



Full wwPDB NMR Structure Validation Report ⓘ

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PDB ID : 7K1Q / pdb_00007k1q
BMRB ID : 30793
Title : Solution structure of lantibiotic from Paenibacillus sp.
Authors : Karczewski, J.; Diehl, C.
Deposited on : 2020-09-08

This is a Full wwPDB NMR Structure Validation Report for a publicly released PDB entry.

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<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
Mogul	:	2022.3.0, CSD as543be (2022)
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

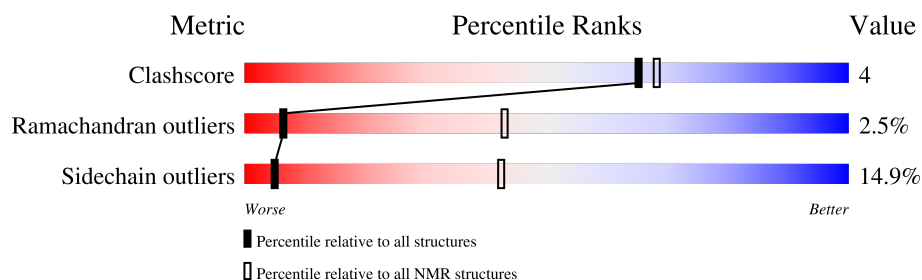
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

SOLUTION NMR

The overall completeness of chemical shifts assignment is 86%.

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	32	

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
1	A	DHA	31	-	8
1	A	DHA	5	-	1

2 Ensemble composition and analysis

This entry contains 15 models. Model 1 is the overall representative, medoid model (most similar to other models).

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:1-A:4, A:6-A:17, A:19-A:30, A:32-A:32 (29)	0.88	1

Ill-defined regions of proteins are excluded from the global statistics.

Ligands and non-protein polymers are included in the analysis.

The models can be grouped into 3 clusters. No single-model clusters were found.

Cluster number	Models
1	1, 2, 3, 4, 5, 6, 8, 10, 13, 14
2	7, 12, 15
3	9, 11

3 Entry composition [i](#)

There is only 1 type of molecule in this entry. The entry contains 454 atoms, of which 221 are hydrogens and 0 are deuteriums.

- Molecule 1 is a protein called Lantibiotic CMB001.

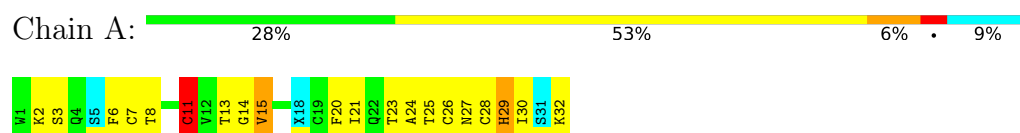
Mol	Chain	Residues	Atoms						Trace
1	A	32	Total	C	H	N	O	S	0
			454	150	221	41	37	5	

4 Residue-property plots [i](#)

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: Lantibiotic CMB001

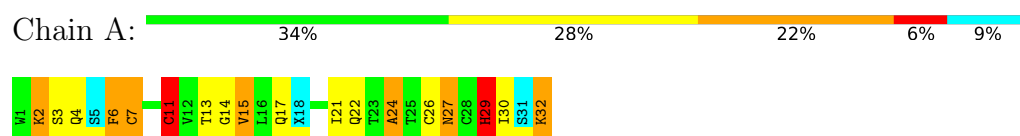


4.2 Scores per residue for each member of the ensemble

Colouring as in section 4.1 above.

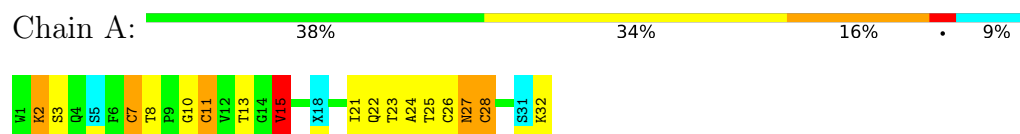
4.2.1 Score per residue for model 1 (medoid)

- Molecule 1: Lantibiotic CMB001



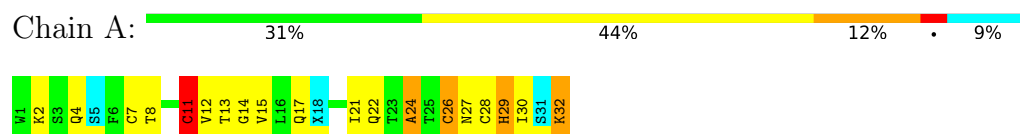
4.2.2 Score per residue for model 2

- Molecule 1: Lantibiotic CMB001



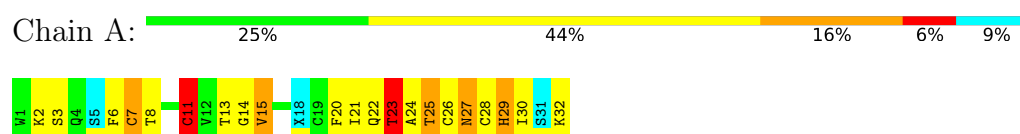
4.2.3 Score per residue for model 3

- Molecule 1: Lantibiotic CMB001



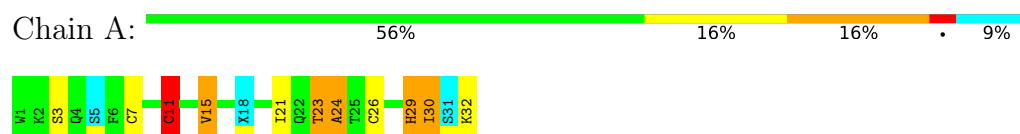
4.2.4 Score per residue for model 4

- Molecule 1: Lantibiotic CMB001



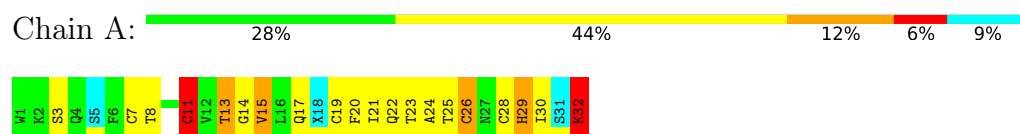
4.2.5 Score per residue for model 5

- Molecule 1: Lantibiotic CMB001



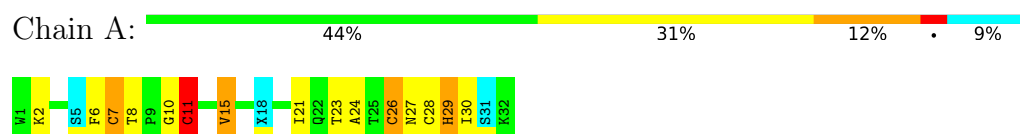
4.2.6 Score per residue for model 6

- Molecule 1: Lantibiotic CMB001



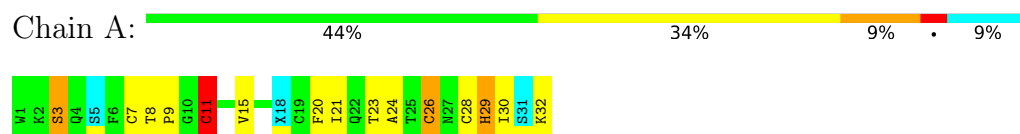
4.2.7 Score per residue for model 7

- Molecule 1: Lantibiotic CMB001



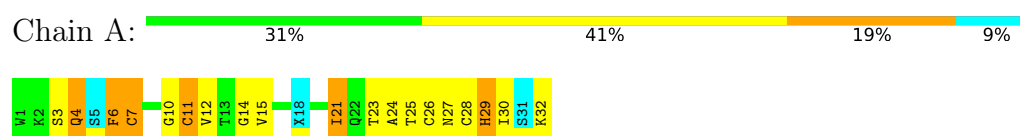
4.2.8 Score per residue for model 8

- Molecule 1: Lantibiotic CMB001



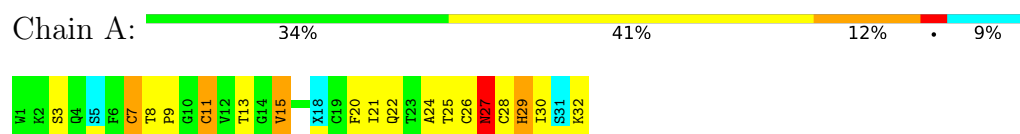
4.2.9 Score per residue for model 9

- Molecule 1: Lantibiotic CMB001



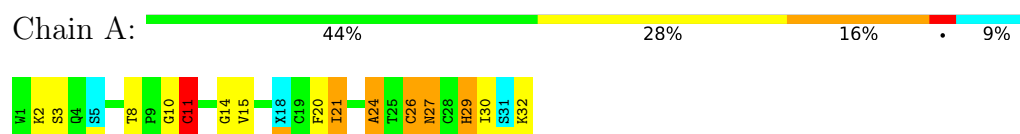
4.2.10 Score per residue for model 10

- Molecule 1: Lantibiotic CMB001



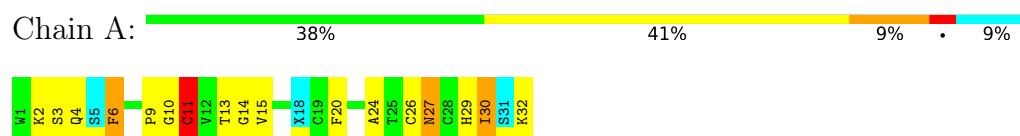
4.2.11 Score per residue for model 11

- Molecule 1: Lantibiotic CMB001



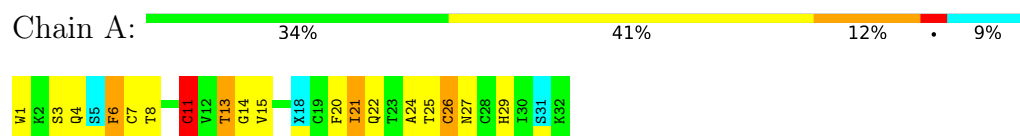
4.2.12 Score per residue for model 12

- Molecule 1: Lantibiotic CMB001



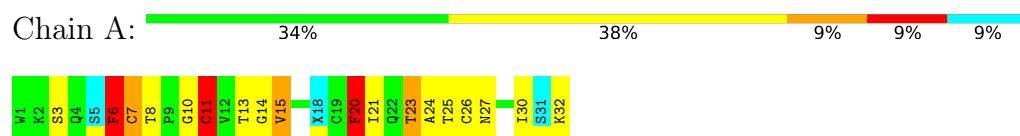
4.2.13 Score per residue for model 13

- Molecule 1: Lantibiotic CMB001



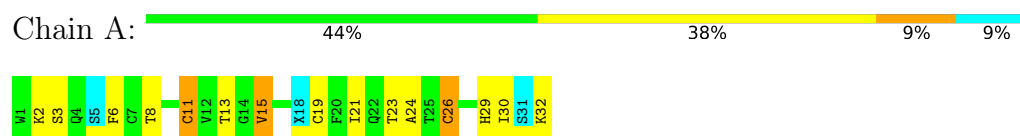
4.2.14 Score per residue for model 14

- Molecule 1: Lantibiotic CMB001



4.2.15 Score per residue for model 15

- Molecule 1: Lantibiotic CMB001



5 Refinement protocol and experimental data overview

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

Of the 60 calculated structures, 15 were deposited, based on the following criterion: *structures with acceptable covalent geometry*.

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

Software name	Classification	Version
GROMACS	refinement	
GROMACS	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	341
Number of shifts mapped to atoms	341
Number of unparsed shifts	0
Number of shifts with mapping errors	0
Number of shifts with mapping warnings	0
Assignment completeness (well-defined parts)	86%

6 Model quality [i](#)

6.1 Standard geometry [i](#)

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

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	1.33±0.02	0±0/219 (0.0± 0.0%)	2.74±0.16	21±6/288 (7.2± 2.0%)
All	All	1.33	0/3285 (0.0%)	2.75	311/4320 (7.2%)

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	6.2±1.2
All	All	0	93

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	11	CYS	N-CA-C	14.51	126.59	111.07	1	15
1	A	15	VAL	CA-C-N	10.69	140.94	121.70	6	12
1	A	15	VAL	C-N-CA	10.69	140.94	121.70	6	12
1	A	27	ASN	CA-CB-CG	-10.02	102.58	112.60	12	4
1	A	11	CYS	O-C-N	-9.84	111.86	122.09	6	6
1	A	20	PHE	O-C-N	-9.44	112.66	123.33	13	1
1	A	14	GLY	CA-C-O	9.35	129.40	119.02	1	4
1	A	2	LYS	CA-C-N	9.31	136.04	122.82	7	4
1	A	2	LYS	C-N-CA	9.31	136.04	122.82	7	4
1	A	15	VAL	N-CA-C	9.30	120.11	110.62	8	9
1	A	13	THR	N-CA-C	-9.20	101.61	112.92	6	4
1	A	7	CYS	CA-C-O	9.19	129.02	118.55	2	3

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)	Models	
								Worst	Total
1	A	26	CYS	N-CA-C	-8.70	95.33	108.99	4	8
1	A	2	LYS	N-CA-C	8.70	120.53	111.14	3	6
1	A	25	THR	CA-C-N	8.57	137.02	121.85	4	2
1	A	25	THR	C-N-CA	8.57	137.02	121.85	4	2
1	A	25	THR	N-CA-CB	8.54	124.78	110.87	14	3
1	A	3	SER	N-CA-C	8.50	123.42	111.52	4	9
1	A	22	GLN	OE1-CD-NE2	-8.44	114.16	122.60	10	3
1	A	15	VAL	O-C-N	-8.33	113.46	121.87	3	5
1	A	8	THR	CB-CA-C	8.07	120.31	109.42	8	2
1	A	27	ASN	OD1-CG-ND2	-7.93	114.67	122.60	10	1
1	A	21	ILE	CA-C-N	7.89	135.90	121.70	10	8
1	A	21	ILE	C-N-CA	7.89	135.90	121.70	10	8
1	A	11	CYS	CA-C-N	7.89	135.90	121.70	5	2
1	A	11	CYS	C-N-CA	7.89	135.90	121.70	5	2
1	A	28	CYS	CA-C-O	7.71	128.88	119.31	7	2
1	A	21	ILE	O-C-N	-7.63	115.11	123.20	7	5
1	A	24	ALA	N-CA-C	7.36	121.84	113.01	5	1
1	A	14	GLY	CA-C-N	7.33	129.80	120.56	9	4
1	A	14	GLY	C-N-CA	7.33	129.80	120.56	9	4
1	A	8	THR	CA-C-N	7.32	127.03	119.56	7	4
1	A	8	THR	C-N-CA	7.32	127.03	119.56	7	4
1	A	8	THR	CA-C-O	-7.22	112.23	120.03	11	5
1	A	23	THR	CA-C-N	7.21	130.66	120.28	14	1
1	A	23	THR	C-N-CA	7.21	130.66	120.28	14	1
1	A	6	PHE	CA-CB-CG	-7.12	106.67	113.80	12	2
1	A	7	CYS	N-CA-C	-7.08	106.55	114.62	10	3
1	A	21	ILE	CA-C-O	-7.04	113.16	120.27	9	3
1	A	29	HIS	CA-C-N	7.00	134.30	121.70	12	3
1	A	29	HIS	C-N-CA	7.00	134.30	121.70	12	3
1	A	10	GLY	CA-C-N	6.98	129.97	120.54	7	3
1	A	10	GLY	C-N-CA	6.98	129.97	120.54	7	3
1	A	21	ILE	N-CA-C	-6.96	97.41	107.78	13	1
1	A	26	CYS	O-C-N	6.93	131.72	123.33	7	2
1	A	3	SER	CA-C-N	6.93	134.17	121.70	14	6
1	A	3	SER	C-N-CA	6.93	134.17	121.70	14	6
1	A	29	HIS	ND1-CG-CD2	6.84	112.94	106.10	3	6
1	A	8	THR	O-C-N	-6.82	113.74	121.79	14	3
1	A	27	ASN	O-C-N	-6.77	113.59	122.59	3	2
1	A	15	VAL	CB-CA-C	6.74	120.60	111.97	2	2
1	A	4	GLN	OE1-CD-NE2	-6.70	115.90	122.60	1	1
1	A	3	SER	CB-CA-C	6.62	120.73	111.86	14	4

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)	Models	
								Worst	Total
1	A	27	ASN	CA-C-N	6.52	129.32	120.38	13	3
1	A	27	ASN	C-N-CA	6.52	129.32	120.38	13	3
1	A	20	PHE	CA-C-N	6.46	132.01	122.71	10	2
1	A	20	PHE	C-N-CA	6.46	132.01	122.71	10	2
1	A	29	HIS	ND1-CE1-NE2	6.44	114.84	108.40	1	3
1	A	32	LYS	CB-CA-C	6.43	122.32	110.10	6	1
1	A	20	PHE	CA-CB-CG	-6.40	107.40	113.80	8	2
1	A	8	THR	N-CA-CB	6.38	122.26	110.27	6	3
1	A	32	LYS	CB-CG-CD	6.37	125.95	111.30	1	2
1	A	3	SER	N-CA-CB	6.37	121.74	112.13	11	3
1	A	24	ALA	CA-C-N	-6.34	113.56	123.13	1	2
1	A	24	ALA	C-N-CA	-6.34	113.56	123.13	1	2
1	A	1	TRP	CA-C-N	6.28	128.61	120.44	13	1
1	A	1	TRP	C-N-CA	6.28	128.61	120.44	13	1
1	A	20	PHE	CA-C-O	6.26	128.01	120.99	13	3
1	A	14	GLY	N-CA-C	-6.26	107.07	115.21	11	2
1	A	28	CYS	CB-CA-C	-6.16	100.39	110.85	2	3
1	A	3	SER	O-C-N	-6.12	114.45	122.59	12	1
1	A	26	CYS	N-CA-CB	6.11	122.48	111.37	6	1
1	A	13	THR	CA-CB-CG2	-6.10	100.13	110.50	3	1
1	A	13	THR	N-CA-CB	6.10	119.46	110.56	6	4
1	A	27	ASN	N-CA-CB	6.05	120.71	110.49	7	4
1	A	28	CYS	N-CA-C	6.00	117.49	111.07	6	1
1	A	9	PRO	O-C-N	6.00	130.37	122.27	12	1
1	A	2	LYS	N-CA-CB	-5.99	101.32	110.01	7	1
1	A	2	LYS	O-C-N	-5.96	115.65	122.09	3	1
1	A	25	THR	CA-C-O	5.93	127.58	120.28	4	1
1	A	13	THR	O-C-N	5.86	129.66	122.34	3	1
1	A	28	CYS	CA-C-N	5.83	131.38	122.11	6	2
1	A	28	CYS	C-N-CA	5.83	131.38	122.11	6	2
1	A	28	CYS	N-CA-CB	5.79	118.70	110.13	8	1
1	A	14	GLY	O-C-N	5.71	129.64	122.39	4	1
1	A	13	THR	CB-CA-C	5.68	120.23	110.01	14	2
1	A	29	HIS	CB-CG-ND1	-5.62	114.27	122.70	10	2
1	A	8	THR	N-CA-C	-5.62	99.65	109.48	13	2
1	A	1	TRP	CB-CG-CD2	-5.58	118.99	126.80	13	1
1	A	15	VAL	CA-CB-CG1	5.55	119.84	110.40	8	1
1	A	9	PRO	CA-C-N	5.53	132.25	121.41	10	1
1	A	9	PRO	C-N-CA	5.53	132.25	121.41	10	1
1	A	22	GLN	CB-CG-CD	5.48	121.92	112.60	1	1
1	A	12	VAL	O-C-N	-5.48	114.23	123.00	3	1

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)	Models	
								Worst	Total
1	A	29	HIS	CA-CB-CG	5.44	119.24	113.80	9	2
1	A	25	THR	CA-CB-CG2	5.42	119.71	110.50	9	1
1	A	11	CYS	CA-C-O	-5.39	115.14	121.07	12	1
1	A	15	VAL	CA-C-O	-5.29	115.24	120.85	15	1
1	A	30	ILE	N-CA-CB	5.27	120.46	111.50	12	1
1	A	19	CYS	O-C-N	-5.22	114.64	123.00	15	1
1	A	23	THR	N-CA-C	5.19	121.86	110.80	4	1
1	A	29	HIS	CA-C-O	5.18	126.86	121.31	13	1
1	A	25	THR	N-CA-C	5.18	118.10	107.69	13	1
1	A	29	HIS	CG-CD2-NE2	-5.16	102.04	107.20	7	1
1	A	2	LYS	CA-C-O	5.14	125.89	119.97	11	1
1	A	4	GLN	CA-CB-CG	5.09	124.29	114.10	3	1
1	A	6	PHE	CB-CA-C	5.05	119.70	110.10	12	1
1	A	22	GLN	CB-CA-C	-5.04	100.52	110.10	3	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	24	ALA	Peptide	15
1	A	26	CYS	Peptide,Mainchain	14
1	A	7	CYS	Peptide	12
1	A	11	CYS	Peptide	11
1	A	6	PHE	Sidechain	7
1	A	23	THR	Peptide	7
1	A	27	ASN	Peptide	6
1	A	21	ILE	Peptide	5
1	A	17	GLN	Peptide	3
1	A	15	VAL	Peptide	2
1	A	10	GLY	Peptide	2
1	A	4	GLN	Peptide	2
1	A	25	THR	Peptide	1
1	A	28	CYS	Peptide	1
1	A	29	HIS	Peptide	1
1	A	13	THR	Peptide	1
1	A	3	SER	Peptide	1
1	A	20	PHE	Sidechain	1

6.2 Too-close contacts [i](#)

In the following table, the Non-H and H(model) columns list the number of non-hydrogen atoms and hydrogen atoms in each chain respectively. The H(added) column lists the number of hydrogen atoms added and optimized by MolProbity. The Clashes column lists the number of clashes averaged over the ensemble.

Mol	Chain	Non-H	H(model)	H(added)	Clashes
1	A	217	210	204	2±1
All	All	3255	3150	3060	25

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 4.

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

Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:11:CYS:H	1:A:13:THR:HG23	0.59	1.56	13	1
1:A:29:HIS:CG	1:A:30:ILE:H	0.56	2.18	8	5
1:A:29:HIS:CG	1:A:30:ILE:N	0.52	2.77	8	8
1:A:29:HIS:CE1	1:A:30:ILE:HD11	0.51	2.40	1	1
1:A:2:LYS:HA	1:A:13:THR:HG22	0.50	1.82	4	3
1:A:29:HIS:CE1	1:A:30:ILE:HG12	0.49	2.42	10	1
1:A:29:HIS:CE1	1:A:30:ILE:CD1	0.45	2.99	1	1
1:A:22:GLN:H	1:A:32:LYS:C	0.45	2.20	6	1
1:A:15:VAL:HG12	1:A:19:CYS:SG	0.44	2.52	6	1
1:A:23:THR:HA	1:A:25:THR:C	0.43	2.38	4	1
1:A:20:PHE:CD2	1:A:23:THR:HG22	0.41	2.50	4	1
1:A:10:GLY:C	1:A:12:VAL:HA	0.40	2.41	9	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	27/32 (84%)	22±2 (80±6%)	5±1 (17±5%)	1±1 (2±2%)	6	43
All	All	405/480 (84%)	325 (80%)	70 (17%)	10 (2%)	6	43

All 4 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	30	ILE	4
1	A	23	THR	3
1	A	4	GLN	2
1	A	27	ASN	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	21/26 (81%)	18±1 (85±5%)	3±1 (15±5%)	5	42
All	All	315/390 (81%)	268 (85%)	47 (15%)	5	42

All 11 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	11	CYS	15
1	A	32	LYS	13
1	A	15	VAL	7
1	A	6	PHE	5
1	A	29	HIS	1
1	A	27	ASN	1
1	A	22	GLN	1
1	A	28	CYS	1
1	A	7	CYS	1
1	A	9	PRO	1
1	A	20	PHE	1

6.3.3 RNA [i](#)

There are no RNA molecules in this entry.

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

3 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	Counts	Bond lengths	
						RMSZ	#Z>2
1	DHA	A	5	1	3,4,5	2.43±0.10	1±0 (48±16%)
1	MDH	A	18	1	3,5,7	1.27±0.12	1±0 (17±16%)
1	DHA	A	31	1	3,4,5	2.43±0.05	2±0 (55±15%)

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	Counts	Bond angles	
						RMSZ	#Z>2
1	DHA	A	5	1	2,4,6	2.65±0.93	1±1 (56±30%)
1	MDH	A	18	1	3,5,8	6.11±2.06	2±1 (75±22%)
1	DHA	A	31	1	2,4,6	3.96±0.59	2±0 (86±22%)

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
1	DHA	A	31	1	-	0±0,0,2,4	-
1	MDH	A	18	1	-	0±0,1,4,8	-
1	DHA	A	5	1	-	0±0,0,2,4	-

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	31	DHA	CB-CA	3.74	1.51	1.34	3	15
1	A	5	DHA	CB-CA	3.73	1.51	1.34	6	15
1	A	5	DHA	C-CA	2.72	1.49	1.45	11	7
1	A	18	MDH	C-CA	2.41	1.49	1.45	6	8
1	A	31	DHA	C-CA	2.34	1.49	1.45	9	10

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	18	MDH	CG-CB-CA	15.66	106.94	126.12	1	15
1	A	18	MDH	CB-CA-N	7.60	109.45	123.25	14	13
1	A	18	MDH	O-C-CA	6.58	117.14	125.39	8	6
1	A	31	DHA	CB-CA-N	6.31	110.55	125.76	3	14
1	A	5	DHA	CB-CA-N	6.21	110.81	125.76	13	11
1	A	5	DHA	O-C-CA	5.03	116.09	125.53	4	6
1	A	31	DHA	O-C-CA	4.73	116.65	125.53	6	12

There are no chirality outliers.

All unique torsion outliers are listed below.

Mol	Chain	Res	Type	Atoms	Models (Total)
1	A	18	MDH	O-C-CA-CB	9

There are no ring outliers.

6.5 Carbohydrates [i](#)

There are no oligosaccharides 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 ⓘ

There are no chain breaks in this entry.

7 Chemical shift validation

The completeness of assignment taking into account all chemical shift lists is 86% for the well-defined parts and 86% 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	341
Number of shifts mapped to atoms	341
Number of unparsed shifts	0
Number of shifts with mapping errors	0
Number of shifts with mapping warnings	0
Number of shift outliers (ShiftChecker)	15

7.1.2 Chemical shift referencing

The following table shows the suggested chemical shift referencing corrections.

Nucleus	# values	Correction $\pm$ precision, ppm	Suggested action
$^{13}\text{C}_\alpha$	29	2.45 ± 0.66	Should be checked
$^{13}\text{C}_\beta$	22	—	None (insufficient data)
$^{13}\text{C}'$	0	—	None (insufficient data)
^{15}N	28	3.76 ± 0.60	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 86%, i.e. 320 atoms were assigned a chemical shift out of a possible 373. 0 out of 3 assigned methyl groups (LEU and VAL) were assigned stereospecifically.

	Total	^1H	^{13}C	^{15}N
Backbone	115/145 (79%)	58/59 (98%)	29/58 (50%)	28/28 (100%)
Sidechain	169/189 (89%)	118/124 (95%)	48/59 (81%)	3/6 (50%)

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	Total	¹ H	¹³ C	¹⁵ N
Aromatic	36/39 (92%)	18/20 (90%)	17/17 (100%)	1/2 (50%)
Overall	320/373 (86%)	194/203 (96%)	94/134 (70%)	32/36 (89%)

The following table shows the completeness of the chemical shift assignments for the full structure. The overall completeness is 86%, i.e. 320 atoms were assigned a chemical shift out of a possible 373. 0 out of 3 assigned methyl groups (LEU and VAL) were assigned stereospecifically.

	Total	¹ H	¹³ C	¹⁵ N
Backbone	115/145 (79%)	58/59 (98%)	29/58 (50%)	28/28 (100%)
Sidechain	169/189 (89%)	118/124 (95%)	48/59 (81%)	3/6 (50%)
Aromatic	36/39 (92%)	18/20 (90%)	17/17 (100%)	1/2 (50%)
Overall	320/373 (86%)	194/203 (96%)	94/134 (70%)	32/36 (89%)

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	3	SER	CB	37.12	56.28 – 71.32	-17.7
1	A	13	THR	CB	40.49	61.12 – 78.27	-17.0
1	A	17	GLN	HB2	0.53	0.80 – 3.29	-6.1
1	A	17	GLN	HG2	0.73	1.01 – 3.62	-6.1
1	A	2	LYS	HE2	1.82	1.95 – 3.88	-5.7
1	A	17	GLN	HG3	0.73	0.91 – 3.68	-5.7
1	A	32	LYS	HE2	1.82	1.95 – 3.88	-5.7
1	A	2	LYS	HE3	1.82	1.92 – 3.89	-5.5
1	A	32	LYS	HE3	1.82	1.92 – 3.89	-5.5
1	A	23	THR	HB	2.43	2.57 – 5.77	-5.4
1	A	17	GLN	HB3	0.60	0.71 – 3.33	-5.4
1	A	13	THR	HB	2.46	2.57 – 5.77	-5.3
1	A	1	TRP	CZ2	121.76	107.20 – 121.33	5.3
1	A	8	THR	HB	2.47	2.57 – 5.77	-5.3
1	A	25	THR	HB	2.51	2.57 – 5.77	-5.2

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:

