



Full wwPDB NMR Structure Validation Report ⓘ

Mar 26, 2026 – 09:54 PM UTC

PDB ID : 2N6J / pdb_00002n6j
BMRB ID : 25766
Title : Solution structure of Zmp1, a zinc-dependent metalloprotease secreted by Clostridium difficile
Authors : Banci, L.; Cantini, F.; Scarselli, M.; Rubino, J.T.; Martinelli, M.
Deposited on : 2015-08-24

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 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 : 4-5-2 with Phenix2.0
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)
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) : 2.49

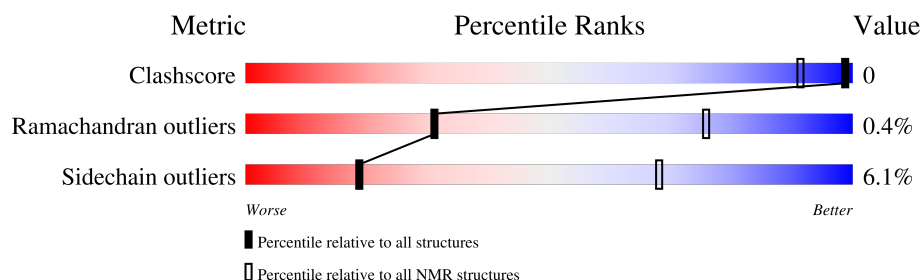
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

SOLUTION NMR

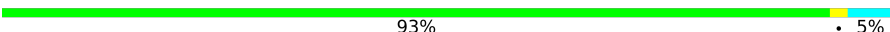
The overall completeness of chemical shifts assignment is 91%.

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	229148	14424
Ramachandran outliers	224038	12848
Sidechain outliers	223484	12823

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	195	 93% • 5%

2 Ensemble composition and analysis

This entry contains 20 models. Model 13 is the overall representative, medoid model (most similar to other models). The authors have identified model 1 as representative, based on the following criterion: *fewest violations*.

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:28-A:100, A:109-A:220 (185)	0.95	13

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 and 6 single-model clusters were found.

Cluster number	Models
1	1, 7, 18, 30
2	5, 8, 14, 17
3	6, 13, 29
4	11, 34, 40
Single-model clusters	2; 23; 24; 36; 38; 28

3 Entry composition

There are 3 unique types of molecules in this entry. The entry contains 3040 atoms, of which 1511 are hydrogens and 0 are deuteriums.

- Molecule 1 is a protein called Zinc metalloprotease Zmp1.

Mol	Chain	Residues	Atoms						Trace
1	A	195	Total	C	H	N	O	S	0
			3036	969	1509	259	297	2	

There is a discrepancy between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	26	GLY	-	expression tag	UNP Q183R7

- Molecule 2 is ZINC ION (CCD ID: ZN) (formula: Zn).

Mol	Chain	Residues	Atoms	
2	A	1	Total	Zn
			1	1

- Molecule 3 is water.

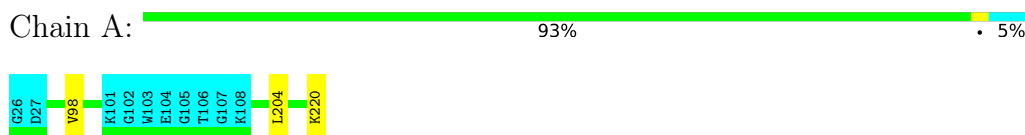
Mol	Chain	Residues	Atoms		
3	A	1	Total	H	O
			3	2	1

4 Residue-property plots

4.1 Average score per residue in the NMR ensemble

These plots are provided for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic is the same as shown in the summary in section 1 of this report. The second graphic shows the sequence where residues are colour-coded according to the number of geometric quality criteria for which they contain at least one outlier: green = 0, yellow = 1, orange = 2 and red = 3 or more. Stretches of 2 or more consecutive residues without any outliers are shown as green connectors. Residues which are classified as ill-defined in the NMR ensemble, are shown in cyan with an underline colour-coded according to the previous scheme. Residues which were present in the experimental sample, but not modelled in the final structure are shown in grey.

- Molecule 1: Zinc metalloprotease Zmp1

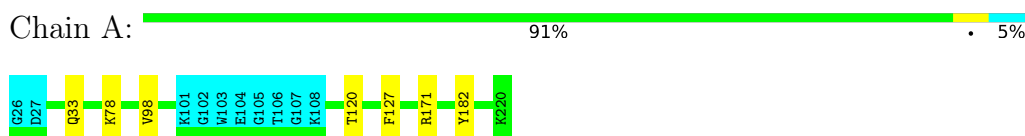


4.2 Scores per residue for each member of the ensemble

Colouring as in section 4.1 above.

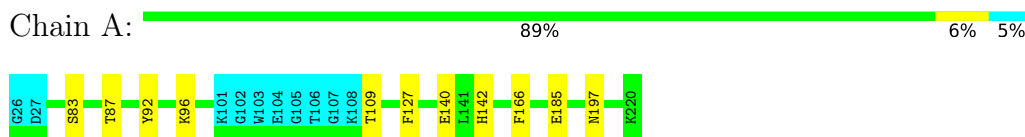
4.2.1 Score per residue for model 1

- Molecule 1: Zinc metalloprotease Zmp1



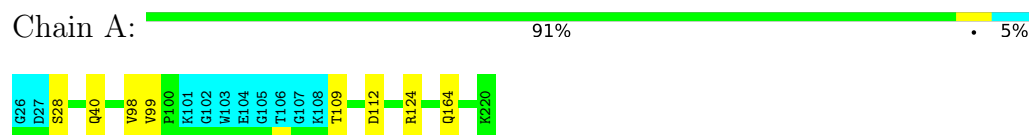
4.2.2 Score per residue for model 2

- Molecule 1: Zinc metalloprotease Zmp1



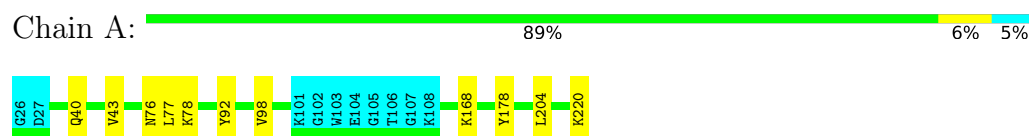
4.2.3 Score per residue for model 5

- Molecule 1: Zinc metalloprotease Zmp1



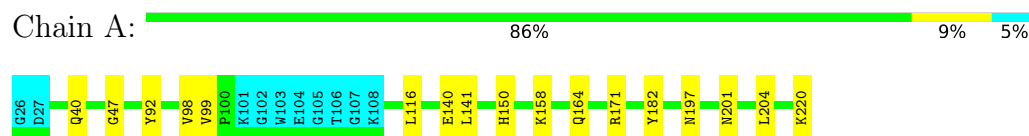
4.2.4 Score per residue for model 6

- Molecule 1: Zinc metalloprotease Zmp1



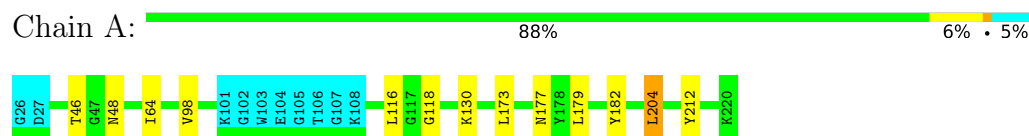
4.2.5 Score per residue for model 7

- Molecule 1: Zinc metalloprotease Zmp1



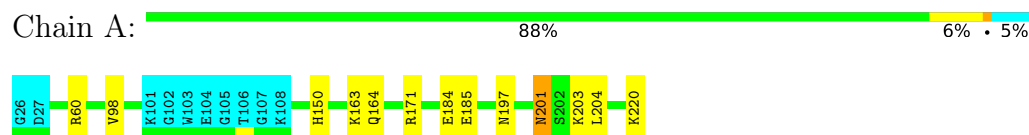
4.2.6 Score per residue for model 8

- Molecule 1: Zinc metalloprotease Zmp1



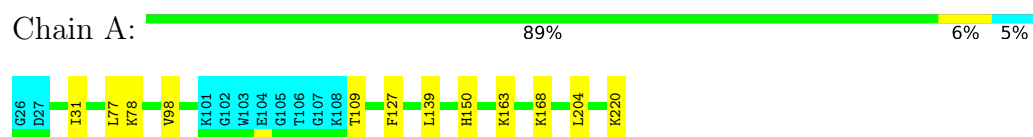
4.2.7 Score per residue for model 11

- Molecule 1: Zinc metalloprotease Zmp1



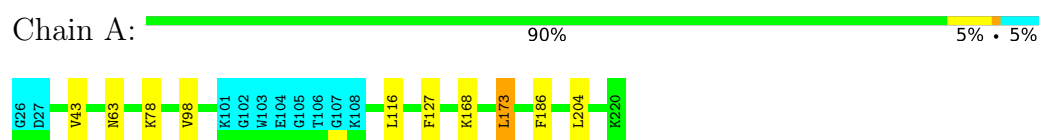
4.2.8 Score per residue for model 13 (medoid)

- Molecule 1: Zinc metalloprotease Zmp1



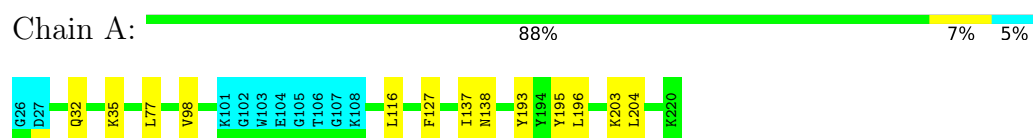
4.2.9 Score per residue for model 14

- Molecule 1: Zinc metalloprotease Zmp1



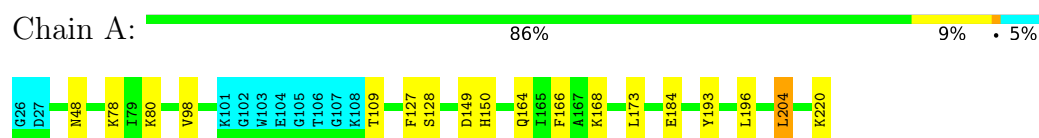
4.2.10 Score per residue for model 17

- Molecule 1: Zinc metalloprotease Zmp1



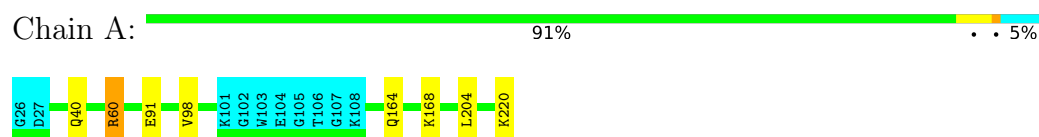
4.2.11 Score per residue for model 18

- Molecule 1: Zinc metalloprotease Zmp1



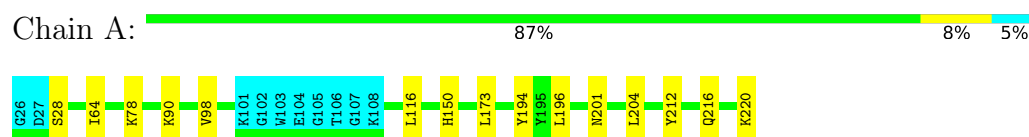
4.2.12 Score per residue for model 23

- Molecule 1: Zinc metalloprotease Zmp1



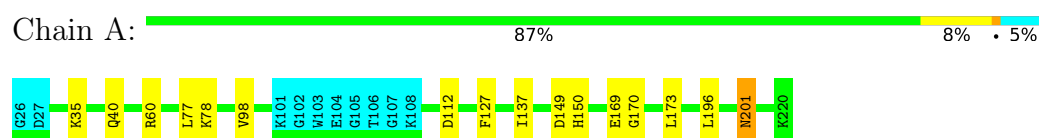
4.2.13 Score per residue for model 24

- Molecule 1: Zinc metalloprotease Zmp1



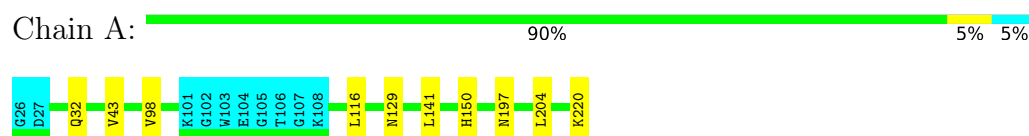
4.2.14 Score per residue for model 29

- Molecule 1: Zinc metalloprotease Zmp1



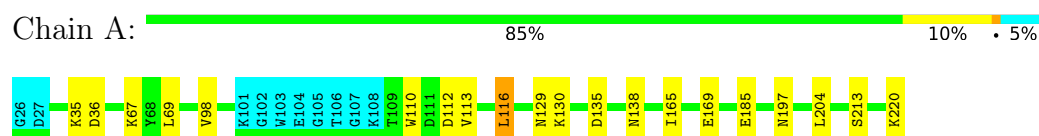
4.2.15 Score per residue for model 30

- Molecule 1: Zinc metalloprotease Zmp1



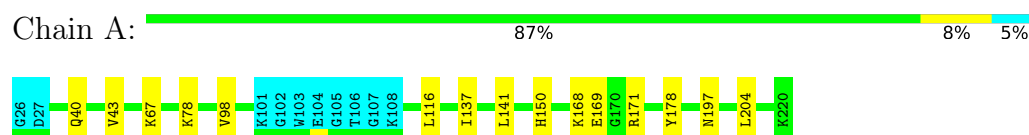
4.2.16 Score per residue for model 34

- Molecule 1: Zinc metalloprotease Zmp1



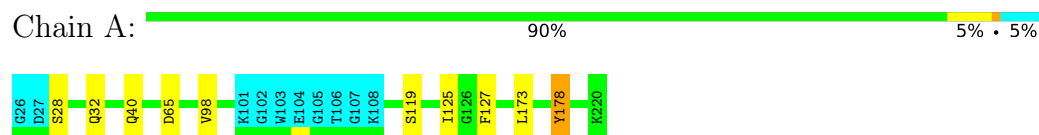
4.2.17 Score per residue for model 36

- Molecule 1: Zinc metalloprotease Zmp1



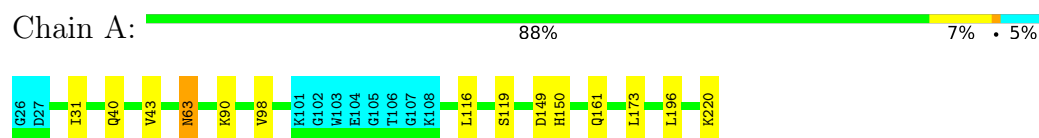
4.2.18 Score per residue for model 38

- Molecule 1: Zinc metalloprotease Zmp1



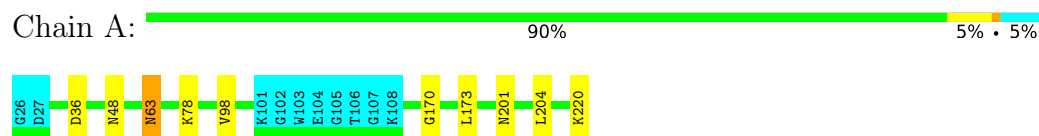
4.2.19 Score per residue for model 40

- Molecule 1: Zinc metalloprotease Zmp1



4.2.20 Score per residue for model 28

- Molecule 1: Zinc metalloprotease Zmp1



5 Refinement protocol and experimental data overview

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

Of the 400 calculated structures, 20 were deposited, based on the following criterion: *target function*.

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

Software name	Classification	Version
CYANA	structure solution	2.1
CYANA	refinement	2.1
PSVS	structure solution	
PSVS	refinement	
Amber	refinement	10
CARA	refinement	2

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	2373
Number of shifts mapped to atoms	2373
Number of unparsed shifts	0
Number of shifts with mapping errors	0
Number of shifts with mapping warnings	0
Assignment completeness (well-defined parts)	91%

6 Model quality

6.1 Standard geometry

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

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	0.84±0.01	0±0/1483 (0.0± 0.0%)	1.40±0.02	2±1/2004 (0.1± 0.1%)
All	All	0.84	0/29660 (0.0%)	1.40	35/40080 (0.1%)

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	0.9±0.8
All	All	0	19

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	201	ASN	CA-CB-CG	7.65	120.25	112.60	11	4
1	A	63	ASN	CA-CB-CG	7.03	119.63	112.60	28	2
1	A	127	PHE	CA-CB-CG	6.85	120.65	113.80	1	6
1	A	166	PHE	CA-CB-CG	6.21	120.01	113.80	2	2
1	A	116	LEU	CA-C-N	6.03	126.25	121.61	34	4
1	A	116	LEU	C-N-CA	6.03	126.25	121.61	34	4
1	A	150	HIS	CA-CB-CG	5.90	119.70	113.80	36	2
1	A	129	ASN	CA-C-N	5.42	131.89	121.54	34	1
1	A	129	ASN	C-N-CA	5.42	131.89	121.54	34	1
1	A	127	PHE	CA-C-N	5.24	130.01	121.74	18	1
1	A	127	PHE	C-N-CA	5.24	130.01	121.74	18	1
1	A	125	ILE	CA-CB-CG1	5.21	119.26	110.40	38	1

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)	Models	
								Worst	Total
1	A	28	SER	CA-C-N	5.20	127.56	120.54	5	1
1	A	28	SER	C-N-CA	5.20	127.56	120.54	5	1
1	A	109	THR	CA-C-N	5.07	127.79	120.38	13	1
1	A	109	THR	C-N-CA	5.07	127.79	120.38	13	1
1	A	142	HIS	CE1-NE2-CD2	-5.04	103.96	109.00	2	1
1	A	33	GLN	OE1-CD-NE2	-5.01	117.59	122.60	1	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	92	TYR	Sidechain	3
1	A	171	ARG	Sidechain,Peptide	2
1	A	173	LEU	Peptide	2
1	A	60	ARG	Sidechain	2
1	A	119	SER	Peptide	2
1	A	182	TYR	Sidechain	1
1	A	124	ARG	Sidechain	1
1	A	212	TYR	Sidechain	1
1	A	193	TYR	Sidechain	1
1	A	195	TYR	Sidechain	1
1	A	168	LYS	Peptide	1
1	A	137	ILE	Peptide	1
1	A	178	TYR	Sidechain	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	1455	1442	1441	0±0
All	All	29140	28880	28820	5

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:173:LEU:HD23	1:A:186:PHE:CD1	0.51	2.40	14	1
1:A:193:TYR:CG	1:A:204:LEU:HD23	0.45	2.46	18	1
1:A:110:TRP:HA	1:A:113:VAL:HG13	0.44	1.88	34	1
1:A:173:LEU:HD13	1:A:204:LEU:HD21	0.43	1.90	8	1
1:A:194:TYR:CZ	1:A:212:TYR:CD2	0.41	3.09	24	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	184/195 (94%)	174±3 (94±1%)	9±3 (5±2%)	1±1 (0±1%)	31	76
All	All	3680/3900 (94%)	3476 (94%)	189 (5%)	15 (0%)	31	76

All 10 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	127	PHE	2
1	A	64	ILE	2
1	A	130	LYS	2
1	A	28	SER	2
1	A	170	GLY	2
1	A	47	GLY	1
1	A	118	GLY	1
1	A	48	ASN	1
1	A	129	ASN	1
1	A	65	ASP	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	157/163 (96%)	147±3 (94±2%)	10±3 (6±2%)	19	68
All	All	3140/3260 (96%)	2949 (94%)	191 (6%)	19	68

All 59 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	98	VAL	19
1	A	204	LEU	14
1	A	220	LYS	11
1	A	78	LYS	9
1	A	40	GLN	8
1	A	150	HIS	7
1	A	197	ASN	6
1	A	116	LEU	6
1	A	164	GLN	5
1	A	43	VAL	5
1	A	168	LYS	5
1	A	196	LEU	5
1	A	173	LEU	5
1	A	77	LEU	4
1	A	109	THR	3
1	A	185	GLU	3
1	A	112	ASP	3
1	A	178	TYR	3
1	A	141	LEU	3
1	A	201	ASN	3
1	A	63	ASN	3
1	A	32	GLN	3
1	A	35	LYS	3
1	A	149	ASP	3
1	A	169	GLU	3
1	A	140	GLU	2
1	A	99	VAL	2
1	A	171	ARG	2
1	A	182	TYR	2
1	A	48	ASN	2
1	A	60	ARG	2
1	A	163	LYS	2
1	A	184	GLU	2
1	A	203	LYS	2
1	A	31	ILE	2
1	A	137	ILE	2

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Models (Total)
1	A	138	ASN	2
1	A	90	LYS	2
1	A	36	ASP	2
1	A	67	LYS	2
1	A	120	THR	1
1	A	83	SER	1
1	A	87	THR	1
1	A	96	LYS	1
1	A	76	ASN	1
1	A	158	LYS	1
1	A	46	THR	1
1	A	177	ASN	1
1	A	179	LEU	1
1	A	139	LEU	1
1	A	80	LYS	1
1	A	128	SER	1
1	A	91	GLU	1
1	A	216	GLN	1
1	A	69	LEU	1
1	A	135	ASP	1
1	A	165	ILE	1
1	A	213	SER	1
1	A	161	GLN	1

6.3.3 RNA ⓘ

There are no RNA molecules in this entry.

6.4 Non-standard residues in protein, DNA, RNA chains ⓘ

There are no non-standard protein/DNA/RNA residues in this entry.

6.5 Carbohydrates ⓘ

There are no oligosaccharides in this entry.

6.6 Ligand geometry ⓘ

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 91% for the well-defined parts and 91% for the entire structure.

7.1 Chemical shift list 1

File name: working_cs.cif

Chemical shift list name: *assigned_chem_shift_list_1*

7.1.1 Bookkeeping

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	2373
Number of shifts mapped to atoms	2373
Number of unparsed shifts	0
Number of shifts with mapping errors	0
Number of shifts with mapping warnings	0
Number of shift outliers (ShiftChecker)	14

7.1.2 Chemical shift referencing

The following table shows the suggested chemical shift referencing corrections.

Nucleus	# values	Correction $\pm$ precision, ppm	Suggested action
$^{13}\text{C}_\alpha$	192	-0.66 ± 0.15	Should be checked
$^{13}\text{C}_\beta$	176	0.38 ± 0.11	None needed (< 0.5 ppm)
$^{13}\text{C}'$	154	-0.28 ± 0.18	None needed (< 0.5 ppm)
^{15}N	184	0.59 ± 0.34	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 91%, i.e. 2285 atoms were assigned a chemical shift out of a possible 2502. 0 out of 30 assigned methyl groups (LEU and VAL) were assigned stereospecifically.

	Total	^1H	^{13}C	^{15}N
Backbone	882/928 (95%)	374/378 (99%)	331/370 (89%)	177/180 (98%)
Sidechain	1249/1360 (92%)	845/881 (96%)	377/427 (88%)	27/52 (52%)

Continued on next page...

Continued from previous page...

	Total	¹ H	¹³ C	¹⁵ N
Aromatic	154/214 (72%)	81/102 (79%)	64/103 (62%)	9/9 (100%)
Overall	2285/2502 (91%)	1300/1361 (96%)	772/900 (86%)	213/241 (88%)

The following table shows the completeness of the chemical shift assignments for the full structure. The overall completeness is 91%, i.e. 2371 atoms were assigned a chemical shift out of a possible 2614. 0 out of 30 assigned methyl groups (LEU and VAL) were assigned stereospecifically.

	Total	¹ H	¹³ C	¹⁵ N
Backbone	921/982 (94%)	391/402 (97%)	346/390 (89%)	184/190 (97%)
Sidechain	1286/1406 (91%)	869/909 (96%)	390/443 (88%)	27/54 (50%)
Aromatic	164/226 (73%)	86/108 (80%)	68/108 (63%)	10/10 (100%)
Overall	2371/2614 (91%)	1346/1419 (95%)	804/941 (85%)	221/254 (87%)

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.

List Id	Chain	Res	Type	Atom	Shift, ppm	Expected range, ppm	Z-score
1	A	124	ARG	NE	137.43	76.53 – 92.65	32.8
1	A	60	ARG	NE	135.95	76.53 – 92.65	31.9
1	A	211	THR	HG1	5.89	0.08 – 2.19	22.5
1	A	106	THR	HG1	5.82	0.08 – 2.19	22.2
1	A	100	PRO	HG3	-0.63	0.33 – 3.48	-8.0
1	A	95	LEU	HG	-0.56	-0.13 – 3.16	-6.3
1	A	194	TYR	HD1	5.18	5.49 – 8.39	-6.1
1	A	194	TYR	HD2	5.18	5.48 – 8.39	-6.0
1	A	100	PRO	HG2	0.12	0.41 – 3.45	-5.9
1	A	65	ASP	H	5.02	5.52 – 11.08	-5.9
1	A	170	GLY	HA2	1.88	2.15 – 5.77	-5.8
1	A	124	ARG	HD3	1.64	1.81 – 4.39	-5.7
1	A	136	ALA	H	11.40	5.31 – 11.08	5.6
1	A	210	GLN	H	11.29	5.39 – 11.05	5.4

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. 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:

