



wwPDB NMR Structure Validation Summary Report ⓘ

Dec 12, 2022 – 08:36 am GMT

PDB ID : 6YEG
EMDB ID : EMD-10792
BMRB ID : 27468
Title : Hybrid structure of the SPP1 tail tube by solid-state NMR and cryo EM - Final EM Refinement
Authors : Zinke, M.; Sachowsky, K.A.A.; Zinn-Justin, S.; Ravelli, R.; Schroder, G.F.; Habeck, M.; Lange, A.
Deposited on : 2020-03-24

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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:

EMDB validation analysis : **NOT EXECUTED**
MolProbity : 4.02b-467
Percentile statistics : 20191225.v01 (using entries in the PDB archive December 25th 2019)
MapQ : **NOT EXECUTED**
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.31.3

1 Overall quality at a glance ⓘ

The following experimental techniques were used to determine the structure:

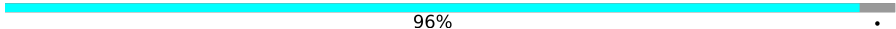
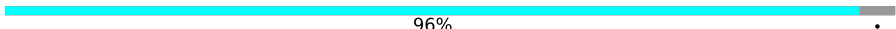
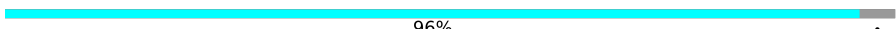
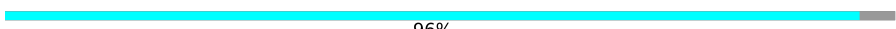
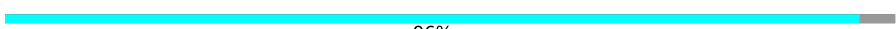






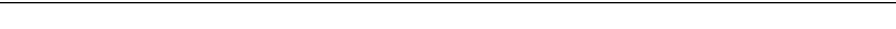
ELECTRON MICROSCOPY, SOLID-STATE NMR

The reported resolution of this entry is 4.00 Å.

The overall completeness of chemical shifts assignment is 4%.

There are no overall percentile quality scores available for this entry.

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	180	 96% .
1	B	180	 96% .
1	C	180	 96% .
1	D	180	 96% .
1	E	180	 96% .
1	F	180	 96% .
1	G	180	 96% .
1	H	180	 96% .
1	I	180	 96% .
1	J	180	 96% .
1	K	180	 96% .
1	L	180	 96% .

2 Ensemble composition and analysis ⓘ

This entry contains 1 models. Identification of well-defined residues and clustering analysis are not possible.

3 Entry composition

There is only 1 type of molecule in this entry. The entry contains 15756 atoms, of which 0 are hydrogens and 0 are deuteriums.

In the tables below, the AltConf column contains the number of residues with at least one atom in alternate conformation and the Trace column contains the number of residues modelled with at most 2 atoms.

- Molecule 1 is a protein called Tail tube protein gp17.1*.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	A	172	Total	C	N	O	S	0	
			1313	821	216	275	1		
1	B	172	Total	C	N	O	S	0	
			1313	821	216	275	1		
1	C	172	Total	C	N	O	S	0	
			1313	821	216	275	1		
1	D	172	Total	C	N	O	S	0	
			1313	821	216	275	1		
1	E	172	Total	C	N	O	S	0	
			1313	821	216	275	1		
1	F	172	Total	C	N	O	S	0	
			1313	821	216	275	1		
1	G	172	Total	C	N	O	S	0	
			1313	821	216	275	1		
1	H	172	Total	C	N	O	S	0	
			1313	821	216	275	1		
1	I	172	Total	C	N	O	S	0	
			1313	821	216	275	1		
1	J	172	Total	C	N	O	S	0	
			1313	821	216	275	1		
1	K	172	Total	C	N	O	S	0	
			1313	821	216	275	1		
1	L	172	Total	C	N	O	S	0	
			1313	821	216	275	1		

There are 84 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	4	MET	-	initiating methionine	UNP O48449
A	178	HIS	-	expression tag	UNP O48449
A	179	HIS	-	expression tag	UNP O48449
A	180	HIS	-	expression tag	UNP O48449
A	181	HIS	-	expression tag	UNP O48449
A	182	HIS	-	expression tag	UNP O48449

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Chain	Residue	Modelled	Actual	Comment	Reference
A	183	HIS	-	expression tag	UNP O48449
B	4	MET	-	initiating methionine	UNP O48449
B	178	HIS	-	expression tag	UNP O48449
B	179	HIS	-	expression tag	UNP O48449
B	180	HIS	-	expression tag	UNP O48449
B	181	HIS	-	expression tag	UNP O48449
B	182	HIS	-	expression tag	UNP O48449
B	183	HIS	-	expression tag	UNP O48449
C	4	MET	-	initiating methionine	UNP O48449
C	178	HIS	-	expression tag	UNP O48449
C	179	HIS	-	expression tag	UNP O48449
C	180	HIS	-	expression tag	UNP O48449
C	181	HIS	-	expression tag	UNP O48449
C	182	HIS	-	expression tag	UNP O48449
C	183	HIS	-	expression tag	UNP O48449
D	4	MET	-	initiating methionine	UNP O48449
D	178	HIS	-	expression tag	UNP O48449
D	179	HIS	-	expression tag	UNP O48449
D	180	HIS	-	expression tag	UNP O48449
D	181	HIS	-	expression tag	UNP O48449
D	182	HIS	-	expression tag	UNP O48449
D	183	HIS	-	expression tag	UNP O48449
E	4	MET	-	initiating methionine	UNP O48449
E	178	HIS	-	expression tag	UNP O48449
E	179	HIS	-	expression tag	UNP O48449
E	180	HIS	-	expression tag	UNP O48449
E	181	HIS	-	expression tag	UNP O48449
E	182	HIS	-	expression tag	UNP O48449
E	183	HIS	-	expression tag	UNP O48449
F	4	MET	-	initiating methionine	UNP O48449
F	178	HIS	-	expression tag	UNP O48449
F	179	HIS	-	expression tag	UNP O48449
F	180	HIS	-	expression tag	UNP O48449
F	181	HIS	-	expression tag	UNP O48449
F	182	HIS	-	expression tag	UNP O48449
F	183	HIS	-	expression tag	UNP O48449
G	4	MET	-	initiating methionine	UNP O48449
G	178	HIS	-	expression tag	UNP O48449
G	179	HIS	-	expression tag	UNP O48449
G	180	HIS	-	expression tag	UNP O48449
G	181	HIS	-	expression tag	UNP O48449
G	182	HIS	-	expression tag	UNP O48449

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Chain	Residue	Modelled	Actual	Comment	Reference
G	183	HIS	-	expression tag	UNP O48449
H	4	MET	-	initiating methionine	UNP O48449
H	178	HIS	-	expression tag	UNP O48449
H	179	HIS	-	expression tag	UNP O48449
H	180	HIS	-	expression tag	UNP O48449
H	181	HIS	-	expression tag	UNP O48449
H	182	HIS	-	expression tag	UNP O48449
H	183	HIS	-	expression tag	UNP O48449
I	4	MET	-	initiating methionine	UNP O48449
I	178	HIS	-	expression tag	UNP O48449
I	179	HIS	-	expression tag	UNP O48449
I	180	HIS	-	expression tag	UNP O48449
I	181	HIS	-	expression tag	UNP O48449
I	182	HIS	-	expression tag	UNP O48449
I	183	HIS	-	expression tag	UNP O48449
J	4	MET	-	initiating methionine	UNP O48449
J	178	HIS	-	expression tag	UNP O48449
J	179	HIS	-	expression tag	UNP O48449
J	180	HIS	-	expression tag	UNP O48449
J	181	HIS	-	expression tag	UNP O48449
J	182	HIS	-	expression tag	UNP O48449
J	183	HIS	-	expression tag	UNP O48449
K	4	MET	-	initiating methionine	UNP O48449
K	178	HIS	-	expression tag	UNP O48449
K	179	HIS	-	expression tag	UNP O48449
K	180	HIS	-	expression tag	UNP O48449
K	181	HIS	-	expression tag	UNP O48449
K	182	HIS	-	expression tag	UNP O48449
K	183	HIS	-	expression tag	UNP O48449
L	4	MET	-	initiating methionine	UNP O48449
L	178	HIS	-	expression tag	UNP O48449
L	179	HIS	-	expression tag	UNP O48449
L	180	HIS	-	expression tag	UNP O48449
L	181	HIS	-	expression tag	UNP O48449
L	182	HIS	-	expression tag	UNP O48449
L	183	HIS	-	expression tag	UNP O48449

i

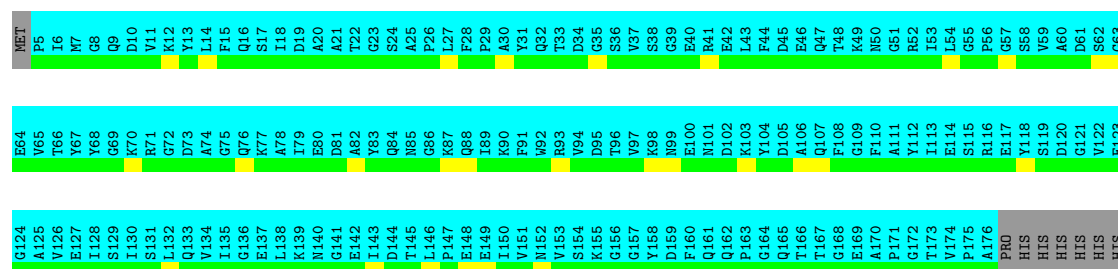
- Molecule 1: Tail tube protein gp17.1*

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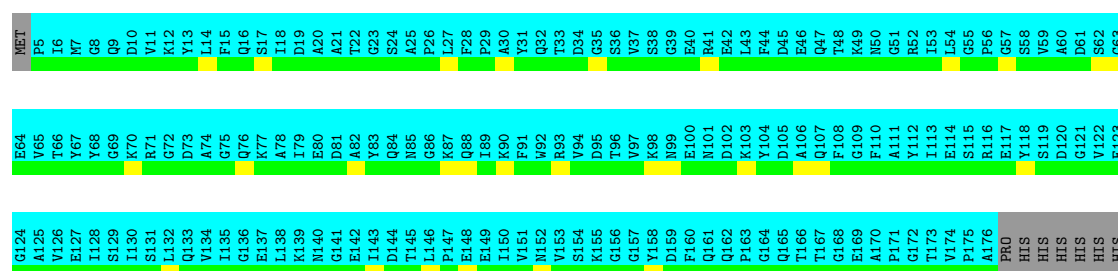
- Molecule 1: Tail tube protein gp17.1*

Chain D:  96%



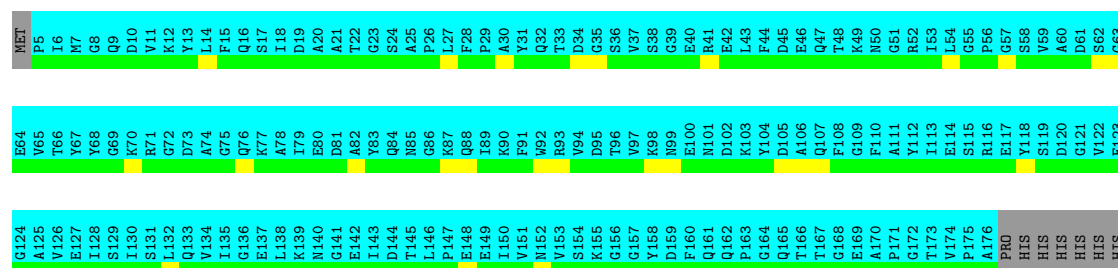
- Molecule 1: Tail tube protein gp17.1*

Chain E:  96%



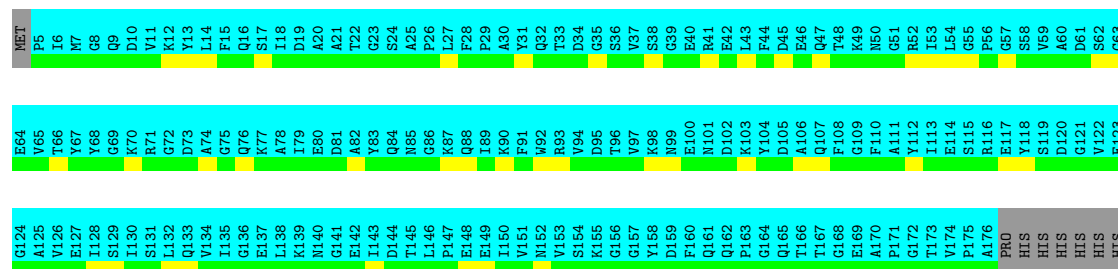
- Molecule 1: Tail tube protein gp17.1*

Chain F:  96%



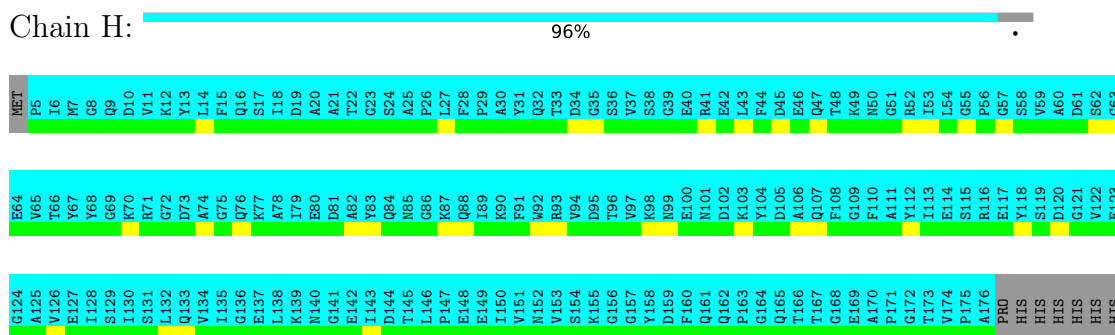
- Molecule 1: Tail tube protein gp17.1*

Chain G:  96%



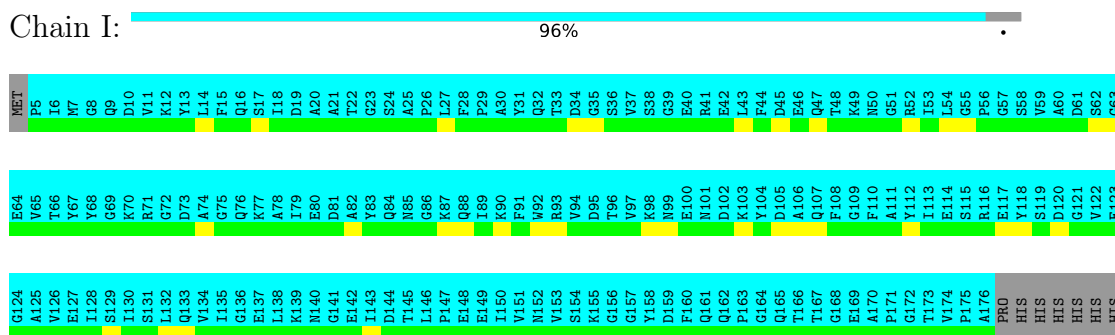
- Molecule 1: Tail tube protein gp17.1*

Chain H:



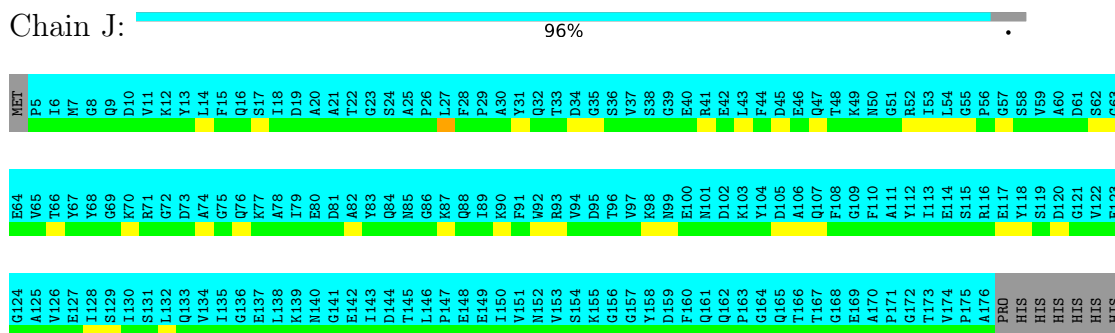
- Molecule 1: Tail tube protein gp17.1*

Chain I:



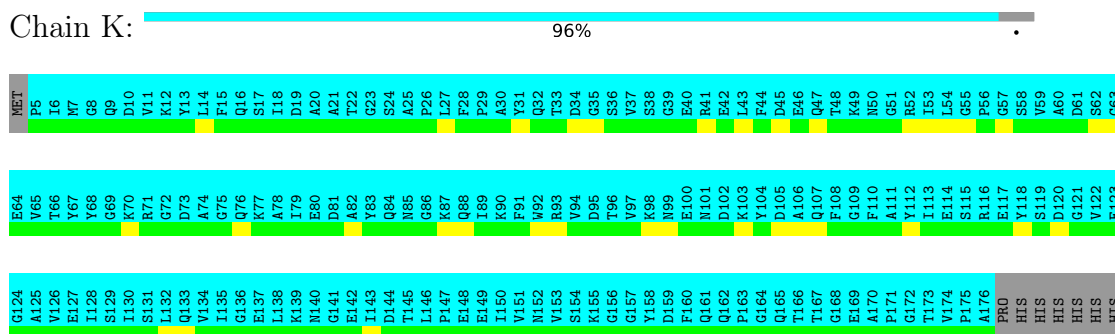
- Molecule 1: Tail tube protein gp17.1*

Chain J:



- Molecule 1: Tail tube protein gp17.1*

Chain K:



- Molecule 1: Tail tube protein gp17.1*

Chain L:

96%

.

MET	P5	I6	M7	G8	Q9	D10	V11	K12	Y13	L14	F15	Q16	S17	I18	D19	A20	A21	T22	G23	S24	A25	P26	L27	F28	P29	A30	Y31	Q32	T33	D34	G35	S36	V37	S38	G39	F40	R41	E42	L43	F44	D45	E46	Q47	F48	K49	N50	G51	R52	I53	L54	G55	P56	G57	S58	V59	A60	D61	S62	G63		
E64	V65	T66	Y67	Y68	G69	K70	R71	G72	D73	A74	G75	G76	K77	A78	I79	E80	D81	A82	Y83	Q84	N85	G86	K87	Q88	I89	K90	F91	W92	R93	V94	D95	T96	V97	K98	N99	E100	N101	D102	K103	Y104	D105	A106	Q107	F108	G109	F110	A111	Y112	I113	E114	S115	R116	E117	Y118	S119	D120	G121	V122	E123		
G124	A125	V126	E127	I128	S129	I130	S131	L132	Q133	V134	I135	G136	E137	L138	K139	N140	G141	E142	I143	D144	T145	L146	P147	E148	E149	I150	V151	N152	V153	S154	K155	G156	G157	Y158	D159	F160	Q161	Q162	P163	G164	Q165	T166	T167	G168	E169	A170	P171	G172	T173	V174	P175	A176	PRO	HIS	HIS	HIS	HIS	HIS	HIS	HIS	HIS

5 Refinement protocol and experimental data overview

The models were refined using the following method: *na*.

Of the 1 calculated structures, 1 were deposited, based on the following criterion: *all calculated structures submitted*.

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

Software name	Classification	Version
Inferential Structure Determination (ISD)	structure calculation	

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	963
Number of shifts mapped to atoms	963
Number of unparsed shifts	0
Number of shifts with mapping errors	0
Number of shifts with mapping warnings	0
Assignment completeness (well-defined parts)	4%

Note: This is a solid-state NMR structure, where hydrogen atoms are typically not assigned a chemical shift value, which may lead to lower completeness of assignment measure.

6 Model quality [i](#)

6.1 Standard geometry [i](#)

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 [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	0	0	0	0
1	B	0	0	0	0
1	C	0	0	0	0
1	D	0	0	0	0
1	E	0	0	0	0
1	F	0	0	0	0
1	G	0	0	0	0
1	H	0	0	0	0
1	I	0	0	0	0
1	J	0	0	0	0
1	K	0	0	0	0
1	L	0	0	0	0
All	All	0	0	0	-

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 -.

There are no clashes.

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	0	-	-	-	-
1	B	0	-	-	-	-
1	C	0	-	-	-	-
1	D	0	-	-	-	-
1	E	0	-	-	-	-
1	F	0	-	-	-	-
1	G	0	-	-	-	-
1	H	0	-	-	-	-
1	I	0	-	-	-	-
1	J	0	-	-	-	-
1	K	0	-	-	-	-
1	L	0	-	-	-	-
All	All	0	-	-	-	-

There are no Ramachandran outliers.

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	0	-	-	-
1	B	0	-	-	-
1	C	0	-	-	-
1	D	0	-	-	-
1	E	0	-	-	-
1	F	0	-	-	-
1	G	0	-	-	-
1	H	0	-	-	-
1	I	0	-	-	-
1	J	0	-	-	-

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
1	K	0	-	-	-
1	L	0	-	-	-
All	All	0	-	-	-

There are no protein residues with a non-rotameric sidechain to report.

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 4% for the well-defined parts and 4% 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	963
Number of shifts mapped to atoms	963
Number of unparsed shifts	0
Number of shifts with mapping errors	0
Number of shifts with mapping warnings	0
Number of shift outliers (ShiftChecker)	0

7.1.2 Chemical shift referencing

The following table shows the suggested chemical shift referencing corrections.

Nucleus	# values	Correction \pm precision, ppm	Suggested action
$^{13}\text{C}_\alpha$	161	-0.10 ± 0.09	None needed (< 0.5 ppm)
$^{13}\text{C}_\beta$	126	0.59 ± 0.16	Should be applied
$^{13}\text{C}'$	161	0.02 ± 0.15	None needed (< 0.5 ppm)
^{15}N	151	0.00 ± 0.27	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 4%, i.e. 861 atoms were assigned a chemical shift out of a possible 23869. 0 out of 228 assigned methyl groups (LEU and VAL) were assigned stereospecifically.

	Total	^1H	^{13}C	^{15}N
Backbone	624/10128 (6%)	151/4032 (4%)	322/4128 (8%)	151/1968 (8%)
Sidechain	235/11988 (2%)	57/6996 (1%)	178/4476 (4%)	0/516 (0%)

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	Total	¹H	¹³C	¹⁵N
Aromatic	2/1753 (0%)	1/924 (0%)	0/828 (0%)	1/1 (100%)
Overall	861/23869 (4%)	209/11952 (2%)	500/9432 (5%)	152/2485 (6%)

Note: This is a solid-state NMR structure, where hydrogen atoms are typically not assigned a chemical shift value, which may lead to lower completeness of assignment measure.

7.1.4 Statistically unusual chemical shifts [i](#)

There are no statistically unusual chemical shifts.

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.

Random coil index (RCI) for chain A:

