



# Full wwPDB X-ray Structure Validation Report ⓘ

Mar 25, 2026 – 08:31 PM UTC

PDB ID : 8JMX / pdb\_00008jmx  
Title : The crystal structure of human aurka kinase domain in complex with AURKA-A2  
Authors : Zhu, C.J.; Zhang, Z.M.  
Deposited on : 2023-06-05  
Resolution : 2.95 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>                                                    |
| Mogul                          | : | 2022.3.0, CSD as543be (2022)                                     |
| Xtriage (Phenix)               | : | 2.0                                                              |
| EDS                            | : | 3.0                                                              |
| Buster-report                  | : | wwPDB partial adaption of 1.1.7 (2018)                           |
| 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                                                             |

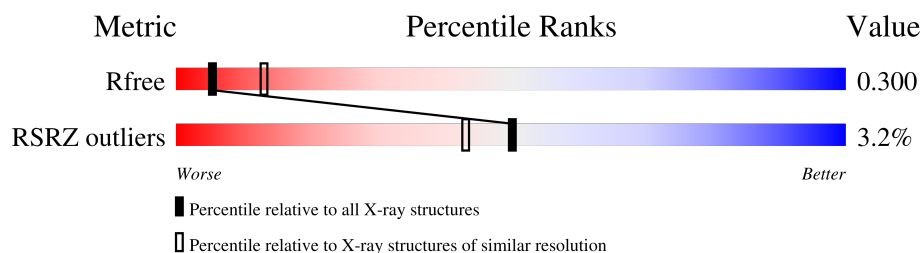
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

The reported resolution of this entry is 2.95 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.



| <b>Metric</b> | <b>Whole archive<br/>(#Entries)</b> | <b>Similar resolution<br/>(#Entries, resolution range(Å))</b> |
|---------------|-------------------------------------|---------------------------------------------------------------|
| $R_{free}$    | 180053                              | 1130 (2.98-2.94)                                              |
| RSRZ outliers | 180081                              | 1130 (2.98-2.94)                                              |

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

## 2 Entry composition [i](#)

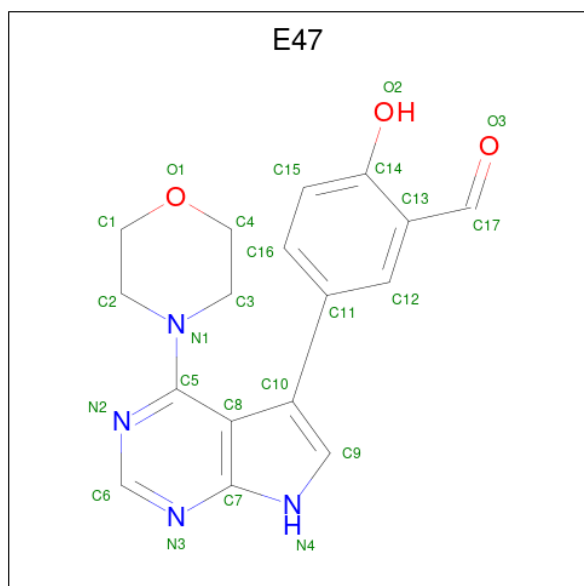
There are 2 unique types of molecules in this entry. The entry contains 1956 atoms, of which 0 are hydrogens and 0 are deuteriums.

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 Aurora kinase A.

| Mol | Chain | Residues | Atoms |      |     |     |   | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|------|-----|-----|---|---------|---------|-------|
| 1   | A     | 250      | Total | C    | N   | O   | S | 0       | 0       | 0     |
|     |       |          | 1933  | 1244 | 327 | 357 | 5 |         |         |       |

- Molecule 2 is 5-(4-morpholin-4-yl-7H-pyrrolo[2,3-d]pyrimidin-5-yl)-2-oxidanyl-benzaldehyde (CCD ID: E47) (formula: C<sub>17</sub>H<sub>16</sub>N<sub>4</sub>O<sub>3</sub>) (labeled as "Ligand of Interest" by depositor).



| Mol | Chain | Residues | Atoms |    |   |   | ZeroOcc | AltConf |
|-----|-------|----------|-------|----|---|---|---------|---------|
| 2   | A     | 1        | Total | C  | N | O | 0       | 0       |
|     |       |          | 23    | 17 | 4 | 2 |         |         |

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### 3 Data and refinement statistics

| Property                                                                | Value                                                       | Source           |
|-------------------------------------------------------------------------|-------------------------------------------------------------|------------------|
| Space group                                                             | P 61 2 2                                                    | Depositor        |
| Cell constants<br>a, b, c, $\alpha$ , $\beta$ , $\gamma$                | 83.13Å 83.13Å 171.45Å<br>90.00° 90.00° 120.00°              | Depositor        |
| Resolution (Å)                                                          | 44.76 – 2.95<br>44.76 – 2.95                                | Depositor<br>EDS |
| % Data completeness<br>(in resolution range)                            | 100.0 (44.76-2.95)<br>100.0 (44.76-2.95)                    | Depositor<br>EDS |
| $R_{merge}$                                                             | 0.18                                                        | Depositor        |
| $R_{sym}$                                                               | (Not available)                                             | Depositor        |
| $\langle I/\sigma(I) \rangle$ <sup>1</sup>                              | 1.52 (at 2.96Å)                                             | Xtriage          |
| Refinement program                                                      | PHENIX 1.9_1692+SVN                                         | Depositor        |
| R, $R_{free}$                                                           | 0.222 , 0.306<br>0.230 , 0.300                              | Depositor<br>DCC |
| $R_{free}$ test set                                                     | 793 reflections (10.00%)                                    | wwPDB-VP         |
| Wilson B-factor (Å <sup>2</sup> )                                       | 94.6                                                        | Xtriage          |
| Anisotropy                                                              | 0.157                                                       | Xtriage          |
| Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> ) | 0.35 , 64.8                                                 | EDS              |
| L-test for twinning <sup>2</sup>                                        | $\langle  L  \rangle = 0.50$ , $\langle L^2 \rangle = 0.33$ | Xtriage          |
| Estimated twinning fraction                                             | No twinning to report.                                      | Xtriage          |
| $F_o, F_c$ correlation                                                  | 0.94                                                        | EDS              |
| Total number of atoms                                                   | 1956                                                        | wwPDB-VP         |
| Average B, all atoms (Å <sup>2</sup> )                                  | 84.0                                                        | wwPDB-VP         |

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.38% 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](#)

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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](#)

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](#)

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   | E47  | A     | 401 | 1    | 26,26,27     | 3.95 | 15 (57%)    | 33,37,38    | 5.46 | 16 (48%)    |

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   | E47  | A     | 401 | 1    | -       | 2/8/16/18 | 0/4/4/4 |

All (15) bond length outliers are listed below:

| Mol | Chain | Res | Type | Atoms   | Z     | Observed(Å) | Ideal(Å) |
|-----|-------|-----|------|---------|-------|-------------|----------|
| 2   | A     | 401 | E47  | C12-C13 | 10.07 | 1.53        | 1.39     |
| 2   | A     | 401 | E47  | C16-C11 | 9.09  | 1.53        | 1.39     |
| 2   | A     | 401 | E47  | C15-C14 | 6.89  | 1.51        | 1.39     |
| 2   | A     | 401 | E47  | C9-C10  | -6.17 | 1.31        | 1.37     |
| 2   | A     | 401 | E47  | C8-C7   | 5.35  | 1.48        | 1.41     |
| 2   | A     | 401 | E47  | C7-N4   | 4.93  | 1.44        | 1.36     |
| 2   | A     | 401 | E47  | C9-N4   | -3.99 | 1.30        | 1.37     |
| 2   | A     | 401 | E47  | C11-C10 | 3.66  | 1.54        | 1.49     |
| 2   | A     | 401 | E47  | O2-C14  | 2.78  | 1.41        | 1.36     |
| 2   | A     | 401 | E47  | C5-N1   | 2.76  | 1.44        | 1.37     |
| 2   | A     | 401 | E47  | C3-N1   | -2.52 | 1.42        | 1.46     |
| 2   | A     | 401 | E47  | C6-N2   | 2.31  | 1.38        | 1.33     |
| 2   | A     | 401 | E47  | C14-C13 | -2.28 | 1.37        | 1.40     |
| 2   | A     | 401 | E47  | C12-C11 | -2.25 | 1.36        | 1.39     |
| 2   | A     | 401 | E47  | C16-C15 | -2.13 | 1.35        | 1.38     |

All (16) bond angle outliers are listed below:

| Mol | Chain | Res | Type | Atoms       | Z      | Observed(°) | Ideal(°) |
|-----|-------|-----|------|-------------|--------|-------------|----------|
| 2   | A     | 401 | E47  | C8-C10-C9   | 19.34  | 118.23      | 105.68   |
| 2   | A     | 401 | E47  | C7-N4-C9    | 16.84  | 116.42      | 108.48   |
| 2   | A     | 401 | E47  | C10-C9-N4   | -12.04 | 102.69      | 110.46   |
| 2   | A     | 401 | E47  | C16-C11-C10 | -6.37  | 113.00      | 120.98   |
| 2   | A     | 401 | E47  | C12-C11-C10 | 4.79   | 126.96      | 120.74   |
| 2   | A     | 401 | E47  | C4-C3-N1    | -3.97  | 102.42      | 109.93   |

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| Mol | Chain | Res | Type | Atoms       | Z     | Observed(°) | Ideal(°) |
|-----|-------|-----|------|-------------|-------|-------------|----------|
| 2   | A     | 401 | E47  | C12-C13-C14 | 3.52  | 121.34      | 117.64   |
| 2   | A     | 401 | E47  | C3-N1-C2    | 3.41  | 119.25      | 111.57   |
| 2   | A     | 401 | E47  | C6-N2-C5    | 3.28  | 119.85      | 111.83   |
| 2   | A     | 401 | E47  | C11-C10-C9  | -3.23 | 118.25      | 124.90   |
| 2   | A     | 401 | E47  | C11-C12-C13 | -2.84 | 118.25      | 121.74   |
| 2   | A     | 401 | E47  | C8-C10-C11  | -2.75 | 122.83      | 129.60   |
| 2   | A     | 401 | E47  | N4-C7-N3    | 2.66  | 131.00      | 126.69   |
| 2   | A     | 401 | E47  | O2-C14-C13  | 2.64  | 122.68      | 117.60   |
| 2   | A     | 401 | E47  | C8-C5-N1    | 2.19  | 125.97      | 122.08   |
| 2   | A     | 401 | E47  | C16-C15-C14 | -2.16 | 118.34      | 120.50   |

There are no chirality outliers.

