# WORLDWIDE wwPDB PROTEIN DATA BANK

# wwPDB X-ray Structure Validation Summary Report (i)

Dec 18, 2023 – 09:17 am GMT

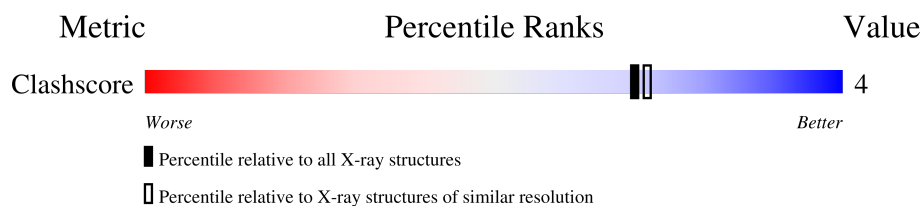| | | |
|---|---|---|
| PDB ID | : | 3ZVD |
| Title | : | 3C protease of Enterovirus 68 complexed with Michael receptor inhibitor 83 |
| Authors | : | Tan, J.; Perbandt, M.; Mesters, J.R.; Hilgenfeld, R. |
| Deposited on | : | 2011-07-24 |
| Resolution | : | 2.25 Å(reported) |

# 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 2.25 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 | Percentile Ranks | Value |
|---|---|---|
| Clashscore | | 4 |

*Worse*                                                                        *Better*

▮ Percentile relative to all X-ray structures

▯ Percentile relative to X-ray structures of similar resolution

| Metric | Whole archive (#Entries) | Similar resolution (#Entries, resolution range(Å)) |
|---|---|---|
| Clashscore | 141614 | 1487 (2.26-2.26) |

# 2 Entry composition (i)

There are 3 unique types of molecules in this entry. The entry contains 1615 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 protein called 3C PROTEASE.

| Mol | Chain | Residues | Atoms | | | | | ZeroOcc | AltConf | Trace |
|---|---|---|---|---|---|---|---|---|---|---|
| | | | Total | C | N | O | S | | | |
| 1 | A | 189 | 1473 | 932 | 263 | 270 | 8 | 0 | 1 | 1 |

There are 7 discrepancies between the modelled and reference sequences:

| Chain | Residue | Modelled | Actual | Comment | Reference |
|---|---|---|---|---|---|
| A | 184 | LYS | - | expression tag | UNP A1E4A3 |
| A | 185 | HIS | - | expression tag | UNP A1E4A3 |
| A | 186 | HIS | - | expression tag | UNP A1E4A3 |
| A | 187 | HIS | - | expression tag | UNP A1E4A3 |
| A | 188 | HIS | - | expression tag | UNP A1E4A3 |
| A | 189 | HIS | - | expression tag | UNP A1E4A3 |
| A | 190 | HIS | - | expression tag | UNP A1E4A3 |

- Molecule 2 is ETHYL (5S,8S,11R)-8-BENZYL-5-(2-TERT-BUTOXY-2-OXOETHYL)-3,6,9 -TRIOXO-11-{[(3S)-2-OXOPYRROLIDIN-3-YL]METHYL}-1-PHENYL-2-OXA-4,7,10-TR IAZATETRADECAN-14-OATE (three-letter code: G83) (formula: $C_{36}H_{48}N_4O_9$).
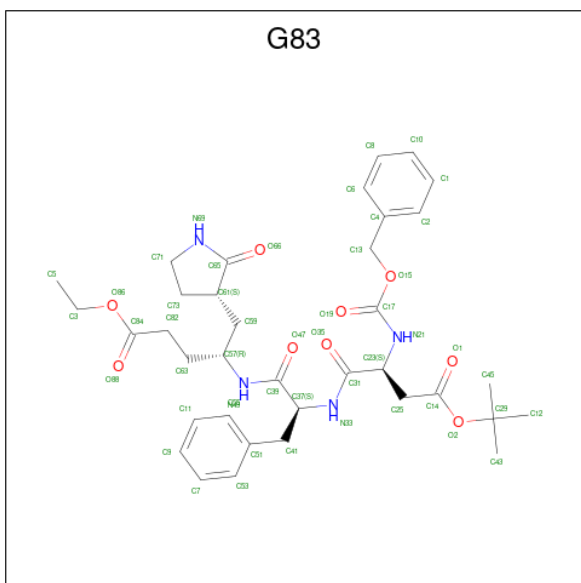
| Mol | Chain | Residues | Atoms | | | | ZeroOcc | AltConf |
|---|---|---|---|---|---|---|---|---|
| 2 | A | 1 | Total<br>49 | C<br>36 | N<br>4 | O<br>9 | 0 | 0 |

- Molecule 3 is water.

| Mol | Chain | Residues | Atoms | | ZeroOcc | AltConf |
|---|---|---|---|---|---|---|
| 3 | A | 93 | Total<br>93 | O<br>93 | 0 | 0 |

