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

Nov 15, 2023 – 01:35 PM JST

| | | |
|---|---|---|
| PDB ID | : | 6J6U |
| Title | : | Rat PTPRZ D1-D2 domain |
| Authors | : | Sugawara, H. |
| Deposited on | : | 2019-01-15 |
| Resolution | : | 3.32 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 (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 (i)) were used in the production of this report:

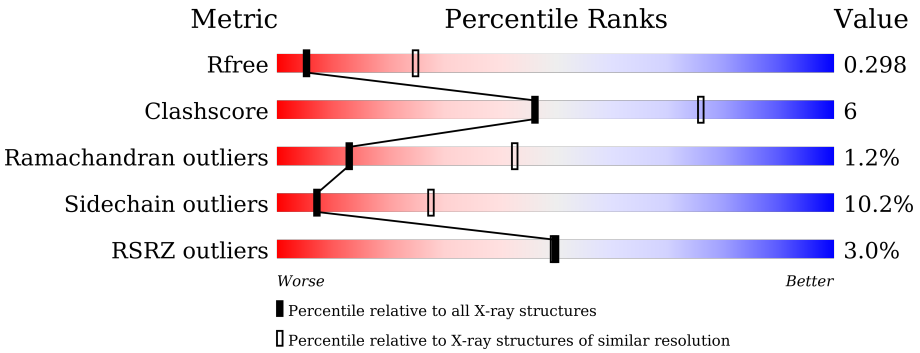
| | | |
|---|---|---|
| MolProbity | : | 4.02b-467 |
| Xtriage (Phenix) | : | 1.13 |
| EDS | : | 2.36 |
| Percentile statistics | : | 20191225.v01 (using entries in the PDB archive December 25th 2019) |
| Refmac | : | 5.8.0158 |
| CCP4 | : | 7.0.044 (Gargrove) |
| Ideal geometry (proteins) | : | Engh & Huber (2001) |
| Ideal geometry (DNA, RNA) | : | Parkinson et al. (1996) |
| Validation Pipeline (wwPDB-VP) | : | 2.36 |

# 1 Overall quality at a glance (i)

The following experimental techniques were used to determine the structure:
*X-RAY DIFFRACTION*

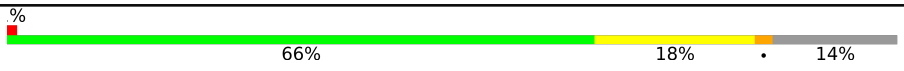
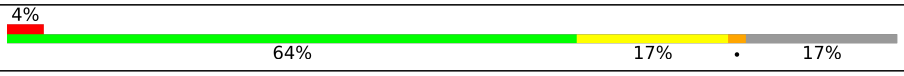
The reported resolution of this entry is 3.32 Å.

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 | 1089 (3.36-3.28) |
| Clashscore | 141614 | 1137 (3.36-3.28) |
| Ramachandran outliers | 138981 | 1115 (3.36-3.28) |
| Sidechain outliers | 138945 | 1114 (3.36-3.28) |
| RSRZ outliers | 127900 | 1059 (3.36-3.28) |

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 | 618 |   |
| 1 | B | 618 |   |

## 2 Entry composition (i)

There is only 1 type of molecule in this entry. The entry contains 8547 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.

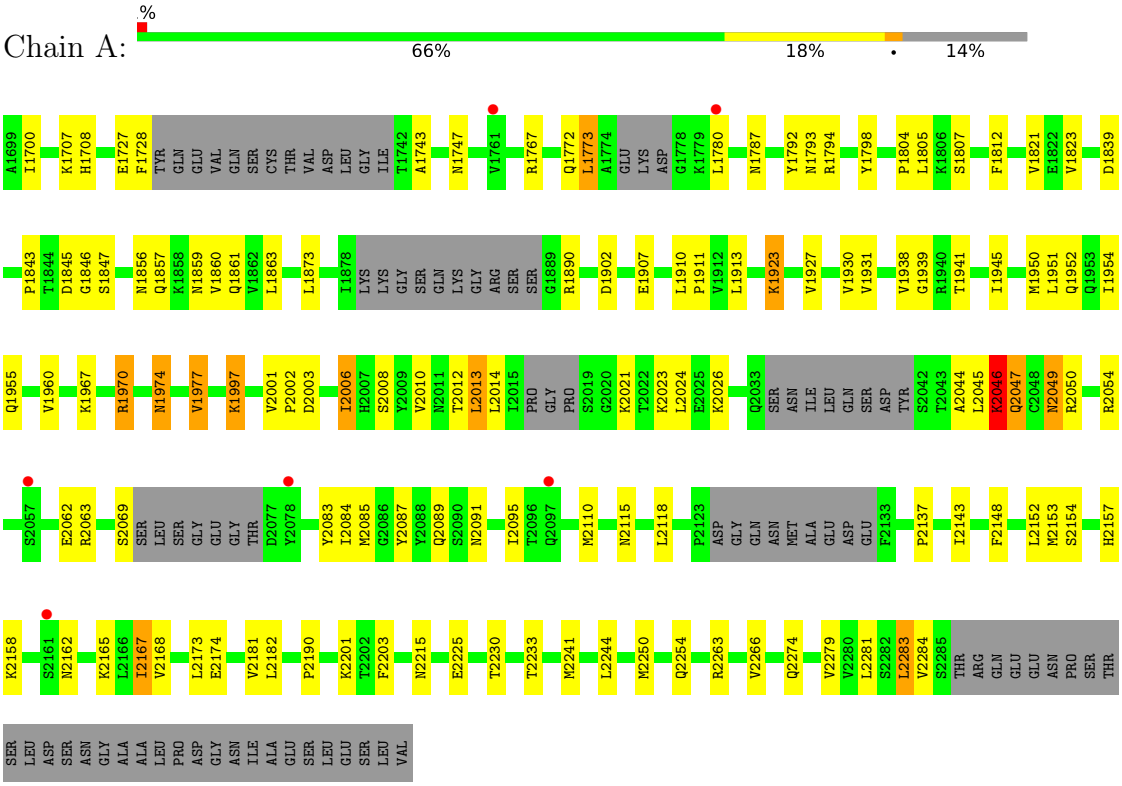
- Molecule 1 is a protein called Receptor-type tyrosine-protein phosphatase zeta.

| Mol | Chain | Residues | Atoms | | | | | ZeroOcc | AltConf | Trace |
|---|---|---|---|---|---|---|---|---|---|---|
| 1 | A | 534 | Total | C | N | O | S | 0 | 0 | 0 |
| | | | 4346 | 2777 | 744 | 805 | 20 | | | |
| 1 | B | 514 | Total | C | N | O | S | 0 | 0 | 0 |
| | | | 4201 | 2682 | 719 | 780 | 20 | | | |

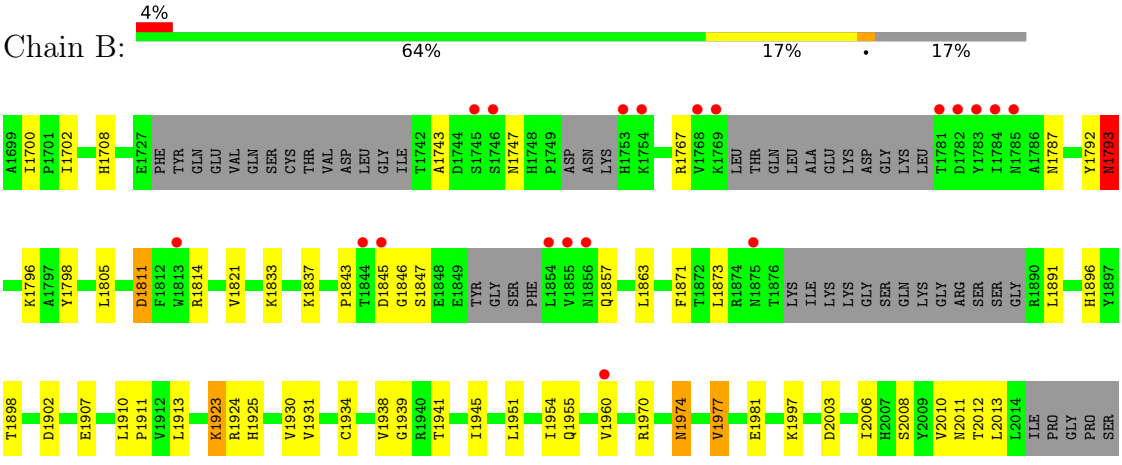
# 3 Residue-property plots (i)

