



Full wwPDB NMR Structure Validation Report ⓘ

May 28, 2020 – 11:49 pm BST

PDB ID : 2MJU
Title : Solution structure of a C terminal fragment of the neuronal isoform of the polypyrimidine tract binding protein (nPTB)
Authors : Esteve, V.; Blatter, M.; Allain, F.H.-T.
Deposited on : 2014-01-16

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

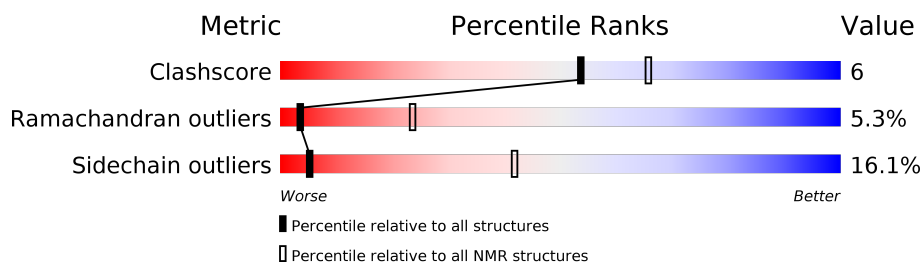
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

SOLUTION NMR

The overall completeness of chemical shifts assignment is 71%.

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	207	<div>68% 14% • 15%</div>

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:333-A:371, A:376-A:410, A:415-A:437, A:450-A:487, A:492-A:531 (175)	0.26	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 3 clusters and 1 single-model cluster was found.

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

3 Entry composition [i](#)

There is only 1 type of molecule in this entry. The entry contains 3232 atoms, of which 1622 are hydrogens and 0 are deuteriums.

- Molecule 1 is a protein called Polypyrimidine tract-binding protein 2.

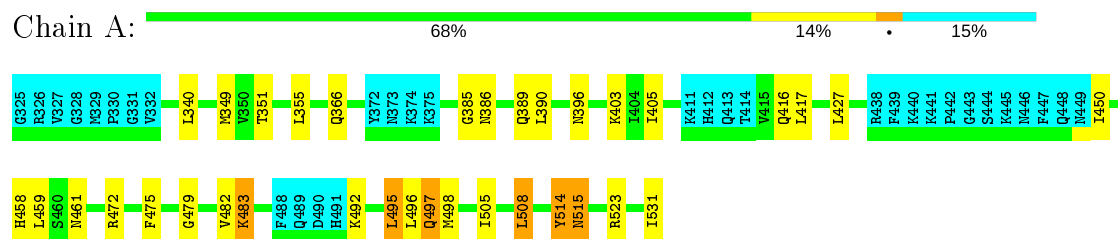
Mol	Chain	Residues	Atoms						Trace
1	A	207	Total	C	H	N	O	S	0
			3232	1018	1622	286	299	7	

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: Polypyrimidine tract-binding protein 2

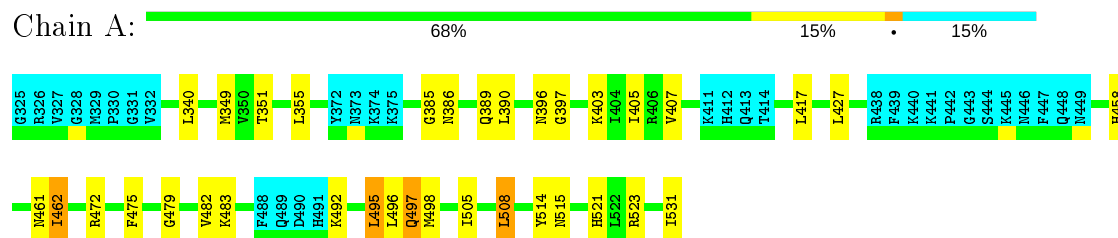


4.2 Scores per residue for each member of the ensemble

Colouring as in section 4.1 above.

4.2.1 Score per residue for model 1 (medoid)

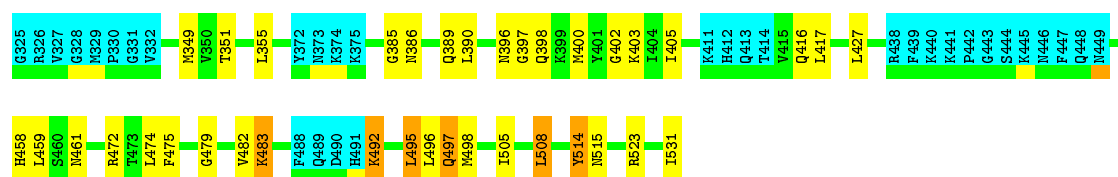
- Molecule 1: Polypyrimidine tract-binding protein 2



4.2.2 Score per residue for model 2

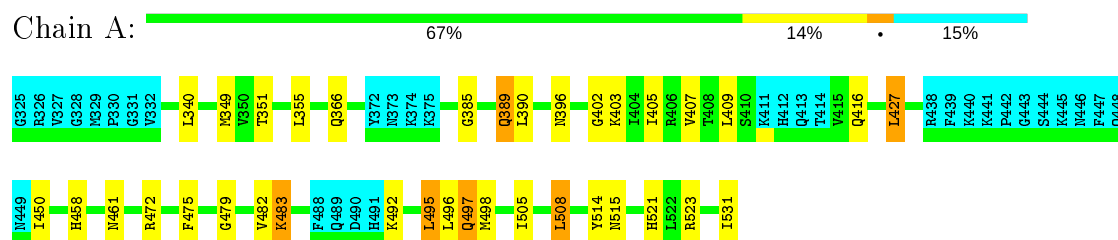
- Molecule 1: Polypyrimidine tract-binding protein 2





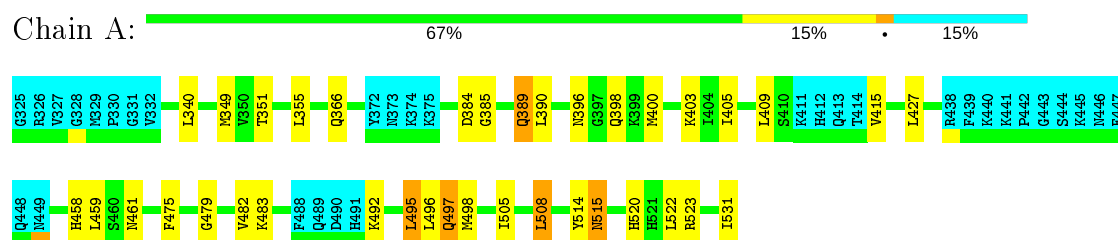
4.2.3 Score per residue for model 3

- Molecule 1: Polypyrimidine tract-binding protein 2



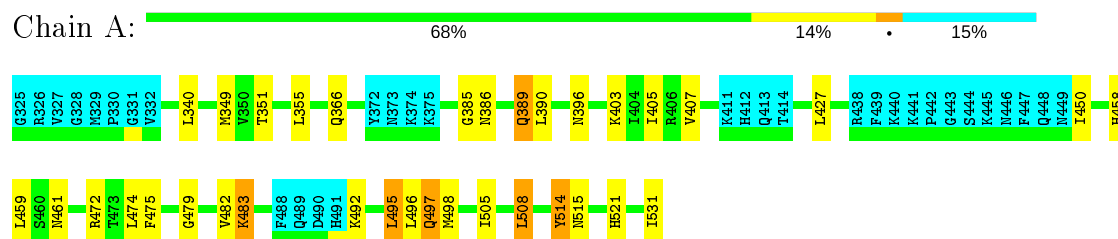
4.2.4 Score per residue for model 4

- Molecule 1: Polypyrimidine tract-binding protein 2



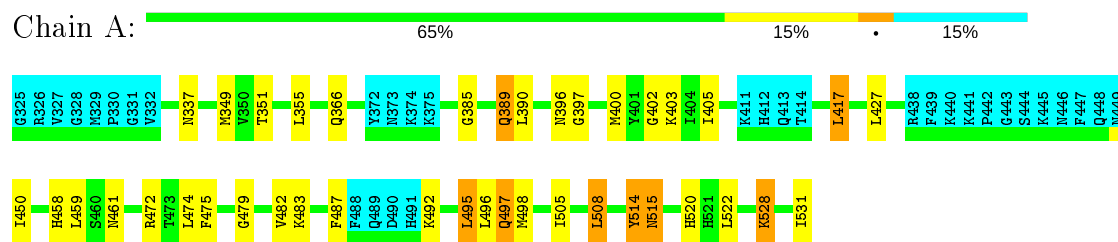
4.2.5 Score per residue for model 5

- Molecule 1: Polypyrimidine tract-binding protein 2



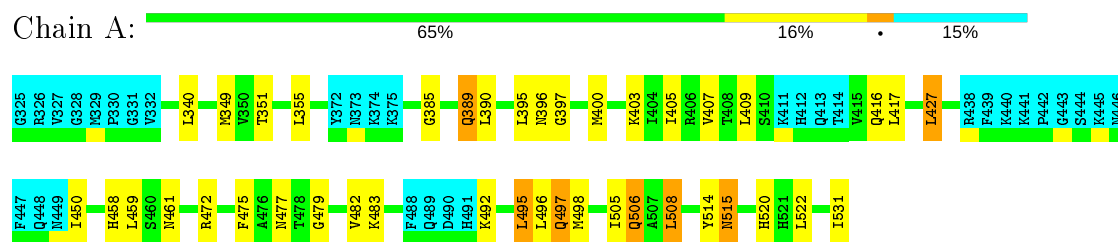
4.2.6 Score per residue for model 6

- Molecule 1: Polypyrimidine tract-binding protein 2



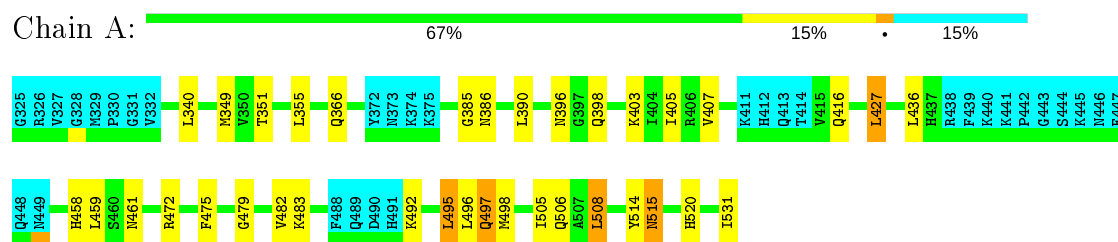
4.2.7 Score per residue for model 7

- Molecule 1: Polypyrimidine tract-binding protein 2



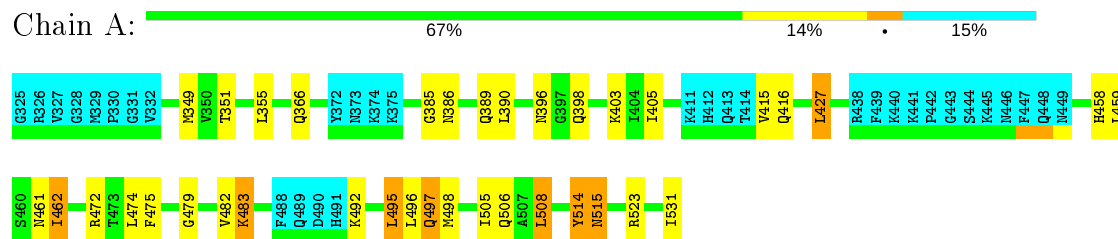
4.2.8 Score per residue for model 8

- Molecule 1: Polypyrimidine tract-binding protein 2



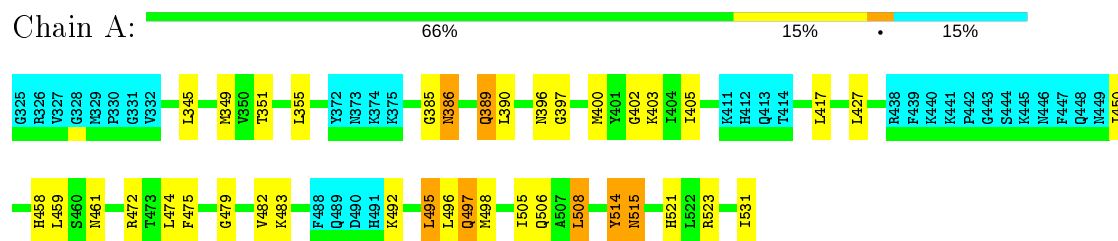
4.2.9 Score per residue for model 9

- Molecule 1: Polypyrimidine tract-binding protein 2

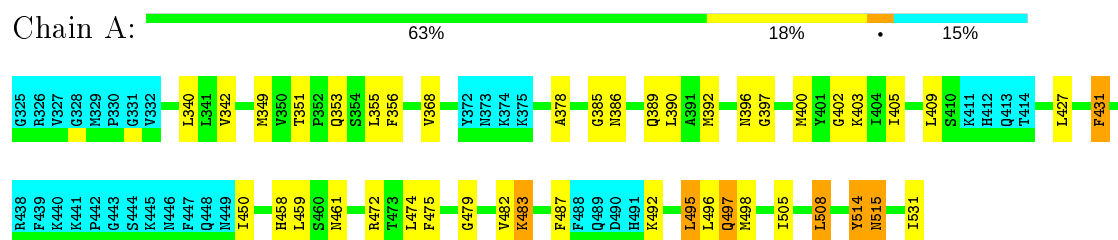


4.2.10 Score per residue for model 10

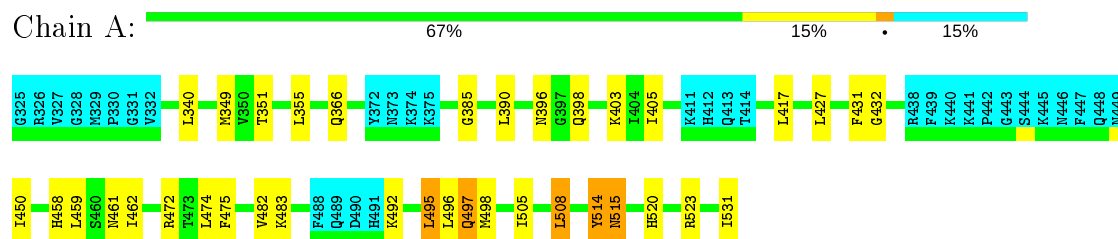
- Molecule 1: Polypyrimidine tract-binding protein 2



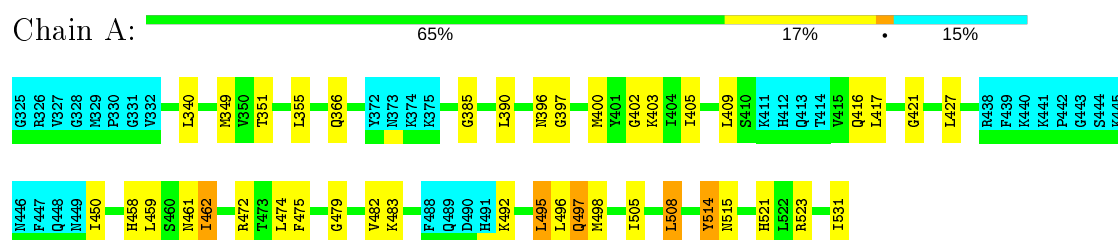
- Molecule 1: Polypyrimidine tract-binding protein 2



- Molecule 1: Polypyrimidine tract-binding protein 2

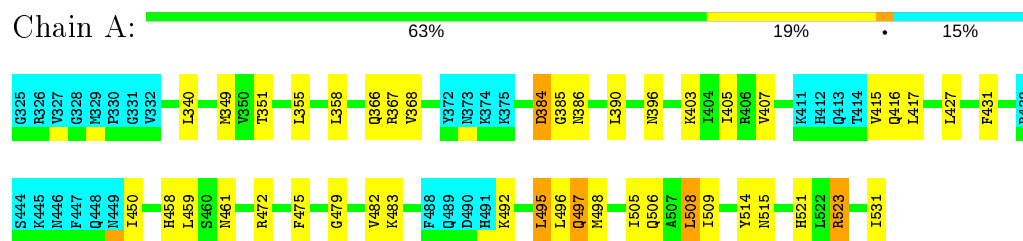


- Molecule 1: Polypyrimidine tract-binding protein 2



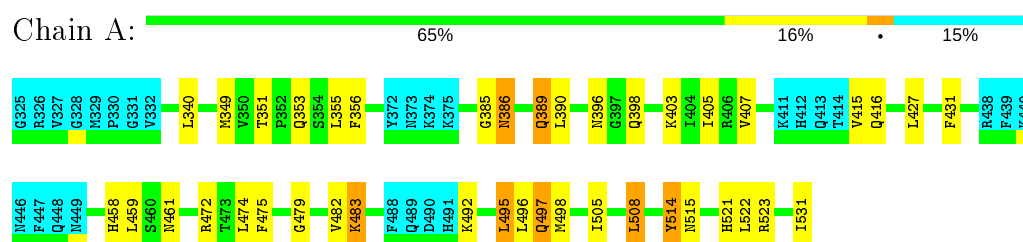
4.2.14 Score per residue for model 14

- Molecule 1: Polypyrimidine tract-binding protein 2



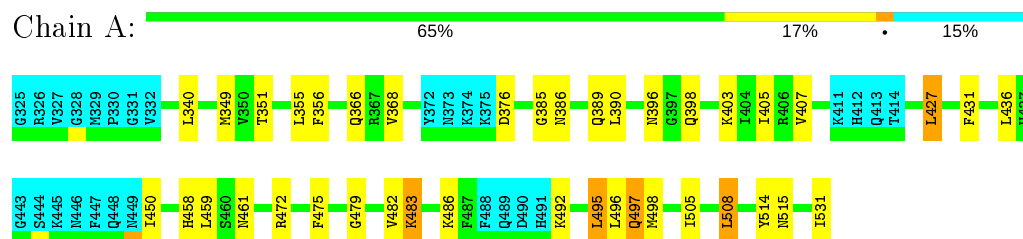
4.2.15 Score per residue for model 15

- Molecule 1: Polypyrimidine tract-binding protein 2



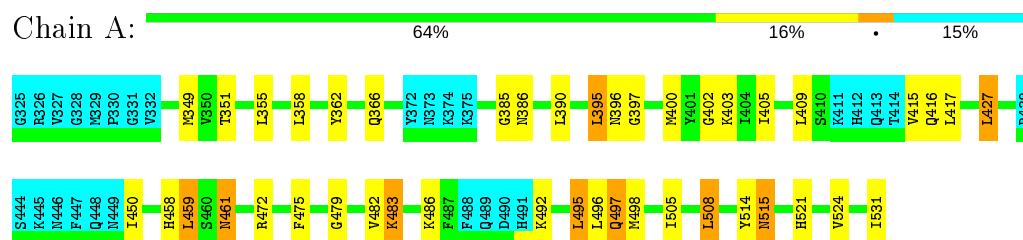
4.2.16 Score per residue for model 16

- Molecule 1: Polypyrimidine tract-binding protein 2



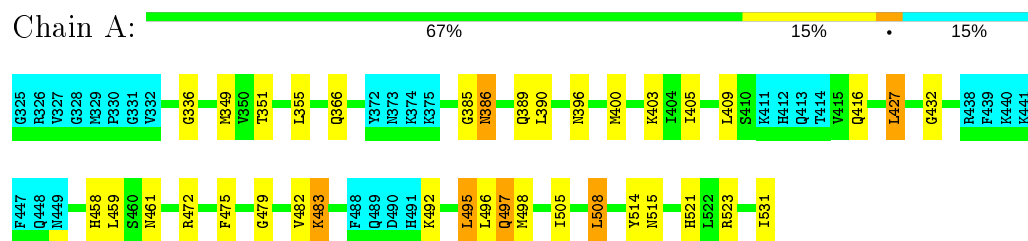
4.2.17 Score per residue for model 17

- Molecule 1: Polypyrimidine tract-binding protein 2

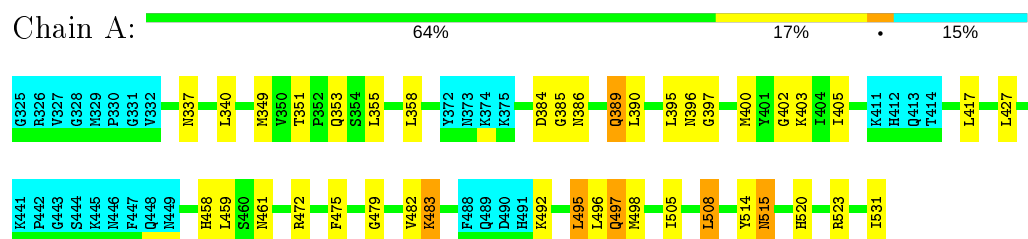


4.2.18 Score per residue for model 18

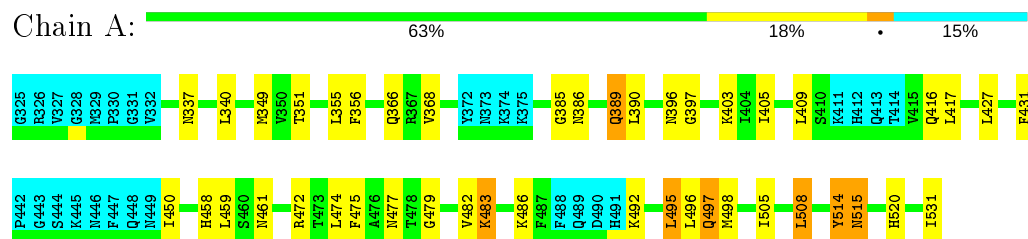
- Molecule 1: Polypyrimidine tract-binding protein 2



- Molecule 1: Polypyrimidine tract-binding protein 2



- Molecule 1: Polypyrimidine tract-binding protein 2



5 Refinement protocol and experimental data overview

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

Of the 250 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
AMBER	refinement	12
CYANA	structure calculation	3.0

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	1769
Number of shifts mapped to atoms	1769
Number of unparsed shifts	0
Number of shifts with mapping errors	0
Number of shifts with mapping warnings	0
Assignment completeness (well-defined parts)	71%

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	1345	1357	1357	15±2
All	All	26900	27140	27140	299

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 6.

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

Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:495:LEU:HD22	1:A:531:ILE:HD11	0.82	1.52	12	20
1:A:495:LEU:CD2	1:A:531:ILE:HD11	0.77	2.10	6	20
1:A:521:HIS:CE1	1:A:524:VAL:HG23	0.67	2.25	17	1
1:A:356:PHE:CE2	1:A:431:PHE:CD2	0.66	2.84	16	1
1:A:497:GLN:CB	1:A:531:ILE:HD12	0.62	2.24	18	20
1:A:495:LEU:HD21	1:A:531:ILE:CG1	0.55	2.31	5	20
1:A:497:GLN:HB2	1:A:531:ILE:HD12	0.52	1.80	18	20
1:A:508:LEU:HD22	1:A:508:LEU:C	0.51	2.26	6	9
1:A:340:LEU:C	1:A:340:LEU:HD23	0.51	2.26	16	6
1:A:474:LEU:HD22	1:A:514:TYR:CE2	0.50	2.41	15	10
1:A:342:VAL:CG2	1:A:378:ALA:HB3	0.50	2.36	11	1
1:A:392:MET:SD	1:A:409:LEU:HD22	0.49	2.47	11	1
1:A:356:PHE:CE2	1:A:431:PHE:HB3	0.49	2.42	15	1
1:A:389:GLN:CD	1:A:389:GLN:H	0.49	2.11	19	4

