# WORLDWIDE wwPDB PROTEIN DATA BANK

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

Aug 7, 2023 – 02:14 PM EDT

|  |  |  |
|---|---|---|
| PDB ID | : | 7FVS |
| Title | : | Crystal Structure of S. aureus gyrase in complex with 4-[[1-[(1-chloro-6,7-dihydro-5H-cyclopenta[c]pyridin-6-yl)methyl]azetidin-3-yl]methylamino]-6-fluorochromen-2-one |
| Authors | : | Xu, B.; Benz, J.; Cumming, J.G.; Kreis, L.; Rudolph, M.G. |
| Deposited on | : | 2023-04-18 |
| Resolution | : | 2.16 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 (i) 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 (i)) 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 | : | 2.35 |
| 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) | : | 2.35 |

# 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 2.16 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.
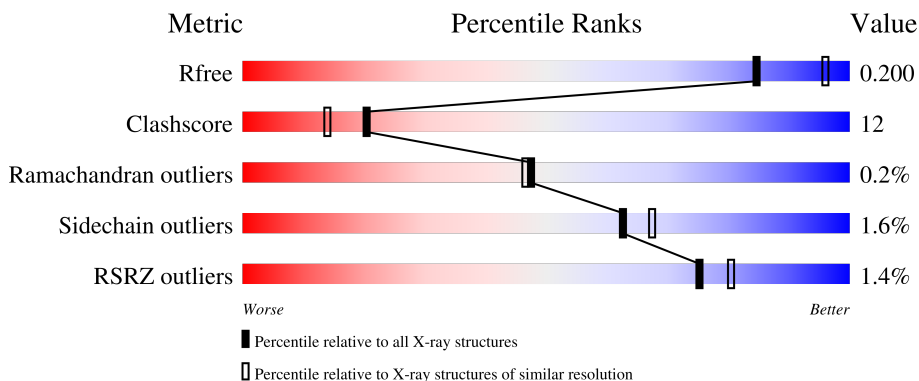


| Metric | Whole archive (#Entries) | Similar resolution (#Entries, resolution range(Å)) |
|---|---|---|
| $R_{free}$ | 130704 | 1479 (2.16-2.16) |
| Clashscore | 141614 | 1585 (2.16-2.16) |
| Ramachandran outliers | 138981 | 1560 (2.16-2.16) |
| Sidechain outliers | 138945 | 1559 (2.16-2.16) |
| RSRZ outliers | 127900 | 1456 (2.16-2.16) |

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 of 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 <=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 | 692 | 71% 25% |
| 1 | B | 692 | 69% 27% |
| 2 | C | 20 | 60% 30% 10% |
| 2 | D | 20 | 45% 35% 20% |

The following table lists non-polymeric compounds, carbohydrate monomers and non-standard residues in protein, DNA, RNA chains that are outliers for geometric or electron-density-fit criteria:

| Mol | Type | Chain | Res | Chirality | Geometry | Clashes | Electron density |
|-----|------|-------|------|-----------|----------|---------|------------------|
| 5 | ACT | B | 1503 | - | - | X | - |

# 2 Entry composition ⓘ

There are 7 unique types of molecules in this entry. The entry contains 11927 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 DNA gyrase subunit B,DNA gyrase subunit A Chimera.

| Mol | Chain | Residues | Atoms | | | | | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|---|---|---|---|---------|---------|-------|
| 1 | A | 670 | Total 5313 | C 3314 | N 957 | O 1017 | S 25 | 0 | 0 | 0 |
| 1 | B | 671 | Total 5318 | C 3316 | N 958 | O 1019 | S 25 | 0 | 0 | 0 |

There are 76 discrepancies between the modelled and reference sequences:

| Chain | Residue | Modelled | Actual | Comment | Reference |
|-------|---------|----------|--------|---------|-----------|
| A | 409 | MET | - | initiating methionine | UNP P66937 |
| A | ? | - | LEU | deletion | UNP P66937 |
| A | ? | - | TYR | deletion | UNP P66937 |
| A | ? | - | LYS | deletion | UNP P66937 |
| A | ? | - | LEU | deletion | UNP P66937 |
| A | ? | - | THR | deletion | UNP P66937 |
| A | ? | - | GLN | deletion | UNP P66937 |
| A | ? | - | GLY | deletion | UNP P66937 |
| A | ? | - | LYS | deletion | UNP P66937 |
| A | ? | - | GLN | deletion | UNP P66937 |
| A | ? | - | LYS | deletion | UNP P66937 |
| A | ? | - | TYR | deletion | UNP P66937 |
| A | ? | - | TYR | deletion | UNP P66937 |
| A | ? | - | VAL | deletion | UNP P66937 |
| A | ? | - | TYR | deletion | UNP P66937 |
| A | ? | - | ASN | deletion | UNP P66937 |
| A | ? | - | ASP | deletion | UNP P66937 |
| A | ? | - | ARG | deletion | UNP P66937 |
| A | ? | - | GLU | deletion | UNP P66937 |
| A | ? | - | LEU | deletion | UNP P66937 |
| A | ? | - | ASP | deletion | UNP P66937 |
| A | ? | - | LYS | deletion | UNP P66937 |
| A | ? | - | LEU | deletion | UNP P66937 |
| A | ? | - | LYS | deletion | UNP P66937 |
| A | ? | - | SER | deletion | UNP P66937 |

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| Chain | Residue | Modelled | Actual | Comment | Reference |
|-------|---------|----------|--------|---------|-----------|
| A | ? | - | GLU | deletion | UNP P66937 |
| A | ? | - | LEU | deletion | UNP P66937 |
| A | ? | - | ASN | deletion | UNP P66937 |
| A | ? | - | PRO | deletion | UNP P66937 |
| A | ? | - | THR | deletion | UNP P66937 |
| A | ? | - | PRO | deletion | UNP P66937 |
| A | ? | - | LYS | deletion | UNP P66937 |
| A | ? | - | TRP | deletion | UNP P66937 |
| A | ? | - | SER | deletion | UNP P66937 |
| A | ? | - | ILE | deletion | UNP P66937 |
| A | 544 | THR | ALA | conflict | UNP P66937 |
| A | 545 | GLY | ARG | conflict | UNP P66937 |
| A | 1123 | PHE | TYR | engineered mutation | UNP Q99XG5 |
| B | 409 | MET | - | initiating methionine | UNP P66937 |
| B | ? | - | LEU | deletion | UNP P66937 |
| B | ? | - | TYR | deletion | UNP P66937 |
| B | ? | - | LYS | deletion | UNP P66937 |
| B | ? | - | LEU | deletion | UNP P66937 |
| B | ? | - | THR | deletion | UNP P66937 |
| B | ? | - | GLN | deletion | UNP P66937 |
| B | ? | - | GLY | deletion | UNP P66937 |
| B | ? | - | LYS | deletion | UNP P66937 |
| B | ? | - | GLN | deletion | UNP P66937 |
| B | ? | - | LYS | deletion | UNP P66937 |
| B | ? | - | TYR | deletion | UNP P66937 |
| B | ? | - | TYR | deletion | UNP P66937 |
| B | ? | - | VAL | deletion | UNP P66937 |
| B | ? | - | TYR | deletion | UNP P66937 |
| B | ? | - | ASN | deletion | UNP P66937 |
| B | ? | - | ASP | deletion | UNP P66937 |
| B | ? | - | ARG | deletion | UNP P66937 |
| B | ? | - | GLU | deletion | UNP P66937 |
| B | ? | - | LEU | deletion | UNP P66937 |
| B | ? | - | ASP | deletion | UNP P66937 |
| B | ? | - | LYS | deletion | UNP P66937 |
| B | ? | - | LEU | deletion | UNP P66937 |
| B | ? | - | LYS | deletion | UNP P66937 |
| B | ? | - | SER | deletion | UNP P66937 |
| B | ? | - | GLU | deletion | UNP P66937 |
| B | ? | - | LEU | deletion | UNP P66937 |
| B | ? | - | ASN | deletion | UNP P66937 |
| B | ? | - | PRO | deletion | UNP P66937 |

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| Chain | Residue | Modelled | Actual | Comment | Reference |
|:---:|:---:|:---:|:---:|:---:|:---|
| B | ? | - | THR | deletion | UNP P66937 |
| B | ? | - | PRO | deletion | UNP P66937 |
| B | ? | - | LYS | deletion | UNP P66937 |
| B | ? | - | TRP | deletion | UNP P66937 |
| B | ? | - | SER | deletion | UNP P66937 |
| B | ? | - | ILE | deletion | UNP P66937 |
| B | 544 | THR | ALA | conflict | UNP P66937 |
| B | 545 | GLY | ARG | conflict | UNP P66937 |
| B | 1123 | PHE | TYR | engineered mutation | UNP Q99XG5 |

- Molecule 2 is a DNA chain called DNA (5'-D(*AP*GP*CP*CP*GP*TP*AP*GP*GP*GP* CP*CP*CP*TP*AP*CP*GP*GP*CP*T)-3').

| Mol | Chain | Residues | Atoms | | | | | ZeroOcc | AltConf | Trace |
|:---:|:---:|:---:|:---:|:---:|:---:|:---:|:---:|:---:|:---:|:---:|
| 2 | C | 20 | Total 407 | C 193 | N 77 | O 118 | P 19 | 0 | 0 | 0 |
| 2 | D | 20 | Total 390 | C 183 | N 75 | O 113 | P 19 | 0 | 0 | 0 |

- Molecule 3 is MANGANESE (II) ION (three-letter code: MN) (formula: Mn).

| Mol | Chain | Residues | Atoms | | ZeroOcc | AltConf |
|:---:|:---:|:---:|:---:|:---:|:---:|:---:|
| 3 | A | 1 | Total 1 | Mn 1 | 0 | 0 |
| 3 | B | 2 | Total 2 | Mn 2 | 0 | 0 |

- Molecule 4 is CHLORIDE ION (three-letter code: CL) (formula: Cl).

| Mol | Chain | Residues | Atoms | | ZeroOcc | AltConf |
|:---:|:---:|:---:|:---:|:---:|:---:|:---:|
| 4 | A | 1 | Total 1 | Cl 1 | 0 | 0 |

- Molecule 5 is ACETATE ION (three-letter code: ACT) (formula: $C_2H_3O_2$).

ACT

| Mol | Chain | Residues | Atoms | | | ZeroOcc | AltConf |
|---|---|---|---|---|---|---|---|
| | | | Total | C | O | | |
| 5 | B | 1 | 4 | 2 | 2 | 0 | 0 |

- Molecule 6 is 4-{[(1-{[(6R)-1-chloro-6,7-dihydro-5H-cyclopenta[c]pyridin-6-yl]methyl}azet idin-3-yl)methyl]amino}-6-fluoro-2H-1-benzopyran-2-one (three-letter code: 61I) (formula: $C_{22}H_{21}ClFN_3O_2$) (labeled as "Ligand of Interest" by depositor).



61I
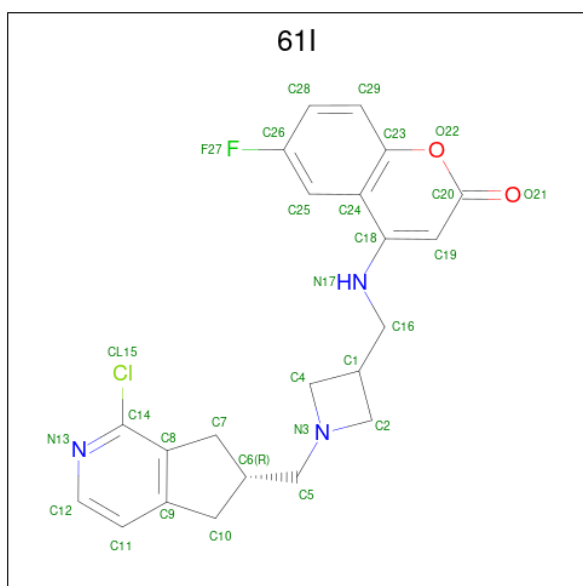
| Mol | Chain | Residues | Atoms | | | | | | ZeroOcc | AltConf |
|---|---|---|---|---|---|---|---|---|---|---|
| | | | Total | C | Cl | F | N | O | | |
| 6 | B | 1 | 29 | 22 | 1 | 1 | 3 | 2 | 0 | 0 |

- Molecule 7 is water.

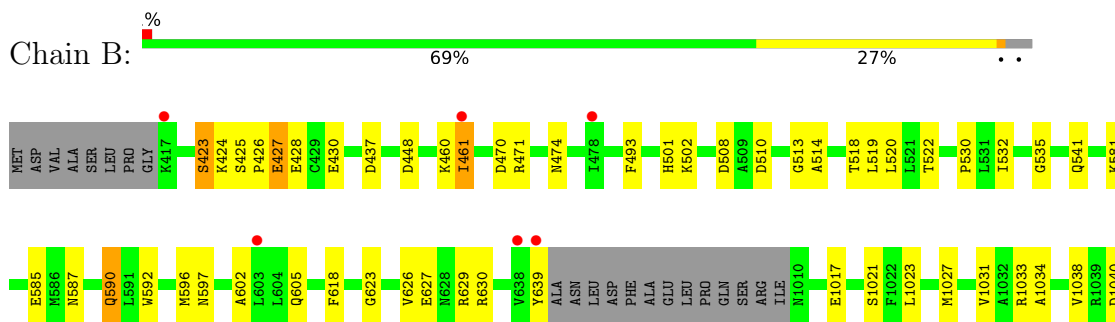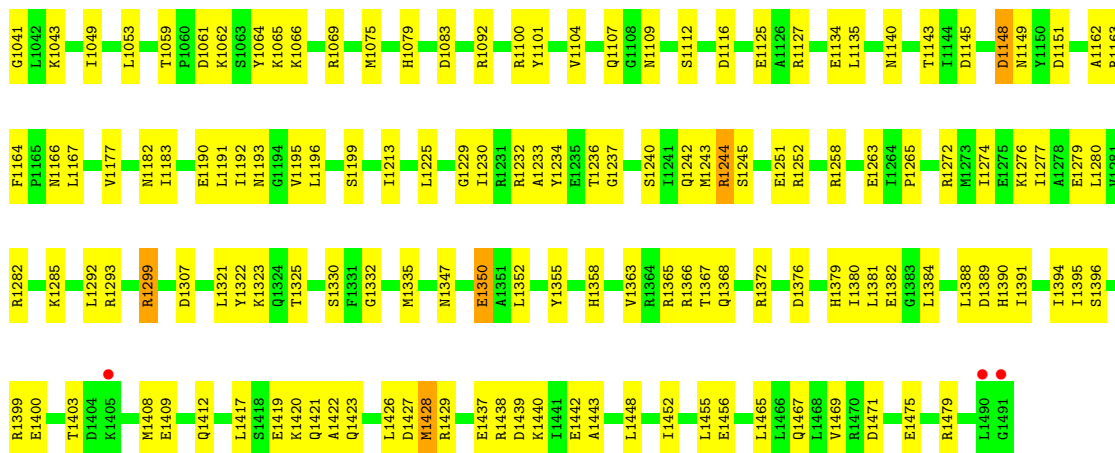| Mol | Chain | Residues | Atoms | | ZeroOcc | AltConf |
|-----|-------|----------|-------|------|---------|---------|
| 7 | A | 205 | Total 205 | O 205 | 0 | 0 |
| 7 | B | 197 | Total 197 | O 197 | 0 | 0 |
| 7 | C | 30 | Total 30 | O 30 | 0 | 0 |
| 7 | D | 30 | Total 30 | O 30 | 0 | 0 |

# 3 Residue-property plots ⓘ

These plots are drawn for all protein, RNA, DNA and oligosaccharide 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.

• Molecule 1: DNA gyrase subunit B,DNA gyrase subunit A Chimera
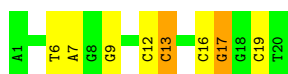


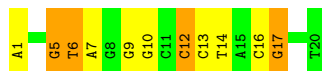• Molecule 1: DNA gyrase subunit B,DNA gyrase subunit A Chimera

G1041 L1042 K1043 I1049 L1053 T1059 P1060 D1061 K1062 S1063 Y1064 K1065 K1066 R1069 M1075 H1079 D1083 R1092 R1100 Y1101 V1104 Q1107 G1108 N1109 S1112 D1116 E1125 A1126 R1127 E1134 L1135 N1140 T1143 I1144 D1145 D1148 N1149 Y1150 D1151 A1162 R1163

F1164 P1165 N1166 L1167 V1177 N1182 I1183 E1190 L1191 I1192 N1193 G1194 V1195 L1196 S1199 I1213 L1225 G1229 I1230 R1231 R1232 A1233 Y1234 E1235 T1236 G1237 S1240 I1241 Q1242 M1243 R1244 S1245 E1251 R1252 R1258 E1263 I1264 P1265 R1272 M1273 I1274 E1275 K1276 I1277 A1278 E1279 L1280 V1281

R1282 K1285 L1292 R1293 R1299 D1307 L1321 Y1322 K1323 Q1324 T1325 S1330 F1331 G1332 M1335 N1347 E1350 A1351 L1352 Y1355 H1358 V1363 R1364 R1365 R1366 T1367 Q1368 R1372 D1376 H1379 I1380 L1381 E1382 G1383 L1384 L1388 D1389 H1390 I1391 I1394 I1395 S1396

R1399 E1400 T1403 D1404 K1405 M1408 E1409 Q1412 L1417 S1418 E1419 K1420 Q1421 A1422 Q1423 L1426 D1427 M1428 R1429 E1437 R1438 D1439 K1440 I1441 E1442 A1443 L1448 I1452 L1455 E1456 L1465 L1466 Q1467 L1468 V1469 R1470 D1471 E1475 R1479 L1490 G1491

• Molecule 2: DNA (5'-D(*AP*GP*CP*CP*GP*TP*AP*GP*GP*GP*CP*CP*CP*TP*AP*CP *GP*GP*CP*T)-3')

Chain C:

A1 T6 A7 G8 G9 C12 C13 C16 G17 G18 C19 T20

• Molecule 2: DNA (5'-D(*AP*GP*CP*CP*GP*TP*AP*GP*GP*GP*CP*CP*CP*TP*AP*CP *GP*GP*CP*T)-3')

Chain D:

A1 G5 T6 A7 G8 G9 G10 C11 C12 C13 T14 A15 C16 G17 T20

# 4 Data and refinement statistics ⓘ

| Property | Value | Source |
|----------|-------|--------|
| Space group | P 61 | Depositor |
| Cell constants<br>a, b, c, $\alpha$, $\beta$, $\gamma$ | 92.92Å   92.92Å   407.58Å<br>90.00°   90.00°   120.00° | Depositor |
| Resolution (Å) | 80.47  –  2.16<br>80.47  –  2.16 | Depositor<br>EDS |
| % Data completeness<br>(in resolution range) | 95.6 (80.47-2.16)<br>94.6 (80.47-2.16) | Depositor<br>EDS |
| $R_{merge}$ | 0.16 | Depositor |
| $R_{sym}$ | (Not available) | Depositor |
| $< I/\sigma(I) >$ [1] | 0.89 (at 2.16Å) | Xtriage |
| Refinement program | PHENIX 1.12rc1_2801 | Depositor |
| R, $R_{free}$ | 0.185  ,  0.221<br>0.175  ,  0.200 | Depositor<br>DCC |
| $R_{free}$ test set | 5099 reflections (5.04%) | wwPDB-VP |
| Wilson B-factor (Å$^2$) | 35.2 | Xtriage |
| Anisotropy | 0.014 | Xtriage |
| Bulk solvent $k_{sol}$(e/Å$^3$), $B_{sol}$(Å$^2$) | 0.38 , 39.3 | EDS |
| L-test for twinning [2] | $< \|L\| > = 0.38$, $< L^2 > = 0.20$ | Xtriage |
| Estimated twinning fraction | 0.356 for h,-h-k,-l | Xtriage |
| Reported twinning fraction | 0.330 for k,h,-l | Depositor |
| Outliers | 0 of 101251 reflections | Xtriage |
| $F_o,F_c$ correlation | 0.95 | EDS |
| Total number of atoms | 11927 | wwPDB-VP |
| Average B, all atoms (Å$^2$) | 32.0 | wwPDB-VP |

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.04% 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.

# 5   Model quality  ⓘ

## 5.1   Standard geometry  ⓘ

Bond lengths and bond angles in the following residue types are not validated in this section: CL, MN, 61I, ACT

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     | 0.47 | 0/5385    | 0.61 | 0/7254    |
| 1   | B     | 0.47 | 0/5390    | 0.60 | 0/7259    |
| 2   | C     | 0.98 | 1/456 (0.2%) | 1.07 | 3/702 (0.4%) |
| 2   | D     | 1.24 | 3/437 (0.7%) | 1.10 | 2/672 (0.3%) |
| All | All   | 0.54 | 4/11668 (0.0%) | 0.66 | 5/15887 (0.0%) |

All (4) bond length outliers are listed below:

| Mol | Chain | Res | Type | Atoms | Z | Observed(Å) | Ideal(Å) |
|-----|-------|-----|------|-------|-----|-------------|----------|
| 2   | D     | 17  | DG   | C3'-O3' | -7.22 | 1.34 | 1.44 |
| 2   | D     | 5   | DG   | C3'-O3' | -6.75 | 1.35 | 1.44 |
| 2   | C     | 17  | DG   | C3'-O3' | -6.13 | 1.35 | 1.44 |
| 2   | D     | 6   | DT   | C3'-O3' | -5.35 | 1.36 | 1.44 |

All (5) bond angle outliers are listed below:

| Mol | Chain | Res | Type | Atoms | Z | Observed($^o$) | Ideal($^o$) |
|-----|-------|-----|------|-------|-----|----------------|-------------|
| 2   | D     | 9   | DG   | O4'-C4'-C3' | -8.46 | 100.92 | 106.00 |
| 2   | C     | 19  | DC   | O4'-C4'-C3' | -6.27 | 101.99 | 104.50 |
| 2   | D     | 12  | DC   | O4'-C4'-C3' | -5.91 | 102.14 | 104.50 |
| 2   | C     | 9   | DG   | O4'-C4'-C3' | -5.90 | 102.14 | 104.50 |
| 2   | C     | 13  | DC   | O4'-C4'-C3' | -5.83 | 102.17 | 104.50 |

There are no chirality outliers.

There are no planarity outliers.

## 5.2 Too-close contacts ⓘ

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 | 5313 | 0 | 5366 | 125 | 0 |
| 1 | B | 5318 | 0 | 5369 | 145 | 0 |
| 2 | C | 407 | 0 | 225 | 7 | 0 |
| 2 | D | 390 | 0 | 212 | 14 | 0 |
| 3 | A | 1 | 0 | 0 | 0 | 0 |
| 3 | B | 2 | 0 | 0 | 0 | 0 |
| 4 | A | 1 | 0 | 0 | 1 | 0 |
| 5 | B | 4 | 0 | 3 | 2 | 0 |
| 6 | B | 29 | 0 | 0 | 0 | 0 |
| 7 | A | 205 | 0 | 0 | 20 | 2 |
| 7 | B | 197 | 0 | 0 | 21 | 2 |
| 7 | C | 30 | 0 | 0 | 2 | 0 |
| 7 | D | 30 | 0 | 0 | 2 | 0 |
| All | All | 11927 | 0 | 11175 | 275 | 2 |

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 12.

The worst 5 of 275 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:447:ARG:NH2 | 1:A:452:GLN:O | 2.11 | 0.83 |
| 1:A:535:GLY:O | 1:A:605:GLN:NE2 | 2.10 | 0.82 |
| 1:B:470:ASP:O | 1:B:474:ASN:ND2 | 2.13 | 0.81 |
| 1:B:1323:LYS:O | 7:B:1601:HOH:O | 1.99 | 0.79 |
| 1:B:1439:ASP:O | 1:B:1443:ALA:N | 2.14 | 0.79 |

All (2) 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) |
|--------|--------|--------------------------|-------------------|
| 7:A:1675:HOH:O | 7:B:1756:HOH:O[5_664] | 2.13 | 0.07 |
| 7:A:1738:HOH:O | 7:B:1792:HOH:O[5_664] | 2.17 | 0.03 |

## 5.3 Torsion angles ⓘ

### 5.3.1 Protein backbone ⓘ

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 | 666/692 (96%) | 632 (95%) | 32 (5%) | 2 (0%) | 41 | 37 |
| 1 | B | 667/692 (96%) | 638 (96%) | 28 (4%) | 1 (0%) | 51 | 53 |
| All | All | 1333/1384 (96%) | 1270 (95%) | 60 (4%) | 3 (0%) | 47 | 46 |

All (3) Ramachandran outliers are listed below:

| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1 | A | 1033 | ARG |
| 1 | A | 1283 | ASP |
| 1 | B | 1033 | ARG |

### 5.3.2 Protein sidechains ⓘ

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 | 574/591 (97%) | 566 (99%) | 8 (1%) | 67 | 72 |
| 1 | B | 574/591 (97%) | 564 (98%) | 10 (2%) | 60 | 65 |
| All | All | 1148/1182 (97%) | 1130 (98%) | 18 (2%) | 62 | 67 |

5 of 18 residues with a non-rotameric sidechain are listed below:

| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1 | B | 1299 | ARG |
| 1 | B | 1428 | MET |
| 1 | B | 1403 | THR |

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| Mol | Chain | Res | Type |
|-----|-------|------|------|
| 1 | B | 423 | SER |
| 1 | B | 1244 | ARG |

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (1) such sidechains are listed below:

| Mol | Chain | Res | Type |
|-----|-------|------|------|
| 1 | A | 1010 | ASN |

### 5.3.3   RNA ⓘ

There are no RNA molecules in this entry.

## 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 monosaccharides in this entry.

## 5.6   Ligand geometry ⓘ

Of 6 ligands modelled in this entry, 4 are monoatomic - leaving 2 for Mogul analysis.

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 | $\#|Z| > 2$ |
| 5 | ACT | B | 1503 | - | 3,3,3 | 1.19 | 0 | 3,3,3 | 1.31 | 0 |
| 6 | 61I | B | 1504 | - | 32,33,33 | 1.87 | 9 (28%) | 31,48,48 | 2.45 | 9 (29%) |

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 |
|-----|------|-------|-----|------|---------|----------|-------|
| 6 | 61I | B | 1504 | - | - | 4/7/25/25 | 0/5/5/5 |

The worst 5 of 9 bond length outliers are listed below:

| Mol | Chain | Res | Type | Atoms | Z | Observed(Å) | Ideal(Å) |
|-----|-------|-----|------|-------|---|-------------|----------|
| 6 | B | 1504 | 61I | C2-N3 | 4.85 | 1.53 | 1.49 |
| 6 | B | 1504 | 61I | C14-CL15 | -3.21 | 1.68 | 1.74 |
| 6 | B | 1504 | 61I | C19-C20 | -3.16 | 1.38 | 1.44 |
| 6 | B | 1504 | 61I | C4-N3 | 3.07 | 1.52 | 1.49 |
| 6 | B | 1504 | 61I | C19-C18 | -2.80 | 1.33 | 1.36 |

The worst 5 of 9 bond angle outliers are listed below:

| Mol | Chain | Res | Type | Atoms | Z | Observed(°) | Ideal(°) |
|-----|-------|-----|------|-------|---|-------------|----------|
| 6 | B | 1504 | 61I | C19-C18-N17 | -7.55 | 112.42 | 124.79 |
| 6 | B | 1504 | 61I | C1-C16-N17 | -6.67 | 100.17 | 112.73 |
| 6 | B | 1504 | 61I | C25-C24-C18 | 3.82 | 127.62 | 120.61 |
| 6 | B | 1504 | 61I | C9-C10-C6 | -3.37 | 100.33 | 103.64 |
| 6 | B | 1504 | 61I | O22-C23-C29 | -3.13 | 112.11 | 116.26 |

There are no chirality outliers.

All (4) torsion outliers are listed below:

| Mol | Chain | Res | Type | Atoms |
|-----|-------|-----|------|-------|
| 6 | B | 1504 | 61I | N3-C5-C6-C10 |
| 6 | B | 1504 | 61I | C19-C18-N17-C16 |
| 6 | B | 1504 | 61I | C24-C18-N17-C16 |
| 6 | B | 1504 | 61I | N3-C5-C6-C7 |

There are no ring outliers.

1 monomer is involved in 2 short contacts:

| Mol | Chain | Res | Type | Clashes | Symm-Clashes |
|-----|-------|-----|------|---------|--------------|
| 5 | B | 1503 | ACT | 2 | 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 then 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.



**Ligand 61I B 1504**

Bond lengths

Bond angles

Torsions

Rings
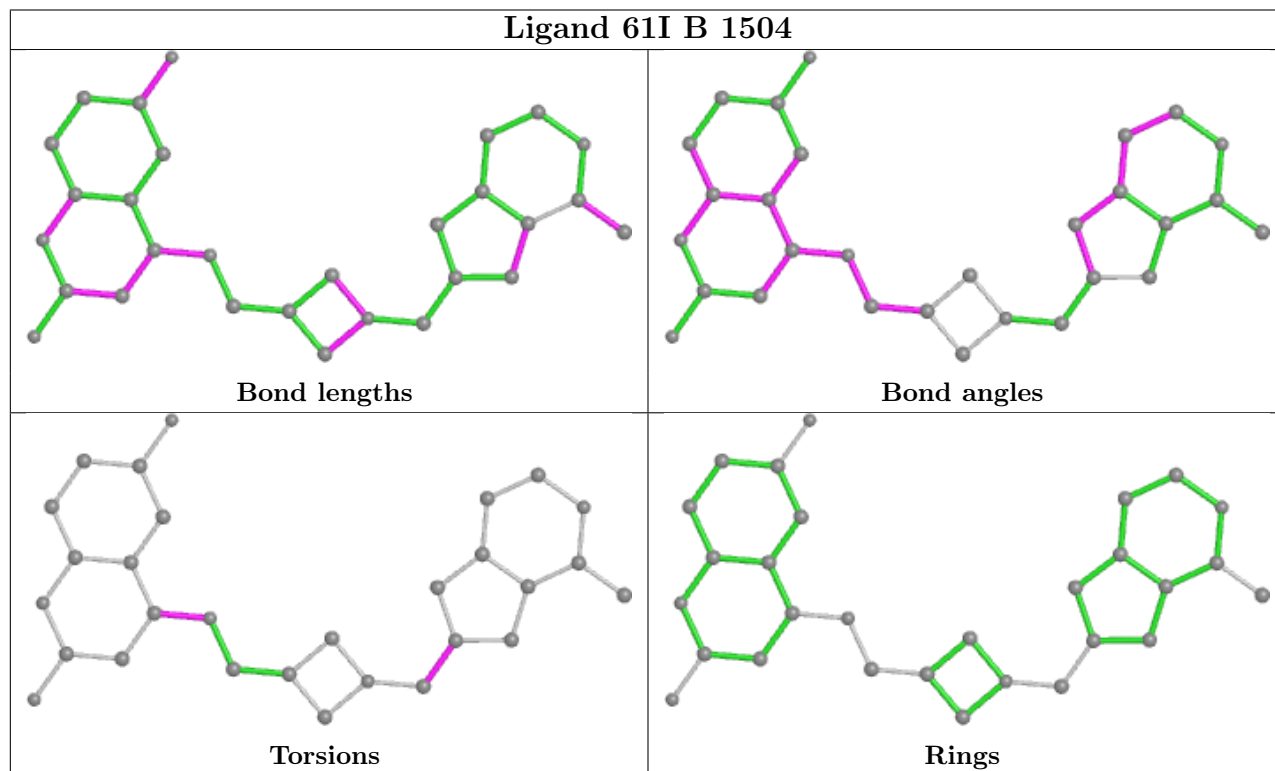
## 5.7 Other polymers ⓘ

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, $95^{th}$ 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 | 670/692 (96%) | 0.24 | 10 (1%) | 73 | 79 | 23, 32, 44, 54 | 0 |
| 1 | B | 671/692 (96%) | 0.24 | 9 (1%) | 77 | 82 | 23, 32, 43, 48 | 0 |
| 2 | C | 20/20 (100%) | -0.25 | 0 | 100 | 100 | 25, 30, 38, 39 | 0 |
| 2 | D | 20/20 (100%) | -0.20 | 0 | 100 | 100 | 24, 30, 40, 50 | 0 |
| All | All | 1381/1424 (96%) | 0.23 | 19 (1%) | 75 | 80 | 23, 32, 44, 54 | 0 |

The worst 5 of 19 RSRZ outliers are listed below:

| Mol | Chain | Res | Type | RSRZ |
| --- | --- | --- | --- | --- |
| 1 | A | 639 | TYR | 4.3 |
| 1 | A | 1490 | LEU | 4.2 |
| 1 | B | 639 | TYR | 3.3 |
| 1 | B | 1490 | LEU | 3.3 |
| 1 | B | 638 | VAL | 2.9 |

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

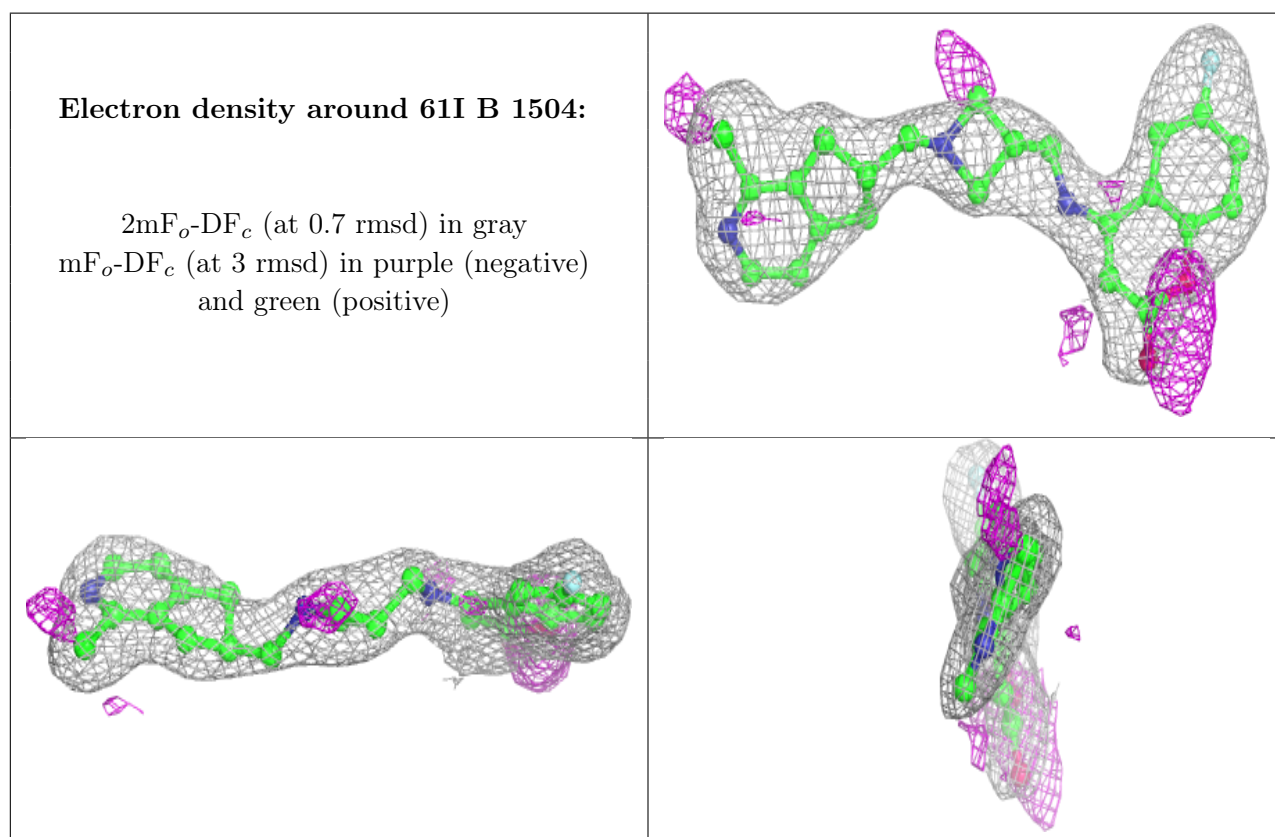There are no non-standard protein/DNA/RNA residues in this entry.

## 6.3 Carbohydrates ⓘ

There are no monosaccharides 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. 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 |
|-----|------|-------|------|-------|------|------|------------------|-------|
| 5 | ACT | B | 1503 | 4/4 | 0.84 | 0.21 | 32,32,34,36 | 0 |
| 6 | 61I | B | 1504 | 29/29 | 0.91 | 0.26 | 30,35,39,47 | 0 |
| 3 | MN | B | 1502 | 1/1 | 0.93 | 0.12 | 46,46,46,46 | 0 |
| 4 | CL | A | 1502 | 1/1 | 0.94 | 0.07 | 43,43,43,43 | 0 |
| 3 | MN | A | 1501 | 1/1 | 0.99 | 0.09 | 31,31,31,31 | 0 |
| 3 | MN | B | 1501 | 1/1 | 1.00 | 0.08 | 32,32,32,32 | 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 61I B 1504:**

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

## 6.5 Other polymers (i)

There are no such residues in this entry.