



# Full wwPDB X-ray Structure Validation Report ⓘ

Mar 8, 2026 – 12:15 PM UTC

PDB ID : 8A55 / pdb\_00008a55  
Title : Structure of N-terminal SARS-CoV-2 nonstructural protein 1 (nsp1) at atomic resolution  
Authors : Ma, S.; Pinotsis, N.; Bowler, M.W.; Kozielski, F.  
Deposited on : 2022-06-14  
Resolution : 0.99 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](mailto: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>.

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

|                                |   |                                                                  |
|--------------------------------|---|------------------------------------------------------------------|
| MolProbity                     | : | <b>FAILED</b>                                                    |
| Xtriage (Phenix)               | : | 2.0                                                              |
| EDS                            | : | 3.0                                                              |
| Percentile statistics          | : | 20250101.v01 (using entries in the PDB archive January 1st 2025) |
| CCP4                           | : | 9.0.010 (Gargrove)                                               |
| Density-Fitness                | : | 1.0.12                                                           |
| Ideal geometry (proteins)      | : | Engh & Huber (2001)                                              |
| Ideal geometry (DNA, RNA)      | : | Parkinson et al. (1996)                                          |
| Validation Pipeline (wwPDB-VP) | : | 2.49                                                             |

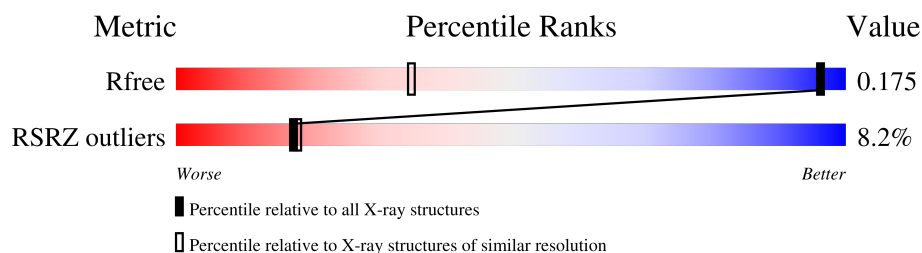
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

The reported resolution of this entry is 0.99 Å.

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) | Similar resolution<br>(#Entries, resolution range(Å)) |
|---------------|-----------------------------|-------------------------------------------------------|
| $R_{free}$    | 180053                      | 1358 (1.04-0.96)                                      |
| RSRZ outliers | 180081                      | 1355 (1.04-0.96)                                      |

MolProbity failed to run properly - the sequence quality summary graphics cannot be shown.

## 2 Entry composition

There are 2 unique types of molecules in this entry. The entry contains 2033 atoms, of which 916 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 protein called Host translation inhibitor nsp1.

| Mol | Chain | Residues | Atoms |     |     |     |     |   | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|-----|---|---------|---------|-------|
| 1   | 1-A   | 110      | Total | C   | H   | N   | O   | S | 8       | 14      | 0     |
|     |       |          | 1805  | 571 | 910 | 154 | 165 | 5 |         |         |       |

There is a discrepancy between the modelled and reference sequences:

| Chain | Residue | Modelled | Actual | Comment               | Reference  |
|-------|---------|----------|--------|-----------------------|------------|
| A     | 9       | MET      | -      | initiating methionine | UNP P0DTD1 |

- Molecule 2 is water.

| Mol | Chain | Residues | Atoms | ZeroOcc | AltConf |
|-----|-------|----------|-------|---------|---------|
|-----|-------|----------|-------|---------|---------|

SEQUENCE-PLOTS INFOmissingINFO

### 3 Data and refinement statistics

| Property                                                                | Value                                                       | Source           |
|-------------------------------------------------------------------------|-------------------------------------------------------------|------------------|
| Space group                                                             | P 43 21 2                                                   | Depositor        |
| Cell constants<br>a, b, c, $\alpha$ , $\beta$ , $\gamma$                | 36.81Å 36.81Å 140.96Å<br>90.00° 90.00° 90.00°               | Depositor        |
| Resolution (Å)                                                          | 32.63 – 0.99<br>32.63 – 0.99                                | Depositor<br>EDS |
| % Data completeness<br>(in resolution range)                            | 99.5 (32.63-0.99)<br>99.5 (32.63-0.99)                      | Depositor<br>EDS |
| $R_{merge}$                                                             | (Not available)                                             | Depositor        |
| $R_{sym}$                                                               | (Not available)                                             | Depositor        |
| $\langle I/\sigma(I) \rangle$ <sup>1</sup>                              | 1.19 (at 0.99Å)                                             | Xtriage          |
| Refinement program                                                      | PHENIX 1.19.1_4122                                          | Depositor        |
| R, $R_{free}$                                                           | 0.153 , 0.173<br>0.154 , 0.175                              | Depositor<br>DCC |
| $R_{free}$ test set                                                     | 2752 reflections (4.41%)                                    | wwPDB-VP         |
| Wilson B-factor (Å <sup>2</sup> )                                       | 13.5                                                        | Xtriage          |
| Anisotropy                                                              | 0.043                                                       | Xtriage          |
| Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> ) | 0.39 , 43.7                                                 | EDS              |
| L-test for twinning <sup>2</sup>                                        | $\langle  L  \rangle = 0.48$ , $\langle L^2 \rangle = 0.32$ | Xtriage          |
| Estimated twinning fraction                                             | No twinning to report.                                      | Xtriage          |
| $F_o, F_c$ correlation                                                  | 0.98                                                        | EDS              |
| Total number of atoms                                                   | 2033                                                        | wwPDB-VP         |
| Average B, all atoms (Å <sup>2</sup> )                                  | 20.0                                                        | wwPDB-VP         |

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 9.18% of the height of the origin peak. No significant pseudotranslation is detected.*

<sup>1</sup>Intensities estimated from amplitudes.

<sup>2</sup>Theoretical 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.

## 4 Model quality [i](#)

### 4.1 Standard geometry [i](#)

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

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

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### 4.3 Torsion angles [i](#)

#### 4.3.1 Protein backbone [i](#)

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

#### 4.3.2 Protein sidechains [i](#)

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

#### 4.3.3 RNA [i](#)

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

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

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

### 4.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

### 4.6 Ligand geometry [i](#)

There are no ligands in this entry.

### 4.7 Other polymers [i](#)

There are no such residues in this entry.

## 4.8 Polymer linkage issues ⓘ

There are no chain breaks in this entry.

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

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

In the following table, the column labelled ‘#RSRZ > 2’ contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 95<sup>th</sup> percentile and maximum values of the occupancy-weighted average B-factor per residue. The column labelled ‘Q < 0.9’ lists the number of (and percentage) of residues with an average occupancy less than 0.9.

| Mol | Chain | Analysed      | <RSRZ> | #RSRZ>2      | OWAB(Å <sup>2</sup> ) | Q<0.9   |
|-----|-------|---------------|--------|--------------|-----------------------|---------|
| 1   | 1-A   | 110/118 (93%) | 0.41   | 9 (8%) 17 18 | 7, 17, 52, 107        | 10 (9%) |

All (9) RSRZ outliers are listed below:

| Mol | Chain | Res   | Type | RSRZ |
|-----|-------|-------|------|------|
| 1   | 1-A   | 78    | THR  | 9.9  |
| 1   | 1-A   | 79    | ALA  | 6.4  |
| 1   | 1-A   | 76    | ALA  | 5.4  |
| 1   | 1-A   | 9     | MET  | 3.7  |
| 1   | 1-A   | 80    | PRO  | 3.7  |
| 1   | 1-A   | 77    | ARG  | 3.6  |
| 1   | 1-A   | 81    | HIS  | 3.2  |
| 1   | 1-A   | 75[A] | ASP  | 2.4  |
| 1   | 1-A   | 82    | GLY  | 2.4  |

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

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

### 5.3 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

### 5.4 Ligands [i](#)

There are no ligands in this entry.

## 5.5 Other polymers [i](#)

There are no such residues in this entry.