



Full wwPDB X-ray Structure Validation Report ⓘ

Apr 22, 2026 – 11:26 AM EDT

PDB ID : 7SPL / pdb_00007spl
Title : [2T3] Self-assembling 3D DNA triangle with three inter-junction base pairs containing the L1 junction and a zero-linked center strand
Authors : Vecchioni, S.; Lu, B.; Sha, R.; Ohayon, Y.P.; Seeman, N.C.
Deposited on : 2021-11-02
Resolution : 6.09 Å (reported)

This is a Full wwPDB X-ray Structure Validation 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/XrayValidationReportHelp>

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)
Xtrriage (Phenix) : 2.0
EDS : **FAILED**
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.49

2 Entry composition i

There are 5 unique types of molecules in this entry. The entry contains 858 atoms, of which 0 are hydrogens and 0 are deuteriums.

In the tables below, the ZeroOcc column contains the number of atoms modelled with zero occupancy, the AltConf column contains the number of residues with at least one atom in alternate conformation and the Trace column contains the number of residues modelled with at most 2 atoms.

- Molecule 1 is a DNA chain called DNA (5'-D(P*GP*AP*GP*CP*AP*GP*CP*CP*TP*GP*TP*GP*AP*CP*AP*TP*CP*A)-3').

| Mol | Chain | Residues | Atoms | | | | | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|-----|----|-----|----|---------|---------|-------|
| | | | Total | C | N | O | P | | | |
| 1 | A | 17 | 349 | 167 | 61 | 104 | 17 | 0 | 0 | 0 |

- Molecule 2 is a DNA chain called DNA (5'-D(*TP*CP*TP*GP*AP*TP*GP*TP*CP*C)-3').

| Mol | Chain | Residues | Atoms | | | | | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|-----|----|----|----|---------|---------|-------|
| | | | Total | C | N | O | P | | | |
| 2 | B | 11 | 223 | 107 | 37 | 68 | 11 | 0 | 0 | 0 |

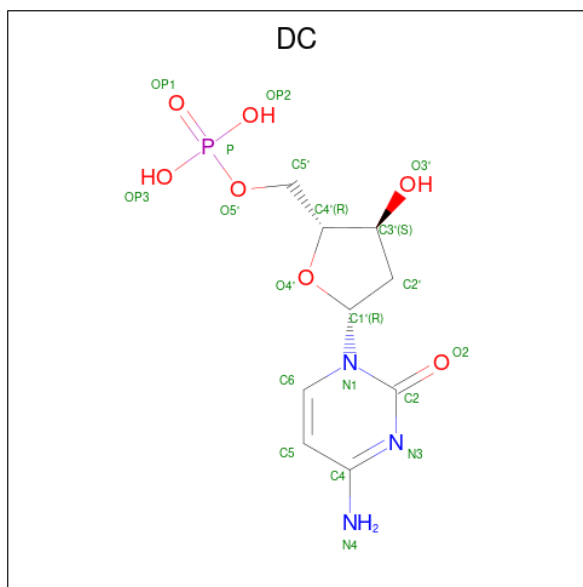
- Molecule 3 is a DNA chain called DNA (5'-D(P*GP*TP*AP*CP*AP*GP*GP*CP*TP*GP*C)-3').

| Mol | Chain | Residues | Atoms | | | | | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|----|----|----|----|---------|---------|-------|
| | | | Total | C | N | O | P | | | |
| 3 | C | 10 | 211 | 99 | 45 | 57 | 10 | 0 | 0 | 0 |

- Molecule 4 is a DNA chain called DNA (5'-D(*GP*AP*C)-3').

| Mol | Chain | Residues | Atoms | | | | | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|----|----|----|---|---------|---------|-------|
| | | | Total | C | N | O | P | | | |
| 4 | D | 3 | 56 | 28 | 11 | 15 | 2 | 0 | 0 | 0 |

- Molecule 5 is 2'-DEOXYCYTIDINE-5'-MONOPHOSPHATE (CCD ID: DC) (formula: C₉H₁₄N₃O₇P).



| Mol | Chain | Residues | Atoms | | | | | ZeroOcc | AltConf |
|-----|-------|----------|-------|---|---|---|---|---------|---------|
| | | | Total | C | N | O | P | | |
| 5 | A | 1 | 19 | 9 | 3 | 6 | 1 | 0 | 0 |

3 Residue-property plots

These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry. Residues are color-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 outlier are shown as a green connector. Residues present in the sample, but not in the model, are shown in grey.


Note EDS failed to run properly.

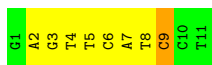
- Molecule 1: DNA (5'-D(P*GP*AP*GP*CP*AP*GP*CP*CP*TP*GP*TP*GP*AP*CP*AP*TP*CP*A)-3')

Chain A: 



- Molecule 2: DNA (5'-D(*TP*CP*TP*GP*AP*TP*GP*TP*CP*C)-3')

Chain B: 



- Molecule 3: DNA (5'-D(P*GP*TP*AP*CP*AP*GP*GP*CP*TP*GP*C)-3')

Chain C: 

There are no outlier residues recorded for this chain.

- Molecule 4: DNA (5'-D(*GP*AP*C)-3')

Chain D: 



4 Data and refinement statistics i

EDS failed to run properly - this section is therefore incomplete.

| Property | Value | Source |
|----------------------------------------------------------|-------------------------------------------------------------|-----------|
| Space group | H 3 | Depositor |
| Cell constants a, b, c, α , β , γ | 87.84Å 87.84Å 140.53Å 90.00° 90.00° 120.00° | Depositor |
| Resolution (Å) | 36.72 – 6.09 | Depositor |
| % Data completeness (in resolution range) | 61.1 (36.72-6.09) | Depositor |
| R_{merge} | (Not available) | Depositor |
| R_{sym} | (Not available) | Depositor |
| $\langle I/\sigma(I) \rangle$ ¹ | 0.20 (at 6.18Å) | Xtrriage |
| Refinement program | PHENIX 1.18.2_3874 | Depositor |
| R, R_{free} | 0.234 , 0.335 | Depositor |
| Wilson B-factor (Å ²) | 348.9 | Xtrriage |
| Anisotropy | 0.331 | Xtrriage |
| L-test for twinning ² | $\langle L \rangle = 0.50$, $\langle L^2 \rangle = 0.33$ | Xtrriage |
| Estimated twinning fraction | 0.239 for h,-h-k,-l | Xtrriage |
| Total number of atoms | 858 | wwPDB-VP |
| Average B, all atoms (Å ²) | 847.0 | wwPDB-VP |

Xtrriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 13.00% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

²Theoretical values of $\langle |L| \rangle$, $\langle L^2 \rangle$ for acentric reflections are 0.5, 0.333 respectively for untwinned datasets, and 0.375, 0.2 for perfectly twinned datasets.

5 Model quality [i](#)

5.1 Standard geometry [i](#)

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 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 | 0.28 | 0/390 | 0.52 | 0/600 |
| 2 | B | 0.27 | 0/248 | 0.85 | 2/380 (0.5%) |
| 3 | C | 0.22 | 0/238 | 0.42 | 0/366 |
| 4 | D | 0.31 | 0/62 | 0.61 | 0/93 |
| All | All | 0.26 | 0/938 | 0.61 | 2/1439 (0.1%) |

There are no bond length outliers.

All (2) bond angle outliers are listed below:

| Mol | Chain | Res | Type | Atoms | Z | Observed(°) | Ideal(°) |
|-----|-------|-----|------|-----------|-------|-------------|----------|
| 2 | B | 9 | DC | OP1-P-O3' | -8.90 | 81.29 | 108.00 |
| 2 | B | 9 | DC | OP2-P-O3' | -7.54 | 85.38 | 108.00 |

There are no chirality outliers.

There are no planarity outliers.

5.2 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 the 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 within the asymmetric unit, whereas Symm-Clashes lists symmetry-related clashes.

| Mol | Chain | Non-H | H(model) | H(added) | Clashes | Symm-Clashes |
|-----|-------|-------|----------|----------|---------|--------------|
| 1 | A | 349 | 0 | 194 | 8 | 0 |
| 2 | B | 223 | 0 | 126 | 9 | 0 |
| 3 | C | 211 | 0 | 112 | 0 | 0 |
| 4 | D | 56 | 0 | 35 | 1 | 0 |
| 5 | A | 19 | 0 | 12 | 2 | 0 |
| All | All | 858 | 0 | 479 | 17 | 0 |

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 13.

All (17) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|----------------|---------------|--------------------------|-------------------|
| 1:A:8:DT:H2' | 1:A:9:DG:C8 | 2.19 | 0.77 |
| 1:A:4:DC:H2'' | 1:A:5:DT:C6 | 2.28 | 0.68 |
| 1:A:2:DC:H2'' | 1:A:3:DT:H5'' | 1.80 | 0.64 |
| 1:A:17:DA:H2'' | 5:A:101:DC:H5 | 1.63 | 0.63 |
| 2:B:3:DG:H2'' | 2:B:4:DT:H72 | 1.85 | 0.58 |
| 2:B:2:DA:H2'' | 2:B:3:DG:H8 | 1.72 | 0.55 |
| 2:B:8:DT:H2'' | 2:B:9:DC:H5'' | 1.89 | 0.54 |
| 2:B:2:DA:H2'' | 2:B:3:DG:C8 | 2.45 | 0.52 |
| 2:B:3:DG:H1' | 2:B:4:DT:OP2 | 2.11 | 0.51 |
| 1:A:15:DG:H2'' | 1:A:16:DA:O5' | 2.12 | 0.48 |
| 1:A:7:DC:H2' | 1:A:8:DT:C1' | 2.45 | 0.46 |
| 1:A:11:DG:O6 | 4:D:1:DA:N6 | 2.49 | 0.45 |
| 1:A:17:DA:H2'' | 5:A:101:DC:C5 | 2.47 | 0.44 |
| 2:B:5:DT:H2'' | 2:B:6:DC:H5'' | 1.99 | 0.43 |
| 2:B:6:DC:H2' | 2:B:7:DA:C8 | 2.55 | 0.41 |
| 2:B:3:DG:C2' | 2:B:4:DT:H72 | 2.49 | 0.41 |
| 2:B:4:DT:H2'' | 2:B:5:DT:OP1 | 2.21 | 0.41 |

There are no symmetry-related clashes.

5.3 Torsion angles [i](#)

5.3.1 Protein backbone [i](#)

There are no protein molecules in this entry.

5.3.2 Protein sidechains [i](#)

There are no protein molecules in this entry.

5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

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

There are no non-standard protein/DNA/RNA residues in this entry.

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

1 ligand is modelled in this entry.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or 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 length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 2$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

| Mol | Type | Chain | Res | Link | Bond lengths | | | Bond angles | | |
|-----|------|-------|-----|------|--------------|------|----------|-------------|------|----------|
| | | | | | Counts | RMSZ | # Z > 2 | Counts | RMSZ | # Z > 2 |
| 5 | DC | A | 101 | - | 17,20,21 | 0.33 | 0 | 23,28,31 | 0.40 | 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 |
|-----|------|-------|-----|------|---------|-----------|---------|
| 5 | DC | A | 101 | - | - | 0/7/21/22 | 0/2/2/2 |

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.

1 monomer is involved in 2 short contacts:

| Mol | Chain | Res | Type | Clashes | Symm-Clashes |
|-----|-------|-----|------|---------|--------------|
| 5 | A | 101 | DC | 2 | 0 |

5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

6 Fit of model and data [i](#)

6.1 Protein, DNA and RNA chains [i](#)

EDS failed to run properly - this section is therefore empty.

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

EDS failed to run properly - this section is therefore empty.

6.3 Carbohydrates [i](#)

EDS failed to run properly - this section is therefore empty.

6.4 Ligands [i](#)

EDS failed to run properly - this section is therefore empty.

6.5 Other polymers [i](#)

EDS failed to run properly - this section is therefore empty.