



wwPDB X-ray Structure Validation Summary Report ⓘ

Mar 25, 2026 – 07:25 AM UTC

PDB ID : 4HTE / pdb_00004hte
Title : Crystal Structure of the C-terminal domain of Nicking Enzyme from Staphylococcus aureus
Authors : Betts, L.
Deposited on : 2012-11-01
Resolution : 3.00 Å(reported)

This is a wwPDB X-ray Structure Validation Summary 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 : **FAILED**
Mogul : 2022.3.0, CSD as543be (2022)
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

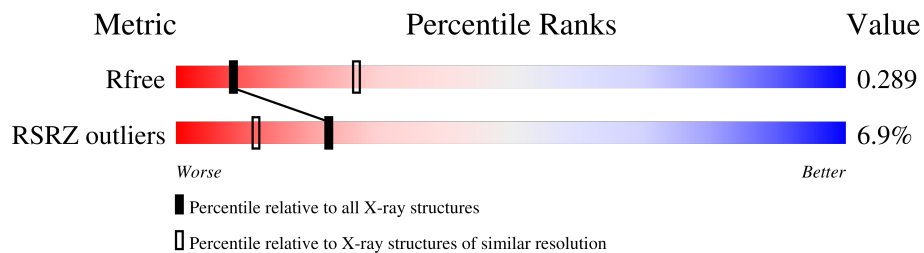
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 3.00 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 (#Entries) | Similar resolution (#Entries, resolution range(Å)) |
|---------------|-----------------------------|---|
| R_{free} | 180053 | 2672 (3.00-3.00) |
| RSRZ outliers | 180081 | 2671 (3.00-3.00) |

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

2 Entry composition [i](#)

There are 2 unique types of molecules in this entry. The entry contains 5081 atoms, of which 2405 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 Nicking enzyme.

| Mol | Chain | Residues | Atoms | | | | | | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|------|------|-----|-----|----|---------|---------|-------|
| | | | Total | C | H | N | O | Se | | | |
| 1 | A | 340 | 5080 | 1685 | 2405 | 433 | 552 | 5 | 0 | 0 | 0 |

There are 13 discrepancies between the modelled and reference sequences:

| Chain | Residue | Modelled | Actual | Comment | Reference |
|-------|---------|----------|--------|----------------|------------|
| A | 242 | LEU | - | expression tag | UNP O87361 |
| A | 243 | MSE | - | expression tag | UNP O87361 |
| A | 244 | PHE | - | expression tag | UNP O87361 |
| A | 245 | ASN | - | expression tag | UNP O87361 |
| A | 246 | GLU | - | expression tag | UNP O87361 |
| A | 247 | VAL | - | expression tag | UNP O87361 |
| A | 248 | ASP | - | expression tag | UNP O87361 |
| A | 249 | ASP | - | expression tag | UNP O87361 |
| A | 250 | MSE | - | expression tag | UNP O87361 |
| A | 251 | LYS | - | expression tag | UNP O87361 |
| A | 252 | SER | - | expression tag | UNP O87361 |
| A | 253 | HIS | - | expression tag | UNP O87361 |
| A | 594 | GLU | - | expression tag | UNP O87361 |

- Molecule 2 is CALCIUM ION (CCD ID: CA) (formula: Ca).

| Mol | Chain | Residues | Atoms | | ZeroOcc | AltConf |
|-----|-------|----------|-------|----|---------|---------|
| 2 | A | 1 | Total | Ca | 0 | 0 |
| | | | 1 | 1 | | |

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3 Data and refinement statistics

| Property | Value | Source |
|---|---|------------------|
| Space group | P 43 21 2 | Depositor |
| Cell constants a, b, c, α , β , γ | 75.28Å 75.28Å 179.85Å 90.00° 90.00° 90.00° | Depositor |
| Resolution (Å) | 45.81 – 3.00 45.81 – 3.00 | Depositor EDS |
| % Data completeness (in resolution range) | 99.8 (45.81-3.00) 99.8 (45.81-3.00) | Depositor EDS |
| R_{merge} | 0.08 | Depositor |
| R_{sym} | (Not available) | Depositor |
| $\langle I/\sigma(I) \rangle$ ¹ | 3.19 (at 3.01Å) | Xtrriage |
| Refinement program | PHENIX 1.7.3_928 | Depositor |
| R, R_{free} | 0.267 , 0.292 0.266 , 0.289 | Depositor DCC |
| R_{free} test set | 1097 reflections (10.01%) | wwPDB-VP |
| Wilson B-factor (Å ²) | 56.4 | Xtrriage |
| Anisotropy | 0.052 | Xtrriage |
| Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²) | 0.35 , 45.8 | EDS |
| L-test for twinning ² | $\langle L \rangle = 0.48$, $\langle L^2 \rangle = 0.32$ | Xtrriage |
| Estimated twinning fraction | No twinning to report. | Xtrriage |
| F_o, F_c correlation | 0.89 | EDS |
| Total number of atoms | 5081 | wwPDB-VP |
| Average B, all atoms (Å ²) | 75.0 | wwPDB-VP |

Xtrriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.54% 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.

4 Model quality [i](#)

4.1 Standard geometry [i](#)

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4.2 Too-close contacts [i](#)

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4.3 Torsion angles [i](#)

4.3.1 Protein backbone [i](#)

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4.3.2 Protein sidechains [i](#)

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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](#)

Of 1 ligands modelled in this entry, 1 is monoatomic - leaving 0 for Mogul analysis.

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.

No monomer is involved in short contacts.

4.7 Other polymers [i](#)

There are no such residues in this entry.

4.8 Polymer linkage issues [i](#)

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, 95th 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 ²) | Q<0.9 |
|-----|-------|---------------|--------|-----------------------------|-----------------------|-------|
| 1 | A | 335/353 (94%) | 0.61 | 23 (6%) 23 12 | 27, 75, 111, 139 | 0 |

The worst 5 of 23 RSRZ outliers are listed below:

| Mol | Chain | Res | Type | RSRZ |
|-----|-------|-----|------|------|
| 1 | A | 564 | TYR | 4.1 |
| 1 | A | 471 | PHE | 3.6 |
| 1 | A | 299 | THR | 3.4 |
| 1 | A | 563 | ASP | 3.3 |
| 1 | A | 365 | ASP | 3.1 |

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](#)

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled ‘Q< 0.9’ lists the number of atoms with occupancy less than 0.9.

| Mol | Type | Chain | Res | Atoms | RSCC | RSR | B-factors(Å ²) | Q<0.9 |
|-----|------|-------|-----|-------|------|------|----------------------------|-------|
| 2 | CA | A | 601 | 1/1 | 0.81 | 0.10 | 62,62,62,62 | 1 |

5.5 Other polymers

There are no such residues in this entry.