



wwPDB NMR Structure Validation Summary Report ⓘ

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

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

Cyrange	:	Kirchner and Güntert (2011)
NmrClust	:	Kelley et al. (1996)
MolProbity	:	4.02b-467
Mogul	:	1.7.3 (157068), CSD as539be (2018)
Percentile statistics	:	20171227.v01 (using entries in the PDB archive December 27th 2017)
RCI	:	v_1n_11_5_13_A (Berjanski et al., 2005)
PANAV	:	Wang et al. (2010)
ShiftChecker	:	trunk30686
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	trunk30686

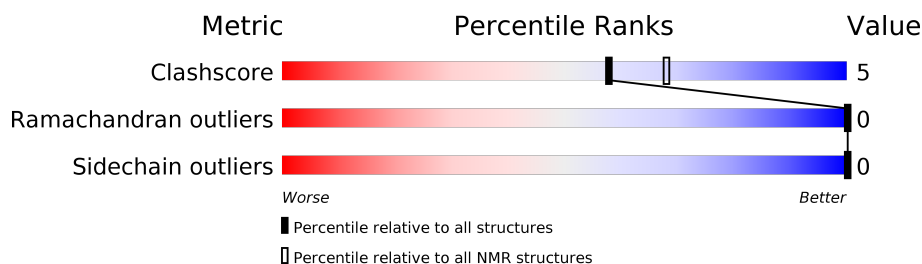
1 Overall quality at a glance

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	Whole archive (#Entries)	NMR archive (#Entries)
Clashscore	136279	12091
Ramachandran outliers	132675	10835
Sidechain outliers	132484	10811

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	18	

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	BB9	13	-	20

2 Ensemble composition and analysis ⓘ

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

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:

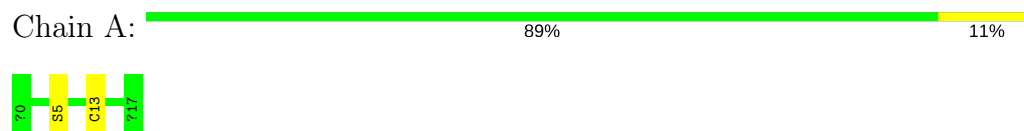
Chain	Residue	Modelled	Actual	Comment	Reference
A	0	QUA	-	SEE REMARK 999	UNP P0C8P8
A	17	NH2	-	AMIDATION	UNP P0C8P8

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.

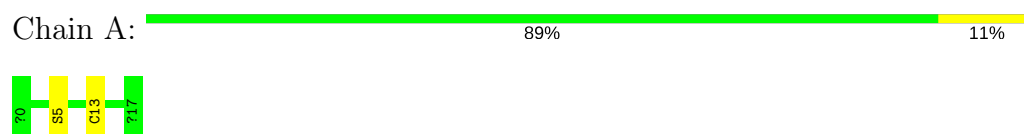
- Molecule 1: Thiostrepton



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

The representative model is number 1. Colouring as in section 4.1 above.

- Molecule 1: Thiostrepton



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 [i](#)

6.1 Standard geometry [i](#)

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 [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	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 [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	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 [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	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 [i](#)

There are no RNA molecules in this entry.

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

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	0.86±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	3,4,6	4.42±0.04	1±0 (33±0%)
1	MH6	A	14	1	3,3,6	1.12±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	2.60±0.05	1±0 (17±11%)
1	DHA	A	3	1	4,4,5	2.61±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	0.73±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	0.37±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	2,4,6	3.14±0.10	0±0 (0±0%)
1	DHA	A	3	1	2,4,6	3.17±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	13	BB9	CB-CA	7.72	1.43	1.33	15	20
1	A	8	DBU	CA-N	5.51	1.47	1.33	8	20
1	A	3	DHA	CA-N	5.22	1.48	1.34	10	20
1	A	16	DHA	CA-N	5.19	1.48	1.34	9	14

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](#)

There are no carbohydrates 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 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. First 5 (of 151) occurrences 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

7.1.2 Chemical shift referencing

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

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 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%)

7.1.4 Statistically unusual chemical shifts [i](#)

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 [i](#)

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.