Full wwPDB NMR Structure Validation Report (i)

Jun 22, 2022 – 01:13 pm BST

PDB ID	:	7ZBQ
Title	:	Structure of the ADP-ribosyltransferase TccC3HVR from Photorhabdus Luminescens
Authors	:	Lindemann, F.; Belyy, A.; Friedrich, D.; Schmieder, P.; Bardiaux, B.; Roderer, D.; Funk, J.; Protze, J.; Bieling, P.; Oschkinat, H.; Raunser, S.
Deposited on	:	2022-03-24

The following versions of software and data (see references (i)) 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)
RCI	:	v_1n_11_5_13_A (Berjanski et al., 2005)
PANAV	:	Wang et al. (2010)
ShiftChecker	:	2.29
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.29

1 Overall quality at a glance ⓘ

The following experimental techniques were used to determine the structure:
SOLUTION NMR

The overall completeness of chemical shifts assignment is 79%.

Percentile scores (ranging between 0-100) for global validation metrics of the entry are shown in the following graphic. The table shows the number of entries on which the scores are based.
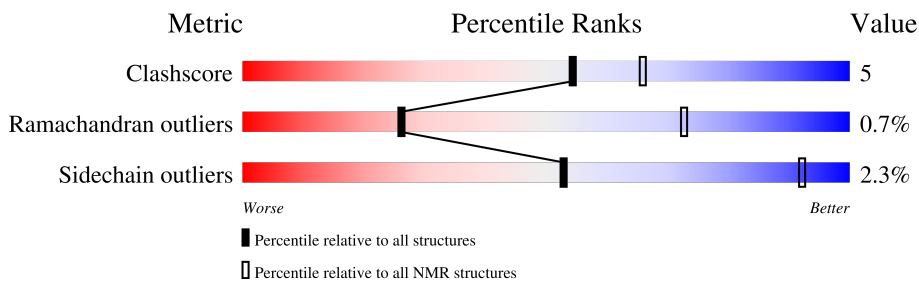
Metric	Whole archive (#Entries)	NMR archive (#Entries)
Clashscore	158937	12864
Ramachandran outliers	154571	11451
Sidechain outliers	154315	11428

The table below summarises the geometric issues observed across the polymeric chains and their fit to the experimental data. The red, orange, yellow and green segments indicate the fraction of residues that contain outliers for >=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 <=5%

Mol	Chain	Length	Quality of chain
1	A	194	78% 7% · 7% 7%

2 Ensemble composition and analysis ⓘ

This entry contains 10 models. Model 2 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:103-A:201, A:207-A:229, A:238-A:281 (166)	0.39	2

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 2 clusters and 2 single-model clusters were found.

Cluster number	Models
1	1, 2, 3, 4, 6, 7
2	9, 10
Single-model clusters	5; 8

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wwPDB
PROTEIN DATA BANK

3 Entry composition ⓘ

There is only 1 type of molecule in this entry. The entry contains 2860 atoms, of which 1441 are hydrogens and 0 are deuteriums.

- Molecule 1 is a protein called TccC3.

Mol	Chain	Residues	Atoms						Trace
			Total	C	H	N	O	S	
1	A	180	2860	905	1441	239	271	4	0

There are 9 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	97	MET	-	initiating methionine	UNP Q8GF97
A	283	GLY	-	expression tag	UNP Q8GF97
A	284	THR	-	expression tag	UNP Q8GF97
A	285	LEU	-	expression tag	UNP Q8GF97
A	286	GLU	-	expression tag	UNP Q8GF97
A	287	VAL	-	expression tag	UNP Q8GF97
A	288	LEU	-	expression tag	UNP Q8GF97
A	289	PHE	-	expression tag	UNP Q8GF97
A	290	GLN	-	expression tag	UNP Q8GF97

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.

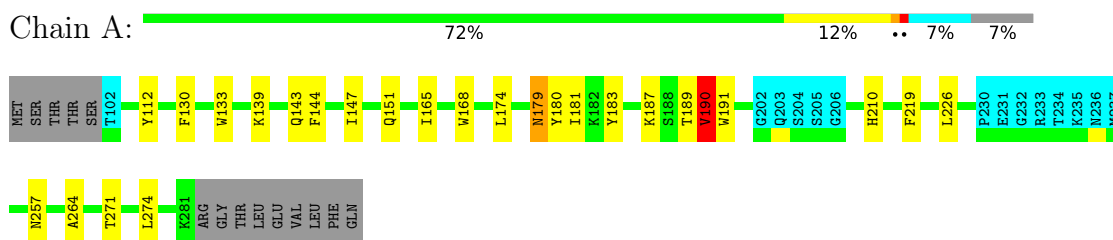• Molecule 1: TccC3

Chain A:
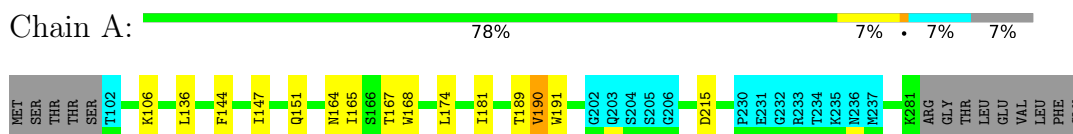
4.2　Scores per residue for each member of the ensemble
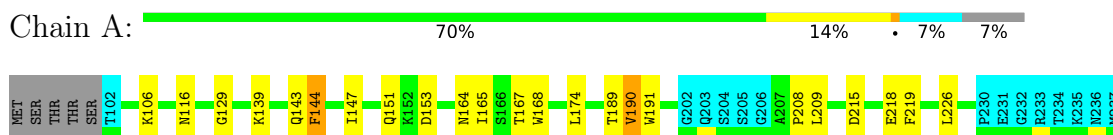
Colouring as in section 4.1 above.

4.2.1　Score per residue for model 1

• Molecule 1: TccC3

Chain A:

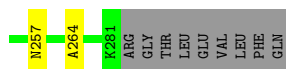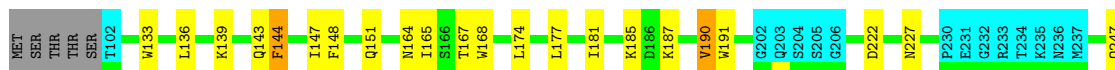### 4.2.2　Score per residue for model 2 (medoid)

• Molecule 1: TccC3

Chain A:

D244 S252 N257 A264 T270 T271 I272 H280 K281 ARG GLY THR LEU GLU VAL LEU PHE GLN

4.2.3 Score per residue for model 3

● Molecule 1: TccC3

Chain A: 73%   11%   •   7%   7%

MET SER THR SER T102 W133 L136 K139 Q143 F144 I147 F148 Q151 N164 I165 S166 T167 W168 L174 L177 I181 K185 D186 K187 V190 W191 G202 Q203 S204 S205 G206 D222 N227 P230 E231 G232 R233 T234 K235 N236 M237 Q247

N257 A264 K281 ARG GLY THR LEU GLU VAL LEU PHE GLN

4.2.4 Score per residue for model 4

● Molecule 1: TccC3

Chain A: 72%   13%   •   7%   7%

MET SER THR SER T102 N103 K107 S108 F109 F119 Q123 W133 L136 F144 I147 F148 Q151 P158 T161 N164 I165 S166 T167 W168 K175 D176 L177 K187 S188 T189 V190 W191 G202 Q203 S204 S205 G206 E218 P228 L229 P230 E231 G232

R233 T234 K235 N236 M237 N257 A264 K281 ARG GLY THR LEU GLU VAL LEU PHE GLN

4.2.5 Score per residue for model 5

● Molecule 1: TccC3

Chain A: 73%   11%   ••   7%   7%

MET SER THR SER T102 K106 G129 F144 A145 S146 I147 Q151 I165 W168 Y180 I181 T189 V190 W191 G202 Q203 S204 S205 G206 D215 E218 F219 L226 L229 P230 E231 G232 T234 K235 N236 M237 V238 P239 G259 I272 P273 L274

V277 K281 ARG GLY THR LEU GLU VAL LEU PHE GLN
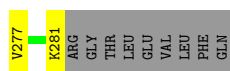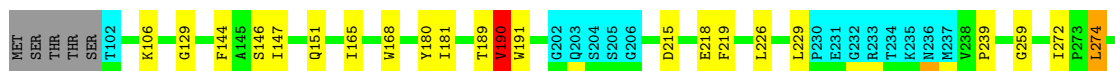
4.2.6 Score per residue for model 6

● Molecule 1: TccC3

Chain A: 69%   16%   •   7%   7%

MET SER THR SER T102 N103 L104 Q105 K106 R117 S118 F119 Q123 G129 T134 P135 L136 K139 Q143 F144 A145 S146 I147 Q151 N164 I165 S166 T167 W168 L174 I181 T189 V190 W191 N197 G202 Q203 S204 S205 G206 D215 L216 Y217 P230

E231 G232 R233 T234 K235 N236 M237 V238 H258 D263 L269 I272 P273 L274 V277 K281 ARG GLY THR LEU GLU VAL LEU PHE GLN
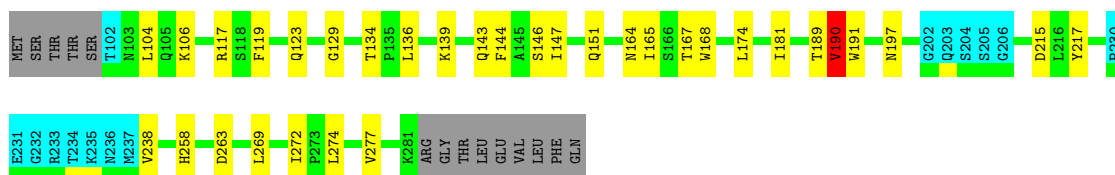
4.2.7 Score per residue for model 7

• Molecule 1: TccC3

Chain A: 65%   20%   •   7%   7%

MET SER THR SER T102 N116 R117 S118 F119 Q123 E128 W133 T134 P135 L136 Q143 F144 I147 Q151 K152 D153 T161 N164 I165 S166 T167 W168 L174 K175 N179 Y180 I181 K182 Y183 K187 S188 T189 V190 W191 N197 G202 Q203 S204 S205 G206

E218 P228 L229 P230 E231 G232 R233 T234 K235 N236 M237 V238 P239 S240 D263 L269 L274 V277 K281 ARG GLY THR LEU GLU VAL LEU PHE GLN
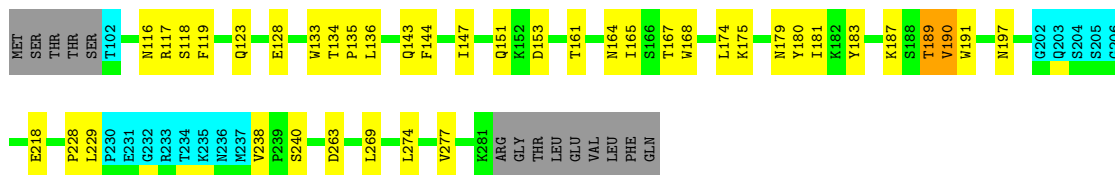
4.2.8 Score per residue for model 8

• Molecule 1: TccC3

Chain A: 73%   12%   •   7%   7%

MET SER THR SER T102 K106 S118 E121 F144 I147 F148 Q151 K152 D153 N164 I165 S166 T167 W168 L174 L177 S178 T189 V190 W191 G202 Q203 S204 S205 G206 D215 P230 E231 G232 R233 T234 K235 N236 M237 V238 P239 Q247 T250

A255 P260 F268 K281 ARG GLY THR LEU GLU VAL LEU PHE GLN
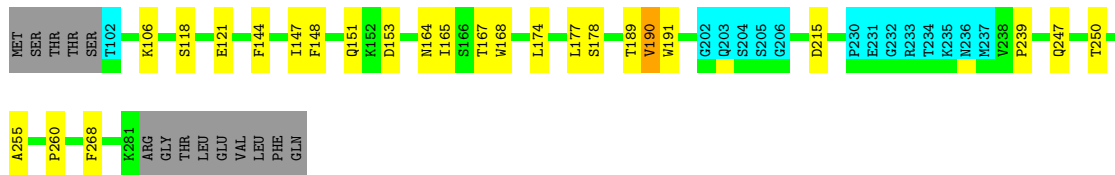
4.2.9 Score per residue for model 9

• Molecule 1: TccC3

Chain A: 71%   14%   •   7%   7%

MET SER THR SER T102 K106 F119 Q123 G129 T134 P135 L136 F144 I147 Q151 T161 N164 I165 S166 T167 W168 K175 I181 K182 K185 T189 V190 W191 G202 Q203 S204 S205 G206 D215 P230 E231 G232 R233 T234 K235 N236 M237

N257 H258 G259 P260 A264 L269 I272 K281 ARG GLY THR LEU GLU VAL LEU PHE GLN

4.2.10 Score per residue for model 10

• Molecule 1: TccC3

Chain A:

69%   16%   • 7%   7%

MET SER THR THR SER T102 Q105 K106 T110 L111 S118 F119 E120 E121 M122 Q123 G129 W133 L136 F144 A145 S146 I147 F148 I149 G150 Q151 S155 N156 T161 I165 K173 D176 N179 Y180 I181 K187 V190 W191 G202 Q203 S204 S205 G206

K211 I212 D215 P228 L229 P230 E231 G232 R233 T234 K235 N236 M237 L269 I272 K281 ARG GLY THR LEU GLU VAL LEU PHE GLN

5 Refinement protocol and experimental data overview ⓘ

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

Of the 400 calculated structures, 10 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
ARIA	structure calculation	2.3.2
CNS	refinement	1.21

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	2067
Number of shifts mapped to atoms	2067
Number of unparsed shifts	0
Number of shifts with mapping errors	0
Number of shifts with mapping warnings	0
Assignment completeness (well-defined parts)	79%

6 Model quality ⓘ

6.1 Standard geometry ⓘ

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	0.36±0.04	1±1/1351 (0.0± 0.1%)	0.42±0.01	0±0/1832 (0.0± 0.0%)
All	All	0.36	6/13510 (0.0%)	0.42	0/18320 (0.0%)

All unique bond 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(Å)	Ideal(Å)	Models	
								Worst	Total
1	A	180	TYR	CE1-CZ	-6.66	1.29	1.38	7	3
1	A	180	TYR	CE2-CZ	6.52	1.47	1.38	7	3

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	1320	1346	1343	14±2
All	All	13200	13460	13430	143

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 5.

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

Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:147:ILE:HA	1:A:151:GLN:O	0.68	1.88	7	8
1:A:181:ILE:HA	1:A:191:TRP:CZ2	0.65	2.27	7	7
1:A:116:ASN:O	1:A:117:ARG:HD2	0.63	1.93	7	1
1:A:136:LEU:HB2	1:A:269:LEU:O	0.60	1.97	9	4
1:A:164:ASN:O	1:A:167:THR:HG22	0.55	2.00	9	7
1:A:134:THR:O	1:A:190:VAL:HA	0.54	2.03	7	3
1:A:165:ILE:HA	1:A:168:TRP:CE3	0.53	2.38	2	9
1:A:106:LYS:HD3	1:A:215:ASP:O	0.53	2.03	9	5
1:A:274:LEU:O	1:A:277:VAL:HG12	0.52	2.05	6	3
1:A:218:GLU:O	1:A:228:PRO:HA	0.51	2.06	4	2
1:A:139:LYS:O	1:A:143:GLN:HG2	0.51	2.05	6	2
1:A:119:PHE:O	1:A:123:GLN:HG2	0.51	2.05	9	5
1:A:257:ASN:OD1	1:A:264:ALA:HB1	0.51	2.06	4	5
1:A:148:PHE:CZ	1:A:177:LEU:HD22	0.51	2.41	3	3
1:A:143:GLN:HB3	1:A:153:ASP:O	0.50	2.06	7	1
1:A:146:SER:HB2	1:A:151:GLN:NE2	0.50	2.22	10	2
1:A:139:LYS:O	1:A:143:GLN:HG3	0.49	2.06	1	2
1:A:129:GLY:HA3	1:A:272:ILE:O	0.49	2.08	10	5
1:A:135:PRO:HA	1:A:190:VAL:O	0.49	2.08	7	1
1:A:133:TRP:CD2	1:A:187:LYS:HD2	0.48	2.43	3	3
1:A:144:PHE:O	1:A:147:ILE:HG12	0.48	2.08	9	7
1:A:189:THR:O	1:A:190:VAL:HB	0.48	2.08	7	2
1:A:110:THR:HA	1:A:212:ILE:O	0.48	2.08	10	1
1:A:219:PHE:CD1	1:A:226:LEU:HG	0.48	2.43	2	3
1:A:133:TRP:CE3	1:A:187:LYS:HD2	0.48	2.44	10	2
1:A:179:ASN:O	1:A:183:TYR:HD2	0.47	1.92	7	2
1:A:146:SER:O	1:A:149:ILE:HG12	0.47	2.09	10	1
1:A:155:SER:O	1:A:156:ASN:HB3	0.46	2.10	10	1
1:A:133:TRP:HB2	1:A:187:LYS:O	0.46	2.09	7	1
1:A:118:SER:HB2	1:A:121:GLU:CB	0.46	2.40	8	2
1:A:136:LEU:H	1:A:136:LEU:HD23	0.46	1.71	3	2
1:A:197:ASN:ND2	1:A:263:ASP:HA	0.45	2.25	6	2
1:A:104:LEU:HG	1:A:217:TYR:CE2	0.45	2.47	6	1
1:A:181:ILE:HA	1:A:191:TRP:CH2	0.44	2.48	6	1
1:A:178:SER:OG	1:A:239:PRO:HG2	0.44	2.13	8	1
1:A:247:GLN:HB3	1:A:250:THR:OG1	0.44	2.13	8	1
1:A:222:ASP:HB2	1:A:227:ASN:ND2	0.43	2.27	3	1
1:A:116:ASN:HA	1:A:208:PRO:CD	0.43	2.44	2	1
1:A:189:THR:HB	1:A:191:TRP:CE2	0.42	2.49	8	3
1:A:146:SER:HB3	1:A:151:GLN:HB2	0.42	1.92	6	1
1:A:173:LYS:HB2	1:A:176:ASP:OD2	0.42	2.14	10	1
1:A:259:GLY:N	1:A:260:PRO:HD3	0.42	2.28	9	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models Worst	Models Total
1:A:174:LEU:H	1:A:174:LEU:HD22	0.42	1.74	1	3
1:A:158:PRO:HG2	1:A:161:THR:OG1	0.42	2.14	4	1
1:A:161:THR:O	1:A:165:ILE:HG13	0.42	2.14	4	4
1:A:274:LEU:O	1:A:274:LEU:HD13	0.42	2.15	7	1
1:A:112:TYR:HA	1:A:210:HIS:O	0.41	2.15	1	1
1:A:106:LYS:HD2	1:A:215:ASP:O	0.41	2.16	2	1
1:A:174:LEU:HD22	1:A:174:LEU:H	0.41	1.75	6	3
1:A:189:THR:O	1:A:190:VAL:HG12	0.41	2.16	1	1
1:A:133:TRP:CD1	1:A:187:LYS:HB3	0.41	2.49	1	2
1:A:111:LEU:O	1:A:211:LYS:HA	0.41	2.15	10	1
1:A:252:SER:O	1:A:270:THR:HG21	0.41	2.15	2	1
1:A:255:ALA:HB2	1:A:268:PHE:CD1	0.41	2.51	8	1
1:A:247:GLN:HA	1:A:247:GLN:OE1	0.41	2.16	3	1
1:A:182:LYS:O	1:A:185:LYS:HE2	0.41	2.15	9	1
1:A:174:LEU:O	1:A:177:LEU:HD23	0.41	2.16	3	1
1:A:107:LYS:HB3	1:A:109:PHE:CE1	0.41	2.51	4	1
1:A:130:PHE:O	1:A:271:THR:HG23	0.40	2.17	1	1
1:A:189:THR:O	1:A:190:VAL:CB	0.40	2.68	5	1
1:A:209:LEU:O	1:A:280:HIS:HB3	0.40	2.16	2	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	165/194 (85%)	159±2 (96±1%)	5±2 (3±1%)	1±0 (1±0%)	26	73
All	All	1650/1940 (85%)	1590 (96%)	48 (3%)	12 (1%)	26	73

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	190	VAL	10
1	A	259	GLY	1
1	A	260	PRO	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	149/173 (86%)	146±1 (98±0%)	4±1 (2±0%)	53	92
All	All	1490/1730 (86%)	1455 (98%)	35 (2%)	53	92

All 16 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	190	VAL	9
1	A	144	PHE	5
1	A	175	LYS	3
1	A	189	THR	3
1	A	179	ASN	2
1	A	274	LEU	2
1	A	153	ASP	2
1	A	244	ASP	1
1	A	185	LYS	1
1	A	103	ASN	1
1	A	281	LYS	1
1	A	117	ARG	1
1	A	258	HIS	1
1	A	118	SER	1
1	A	128	GLU	1
1	A	105	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 monosaccharides in this entry.

6.6   Ligand geometry ⓘ

There are no ligands in this entry.

6.7   Other polymers ⓘ

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 79% for the well-defined parts and 78% for the entire structure.

7.1 Chemical shift list 1

File name: working_cs.cif

Chemical shift list name: *assigned_chem_shift_list*

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	2067
Number of shifts mapped to atoms	2067
Number of unparsed shifts	0
Number of shifts with mapping errors	0
Number of shifts with mapping warnings	0
Number of shift outliers (ShiftChecker)	10

7.1.2 Chemical shift referencing ⓘ

The following table shows the suggested chemical shift referencing corrections.

Nucleus	# values	Correction ± precision, *ppm*	Suggested action
$^{13}C_\alpha$	187	0.30 ± 0.11	None needed (< 0.5 ppm)
$^{13}C_\beta$	176	0.03 ± 0.10	None needed (< 0.5 ppm)
$^{13}C'$	0	—	None (insufficient data)
^{15}N	171	0.54 ± 0.18	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 79%, i.e. 1647 atoms were assigned a chemical shift out of a possible 2081. 0 out of 22 assigned methyl groups (LEU and VAL) were assigned stereospecifically.

	Total	^1H	^{13}C	^{15}N
Backbone	634/808 (78%)	318/321 (99%)	165/332 (50%)	151/155 (97%)
Sidechain	867/1109 (78%)	529/653 (81%)	320/412 (78%)	18/44 (41%)

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	Total	**^{1}H**	**^{13}C**	**^{15}N**
Aromatic	146/164 (89%)	77/86 (90%)	66/69 (96%)	3/9 (33%)
Overall	1647/2081 (79%)	924/1060 (87%)	551/813 (68%)	172/208 (83%)

The following table shows the completeness of the chemical shift assignments for the full structure. The overall completeness is 78%, i.e. 1737 atoms were assigned a chemical shift out of a possible 2235. 0 out of 22 assigned methyl groups (LEU and VAL) were assigned stereospecifically.

	Total	**^{1}H**	**^{13}C**	**^{15}N**
Backbone	680/876 (78%)	340/348 (98%)	178/360 (49%)	162/168 (96%)
Sidechain	911/1195 (76%)	556/705 (79%)	335/440 (76%)	20/50 (40%)
Aromatic	146/164 (89%)	77/86 (90%)	66/69 (96%)	3/9 (33%)
Overall	1737/2235 (78%)	973/1139 (85%)	579/869 (67%)	185/227 (81%)

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	181	ILE	HG13	-2.37	3.26 − -0.84	-8.7
1	A	176	ASP	HB2	0.64	4.07 − 1.37	-7.7
1	A	113	ARG	HD2	1.67	4.27 − 1.97	-6.3
1	A	106	LYS	HG2	-0.27	2.67 − 0.07	-6.3
1	A	189	THR	HB	2.32	5.82 − 2.52	-5.6
1	A	187	LYS	HE3	1.85	3.86 − 1.96	-5.6
1	A	255	ALA	HB2	-0.02	2.61 − 0.11	-5.5
1	A	255	ALA	HB3	-0.02	2.61 − 0.11	-5.5
1	A	255	ALA	HB1	-0.02	2.61 − 0.11	-5.5
1	A	164	ASN	HB2	1.25	4.36 − 1.26	-5.0

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: