Full wwPDB NMR Structure Validation Report (i)

Feb 13, 2017 – 12:25 am GMT

PDB ID : 2L2X

Title : Thiostrepton, oxidized at CA-CB bond of residue 9

Authors : Jonker, H.R.A.; Baumann, S.; Wolf, A.; Schoof, S.; Hiller, F.; Schulte, K.W.; Kirschner, K.N.; Schwalbe, H.; Arndt, H.-D.

Deposited on : 2010-08-27

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

We welcome your comments at *validation@mail.wwpdb.org*
A user guide is available at
http://wwpdb.org/validation/2016/NMRValidationReportHelp
with specific help available everywhere you see the (i) symbol.

The following versions of software and data (see references (i)) were used in the production of this report:

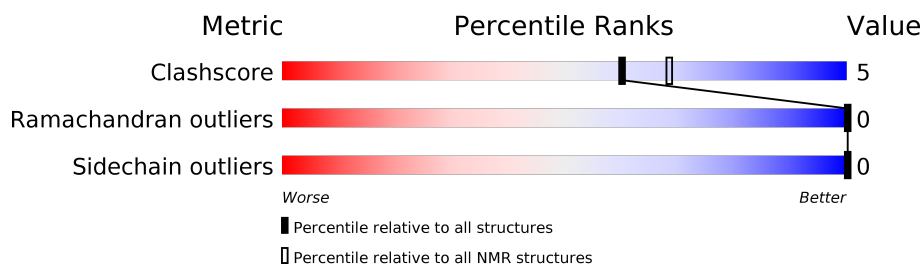|		
Cyrange	:	Kirchner and Güntert (2011)
NmrClust	:	Kelley et al. (1996)
MolProbity	:	4.02b-467
Mogul	:	1.7.2 (RC1), CSD as538be (2017)
Percentile statistics	:	20161228.v01 (using entries in the PDB archive December 28th 2016)
RCI	:	v_1n_11_5_13_A (Berjanski et al., 2005)
PANAV	:	Wang et al. (2010)
ShiftChecker	:	trunk28760
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	recalc28949

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 was not calculated.

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	Percentile Ranks	Value
Clashscore		5
Ramachandran outliers		0
Sidechain outliers		0

Worse   *Better*

▌ Percentile relative to all structures
⫿ Percentile relative to all NMR structures

Metric	Whole archive (#Entries)	NMR archive (#Entries)
Clashscore	125131	11601
Ramachandran outliers	121729	10391
Sidechain outliers	121581	10367

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	18	89% 11%

2 Ensemble composition and analysis (i)

This entry contains 20 models.

Cyrange was unable to find well-defined residues.

Error message: The number of core atoms (6) was below the domain threshold value (8).

NmrClust was unable to cluster the ensemble.

Error message: Wrapper check: not enough residues in core to run NmrClust

3 Entry composition (i)

There is only 1 type of molecule in this entry. The entry contains 189 atoms, of which 80 are hydrogens and 0 are deuteriums.

- Molecule 1 is a protein called Thiostrepton.

Mol	Chain	Residues	Atoms						Trace
1	A	18	Total	C	H	N	O	S	1
			189	69	80	18	17	5	

There are 2 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	0	QUA	-	SEE REMARK 999	UNP P0C8P8
A	17	NH2	-	AMIDATION	UNP P0C8P8

4 Residue-property plots ⓘ

4.1 Average score per residue in the NMR ensemble

These plots are provided for all protein, RNA and DNA 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.
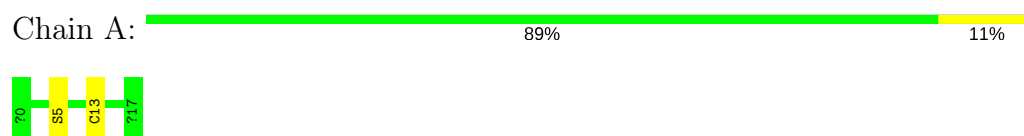
• Molecule 1: Thiostrepton

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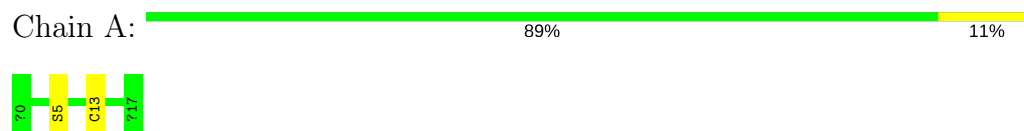
4.2 Scores per residue for each member of the ensemble
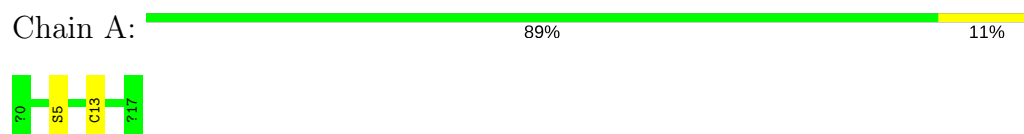
Colouring as in section 4.1 above.

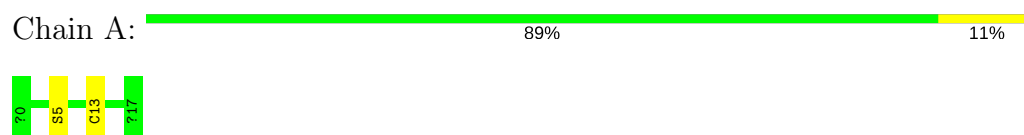### 4.2.1 Score per residue for model 1

• Molecule 1: Thiostrepton

Chain A:

4.2.2 Score per residue for model 2

• Molecule 1: Thiostrepton

Chain A:

4.2.3 Score per residue for model 3

• Molecule 1: Thiostrepton

Chain A:
89%   11%

4.2.4 Score per residue for model 4

• Molecule 1: Thiostrepton

Chain A:
89%   11%

4.2.5 Score per residue for model 5

• Molecule 1: Thiostrepton

Chain A:
89%   11%
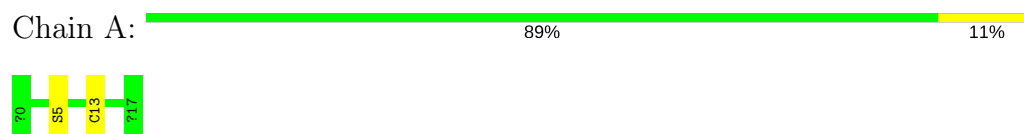
4.2.6 Score per residue for model 6

• Molecule 1: Thiostrepton

Chain A:
89%   11%

4.2.7 Score per residue for model 7

• Molecule 1: Thiostrepton

Chain A:
89%   11%
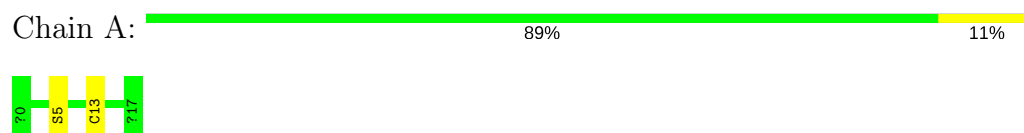
4.2.8 Score per residue for model 8

• Molecule 1: Thiostrepton

Chain A:

89%   11%

?0 S5 C13 ?17
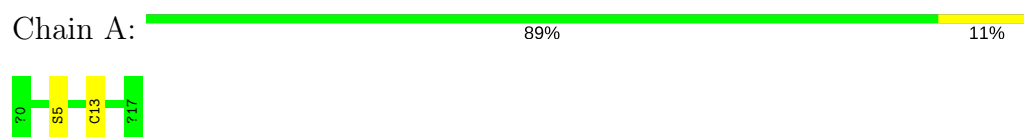
4.2.9 Score per residue for model 9

• Molecule 1: Thiostrepton

Chain A:

89%   11%

?0 S5 C13 ?17
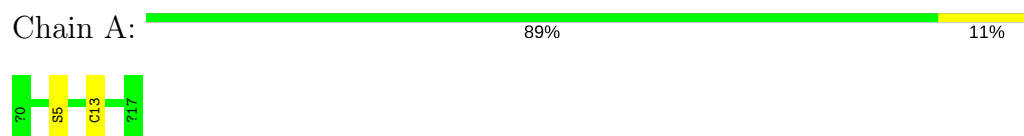
4.2.10 Score per residue for model 10

• Molecule 1: Thiostrepton

Chain A:

89%   11%

?0 S5 C13 ?17
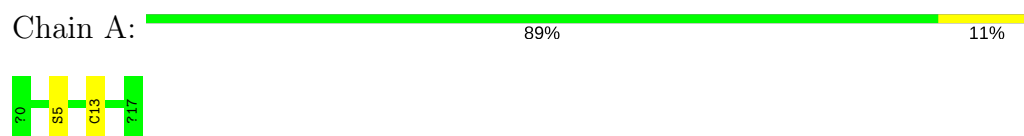
4.2.11 Score per residue for model 11

• Molecule 1: Thiostrepton

Chain A:

89%   11%

?0 S5 C13 ?17
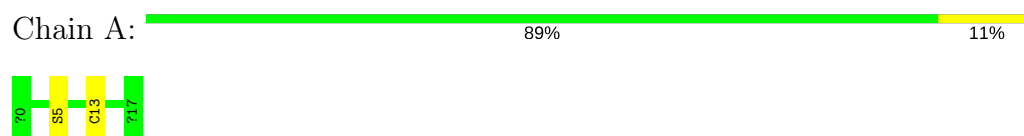
4.2.12 Score per residue for model 12

• Molecule 1: Thiostrepton

Chain A:

89%   11%

?0 S5 C13 ?17
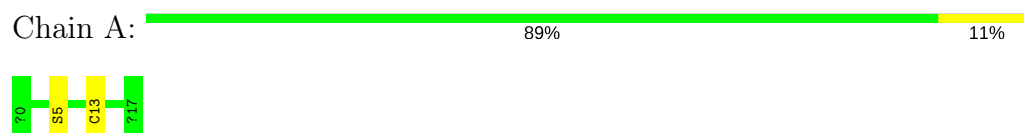
4.2.13 Score per residue for model 13

• Molecule 1: Thiostrepton

Chain A:
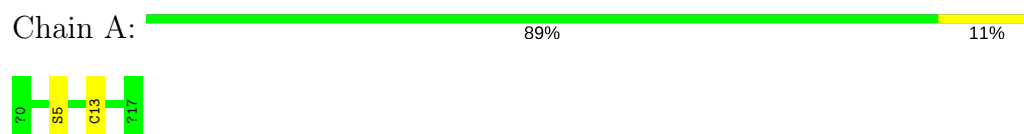
89%   6%   6%
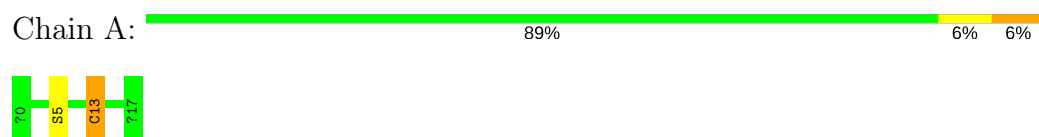
4.2.14 Score per residue for model 14

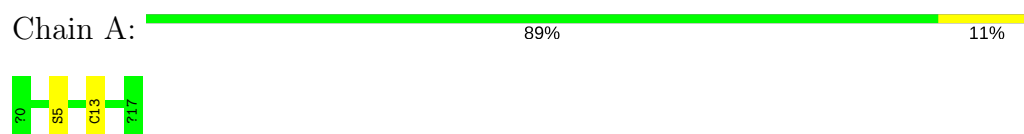• Molecule 1: Thiostrepton

Chain A:

89%   11%
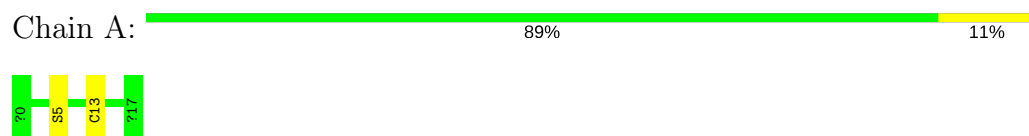
4.2.15 Score per residue for model 15

• Molecule 1: Thiostrepton

Chain A:

89%   11%
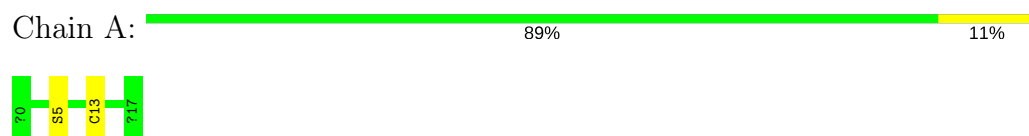
4.2.16 Score per residue for model 16

• Molecule 1: Thiostrepton

Chain A:

89%   11%
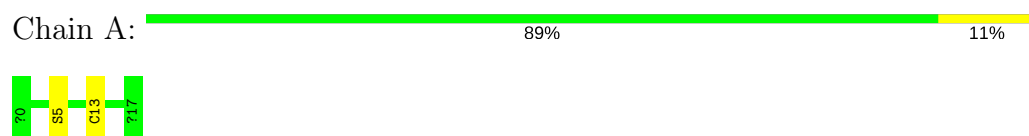
4.2.17 Score per residue for model 17

• Molecule 1: Thiostrepton

Chain A:

89%   11%
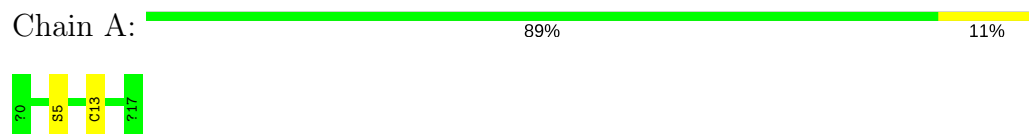
4.2.18 Score per residue for model 18

• Molecule 1: Thiostrepton

Chain A:

89%   11%
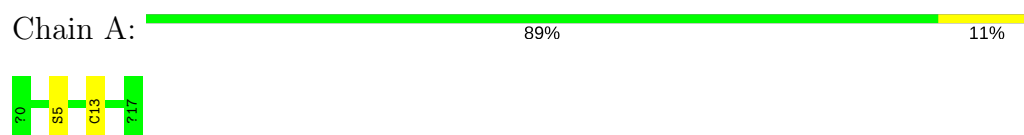
4.2.19 Score per residue for model 19

• Molecule 1: Thiostrepton

Chain A:

89%   11%
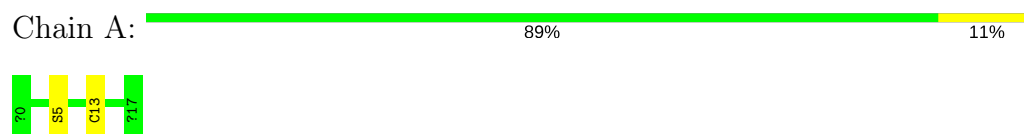
4.2.20 Score per residue for model 20

• Molecule 1: Thiostrepton

Chain A:

89%   11%
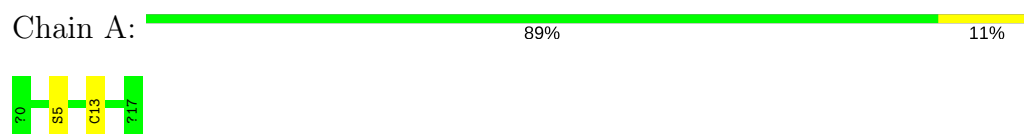
5 Refinement protocol and experimental data overview ⓘ

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

Of the 200 calculated structures, 20 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	refinement	1.2
CNS	structure solution	1.1

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)	BMRB entry 17154
Number of chemical shift lists	1
Total number of shifts	151
Number of shifts mapped to atoms	0
Number of unparsed shifts	0
Number of shifts with mapping errors	151
Number of shifts with mapping warnings	0
Assignment completeness (well-defined parts)	0%

No validations of the models with respect to experimental NMR restraints is performed at this time.

6 Model quality ⓘ

6.1 Standard geometry ⓘ

Bond lengths and bond angles in the following residue types are not validated in this section: TS9, DHA, QUA, BB9, NH2, MH6, DBU

There are no covalent bond-length or bond-angle outliers.

Chiral center outliers are detected by calculating the chiral volume of a chiral center and verifying if the center is modelled as a planar moiety or with the opposite hand. A planarity outlier is detected by checking planarity of atoms in a peptide group, atoms in a mainchain group or atoms of a sidechain that are expected to be planar.

Mol	Chain	Chirality	Planarity
1	A	0.0±0.0	0.1±0.2
All	All	0	1

There are no bond-length outliers.

There are no bond-angle outliers.

There are no chirality outliers.

All unique planar outliers are listed below.

Mol	Chain	Res	Type	Group	Models (Total)
1	A	13	BB9	Peptide	1

6.2 Too-close contacts ⓘ

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes
1	A	109	80	77	1±0
All	All	2180	1600	1540	20

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:5:SER:H	1:A:13:BB9:HN1	0.55	1.43	13	20

6.3 Torsion angles ⓘ

6.3.1 Protein backbone ⓘ

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	5/18 (28%)	4±0 (78±6%)	1±0 (22±6%)	0±0 (0±0%)	100	100
All	All	100/360 (28%)	78 (78%)	22 (22%)	0 (0%)	100	100

There are no Ramachandran outliers.

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	3/4 (75%)	3±0 (100±0%)	0±0 (0±0%)	100	100
All	All	60/80 (75%)	60 (100%)	0 (0%)	100	100

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

6.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

10 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
1	TS9	A	10	1	6,8,10	0.85±0.01	0±0 (0±0%)
1	BB9	A	11	1	3,5,6	0.45±0.02	0±0 (0±0%)
1	BB9	A	13	1	2,4,6	0.63±0.02	0±0 (0±0%)
1	MH6	A	14	1	3,3,6	1.13±0.03	0±0 (0±0%)
1	BB9	A	15	1	3,5,6	0.40±0.02	0±0 (0±0%)
1	DHA	A	16	1	4,4,5	2.62±0.05	1±0 (25±0%)
1	DHA	A	3	1	4,4,5	2.64±0.02	1±0 (25±0%)
1	BB9	A	6	1	3,5,6	0.43±0.02	0±0 (0±0%)
1	DBU	A	8	1	4,4,6	2.78±0.02	1±0 (25±0%)
1	BB9	A	9	1	3,5,6	0.46±0.02	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
1	TS9	A	10	1	5,12,15	0.71±0.01	0±0 (0±0%)
1	BB9	A	11	1	1,5,7	0.88±0.06	0±0 (0±0%)
1	BB9	A	13	1	3,4,7	2.63±0.01	0±0 (0±0%)
1	MH6	A	14	1	1,3,7	0.36±0.04	0±0 (0±0%)
1	BB9	A	15	1	1,5,7	0.98±0.09	0±0 (0±0%)
1	DHA	A	16	1	3,4,6	2.56±0.09	0±0 (0±0%)
1	DHA	A	3	1	3,4,6	2.58±0.02	0±0 (0±0%)
1	BB9	A	6	1	1,5,7	0.74±0.04	0±0 (0±0%)
1	DBU	A	8	1	4,4,7	1.31±0.04	0±0 (0±0%)
1	BB9	A	9	1	1,5,7	0.82±0.06	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
1	TS9	A	10	1	-	0±0,9,12,16	0±0,0,0,0
1	BB9	A	11	1	-	0±0,0,4,6	0±0,0,0,0
1	BB9	A	13	1	-	0±0,0,2,6	0±0,0,0,0
1	MH6	A	14	1	-	0±0,0,0,6	0±0,0,0,0
1	BB9	A	15	1	-	0±0,0,4,6	0±0,0,0,0
1	DHA	A	16	1	-	0±0,0,2,4	0±0,0,0,0
1	DHA	A	3	1	-	0±0,0,2,4	0±0,0,0,0
1	BB9	A	6	1	-	0±0,0,4,6	0±0,0,0,0
1	DBU	A	8	1	-	0±0,1,2,6	0±0,0,0,0
1	BB9	A	9	1	-	0±0,0,4,6	0±0,0,0,0

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	8	DBU	CA-N	5.51	1.47	1.33	8	20
1	A	3	DHA	CA-N	5.27	1.48	1.34	10	20
1	A	16	DHA	CA-N	5.24	1.48	1.34	9	20

There are no bond-angle outliers.

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

6.5　Carbohydrates　ⓘ

There are no carbohydrates 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 (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 0% for the well-defined parts and 0% for the entire structure.

7.1 Chemical shift list 1

File name: BMRB entry 17154

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	151
Number of shifts mapped to atoms	0
Number of unparsed shifts	0
Number of shifts with mapping errors	151
Number of shifts with mapping warnings	0
Number of shift outliers (ShiftChecker)	4

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

- Chain not found in structure. All 151 occurences are reported below.

Chain	Res	Type	Atom	Shift Data		
				Value	Uncertainty	Ambiguity
UNMAPPED	2	ILE	HD12	0.93	0.02	1
UNMAPPED	5	ALA	CA	55.0	0.05	1
UNMAPPED	10	BB9	CB	127.5	0.05	1
UNMAPPED	11	TS9	CG2	20.8	0.05	1
UNMAPPED	18	NH2	HN2	6.43	0.02	2
UNMAPPED	9	DBU	HG2	1.69	0.02	1
UNMAPPED	9	DBU	HG1	1.69	0.02	1
UNMAPPED	7	BB9	C	164.5	0.05	1
UNMAPPED	4	DHA	HB2	5.36	0.02	2
UNMAPPED	4	DHA	HB1	5.82	0.02	2
UNMAPPED	2	ILE	CG1	27.8	0.05	1
UNMAPPED	16	BB9	C	162.4	0.05	1
UNMAPPED	3	ALA	HB2	1.22	0.02	1
UNMAPPED	2	ILE	CG2	18.5	0.05	1

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Chain	Res	Type	Atom	Shift Data		
				Value	Uncertainty	Ambiguity
UNMAPPED	1	QUA	C9	157.3	0.05	1
UNMAPPED	10	BB9	HB	8.06	0.02	1
UNMAPPED	5	ALA	HB3	1.47	0.02	1
UNMAPPED	1	QUA	C3	125.0	0.05	1
UNMAPPED	9	DBU	H1	8.57	0.02	1
UNMAPPED	5	ALA	C	176.0	0.05	1
UNMAPPED	9	DBU	N	122.0	0.05	1
UNMAPPED	1	QUA	C5	126.0	0.05	1
UNMAPPED	2	ILE	CA	68.9	0.05	1
UNMAPPED	17	DHA	H	10.05	0.02	1
UNMAPPED	13	THR	CG2	21.5	0.05	1
UNMAPPED	15	MH6	CB	27.4	0.05	1
UNMAPPED	6	SER	CA	60.4	0.05	1
UNMAPPED	15	MH6	CA	164.7	0.05	1
UNMAPPED	6	SER	CB	32.2	0.05	1
UNMAPPED	7	BB9	CA	149.2	0.05	1
UNMAPPED	11	TS9	CA	56.2	0.05	1
UNMAPPED	1	QUA	H141	1.39	0.02	1
UNMAPPED	5	ALA	H	7.15	0.02	1
UNMAPPED	8	THR	H	7.03	0.02	1
UNMAPPED	11	TS9	N	116.9	0.05	1
UNMAPPED	1	QUA	H142	1.39	0.02	1
UNMAPPED	13	THR	CB	75.2	0.05	1
UNMAPPED	11	TS9	HD11	1.34	0.02	1
UNMAPPED	2	ILE	HB	1.81	0.02	1
UNMAPPED	16	BB9	HB	8.29	0.02	1
UNMAPPED	8	THR	C	169.4	0.05	1
UNMAPPED	4	DHA	C	166.0	0.05	1
UNMAPPED	14	BB9	C	67.0	0.05	1
UNMAPPED	1	QUA	C11	163.7	0.05	1
UNMAPPED	11	TS9	HG23	1.24	0.02	1
UNMAPPED	6	SER	C	172.6	0.05	1
UNMAPPED	2	ILE	HG22	0.97	0.02	1
UNMAPPED	15	MH6	HB3	3.48	0.02	2
UNMAPPED	3	ALA	CB	21.8	0.05	1
UNMAPPED	11	TS9	CD1	19.1	0.05	1
UNMAPPED	6	SER	HB2	4.11	0.02	2
UNMAPPED	3	ALA	CA	52.1	0.05	1
UNMAPPED	4	DHA	CB	105.1	0.05	1
UNMAPPED	17	DHA	HB1	6.69	0.02	2
UNMAPPED	17	DHA	CA	136.1	0.05	1

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Chain	Res	Type	Atom	Shift Data		
				Value	Uncertainty	Ambiguity
UNMAPPED	17	DHA	HB2	5.65	0.02	2
UNMAPPED	2	ILE	HD13	0.93	0.02	1
UNMAPPED	11	TS9	HD12	1.34	0.02	1
UNMAPPED	8	THR	N	112.5	0.05	1
UNMAPPED	11	TS9	H	8.08	0.02	1
UNMAPPED	8	THR	CA	58.4	0.05	1
UNMAPPED	11	TS9	HD13	1.34	0.02	1
UNMAPPED	10	BB9	CA	151.4	0.05	1
UNMAPPED	12	BB9	CB	127.7	0.05	1
UNMAPPED	12	BB9	CA	152.9	0.05	1
UNMAPPED	1	QUA	HC71	3.61	0.02	1
UNMAPPED	3	ALA	HB1	1.22	0.02	1
UNMAPPED	8	THR	HG21	1.14	0.02	1
UNMAPPED	13	THR	C	173.0	0.05	1
UNMAPPED	8	THR	HG22	1.14	0.02	1
UNMAPPED	5	ALA	HB2	1.47	0.02	1
UNMAPPED	5	ALA	HB1	1.47	0.02	1
UNMAPPED	1	QUA	HC3	7.32	0.02	1
UNMAPPED	9	DBU	HB1	6.28	0.02	1
UNMAPPED	1	QUA	C6	132.8	0.05	1
UNMAPPED	1	QUA	HC6	6.36	0.02	1
UNMAPPED	2	ILE	CB	41.4	0.05	1
UNMAPPED	1	QUA	HC5	6.9	0.02	1
UNMAPPED	1	QUA	HC8	4.62	0.02	1
UNMAPPED	7	BB9	CB	128.0	0.05	1
UNMAPPED	6	SER	N	121.9	0.05	1
UNMAPPED	1	QUA	H143	1.39	0.02	1
UNMAPPED	13	THR	HA	5.89	0.02	1
UNMAPPED	9	DBU	C	169.9	0.05	1
UNMAPPED	13	THR	HB	6.37	0.02	1
UNMAPPED	2	ILE	C	177.1	0.05	1
UNMAPPED	13	THR	CA	58.4	0.05	1
UNMAPPED	14	BB9	CB	120.4	0.05	1
UNMAPPED	13	THR	N	110.4	0.05	1
UNMAPPED	2	ILE	HG13	1.18	0.02	2
UNMAPPED	14	BB9	HB	7.55	0.02	1
UNMAPPED	11	TS9	HG22	1.24	0.02	1
UNMAPPED	11	TS9	HG21	1.24	0.02	1
UNMAPPED	2	ILE	HG23	0.97	0.02	1
UNMAPPED	11	TS9	HA	5.89	0.02	1
UNMAPPED	1	QUA	C14	25.7	0.05	1

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Chain	Res	Type	Atom	Shift Data		
				Value	Uncertainty	Ambiguity
UNMAPPED	6	SER	HB3	2.3	0.02	2
UNMAPPED	13	THR	HG23	1.74	0.02	1
UNMAPPED	4	DHA	CA	135.1	0.05	1
UNMAPPED	17	DHA	CB	106.6	0.05	1
UNMAPPED	12	BB9	HB	8.27	0.02	1
UNMAPPED	5	ALA	N	111.7	0.05	1
UNMAPPED	17	DHA	N	123.0	0.05	1
UNMAPPED	6	SER	H	9.94	0.02	1
UNMAPPED	2	ILE	HD11	0.93	0.02	1
UNMAPPED	7	BB9	HB	8.2	0.02	1
UNMAPPED	5	ALA	CB	21.7	0.05	1
UNMAPPED	8	THR	CB	69.5	0.05	1
UNMAPPED	5	ALA	HA	4.8	0.02	1
UNMAPPED	13	THR	H	8.73	0.02	1
UNMAPPED	2	ILE	HG21	0.97	0.02	1
UNMAPPED	18	NH2	HN1	7.43	0.02	2
UNMAPPED	2	ILE	HA	2.98	0.02	1
UNMAPPED	3	ALA	HA	3.82	0.02	1
UNMAPPED	9	DBU	HG3	1.69	0.02	1
UNMAPPED	8	THR	CG2	21.6	0.05	1
UNMAPPED	3	ALA	HB3	1.22	0.02	1
UNMAPPED	8	THR	HG23	1.14	0.02	1
UNMAPPED	1	QUA	C8	69.9	0.05	1
UNMAPPED	9	DBU	CG	17.5	0.05	1
UNMAPPED	11	TS9	C	169.2	0.05	1
UNMAPPED	3	ALA	H	7.74	0.02	1
UNMAPPED	1	QUA	C7	62.1	0.05	1
UNMAPPED	11	TS9	CG1	70.6	0.05	1
UNMAPPED	4	DHA	N	120.7	0.05	1
UNMAPPED	1	QUA	C4	156.3	0.05	1
UNMAPPED	4	DHA	H	7.88	0.02	1
UNMAPPED	11	TS9	HG1	3.9	0.02	1
UNMAPPED	15	MH6	C	171.1	0.05	1
UNMAPPED	1	QUA	H13	5.34	0.02	1
UNMAPPED	11	TS9	CB	80.3	0.05	1
UNMAPPED	8	THR	HB	1.39	0.02	1
UNMAPPED	12	BB9	C	165.0	0.05	1
UNMAPPED	8	THR	HA	4.59	0.02	1
UNMAPPED	9	DBU	CB	130.1	0.05	1
UNMAPPED	14	BB9	CA	160.3	0.05	1
UNMAPPED	2	ILE	HG12	1.43	0.02	2

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Chain	Res	Type	Atom	Shift Data		
				Value	Uncertainty	Ambiguity
UNMAPPED	16	BB9	CB	130.3	0.05	1
UNMAPPED	14	BB9	HC	5.32	0.02	1
UNMAPPED	9	DBU	CA	130.7	0.05	1
UNMAPPED	3	ALA	C	171.3	0.05	1
UNMAPPED	3	ALA	N	121.0	0.05	1
UNMAPPED	17	DHA	C	169.0	0.05	1
UNMAPPED	1	QUA	C13	67.2	0.05	1
UNMAPPED	1	QUA	C10	130.0	0.05	1
UNMAPPED	16	BB9	CA	153.0	0.05	1
UNMAPPED	2	ILE	CD1	14.2	0.05	1
UNMAPPED	15	MH6	HB2	2.94	0.02	2
UNMAPPED	13	THR	HG22	1.74	0.02	1
UNMAPPED	13	THR	HG21	1.74	0.02	1
UNMAPPED	10	BB9	C	164.3	0.05	1

7.1.2 Chemical shift referencing ⓘ

No chemical shift referencing corrections were calculated (not enough data).

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 0%, i.e. 0 atoms were assigned a chemical shift out of a possible 54. 0 out of 0 assigned methyl groups (LEU and VAL) were assigned stereospecifically.

	Total	^{1}H	^{13}C	^{15}N
Backbone	0/30 (0%)	0/12 (0%)	0/12 (0%)	0/6 (0%)
Sidechain	0/24 (0%)	0/13 (0%)	0/11 (0%)	0/0 (—%)
Aromatic	0/0 (—%)	0/0 (—%)	0/0 (—%)	0/0 (—%)
Overall	0/54 (0%)	0/25 (0%)	0/23 (0%)	0/6 (0%)

The following table shows the completeness of the chemical shift assignments for the full structure. The overall completeness is 0%, i.e. 0 atoms were assigned a chemical shift out of a possible 54. 0 out of 0 assigned methyl groups (LEU and VAL) were assigned stereospecifically.

	Total	^{1}H	^{13}C	^{15}N
Backbone	0/30 (0%)	0/12 (0%)	0/12 (0%)	0/6 (0%)
Sidechain	0/24 (0%)	0/13 (0%)	0/11 (0%)	0/0 (—%)
Aromatic	0/0 (—%)	0/0 (—%)	0/0 (—%)	0/0 (—%)

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	Total	^{1}H	^{13}C	^{15}N
Overall	0/54 (0%)	0/25 (0%)	0/23 (0%)	0/6 (0%)

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
???	UNMAPPED	6	SER	CB	32.20	71.24 − 56.34	-21.2
???	UNMAPPED	8	THR	HB	1.39	5.82 − 2.52	-8.4
???	UNMAPPED	13	THR	HB	6.37	5.82 − 2.52	6.7
???	UNMAPPED	6	SER	HB3	2.30	5.25 − 2.45	-5.5

7.1.5 Random Coil Index (RCI) plots ⓘ

No *random coil index* (RCI) plot could be generated from the current chemical shift list (assigned_chem_shift_list_1). RCI is only applicable to proteins.