



wwPDB X-ray Structure Validation Summary Report ⓘ

May 23, 2020 – 04:47 pm BST

PDB ID : 2WXJ
Title : The crystal structure of the murine class IA PI 3-kinase p110delta in complex with INK654.
Authors : Berndt, A.; Miller, S.; Williams, O.; Lee, D.D.; Houseman, B.T.; Pacold, J.I.; Gorrec, F.; Hon, W.-C.; Liu, Y.; Rommel, C.; Gaillard, P.; Ruckle, T.; Schwarz, M.K.; Shokat, K.M.; Shaw, J.P.; Williams, R.L.
Deposited on : 2009-11-09
Resolution : 2.60 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 following versions of software and data (see [references ⓘ](#)) were used in the production of this report:

MolProbity : 4.02b-467
Mogul : 1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix) : 1.13
EDS : 2.11
buster-report : 1.1.7 (2018)
Percentile statistics : 20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac : 5.8.0158
CCP4 : 7.0.044 (Gargrove)
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.11

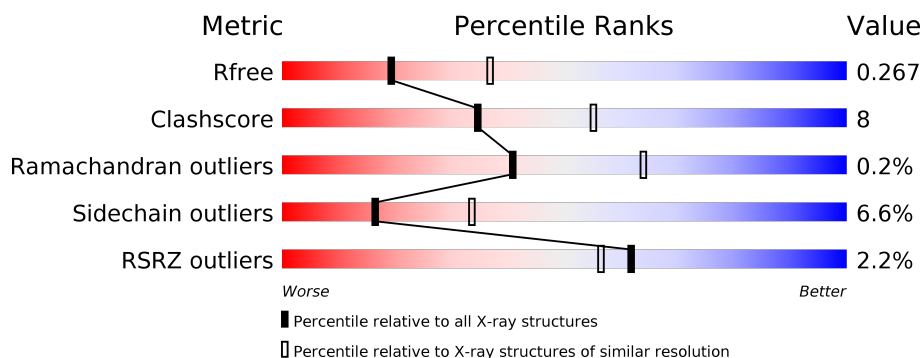
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.60 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} | 130704 | 3163 (2.60-2.60) |
| Clashscore | 141614 | 3518 (2.60-2.60) |
| Ramachandran outliers | 138981 | 3455 (2.60-2.60) |
| Sidechain outliers | 138945 | 3455 (2.60-2.60) |
| RSRZ outliers | 127900 | 3104 (2.60-2.60) |

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments on the lower bar indicate the fraction of residues that contain outliers for ≥ 3 , 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions $\leq 5\%$. The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density. The numeric value is given above the bar.

| Mol | Chain | Length | Quality of chain |
|-----|-------|--------|---|
| 1 | A | 940 | <div> <div>2%</div> <div>69%</div> <div>16%</div> <div>13%</div> </div> |

2 Entry composition [i](#)

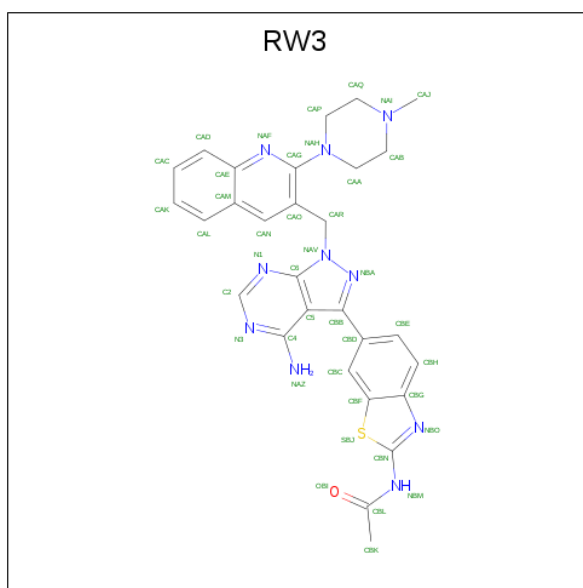
There are 3 unique types of molecules in this entry. The entry contains 6723 atoms, of which 0 are hydrogens and 0 are deuteriums.

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 PHOSPHATIDYLINOSITOL-4,5-BISPHOSPHATE 3-KINASE CATALYTIC SUBUNIT DELTA ISOFORM.

| Mol | Chain | Residues | Atoms | | | | | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|------|------|------|----|---------|---------|-------|
| 1 | A | 822 | Total | C | N | O | S | 0 | 0 | 0 |
| | | | 6633 | 4254 | 1126 | 1199 | 54 | | | |

- Molecule 2 is N-[6-(4-amino-1-{{2-(4-methylpiperazin-1-yl)quinolin-3-yl}methyl}-1H-pyrazol-3-yl)-1,3-benzothiazol-2-yl]acetamide (three-letter code: RW3) (formula: C₂₉H₂₈N₁₀OS).



| Mol | Chain | Residues | Atoms | | | | | ZeroOcc | AltConf |
|-----|-------|----------|-------|----|----|---|---|---------|---------|
| 2 | A | 1 | Total | C | N | O | S | 0 | 0 |
| | | | 41 | 29 | 10 | 1 | 1 | | |

- Molecule 3 is water.

| Mol | Chain | Residues | Atoms | ZeroOcc | AltConf |
|-----|-------|----------|---------------------|---------|---------|
| 3 | A | 49 | Total 49 O 49 | 0 | 0 |

These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. Residues are color-coded according to the number of geometric quality criteria for which they contain at least one outlier: green = 0, yellow = 1, orange = 2 and red = 3 or more. A red dot above a residue indicates a poor fit to the electron density ($RSRZ > 2$). Stretches of 2 or more consecutive residues without any outlier are shown as a green connector. Residues present in the sample, but not in the model, are shown in grey.

Chain A:

2.00
1.50
1.00
0.50
0.00

69% 16% 13%

1 2 3 4 5 6 7 8 9 10 11 12 13 14 15 16 17 18 19 20 21 22 23 24 25 26 27 28 29 30 31 32 33 34 35 36 37 38 39 40 41 42 43 44 45 46 47 48 49 50 51 52 53 54 55 56 57 58 59 60 61 62 63 64 65 66 67 68 69 70 71 72 73 74 75 76 77 78 79 80 81 82 83 84 85 86 87 88 89 90 91 92 93 94 95 96 97 98 99 100

GLY
GLY
ASP
GLY
ARG
Y109
K110
K111
Q235
P236
E237
N244
Q245
N253
L256
C257
I262
L270
T271
P272
H273
Q289
S290
N291
P300
ALA
ARG
GLY
TRP
ARG
ALA
GLY
LEU
LEU
ARG
VAL
SER
N187
R188
A189
L190
F203
D211
P212
P213
L214
N217
I316
W317
S318
L319
P322
F323
T226
S324
I325
E326
L327
I328
P329
C320
GLY
GLY
ASP
GLY
ARG
N334
A335
ASP
GLU
ARG
N339
K340
GLY
GLU
L452
A470
Y474
L475
P476
E477
S586
F587
P588
D589
C590
Y591
G592
G593
S594
S599
L600
L603
D632
T633
N636
I637
Q620
Y621
L629
T630
K631
L634
A637
L655
L656
N657
W658
L659
R670
K1006
T1007
E1010
A1011
V1012

4 Data and refinement statistics

| Property | Value | Source |
|---|---|------------------|
| Space group | C 1 2 1 | Depositor |
| Cell constants a, b, c, α , β , γ | 142.88Å 64.79Å 117.71Å 90.00° 103.21° 90.00° | Depositor |
| Resolution (Å) | 66.52 – 2.60 58.73 – 2.60 | Depositor EDS |
| % Data completeness (in resolution range) | 99.2 (66.52-2.60) 99.3 (58.73-2.60) | Depositor EDS |
| R_{merge} | 0.09 | Depositor |
| R_{sym} | (Not available) | Depositor |
| $\langle I/\sigma(I) \rangle$ ¹ | 4.32 (at 2.58Å) | Xtriage |
| Refinement program | REFMAC 5.5.0046 | Depositor |
| R, R_{free} | 0.210 , 0.264 0.213 , 0.267 | Depositor DCC |
| R_{free} test set | 1018 reflections (3.14%) | wwPDB-VP |
| Wilson B-factor (Å ²) | 39.8 | Xtriage |
| Anisotropy | 0.644 | Xtriage |
| Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²) | 0.34 , 61.6 | EDS |
| L-test for twinning ² | $\langle L \rangle = 0.46$, $\langle L^2 \rangle = 0.29$ | Xtriage |
| Estimated twinning fraction | No twinning to report. | Xtriage |
| F_o, F_c correlation | 0.92 | EDS |
| Total number of atoms | 6723 | wwPDB-VP |
| Average B, all atoms (Å ²) | 12.0 | wwPDB-VP |

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.31% 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.

5 Model quality [i](#)

5.1 Standard geometry [i](#)

Bond lengths and bond angles in the following residue types are not validated in this section: RW3

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 | 0.59 | 2/6776 (0.0%) | 0.64 | 2/9142 (0.0%) |

All (2) bond length outliers are listed below:

| Mol | Chain | Res | Type | Atoms | Z | Observed(Å) | Ideal(Å) |
|-----|-------|-----|------|-------|-------|-------------|----------|
| 1 | A | 257 | CYS | CB-SG | -6.08 | 1.72 | 1.82 |
| 1 | A | 478 | VAL | C-N | 5.48 | 1.46 | 1.34 |

All (2) bond angle outliers are listed below:

| Mol | Chain | Res | Type | Atoms | Z | Observed($^{\circ}$) | Ideal($^{\circ}$) |
|-----|-------|-----|------|----------|------|------------------------|---------------------|
| 1 | A | 907 | LEU | CA-CB-CG | 5.66 | 128.31 | 115.30 |
| 1 | A | 423 | LEU | CA-CB-CG | 5.47 | 127.88 | 115.30 |

There are no chirality outliers.

There are no planarity outliers.

5.2 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 | 6633 | 0 | 6615 | 108 | 0 |
| 2 | A | 41 | 0 | 28 | 3 | 0 |
| 3 | A | 49 | 0 | 0 | 3 | 0 |
| All | All | 6723 | 0 | 6643 | 111 | 0 |

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 8.

The worst 5 of 111 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) |
|------------------|------------------|--------------------------|-------------------|
| 1:A:837:ILE:CD1 | 1:A:901:ILE:HD11 | 1.95 | 0.95 |
| 1:A:110:LYS:HG3 | 1:A:110:LYS:O | 1.65 | 0.93 |
| 1:A:962:ARG:HG2 | 1:A:962:ARG:HH11 | 1.34 | 0.92 |
| 2:A:1500:RW3:OBI | 2:A:1500:RW3:SBJ | 2.30 | 0.88 |
| 1:A:837:ILE:HD11 | 1:A:901:ILE:HD11 | 1.58 | 0.86 |

There are no symmetry-related clashes.

5.3 Torsion angles [i](#)

5.3.1 Protein backbone [i](#)

In the following table, the Percentiles column shows the percent Ramachandran outliers of the chain as a percentile score with respect to all X-ray entries followed by that with respect to entries of similar resolution.

The Analysed column shows the number of residues for which the backbone conformation was analysed, and the total number of residues.

| Mol | Chain | Analysed | Favoured | Allowed | Outliers | Percentiles |
|-----|-------|---------------|-----------|---------|----------|-------------|
| 1 | A | 800/940 (85%) | 759 (95%) | 39 (5%) | 2 (0%) | 41 64 |

All (2) Ramachandran outliers are listed below:

| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1 | A | 755 | LYS |
| 1 | A | 770 | SER |

5.3.2 Protein sidechains [i](#)

In the following table, the Percentiles column shows the percent sidechain outliers of the chain as a percentile score with respect to all X-ray entries followed by that with respect to entries of similar resolution.

The Analysed column shows the number of residues for which the sidechain conformation was analysed, and the total number of residues.

| Mol | Chain | Analysed | Rotameric | Outliers | Percentiles | |
|-----|-------|---------------|-----------|----------|-------------|----|
| 1 | A | 728/827 (88%) | 680 (93%) | 48 (7%) | 16 | 33 |

5 of 48 residues with a non-rotameric sidechain are listed below:

| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1 | A | 523 | LEU |
| 1 | A | 594 | SER |
| 1 | A | 937 | ASP |
| 1 | A | 525 | GLU |
| 1 | A | 563 | GLN |

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 11 such sidechains are listed below:

| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1 | A | 344 | GLN |
| 1 | A | 431 | GLN |
| 1 | A | 898 | ASN |
| 1 | A | 291 | ASN |
| 1 | A | 786 | GLN |

5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates [i](#)

There are no carbohydrates in this entry.

5.6 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 | RW3 | A | 1500 | - | 42,47,47 | 3.38 | 16 (38%) | 48,69,69 | 2.14 | 13 (27%) |

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 | RW3 | A | 1500 | - | - | 2/14/26/26 | 0/7/7/7 |

The worst 5 of 16 bond length outliers are listed below:

| Mol | Chain | Res | Type | Atoms | Z | Observed(Å) | Ideal(Å) |
|-----|-------|------|------|---------|--------|-------------|----------|
| 2 | A | 1500 | RW3 | NBA-NAV | -15.37 | 1.20 | 1.37 |
| 2 | A | 1500 | RW3 | CBD-CBB | -6.77 | 1.39 | 1.49 |
| 2 | A | 1500 | RW3 | CBB-NBA | -6.53 | 1.29 | 1.35 |
| 2 | A | 1500 | RW3 | CAM-CAE | -4.33 | 1.35 | 1.42 |
| 2 | A | 1500 | RW3 | CBH-CBG | -3.83 | 1.35 | 1.41 |

The worst 5 of 13 bond angle outliers are listed below:

| Mol | Chain | Res | Type | Atoms | Z | Observed(°) | Ideal(°) |
|-----|-------|------|------|-------------|-------|-------------|----------|
| 2 | A | 1500 | RW3 | CBC-CBF-SBJ | 5.87 | 136.85 | 125.10 |
| 2 | A | 1500 | RW3 | NAF-CAG-NAH | -5.29 | 113.86 | 117.62 |
| 2 | A | 1500 | RW3 | CBG-CBF-SBJ | -5.10 | 105.09 | 111.85 |
| 2 | A | 1500 | RW3 | CAP-NAH-CAA | 4.32 | 121.06 | 111.52 |
| 2 | A | 1500 | RW3 | N1-C2-N3 | -4.30 | 121.95 | 128.68 |

There are no chirality outliers.

All (2) torsion outliers are listed below:

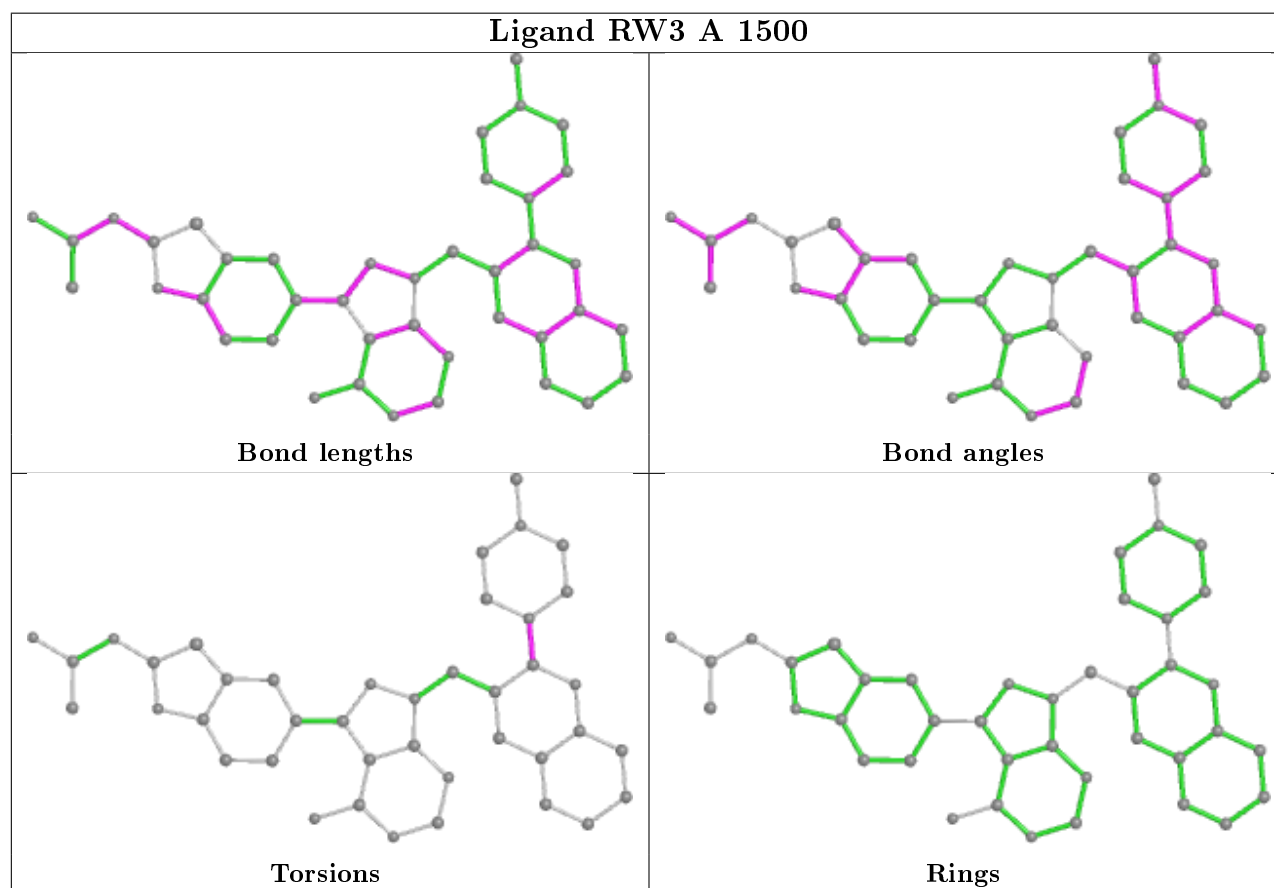
| Mol | Chain | Res | Type | Atoms |
|-----|-------|------|------|-----------------|
| 2 | A | 1500 | RW3 | NAF-CAG-NAH-CAP |
| 2 | A | 1500 | RW3 | CAO-CAG-NAH-CAP |

There are no ring outliers.

1 monomer is involved in 3 short contacts:

| Mol | Chain | Res | Type | Clashes | Symm-Clashes |
|-----|-------|------|------|---------|--------------|
| 2 | A | 1500 | RW3 | 3 | 0 |

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.



5.7 Other polymers [i](#)

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 [i](#)

6.1 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 | 822/940 (87%) | -0.07 | 18 (2%) 62 56 | 2, 11, 23, 35 | 0 |

The worst 5 of 18 RSRZ outliers are listed below:

| Mol | Chain | Res | Type | RSRZ |
|-----|-------|-----|------|------|
| 1 | A | 317 | TRP | 6.2 |
| 1 | A | 319 | LEU | 3.6 |
| 1 | A | 341 | LEU | 3.5 |
| 1 | A | 270 | LEU | 3.3 |
| 1 | A | 322 | PRO | 3.2 |

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

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

6.3 Carbohydrates [i](#)

There are no carbohydrates in this entry.

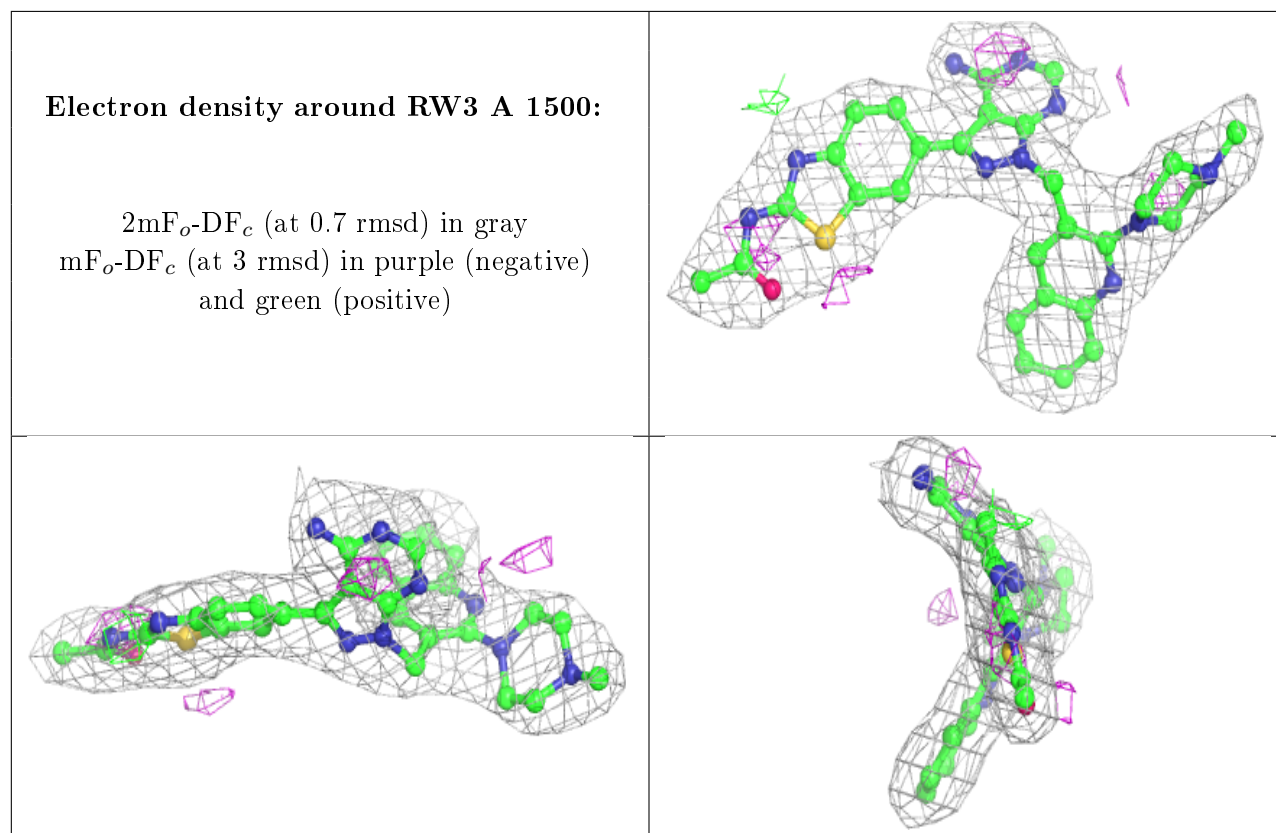
6.4 Ligands [i](#)

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 | RW3 | A | 1500 | 41/41 | 0.96 | 0.14 | 19,25,31,34 | 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.



6.5 Other polymers [i](#)

There are no such residues in this entry.