



wwPDB X-ray Structure Validation Summary Report

Sep 26, 2014 – 04:00 PM EDT

PDB ID : 4QAS
Title : 1.27 Å resolution structure of CT263-D161N (MTAN) from Chlamydia trachomatis
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Deposited on : 2014-05-05
Resolution : 1.25 Å(reported)

This is a wwPDB validation summary report for a publicly released PDB entry.
We welcome your comments at validation@mail.wwpdb.org
A user guide is available at <http://wwpdb.org/ValidationPDFNotes.html>

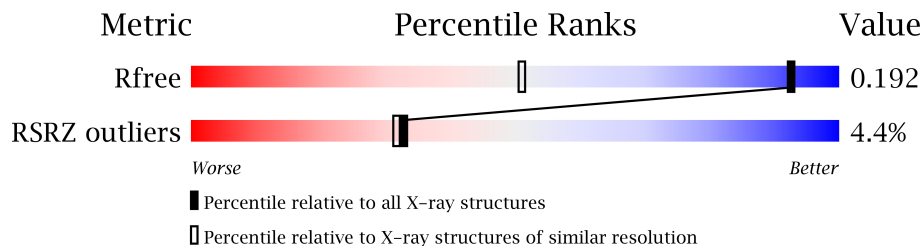
The following versions of software and data (see [references](#)) were used in the production of this report:

MolProbity : **FAILED**
Mogul : 1.16 November 2013
Xtriage (Phenix) : dev-1439
EDS : stable23828
Percentile statistics : 21963
Refmac : 5.8.0049
CCP4 : 6.3.0 (Settle)
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et. al. (1996)
Validation Pipeline (wwPDB-VP) : stable23828

1 Overall quality at a glance

The reported resolution of this entry is 1.25 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} | 66092 | 1021 (1.30-1.22) |
| RSRZ outliers | 66119 | 1021 (1.30-1.22) |

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

2 Entry composition

There are 3 unique types of molecules in this entry. The entry contains 6479 atoms, of which 3085 are hydrogens and 0 are deuterium.

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 CT263.

| Mol | Chain | Residues | Atoms | | | | | | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|------|------|-----|-----|---|---------|---------|-------|
| 1 | A | 197 | Total | C | H | N | O | S | 0 | 7 | 0 |
| | | | 3150 | 1026 | 1585 | 244 | 288 | 7 | | | |
| 1 | B | 187 | Total | C | H | N | O | S | 0 | 6 | 0 |
| | | | 2972 | 967 | 1500 | 229 | 268 | 8 | | | |

There are 12 discrepancies between the modelled and reference sequences:

| Chain | Residue | Modelled | Actual | Comment | Reference |
|-------|---------|----------|--------|---------------------|------------|
| A | -4 | GLY | - | EXPRESSION TAG | UNP B0B7H9 |
| A | -3 | SER | - | EXPRESSION TAG | UNP B0B7H9 |
| A | -2 | THR | - | EXPRESSION TAG | UNP B0B7H9 |
| A | -1 | GLY | - | EXPRESSION TAG | UNP B0B7H9 |
| A | 0 | SER | - | EXPRESSION TAG | UNP B0B7H9 |
| A | 161 | ASN | ASP | ENGINEERED MUTATION | UNP B0B7H9 |
| B | -4 | GLY | - | EXPRESSION TAG | UNP B0B7H9 |
| B | -3 | SER | - | EXPRESSION TAG | UNP B0B7H9 |
| B | -2 | THR | - | EXPRESSION TAG | UNP B0B7H9 |
| B | -1 | GLY | - | EXPRESSION TAG | UNP B0B7H9 |
| B | 0 | SER | - | EXPRESSION TAG | UNP B0B7H9 |
| B | 161 | ASN | ASP | ENGINEERED MUTATION | UNP B0B7H9 |

- Molecule 2 is SULFATE ION (three-letter code: SO4) (formula: O₄S).



| Mol | Chain | Residues | Atoms | | | ZeroOcc | AltConf |
|-----|-------|----------|-------|---|---|---------|---------|
| 2 | A | 1 | Total | O | S | 0 | 0 |
| | | | 5 | 4 | 1 | | |

- Molecule 3 is water.

| Mol | Chain | Residues | Atoms | | ZeroOcc | AltConf |
|-----|-------|----------|-------|-----|---------|---------|
| 3 | A | 193 | Total | O | 0 | 0 |
| | | | 193 | 193 | | |
| 3 | B | 159 | Total | O | 0 | 0 |
| | | | 159 | 159 | | |

3 Residue-property plots

MolProbity failed to run properly - this section will therefore be empty.

4 Data and refinement statistics

| Property | Value | Source |
|---|---|------------------|
| Space group | P 21 21 2 | Depositor |
| Cell constants a, b, c, α , β , γ | 65.44Å 104.15Å 58.15Å 90.00° 90.00° 90.00° | Depositor |
| Resolution (Å) | 33.37 – 1.25 55.41 – 1.25 | Depositor EDS |
| % Data completeness (in resolution range) | 99.9 (33.37-1.25) 99.9 (55.41-1.25) | Depositor EDS |
| R_{merge} | 0.05 | Depositor |
| R_{sym} | (Not available) | Depositor |
| $\langle I/\sigma(I) \rangle$ ¹ | 1.86 (at 1.25Å) | Xtriage |
| Refinement program | PHENIX (phenix.refine: 1.8.4_1496) | Depositor |
| R, R_{free} | 0.174 , 0.192 0.174 , 0.192 | Depositor DCC |
| R_{free} test set | 5516 reflections (5.00%) | DCC |
| Wilson B-factor (Å ²) | 16.3 | Xtriage |
| Anisotropy | 0.298 | Xtriage |
| Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²) | 0.41 , 44.5 | EDS |
| Estimated twinning fraction | No twinning to report. | Xtriage |
| L-test for twinning | $\langle L \rangle = 0.48$, $\langle L^2 \rangle = 0.31$ | Xtriage |
| Outliers | 0 of 110328 reflections | Xtriage |
| F_o, F_c correlation | 0.97 | EDS |
| Total number of atoms | 6479 | wwPDB-VP |
| Average B, all atoms (Å ²) | 30.0 | wwPDB-VP |

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 6.40% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

5 Model quality

5.1 Standard geometry

MolProbity failed to run properly - this section will therefore be empty.

5.2 Close contacts

MolProbity failed to run properly - this section will therefore be empty.

5.3 Torsion angles

5.3.1 Protein backbone

MolProbity failed to run properly - this section will therefore be empty.

5.3.2 Protein sidechains

MolProbity failed to run properly - this section will therefore be empty.

5.3.3 RNA

MolProbity failed to run properly - this section will therefore be empty.

5.4 Non-standard residues in protein, DNA, RNA chains

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

5.5 Carbohydrates

There are no carbohydrates in this entry.

5.6 Ligand geometry

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 | $\# Z > 2$ |
| 2 | SO4 | A | 201 | - | 4,4,4 | 0.18 | 0 | 6,6,6 | 0.09 | 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 |
|-----|------|-------|-----|------|---------|----------|---------|
| 2 | SO4 | A | 201 | - | - | 0/0/0/0 | 0/0/0/0 |

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.

5.7 Other polymers ⓘ

There are no such residues in this entry.

5.8 Polymer linkage issues

There are no chain breaks in this entry.

6 Fit of model and data

6.1 Protein, DNA and RNA chains

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 | 197/201 (98%) | 0.01 | 7 (3%) 41 41 | 12, 21, 53, 88 | 0 |
| 1 | B | 187/201 (93%) | -0.01 | 10 (5%) 25 25 | 13, 20, 56, 108 | 0 |
| All | All | 384/402 (95%) | 0.00 | 17 (4%) 33 32 | 12, 21, 55, 108 | 0 |

The worst 5 of 17 RSRZ outliers are listed below:

| Mol | Chain | Res | Type | RSRZ |
|-----|-------|-----|------|------|
| 1 | A | 196 | VAL | 7.9 |
| 1 | B | 194 | ILE | 5.2 |
| 1 | B | 96 | PRO | 5.1 |
| 1 | A | 124 | TYR | 4.6 |
| 1 | B | 95 | THR | 4.5 |

6.2 Non-standard residues in protein, DNA, RNA chains

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

6.3 Carbohydrates

There are no carbohydrates in this entry.

6.4 Ligands

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. LLDF column lists the quality of electron density of the group with respect to its neighbouring residues in protein, DNA or RNA chains. 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 | RSR | LLDF | B-factors(\AA^2) | Q<0.9 |
|-----|------|-------|-----|-------|------|------|-----------------------------|-------|
| 2 | SO4 | A | 201 | 5/5 | 0.14 | 0.94 | 68,76,84,84 | 0 |

6.5 Other polymers ⓘ

There are no such residues in this entry.