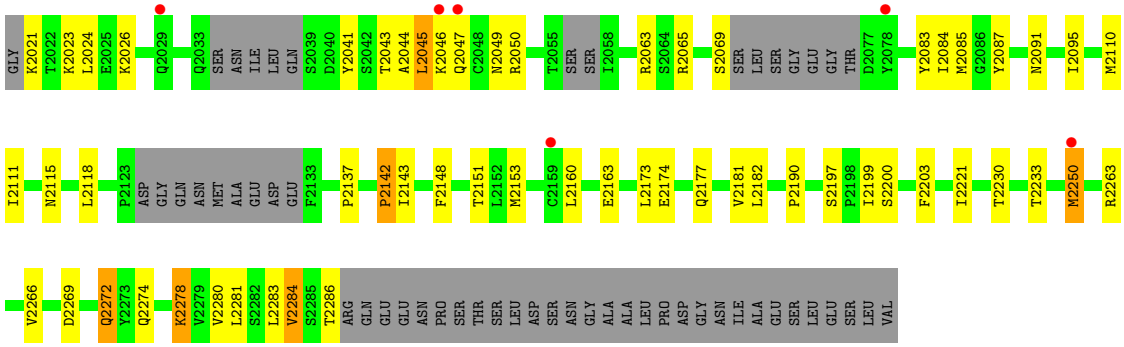
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. 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: Receptor-type tyrosine-protein phosphatase zeta




• Molecule 1: Receptor-type tyrosine-protein phosphatase zeta




GLY K2021 T2022 K2023 L2024 E2025 K2026 Q2029 Q2033 SER ASN ILE LEU GLN S2039 D2040 Y2041 S2042 T2043 A2044 L2045 K2046 Q2047 C2048 N2049 R2050 T2055 SER SER I2058 R2063 S2064 R2065 S2069 SER LEU SER GLY GLU GLY THR D2077 Y2078 Y2083 I2084 M2085 G2086 Y2087 N2091 I2095 M2110
I2111 N2115 L2118 P2123 ASP GLY GLN ASN MET ALA GLU ASP GLU F2133 P2137 P2142 I2143 F2148 T2151 L2152 M2153 C2159 L2160 E2163 L2173 E2174 Q2177 V2181 L2182 P2190 S2197 P2198 I2199 S2200 F2203 I2221 T2230 T2233 M2250 R2263
V2266 D2269 Q2272 Y2273 Q2274 K2278 V2279 V2280 L2281 S2282 L2283 V2284 S2285 T2286 ARG GLN GLU GLU ASN PRO SER THR SER LEU ASP SER ASN GLY ALA ALA LEU PRO ASP GLY ASN ILE ALA GLU SER LEU GLU SER LEU VAL

# 4 Data and refinement statistics (i)

| Property | Value | Source |
|---|---|---|
| Space group | P 21 21 2 | Depositor |
| Cell constants<br>a, b, c, $\alpha$, $\beta$, $\gamma$ | 127.72Å 147.59Å 65.68Å<br>90.00° 90.00° 90.00° | Depositor |
| Resolution (Å) | 38.97 – 3.32<br>38.97 – 3.33 | Depositor<br>EDS |
| % Data completeness<br>(in resolution range) | 83.3 (38.97-3.32)<br>83.4 (38.97-3.33) | Depositor<br>EDS |
| $R_{merge}$ | (Not available) | Depositor |
| $R_{sym}$ | (Not available) | Depositor |
| $< I/\sigma(I) >$ [1] | 4.47 (at 3.32Å) | Xtriage |
| Refinement program | REFMAC 5.8.0158 | Depositor |
| R, $R_{free}$ | 0.235 , 0.318<br>0.218 , 0.298 | Depositor<br>DCC |
| $R_{free}$ test set | 859 reflections (5.45%) | wwPDB-VP |
| Wilson B-factor (Å$^2$) | 66.4 | Xtriage |
| Anisotropy | 0.350 | Xtriage |
| Bulk solvent $k_{sol}$(e/Å$^3$), $B_{sol}$(Å$^2$) | 0.28 , 34.8 | EDS |
| L-test for twinning[2] | $< \|L\| > = 0.39$, $< L^2 > = 0.21$ | Xtriage |
| Estimated twinning fraction | No twinning to report. | Xtriage |
| $F_o$,$F_c$ correlation | 0.88 | EDS |
| Total number of atoms | 8547 | wwPDB-VP |
| Average B, all atoms (Å$^2$) | 85.0 | wwPDB-VP |

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.86% 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.

# 5 Model quality

## 5.1 Standard geometry

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 | 0.52 | 0/4447 | 0.76 | 1/6026 (0.0%) |
| 1 | B | 0.51 | 0/4297 | 0.74 | 1/5823 (0.0%) |
| All | All | 0.52 | 0/8744 | 0.75 | 2/11849 (0.0%) |

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 | 1 |

There are no bond length outliers.

All (2) bond angle outliers are listed below:

| Mol | Chain | Res | Type | Atoms | Z | Observed($^o$) | Ideal($^o$) |
|---|---|---|---|---|---|---|---|
| 1 | B | 1811 | ASP | CB-CG-OD1 | 6.67 | 124.31 | 118.30 |
| 1 | A | 1970 | ARG | NE-CZ-NH2 | 5.26 | 122.93 | 120.30 |

There are no chirality outliers.

All (1) planarity outliers are listed below:

| Mol | Chain | Res | Type | Group |
|---|---|---|---|---|
| 1 | B | 2045 | LEU | Peptide |

## 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 | 4346 | 0 | 4274 | 58 | 0 |
| 1 | B | 4201 | 0 | 4113 | 48 | 0 |
| All | All | 8547 | 0 | 8387 | 106 | 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 6.

All (106) 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:2203:PHE:CZ | 1:A:2279:VAL:HG12 | 2.22 | 0.74 |
| 1:B:2006:ILE:HD13 | 1:B:2284:VAL:HG21 | 1.68 | 0.74 |
| 1:B:1821:VAL:HG11 | 1:B:1931:VAL:HG23 | 1.72 | 0.71 |
| 1:B:2269:ASP:H | 1:B:2272:GLN:HE22 | 1.36 | 0.71 |
| 1:A:2002:PRO:O | 1:A:2006:ILE:HD13 | 1.92 | 0.70 |
| 1:B:2269:ASP:O | 1:B:2272:GLN:NE2 | 2.25 | 0.69 |
| 1:A:1821:VAL:HG11 | 1:A:1931:VAL:HG23 | 1.76 | 0.67 |
| 1:B:2013:LEU:HA | 1:B:2023:LYS:HB2 | 1.75 | 0.67 |
| 1:A:1767:ARG:HA | 1:A:1787:ASN:HD22 | 1.61 | 0.66 |
| 1:B:2142:PRO:HG3 | 1:B:2151:THR:HG23 | 1.78 | 0.66 |
| 1:B:2003:ASP:O | 1:B:2006:ILE:HD12 | 1.96 | 0.65 |
| 1:B:1767:ARG:HA | 1:B:1787:ASN:HD22 | 1.62 | 0.65 |
| 1:A:1941:THR:O | 1:A:1945:ILE:HD12 | 1.97 | 0.64 |
| 1:A:2244:LEU:HB2 | 1:A:2250:MET:SD | 2.38 | 0.64 |
| 1:B:1941:THR:O | 1:B:1945:ILE:HD12 | 1.97 | 0.64 |
| 1:A:2003:ASP:HA | 1:A:2006:ILE:HD11 | 1.80 | 0.62 |
| 1:A:2006:ILE:HG13 | 1:A:2284:VAL:HG11 | 1.82 | 0.61 |
| 1:A:2203:PHE:CZ | 1:A:2283:LEU:HD12 | 2.35 | 0.60 |
| 1:B:1934:CYS:HG | 1:B:1941:THR:HG1 | 1.49 | 0.60 |
| 1:A:2044:ALA:HB1 | 1:A:2046:LYS:CG | 2.32 | 0.60 |
| 1:B:2111:ILE:HD13 | 1:B:2221:ILE:HG13 | 1.87 | 0.57 |
| 1:B:2174:GLU:HG2 | 1:B:2181:VAL:HG22 | 1.86 | 0.57 |
| 1:A:1950:MET:O | 1:A:1954:ILE:HD12 | 2.04 | 0.57 |
| 1:A:2013:LEU:HA | 1:A:2023:LYS:HB2 | 1.86 | 0.57 |
| 1:B:1793:ASN:C | 1:B:1793:ASN:HD22 | 2.08 | 0.56 |
| 1:A:1974:ASN:HD22 | 1:A:1974:ASN:N | 2.04 | 0.56 |
| 1:B:2200:SER:O | 1:B:2203:PHE:CZ | 2.58 | 0.56 |
| 1:B:2006:ILE:CD1 | 1:B:2284:VAL:HG21 | 2.35 | 0.56 |
| 1:A:1847:SER:OG | 1:A:1856:ASN:ND2 | 2.39 | 0.55 |
| 1:B:2045:LEU:HA | 1:B:2046:LYS:HB2 | 1.89 | 0.55 |
| 1:B:2200:SER:O | 1:B:2203:PHE:CE2 | 2.60 | 0.55 |
| 1:A:2049:ASN:HD22 | 1:A:2049:ASN:C | 2.10 | 0.54 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 1:A:2006:ILE:HG13 | 1:A:2284:VAL:HG21 | 1.90 | 0.54 |
| 1:B:1923:LYS:HD2 | 1:B:1930:VAL:HG21 | 1.90 | 0.54 |
| 1:A:1923:LYS:HD2 | 1:A:1930:VAL:HG21 | 1.90 | 0.53 |
| 1:A:2157:HIS:HB3 | 1:A:2165:LYS:CE | 2.39 | 0.53 |
| 1:B:2008:SER:O | 1:B:2011:ASN:OD1 | 2.25 | 0.53 |
| 1:A:1859:ASN:OD1 | 1:A:1860:VAL:N | 2.42 | 0.53 |
| 1:A:2162:ASN:HD21 | 1:A:2201:LYS:HD3 | 1.73 | 0.53 |
| 1:B:1974:ASN:HD22 | 1:B:1974:ASN:N | 2.05 | 0.53 |
| 1:B:1843:PRO:HB2 | 1:B:1845:ASP:O | 2.10 | 0.52 |
| 1:A:1863:LEU:HD22 | 1:A:2087:TYR:CE2 | 2.44 | 0.51 |
| 1:B:1970:ARG:NH1 | 1:B:1977:VAL:O | 2.44 | 0.51 |
| 1:B:1863:LEU:HD22 | 1:B:2087:TYR:CE2 | 2.45 | 0.51 |
| 1:A:2045:LEU:HD13 | 1:A:2047:GLN:HE22 | 1.76 | 0.50 |
| 1:A:2083:TYR:O | 1:A:2084:ILE:HD13 | 2.11 | 0.50 |
| 1:B:2083:TYR:O | 1:B:2084:ILE:HD13 | 2.10 | 0.50 |
| 1:A:1970:ARG:NH1 | 1:A:1977:VAL:O | 2.44 | 0.50 |
| 1:A:2203:PHE:CE1 | 1:A:2283:LEU:HD12 | 2.47 | 0.50 |
| 1:A:2174:GLU:HG2 | 1:A:2181:VAL:HG22 | 1.94 | 0.50 |
| 1:B:2024:LEU:HD21 | 1:B:2274:GLN:HB2 | 1.94 | 0.50 |
| 1:B:2199:ILE:HD13 | 1:B:2278:LYS:HD3 | 1.94 | 0.50 |
| 1:A:2008:SER:O | 1:A:2012:THR:HG23 | 2.13 | 0.49 |
| 1:B:2115:ASN:ND2 | 1:B:2182:LEU:HD13 | 2.27 | 0.49 |
| 1:A:1843:PRO:HB2 | 1:A:1845:ASP:O | 2.13 | 0.49 |
| 1:A:2044:ALA:HB1 | 1:A:2046:LYS:HG3 | 1.95 | 0.48 |
| 1:B:2008:SER:O | 1:B:2012:THR:HG23 | 2.13 | 0.48 |
| 1:B:2284:VAL:HG12 | 1:B:2284:VAL:O | 2.13 | 0.48 |
| 1:A:2045:LEU:HD23 | 1:A:2062:GLU:OE2 | 2.14 | 0.48 |
| 1:A:2006:ILE:O | 1:A:2010:VAL:HG23 | 2.14 | 0.48 |
| 1:B:2200:SER:HA | 1:B:2203:PHE:CE1 | 2.50 | 0.47 |
| 1:A:2044:ALA:HB1 | 1:A:2046:LYS:HG2 | 1.96 | 0.47 |
| 1:A:2045:LEU:HD13 | 1:A:2047:GLN:NE2 | 2.29 | 0.47 |
| 1:A:2115:ASN:ND2 | 1:A:2182:LEU:HD13 | 2.29 | 0.47 |
| 1:B:1871:PHE:O | 1:B:1891:LEU:HD12 | 2.15 | 0.47 |
| 1:B:2250:MET:SD | 1:B:2280:VAL:HG13 | 2.55 | 0.47 |
| 1:B:2084:ILE:HG13 | 1:B:2095:ILE:HD12 | 1.97 | 0.46 |
| 1:B:1743:ALA:O | 1:B:1747:ASN:ND2 | 2.44 | 0.46 |
| 1:B:1833:LYS:HG2 | 1:B:1902:ASP:OD1 | 2.15 | 0.46 |
| 1:A:1743:ALA:O | 1:A:1747:ASN:ND2 | 2.43 | 0.46 |
| 1:B:2045:LEU:HA | 1:B:2046:LYS:CB | 2.45 | 0.46 |
| 1:A:2084:ILE:HG13 | 1:A:2095:ILE:HD12 | 1.97 | 0.45 |
| 1:A:2167:ILE:HD13 | 1:A:2167:ILE:N | 2.32 | 0.45 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 1:A:2010:VAL:O | 1:A:2013:LEU:HD22 | 2.16 | 0.45 |
| 1:A:2024:LEU:HD21 | 1:A:2274:GLN:HB2 | 1.98 | 0.44 |
| 1:B:2044:ALA:O | 1:B:2045:LEU:HD23 | 2.18 | 0.44 |
| 1:A:1794:ARG:NH1 | 1:A:1952:GLN:OE1 | 2.51 | 0.44 |
| 1:A:1974:ASN:N | 1:A:1974:ASN:ND2 | 2.66 | 0.43 |
| 1:B:2006:ILE:O | 1:B:2010:VAL:HG23 | 2.18 | 0.43 |
| 1:A:1727:GLU:HA | 1:A:1728:PHE:C | 2.39 | 0.43 |
| 1:A:1823:VAL:HB | 1:A:1930:VAL:HG22 | 2.01 | 0.43 |
| 1:A:2162:ASN:HD21 | 1:A:2201:LYS:CD | 2.32 | 0.43 |
| 1:A:2137:PRO:HD3 | 1:A:2143:ILE:HD12 | 2.01 | 0.43 |
| 1:B:1798:TYR:CE2 | 1:B:1945:ILE:HG23 | 2.54 | 0.43 |
| 1:B:1974:ASN:N | 1:B:1974:ASN:ND2 | 2.66 | 0.43 |
| 1:B:1896:HIS:O | 1:B:1898:THR:HG23 | 2.19 | 0.42 |
| 1:A:1700:ILE:HG13 | 1:A:1708:HIS:CD2 | 2.54 | 0.42 |
| 1:A:2244:LEU:HD23 | 1:A:2283:LEU:HD22 | 2.01 | 0.42 |
| 1:B:1938:VAL:HG23 | 1:B:1939:GLY:H | 1.85 | 0.42 |
| 1:A:1804:PRO:HG3 | 1:A:1812:PHE:CD2 | 2.54 | 0.42 |
| 1:B:2137:PRO:HD3 | 1:B:2143:ILE:HD12 | 2.01 | 0.42 |
| 1:A:2152:LEU:HD11 | 1:A:2154:SER:O | 2.20 | 0.42 |
| 1:A:2241:MET:HG2 | 1:A:2283:LEU:HD11 | 2.01 | 0.42 |
| 1:A:2001:VAL:HG11 | 1:A:2006:ILE:HA | 2.02 | 0.41 |
| 1:A:1773:LEU:HD13 | 1:A:1773:LEU:N | 2.35 | 0.41 |
| 1:B:1910:LEU:N | 1:B:1911:PRO:HD2 | 2.35 | 0.41 |
| 1:B:2263:ARG:O | 1:B:2266:VAL:HG23 | 2.20 | 0.41 |
| 1:A:1798:TYR:CE2 | 1:A:1945:ILE:HG23 | 2.54 | 0.41 |
| 1:A:2158:LYS:HE3 | 1:A:2168:VAL:HG21 | 2.02 | 0.41 |
| 1:A:1910:LEU:HB3 | 1:A:1911:PRO:HD3 | 2.02 | 0.41 |
| 1:B:2148:PHE:CD1 | 1:B:2173:LEU:HD23 | 2.56 | 0.41 |
| 1:B:1702:ILE:HG21 | 1:B:1954:ILE:HG23 | 2.03 | 0.40 |
| 1:A:1938:VAL:HG23 | 1:A:1939:GLY:H | 1.86 | 0.40 |
| 1:A:2148:PHE:CE1 | 1:A:2173:LEU:HD23 | 2.56 | 0.40 |
| 1:A:2263:ARG:O | 1:A:2266:VAL:HG23 | 2.21 | 0.40 |
| 1:B:1700:ILE:HG13 | 1:B:1708:HIS:CD2 | 2.57 | 0.40 |

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 | 518/618 (84%) | 473 (91%) | 39 (8%) | 6 (1%) | 13 | 43 |
| 1 | B | 492/618 (80%) | 455 (92%) | 31 (6%) | 6 (1%) | 13 | 43 |
| All | All | 1010/1236 (82%) | 928 (92%) | 70 (7%) | 12 (1%) | 13 | 43 |

All (12) Ramachandran outliers are listed below:

| Mol | Chain | Res | Type |
|---|---|---|---|
| 1 | A | 1793 | ASN |
| 1 | B | 1793 | ASN |
| 1 | A | 2046 | LYS |
| 1 | B | 1846 | GLY |
| 1 | A | 1846 | GLY |
| 1 | A | 1997 | LYS |
| 1 | B | 1997 | LYS |
| 1 | A | 1977 | VAL |
| 1 | A | 2190 | PRO |
| 1 | B | 1977 | VAL |
| 1 | B | 2190 | PRO |
| 1 | B | 2284 | VAL |

### 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 | 484/555 (87%) | 435 (90%) | 49 (10%) | 7 | 28 |

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| Mol | Chain | Analysed | Rotameric | Outliers | Percentiles |
|---|---|---|---|---|---|
| 1 | B | 469/555 (84%) | 421 (90%) | 48 (10%) | 7 27 |
| All | All | 953/1110 (86%) | 856 (90%) | 97 (10%) | 7 27 |

All (97) residues with a non-rotameric sidechain are listed below:

| Mol | Chain | Res | Type |
|---|---|---|---|
| 1 | A | 1707 | LYS |
| 1 | A | 1772 | GLN |
| 1 | A | 1773 | LEU |
| 1 | A | 1780 | LEU |
| 1 | A | 1792 | TYR |
| 1 | A | 1805 | LEU |
| 1 | A | 1807 | SER |
| 1 | A | 1839 | ASP |
| 1 | A | 1857 | GLN |
| 1 | A | 1861 | GLN |
| 1 | A | 1873 | LEU |
| 1 | A | 1890 | ARG |
| 1 | A | 1902 | ASP |
| 1 | A | 1907 | GLU |
| 1 | A | 1913 | LEU |
| 1 | A | 1923 | LYS |
| 1 | A | 1927 | VAL |
| 1 | A | 1951 | LEU |
| 1 | A | 1955 | GLN |
| 1 | A | 1960 | VAL |
| 1 | A | 1967 | LYS |
| 1 | A | 1974 | ASN |
| 1 | A | 1997 | LYS |
| 1 | A | 2006 | ILE |
| 1 | A | 2013 | LEU |
| 1 | A | 2014 | LEU |
| 1 | A | 2021 | LYS |
| 1 | A | 2026 | LYS |
| 1 | A | 2046 | LYS |
| 1 | A | 2047 | GLN |
| 1 | A | 2049 | ASN |
| 1 | A | 2050 | ARG |
| 1 | A | 2054 | ARG |
| 1 | A | 2063 | ARG |
| 1 | A | 2069 | SER |
| 1 | A | 2085 | MET |

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| Mol | Chain | Res | Type |
|---|---|---|---|
| 1 | A | 2089 | GLN |
| 1 | A | 2091 | ASN |
| 1 | A | 2110 | MET |
| 1 | A | 2118 | LEU |
| 1 | A | 2153 | MET |
| 1 | A | 2167 | ILE |
| 1 | A | 2215 | ASN |
| 1 | A | 2225 | GLU |
| 1 | A | 2230 | THR |
| 1 | A | 2233 | THR |
| 1 | A | 2254 | GLN |
| 1 | A | 2281 | LEU |
| 1 | A | 2283 | LEU |
| 1 | B | 1792 | TYR |
| 1 | B | 1793 | ASN |
| 1 | B | 1796 | LYS |
| 1 | B | 1805 | LEU |
| 1 | B | 1811 | ASP |
| 1 | B | 1814 | ARG |
| 1 | B | 1837 | LYS |
| 1 | B | 1847 | SER |
| 1 | B | 1857 | GLN |
| 1 | B | 1873 | LEU |
| 1 | B | 1907 | GLU |
| 1 | B | 1913 | LEU |
| 1 | B | 1923 | LYS |
| 1 | B | 1924 | ARG |
| 1 | B | 1925 | HIS |
| 1 | B | 1951 | LEU |
| 1 | B | 1955 | GLN |
| 1 | B | 1960 | VAL |
| 1 | B | 1974 | ASN |
| 1 | B | 1981 | GLU |
| 1 | B | 2021 | LYS |
| 1 | B | 2026 | LYS |
| 1 | B | 2041 | TYR |
| 1 | B | 2043 | THR |
| 1 | B | 2047 | GLN |
| 1 | B | 2049 | ASN |
| 1 | B | 2050 | ARG |
| 1 | B | 2063 | ARG |
| 1 | B | 2065 | ARG |

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| Mol | Chain | Res | Type |
|---|---|---|---|
| 1 | B | 2069 | SER |
| 1 | B | 2085 | MET |
| 1 | B | 2091 | ASN |
| 1 | B | 2110 | MET |
| 1 | B | 2118 | LEU |
| 1 | B | 2142 | PRO |
| 1 | B | 2153 | MET |
| 1 | B | 2160 | LEU |
| 1 | B | 2163 | GLU |
| 1 | B | 2177 | GLN |
| 1 | B | 2197 | SER |
| 1 | B | 2230 | THR |
| 1 | B | 2233 | THR |
| 1 | B | 2250 | MET |
| 1 | B | 2272 | GLN |
| 1 | B | 2278 | LYS |
| 1 | B | 2281 | LEU |
| 1 | B | 2283 | LEU |
| 1 | B | 2286 | THR |

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (19) such sidechains are listed below:

| Mol | Chain | Res | Type |
|---|---|---|---|
| 1 | A | 1708 | HIS |
| 1 | A | 1716 | ASN |
| 1 | A | 1856 | ASN |
| 1 | A | 1953 | GLN |
| 1 | A | 1974 | ASN |
| 1 | A | 2047 | GLN |
| 1 | A | 2049 | ASN |
| 1 | A | 2115 | ASN |
| 1 | A | 2169 | GLN |
| 1 | A | 2254 | GLN |
| 1 | B | 1708 | HIS |
| 1 | B | 1716 | ASN |
| 1 | B | 1753 | HIS |
| 1 | B | 1793 | ASN |
| 1 | B | 1953 | GLN |
| 1 | B | 1974 | ASN |
| 1 | B | 2115 | ASN |
| 1 | B | 2169 | GLN |
| 1 | B | 2272 | GLN |

#### 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

There are no ligands in this entry.

## 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 | 534/618 (86%) | -0.12 | 6 (1%) | 80 | 81 | 43, 75, 112, 173 | 5 (0%) |
| 1 | B | 514/618 (83%) | 0.24 | 25 (4%) | 29 | 29 | 50, 87, 131, 179 | 5 (0%) |
| All | All | 1048/1236 (84%) | 0.06 | 31 (2%) | 50 | 49 | 43, 81, 125, 179 | 10 (0%) |

All (31) RSRZ outliers are listed below:

| Mol | Chain | Res | Type | RSRZ |
|---|---|---|---|---|
| 1 | B | 1875 | ASN | 5.3 |
| 1 | B | 1753 | HIS | 5.2 |
| 1 | B | 2250 | MET | 4.4 |
| 1 | B | 1854 | LEU | 4.0 |
| 1 | A | 1761 | VAL | 3.2 |
| 1 | A | 2161 | SER | 3.2 |
| 1 | B | 1754 | LYS | 3.0 |
| 1 | A | 2097 | GLN | 2.9 |
| 1 | B | 1855 | VAL | 2.8 |
| 1 | B | 1768 | VAL | 2.7 |
| 1 | B | 1785 | ASN | 2.7 |
| 1 | B | 1769 | LYS | 2.6 |
| 1 | B | 1844 | THR | 2.6 |
| 1 | B | 1746 | SER | 2.6 |
| 1 | A | 2057 | SER | 2.5 |
| 1 | B | 1845 | ASP | 2.5 |
| 1 | B | 2159 | CYS | 2.5 |
| 1 | B | 1813 | TRP | 2.4 |
| 1 | B | 1960 | VAL | 2.4 |
| 1 | B | 1783 | TYR | 2.3 |
| 1 | B | 1781 | THR | 2.2 |
| 1 | B | 1856 | ASN | 2.2 |
| 1 | B | 2047 | GLN | 2.2 |
| 1 | B | 1784 | ILE | 2.2 |

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| Mol | Chain | Res | Type | RSRZ |
|---|---|---|---|---|
| 1 | B | 2078 | TYR | 2.2 |
| 1 | A | 2078 | TYR | 2.2 |
| 1 | B | 2029 | GLN | 2.1 |
| 1 | B | 2046 | LYS | 2.1 |
| 1 | A | 1780 | LEU | 2.1 |
| 1 | B | 1745 | SER | 2.1 |
| 1 | B | 1782 | ASP | 2.0 |

## 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)

There are no ligands in this entry.

## 6.5 Other polymers (i)

There are no such residues in this entry.