# Full wwPDB X-ray Structure Validation Report ⓘ

Dec 4, 2023 – 09:44 am GMT

| | | |
|---|---|---|
| PDB ID | : | 1VYQ |
| Title | : | Novel inhibitors of Plasmodium Falciparum dUTPase provide a platform for anti-malarial drug design |
| Authors | : | Whittingham, J.L.; Leal, I.; Kasinathan, G.; Nguyen, C.; Bell, E.; Jones, A.F.; Berry, C.; Benito, A.; Turkenburg, J.P.; Dodson, E.J.; Ruiz Perez, L.M.; Wilkinson, A.J.; Johansson, N.G.; Brun, R.; Gilbert, I.H.; Gonzalez Pacanowska, D.; Wilson, K.S. |
| Deposited on | : | 2004-05-05 |
| Resolution | : | 2.40 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*
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 | : | 4.02b-467 |
| Mogul | : | 1.8.4, CSD as541be (2020) |
| Xtriage (Phenix) | : | 1.13 |
| EDS | : | 2.36 |
| 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) |

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Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.36

# 1 Entry composition

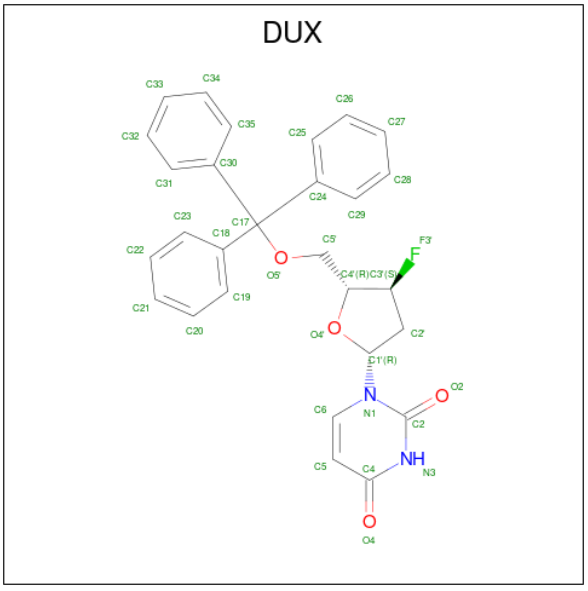
There are 3 unique types of molecules in this entry. The entry contains 3330 atoms, of which 0 are hydrogens and 0 are deuteriums.

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 DEOXYURIDINE 5'-TRIPHOSPHATE NUCLEOTIDOHYDROLASE.

| Mol | Chain | Residues | Atoms | | | | | ZeroOcc | AltConf | Trace |
|---|---|---|---|---|---|---|---|---|---|---|
| 1 | A | 142 | Total | C | N | O | S | 0 | 0 | 4 |
| | | | 1058 | 677 | 176 | 202 | 3 | | | |
| 1 | B | 140 | Total | C | N | O | S | 0 | 1 | 1 |
| | | | 1002 | 643 | 163 | 193 | 3 | | | |
| 1 | C | 141 | Total | C | N | O | S | 0 | 0 | 2 |
| | | | 1046 | 674 | 171 | 198 | 3 | | | |

- Molecule 2 is 2,3-DEOXY-3-FLUORO-5-O-TRITYLURIDINE (three-letter code: DUX) (formula: $C_{28}H_{25}FN_2O_4$).




| Mol | Chain | Residues | Atoms | | | | | ZeroOcc | AltConf |
|---|---|---|---|---|---|---|---|---|---|
| 2 | A | 1 | Total | C | F | N | O | 0 | 0 |
| | | | 35 | 28 | 1 | 2 | 4 | | |
| 2 | B | 1 | Total | C | F | N | O | 0 | 0 |
| | | | 35 | 28 | 1 | 2 | 4 | | |

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| Mol | Chain | Residues | Atoms | | | | | ZeroOcc | AltConf |
|---|---|---|---|---|---|---|---|---|---|
| 2 | C | 1 | Total | C | F | N | O | 0 | 0 |
| | | | 35 | 28 | 1 | 2 | 4 | | |

- Molecule 3 is water.

| Mol | Chain | Residues | Atoms | | ZeroOcc | AltConf |
|---|---|---|---|---|---|---|
| 3 | A | 52 | Total | O | 0 | 0 |
| | | | 52 | 52 | | |
| 3 | B | 25 | Total | O | 0 | 0 |
| | | | 25 | 25 | | |
| 3 | C | 42 | Total | O | 0 | 0 |
| | | | 42 | 42 | | |

SEQUENCE-PLOTS INFOmissingINFO

## 2 Data and refinement statistics (i)

| Property | Value | Source |
|---|---|---|
| Space group | P 41 | Depositor |
| Cell constants<br>a, b, c, $\alpha$, $\beta$, $\gamma$ | 62.83Å 62.83Å 121.53Å<br>90.00° 90.00° 90.00° | Depositor |
| Resolution (Å) | 40.00 – 2.40<br>24.82 – 2.41 | Depositor<br>EDS |
| % Data completeness<br>(in resolution range) | 100.0 (40.00-2.40)<br>99.6 (24.82-2.41) | Depositor<br>EDS |
| $R_{merge}$ | 0.10 | Depositor |
| $R_{sym}$ | (Not available) | Depositor |
| $< I/\sigma(I) >$ [1] | 1.97 (at 2.41Å) | Xtriage |
| Refinement program | REFMAC | Depositor |
| R, $R_{free}$ | 0.191 , 0.295<br>0.198 , 0.298 | Depositor<br>DCC |
| $R_{free}$ test set | 934 reflections (5.13%) | wwPDB-VP |
| Wilson B-factor (Å$^2$) | 42.0 | Xtriage |
| Anisotropy | 0.068 | Xtriage |
| Bulk solvent $k_{sol}$(e/Å$^3$), $B_{sol}$(Å$^2$) | 0.31 , 40.4 | EDS |
| L-test for twinning[2] | $< \|L\| > = 0.49$, $< L^2 > = 0.32$ | Xtriage |
| Estimated twinning fraction | 0.056 for h,-k,-l | Xtriage |
| $F_o$,$F_c$ correlation | 0.94 | EDS |
| Total number of atoms | 3330 | wwPDB-VP |
| Average B, all atoms (Å$^2$) | 44.0 | wwPDB-VP |

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 5.10% of the height of the origin peak. No significant pseudotranslation is detected.*

[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.

# 3 Model quality (i)

## 3.1 Standard geometry (i)

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

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 | 0.87 | 1/1073 (0.1%) | 1.00 | 3/1446 (0.2%) |
| 1 | B | 0.81 | 0/1025 | 1.13 | 8/1390 (0.6%) |
| 1 | C | 0.91 | 0/1063 | 1.14 | 7/1437 (0.5%) |
| All | All | 0.86 | 1/3161 (0.0%) | 1.09 | 18/4273 (0.4%) |

Chiral center outliers are detected by calculating the chiral volume of a chiral center and verifying if the center is modelled as a planar moiety or with the opposite hand.A planarity outlier is detected by checking planarity of atoms in a peptide group, atoms in a mainchain group or atoms of a sidechain that are expected to be planar.

| Mol | Chain | #Chirality outliers | #Planarity outliers |
|---|---|---|---|
| 1 | B | 0 | 2 |

All (1) bond length outliers are listed below:

| Mol | Chain | Res | Type | Atoms | Z | Observed(Å) | Ideal(Å) |
|---|---|---|---|---|---|---|---|
| 1 | A | 152 | VAL | CB-CG1 | -5.24 | 1.41 | 1.52 |

All (18) bond angle outliers are listed below:

| Mol | Chain | Res | Type | Atoms | Z | Observed($^o$) | Ideal($^o$) |
|---|---|---|---|---|---|---|---|
| 1 | B | 22 | HIS | C-N-CA | -12.40 | 90.70 | 121.70 |
| 1 | C | 26 | ASP | CA-C-N | -9.48 | 96.35 | 117.20 |
| 1 | C | 26 | ASP | O-C-N | 9.13 | 137.31 | 122.70 |
| 1 | B | 26 | ASP | O-C-N | 8.82 | 136.81 | 122.70 |
| 1 | B | 26 | ASP | CA-C-N | -8.48 | 98.55 | 117.20 |
| 1 | B | 109[A] | ASP | CB-CG-OD2 | 8.40 | 125.86 | 118.30 |
| 1 | B | 109[B] | ASP | CB-CG-OD2 | 8.40 | 125.86 | 118.30 |
| 1 | B | 25 | GLY | C-N-CA | -7.61 | 102.67 | 121.70 |
| 1 | A | 121 | ASP | CB-CG-OD2 | 7.16 | 124.74 | 118.30 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed($^o$) | Ideal($^o$) |
|---|---|---|---|---|---|---|---|
| 1 | B | 30 | ASP | CB-CG-OD2 | 6.57 | 124.22 | 118.30 |
| 1 | C | 30 | ASP | CB-CG-OD2 | 6.45 | 124.10 | 118.30 |
| 1 | B | 121 | ASP | CB-CG-OD2 | 6.31 | 123.98 | 118.30 |
| 1 | C | 36 | ASP | CB-CG-OD1 | 6.09 | 123.78 | 118.30 |
| 1 | A | 10 | ASP | CB-CG-OD2 | 6.08 | 123.77 | 118.30 |
| 1 | C | 35 | LYS | O-C-N | -5.84 | 113.36 | 122.70 |
| 1 | C | 38 | VAL | CB-CA-C | -5.18 | 101.56 | 111.40 |
| 1 | C | 10 | ASP | CB-CG-OD2 | 5.13 | 122.92 | 118.30 |
| 1 | A | 26 | ASP | CB-CG-OD2 | 5.06 | 122.85 | 118.30 |

There are no chirality outliers.

All (2) planarity outliers are listed below:

| Mol | Chain | Res | Type | Group |
|---|---|---|---|---|
| 1 | B | 23 | HIS | Peptide,Mainchain |

## 3.2 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 | 1058 | 0 | 1044 | 20 | 0 |
| 1 | B | 1002 | 0 | 921 | 19 | 0 |
| 1 | C | 1046 | 0 | 1012 | 18 | 0 |
| 2 | A | 35 | 0 | 25 | 0 | 0 |
| 2 | B | 35 | 0 | 25 | 3 | 0 |
| 2 | C | 35 | 0 | 25 | 3 | 0 |
| 3 | A | 52 | 0 | 0 | 0 | 0 |
| 3 | B | 25 | 0 | 0 | 0 | 0 |
| 3 | C | 42 | 0 | 0 | 1 | 0 |
| All | All | 3330 | 0 | 3052 | 60 | 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 10.

All (60) 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:B:103:ASN:H | 1:B:103:ASN:HD22 | 1.16 | 0.92 |
| 1:B:31:LEU:HD11 | 1:B:139:LEU:HD13 | 1.59 | 0.85 |
| 2:B:1160:DUX:H34 | 1:C:96:LYS:CD | 2.08 | 0.83 |
| 1:B:27:SER:OG | 1:B:144:GLY:O | 2.06 | 0.72 |
| 1:B:88:LEU:HD11 | 1:B:137:VAL:HG13 | 1.72 | 0.69 |
| 1:A:31:LEU:HD11 | 1:A:139:LEU:HD13 | 1.75 | 0.68 |
| 1:B:103:ASN:HD22 | 1:B:103:ASN:N | 1.86 | 0.67 |
| 1:A:97:THR:HB | 1:A:98:PRO:HD2 | 1.78 | 0.66 |
| 1:B:103:ASN:H | 1:B:103:ASN:ND2 | 1.92 | 0.63 |
| 2:B:1160:DUX:H31 | 2:B:1160:DUX:H5'2 | 1.80 | 0.62 |
| 1:A:12:VAL:HG22 | 1:A:34:VAL:HG22 | 1.81 | 0.62 |
| 1:A:100:ARG:NH2 | 1:C:121:ASP:OD2 | 2.32 | 0.60 |
| 1:C:97:THR:CG2 | 1:C:99:LEU:H | 2.14 | 0.60 |
| 1:B:38:VAL:HG22 | 1:B:129:HIS:ND1 | 2.18 | 0.58 |
| 1:C:97:THR:HG23 | 1:C:99:LEU:HG | 1.86 | 0.58 |
| 1:B:112:TYR:C | 1:B:113:ARG:HG2 | 2.24 | 0.57 |
| 2:B:1160:DUX:H31 | 2:B:1160:DUX:C5' | 2.34 | 0.57 |
| 1:A:53:ALA:HB3 | 1:A:116:ILE:HD11 | 1.84 | 0.57 |
| 1:A:91:ARG:HD3 | 1:A:135:LYS:O | 2.04 | 0.57 |
| 1:B:30:ASP:HB3 | 1:B:135:LYS:HG2 | 1.86 | 0.56 |
| 1:C:16:TYR:CE1 | 1:C:51:ILE:CD1 | 2.90 | 0.55 |
| 1:C:97:THR:HG23 | 1:C:99:LEU:H | 1.73 | 0.54 |
| 1:A:83:ASN:ND2 | 1:A:110:ALA:O | 2.43 | 0.52 |
| 1:A:31:LEU:HD11 | 1:A:139:LEU:CD1 | 2.39 | 0.52 |
| 1:C:115:GLU:O | 1:C:117:ILE:HD12 | 2.10 | 0.52 |
| 1:B:88:LEU:HD11 | 1:B:137:VAL:CG1 | 2.38 | 0.51 |
| 1:B:44:THR:HB | 1:B:121:ASP:OD2 | 2.10 | 0.51 |
| 1:C:47:VAL:HG21 | 1:C:120:LEU:HD12 | 1.91 | 0.50 |
| 1:A:54:ILE:HD11 | 1:A:83:ASN:OD1 | 2.11 | 0.50 |
| 2:C:1160:DUX:C25 | 2:C:1160:DUX:C35 | 2.86 | 0.50 |
| 1:A:22:HIS:CD2 | 1:A:29:LEU:HD13 | 2.49 | 0.48 |
| 1:A:88:LEU:HD11 | 1:A:137:VAL:HG13 | 1.95 | 0.47 |
| 1:C:94:ILE:HG12 | 1:C:99:LEU:O | 2.14 | 0.47 |
| 1:A:143:THR:HG1 | 1:A:145:GLU:CD | 2.18 | 0.47 |
| 1:A:2:HIS:HE2 | 1:A:150:GLU:CG | 2.27 | 0.47 |
| 1:A:90:PRO:HD3 | 1:A:101:LEU:HD12 | 1.97 | 0.47 |
| 2:C:1160:DUX:C35 | 2:C:1160:DUX:H25 | 2.45 | 0.47 |
| 1:B:49:LEU:HD11 | 1:B:118:ALA:HB2 | 1.98 | 0.46 |
| 1:B:12:VAL:HG22 | 1:B:34:VAL:HG22 | 1.97 | 0.46 |
| 1:B:49:LEU:HD12 | 1:B:116:ILE:HG22 | 1.98 | 0.45 |
| 1:A:143:THR:OG1 | 1:A:145:GLU:OE2 | 2.30 | 0.44 |
| 1:C:94:ILE:O | 1:C:97:THR:HB | 2.17 | 0.43 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 1:B:47:VAL:HG21 | 1:B:120:LEU:HD12 | 2.00 | 0.43 |
| 1:C:30:ASP:OD1 | 1:C:91:ARG:NE | 2.50 | 0.43 |
| 1:C:89:PHE:CD1 | 1:C:140:VAL:HG13 | 2.53 | 0.43 |
| 1:A:3:LEU:O | 1:A:149:PHE:HA | 2.19 | 0.43 |
| 2:C:1160:DUX:C25 | 2:C:1160:DUX:H35 | 2.48 | 0.43 |
| 1:C:97:THR:HG22 | 1:C:99:LEU:H | 1.83 | 0.43 |
| 1:C:99:LEU:HD23 | 1:C:99:LEU:N | 2.33 | 0.43 |
| 1:A:19:HIS:HE1 | 1:A:30:ASP:O | 2.02 | 0.42 |
| 1:B:152:VAL:HG13 | 1:B:154:GLU:H | 1.85 | 0.42 |
| 1:B:99:LEU:HA | 1:B:121:ASP:O | 2.19 | 0.42 |
| 1:B:44:THR:HG21 | 1:C:100:ARG:NH2 | 2.34 | 0.42 |
| 1:A:97:THR:HB | 1:A:98:PRO:CD | 2.47 | 0.42 |
| 1:B:112:TYR:O | 1:B:113:ARG:HG2 | 2.20 | 0.41 |
| 1:A:94:ILE:HG13 | 1:A:136:LEU:HD22 | 2.01 | 0.41 |
| 1:C:86:PHE:CZ | 1:C:108:ILE:HG21 | 2.56 | 0.41 |
| 1:C:80:ASN:ND2 | 3:C:2024:HOH:O | 2.52 | 0.41 |
| 1:C:132:LYS:O | 1:C:133:ASN:HB2 | 2.20 | 0.41 |
| 1:A:91:ARG:HG3 | 1:A:137:VAL:N | 2.37 | 0.40 |

There are no symmetry-related clashes.

## 3.3 Torsion angles (i)

### 3.3.1 Protein backbone (i)

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

### 3.3.2 Protein sidechains (i)

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

### 3.3.3 RNA (i)

There are no RNA molecules in this entry.

## 3.4 Non-standard residues in protein, DNA, RNA chains (i)

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

## 3.5 Carbohydrates (i)

There are no monosaccharides in this entry.

## 3.6 Ligand geometry (i)

3 ligands are 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 | DUX | A | 1160 | - | 39,39,39 | 1.21 | 3 (7%) | 55,55,55 | 1.83 | 10 (18%) |
| 2 | DUX | B | 1160 | - | 39,39,39 | 1.12 | 2 (5%) | 55,55,55 | 2.74 | 16 (29%) |
| 2 | DUX | C | 1160 | - | 39,39,39 | 1.38 | 5 (12%) | 55,55,55 | 2.01 | 14 (25%) |

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 | DUX | A | 1160 | - | - | 10/28/40/40 | 0/5/5/5 |
| 2 | DUX | B | 1160 | - | - | 13/28/40/40 | 0/5/5/5 |
| 2 | DUX | C | 1160 | - | - | 4/28/40/40 | 0/5/5/5 |

All (10) bond length outliers are listed below:

| Mol | Chain | Res | Type | Atoms | Z | Observed(Å) | Ideal(Å) |
|---|---|---|---|---|---|---|---|
| 2 | C | 1160 | DUX | O5'-C17 | -4.08 | 1.41 | 1.45 |
| 2 | B | 1160 | DUX | C2-N1 | 3.21 | 1.43 | 1.38 |
| 2 | C | 1160 | DUX | C17-C24 | -3.09 | 1.48 | 1.53 |
| 2 | C | 1160 | DUX | C6-C5 | 3.07 | 1.42 | 1.35 |
| 2 | A | 1160 | DUX | F3'-C3' | -2.82 | 1.33 | 1.40 |
| 2 | A | 1160 | DUX | C2-N1 | 2.56 | 1.42 | 1.38 |
| 2 | B | 1160 | DUX | C6-C5 | 2.53 | 1.40 | 1.35 |
| 2 | C | 1160 | DUX | C17-C30 | -2.50 | 1.49 | 1.53 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(Å) | Ideal(Å) |
|---|---|---|---|---|---|---|---|
| 2 | A | 1160 | DUX | C6-C5 | 2.28 | 1.40 | 1.35 |
| 2 | C | 1160 | DUX | C2-N3 | -2.20 | 1.34 | 1.38 |

All (40) bond angle outliers are listed below:

| Mol | Chain | Res | Type | Atoms | Z | Observed($^o$) | Ideal($^o$) |
|---|---|---|---|---|---|---|---|
| 2 | B | 1160 | DUX | C5'-C4'-C3' | -9.39 | 106.08 | 114.70 |
| 2 | B | 1160 | DUX | O5'-C17-C30 | 7.40 | 127.13 | 107.77 |
| 2 | B | 1160 | DUX | O5'-C17-C18 | -7.05 | 89.33 | 107.77 |
| 2 | C | 1160 | DUX | N3-C2-N1 | 6.34 | 123.30 | 114.89 |
| 2 | A | 1160 | DUX | C2'-C3'-C4' | 6.24 | 108.39 | 104.23 |
| 2 | B | 1160 | DUX | F3'-C3'-C4' | -6.07 | 104.90 | 108.84 |
| 2 | C | 1160 | DUX | O2-C2-N1 | -5.76 | 115.13 | 122.79 |
| 2 | C | 1160 | DUX | F3'-C3'-C4' | 5.68 | 112.52 | 108.84 |
| 2 | B | 1160 | DUX | F3'-C3'-C2' | 5.17 | 119.92 | 109.06 |
| 2 | B | 1160 | DUX | N3-C2-N1 | 4.74 | 121.18 | 114.89 |
| 2 | B | 1160 | DUX | O4'-C1'-N1 | -4.67 | 99.52 | 107.86 |
| 2 | C | 1160 | DUX | C4-N3-C2 | -4.63 | 120.47 | 126.58 |
| 2 | B | 1160 | DUX | C4-N3-C2 | -4.42 | 120.75 | 126.58 |
| 2 | A | 1160 | DUX | O4-C4-C5 | -4.21 | 117.75 | 125.16 |
| 2 | A | 1160 | DUX | C5-C4-N3 | 4.01 | 120.84 | 114.84 |
| 2 | A | 1160 | DUX | F3'-C3'-C4' | -3.98 | 106.25 | 108.84 |
| 2 | A | 1160 | DUX | C5'-C4'-C3' | -3.85 | 111.17 | 114.70 |
| 2 | A | 1160 | DUX | C4-N3-C2 | -3.79 | 121.58 | 126.58 |
| 2 | C | 1160 | DUX | C5'-O5'-C17 | 3.69 | 122.84 | 117.01 |
| 2 | A | 1160 | DUX | N3-C2-N1 | 3.49 | 119.53 | 114.89 |
| 2 | A | 1160 | DUX | O2-C2-N1 | -3.17 | 118.57 | 122.79 |
| 2 | B | 1160 | DUX | C2'-C1'-N1 | 3.11 | 120.94 | 113.77 |
| 2 | B | 1160 | DUX | O5'-C5'-C4' | 2.99 | 114.26 | 107.68 |
| 2 | B | 1160 | DUX | C5-C4-N3 | 2.97 | 119.29 | 114.84 |
| 2 | C | 1160 | DUX | C2'-C3'-C4' | 2.86 | 106.14 | 104.23 |
| 2 | C | 1160 | DUX | C1'-N1-C6 | 2.70 | 126.88 | 121.55 |
| 2 | A | 1160 | DUX | C5'-O5'-C17 | 2.62 | 121.14 | 117.01 |
| 2 | A | 1160 | DUX | O4'-C4'-C3' | -2.60 | 104.27 | 105.56 |
| 2 | C | 1160 | DUX | O4-C4-C5 | -2.58 | 120.62 | 125.16 |
| 2 | B | 1160 | DUX | O4-C4-C5 | -2.57 | 120.64 | 125.16 |
| 2 | C | 1160 | DUX | C5-C4-N3 | 2.48 | 118.55 | 114.84 |
| 2 | B | 1160 | DUX | C3'-C2'-C1' | 2.46 | 104.54 | 102.36 |
| 2 | C | 1160 | DUX | C6-N1-C2 | -2.44 | 117.86 | 120.99 |
| 2 | B | 1160 | DUX | O4'-C4'-C5' | 2.42 | 117.35 | 109.37 |
| 2 | C | 1160 | DUX | C5'-C4'-C3' | -2.38 | 112.52 | 114.70 |
| 2 | C | 1160 | DUX | O5'-C17-C18 | -2.28 | 101.80 | 107.77 |

*Continued on next page...*

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| Mol | Chain | Res | Type | Atoms | Z | Observed($^o$) | Ideal($^o$) |
|---|---|---|---|---|---|---|---|
| 2 | B | 1160 | DUX | O2-C2-N1 | -2.26 | 119.79 | 122.79 |
| 2 | C | 1160 | DUX | O4'-C4'-C3' | 2.13 | 106.61 | 105.56 |
| 2 | B | 1160 | DUX | O5'-C17-C24 | -2.05 | 102.41 | 107.77 |
| 2 | C | 1160 | DUX | C28-C29-C24 | -2.02 | 118.63 | 120.76 |

There are no chirality outliers.

All (27) torsion outliers are listed below:

| Mol | Chain | Res | Type | Atoms |
|---|---|---|---|---|
| 2 | A | 1160 | DUX | C2'-C1'-N1-C6 |
| 2 | B | 1160 | DUX | C2'-C1'-N1-C6 |
| 2 | B | 1160 | DUX | C2'-C1'-N1-C2 |
| 2 | B | 1160 | DUX | C18-C17-O5'-C5' |
| 2 | B | 1160 | DUX | O4'-C1'-N1-C6 |
| 2 | A | 1160 | DUX | O4'-C1'-N1-C6 |
| 2 | A | 1160 | DUX | C3'-C4'-C5'-O5' |
| 2 | A | 1160 | DUX | C2'-C1'-N1-C2 |
| 2 | B | 1160 | DUX | O4'-C1'-N1-C2 |
| 2 | B | 1160 | DUX | C24-C17-O5'-C5' |
| 2 | C | 1160 | DUX | C2'-C1'-N1-C6 |
| 2 | B | 1160 | DUX | O5'-C17-C24-C25 |
| 2 | B | 1160 | DUX | O5'-C17-C18-C23 |
| 2 | A | 1160 | DUX | C30-C17-C24-C25 |
| 2 | B | 1160 | DUX | C30-C17-C24-C25 |
| 2 | A | 1160 | DUX | O4'-C1'-N1-C2 |
| 2 | C | 1160 | DUX | O4'-C1'-N1-C6 |
| 2 | B | 1160 | DUX | C30-C17-C24-C29 |
| 2 | A | 1160 | DUX | C30-C17-C24-C29 |
| 2 | A | 1160 | DUX | O5'-C17-C24-C25 |
| 2 | C | 1160 | DUX | O4'-C1'-N1-C2 |
| 2 | C | 1160 | DUX | C2'-C1'-N1-C2 |
| 2 | B | 1160 | DUX | C30-C17-O5'-C5' |
| 2 | B | 1160 | DUX | O5'-C17-C18-C19 |
| 2 | B | 1160 | DUX | O5'-C17-C24-C29 |
| 2 | A | 1160 | DUX | O5'-C17-C18-C23 |
| 2 | A | 1160 | DUX | O5'-C17-C24-C29 |

There are no ring outliers.

2 monomers are involved in 6 short contacts:

| Mol | Chain | Res | Type | Clashes | Symm-Clashes |
|---|---|---|---|---|---|
| 2 | B | 1160 | DUX | 3 | 0 |
| 2 | C | 1160 | DUX | 3 | 0 |

## 3.7 Other polymers (i)

There are no such residues in this entry.

## 3.8 Polymer linkage issues (i)

There are no chain breaks in this entry.

# 4 Fit of model and data

## 4.1 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, $95^{th}$ 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 | 142/173 (82%) | -0.19 | 4 (2%) | 53 | 51 | 27, 39, 58, 64 | 0 |
| 1 | B | 140/173 (80%) | -0.12 | 6 (4%) | 35 | 33 | 34, 51, 72, 75 | 0 |
| 1 | C | 141/173 (81%) | -0.24 | 3 (2%) | 63 | 61 | 25, 41, 60, 71 | 0 |
| All | All | 423/519 (81%) | -0.18 | 13 (3%) | 49 | 47 | 25, 43, 67, 75 | 0 |

All (13) RSRZ outliers are listed below:

| Mol | Chain | Res | Type | RSRZ |
|---|---|---|---|---|
| 1 | A | 159 | SER | 5.4 |
| 1 | C | 20 | LYS | 4.6 |
| 1 | B | 62 | TYR | 4.6 |
| 1 | C | 61 | ASN | 4.5 |
| 1 | A | 80 | ASN | 4.4 |
| 1 | C | 21 | THR | 3.0 |
| 1 | A | 63 | TYR | 2.8 |
| 1 | B | 111 | GLY | 2.7 |
| 1 | B | 126 | GLN | 2.5 |
| 1 | B | 61 | ASN | 2.4 |
| 1 | A | 62 | TYR | 2.3 |
| 1 | B | 125 | ASP | 2.3 |
| 1 | B | 25 | GLY | 2.1 |

## 4.2 Non-standard residues in protein, DNA, RNA chains

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

## 4.3 Carbohydrates

There are no monosaccharides in this entry.

## 4.4 Ligands (i)

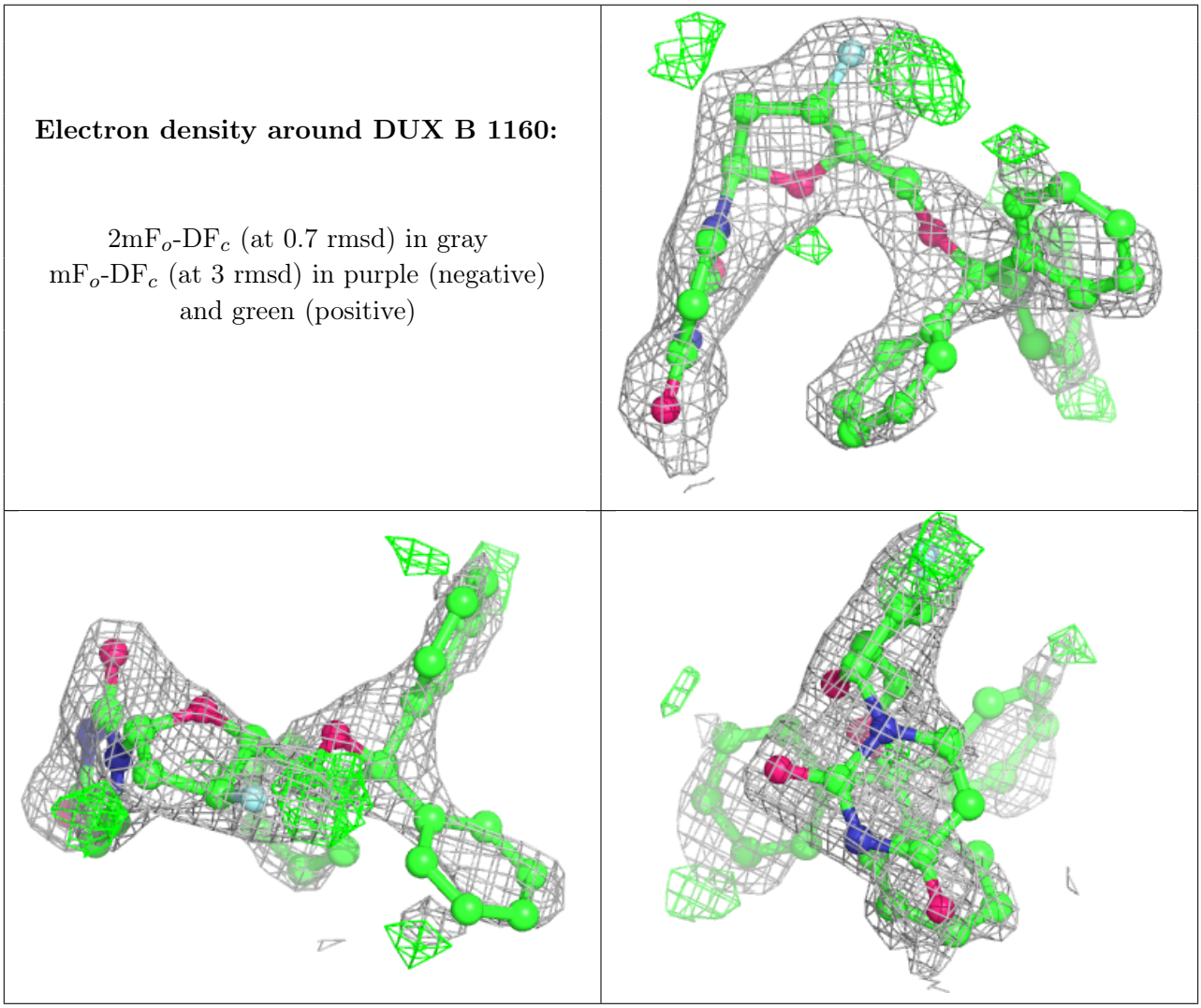
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, $95^{th}$ percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' 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 | DUX | B | 1160 | 35/35 | 0.75 | 0.29 | 33,41,44,44 | 35 |
| 2 | DUX | A | 1160 | 35/35 | 0.93 | 0.12 | 33,41,50,51 | 0 |
| 2 | DUX | C | 1160 | 35/35 | 0.98 | 0.10 | 22,25,30,33 | 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.

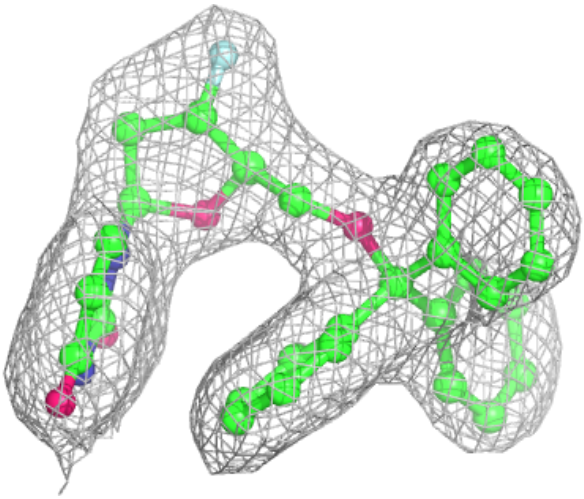
**Electron density around DUX B 1160:**

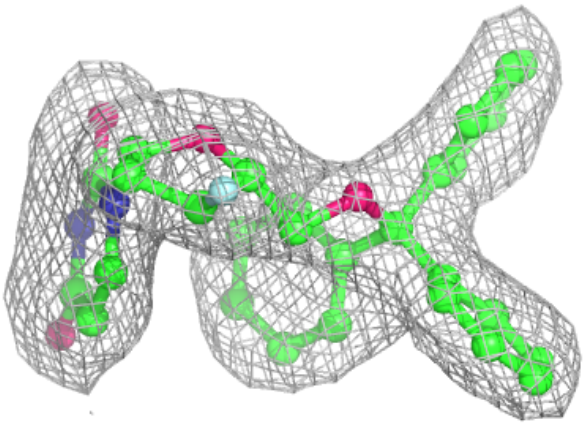
$2mF_o$-$DF_c$ (at 0.7 rmsd) in gray
$mF_o$-$DF_c$ (at 3 rmsd) in purple (negative) and green (positive)

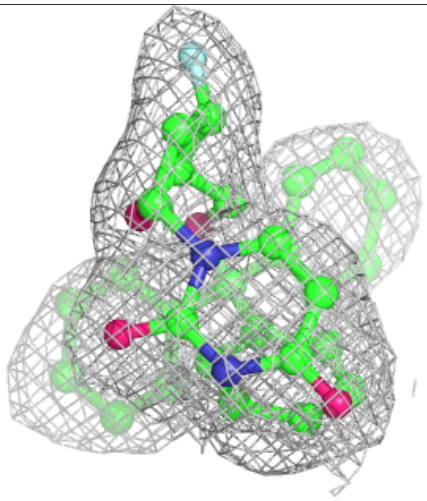


**Electron density around DUX A 1160:**

$2mF_o$-$DF_c$ (at 0.7 rmsd) in gray
$mF_o$-$DF_c$ (at 3 rmsd) in purple (negative) and green (positive)

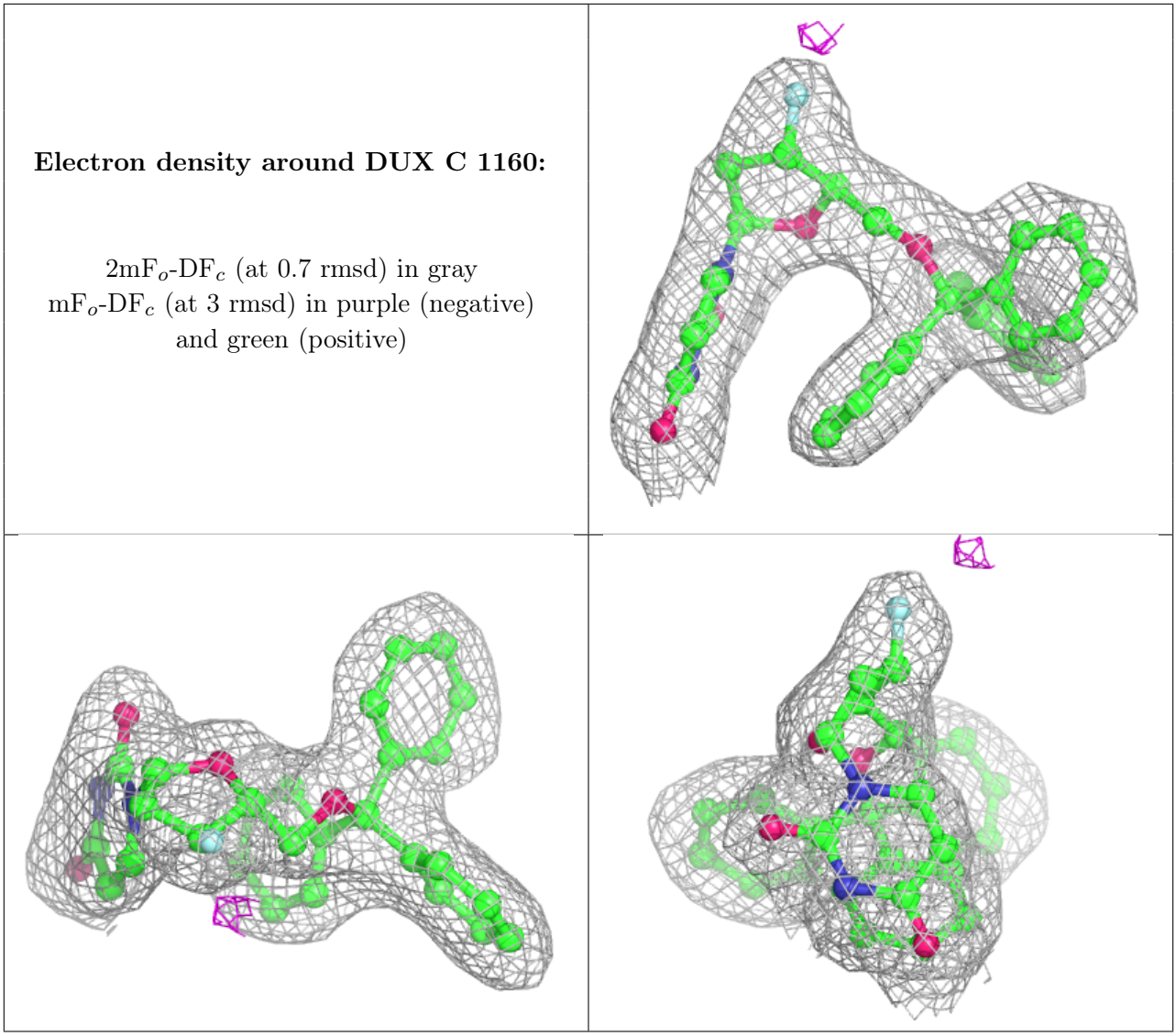






**Electron density around DUX C 1160:**

$2mF_o$-$DF_c$ (at 0.7 rmsd) in gray
$mF_o$-$DF_c$ (at 3 rmsd) in purple (negative) and green (positive)



## 4.5 Other polymers

There are no such residues in this entry.