SEQUENCE-PLOTS INFOmissingINFO

# 3 Data and refinement statistics ⓘ

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

| Property | Value | Source |
|---|---|---|
| Space group | P 31 2 1 | Depositor |
| Cell constants<br>a, b, c, $\alpha$, $\beta$, $\gamma$ | 56.31Å 56.31Å 170.35Å<br>90.00° 90.00° 120.00° | Depositor |
| Resolution (Å) | 56.78 – 2.25 | Depositor |
| % Data completeness<br>(in resolution range) | 99.9 (56.78-2.25) | Depositor |
| $R_{merge}$ | 0.11 | Depositor |
| $R_{sym}$ | (Not available) | Depositor |
| $<I/\sigma(I)>$ [1] | 3.41 (at 2.24Å) | Xtriage |
| Refinement program | REFMAC 5.5.0110 | Depositor |
| R, $R_{free}$ | 0.195 , 0.247 | Depositor |
| Wilson B-factor (Å$^2$) | 29.0 | Xtriage |
| Anisotropy | 0.179 | Xtriage |
| L-test for twinning[2] | $<|L|>\ =\ 0.48,\ <L^2>\ =\ 0.32$ | Xtriage |
| Estimated twinning fraction | 0.046 for -h,-k,l | Xtriage |
| Total number of atoms | 1615 | wwPDB-VP |
| Average B, all atoms (Å$^2$) | 26.0 | wwPDB-VP |

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 7.61% of the height of the origin peak. No significant pseudotranslation is detected.*

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[1]Intensities estimated from amplitudes.

[2]Theoretical values of $<|L|>$, $<L^2>$ 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)

Bond lengths and bond angles in the following residue types are not validated in this section: G83

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 | 0.91 | 1/1510 (0.1%) | 0.82 | 2/2049 (0.1%) |

All (1) bond length outliers are listed below:

| Mol | Chain | Res | Type | Atoms | Z | Observed(Å) | Ideal(Å) |
|-----|-------|-----|------|-------|------|-------------|----------|
| 1 | A | 34 | VAL | CB-CG2 | 5.49 | 1.64 | 1.52 |

All (2) bond angle outliers are listed below:

| Mol | Chain | Res | Type | Atoms | Z | Observed(°) | Ideal(°) |
|-----|-------|-----|------|-------|-------|-------------|----------|
| 1 | A | 79 | ARG | NE-CZ-NH2 | -7.50 | 116.55 | 120.30 |
| 1 | A | 79 | ARG | NE-CZ-NH1 | 6.45 | 123.53 | 120.30 |

There are no chirality outliers.

There are no planarity outliers.

### 4.2 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 | 1473 | 0 | 1450 | 10 | 0 |
| 2 | A | 49 | 0 | 47 | 1 | 0 |
| 3 | A | 93 | 0 | 0 | 2 | 1 |
| All | All | 1615 | 0 | 1497 | 11 | 1 |

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 4.

The worst 5 of 11 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) |
|---|---|---|---|
| 2:A:1190:G83:H6 | 3:A:2087:HOH:O | 1.48 | 1.10 |
| 1:A:183:GLN:HG3 | 1:A:184:LYS:HG2 | 1.60 | 0.82 |
| 1:A:109:PHE:CD1 | 1:A:112:MET:HE3 | 2.44 | 0.53 |
| 1:A:7:ALA:O | 1:A:11:MET:HG2 | 2.12 | 0.48 |
| 1:A:109:PHE:CD1 | 1:A:112:MET:CE | 2.98 | 0.47 |

All (1) symmetry-related close contacts are listed below. The label for Atom-2 includes the symmetry operator and encoded unit-cell translations to be applied.

| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 3:A:2061:HOH:O | 3:A:2091:HOH:O[4_565] | 1.46 | 0.74 |

## 4.3 Torsion angles ⓘ

### 4.3.1 Protein backbone ⓘ

There are no protein backbone outliers to report in this entry.

### 4.3.2 Protein sidechains ⓘ

There are no protein residues with a non-rotameric sidechain to report in this entry.

### 4.3.3 RNA ⓘ

There are no RNA molecules in this entry.

## 4.4 Non-standard residues in protein, DNA, RNA chains ⓘ

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

## 4.5 Carbohydrates ⓘ

There are no monosaccharides in this entry.

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## 4.6 Ligand geometry ⓘ

1 ligand is modelled in this entry.

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 ⓘ

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 ⓘ

## 5.1 Protein, DNA and RNA chains ⓘ

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

## 5.2 Non-standard residues in protein, DNA, RNA chains ⓘ

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

## 5.3 Carbohydrates ⓘ

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

## 5.4 Ligands ⓘ

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

## 5.5 Other polymers ⓘ

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