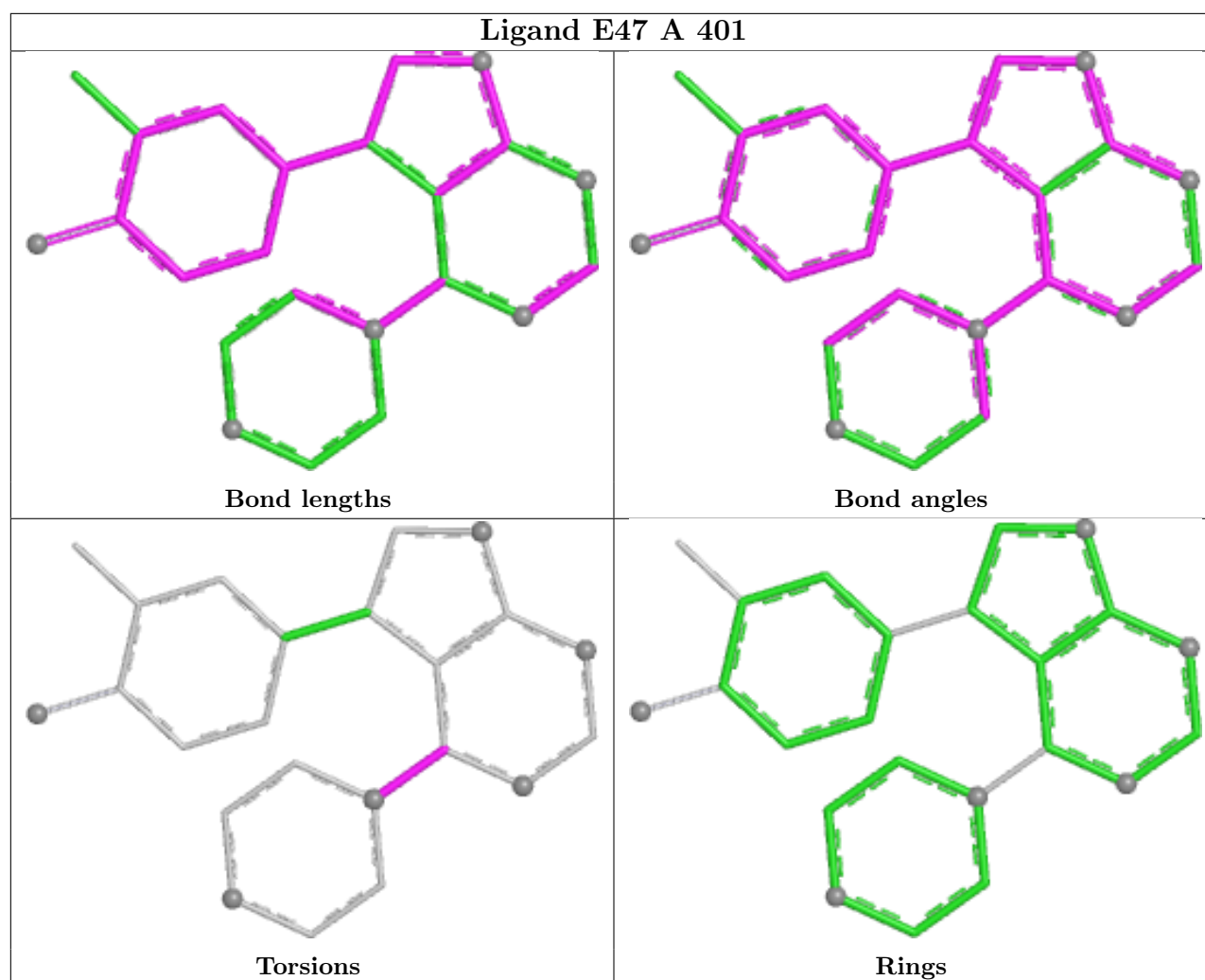
All (2) torsion outliers are listed below:

| Mol | Chain | Res | Type | Atoms       |
|-----|-------|-----|------|-------------|
| 2   | A     | 401 | E47  | N2-C5-N1-C3 |
| 2   | A     | 401 | E47  | C8-C5-N1-C3 |

There are no ring outliers.

No monomer is involved in short contacts.

The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. For torsion angles, if less than 5% of the Mogul distribution of torsion angles is within 10 degrees of the torsion angle in question, then that torsion angle is considered an outlier. Any bond that is central to one or more torsion angles identified as an outlier by Mogul will be highlighted in the graph. For rings, the root-mean-square deviation (RMSD) between the ring in question and similar rings identified by Mogul is calculated over all ring torsion angles. If the average RMSD is greater than 60 degrees and the minimal RMSD between the ring in question and any Mogul-identified rings is also greater than 60 degrees, then that ring is considered an outlier. The outliers are highlighted in purple. The color gray indicates Mogul did not find sufficient equivalents in the CSD to analyse the geometry.



#### 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, 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   | A     | 250/263 (95%) | 0.21   | 8 (3%) 50 43 | 58, 78, 128, 151      | 0     |

All (8) RSRZ outliers are listed below:

| Mol | Chain | Res | Type | RSRZ |
|-----|-------|-----|------|------|
| 1   | A     | 176 | HIS  | 3.3  |
| 1   | A     | 178 | LEU  | 3.1  |
| 1   | A     | 177 | GLN  | 3.0  |
| 1   | A     | 294 | ASP  | 2.9  |
| 1   | A     | 181 | GLU  | 2.8  |
| 1   | A     | 292 | THR  | 2.8  |
| 1   | A     | 276 | GLY  | 2.7  |
| 1   | A     | 256 | ASP  | 2.3  |

### 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](#)

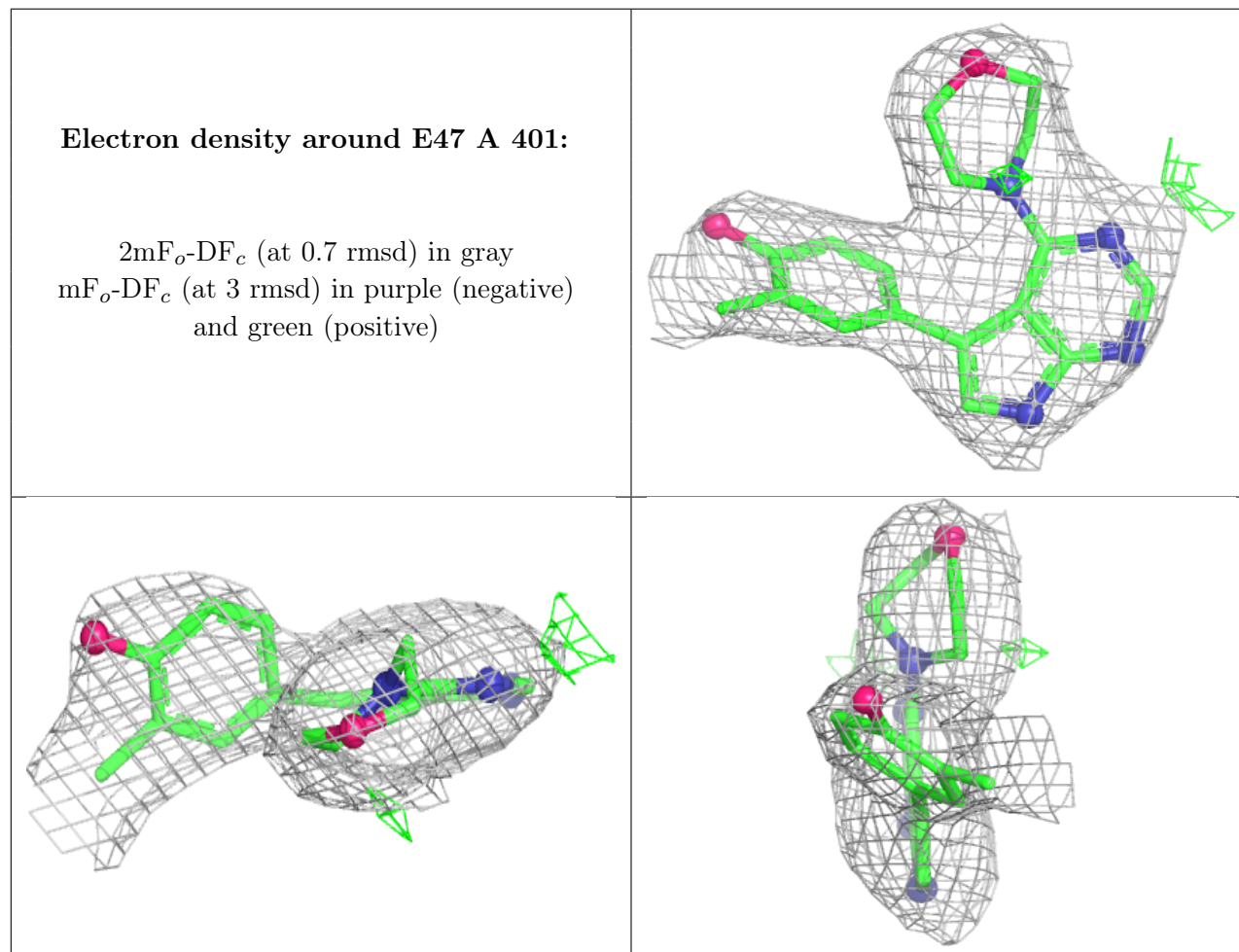
There are no oligosaccharides in this entry.

### 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, 95<sup>th</sup> 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( $\text{\AA}^2$ ) | Q<0.9 |
|-----|------|-------|-----|-------|------|------|-----------------------------|-------|
| 2   | E47  | A     | 401 | 23/24 | 0.93 | 0.12 | 58,63,70,78                 | 0     |

The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation to approximate a three-dimensional view.



## 5.5 Other polymers ⓘ

There are no such residues in this entry.