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:356:PHE:CE2	1:A:431:PHE:CG	0.48	3.01	11	2
1:A:508:LEU:C	1:A:508:LEU:HD22	0.48	2.28	10	11
1:A:340:LEU:HD23	1:A:340:LEU:C	0.48	2.28	3	6
1:A:340:LEU:HD21	1:A:407:VAL:HG13	0.48	1.85	16	7
1:A:390:LEU:C	1:A:390:LEU:HD13	0.47	2.28	9	10
1:A:390:LEU:HD13	1:A:390:LEU:C	0.47	2.29	15	10
1:A:340:LEU:HD11	1:A:407:VAL:CG1	0.47	2.40	8	1
1:A:356:PHE:CD2	1:A:368:VAL:HG21	0.47	2.45	16	1
1:A:458:HIS:CD2	1:A:495:LEU:CB	0.46	2.99	9	20
1:A:528:LYS:HE2	1:A:528:LYS:HA	0.46	1.88	6	1
1:A:389:GLN:H	1:A:389:GLN:CD	0.46	2.13	3	7
1:A:497:GLN:CG	1:A:531:ILE:HD12	0.46	2.41	11	18
1:A:459:LEU:CB	1:A:524:VAL:HG22	0.45	2.41	17	1
1:A:340:LEU:HD21	1:A:407:VAL:CG1	0.45	2.42	3	2
1:A:356:PHE:CE2	1:A:368:VAL:HG21	0.45	2.47	20	2
1:A:462:ILE:O	1:A:462:ILE:HG23	0.45	2.11	1	3
1:A:389:GLN:NE2	1:A:389:GLN:H	0.44	2.10	20	1
1:A:459:LEU:HB3	1:A:524:VAL:HG22	0.44	1.89	17	1
1:A:495:LEU:CD2	1:A:531:ILE:CD1	0.43	2.92	5	17
1:A:458:HIS:CD2	1:A:495:LEU:HB3	0.43	2.49	12	4
1:A:427:LEU:H	1:A:427:LEU:CD1	0.43	2.26	16	4
1:A:483:LYS:N	1:A:497:GLN:O	0.42	2.52	16	20
1:A:427:LEU:CD1	1:A:427:LEU:H	0.42	2.28	18	3
1:A:415:VAL:HG12	1:A:416:GLN:H	0.42	1.75	15	4
1:A:506:GLN:CD	1:A:506:GLN:C	0.41	2.79	7	1
1:A:340:LEU:HG	1:A:392:MET:SD	0.41	2.55	11	1
1:A:461:ASN:CB	1:A:521:HIS:HA	0.41	2.46	17	1
1:A:389:GLN:H	1:A:389:GLN:NE2	0.41	2.13	6	1
1:A:362:TYR:CE2	1:A:395:LEU:HD11	0.41	2.50	17	1
1:A:459:LEU:HB2	1:A:523:ARG:O	0.41	2.16	14	1
1:A:367:ARG:CG	1:A:368:VAL:N	0.41	2.84	14	1
1:A:459:LEU:N	1:A:459:LEU:HD23	0.41	2.31	14	1
1:A:345:LEU:H	1:A:345:LEU:HD22	0.40	1.76	10	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	174/207 (84%)	134±3 (77±2%)	31±4 (18±2%)	9±2 (5±1%)	3	23
All	All	3480/4140 (84%)	2684 (77%)	610 (18%)	186 (5%)	3	23

All 20 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	385	GLY	20
1	A	482	VAL	20
1	A	405	ILE	20
1	A	461	ASN	20
1	A	351	THR	20
1	A	479	GLY	19
1	A	450	ILE	12
1	A	515	ASN	11
1	A	397	GLY	10
1	A	402	GLY	8
1	A	520	HIS	7
1	A	386	ASN	5
1	A	431	PHE	3
1	A	384	ASP	3
1	A	521	HIS	2
1	A	432	GLY	2
1	A	417	LEU	1
1	A	421	GLY	1
1	A	336	GLY	1
1	A	376	ASP	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	150/178 (84%)	126±2 (84±1%)	24±2 (16±1%)	5	42
All	All	3000/3560 (84%)	2518 (84%)	482 (16%)	5	42

All 43 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	496	LEU	20
1	A	495	LEU	20
1	A	508	LEU	20
1	A	349	MET	20
1	A	515	ASN	20
1	A	505	ILE	20
1	A	403	LYS	20
1	A	498	MET	20
1	A	396	ASN	20
1	A	475	PHE	20
1	A	427	LEU	20
1	A	492	LYS	20
1	A	514	TYR	20
1	A	497	GLN	20
1	A	355	LEU	20
1	A	472	ARG	19
1	A	459	LEU	17
1	A	366	GLN	13
1	A	386	ASN	12
1	A	523	ARG	12
1	A	417	LEU	11
1	A	389	GLN	11
1	A	483	LYS	11
1	A	400	MET	10
1	A	416	GLN	7
1	A	409	LEU	7
1	A	398	GLN	7
1	A	521	HIS	6
1	A	506	GLN	5
1	A	522	LEU	4
1	A	462	ILE	4
1	A	358	LEU	3
1	A	337	ASN	3
1	A	395	LEU	3
1	A	486	LYS	3
1	A	353	GLN	3
1	A	436	LEU	3
1	A	487	PHE	2
1	A	477	ASN	2
1	A	528	LYS	1
1	A	509	ILE	1
1	A	415	VAL	1

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Mol	Chain	Res	Type	Models (Total)
1	A	384	ASP	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 [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 71% for the well-defined parts and 60% 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	1769
Number of shifts mapped to atoms	1769
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
$^{13}\text{C}_\alpha$	171	-0.07 ± 0.12	None needed (< 0.5 ppm)
$^{13}\text{C}_\beta$	152	0.01 ± 0.12	None needed (< 0.5 ppm)
$^{13}\text{C}'$	0	—	None (insufficient data)
^{15}N	172	1.22 ± 0.41	Should be applied

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 71%, i.e. 1500 atoms were assigned a chemical shift out of a possible 2103. 26 out of 36 assigned methyl groups (LEU and VAL) were assigned stereospecifically.

	Total	^1H	^{13}C	^{15}N
Backbone	666/861 (77%)	333/343 (97%)	167/350 (48%)	166/168 (99%)
Sidechain	794/1104 (72%)	487/642 (76%)	286/417 (69%)	21/45 (47%)

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	Total	¹H	¹³C	¹⁵N
Aromatic	40/138 (29%)	40/76 (53%)	0/56 (0%)	0/6 (0%)
Overall	1500/2103 (71%)	860/1061 (81%)	453/823 (55%)	187/219 (85%)

The following table shows the completeness of the chemical shift assignments for the full structure. The overall completeness is 60%, i.e. 1534 atoms were assigned a chemical shift out of a possible 2540. 26 out of 38 assigned methyl groups (LEU and VAL) were assigned stereospecifically.

	Total	¹H	¹³C	¹⁵N
Backbone	686/1017 (67%)	343/405 (85%)	171/414 (41%)	172/198 (87%)
Sidechain	806/1336 (60%)	494/783 (63%)	290/490 (59%)	22/63 (35%)
Aromatic	42/187 (22%)	42/103 (41%)	0/76 (0%)	0/8 (0%)
Overall	1534/2540 (60%)	879/1291 (68%)	461/980 (47%)	194/269 (72%)

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	345	LEU	CD2	5.97	32.60 – 15.60	-10.7
1	A	453	PRO	HA	1.45	6.05 – 2.75	-8.9

7.1.5 Random Coil Index (RCI) plots ⓘ

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

Random coil index (RCI) for chain A:

