

wwPDB X-ray Structure Validation Summary Report (i)

Oct 4, 2023 – 12:11 PM EDT

| PDB ID | : | 6OQ5 |
|--------------|---|------------------------------------------------------------------------------|
| Title | : | Structure of the full-length Clostridium difficile toxin B in complex with 3 |
| | | VHHs |
| Authors | : | Chen, P.; Lam, K.; Jin, R. |
| Deposited on | : | 2019-04-25 |
| Resolution | : | 3.87 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.

The following versions of software and data (see references (1)) were used in the production of this report:

| MolProbity | : | 4.02b-467 |
|--------------------------------|---|--------------------------------------------------------------------|
| Xtriage (Phenix) | : | 1.13 |
| EDS | : | 2.35.1 |
| 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 |

1 Overall quality at a glance (i)

The following experimental techniques were used to determine the structure: $X\text{-}RAY \, DIFFRACTION$

The reported resolution of this entry is 3.87 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.



| Motric | Whole archive | Similar resolution |
|-----------------------|---------------------|-------------------------------------------------------------|
| WIEthte | $(\# { m Entries})$ | $(\# { m Entries}, { m resolution} { m range}({ m \AA}))$ |
| R_{free} | 130704 | 1026 (4.12-3.64) |
| Clashscore | 141614 | 1045 (4.10-3.66) |
| Ramachandran outliers | 138981 | 1008 (4.10-3.66) |
| Sidechain outliers | 138945 | 1001 (4.10-3.66) |
| RSRZ outliers | 127900 | 1213 (4.16-3.60) |

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 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 cha | in | | |
|-----|-------|--------|------------------|-----|-----|-----|
| 1 | А | 2373 | % 62% | | 35% | |
| 2 | D | 153 | 53% | 25% | • | 18% |
| 3 | Е | 137 | <u>9%</u> 56% | 21% | • | 22% |
| 4 | F | 142 | 54% | 26% | • | 18% |



6OQ5

2 Entry composition (i)

There are 6 unique types of molecules in this entry. The entry contains 21503 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 Toxin B.

| Mol | Chain | Residues | | At | oms | | | ZeroOcc | AltConf | Trace |
|-----|-------|----------|----------------|------------|-----------|-----------|---------|---------|---------|-------|
| 1 | А | 2346 | Total 18837 | C 12009 | N 2961 | O 3820 | S 47 | 0 | 0 | 0 |

There are 6 discrepancies between the modelled and reference sequences:

| Chain | Residue | Modelled | Actual | Comment | Reference |
|-------|---------|----------|--------|----------------|------------|
| А | 2368 | HIS | - | expression tag | UNP M4NKV9 |
| А | 2369 | HIS | - | expression tag | UNP M4NKV9 |
| А | 2370 | HIS | - | expression tag | UNP M4NKV9 |
| А | 2371 | HIS | - | expression tag | UNP M4NKV9 |
| А | 2372 | HIS | - | expression tag | UNP M4NKV9 |
| А | 2373 | HIS | - | expression tag | UNP M4NKV9 |

• Molecule 2 is a protein called 5D.

| Mol | Chain | Residues | | At | oms | | | ZeroOcc | AltConf | Trace |
|-----|-------|----------|--------------|----------|----------|----------|-----------------|---------|---------|-------|
| 2 | D | 126 | Total 986 | C 617 | N 179 | 0 187 | ${ m S} { m 3}$ | 0 | 0 | 0 |

• Molecule 3 is a protein called E3.

| Mol | Chain | Residues | | At | oms | | | ZeroOcc | AltConf | Trace |
|-----|-------|----------|--------------|----------|----------|----------|---------------|---------|---------|-------|
| 3 | Е | 107 | Total 802 | C 498 | N 141 | 0 159 | ${S \atop 4}$ | 0 | 0 | 0 |

• Molecule 4 is a protein called 7F.

| Mol | Chain | Residues | | At | oms | | | ZeroOcc | AltConf | Trace |
|-----|-------|----------|--------------|----------|----------|----------|--------|---------|---------|-------|
| 4 | F | 116 | Total 876 | C 544 | N 154 | 0 172 | S 6 | 0 | 0 | 0 |

• Molecule 5 is ZINC ION (three-letter code: ZN) (formula: Zn) (labeled as "Ligand of Inter-



est" by depositor).

| Mol | Chain | Residues | Atoms | ZeroOcc | AltConf |
|-----|-------|----------|-----------------|---------|---------|
| 5 | А | 1 | Total Zn 1 1 | 0 | 0 |

• Molecule 6 is MAGNESIUM ION (three-letter code: MG) (formula: Mg).

| Mol | Chain | Residues | Atoms | ZeroOcc | AltConf |
|-----|-------|----------|-----------------|---------|---------|
| 6 | А | 1 | Total Mg 1 1 | 0 | 0 |



3 Residue-property plots (i)

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: Toxin B



| LIOSE BIO27 BIO27 FIO31 TILE TILE TILE ALA TILE ALA ALA ALA ALA ALA ALA ALA ALA TIO55 EIO66 EIO65 EIO65 EIO65 EIO65 EIO65 EIO65 EIO65 EIO65 EIO65 EIO65 EIO65 EIO65 TIO55 TIO55 TIO55 TIO55 TIO55 TIO55 TIO55 TIO55 TIO55 TIO55 TIO55 TIO55 TIO55 TIO55 TIO55 TIO55 TIO55 TIO55 TIO55 TIO55 TIO55 TIO55 TIO55 TIO55 TIO55 TIO55 TIO55 TIO55 TIO55 TIO55 TIO55 TIO55 TIO55 TIO55 TIO55 TIO55 TIO55 TIO55 TIO55 TIO55 TIO55 TIO55 TIO55 TIO55 TIO55 TIO55 TIO55 TIO55 TIO55 TIO55 TIO55 TIO55 TIO55 TIO55 TIO55 TIO55 TIO55 TIO55 TIO55 TIO55 TIO55 TIO55 TIO55 TIO55 TIO55 TIO55 TIO55 TIO55 TIO55 TIO55 TIO55 TIO55 TIO55 TIO55 TIO55 TIO55 TIO55 TIO55 TIO55 TIO55 TIO55 TIO55 TIO55 TIO55 TIO55 TIO55 TIO55 TIO55 TIO55 TIO55 TIO55 TIO55 TIO55 TIO55 TIO55 TIO55 TIO55 TIO55 TIO55 TIO55 TIO55 TIO55 TIO55 TIO55 TIO55 TIO55 TIO55 TIO55 TIO55 TIO55 TIO55 TIO55 TIO55 TIO55 TIO55 TIO55 TIO55 TIO55 TIO55 TIO55 TIO55 TIO55 TIO55 TIO55 TIO55 TIO55 TIO55 TIO55 TIO55 TIO55 TIO55 TIO55 TIO55 TIO55 TIO55 TIO55 TIO55 TIO55 TIO55 TIO55 TIO55 TIO55 TIO55 TIO55 TIO55 TIO55 TIO55 TIO55 TIO55 TIO55 TIO55 TIO55 TIO55 TIO55 TIO55 TIO55 TIO55 TIO55 TIO55 TIO55 TIO55 TIO55 TIO55 TIO55 TIO55 TIO55 TIO55 TIO55 TIO55 TIO55 TIO55 TIO55 TIO55 TIO55 TIO55 TIO55 TIO55 TIO55 TIO55 TIO55 TIO55 TIO55 TIO55 TIO55 TIO55 TIO55 TIO55 TIO55 TIO55 TIO55 TIO55 TIO55 TIO55 TIO55 TIO55 TIO55 TIO55 TIO55 TIO55 TIO55 TIO55 TIO55 TIO55 TIO55 TIO55 TIO55 TIO55 TIO55 TIO55 TIO55 TIO55 TIO55 TIO55 TIO55 TIO55 TIO55 TIO55 TIO55 TIO55 TIO55 TIO55 TIO55 TIO55 TIO55 TIO55 TIO55 TIO55 TIO55 TIO55 TIO55 TIO55 TIO55 TIO55 TIO55 TIO55 TIO55 TIO55 TIO55 TIO55 TIO55 TIO55 TIO55 TIO55 TIO55 TIO55 TIO55 TIO55 TIO55 TIO55 TIO55 TIO55 TIO55 TIO55 TIO55 TIO55 TIO55 TIO55 TIO55 TIO55 TIO55 TIO55 TIO55 TIO55 TIO55 TIO55 TIO55 TIO55 TIO55 TIO55 TIO55 TIO55 TIO55 TIO55 TIO55 TIO55 TIO55 TIO55 TIO55 TIO55 TIO55 TIO55 TIO55 TIO55 TIO55 TIO55 TIO55 TIO55 TIO55 TIO55 TIO55 TIO55 TIO55 TIO55 TIO55 TIO55 TIO55 TIO55 TIO55 TIO55 TIO55 TIO55 TIO55 TIO55 TIO55 TIO55 TIO55 TIO55 TIO55 TIO55 TIO55 TIO55 TIO55 TIO55 TIO5 | 11080 [1084 [1084 [1092] [1092] [1092] [1109 [1100] [1104 [1107] [1104] [1104] [1104] [1104] [1104] [1104] [1106] [1106] [1106] [1106] [1106] [1106] [1106] [1106] [1106] [1106] [1106] [1106] [1106] [1106] [1106] [1106] [1106] [1106] [1106] [1106] [1106] [1106] [1106] [1106] [1106] [1106] [1106] [1106] [1106] [1106] [1106] [1106] [1106] [1106] [1106] [1106] [1106] [1106] [1106] [1106] [1106] [1106] [1106] [1106] [1106] [1106] [1106] [1106] [1106] [1106] [1106] [1106] [1106] [1106] [1106] [1106] [1106] [1106] [1106] [1106] [1106] [1106] [1106] [1106] [1106] [1106] [1106] [1106] [1106] [1106] [1106] [1106] [1106] [1106] [1106] [1106] [1106] [1106] [1106] [1106] [1106] [1106] [1106] [1106] [1106] [1106] [1106] [1106] [1106] [1106] [1106] [1106] [1106] [1106] [1106] [1106] [1106] [1106] [1106] [1106] [1106] [1106] [1106] [1106] [1106] [1106] [1106] [1106] [1106] [1106] [1106] [1106] [1106] [1106] [1106] [1106] [1106] [1106] [1106] [1106] [1106] [1106] [1106] [1106] [1106] [1106] [1106] [1106] [1106] [1106] [1106] [1106] [1106] [1106] [1106] [1106] [1106] [1106] [1106] [1106] [1106] [1106] [1106] [1106] [1106] [1106] [1106] [1106] [1106] [1106] [1106] [1106] [1106] [1106] [1106] [1106] [1106] [1106] [1106] [1106] [1106] [1106] [1106] [1106] [1106] [1106] [1106] [1106] [1106] [1106] [1106] [1106] [1106] [1106] [1106] [1106] [1106] [1106] [1106] [1106] [1106] [1106] [1106] [1106] [1106] [1106] [1106] [1106] [1106] [1106] [1106] [1106] [1106] [1106] [1106] [1106] [1106] [1106] [1106] [1106] [1106] [1106] [1106] [1106] [1106] [1106] [1106] [1106] [1106] [1106] [1106] [1106] [1106] [1106] [1106] [1106] [1106] [1106] [1106] [1106] [1106] [1106] [1106] [1106] [1106] [1106] [1106] [1106] [1106] [1106] [1106] [1106] [1106] [1106] [1106] [1106] [1106] [1106] [1106] [1106] [1106] [1106] [1106] [1106] [1106] [1106] [1106] [1106] [1106] [1106] [1106] [1106] [1106] [1106] [1106] [1106] [1106] [1106] [1106] [1106] [1106] [1106] [1106] [1106] [1106] [1106] [1106] [1106] [1106] [1106] [1106] [1106] [1106] [1106] [1106] [1106] [1106] |
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| CI530 Y1531 Y1532 Y1533 Y1533 L1533 L1533 L1545 L1546 L1546 L1546 L1546 L1548 L1549 L1549 </td <td>F1639 E1643 E1643 F1646 T1647 T1647 T1647 T1648 M1650 M1652 M1655 M1655 M1655</td> | F1639 E1643 E1643 F1646 T1647 T1647 T1647 T1648 M1650 M1652 M1655 M1655 M1655 |
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| Y2010 Y2010 72018 L11 72019 L11 72020 D10 72020 N0022 72020 L11 72020 L11 72020 L11 72020 L11 72020 L2021 12022 L11 12023 L11 12035 L11 12036 L11 12036 L11 12047 L2047 12053 L11 12036 L11 12047 L11 12056 L11 12056 L11 12056 L11 <td< td=""><td>G2101 V1985 L2102 N1996 L2103 N1996 L2104 L1993 L2105 N1996 L2106 N1994 L2106 N1995 L2106 N1994 L2106 N1994 L2106 N1994 D2107 N1996 V2110 Y1998 V2111 Y1998 V2113 Y2000 D2145 D2146 D2146 N2005</td></td<> | G2101 V1985 L2102 N1996 L2103 N1996 L2104 L1993 L2105 N1996 L2106 N1994 L2106 N1995 L2106 N1994 L2106 N1994 L2106 N1994 D2107 N1996 V2110 Y1998 V2111 Y1998 V2113 Y2000 D2145 D2146 D2146 N2005 |
| 12117 72010 M2118 72016 M2120 72018 02113 72018 72121 72019 72121 72020 72121 72020 72121 72020 72131 72020 72131 72020 72131 72020 72131 72020 72131 72020 72131 72020 72131 72024 72131 72024 72131 72024 72131 72024 72131 72024 72132 72024 72131 72024 72132 72024 72133 72034 72145 72034 72145 72034 72145 72034 72146 72034 72147 72034 72148 72034 72149 72034 72141 72034 72145 72034 72146 72034 72147 72034 72148 72034 72149 72034 72149 72034 72149 72034 72149 | Q2211 Q2101 V1986 W2212 L2102 N1966 W2213 L2103 N1966 Y2214 L2103 11993 W2215 N2106 11993 W2216 N2106 11993 W2216 N2106 11993 W2216 N2106 11993 W2216 N2106 11994 W2106 N2106 11994 W2221 N2106 N1996 S2220 Q2108 N1996 S2220 V2111 Y1998 Y2224 Y2110 Y1998 Y2224 Y2111 Y1998 Y2226 D2113 Y2006 Y2226 D2113 Y2006 P2276 D2116 M2006 P2277 C2116 M2006 |
| E2228 12117 Y2010 T2239 Q2113 Y2019 K2231 Q2130 Y2019 K2231 Q2130 Y2009 A2232 Q2131 Y2009 A2233 Q2130 Y2009 A2234 T2122 R0021 A2235 T2122 F2020 C2235 T2122 F2023 T2236 V2133 F2023 N2224 V2133 P2024 N2224 V2133 P2025 T2234 T2138 P2032 N2246 T2138 P2035 T2245 T2138 P2036 P2246 T2138 P2036 P2246 T2138 P2036 P2245 T2138 P2036 P2246 T2145 P2036 <td< td=""><td>C2211 C2101 V1365 F2303 V2222 L2102 M1366 Y2305 Y2213 S2104 11963 Y2305 Y2214 L2104 11963 Y2306 Y2214 L2104 11963 Y2305 D2215 S2104 11993 Y2305 D2216 N2106 11993 Y2305 D2216 N2106 11993 M2310 E2219 C2108 N1996 Y2311 S2220 Y2111 Y1996 Y2315 K2223 Y2111 Y1996 Y2315 Y224 Y2111 Y1996 Y2315 Y2223 Y2111 Y1996 Y2316 Y2224 Y2111 Y1996 Y2315 Y2224 Y2111 Y1996 Y2316 Y2223 Y2111 Y1996 Y2317 Y2224 Y2111 Y1996 Y2321 Y2224 Y2114 Y2006 Y2321 Y2226 Y21</td></td<> | C2211 C2101 V1365 F2303 V2222 L2102 M1366 Y2305 Y2213 S2104 11963 Y2305 Y2214 L2104 11963 Y2306 Y2214 L2104 11963 Y2305 D2215 S2104 11993 Y2305 D2216 N2106 11993 Y2305 D2216 N2106 11993 M2310 E2219 C2108 N1996 Y2311 S2220 Y2111 Y1996 Y2315 K2223 Y2111 Y1996 Y2315 Y224 Y2111 Y1996 Y2315 Y2223 Y2111 Y1996 Y2316 Y2224 Y2111 Y1996 Y2315 Y2224 Y2111 Y1996 Y2316 Y2223 Y2111 Y1996 Y2317 Y2224 Y2111 Y1996 Y2321 Y2224 Y2114 Y2006 Y2321 Y2226 Y21 |







4 Data and refinement statistics (i)

| Property | Value | Source |
|---------------------------------------------|-------------------------------------------------|-----------|
| Space group | P 21 21 21 | Depositor |
| Cell constants | 149.62Å 168.56Å 179.92Å | Depositor |
| a, b, c, α , β , γ | 90.00° 90.00° 90.00° | Depositor |
| Bosolution(A) | 48.91 - 3.87 | Depositor |
| Resolution (A) | 48.87 - 3.87 | EDS |
| % Data completeness | 99.2 (48.91-3.87) | Depositor |
| (in resolution range) | 99.3 (48.87-3.87) | EDS |
| R_{merge} | 0.14 | Depositor |
| R_{sym} | (Not available) | Depositor |
| $< I/\sigma(I) > 1$ | $1.37 (at 3.88 \text{\AA})$ | Xtriage |
| Refinement program | REFMAC 5.8.0232 | Depositor |
| D D | 0.263 , 0.315 | Depositor |
| n, n_{free} | 0.263 , 0.315 | DCC |
| R_{free} test set | 2203 reflections $(5.13%)$ | wwPDB-VP |
| Wilson B-factor $(Å^2)$ | 135.9 | Xtriage |
| Anisotropy | 0.169 | Xtriage |
| Bulk solvent $k_{sol}(e/Å^3), B_{sol}(Å^2)$ | 0.24 , 78.4 | EDS |
| L-test for $twinning^2$ | $ < L >=0.44, < L^2>=0.26$ | Xtriage |
| Estimated twinning fraction | No twinning to report. | Xtriage |
| F_o, F_c correlation | 0.93 | EDS |
| Total number of atoms | 21503 | wwPDB-VP |
| Average B, all atoms $(Å^2)$ | 169.0 | wwPDB-VP |

Xtriage's analysis on translational NCS is as follows: The largest off-origin peak in the Patterson function is 1.86% of the height of the origin peak. No significant pseudotranslation is detected.

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.



¹Intensities estimated from amplitudes.

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: MG, ZN

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).

| Mal | Chain | Bond | lengths | Bond angles | | |
|-----|-------|----------|---------|-------------|---------|--|
| | RMSZ | # Z > 5 | RMSZ | # Z > 5 | | |
| 1 | А | 0.26 | 0/19208 | 0.64 | 0/26012 | |
| 2 | D | 0.29 | 0/1006 | 0.65 | 0/1360 | |
| 3 | Е | 0.29 | 0/814 | 0.61 | 0/1098 | |
| 4 | F | 0.32 | 0/893 | 0.65 | 0/1206 | |
| All | All | 0.27 | 0/21921 | 0.64 | 0/29676 | |

There are no bond length outliers.

There are no bond angle outliers.

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 | А | 18837 | 0 | 18156 | 803 | 0 |
| 2 | D | 986 | 0 | 959 | 87 | 0 |
| 3 | Е | 802 | 0 | 797 | 30 | 0 |
| 4 | F | 876 | 0 | 856 | 40 | 0 |
| 5 | А | 1 | 0 | 0 | 0 | 0 |
| 6 | А | 1 | 0 | 0 | 0 | 0 |
| All | All | 21503 | 0 | 20768 | 944 | 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 22.



| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) | |
|------------------|-------------------|-----------------------------|----------------------|--|
| 1:A:2107:ASP:CB | 1:A:2137:ILE:HG22 | 1.73 | 1.19 | |
| 1:A:1847:LYS:HG3 | 1:A:1848:PRO:HD2 | 1.27 | 1.16 | |
| 1:A:2025:GLU:O | 1:A:2026:MET:HG2 | 1.44 | 1.14 | |
| 1:A:120:ASP:HB3 | 1:A:357:LYS:HD2 | 1.18 | 1.14 | |
| 1:A:625:THR:HB | 1:A:628:GLU:HG2 | 1.25 | 1.14 | |

The worst 5 of 944 close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

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 | Perce | ntiles |
|-----|-------|-----------------|------------|-----------|----------|-------|--------|
| 1 | А | 2340/2373~(99%) | 2001 (86%) | 319 (14%) | 20 (1%) | 17 | 54 |
| 2 | D | 124/153~(81%) | 112 (90%) | 12 (10%) | 0 | 100 | 100 |
| 3 | Ε | 105/137~(77%) | 94 (90%) | 11 (10%) | 0 | 100 | 100 |
| 4 | F | 114/142~(80%) | 98~(86%) | 16 (14%) | 0 | 100 | 100 |
| All | All | 2683/2805~(96%) | 2305~(86%) | 358 (13%) | 20 (1%) | 22 | 60 |

5 of 20 Ramachandran outliers are listed below:

| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1 | А | 164 | PRO |
| 1 | А | 306 | SER |
| 1 | А | 307 | VAL |
| 1 | А | 574 | SER |
| 1 | А | 576 | ARG |



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 side chain conformation was analysed, and the total number of residues.

| Mol | Chain | Analysed | Rotameric | Outliers | Percen | tiles |
|-----|-------|-----------------|------------|----------|--------|-------|
| 1 | А | 2113/2142~(99%) | 2030~(96%) | 83 (4%) | 32 | 59 |
| 2 | D | 102/127~(80%) | 93 (91%) | 9 (9%) | 10 | 37 |
| 3 | Ε | 89/117~(76%) | 86~(97%) | 3(3%) | 37 | 62 |
| 4 | F | 95/119 (80%) | 92~(97%) | 3(3%) | 39 | 63 |
| All | All | 2399/2505~(96%) | 2301 (96%) | 98 (4%) | 30 | 58 |

5 of 98 residues with a non-rotameric sidechain are listed below:

| Mol | Chain | \mathbf{Res} | Type |
|-----|-------|----------------|------|
| 1 | А | 1940 | GLU |
| 1 | А | 2112 | PHE |
| 1 | А | 1973 | ILE |
| 1 | А | 2100 | ILE |
| 1 | А | 2192 | LEU |

Sometimes side chains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 43 such side chains are listed below:

| Mol | Chain | Res | Type |
|-----|-------|------|------|
| 1 | А | 1727 | ASN |
| 1 | А | 1935 | ASN |
| 1 | А | 1735 | ASN |
| 1 | А | 1851 | ASN |
| 1 | А | 1987 | 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 monosaccharides in this entry.

5.6 Ligand geometry (i)

Of 2 ligands modelled in this entry, 2 are monoatomic - leaving 0 for Mogul analysis.

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

No monomer is involved in short contacts.

5.7 Other polymers (i)

There are no such residues in this entry.

5.8 Polymer linkage issues (i)

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, 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 | $\langle RSRZ \rangle$ | #RSRZ>2 | $OWAB(Å^2)$ | Q<0.9 |
|-----|-------|-----------------|------------------------|---------------|--------------------|-------|
| 1 | А | 2346/2373~(98%) | -0.33 | 16 (0%) 87 82 | 80, 160, 233, 324 | 0 |
| 2 | D | 126/153~(82%) | -0.19 | 2 (1%) 72 63 | 147, 200, 255, 290 | 0 |
| 3 | Ε | 107/137~(78%) | 0.62 | 12 (11%) 5 5 | 213, 260, 307, 341 | 0 |
| 4 | F | 116/142~(81%) | -0.42 | 0 100 100 | 117, 166, 214, 240 | 0 |
| All | All | 2695/2805~(96%) | -0.29 | 30 (1%) 80 73 | 80, 165, 249, 341 | 0 |

The worst 5 of 30 RSRZ outliers are listed below:

| Mol | Chain | Res | Type | RSRZ |
|-----|-------|----------------------|------|------|
| 3 | Е | 108 | THR | 4.1 |
| 1 | А | 1810 | ILE | 3.7 |
| 3 | Е | 107 | VAL | 3.6 |
| 1 | А | 317 | GLN | 3.5 |
| 3 | Е | 93 | TYR | 3.4 |

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 monosaccharides 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, 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 |
|-----|------|-------|------|-------|------|------|------------------|-------|
| 6 | MG | А | 2802 | 1/1 | 0.80 | 0.47 | 119,119,119,119 | 0 |
| 5 | ZN | А | 2801 | 1/1 | 0.98 | 0.20 | 120,120,120,120 | 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.

