



# wwPDB NMR Structure Validation Summary Report ⓘ

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PDB ID : 2L2W  
Title : Thiostrepton  
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This is a wwPDB NMR Structure Validation Summary Report for a publicly released PDB entry.  
We welcome your comments at [validation@mail.wwpdb.org](mailto:validation@mail.wwpdb.org)  
A user guide is available at  
<http://wwpdb.org/validation/2016/NMRValidationReportHelp>  
with specific help available everywhere you see the ⓘ symbol.

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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 : 1.7.1 (RC1), CSD as537be (2016)  
Percentile statistics : 20151230.v01 (using entries in the PDB archive December 30th 2015)  
RCI : v\_1n\_11\_5\_13\_A (Berjanski et al., 2005)  
PANAV : Wang et al. (2010)  
ShiftChecker : rb-20027457  
Ideal geometry (proteins) : Engh & Huber (2001)  
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)  
Validation Pipeline (wwPDB-VP) : rb-20027457

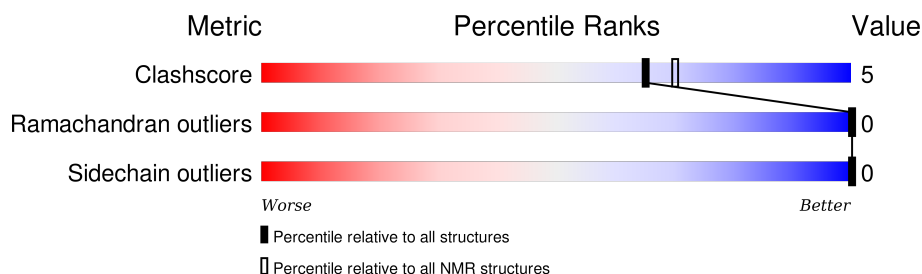
# 1 Overall quality at a glance

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<br>(#Entries) | NMR archive<br>(#Entries) |
|-----------------------|-----------------------------|---------------------------|
| Clashscore            | 114402                      | 11133                     |
| Ramachandran outliers | 111179                      | 9975                      |
| Sidechain outliers    | 111093                      | 9958                      |

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  $\geq 3$ , 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     | 19     | <div> <div></div> <div>89%</div> <div>11%</div> </div> |

## 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 199 atoms, of which 85 are hydrogens and 0 are deuteriums.

- Molecule 1 is a protein called Thiostrepton.

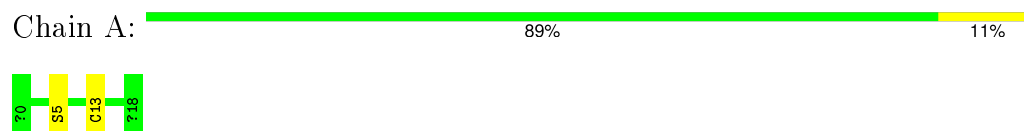
| Mol | Chain | Residues | Atoms |    |    |    |    |   | Trace |
|-----|-------|----------|-------|----|----|----|----|---|-------|
| 1   | A     | 19       | Total | C  | H  | N  | O  | S | 1     |
|     |       |          | 199   | 72 | 85 | 19 | 18 | 5 |       |

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     | 18      | NH2      | -      | AMIDATION      | UNP P0C8P8 |

#### 4.1 Average score per residue in the NMR ensemble

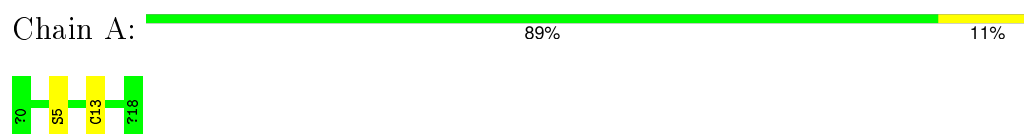
- Molecule 1: Thiostrepton



#### 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 17153 |
| Number of chemical shift lists               | 1                |
| Total number of shifts                       | 161              |
| Number of shifts mapped to atoms             | 0                |
| Number of unparsed shifts                    | 0                |
| Number of shifts with mapping errors         | 161              |
| 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, DCY, DBU

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

There are no bond-length outliers.

There are no bond-angle outliers.

There are no chirality outliers.

There are no planarity outliers.

### 6.2 Too-close contacts [i](#)

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

| Mol | Chain | Non-H | H(model) | H(added) | Clashes |
|-----|-------|-------|----------|----------|---------|
| 1   | A     | 114   | 85       | 82       | 1±0     |
| All | All   | 2280  | 1700     | 1640     | 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 | 0.69     | 1.30        | 12     | 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     | 5/19 (26%)    | 3±0 (60±0%) | 2±0 (40±0%) | 0±0 (0±0%) | 100         | 100 |
| All | All   | 100/380 (26%) | 60 (60%)    | 40 (40%)    | 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 ⓘ

11 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    | 7,8,10       | 0.86±0.01 | 0±0 (0±0%) |
| 1   | BB9  | A     | 11  | 1    | 3,5,6        | 0.47±0.02 | 0±0 (0±0%) |
| 1   | BB9  | A     | 13  | 1    | 2,4,6        | 0.36±0.02 | 0±0 (0±0%) |
| 1   | MH6  | A     | 14  | 1    | 3,3,6        | 1.02±0.03 | 0±0 (0±0%) |
| 1   | BB9  | A     | 15  | 1    | 3,5,6        | 0.39±0.01 | 0±0 (0±0%) |



| Mol | Type | Chain | Res | Link | Bond lengths |           |             |
|-----|------|-------|-----|------|--------------|-----------|-------------|
|     |      |       |     |      | Counts       | RMSZ      | #Z>2        |
| 1   | DHA  | A     | 16  | 1    | 4,4,5        | 2.63±0.01 | 1±0 (25±0%) |
| 1   | DHA  | A     | 17  | 1    | 4,4,5        | 2.63±0.01 | 1±0 (25±0%) |
| 1   | DHA  | A     | 3   | 1    | 4,4,5        | 2.54±0.02 | 1±0 (22±7%) |
| 1   | BB9  | A     | 6   | 1    | 3,5,6        | 0.39±0.01 | 0±0 (0±0%)  |
| 1   | DBU  | A     | 8   | 1    | 4,4,6        | 2.59±0.01 | 1±0 (22±7%) |
| 1   | DCY  | A     | 9   | 1    | 3,5,6        | 0.64±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    | 7,12,15     | 0.70±0.01 | 0±0 (0±0%) |
| 1   | BB9  | A     | 11  | 1    | 1,5,7       | 1.21±0.05 | 0±0 (0±0%) |
| 1   | BB9  | A     | 13  | 1    | 3,4,7       | 3.17±0.02 | 0±0 (0±0%) |
| 1   | MH6  | A     | 14  | 1    | 1,3,7       | 0.45±0.05 | 0±0 (0±0%) |
| 1   | BB9  | A     | 15  | 1    | 1,5,7       | 0.90±0.06 | 0±0 (0±0%) |
| 1   | DHA  | A     | 16  | 1    | 3,4,6       | 2.49±0.02 | 0±0 (0±0%) |
| 1   | DHA  | A     | 17  | 1    | 3,4,6       | 2.33±0.01 | 0±0 (0±0%) |
| 1   | DHA  | A     | 3   | 1    | 3,4,6       | 2.37±0.01 | 0±0 (0±0%) |
| 1   | BB9  | A     | 6   | 1    | 1,5,7       | 0.67±0.06 | 0±0 (0±0%) |
| 1   | DBU  | A     | 8   | 1    | 1,4,7       | 1.10±0.06 | 0±0 (0±0%) |
| 1   | DCY  | A     | 9   | 1    | 3,5,7       | 3.07±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     |
|-----|------|-------|-----|------|---------|-------------|-----------|
| 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 |

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| Mol | Type | Chain | Res | Link | Chirals | Torsions  | Rings     |
|-----|------|-------|-----|------|---------|-----------|-----------|
| 1   | DHA  | A     | 17  | 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   | DCY  | A     | 9   | 1    | -       | 0±0,1,4,6 | 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     | 16  | DHA  | CA-N  | 5.27 | 1.48        | 1.35     | 15     | 20    |
| 1   | A     | 17  | DHA  | CA-N  | 5.23 | 1.48        | 1.35     | 16     | 20    |
| 1   | A     | 3   | DHA  | CA-N  | 5.11 | 1.47        | 1.35     | 3      | 18    |
| 1   | A     | 8   | DBU  | CA-N  | 5.08 | 1.47        | 1.33     | 4      | 18    |

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 [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 17153

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                  | 161 |
| Number of shifts mapped to atoms        | 0   |
| Number of unparsed shifts               | 0   |
| Number of shifts with mapping errors    | 161 |
| 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 161) occurrences are reported below.

| Chain    | Res | Type | Atom | Shift Data |             |           |
|----------|-----|------|------|------------|-------------|-----------|
|          |     |      |      | Value      | Uncertainty | Ambiguity |
| UNMAPPED | 18  | DHA  | HB2  | 5.69       | 0.02        | 2         |
| UNMAPPED | 2   | ILE  | HD12 | 0.92       | 0.02        | 1         |
| UNMAPPED | 18  | DHA  | HB1  | 6.59       | 0.02        | 2         |
| UNMAPPED | 5   | ALA  | CA   | 54.8       | 0.05        | 1         |
| UNMAPPED | 11  | TS9  | CG2  | 20.4       | 0.05        | 1         |

#### 7.1.2 Chemical shift referencing

The following table shows the suggested chemical shift referencing corrections.

| Nucleus                | # values | Correction $\pm$ precision, ppm | Suggested action           |
|------------------------|----------|---------------------------------|----------------------------|
| $^{13}\text{C}_\alpha$ | 17       | 0.00 $\pm$ 0.00                 | None needed ( $< 0.5$ ppm) |
| $^{13}\text{C}_\beta$  | 17       | 0.00 $\pm$ 0.00                 | None needed ( $< 0.5$ ppm) |
| $^{13}\text{C}'$       | 17       | 0.00 $\pm$ 0.00                 | None needed ( $< 0.5$ ppm) |

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| Nucleus         | # values | Correction $\pm$ precision, ppm | Suggested action           |
|-----------------|----------|---------------------------------|----------------------------|
| $^{15}\text{N}$ | 11       | 0.00 $\pm$ 0.00                 | 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 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     | $^1\text{H}$ | $^{13}\text{C}$ | $^{15}\text{N}$ |
|-----------|-----------|--------------|-----------------|-----------------|
| 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   | 32.00      | 71.24 – 56.34       | -21.3   |
| ??? | UNMAPPED | 8   | THR  | HB   | 1.35       | 5.82 – 2.52         | -8.5    |
| ??? | 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.