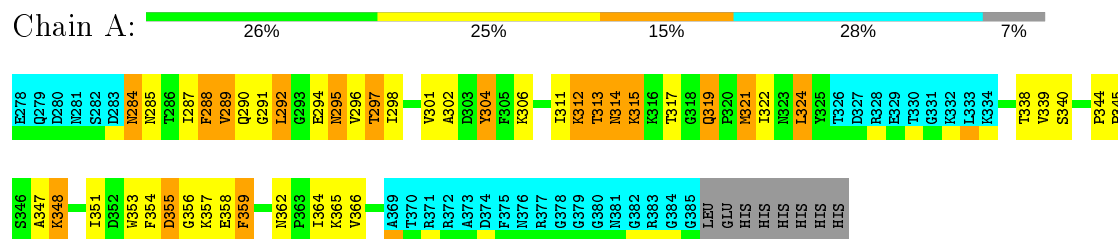
4.2.19 Score per residue for model 19

- Molecule 1: RNA-binding protein FUS



4.2.20 Score per residue for model 20

- Molecule 1: RNA-binding protein FUS



5 Refinement protocol and experimental data overview

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

Of the 400 calculated structures, 20 were deposited, based on the following criterion: *structures with the lowest energy and the least restraint violations*.

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

Software name	Classification	Version
CNS	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	1220
Number of shifts mapped to atoms	1220
Number of unparsed shifts	0
Number of shifts with mapping errors	0
Number of shifts with mapping warnings	0
Assignment completeness (well-defined parts)	95%

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

6 Model quality ⓘ

6.1 Standard geometry ⓘ

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

There are no bond-length outliers.

There are no bond-angle outliers.

There are no chirality outliers.

There are no planarity outliers.

6.2 Too-close contacts ⓘ

In the following table, the Non-H and H(model) columns list the number of non-hydrogen atoms and hydrogen atoms in each chain respectively. The H(added) column lists the number of hydrogen atoms added and optimized by MolProbity. The Clashes column lists the number of clashes averaged over the ensemble.

Mol	Chain	Non-H	H(model)	H(added)	Clashes
1	A	587	575	575	46±7
All	All	11740	11500	11500	910

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 39.

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

Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:296:VAL:HG22	1:A:324:LEU:HD23	1.05	1.24	10	1
1:A:296:VAL:HG12	1:A:324:LEU:HD23	0.91	1.35	3	1
1:A:287:ILE:HD12	1:A:366:VAL:HG13	0.84	1.48	7	12
1:A:297:THR:O	1:A:301:VAL:HG23	0.80	1.76	9	20
1:A:311:ILE:HG23	1:A:340:SER:O	0.79	1.78	16	12
1:A:289:VAL:HG13	1:A:366:VAL:HG22	0.79	1.54	13	8
1:A:316:LYS:HD3	1:A:317:THR:HG23	0.79	1.53	7	1
1:A:348:LYS:HA	1:A:351:ILE:HD12	0.78	1.56	3	20
1:A:305:PHE:CD2	1:A:339:VAL:HG21	0.78	2.14	18	2
1:A:292:LEU:HD12	1:A:295:ASN:ND2	0.78	1.94	12	1
1:A:296:VAL:HG12	1:A:324:LEU:HD22	0.75	1.56	6	2
1:A:292:LEU:HD21	1:A:359:PHE:CE2	0.75	2.16	13	1
1:A:301:VAL:HG11	1:A:339:VAL:CG2	0.75	2.12	1	9
1:A:285:ASN:O	1:A:347:ALA:HB2	0.75	1.82	18	5

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:298:ILE:HD11	1:A:324:LEU:HD11	0.75	1.56	3	4
1:A:296:VAL:O	1:A:324:LEU:HD13	0.75	1.82	4	3
1:A:287:ILE:HD12	1:A:366:VAL:CG1	0.74	2.12	5	10
1:A:291:GLY:C	1:A:292:LEU:HD13	0.74	2.02	3	2
1:A:287:ILE:HD11	1:A:305:PHE:CE2	0.73	2.18	2	3
1:A:291:GLY:O	1:A:364:ILE:HG22	0.73	1.83	10	6
1:A:322:ILE:HG23	1:A:338:THR:O	0.73	1.83	4	10
1:A:314:ASN:ND2	1:A:317:THR:OG1	0.72	2.23	12	2
1:A:292:LEU:HD21	1:A:336:GLU:HA	0.72	1.59	3	1
1:A:298:ILE:CD1	1:A:324:LEU:HD11	0.72	2.15	1	4
1:A:292:LEU:HD12	1:A:296:VAL:HG22	0.72	1.60	6	3
1:A:305:PHE:O	1:A:311:ILE:HD11	0.70	1.85	17	4
1:A:324:LEU:HD23	1:A:337:ALA:CB	0.70	2.16	18	4
1:A:292:LEU:HD22	1:A:359:PHE:CD2	0.70	2.20	15	3
1:A:358:GLU:HA	1:A:362:ASN:O	0.69	1.87	10	15
1:A:296:VAL:O	1:A:296:VAL:HG12	0.69	1.85	19	2
1:A:288:PHE:CE1	1:A:338:THR:HG22	0.68	2.23	16	6
1:A:287:ILE:HD12	1:A:366:VAL:HG11	0.68	1.64	18	2
1:A:351:ILE:HD13	1:A:368:PHE:CE1	0.68	2.24	9	1
1:A:289:VAL:CG1	1:A:364:ILE:HD12	0.67	2.20	9	3
1:A:322:ILE:HG12	1:A:339:VAL:HG23	0.67	1.66	18	1
1:A:288:PHE:CD1	1:A:338:THR:HG22	0.66	2.26	10	9
1:A:316:LYS:CD	1:A:317:THR:HG23	0.66	2.19	7	1
1:A:305:PHE:HB3	1:A:311:ILE:HD11	0.66	1.67	3	3
1:A:323:ASN:O	1:A:337:ALA:HB1	0.66	1.90	11	8
1:A:351:ILE:HG23	1:A:366:VAL:O	0.66	1.90	13	1
1:A:287:ILE:CG2	1:A:347:ALA:HB1	0.65	2.21	5	6
1:A:296:VAL:CG1	1:A:324:LEU:HD22	0.65	2.22	6	3
1:A:292:LEU:N	1:A:292:LEU:CD2	0.65	2.60	14	2
1:A:322:ILE:HG12	1:A:339:VAL:HG22	0.64	1.69	9	9
1:A:354:PHE:HB3	1:A:364:ILE:HD11	0.63	1.69	15	1
1:A:314:ASN:HD21	1:A:317:THR:HG23	0.62	1.54	3	2
1:A:301:VAL:HG11	1:A:339:VAL:HG21	0.61	1.72	10	3
1:A:296:VAL:CG1	1:A:337:ALA:HB2	0.61	2.25	3	2
1:A:354:PHE:O	1:A:356:GLY:N	0.61	2.34	12	10
1:A:292:LEU:HD12	1:A:359:PHE:CD2	0.61	2.30	3	3
1:A:292:LEU:HD13	1:A:292:LEU:N	0.61	2.10	16	3
1:A:354:PHE:HB2	1:A:366:VAL:HG21	0.61	1.72	8	10
1:A:353:TRP:CD1	1:A:353:TRP:C	0.61	2.74	12	10
1:A:296:VAL:HG13	1:A:324:LEU:HD22	0.60	1.72	18	1
1:A:302:ALA:HA	1:A:311:ILE:HD13	0.60	1.73	6	11

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:298:ILE:HD13	1:A:324:LEU:HD21	0.60	1.73	13	1
1:A:298:ILE:HD12	1:A:298:ILE:N	0.60	2.11	19	1
1:A:288:PHE:O	1:A:288:PHE:CD1	0.60	2.55	4	2
1:A:314:ASN:OD1	1:A:317:THR:OG1	0.60	2.19	13	1
1:A:353:TRP:C	1:A:353:TRP:CD1	0.60	2.76	14	10
1:A:296:VAL:HG22	1:A:324:LEU:HD13	0.60	1.74	12	1
1:A:296:VAL:HG13	1:A:296:VAL:O	0.59	1.97	1	7
1:A:288:PHE:CZ	1:A:338:THR:HG21	0.59	2.32	3	5
1:A:359:PHE:CD1	1:A:364:ILE:HG21	0.59	2.33	8	2
1:A:313:THR:HA	1:A:320:PRO:HA	0.59	1.74	19	8
1:A:289:VAL:HG13	1:A:366:VAL:CG2	0.59	2.26	13	2
1:A:298:ILE:HG23	1:A:322:ILE:HD12	0.59	1.74	10	6
1:A:296:VAL:O	1:A:296:VAL:HG13	0.59	1.98	14	2
1:A:313:THR:HG23	1:A:319:GLN:C	0.58	2.18	15	4
1:A:324:LEU:HD23	1:A:337:ALA:HB1	0.58	1.74	17	5
1:A:298:ILE:HG23	1:A:322:ILE:HB	0.58	1.75	4	3
1:A:314:ASN:OD1	1:A:321:MET:CG	0.58	2.52	6	7
1:A:301:VAL:HG11	1:A:339:VAL:HG22	0.58	1.74	2	4
1:A:358:GLU:CA	1:A:362:ASN:O	0.57	2.51	10	12
1:A:298:ILE:HD12	1:A:324:LEU:HD21	0.57	1.75	19	1
1:A:292:LEU:CB	1:A:296:VAL:HG22	0.57	2.29	7	1
1:A:351:ILE:HD13	1:A:368:PHE:CD2	0.57	2.35	5	1
1:A:296:VAL:CG2	1:A:337:ALA:HB2	0.57	2.30	8	2
1:A:287:ILE:HD11	1:A:305:PHE:CZ	0.57	2.35	5	3
1:A:288:PHE:CD2	1:A:338:THR:HG22	0.57	2.35	5	1
1:A:359:PHE:HD2	1:A:364:ILE:HG21	0.56	1.60	6	3
1:A:292:LEU:HD22	1:A:292:LEU:N	0.56	2.15	3	2
1:A:353:TRP:CD1	1:A:354:PHE:CD1	0.56	2.93	3	5
1:A:324:LEU:HD12	1:A:324:LEU:N	0.56	2.15	16	2
1:A:292:LEU:HD12	1:A:295:ASN:HD21	0.56	1.61	12	1
1:A:354:PHE:O	1:A:355:ASP:C	0.56	2.44	1	19
1:A:292:LEU:HD22	1:A:292:LEU:H	0.56	1.61	3	1
1:A:292:LEU:HD22	1:A:296:VAL:CB	0.56	2.30	13	1
1:A:351:ILE:HD11	1:A:368:PHE:CD1	0.56	2.36	15	1
1:A:359:PHE:N	1:A:362:ASN:O	0.56	2.38	3	15
1:A:305:PHE:CZ	1:A:354:PHE:CE2	0.56	2.94	8	6
1:A:292:LEU:N	1:A:292:LEU:HD12	0.56	2.16	19	1
1:A:292:LEU:H	1:A:292:LEU:HD22	0.56	1.61	16	1
1:A:359:PHE:HB2	1:A:364:ILE:HD13	0.56	1.76	18	1
1:A:296:VAL:O	1:A:297:THR:HG23	0.56	2.01	12	3
1:A:308:ILE:HG23	1:A:341:PHE:CE2	0.55	2.36	19	2

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:296:VAL:HG22	1:A:324:LEU:HD22	0.55	1.77	14	1
1:A:292:LEU:HD22	1:A:335:GLY:O	0.55	2.00	2	2
1:A:288:PHE:CD1	1:A:288:PHE:O	0.55	2.58	11	2
1:A:284:ASN:OD1	1:A:368:PHE:CD1	0.55	2.59	7	1
1:A:351:ILE:CD1	1:A:368:PHE:CE1	0.55	2.89	7	4
1:A:324:LEU:HD23	1:A:324:LEU:N	0.55	2.17	2	2
1:A:302:ALA:HB1	1:A:320:PRO:HG2	0.55	1.77	1	5
1:A:292:LEU:HD22	1:A:296:VAL:HB	0.55	1.78	13	1
1:A:311:ILE:HD13	1:A:339:VAL:CG1	0.55	2.31	19	1
1:A:344:PRO:N	1:A:345:PRO:HD2	0.54	2.17	4	20
1:A:304:TYR:CE1	1:A:359:PHE:CZ	0.54	2.95	16	12
1:A:314:ASN:ND2	1:A:319:GLN:O	0.54	2.41	15	2
1:A:301:VAL:O	1:A:305:PHE:HB2	0.54	2.01	12	15
1:A:302:ALA:HA	1:A:311:ILE:HD12	0.54	1.78	14	2
1:A:289:VAL:HG13	1:A:364:ILE:HD12	0.54	1.79	9	2
1:A:288:PHE:HD1	1:A:338:THR:HG22	0.54	1.63	12	1
1:A:354:PHE:CB	1:A:366:VAL:HG21	0.54	2.33	8	5
1:A:351:ILE:O	1:A:355:ASP:CB	0.54	2.56	11	8
1:A:291:GLY:C	1:A:292:LEU:HD23	0.54	2.23	15	1
1:A:353:TRP:CE3	1:A:354:PHE:CZ	0.53	2.96	2	6
1:A:304:TYR:CZ	1:A:305:PHE:CD1	0.53	2.97	15	4
1:A:312:LYS:O	1:A:321:MET:N	0.53	2.41	18	8
1:A:304:TYR:CZ	1:A:305:PHE:CE1	0.53	2.97	2	3
1:A:353:TRP:CZ3	1:A:354:PHE:CZ	0.53	2.96	8	5
1:A:305:PHE:CZ	1:A:354:PHE:CD2	0.53	2.95	11	3
1:A:305:PHE:CE1	1:A:354:PHE:CE2	0.53	2.97	1	10
1:A:308:ILE:HG21	1:A:354:PHE:CE2	0.53	2.39	11	1
1:A:301:VAL:CG1	1:A:339:VAL:HG21	0.53	2.34	13	5
1:A:315:LYS:HD2	1:A:315:LYS:N	0.53	2.19	11	1
1:A:305:PHE:CE1	1:A:354:PHE:CZ	0.53	2.96	12	2
1:A:304:TYR:CE2	1:A:359:PHE:CZ	0.53	2.97	20	2
1:A:292:LEU:N	1:A:292:LEU:HD23	0.52	2.19	20	1
1:A:314:ASN:OD1	1:A:318:GLY:N	0.52	2.42	18	1
1:A:288:PHE:CE1	1:A:338:THR:HG21	0.52	2.40	3	3
1:A:351:ILE:O	1:A:355:ASP:HB3	0.52	2.04	9	9
1:A:353:TRP:CD1	1:A:354:PHE:CD2	0.52	2.97	9	1
1:A:304:TYR:CZ	1:A:359:PHE:CE2	0.52	2.98	17	2
1:A:295:ASN:O	1:A:296:VAL:C	0.52	2.48	2	4
1:A:289:VAL:HG12	1:A:364:ILE:HB	0.52	1.80	13	2
1:A:288:PHE:CE2	1:A:367:SER:CB	0.52	2.93	9	1
1:A:308:ILE:HD11	1:A:349:ALA:O	0.52	2.05	9	3

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:301:VAL:HB	1:A:322:ILE:HD13	0.52	1.81	16	3
1:A:314:ASN:O	1:A:318:GLY:N	0.52	2.40	11	8
1:A:287:ILE:HG23	1:A:347:ALA:HB1	0.52	1.81	15	3
1:A:292:LEU:CD1	1:A:296:VAL:HG13	0.52	2.35	6	1
1:A:296:VAL:CG2	1:A:324:LEU:HD23	0.51	2.16	10	1
1:A:296:VAL:HG12	1:A:296:VAL:O	0.51	2.04	18	1
1:A:298:ILE:HG21	1:A:319:GLN:HE22	0.51	1.65	19	1
1:A:304:TYR:CE1	1:A:305:PHE:CD2	0.51	2.98	6	2
1:A:295:ASN:O	1:A:295:ASN:CG	0.51	2.47	20	1
1:A:305:PHE:CE1	1:A:354:PHE:CE1	0.51	2.98	9	1
1:A:304:TYR:CE1	1:A:305:PHE:CD1	0.51	2.99	2	3
1:A:314:ASN:HB3	1:A:317:THR:OG1	0.50	2.06	11	1
1:A:321:MET:O	1:A:340:SER:OG	0.50	2.29	18	2
1:A:298:ILE:N	1:A:298:ILE:CD1	0.50	2.74	19	1
1:A:288:PHE:HD2	1:A:338:THR:HG22	0.50	1.65	5	1
1:A:311:ILE:HD13	1:A:339:VAL:HG13	0.50	1.83	19	1
1:A:304:TYR:CE1	1:A:359:PHE:CE2	0.50	2.99	2	4
1:A:289:VAL:HA	1:A:365:LYS:O	0.50	2.07	16	1
1:A:292:LEU:HD23	1:A:295:ASN:HD21	0.50	1.66	19	1
1:A:290:GLN:O	1:A:364:ILE:HA	0.50	2.06	6	5
1:A:292:LEU:HD22	1:A:359:PHE:HD2	0.49	1.66	18	1
1:A:311:ILE:HB	1:A:320:PRO:HB3	0.49	1.84	19	6
1:A:292:LEU:HD12	1:A:359:PHE:HD2	0.49	1.66	3	2
1:A:304:TYR:CE2	1:A:305:PHE:CE1	0.49	3.01	11	1
1:A:359:PHE:CD2	1:A:364:ILE:HG21	0.49	2.43	1	6
1:A:287:ILE:CD1	1:A:305:PHE:CZ	0.49	2.96	19	7
1:A:284:ASN:O	1:A:285:ASN:ND2	0.49	2.45	2	1
1:A:301:VAL:HG22	1:A:359:PHE:HZ	0.49	1.68	14	2
1:A:313:THR:HA	1:A:320:PRO:CA	0.49	2.36	19	1
1:A:314:ASN:ND2	1:A:317:THR:HG23	0.49	2.21	3	1
1:A:284:ASN:ND2	1:A:368:PHE:CD1	0.49	2.80	17	2
1:A:285:ASN:HA	1:A:347:ALA:HB2	0.48	1.84	4	2
1:A:296:VAL:HG22	1:A:324:LEU:CD2	0.48	2.38	15	1
1:A:288:PHE:CD2	1:A:290:GLN:OE1	0.48	2.66	4	3
1:A:314:ASN:OD1	1:A:316:LYS:HB2	0.48	2.08	19	1
1:A:288:PHE:CE1	1:A:338:THR:CG2	0.48	2.96	14	9
1:A:351:ILE:O	1:A:355:ASP:HB2	0.48	2.07	2	7
1:A:348:LYS:C	1:A:348:LYS:CD	0.48	2.82	16	3
1:A:287:ILE:HD13	1:A:341:PHE:HE2	0.48	1.67	6	1
1:A:319:GLN:HG2	1:A:320:PRO:N	0.48	2.22	18	2
1:A:296:VAL:HG23	1:A:337:ALA:HB2	0.48	1.86	8	1

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:287:ILE:HG12	1:A:339:VAL:HG12	0.48	1.86	18	1
1:A:317:THR:HG22	1:A:319:GLN:H	0.47	1.68	10	2
1:A:288:PHE:CE2	1:A:290:GLN:CG	0.47	2.97	13	1
1:A:317:THR:HG21	1:A:319:GLN:HG2	0.47	1.86	19	1
1:A:296:VAL:O	1:A:296:VAL:CG1	0.47	2.56	19	1
1:A:339:VAL:CG1	1:A:341:PHE:CE1	0.47	2.97	7	1
1:A:288:PHE:CZ	1:A:338:THR:CG2	0.47	2.98	15	4
1:A:343:ASP:N	1:A:343:ASP:OD1	0.47	2.48	9	1
1:A:289:VAL:CG2	1:A:339:VAL:HG23	0.47	2.40	1	2
1:A:314:ASN:OD1	1:A:319:GLN:O	0.47	2.32	17	1
1:A:347:ALA:HB3	1:A:368:PHE:CE1	0.47	2.44	3	2
1:A:351:ILE:HD13	1:A:368:PHE:CD1	0.47	2.45	9	1
1:A:289:VAL:HG22	1:A:366:VAL:HG22	0.47	1.85	11	1
1:A:285:ASN:ND2	1:A:341:PHE:CB	0.47	2.78	16	1
1:A:298:ILE:HD13	1:A:324:LEU:HD11	0.47	1.87	18	1
1:A:323:ASN:O	1:A:324:LEU:HD23	0.47	2.10	4	1
1:A:308:ILE:HD13	1:A:350:ALA:HA	0.47	1.87	1	1
1:A:301:VAL:O	1:A:305:PHE:CB	0.47	2.63	10	3
1:A:314:ASN:OD1	1:A:316:LYS:N	0.46	2.49	10	1
1:A:304:TYR:CZ	1:A:359:PHE:CZ	0.46	3.02	11	1
1:A:312:LYS:HB2	1:A:340:SER:CB	0.46	2.40	1	1
1:A:292:LEU:CD2	1:A:359:PHE:CE1	0.46	2.98	8	1
1:A:312:LYS:CE	1:A:341:PHE:O	0.46	2.64	9	1
1:A:290:GLN:CD	1:A:290:GLN:N	0.46	2.68	4	1
1:A:322:ILE:HG12	1:A:339:VAL:HG13	0.46	1.86	4	1
1:A:292:LEU:CD2	1:A:359:PHE:CD2	0.46	2.98	10	2
1:A:301:VAL:HG22	1:A:359:PHE:CZ	0.46	2.45	13	4
1:A:317:THR:OG1	1:A:319:GLN:HG3	0.46	2.11	20	2
1:A:295:ASN:C	1:A:295:ASN:ND2	0.46	2.68	15	1
1:A:359:PHE:HD1	1:A:364:ILE:HG21	0.46	1.68	8	2
1:A:356:GLY:HA2	1:A:364:ILE:O	0.46	2.11	6	2
1:A:313:THR:CA	1:A:320:PRO:HA	0.46	2.40	19	2
1:A:353:TRP:CZ2	1:A:354:PHE:CE1	0.45	3.04	8	1
1:A:311:ILE:CG2	1:A:320:PRO:CB	0.45	2.94	14	3
1:A:305:PHE:CE1	1:A:354:PHE:CD2	0.45	3.04	11	1
1:A:319:GLN:NE2	1:A:320:PRO:O	0.45	2.50	19	1
1:A:298:ILE:CD1	1:A:324:LEU:HD21	0.45	2.41	19	1
1:A:296:VAL:CG2	1:A:337:ALA:CB	0.45	2.95	2	1
1:A:292:LEU:CD2	1:A:359:PHE:CD1	0.45	2.98	8	1
1:A:351:ILE:CD1	1:A:368:PHE:CE2	0.45	2.99	16	1
1:A:287:ILE:HD13	1:A:341:PHE:CE2	0.45	2.47	18	2

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:284:ASN:ND2	1:A:368:PHE:CE1	0.45	2.84	2	1
1:A:324:LEU:N	1:A:324:LEU:HD12	0.45	2.27	3	1
1:A:354:PHE:HB3	1:A:357:LYS:HG2	0.45	1.89	17	3
1:A:292:LEU:CD1	1:A:359:PHE:CE2	0.45	3.00	7	1
1:A:324:LEU:HB3	1:A:337:ALA:HB2	0.44	1.88	2	1
1:A:314:ASN:O	1:A:315:LYS:CB	0.44	2.65	8	1
1:A:287:ILE:CD1	1:A:305:PHE:CE2	0.44	3.00	10	1
1:A:313:THR:HG23	1:A:319:GLN:CA	0.44	2.42	17	1
1:A:314:ASN:OD1	1:A:317:THR:N	0.44	2.44	10	1
1:A:285:ASN:ND2	1:A:285:ASN:N	0.44	2.63	12	1
1:A:292:LEU:N	1:A:292:LEU:HD22	0.44	2.25	14	1
1:A:351:ILE:HD12	1:A:368:PHE:CE1	0.44	2.47	7	1
1:A:292:LEU:HG	1:A:296:VAL:HG22	0.44	1.89	7	1
1:A:323:ASN:O	1:A:337:ALA:CB	0.44	2.66	8	3
1:A:292:LEU:HD13	1:A:295:ASN:ND2	0.44	2.28	11	1
1:A:288:PHE:CG	1:A:290:GLN:OE1	0.44	2.70	4	1
1:A:296:VAL:CG1	1:A:324:LEU:CB	0.44	2.96	6	2
1:A:351:ILE:CD1	1:A:368:PHE:CD1	0.44	3.00	15	1
1:A:296:VAL:HG13	1:A:324:LEU:CB	0.44	2.43	18	1
1:A:314:ASN:HB2	1:A:321:MET:CG	0.44	2.43	5	2
1:A:298:ILE:HD12	1:A:322:ILE:O	0.44	2.12	16	1
1:A:288:PHE:CD1	1:A:338:THR:CG2	0.44	3.00	7	1
1:A:353:TRP:CD1	1:A:357:LYS:HG3	0.44	2.47	11	1
1:A:302:ALA:O	1:A:306:LYS:HB3	0.44	2.13	14	1
1:A:296:VAL:CG2	1:A:337:ALA:HB3	0.43	2.43	2	1
1:A:294:GLU:HG3	1:A:294:GLU:O	0.43	2.13	3	1
1:A:354:PHE:CD2	1:A:357:LYS:HD3	0.43	2.48	12	1
1:A:288:PHE:CE2	1:A:367:SER:HB2	0.43	2.49	9	1
1:A:296:VAL:O	1:A:297:THR:CG2	0.43	2.67	16	1
1:A:324:LEU:HD23	1:A:337:ALA:HB2	0.43	1.86	18	1
1:A:284:ASN:OD1	1:A:368:PHE:CZ	0.43	2.71	3	1
1:A:314:ASN:OD1	1:A:321:MET:HG3	0.43	2.13	6	1
1:A:292:LEU:HD22	1:A:359:PHE:CE2	0.43	2.48	5	1
1:A:314:ASN:OD1	1:A:321:MET:CB	0.43	2.67	1	1
1:A:292:LEU:CD2	1:A:292:LEU:N	0.43	2.82	12	1
1:A:296:VAL:CG1	1:A:324:LEU:HD23	0.43	2.26	3	1
1:A:295:ASN:ND2	1:A:296:VAL:N	0.43	2.67	16	1
1:A:288:PHE:CE2	1:A:367:SER:HB3	0.43	2.48	9	1
1:A:304:TYR:OH	1:A:364:ILE:HD13	0.42	2.13	1	1
1:A:292:LEU:N	1:A:292:LEU:CD1	0.42	2.82	19	1
1:A:354:PHE:HB2	1:A:366:VAL:CG2	0.42	2.43	8	1

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:359:PHE:HB2	1:A:364:ILE:CG2	0.42	2.44	9	1
1:A:292:LEU:HD12	1:A:296:VAL:HG13	0.42	1.90	6	1
1:A:290:GLN:NE2	1:A:336:GLU:HB2	0.42	2.29	16	1
1:A:298:ILE:CD1	1:A:322:ILE:O	0.42	2.66	1	1
1:A:314:ASN:OD1	1:A:314:ASN:N	0.42	2.53	6	1
1:A:314:ASN:O	1:A:316:LYS:N	0.42	2.52	11	1
1:A:296:VAL:HG22	1:A:324:LEU:HB3	0.42	1.92	8	1
1:A:285:ASN:HD22	1:A:347:ALA:HB2	0.42	1.74	16	1
1:A:289:VAL:O	1:A:290:GLN:NE2	0.42	2.52	19	2
1:A:314:ASN:ND2	1:A:317:THR:N	0.42	2.66	20	2
1:A:292:LEU:CD1	1:A:359:PHE:CD2	0.42	3.03	2	1
1:A:314:ASN:C	1:A:316:LYS:N	0.42	2.73	11	1
1:A:286:THR:OG1	1:A:340:SER:HA	0.42	2.14	18	1
1:A:284:ASN:ND2	1:A:284:ASN:N	0.42	2.68	6	2
1:A:289:VAL:HG21	1:A:305:PHE:CE2	0.42	2.50	11	1
1:A:295:ASN:O	1:A:297:THR:N	0.42	2.52	16	2
1:A:292:LEU:HD23	1:A:296:VAL:CG2	0.42	2.45	3	1
1:A:317:THR:HG21	1:A:319:GLN:CD	0.42	2.35	10	1
1:A:351:ILE:HD13	1:A:368:PHE:CZ	0.42	2.50	16	1
1:A:313:THR:OG1	1:A:319:GLN:N	0.42	2.53	19	1
1:A:288:PHE:CE1	1:A:290:GLN:OE1	0.42	2.72	9	1
1:A:311:ILE:CG2	1:A:320:PRO:HB3	0.42	2.45	18	2
1:A:287:ILE:CD1	1:A:366:VAL:HG13	0.42	2.35	7	1
1:A:290:GLN:O	1:A:365:LYS:N	0.41	2.53	9	1
1:A:317:THR:CG2	1:A:319:GLN:CG	0.41	2.98	19	1
1:A:339:VAL:HG12	1:A:341:PHE:CZ	0.41	2.50	7	1
1:A:339:VAL:HG12	1:A:341:PHE:CE1	0.41	2.49	7	1
1:A:348:LYS:C	1:A:348:LYS:HD3	0.41	2.36	10	1
1:A:351:ILE:O	1:A:355:ASP:CG	0.41	2.58	19	1
1:A:301:VAL:HG11	1:A:339:VAL:HG23	0.41	1.92	12	1
1:A:339:VAL:CG1	1:A:341:PHE:CZ	0.41	3.03	7	2
1:A:301:VAL:CG1	1:A:339:VAL:CG2	0.41	2.98	13	2
1:A:344:PRO:N	1:A:345:PRO:CD	0.41	2.84	7	2
1:A:343:ASP:OD1	1:A:346:SER:CB	0.41	2.68	9	1
1:A:306:LYS:CG	1:A:306:LYS:O	0.41	2.68	11	1
1:A:339:VAL:HG11	1:A:341:PHE:CZ	0.41	2.50	12	1
1:A:314:ASN:ND2	1:A:321:MET:HG2	0.41	2.30	2	1
1:A:314:ASN:ND2	1:A:317:THR:H	0.41	2.13	5	1
1:A:312:LYS:HB3	1:A:340:SER:CB	0.41	2.46	6	1
1:A:351:ILE:HG23	1:A:355:ASP:HB2	0.41	1.91	8	1
1:A:311:ILE:O	1:A:313:THR:N	0.41	2.53	9	1

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:312:LYS:O	1:A:321:MET:HB2	0.41	2.16	12	1
1:A:315:LYS:CD	1:A:315:LYS:N	0.41	2.84	18	1
1:A:311:ILE:CB	1:A:320:PRO:HB3	0.41	2.45	3	2
1:A:296:VAL:HG13	1:A:324:LEU:CD2	0.41	2.45	18	1
1:A:296:VAL:CG1	1:A:296:VAL:O	0.41	2.68	2	2
1:A:284:ASN:O	1:A:285:ASN:CB	0.41	2.68	2	1
1:A:313:THR:HG22	1:A:318:GLY:C	0.41	2.36	3	1
1:A:348:LYS:CD	1:A:348:LYS:C	0.41	2.88	13	2
1:A:312:LYS:N	1:A:340:SER:O	0.41	2.53	6	1
1:A:353:TRP:CE2	1:A:354:PHE:CE1	0.41	3.09	8	1
1:A:288:PHE:C	1:A:288:PHE:CD1	0.41	2.93	9	1
1:A:341:PHE:CD2	1:A:347:ALA:HA	0.41	2.51	9	1
1:A:289:VAL:CG1	1:A:366:VAL:HG22	0.41	2.36	13	1
1:A:291:GLY:O	1:A:364:ILE:CG2	0.41	2.66	14	1
1:A:314:ASN:ND2	1:A:317:THR:CB	0.41	2.84	15	1
1:A:295:ASN:ND2	1:A:359:PHE:CD1	0.41	2.89	1	1
1:A:323:ASN:O	1:A:337:ALA:CA	0.41	2.69	9	2
1:A:292:LEU:HD12	1:A:296:VAL:CG2	0.41	2.39	6	1
1:A:296:VAL:HG23	1:A:324:LEU:HB3	0.41	1.92	12	1
1:A:290:GLN:NE2	1:A:336:GLU:CB	0.41	2.84	16	1
1:A:297:THR:O	1:A:301:VAL:CG2	0.41	2.69	18	1
1:A:296:VAL:HG12	1:A:324:LEU:HB3	0.41	1.93	7	1
1:A:292:LEU:HD22	1:A:335:GLY:C	0.40	2.35	4	1
1:A:287:ILE:HD13	1:A:305:PHE:CE2	0.40	2.51	10	1
1:A:312:LYS:CG	1:A:341:PHE:O	0.40	2.69	13	1
1:A:311:ILE:HG22	1:A:320:PRO:CB	0.40	2.46	14	1
1:A:285:ASN:OD1	1:A:344:PRO:CD	0.40	2.69	7	1
1:A:292:LEU:HB3	1:A:295:ASN:ND2	0.40	2.31	20	1
1:A:287:ILE:CD1	1:A:366:VAL:CG1	0.40	2.99	7	1
1:A:292:LEU:HD13	1:A:364:ILE:HG22	0.40	1.93	2	1
1:A:296:VAL:CG2	1:A:324:LEU:CB	0.40	3.00	9	1
1:A:323:ASN:O	1:A:337:ALA:HA	0.40	2.16	9	1
1:A:288:PHE:O	1:A:288:PHE:CG	0.40	2.75	13	2
1:A:306:LYS:CD	1:A:306:LYS:O	0.40	2.69	11	1
1:A:296:VAL:HG13	1:A:324:LEU:HB3	0.40	1.93	18	1
1:A:302:ALA:HB1	1:A:320:PRO:CG	0.40	2.46	19	1
1:A:292:LEU:CG	1:A:296:VAL:HG22	0.40	2.46	7	1
1:A:353:TRP:CD1	1:A:357:LYS:HD2	0.40	2.51	2	1
1:A:302:ALA:CA	1:A:311:ILE:HD13	0.40	2.44	6	1
1:A:288:PHE:CZ	1:A:325:TYR:OH	0.40	2.73	14	1
1:A:312:LYS:O	1:A:321:MET:CB	0.40	2.70	15	1

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:314:ASN:CG	1:A:317:THR:OG1	0.40	2.59	17	1
1:A:313:THR:OG1	1:A:314:ASN:N	0.40	2.55	19	1
1:A:302:ALA:O	1:A:306:LYS:CG	0.40	2.69	7	1
1:A:304:TYR:OH	1:A:359:PHE:CE1	0.40	2.71	19	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	76/116 (66%)	61±2 (80±2%)	12±2 (16±3%)	3±1 (5±2%)	4	28
All	All	1520/2320 (66%)	1215 (80%)	236 (16%)	69 (5%)	4	28

All 13 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	355	ASP	18
1	A	312	LYS	15
1	A	296	VAL	9
1	A	292	LEU	6
1	A	284	ASN	5
1	A	320	PRO	4
1	A	315	LYS	3
1	A	354	PHE	2
1	A	295	ASN	2
1	A	285	ASN	2
1	A	343	ASP	1
1	A	360	SER	1
1	A	293	GLY	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	64/95 (67%)	41±3 (64±5%)	23±3 (36±5%)	1	8
All	All	1280/1900 (67%)	820 (64%)	460 (36%)	1	8

All 49 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	304	TYR	20
1	A	359	PHE	20
1	A	295	ASN	19
1	A	319	GLN	19
1	A	297	THR	18
1	A	306	LYS	18
1	A	313	THR	18
1	A	305	PHE	17
1	A	289	VAL	16
1	A	348	LYS	16
1	A	314	ASN	16
1	A	324	LEU	16
1	A	357	LYS	14
1	A	315	LYS	14
1	A	288	PHE	12
1	A	343	ASP	11
1	A	312	LYS	11
1	A	292	LEU	11
1	A	290	GLN	10
1	A	316	LYS	10
1	A	365	LYS	10
1	A	284	ASN	10
1	A	321	MET	10
1	A	285	ASN	10
1	A	342	ASP	8
1	A	308	ILE	7
1	A	352	ASP	7
1	A	360	SER	7
1	A	362	ASN	7
1	A	368	PHE	7
1	A	303	ASP	6
1	A	367	SER	6
1	A	346	SER	6

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Models (Total)
1	A	336	GLU	6
1	A	307	GLN	5
1	A	358	GLU	5
1	A	294	GLU	5
1	A	299	GLU	5
1	A	317	THR	5
1	A	323	ASN	4
1	A	300	SER	4
1	A	354	PHE	3
1	A	340	SER	3
1	A	353	TRP	3
1	A	286	THR	1
1	A	341	PHE	1
1	A	338	THR	1
1	A	339	VAL	1
1	A	310	ILE	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](#)

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 ⓘ

There are no chain breaks in this entry.

7 Chemical shift validation

The completeness of assignment taking into account all chemical shift lists is 95% for the well-defined parts and 91% 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	1220
Number of shifts mapped to atoms	1220
Number of unparsed shifts	0
Number of shifts with mapping errors	0
Number of shifts with mapping warnings	0
Number of shift outliers (ShiftChecker)	1

7.1.2 Chemical shift referencing

The following table shows the suggested chemical shift referencing corrections.

Nucleus	# values	Correction \pm precision, ppm	Suggested action
$^{13}\text{C}_\alpha$	108	-0.52 ± 0.20	Should be applied
$^{13}\text{C}_\beta$	94	0.05 ± 0.22	None needed (< 0.5 ppm)
$^{13}\text{C}'$	107	0.70 ± 0.31	Should be applied
^{15}N	103	0.51 ± 0.27	None needed (imprecise)

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 95%, i.e. 858 atoms were assigned a chemical shift out of a possible 901. 0 out of 7 assigned methyl groups (LEU and VAL) were assigned stereospecifically.

	Total	^1H	^{13}C	^{15}N
Backbone	371/372 (100%)	148/148 (100%)	151/152 (99%)	72/72 (100%)
Sidechain	420/447 (94%)	256/261 (98%)	155/170 (91%)	9/16 (56%)

Continued on next page...

Continued from previous page...

	Total	¹ H	¹³ C	¹⁵ N
Aromatic	67/82 (82%)	36/44 (82%)	30/37 (81%)	1/1 (100%)
Overall	858/901 (95%)	440/453 (97%)	336/359 (94%)	82/89 (92%)

The following table shows the completeness of the chemical shift assignments for the full structure. The overall completeness is 91%, i.e. 1166 atoms were assigned a chemical shift out of a possible 1278. 0 out of 8 assigned methyl groups (LEU and VAL) were assigned stereospecifically.

	Total	¹ H	¹³ C	¹⁵ N
Backbone	529/532 (99%)	211/212 (100%)	215/216 (100%)	103/104 (99%)
Sidechain	568/655 (87%)	350/383 (91%)	205/235 (87%)	13/37 (35%)
Aromatic	69/91 (76%)	38/49 (78%)	30/41 (73%)	1/1 (100%)
Overall	1166/1278 (91%)	599/644 (93%)	450/492 (91%)	117/142 (82%)

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	353	TRP	HD1	5.24	8.95 – 5.35	-5.3

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:

