



Full wwPDB NMR Structure Validation Report ⓘ

Jun 23, 2024 – 01:03 AM EDT

PDB ID : 6RH5
BMRB ID : 34394
Title : Solution structure and ¹H, ¹³C and ¹⁵N chemical shift assignments for
NECAP1 PHear domain
Authors : Owen, D.J.; Neuhaus, D.; Yang, J.-C.; Herrmann, T.
Deposited on : 2019-04-18

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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 types of validation reports are described at

<http://www.wwpdb.org/validation/2017/FAQs#types>.

The following versions of software and data (see [references ⓘ](#)) 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) : 2.37.1

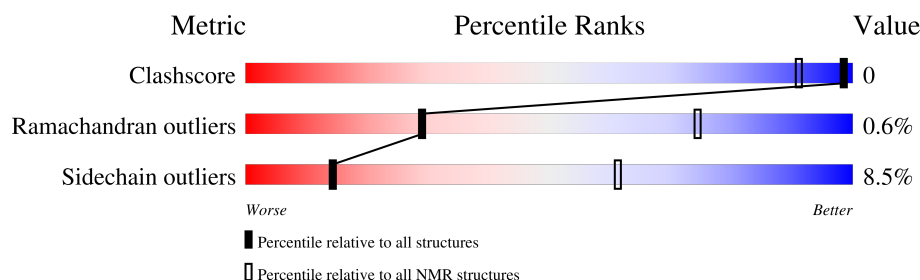
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

SOLUTION NMR

The overall completeness of chemical shifts assignment is 85%.

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	138	

2 Ensemble composition and analysis

This entry contains 30 models. Model 6 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:9-A:22, A:31-A:97, A:103-A:128 (107)	0.34	6

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 3 single-model clusters were found.

Cluster number	Models
1	1, 2, 3, 4, 5, 6, 8, 9, 10, 11, 12, 14, 15, 16, 17, 20, 23, 25, 26, 27
2	7, 13, 18, 19, 28
3	22, 24
Single-model clusters	21; 29; 30

3 Entry composition

There is only 1 type of molecule in this entry. The entry contains 2168 atoms, of which 1069 are hydrogens and 0 are deuteriums.

- Molecule 1 is a protein called Adaptin ear-binding coat-associated protein 1.

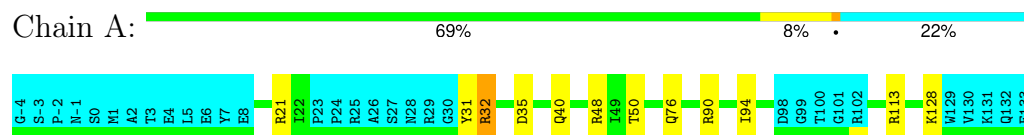
Mol	Chain	Residues	Atoms						Trace
1	A	138	Total	C	H	N	O	S	0
			2168	695	1069	190	212	2	

There are 5 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	-4	GLY	-	expression tag	UNP Q8NC96
A	-3	SER	-	expression tag	UNP Q8NC96
A	-2	PRO	-	expression tag	UNP Q8NC96
A	-1	ASN	-	expression tag	UNP Q8NC96
A	0	SER	-	expression tag	UNP Q8NC96

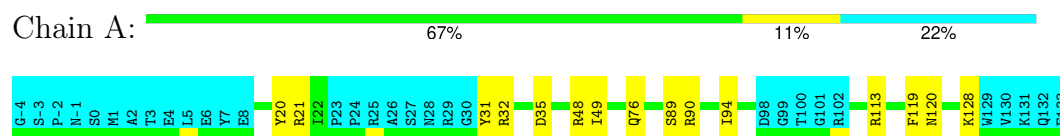
4.2.3 Score per residue for model 3

- Molecule 1: Adaptin ear-binding coat-associated protein 1



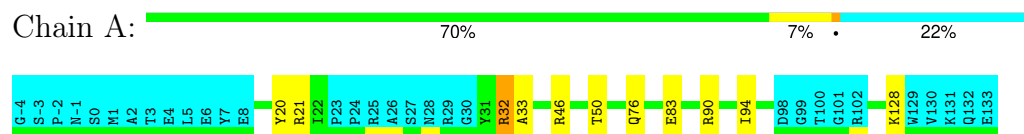
4.2.4 Score per residue for model 4

- Molecule 1: Adaptin ear-binding coat-associated protein 1



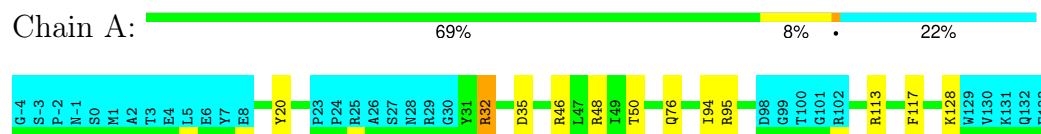
4.2.5 Score per residue for model 5

- Molecule 1: Adaptin ear-binding coat-associated protein 1



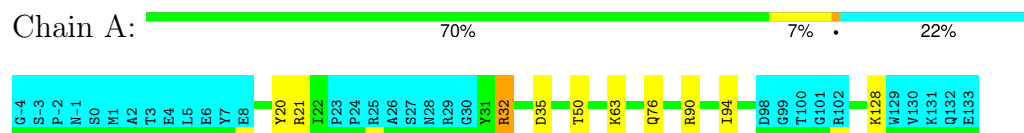
4.2.6 Score per residue for model 6 (medoid)

- Molecule 1: Adaptin ear-binding coat-associated protein 1



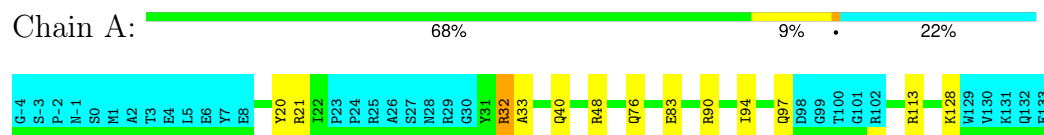
4.2.7 Score per residue for model 7

- Molecule 1: Adaptin ear-binding coat-associated protein 1



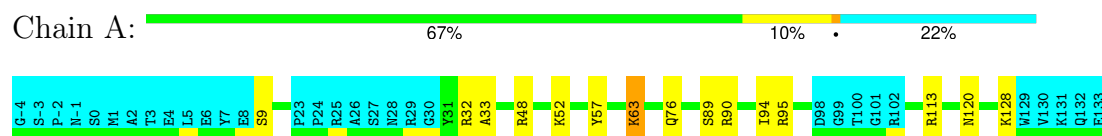
4.2.8 Score per residue for model 8

- Molecule 1: Adaptin ear-binding coat-associated protein 1



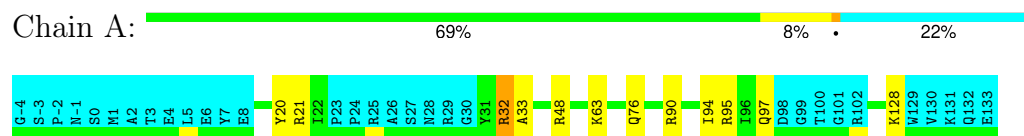
4.2.9 Score per residue for model 9

- Molecule 1: Adaptin ear-binding coat-associated protein 1



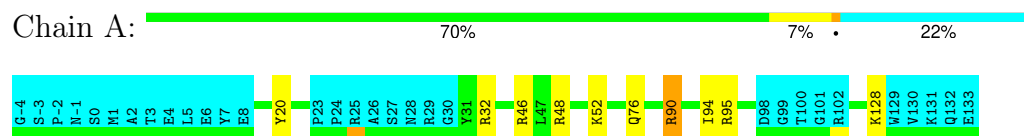
4.2.10 Score per residue for model 10

- Molecule 1: Adaptin ear-binding coat-associated protein 1



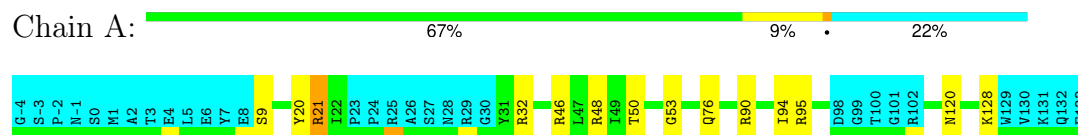
4.2.11 Score per residue for model 11

- Molecule 1: Adaptin ear-binding coat-associated protein 1



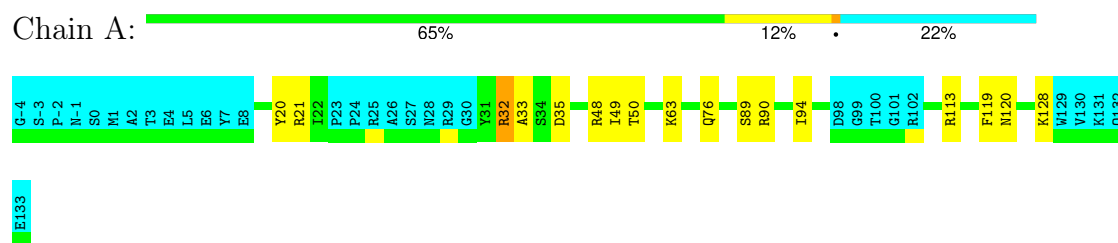
4.2.12 Score per residue for model 12

- Molecule 1: Adaptin ear-binding coat-associated protein 1



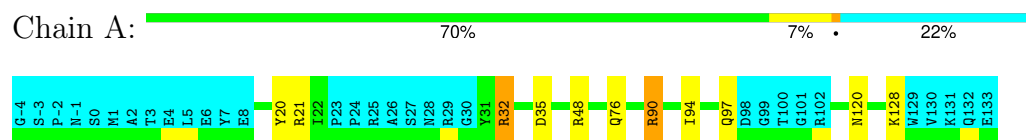
4.2.13 Score per residue for model 13

- Molecule 1: Adaptin ear-binding coat-associated protein 1



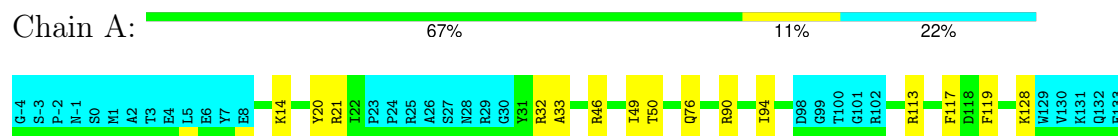
4.2.14 Score per residue for model 14

- Molecule 1: Adaptin ear-binding coat-associated protein 1



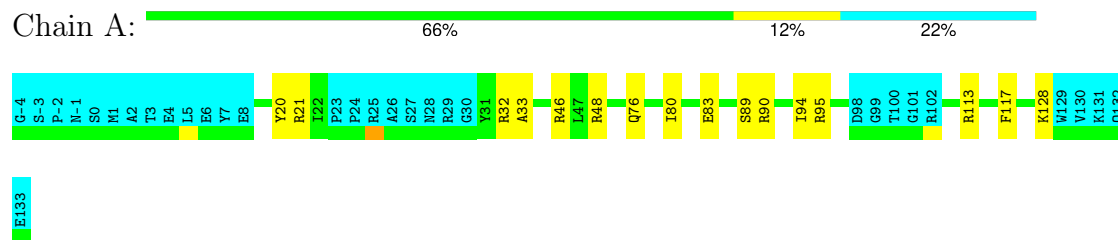
4.2.15 Score per residue for model 15

- Molecule 1: Adaptin ear-binding coat-associated protein 1



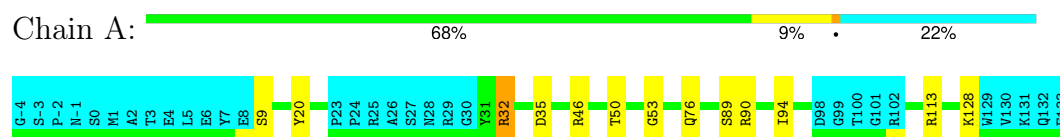
4.2.16 Score per residue for model 16

- Molecule 1: Adaptin ear-binding coat-associated protein 1



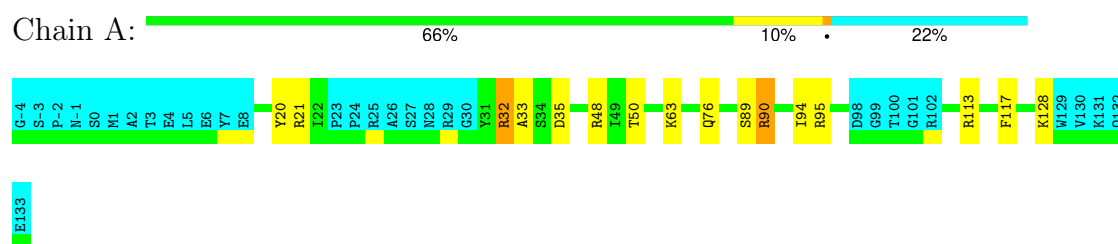
4.2.17 Score per residue for model 17

- Molecule 1: Adaptin ear-binding coat-associated protein 1



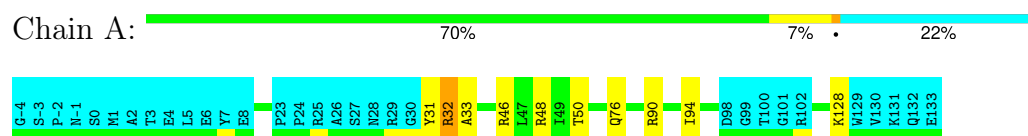
4.2.18 Score per residue for model 18

- Molecule 1: Adaptin ear-binding coat-associated protein 1



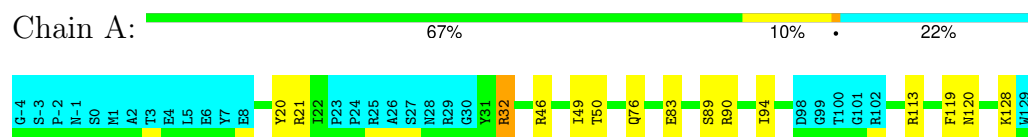
4.2.19 Score per residue for model 19

- Molecule 1: Adaptin ear-binding coat-associated protein 1



4.2.20 Score per residue for model 20

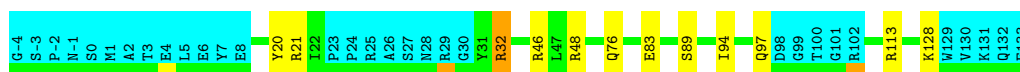
- Molecule 1: Adaptin ear-binding coat-associated protein 1



4.2.21 Score per residue for model 21

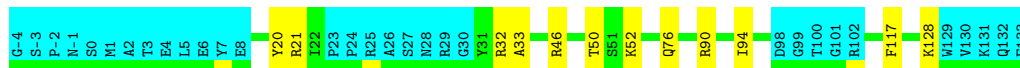
- Molecule 1: Adaptin ear-binding coat-associated protein 1





4.2.22 Score per residue for model 22

- Molecule 1: Adaptin ear-binding coat-associated protein 1



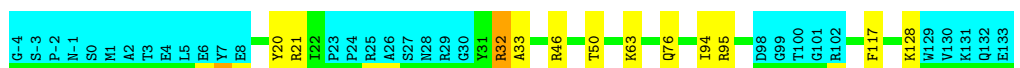
4.2.23 Score per residue for model 23

- Molecule 1: Adaptin ear-binding coat-associated protein 1



4.2.24 Score per residue for model 24

- Molecule 1: Adaptin ear-binding coat-associated protein 1



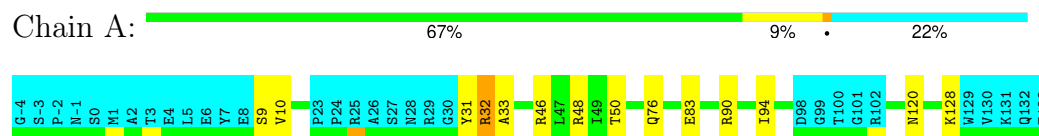
4.2.25 Score per residue for model 25

- Molecule 1: Adaptin ear-binding coat-associated protein 1



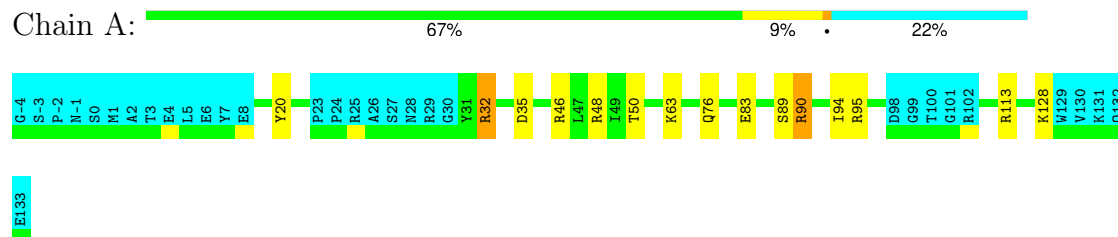
4.2.26 Score per residue for model 26

- Molecule 1: Adaptin ear-binding coat-associated protein 1



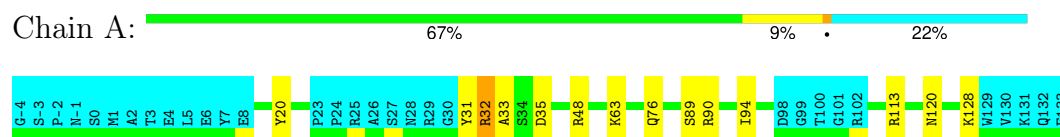
4.2.27 Score per residue for model 27

- Molecule 1: Adaptin ear-binding coat-associated protein 1



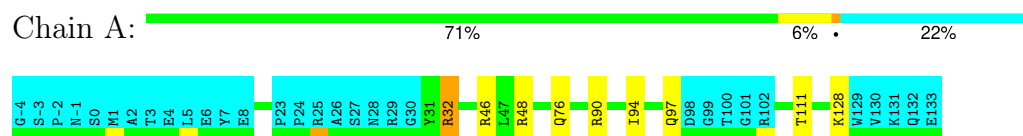
4.2.28 Score per residue for model 28

- Molecule 1: Adaptin ear-binding coat-associated protein 1



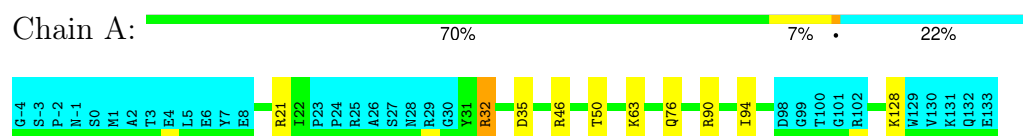
4.2.29 Score per residue for model 29

- Molecule 1: Adaptin ear-binding coat-associated protein 1



4.2.30 Score per residue for model 30

- Molecule 1: Adaptin ear-binding coat-associated protein 1



5 Refinement protocol and experimental data overview

The models were refined using the following method: *torsion angle dynamics, simulated annealing, molecular dynamics*.

Of the 50 calculated structures, 30 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
UNIO	structure calculation	2.8.1
Xplor-NIH	structure calculation	2.28
Amber	structure calculation	11

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	1580
Number of shifts mapped to atoms	1580
Number of unparsed shifts	0
Number of shifts with mapping errors	0
Number of shifts with mapping warnings	0
Assignment completeness (well-defined parts)	85%

6 Model quality i

6.1 Standard geometry i

The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 5$ is considered an outlier worth inspection. RMSZ is the (average) root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	#Z>5	RMSZ	#Z>5
1	A	0.73±0.00	0±0/880 (0.0± 0.0%)	1.05±0.02	5±1/1194 (0.4± 0.1%)
All	All	0.73	0/26400 (0.0%)	1.05	149/35820 (0.4%)

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±0.3
All	All	0	3

There are no bond-length outliers.

All unique angle outliers are listed below. They are sorted according to the Z-score of the worst occurrence in the ensemble.

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)	Models	
								Worst	Total
1	A	46	ARG	NE-CZ-NH2	9.34	124.97	120.30	23	19
1	A	48	ARG	NE-CZ-NH2	8.04	124.32	120.30	21	22
1	A	21	ARG	NE-CZ-NH2	7.34	123.97	120.30	7	19
1	A	31	TYR	CB-CG-CD2	-6.84	116.89	121.00	3	4
1	A	31	TYR	CB-CG-CD1	-6.44	117.14	121.00	19	3
1	A	90	ARG	NE-CZ-NH2	6.38	123.49	120.30	15	24
1	A	32	ARG	NE-CZ-NH2	6.28	123.44	120.30	1	22
1	A	90	ARG	NE-CZ-NH1	6.24	123.42	120.30	1	1
1	A	113	ARG	NE-CZ-NH2	5.84	123.22	120.30	9	15
1	A	21	ARG	NE-CZ-NH1	-5.70	117.45	120.30	10	5
1	A	48	ARG	NE-CZ-NH1	-5.64	117.48	120.30	21	2
1	A	95	ARG	NE-CZ-NH2	5.48	123.04	120.30	27	9
1	A	32	ARG	NE-CZ-NH1	-5.46	117.57	120.30	7	3
1	A	32	ARG	CD-NE-CZ	5.06	130.69	123.60	21	1

There are no chirality outliers.

All unique planar outliers are listed below. They are sorted by the frequency of occurrence in the ensemble.

Mol	Chain	Res	Type	Group	Models (Total)
1	A	117	PHE	Peptide	2
1	A	111	THR	Peptide	1

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	859	847	847	0±0
All	All	25770	25410	25410	7

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 0.

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

Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:63:LYS:H	1:A:63:LYS:CD	0.49	2.20	9	1
1:A:49:ILE:HD11	1:A:119:PHE:CD1	0.46	2.46	20	4
1:A:52:LYS:HE3	1:A:57:TYR:CE1	0.41	2.49	9	1
1:A:49:ILE:HD11	1:A:119:PHE:CD2	0.40	2.51	15	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	107/138 (78%)	101±2 (94±1%)	5±2 (5±2%)	1±0 (1±0%)	29	74
All	All	3210/4140 (78%)	3031 (94%)	161 (5%)	18 (1%)	29	74

All 3 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	33	ALA	15
1	A	53	GLY	2
1	A	52	LYS	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	93/118 (79%)	85±1 (92±2%)	8±1 (8±2%)	14	61
All	All	2790/3540 (79%)	2553 (92%)	237 (8%)	14	61

All 22 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	ARG	30
1	A	76	GLN	30
1	A	94	ILE	30
1	A	128	LYS	30
1	A	20	TYR	22
1	A	50	THR	17
1	A	35	ASP	12
1	A	89	SER	12
1	A	120	ASN	11
1	A	63	LYS	9
1	A	83	GLU	7
1	A	97	GLN	6
1	A	9	SER	4
1	A	90	ARG	4
1	A	117	PHE	4
1	A	40	GLN	3
1	A	113	ARG	1
1	A	21	ARG	1
1	A	14	LYS	1
1	A	80	ILE	1
1	A	52	LYS	1

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Mol	Chain	Res	Type	Models (Total)
1	A	10	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

The completeness of assignment taking into account all chemical shift lists is 85% for the well-defined parts and 84% for the entire structure.

7.1 Chemical shift list 1

File name: `working_cs.cif`

Chemical shift list name: *starch_output*

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	1580
Number of shifts mapped to atoms	1580
Number of unparsed shifts	0
Number of shifts with mapping errors	0
Number of shifts with mapping warnings	0
Number of shift outliers (ShiftChecker)	4

7.1.2 Chemical shift referencing

The following table shows the suggested chemical shift referencing corrections.

Nucleus	# values	Correction \pm precision, ppm	Suggested action
$^{13}\text{C}_\alpha$	138	-0.10 ± 0.12	None needed (< 0.5 ppm)
$^{13}\text{C}_\beta$	126	-0.24 ± 0.14	None needed (< 0.5 ppm)
$^{13}\text{C}'$	0	—	None (insufficient data)
^{15}N	128	0.36 ± 0.36	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 85%, i.e. 1264 atoms were assigned a chemical shift out of a possible 1479. 0 out of 16 assigned methyl groups (LEU and VAL) were assigned stereospecifically.

	Total	^1H	^{13}C	^{15}N
Backbone	425/534 (80%)	216/217 (100%)	107/214 (50%)	102/103 (99%)
Sidechain	705/799 (88%)	481/518 (93%)	218/247 (88%)	6/34 (18%)

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	Total	¹H	¹³C	¹⁵N
Aromatic	134/146 (92%)	67/71 (94%)	65/72 (90%)	2/3 (67%)
Overall	1264/1479 (85%)	764/806 (95%)	390/533 (73%)	110/140 (79%)

The following table shows the completeness of the chemical shift assignments for the full structure. The overall completeness is 84%, i.e. 1580 atoms were assigned a chemical shift out of a possible 1871. 0 out of 18 assigned methyl groups (LEU and VAL) were assigned stereospecifically.

	Total	¹H	¹³C	¹⁵N
Backbone	543/687 (79%)	277/280 (99%)	138/276 (50%)	128/131 (98%)
Sidechain	883/1017 (87%)	601/656 (92%)	273/314 (87%)	9/47 (19%)
Aromatic	154/167 (92%)	77/81 (95%)	74/82 (90%)	3/4 (75%)
Overall	1580/1871 (84%)	955/1017 (94%)	485/672 (72%)	140/182 (77%)

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	33	ALA	HA	1.48	2.13 – 6.34	-6.6
1	A	33	ALA	HB1	-0.07	0.14 – 2.58	-5.9
1	A	33	ALA	HB2	-0.07	0.14 – 2.58	-5.9
1	A	33	ALA	HB3	-0.07	0.14 – 2.58	-5.9

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:

