wwPDB NMR Structure Validation Summary Report

Nov 6, 2023 – 08:12 AM EST

PDB ID	:	2MTZ
BMRB ID	:	25192
Title	:	Haddock model of Bacillus subtilis L,D-transpeptidase in complex with a peptidoglycan hexamuropeptide
Authors	:	Schanda, P.; Triboulet, S.; Laguri, C.; Bougault, C.; Ayala, I.; Callon, M.; Arthur, M.; Simorre, J.
Deposited on	:	2014-09-02

This is a wwPDB NMR Structure Validation Summary 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 (i) 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 (i)) were used in the production of this report:

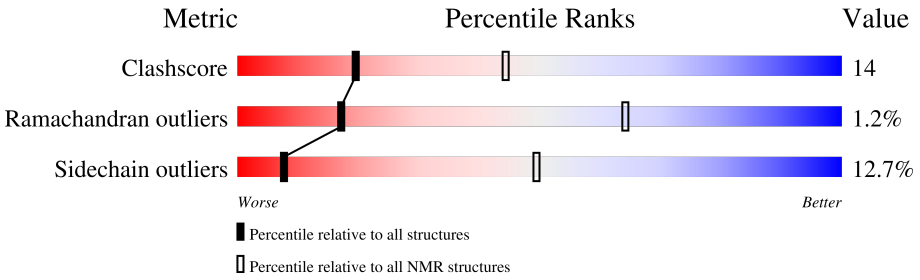
Cyrange	:	Kirchner and Güntert (2011)
NmrClust	:	Kelley et al. (1996)
MolProbity	:	4.02b-467
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
wwPDB-RCI	:	v_1n_11_5_13_A (Berjanski et al., 2005)
PANAV	:	Wang et al. (2010)
wwPDB-ShiftChecker	:	v1.2
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.36

1 Overall quality at a glance (i)

The following experimental techniques were used to determine the structure:
SOLID-STATE NMR

The overall completeness of chemical shifts assignment is 13%.

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	175	73% 21%
2	B	4	100%
2	C	4	100%
2	D	4	100%
2	E	4	100%
2	F	4	100%
2	G	4	100%
3	H	12	58% 42%

The following table lists non-polymeric compounds, carbohydrate monomers and non-standard residues in protein, DNA and RNA chains that are outliers for geometric criteria:

Mol	Chain	Compound	Res	Total models with violations	
				Chirality	Geometry
3	H	NAG	4	1	-
3	H	NAG	8	1	-

2 Ensemble composition and analysis

This entry contains 5 models. Model 5 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:3-A:166 (164)	0.70	5

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 1 clusters. No single-model clusters were found.

Cluster number	Models
1	1, 2, 3, 4, 5

3 Entry composition (i)

There are 3 unique types of molecules in this entry. The entry contains 1661 atoms, of which 0 are hydrogens and 0 are deuteriums.

- Molecule 1 is a protein called Putative L,D-transpeptidase YkuD.

Mol	Chain	Residues	Atoms					Trace
1	A	169	Total	C	N	O	S	0
			1276	810	230	233	3	

There are 12 discrepancies between the modelled and reference sequences:

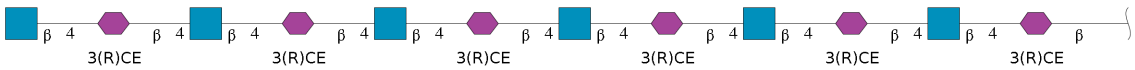
Chain	Residue	Modelled	Actual	Comment	Reference
A	1	GLY	-	expression tag	UNP O34816
A	2	ARG	-	expression tag	UNP O34816
A	3	LYS	-	expression tag	UNP O34816
A	4	LEU	-	expression tag	UNP O34816
A	168	GLY	-	expression tag	UNP O34816
A	169	SER	-	expression tag	UNP O34816
A	170	HIS	-	expression tag	UNP O34816
A	171	HIS	-	expression tag	UNP O34816
A	172	HIS	-	expression tag	UNP O34816
A	173	HIS	-	expression tag	UNP O34816
A	174	HIS	-	expression tag	UNP O34816
A	175	HIS	-	expression tag	UNP O34816

- Molecule 2 is a protein called intact bacterial peptidoglycan.

Mol	Chain	Residues	Atoms				Trace
2	B	4	Total	C	N	O	0
			32	18	5	9	
2	C	4	Total	C	N	O	0
			32	18	5	9	
2	D	4	Total	C	N	O	0
			32	18	5	9	
2	E	4	Total	C	N	O	0
			32	18	5	9	
2	F	4	Total	C	N	O	0
			32	18	5	9	
2	G	4	Total	C	N	O	0
			32	18	5	9	

- Molecule 3 is an oligosaccharide called 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-N-acetyl-beta-muramic acid-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-N-acetyl-b

eta-muramic acid-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-N-acetyl-beta-muramic acid-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-N-acetyl-beta-muramic acid-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-N-acetyl-beta-muramic acid-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-N-acetyl-beta-muramic acid.



Mol	Chain	Residues	Atoms				Trace
3	H	12	Total	C	N	O	0
			193	114	12	67	

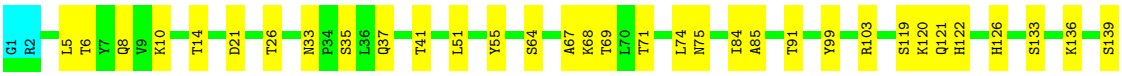
4 Residue-property plots

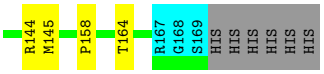
4.1 Average score per residue in the NMR ensemble

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: Putative L,D-transpeptidase YkuD

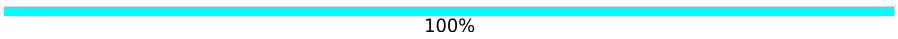
Chain A:





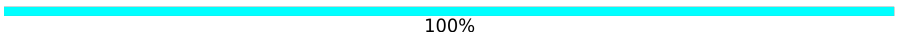
• Molecule 2: intact bacterial peptidoglycan

Chain B:



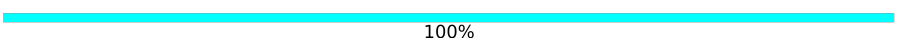
• Molecule 2: intact bacterial peptidoglycan

Chain C:



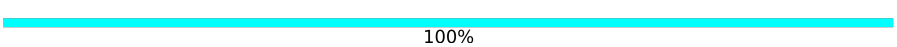
• Molecule 2: intact bacterial peptidoglycan

Chain D:



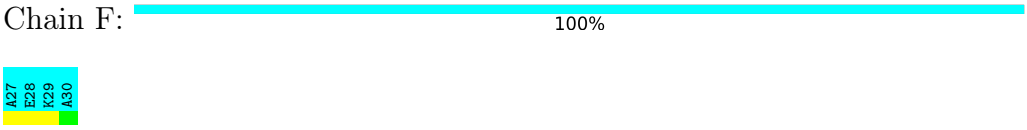
• Molecule 2: intact bacterial peptidoglycan

Chain E:



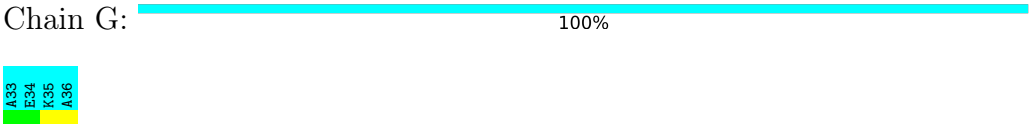
• Molecule 2: intact bacterial peptidoglycan

Chain F:



• Molecule 2: intact bacterial peptidoglycan

Chain G:



• Molecule 3: 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-N-acetyl-beta-muramic acid-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-N-acetyl-beta-muramic acid-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-N-acetyl-beta-muramic acid-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-N-acetyl-beta-muramic acid-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-N-acetyl-beta-muramic acid-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-N-acetyl-beta-muramic acid

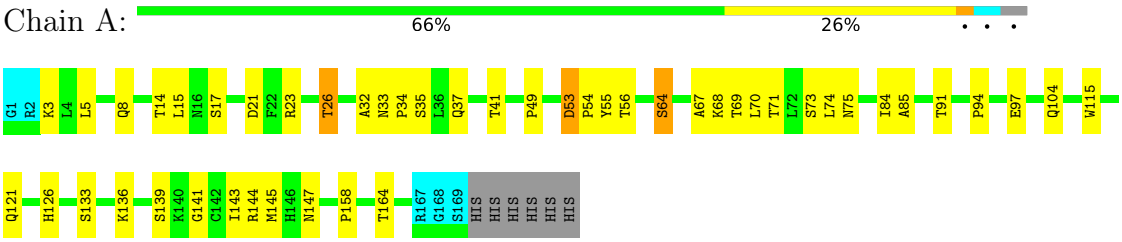
Chain H:

4.2 Residue scores for the representative (medoid) model from the NMR ensemble

The representative model is number 5. Colouring as in section 4.1 above.

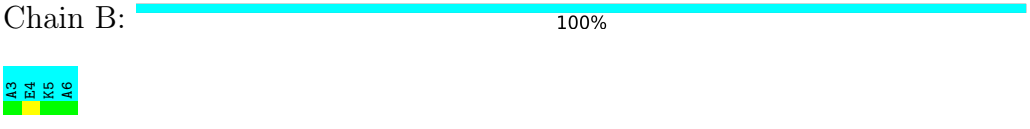
• Molecule 1: Putative L,D-transpeptidase YkuD

Chain A:



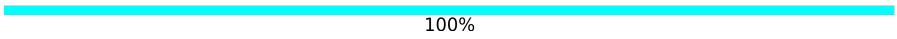
• Molecule 2: intact bacterial peptidoglycan

Chain B:



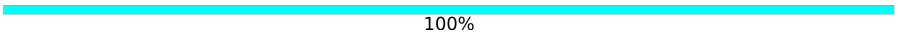
• Molecule 2: intact bacterial peptidoglycan

Chain C:



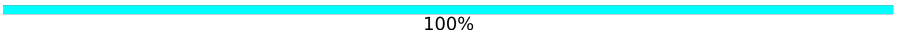
• Molecule 2: intact bacterial peptidoglycan

Chain D:



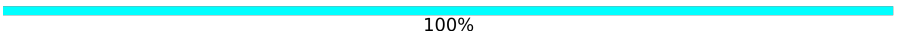
• Molecule 2: intact bacterial peptidoglycan

Chain E:



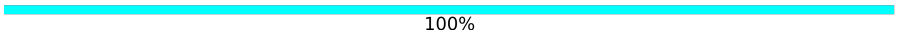
• Molecule 2: intact bacterial peptidoglycan

Chain F:



• Molecule 2: intact bacterial peptidoglycan

Chain G:



• Molecule 3: 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-N-acetyl-beta-muramic acid-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-N-acetyl-beta-muramic acid-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-N-acetyl-beta-muramic acid-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-N-acetyl-beta-muramic acid-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-N-acetyl-beta-muramic acid

Chain H:

5 Refinement protocol and experimental data overview

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

Of the 200 calculated structures, 5 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
HADDOCK	structure solution	2.1
HADDOCK	refinement	2.1

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	2
Total number of shifts	576
Number of shifts mapped to atoms	384
Number of unparsed shifts	0
Number of shifts with mapping errors	192
Number of shifts with mapping warnings	0
Assignment completeness (well-defined parts)	13%

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

6.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: DAL, NAG, AMU, FGA, API

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	1240	0	1282	17±4
2	C	0	0	0	0±0
2	D	0	0	0	0±0
2	E	0	0	0	0±0
2	F	0	0	0	0±0
2	G	0	0	0	0±0
2	B	0	0	0	0±0
3	H	193	0	165	27±4
All	All	7165	0	7235	201

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 14.

5 of 122 unique clashes are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
3:H:3:AMU:C10	3:H:3:AMU:H4	0.92	1.93	3	4
3:H:1:AMU:C11	3:H:1:AMU:H4	0.89	1.98	5	5
3:H:3:AMU:H4	3:H:3:AMU:O10	0.84	1.70	4	2
3:H:6:NAG:H62	3:H:7:AMU:C1	0.78	2.08	5	1
3:H:5:AMU:H3	3:H:5:AMU:O10	0.76	1.77	2	2

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	164/175 (94%)	152±1 (93±0%)	10±2 (6±1%)	2±1 (1±1%)	17 64
2	B	0	-	-	-	-
2	C	0	-	-	-	-
2	D	0	-	-	-	-
2	E	0	-	-	-	-
2	F	0	-	-	-	-
2	G	0	-	-	-	-
All	All	820/995 (82%)	762 (93%)	48 (6%)	10 (1%)	17 64

All 5 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	139	SER	4
1	A	158	PRO	3
1	A	67	ALA	1
1	A	121	GLN	1
1	A	94	PRO	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	135/144 (94%)	118±3 (87±2%)	17±3 (13±2%)	8 49
2	B	0	-	-	-
2	C	0	-	-	-
2	D	0	-	-	-
2	E	0	-	-	-
2	F	0	-	-	-

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
2	G	0	-	-	-
All	All	675/720 (94%)	589 (87%)	86 (13%)	8 49

5 of 38 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	69	THR	5
1	A	74	LEU	5
1	A	91	THR	5
1	A	21	ASP	4
1	A	68	LYS	4

6.3.3 RNA (i)

There are no RNA molecules in this entry.

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

18 non-standard protein/DNA/RNA residues are modelled in this entry.

In the following table, the Counts columns list the number of bonds for which Mogul statistics could be retrieved, the number of bonds that are observed in the model and the number of bonds that are defined in the chemical component dictionary. The Link column lists molecule types, if any, to which the group is linked. The Z score for a bond length is the number of standard deviations the observed value is removed from the expected value. A bond length with $|Z| > 2$ is considered an outlier worth inspection. RMSZ is the average root-mean-square of all Z scores of the bond lengths.

Mol	Type	Chain	Res	Link	Bond lengths		
					Counts	RMSZ	#Z>2
2	FGA	E	22	2	7,8,9	0.82±0.01	0±0 (0±0%)
2	API	B	5	2	9,11,12	0.73±0.01	0±0 (0±0%)
2	FGA	B	4	2	7,8,9	0.81±0.01	0±0 (0±0%)
2	API	G	35	2	9,11,12	0.73±0.01	0±0 (0±0%)
2	FGA	F	28	2	7,8,9	0.82±0.01	0±0 (0±0%)
2	API	E	23	2	9,11,12	0.73±0.01	0±0 (0±0%)
2	API	D	17	2	9,11,12	0.73±0.01	0±0 (0±0%)
2	API	F	29	2	9,11,12	0.73±0.00	0±0 (0±0%)
2	FGA	G	34	2	7,8,9	0.82±0.01	0±0 (0±0%)
2	FGA	D	16	2	7,8,9	0.82±0.01	0±0 (0±0%)
2	API	C	11	2	9,11,12	0.73±0.01	0±0 (0±0%)

Mol	Type	Chain	Res	Link	Bond lengths		
					Counts	RMSZ	#Z>2
2	FGA	C	10	2	7,8,9	0.82±0.00	0±0 (0±0%)

In the following table, the Counts columns list the number of angles for which Mogul statistics could be retrieved, the number of angles that are observed in the model and the number of angles that are defined in the chemical component dictionary. The Link column lists molecule types, if any, to which the group is linked. The Z score for a bond angle is the number of standard deviations the observed value is removed from the expected value. A bond angle with $|Z| > 2$ is considered an outlier worth inspection. RMSZ is the average root-mean-square of all Z scores of the bond angles.

Mol	Type	Chain	Res	Link	Bond angles		
					Counts	RMSZ	#Z>2
2	FGA	E	22	2	7,9,11	0.94±0.01	0±0 (0±0%)
2	API	B	5	2	7,13,15	0.91±0.03	0±0 (0±0%)
2	FGA	B	4	2	7,9,11	0.90±0.02	0±0 (0±0%)
2	API	G	35	2	7,13,15	0.93±0.03	0±0 (0±0%)
2	FGA	F	28	2	7,9,11	0.92±0.02	0±0 (0±0%)
2	API	E	23	2	7,13,15	0.91±0.04	0±0 (0±0%)
2	API	D	17	2	7,13,15	0.89±0.05	0±0 (0±0%)
2	API	F	29	2	7,13,15	0.89±0.07	0±0 (0±0%)
2	FGA	G	34	2	7,9,11	0.92±0.03	0±0 (0±0%)
2	FGA	D	16	2	7,9,11	0.93±0.02	0±0 (0±0%)
2	API	C	11	2	7,13,15	0.89±0.05	0±0 (0±0%)
2	FGA	C	10	2	7,9,11	0.90±0.03	0±0 (0±0%)

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral centers analysed, the number of these observed in the model and the number defined in the chemical component dictionary. Similar counts are reported in the Torsion and Rings columns. '-' means no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	FGA	B	4	2	-	0±0,7,8,9	-
2	API	E	23	2	-	0±0,11,12,14	-
2	API	F	29	2	-	0±0,11,12,14	-
2	API	D	17	2	-	0±0,11,12,14	-
2	FGA	G	34	2	-	0±0,7,8,9	-
2	API	B	5	2	-	0±0,11,12,14	-
2	API	C	11	2	-	0±0,11,12,14	-
2	FGA	D	16	2	-	0±0,7,8,9	-
2	API	G	35	2	-	0±0,11,12,14	-
2	FGA	F	28	2	-	0±0,7,8,9	-
2	FGA	E	22	2	-	0±0,7,8,9	-
2	FGA	C	10	2	-	0±0,7,8,9	-

There are no bond-length outliers.

There are no bond-angle outliers.

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

6.5 Carbohydrates (i)

12 monosaccharides are modelled in this entry.

In the following table, the Counts columns list the number of bonds for which Mogul statistics could be retrieved, the number of bonds that are observed in the model and the number of bonds that are defined in the chemical component dictionary. The Link column lists molecule types, if any, to which the group is linked. The Z score for a bond length is the number of standard deviations the observed value is removed from the expected value. A bond length with $|Z| > 2$ is considered an outlier worth inspection. RMSZ is the average root-mean-square of all Z scores of the bond lengths.

Mol	Type	Chain	Res	Link	Bond lengths		
					Counts	RMSZ	#Z>2
3	AMU	H	1	3,2	18,19,20	0.49±0.01	0±0 (0±0%)
3	NAG	H	10	3	14,14,15	0.33±0.03	0±0 (0±0%)
3	AMU	H	11	3,2	17,18,20	0.50±0.01	0±0 (0±0%)
3	NAG	H	12	3	14,14,15	0.26±0.02	0±0 (0±0%)
3	NAG	H	2	3	14,14,15	0.32±0.02	0±0 (0±0%)
3	AMU	H	3	3,2	17,18,20	0.50±0.02	0±0 (0±0%)
3	NAG	H	4	3	14,14,15	0.32±0.01	0±0 (0±0%)
3	AMU	H	5	3,2	17,18,20	0.51±0.02	0±0 (0±0%)
3	NAG	H	6	3	14,14,15	0.34±0.03	0±0 (0±0%)
3	AMU	H	7	3,2	17,18,20	0.51±0.02	0±0 (0±0%)
3	NAG	H	8	3	14,14,15	0.33±0.03	0±0 (0±0%)
3	AMU	H	9	3,2	17,18,20	0.52±0.01	0±0 (0±0%)

In the following table, the Counts columns list the number of angles for which Mogul statistics could be retrieved, the number of angles that are observed in the model and the number of angles that are defined in the chemical component dictionary. The Link column lists molecule types, if any, to which the group is linked. The Z score for a bond angle is the number of standard deviations the observed value is removed from the expected value. A bond angle with $|Z| > 2$ is considered an outlier worth inspection. RMSZ is the average root-mean-square of all Z scores of the bond angles.

Mol	Type	Chain	Res	Link	Bond angles		
					Counts	RMSZ	#Z>2

Mol	Type	Chain	Res	Link	Bond angles		
					Counts	RMSZ	#Z>2
3	AMU	H	1	3,2	21,26,28	0.88±0.04	1±0 (3±1%)
3	NAG	H	10	3	17,19,21	0.75±0.09	1±0 (3±2%)
3	AMU	H	11	3,2	21,24,28	0.75±0.11	1±0 (2±2%)
3	NAG	H	12	3	17,19,21	0.73±0.03	1±0 (4±2%)
3	NAG	H	2	3	17,19,21	0.67±0.02	0±0 (2±2%)
3	AMU	H	3	3,2	21,24,28	0.69±0.05	0±0 (0±0%)
3	NAG	H	4	3	17,19,21	0.70±0.02	1±0 (4±2%)
3	AMU	H	5	3,2	21,24,28	0.68±0.03	1±0 (4±0%)
3	NAG	H	6	3	17,19,21	0.73±0.04	1±0 (3±2%)
3	AMU	H	7	3,2	21,24,28	0.82±0.08	1±0 (2±2%)
3	NAG	H	8	3	17,19,21	0.74±0.09	1±0 (3±2%)
3	AMU	H	9	3,2	21,24,28	0.72±0.08	0±0 (0±1%)

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral centers analysed, the number of these observed in the model and the number defined in the chemical component dictionary. Similar counts are reported in the Torsion and Rings columns. '-' means no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
3	AMU	H	1	3,2	-	0±0,10,32,34	0±0,1,1,1
3	NAG	H	10	3	-	0±0,6,23,26	0±0,1,1,1
3	AMU	H	11	3,2	-	0±0,10,29,34	0±0,1,1,1
3	NAG	H	12	3	-	0±0,6,23,26	0±0,1,1,1
3	NAG	H	2	3	-	0±0,6,23,26	0±0,1,1,1
3	AMU	H	3	3,2	-	0±0,10,29,34	0±0,1,1,1
3	NAG	H	4	3	-	0±0,6,23,26	0±0,1,1,1
3	AMU	H	5	3,2	-	0±0,10,29,34	0±0,1,1,1
3	NAG	H	6	3	-	0±0,6,23,26	0±0,1,1,1
3	AMU	H	7	3,2	-	0±0,10,29,34	0±0,1,1,1
3	NAG	H	8	3	-	0±0,6,23,26	0±0,1,1,1
3	AMU	H	9	3,2	-	0±0,10,29,34	0±0,1,1,1

There are no bond-length outliers.

5 of 11 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(^{o})	Ideal(^{o})	Models	
								Worst	Total
3	H	7	AMU	O3-C3-C4	2.99	115.23	107.28	1	3
3	H	11	AMU	C4-C3-C2	2.71	106.45	111.18	5	3
3	H	10	NAG	C4-C3-C2	2.70	107.07	111.02	5	3
3	H	8	NAG	C4-C3-C2	2.59	107.22	111.02	3	3
3	H	6	NAG	C4-C3-C2	2.45	107.42	111.02	1	3

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

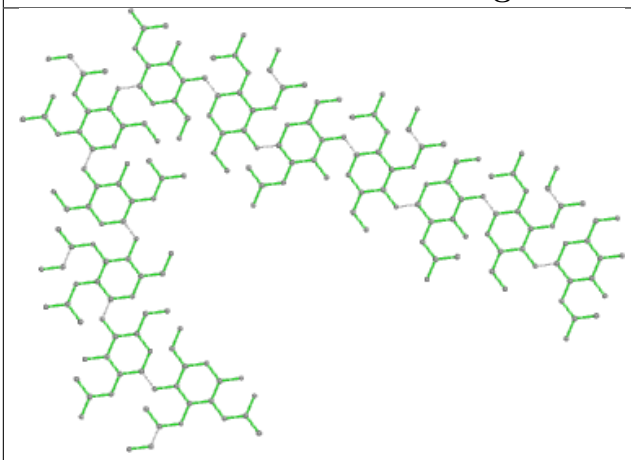
Mol	Chain	Res	Type	Atoms	Models (Total)
3	H	4	NAG	C1	1
3	H	8	NAG	C1	1

There are no torsion outliers.

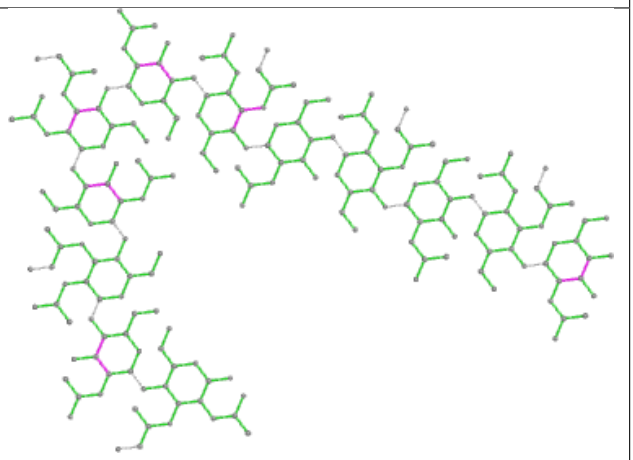
There are no ring outliers.

The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for oligosaccharide.

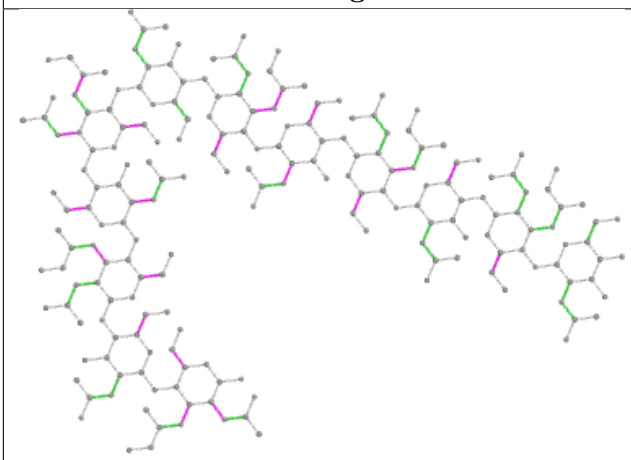
Oligosaccharide Chain H



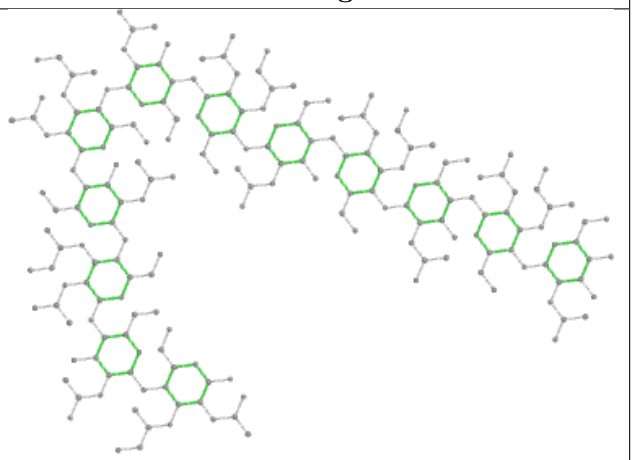
Bond lengths



Bond angles



Torsions



Rings

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 13% for the well-defined parts and 12% for the entire structure.

7.1 Chemical shift list 1

File name: working_cs.cif

Chemical shift list name: *protein_interacting_with_peptidoglycan*

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	288
Number of shifts mapped to atoms	192
Number of unparsed shifts	0
Number of shifts with mapping errors	96
Number of shifts with mapping warnings	0
Number of shift outliers (ShiftChecker)	0

The following assigned chemical shifts were not mapped to the molecules present in the coordinate file.

- No matching atom found in the structure. First 5 (of 96) occurrences are reported below.

List ID	Chain	Res	Type	Atom	Shift Data		
					Value	Uncertainty	Ambiguity
1	A	2	ARG	H	8.24	0.040	1
1	A	5	LEU	H	7.721	0.040	1
1	A	6	THR	H	7.96	0.040	1
1	A	7	TYR	H	9.355	0.040	1
1	A	8	GLN	H	7.609	0.040	1
1	A	9	VAL	H	8.49	0.040	1
1	A	10	LYS	H	9.092	0.040	1
1	A	11	GLN	H	8.855	0.040	1
1	A	13	ASP	H	7.891	0.040	1
1	A	15	LEU	H	9.012	0.040	1
1	A	17	SER	H	8.745	0.040	1
1	A	19	ALA	H	7.805	0.040	1
1	A	20	ALA	H	7.862	0.040	1
1	A	21	ASP	H	8.431	0.040	1

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List ID	Chain	Res	Type	Atom	Shift Data		
					Value	Uncertainty	Ambiguity
1	A	22	PHE	H	7.833	0.040	1
1	A	28	ALA	H	8.093	0.040	1
1	A	29	LEU	H	7.679	0.040	1
1	A	30	LEU	H	8.357	0.040	1
1	A	31	GLN	H	8.14	0.040	1
1	A	32	ALA	H	7.202	0.040	1
1	A	40	LEU	H	8.241	0.040	1
1	A	41	THR	H	8.584	0.040	1
1	A	42	ALA	H	8.555	0.040	1
1	A	43	GLY	H	8.914	0.040	1
1	A	44	GLN	H	7.627	0.040	1
1	A	45	SER	H	8.585	0.040	1
1	A	46	ILE	H	9.168	0.040	1
1	A	47	VAL	H	9.274	0.040	1
1	A	48	ILE	H	8.221	0.040	1
1	A	50	GLY	H	8.07	0.040	1
1	A	51	LEU	H	7.228	0.040	1
1	A	53	ASP	H	7.57	0.040	1
1	A	56	THR	H	8.046	0.040	1
1	A	60	HIS	H	8.494	0.040	1
1	A	62	ALA	H	8.955	0.040	1
1	A	63	VAL	H	9.513	0.040	1
1	A	64	SER	H	8.747	0.040	1
1	A	65	ILE	H	8.731	0.040	1
1	A	69	THR	H	7.623	0.040	1
1	A	70	LEU	H	9.332	0.040	1
1	A	71	THR	H	9.723	0.040	1
1	A	72	LEU	H	9.286	0.040	1
1	A	73	SER	H	9.228	0.040	1
1	A	74	LEU	H	8.728	0.040	1
1	A	75	ASN	H	9.085	0.040	1
1	A	77	ARG	H	7.85	0.040	1
1	A	78	VAL	H	8.779	0.040	1
1	A	80	LYS	H	7.713	0.040	1
1	A	81	THR	H	7.997	0.040	1
1	A	84	ILE	H	7.358	0.040	1
1	A	85	ALA	H	9.329	0.040	1
1	A	86	VAL	H	7.753	0.040	1
1	A	88	LYS	H	7.539	0.040	1
1	A	96	GLY	H	8.167	0.040	1
1	A	97	GLU	H	7.649	0.040	1

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List ID	Chain	Res	Type	Atom	Shift Data		
					Value	Uncertainty	Ambiguity
1	A	98	PHE	H	8.956	0.040	1
1	A	99	TYR	H	8.472	0.040	1
1	A	100	ILE	H	8.485	0.040	1
1	A	101	ILE	H	8.642	0.040	1
1	A	104	GLN	H	9.536	0.040	1
1	A	105	ARG	H	8.801	0.040	1
1	A	114	TYR	H	7.92	0.040	1
1	A	115	TRP	H	8.604	0.040	1
1	A	116	LEU	H	9.389	0.040	1
1	A	117	SER	H	8.4	0.040	1
1	A	118	LEU	H	7.929	0.040	1
1	A	119	SER	H	7.591	0.040	1
1	A	120	LYS	H	8.169	0.040	1
1	A	121	GLN	H	8.711	0.040	1
1	A	122	HIS	H	8.497	0.040	1
1	A	123	TYR	H	8.772	0.040	1
1	A	124	GLY	H	7.38	0.040	1
1	A	125	ILE	H	8.325	0.040	1
1	A	126	HIS	H	8.866	0.040	1
1	A	127	GLY	H	8.389	0.040	1
1	A	128	THR	H	7.687	0.040	1
1	A	132	ALA	H	7.766	0.040	1
1	A	134	ILE	H	6.867	0.040	1
1	A	137	ALA	H	8.339	0.040	1
1	A	138	VAL	H	8.284	0.040	1
1	A	140	LYS	H	8.1	0.040	1
1	A	143	ILE	H	7.472	0.040	1
1	A	144	ARG	H	8.102	0.040	1
1	A	145	MET	H	8.963	0.040	1
1	A	148	LYS	H	9.226	0.040	1
1	A	149	ASP	H	6.759	0.040	1
1	A	151	ILE	H	7.853	0.040	1
1	A	152	GLU	H	7.347	0.040	1
1	A	156	ILE	H	7.357	0.040	1
1	A	159	ASN	H	9.143	0.040	1
1	A	160	GLY	H	9.861	0.040	1
1	A	161	THR	H	7.075	0.040	1
1	A	162	ARG	H	8.829	0.040	1
1	A	164	THR	H	9.274	0.040	1
1	A	165	ILE	H	9.107	0.040	1
1	A	169	SER	H	8.262	0.040	1

7.1.2 Chemical shift referencing (i)

The following table shows the suggested chemical shift referencing corrections.

Nucleus	# values	Correction ± precision, *ppm*	Suggested action
$^{13}C_{\alpha}$	96	0.20 ± 0.08	None needed (< 0.5 ppm)
$^{13}C_{\beta}$	0	—	None (insufficient data)
$^{13}C'$	0	—	None (insufficient data)
^{15}N	96	-0.32 ± 0.35	None needed (< 0.5 ppm)

7.1.3 Completeness of resonance assignments (i)

The following table shows the completeness of the chemical shift assignments for the well-defined regions of the structure. The overall completeness is 13%, i.e. 282 atoms were assigned a chemical shift out of a possible 2199. 0 out of 24 assigned methyl groups (LEU and VAL) were assigned stereospecifically.

	Total	^{1}H	^{13}C	^{15}N
Backbone	282/813 (35%)	94/332 (28%)	94/328 (29%)	94/153 (61%)
Sidechain	0/1258 (0%)	0/829 (0%)	0/383 (0%)	0/46 (0%)
Aromatic	0/128 (0%)	0/65 (0%)	0/63 (0%)	0/0 (—%)
Overall	282/2199 (13%)	94/1226 (8%)	94/774 (12%)	94/199 (47%)

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.

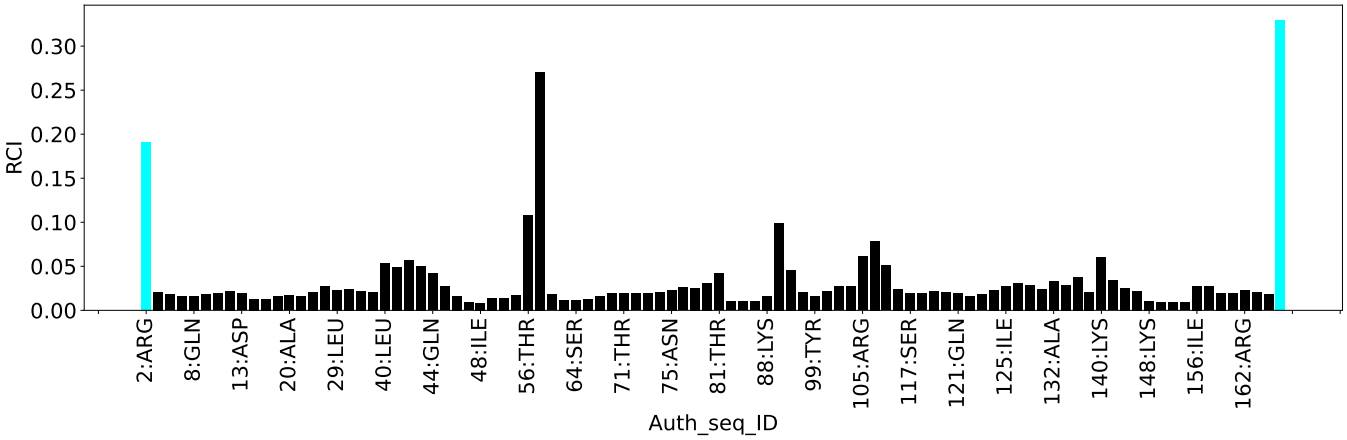
7.1.4 Statistically unusual chemical shifts (i)

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.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:



7.2 Chemical shift list 2

File name: working_cs.cif

Chemical shift list name: *protein_free_in_solution*

7.2.1 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	288
Number of shifts mapped to atoms	192
Number of unparsed shifts	0
Number of shifts with mapping errors	96
Number of shifts with mapping warnings	0
Number of shift outliers (ShiftChecker)	0

The following assigned chemical shifts were not mapped to the molecules present in the coordinate file.

- No matching atom found in the structure. First 5 (of 96) occurrences are reported below.

List ID	Chain	Res	Type	Atom	Shift Data		
					Value	Uncertainty	Ambiguity
2	A	2	ARG	H	8.281	0.030	1
2	A	5	LEU	H	7.786	0.030	1
2	A	6	THR	H	7.986	0.030	1
2	A	7	TYR	H	9.304	0.030	1
2	A	8	GLN	H	7.611	0.030	1
2	A	9	VAL	H	8.529	0.030	1
2	A	10	LYS	H	9.112	0.030	1

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List ID	Chain	Res	Type	Atom	Shift Data		
					Value	Uncertainty	Ambiguity
2	A	11	GLN	H	8.835	0.030	1
2	A	13	ASP	H	7.871	0.030	1
2	A	15	LEU	H	9.015	0.030	1
2	A	17	SER	H	8.715	0.030	1
2	A	19	ALA	H	7.787	0.030	1
2	A	20	ALA	H	7.763	0.030	1
2	A	21	ASP	H	8.513	0.030	1
2	A	22	PHE	H	7.813	0.030	1
2	A	28	ALA	H	8.073	0.030	1
2	A	29	LEU	H	7.654	0.030	1
2	A	30	LEU	H	8.335	0.030	1
2	A	31	GLN	H	8.121	0.030	1
2	A	32	ALA	H	7.185	0.030	1
2	A	40	LEU	H	8.221	0.030	1
2	A	41	THR	H	8.561	0.030	1
2	A	42	ALA	H	8.626	0.030	1
2	A	43	GLY	H	8.884	0.030	1
2	A	44	GLN	H	7.607	0.030	1
2	A	45	SER	H	8.562	0.030	1
2	A	46	ILE	H	9.233	0.030	1
2	A	47	VAL	H	9.288	0.030	1
2	A	48	ILE	H	8.217	0.030	1
2	A	50	GLY	H	8.041	0.030	1
2	A	51	LEU	H	7.208	0.030	1
2	A	53	ASP	H	7.544	0.030	1
2	A	56	THR	H	8.014	0.030	1
2	A	60	HIS	H	8.538	0.030	1
2	A	62	ALA	H	8.928	0.030	1
2	A	63	VAL	H	9.477	0.030	1
2	A	64	SER	H	8.76	0.030	1
2	A	65	ILE	H	8.706	0.030	1
2	A	69	THR	H	7.603	0.030	1
2	A	70	LEU	H	9.406	0.030	1
2	A	71	THR	H	9.653	0.030	1
2	A	72	LEU	H	9.333	0.030	1
2	A	73	SER	H	9.33	0.030	1
2	A	74	LEU	H	8.697	0.030	1
2	A	75	ASN	H	9.054	0.030	1
2	A	77	ARG	H	7.83	0.030	1
2	A	78	VAL	H	8.727	0.030	1
2	A	80	LYS	H	7.695	0.030	1

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List ID	Chain	Res	Type	Atom	Shift Data		
					Value	Uncertainty	Ambiguity
2	A	81	THR	H	7.998	0.030	1
2	A	84	ILE	H	7.344	0.030	1
2	A	85	ALA	H	9.304	0.030	1
2	A	86	VAL	H	7.785	0.030	1
2	A	88	LYS	H	7.476	0.030	1
2	A	96	GLY	H	8.23	0.030	1
2	A	97	GLU	H	7.642	0.030	1
2	A	98	PHE	H	9.007	0.030	1
2	A	99	TYR	H	8.377	0.030	1
2	A	100	ILE	H	8.381	0.030	1
2	A	101	ILE	H	8.613	0.030	1
2	A	104	GLN	H	9.512	0.030	1
2	A	105	ARG	H	8.806	0.030	1
2	A	114	TYR	H	7.9	0.030	1
2	A	115	TRP	H	8.616	0.030	1
2	A	116	LEU	H	9.322	0.030	1
2	A	117	SER	H	8.373	0.030	1
2	A	118	LEU	H	7.936	0.030	1
2	A	119	SER	H	7.579	0.030	1
2	A	120	LYS	H	8.117	0.030	1
2	A	121	GLN	H	8.76	0.030	1
2	A	122	HIS	H	8.485	0.030	1
2	A	123	TYR	H	8.743	0.030	1
2	A	124	GLY	H	7.389	0.030	1
2	A	125	ILE	H	8.328	0.030	1
2	A	126	HIS	H	8.853	0.030	1
2	A	127	GLY	H	8.352	0.030	1
2	A	128	THR	H	7.684	0.030	1
2	A	132	ALA	H	7.749	0.030	1
2	A	134	ILE	H	6.847	0.030	1
2	A	137	ALA	H	8.303	0.030	1
2	A	138	VAL	H	8.277	0.030	1
2	A	140	LYS	H	8.08	0.030	1
2	A	143	ILE	H	7.479	0.030	1
2	A	144	ARG	H	8.044	0.030	1
2	A	145	MET	H	8.945	0.030	1
2	A	148	LYS	H	9.202	0.030	1
2	A	149	ASP	H	6.737	0.030	1
2	A	151	ILE	H	7.887	0.030	1
2	A	152	GLU	H	7.358	0.030	1
2	A	156	ILE	H	7.331	0.030	1

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List ID	Chain	Res	Type	Atom	Shift Data		
					Value	Uncertainty	Ambiguity
2	A	159	ASN	H	9.094	0.030	1
2	A	160	GLY	H	9.801	0.030	1
2	A	161	THR	H	7.037	0.030	1
2	A	162	ARG	H	8.805	0.030	1
2	A	164	THR	H	9.267	0.030	1
2	A	165	ILE	H	9.096	0.030	1
2	A	169	SER	H	8.18	0.030	1

7.2.2 Chemical shift referencing (i)

The following table shows the suggested chemical shift referencing corrections.

Nucleus	# values	Correction ± precision, *ppm*	Suggested action
$^{13}C_{\alpha}$	96	0.23 ± 0.25	None needed (< 0.5 ppm)
$^{13}C_{\beta}$	0	—	None (insufficient data)
$^{13}C'$	0	—	None (insufficient data)
^{15}N	96	-0.32 ± 0.27	None needed (< 0.5 ppm)

7.2.3 Completeness of resonance assignments (i)

The following table shows the completeness of the chemical shift assignments for the well-defined regions of the structure. The overall completeness is 13%, i.e. 282 atoms were assigned a chemical shift out of a possible 2199. 0 out of 24 assigned methyl groups (LEU and VAL) were assigned stereospecifically.

	Total	^{1}H	^{13}C	^{15}N
Backbone	282/813 (35%)	94/332 (28%)	94/328 (29%)	94/153 (61%)
Sidechain	0/1258 (0%)	0/829 (0%)	0/383 (0%)	0/46 (0%)
Aromatic	0/128 (0%)	0/65 (0%)	0/63 (0%)	0/0 (—%)
Overall	282/2199 (13%)	94/1226 (8%)	94/774 (12%)	94/199 (47%)

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.

7.2.4 Statistically unusual chemical shifts (i)

There are no statistically unusual chemical shifts.

7.2.5 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: