# Full wwPDB X-ray Structure Validation Report ⓘ

May 16, 2020 – 07:23 am BST

| | | |
|---|---|---|
| PDB ID | : | 1M8X |
| Title | : | CRYSTAL STRUCTURE OF THE PUMILIO-HOMOLOGY DOMAIN FROM HUMAN PUMILIO1 IN COMPLEX WITH NRE1-14 RNA |
| Authors | : | Wang, X.; McLachlan, J.; Zamore, P.D.; Hall, T.M.T. |
| Deposited on | : | 2002-07-26 |
| Resolution | : | 2.20 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 following versions of software and data (see references ⓘ) were used in the production of this report:

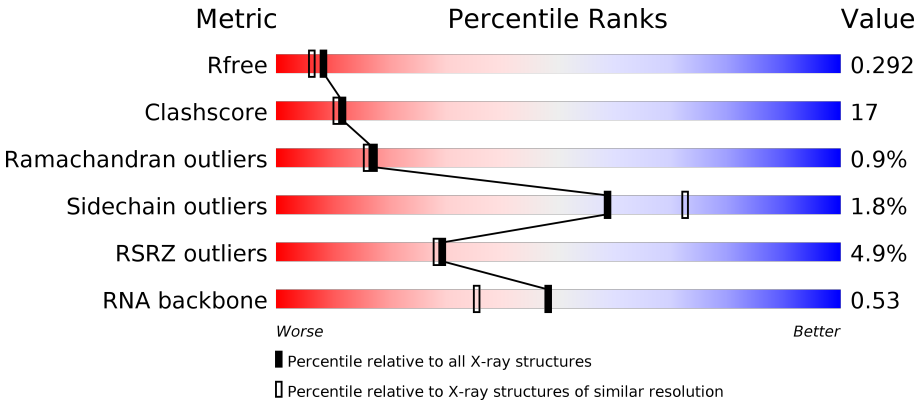
| | | |
|---|---|---|
| MolProbity | : | 4.02b-467 |
| Xtriage (Phenix) | : | 1.13 |
| EDS | : | 2.11 |
| Percentile statistics | : | 20191225.v01 (using entries in the PDB archive December 25th 2019) |
| Refmac | : | 5.8.0158 |
| CCP4 | : | 7.0.044 (Gargrove) |
| Ideal geometry (proteins) | : | Engh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

# 1 Overall quality at a glance

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

The reported resolution of this entry is 2.20 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 | 4898 (2.20-2.20) |
| Clashscore | 141614 | 5594 (2.20-2.20) |
| Ramachandran outliers | 138981 | 5503 (2.20-2.20) |
| Sidechain outliers | 138945 | 5504 (2.20-2.20) |
| RSRZ outliers | 127900 | 4800 (2.20-2.20) |
| RNA backbone | 3102 | 1032 (2.60-1.80) |

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments on the lower bar indicate the fraction of residues that contain outliers for >=3, 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions <=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 | C | 8 | 13% 88% 13% |
| 2 | D | 7 | 29% 57% 14% |
| 3 | A | 349 | 3% 68% 28% •• |
| 3 | B | 349 | 7% 58% 38% •• |

# 2 Entry composition

There are 4 unique types of molecules in this entry. The entry contains 6357 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 RNA chain called 5'-R(P*UP*UP*GP*UP*AP*UP*AP*U)-3'.

| Mol | Chain | Residues | Atoms | | | | | ZeroOcc | AltConf | Trace |
|---|---|---|---|---|---|---|---|---|---|---|
| 1 | C | 8 | Total | C | N | O | P | 0 | 0 | 0 |
| | | | 167 | 75 | 25 | 59 | 8 | | | |

- Molecule 2 is a RNA chain called 5'-R(P*UP*GP*UP*AP*UP*AP*U)-3'.

| Mol | Chain | Residues | Atoms | | | | | ZeroOcc | AltConf | Trace |
|---|---|---|---|---|---|---|---|---|---|---|
| 2 | D | 7 | Total | C | N | O | P | 0 | 0 | 0 |
| | | | 147 | 66 | 23 | 51 | 7 | | | |

- Molecule 3 is a protein called Pumilio 1.

| Mol | Chain | Residues | Atoms | | | | | ZeroOcc | AltConf | Trace |
|---|---|---|---|---|---|---|---|---|---|---|
| 3 | A | 341 | Total | C | N | O | S | 0 | 0 | 0 |
| | | | 2775 | 1758 | 501 | 499 | 17 | | | |
| 3 | B | 341 | Total | C | N | O | S | 0 | 0 | 0 |
| | | | 2775 | 1758 | 501 | 499 | 17 | | | |

- Molecule 4 is water.

| Mol | Chain | Residues | Atoms | | ZeroOcc | AltConf |
|---|---|---|---|---|---|---|
| 4 | C | 16 | Total | O | 0 | 0 |
| | | | 16 | 16 | | |
| 4 | D | 11 | Total | O | 0 | 0 |
| | | | 11 | 11 | | |
| 4 | A | 295 | Total | O | 0 | 0 |
| | | | 295 | 295 | | |
| 4 | B | 171 | Total | O | 0 | 0 |
| | | | 171 | 171 | | |

# 3 Residue-property plots

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

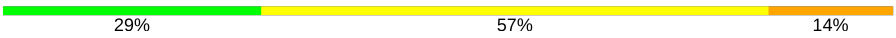
- Molecule 1: 5'-R(P*UP*UP*GP*UP*AP*UP*AP*U)-3'

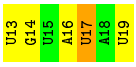
Chain C:



- Molecule 2: 5'-R(P*UP*GP*UP*AP*UP*AP*U)-3'

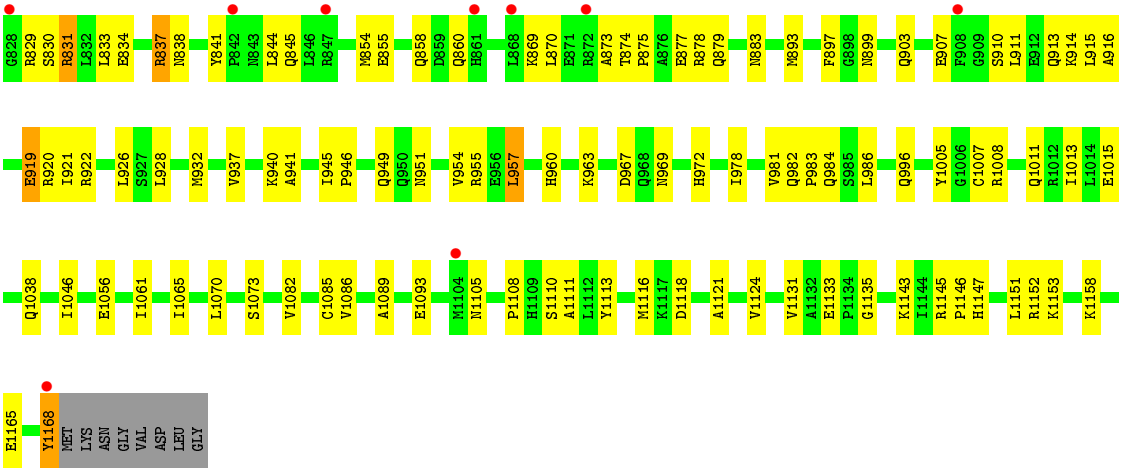
Chain D:



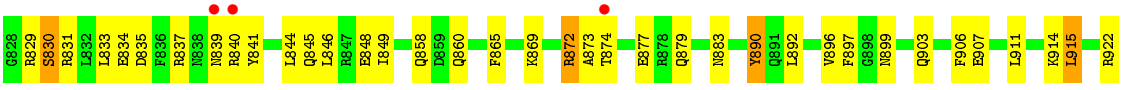

- Molecule 3: Pumilio 1

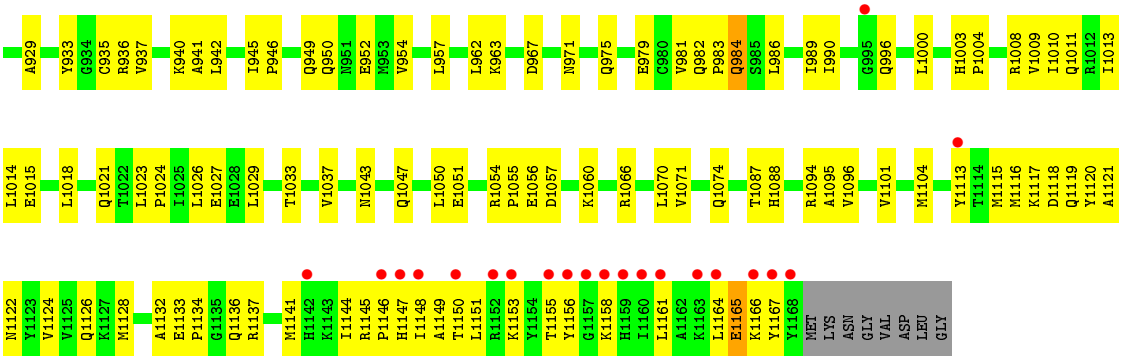
Chain A:


- Molecule 3: Pumilio 1

Chain B:


A929 Y933 G934 C935 R936 V937 K940 A941 L942 I945 P946 Q949 Q950 N951 E952 N953 V954 L957 L962 K963 D967 N971 Q975 E979 C980 V981 Q982 P983 Q984 S985 L986 I989 I990 G995 Q996 L1000 H1003 P1004 R1008 V1009 I1010 Q1011 R1012 I1013
L1014 E1015 L1018 Q1021 T1022 L1023 P1024 I1025 L1026 E1027 E1028 L1029 T1033 V1037 N1043 Q1047 L1050 E1051 R1054 P1055 E1056 D1057 K1060 R1066 L1070 V1071 Q1074 T1087 H1088 R1094 A1095 V1096 V1101 M1104 Y1113 T1114 M1115 M1116 K1117 D1118 Q1119 Y1120 A1121
N1122 Y1123 V1124 V1125 Q1126 K1127 M1128 A1132 E1133 P1134 G1135 Q1136 R1137 M1141 H1142 K1143 I1144 R1145 P1146 H1147 I1148 A1149 T1150 L1151 R1152 K1153 Y1154 T1155 Y1156 G1157 K1158 H1159 I1160 L1161 A1162 K1163 L1164 E1165 K1166 Y1167 Y1168 MET LYS ASN GLY VAL ASP LEU GLY

# 4 Data and refinement statistics (i)

| Property | Value | Source |
|---|---|---|
| Space group | C 1 2 1 | Depositor |
| Cell constants<br>a, b, c, $\alpha$, $\beta$, $\gamma$ | 262.73Å 37.73Å 82.52Å<br>90.00° 102.95° 90.00° | Depositor |
| Resolution (Å) | 34.29 – 2.20<br>34.29 – 2.19 | Depositor<br>EDS |
| % Data completeness<br>(in resolution range) | 92.7 (34.29-2.20)<br>92.0 (34.29-2.19) | Depositor<br>EDS |
| $R_{merge}$ | (Not available) | Depositor |
| $R_{sym}$ | 0.08 | Depositor |
| $< I/\sigma(I) >$ [1] | 1.76 (at 2.20Å) | Xtriage |
| Refinement program | CNS 1.0 | Depositor |
| R, $R_{free}$ | 0.236 , 0.293<br>0.236 , 0.292 | Depositor<br>DCC |
| $R_{free}$ test set | 2381 reflections (6.03%) | wwPDB-VP |
| Wilson B-factor (Å$^2$) | 35.4 | Xtriage |
| Anisotropy | 0.374 | Xtriage |
| Bulk solvent $k_{sol}$(e/Å$^3$), $B_{sol}$(Å$^2$) | 0.32 , 60.2 | EDS |
| L-test for twinning[2] | $< \|L\| > = 0.49$, $< L^2 > = 0.32$ | Xtriage |
| Estimated twinning fraction | No twinning to report. | Xtriage |
| $F_o$,$F_c$ correlation | 0.93 | EDS |
| Total number of atoms | 6357 | wwPDB-VP |
| Average B, all atoms (Å$^2$) | 48.0 | wwPDB-VP |

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 5.14% 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 | C | 0.56 | 0/185 | 0.72 | 0/285 |
| 2 | D | 0.46 | 0/163 | 0.68 | 0/251 |
| 3 | A | 0.40 | 0/2829 | 0.58 | 0/3815 |
| 3 | B | 0.33 | 0/2829 | 0.54 | 0/3815 |
| All | All | 0.38 | 0/6006 | 0.57 | 0/8166 |

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

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 | C | 167 | 0 | 84 | 1 | 0 |
| 2 | D | 147 | 0 | 74 | 6 | 0 |
| 3 | A | 2775 | 0 | 2790 | 75 | 0 |
| 3 | B | 2775 | 0 | 2790 | 123 | 0 |
| 4 | A | 295 | 0 | 0 | 8 | 0 |
| 4 | B | 171 | 0 | 0 | 8 | 0 |
| 4 | C | 16 | 0 | 0 | 0 | 0 |
| 4 | D | 11 | 0 | 0 | 0 | 0 |
| All | All | 6357 | 0 | 5738 | 202 | 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 17.

All (202) 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) |
|---|---|---|---|
| 3:B:879:GLN:HE21 | 3:B:883:ASN:HD21 | 0.98 | 0.91 |
| 3:B:879:GLN:HE21 | 3:B:883:ASN:ND2 | 1.70 | 0.89 |
| 3:B:879:GLN:NE2 | 3:B:883:ASN:HD21 | 1.77 | 0.82 |
| 3:A:879:GLN:HE21 | 3:A:883:ASN:HD21 | 1.26 | 0.80 |
| 3:B:1101:VAL:HG11 | 3:B:1115:MET:SD | 2.24 | 0.78 |
| 3:A:874:THR:HG22 | 3:A:877:GLU:OE1 | 1.85 | 0.77 |
| 3:B:846:LEU:HG | 3:B:869:LYS:HG2 | 1.68 | 0.75 |
| 3:A:893:MET:HE1 | 3:A:928:LEU:HD13 | 1.72 | 0.72 |
| 3:B:1043:ASN:O | 3:B:1047:GLN:HG3 | 1.90 | 0.70 |
| 3:B:879:GLN:NE2 | 3:B:883:ASN:ND2 | 2.38 | 0.70 |
| 3:A:910:SER:OG | 3:A:913:GLN:HG3 | 1.94 | 0.68 |
| 3:B:954:VAL:HG11 | 3:B:981:VAL:HG21 | 1.75 | 0.68 |
| 3:B:983:PRO:HG2 | 3:B:984:GLN:OE1 | 1.95 | 0.67 |
| 3:B:1118:ASP:HB3 | 3:B:1121:ALA:HB3 | 1.77 | 0.66 |
| 2:D:16:A:H2' | 2:D:17:U:H5" | 1.78 | 0.66 |
| 3:B:1000:LEU:HB2 | 3:B:1010:ILE:HD11 | 1.77 | 0.65 |
| 3:B:874:THR:HG23 | 3:B:877:GLU:H | 1.62 | 0.65 |
| 3:A:1118:ASP:HB3 | 3:A:1121:ALA:HB3 | 1.77 | 0.65 |
| 3:B:860:GLN:HA | 3:B:897:PHE:CD2 | 2.32 | 0.65 |
| 3:B:869:LYS:O | 3:B:873:ALA:HB2 | 1.98 | 0.64 |
| 3:B:1054:ARG:HB3 | 3:B:1057:ASP:OD2 | 1.97 | 0.64 |
| 3:A:833:LEU:HD22 | 3:A:855:GLU:HG2 | 1.78 | 0.63 |
| 2:D:19:U:O2 | 3:B:933:TYR:HD2 | 1.82 | 0.63 |
| 3:B:1051:GLU:HA | 3:B:1088:HIS:ND1 | 2.13 | 0.63 |
| 3:A:879:GLN:HE21 | 3:A:883:ASN:ND2 | 1.96 | 0.63 |
| 3:B:982:GLN:HG3 | 4:B:294:HOH:O | 1.99 | 0.62 |
| 3:B:1051:GLU:HA | 3:B:1088:HIS:CE1 | 2.34 | 0.62 |
| 3:B:1161:LEU:O | 3:B:1165:GLU:HG3 | 1.99 | 0.62 |
| 3:B:1151:LEU:HD22 | 3:B:1161:LEU:HD13 | 1.82 | 0.61 |
| 3:B:1150:THR:HG22 | 3:B:1153:LYS:NZ | 2.16 | 0.60 |
| 3:B:1023:LEU:O | 3:B:1027:GLU:HG3 | 2.02 | 0.60 |
| 3:B:981:VAL:HG12 | 3:B:982:GLN:N | 2.16 | 0.60 |
| 3:B:1051:GLU:HA | 3:B:1088:HIS:HD1 | 1.65 | 0.59 |
| 3:B:1158:LYS:NZ | 3:B:1158:LYS:HB2 | 2.17 | 0.59 |
| 3:A:1011:GLN:O | 3:A:1015:GLU:HG3 | 2.03 | 0.58 |
| 3:A:932:MET:HG3 | 4:B:121:HOH:O | 2.02 | 0.58 |
| 3:A:870:LEU:HD22 | 3:A:878:ARG:HG2 | 1.86 | 0.58 |
| 3:A:1133:GLU:CD | 3:A:1135:GLY:H | 2.06 | 0.58 |
| 3:B:1151:LEU:HD23 | 3:B:1151:LEU:O | 2.03 | 0.58 |
| 3:B:896:VAL:HG13 | 3:B:897:PHE:CD1 | 2.39 | 0.57 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 3:A:874:THR:HG23 | 3:A:877:GLU:H | 1.69 | 0.57 |
| 3:A:945:ILE:HD12 | 3:A:949:GLN:HB3 | 1.87 | 0.57 |
| 3:B:1056:GLU:H | 3:B:1056:GLU:CD | 2.08 | 0.57 |
| 3:B:963:LYS:O | 3:B:967:ASP:HB2 | 2.05 | 0.56 |
| 3:A:879:GLN:NE2 | 3:A:883:ASN:HD21 | 2.00 | 0.56 |
| 3:B:1055:PRO:HB2 | 3:B:1056:GLU:OE2 | 2.05 | 0.56 |
| 3:B:945:ILE:HD12 | 3:B:949:GLN:HB3 | 1.88 | 0.56 |
| 3:B:946:PRO:HB2 | 3:B:949:GLN:HE21 | 1.70 | 0.56 |
| 3:B:872:ARG:H | 3:B:872:ARG:HD2 | 1.70 | 0.56 |
| 3:B:1113:TYR:CD1 | 3:B:1147:HIS:HB3 | 2.41 | 0.56 |
| 3:B:829:ARG:HG3 | 3:B:833:LEU:HD23 | 1.87 | 0.56 |
| 3:B:874:THR:HG22 | 3:B:877:GLU:CG | 2.36 | 0.55 |
| 3:A:967:ASP:OD1 | 3:A:969:ASN:N | 2.37 | 0.55 |
| 3:B:1066:ARG:CZ | 3:B:1096:VAL:HG11 | 2.37 | 0.55 |
| 3:B:1071:VAL:HG23 | 4:B:90:HOH:O | 2.06 | 0.55 |
| 3:B:971:ASN:O | 3:B:975:GLN:HG3 | 2.07 | 0.54 |
| 3:B:1155:THR:HA | 3:B:1158:LYS:NZ | 2.21 | 0.54 |
| 3:A:919:GLU:HB2 | 3:A:922:ARG:NH2 | 2.23 | 0.54 |
| 3:A:893:MET:HE1 | 3:A:921:ILE:HG12 | 1.89 | 0.54 |
| 3:B:845:GLN:HG2 | 3:B:848:GLU:OE1 | 2.08 | 0.54 |
| 3:B:941:ALA:O | 3:B:945:ILE:HG12 | 2.07 | 0.53 |
| 3:A:841:TYR:HB3 | 3:A:844:LEU:HB2 | 1.90 | 0.53 |
| 3:B:1026:LEU:HD23 | 3:B:1029:LEU:HD12 | 1.90 | 0.53 |
| 3:A:1089:ALA:HB1 | 3:A:1093:GLU:HB2 | 1.91 | 0.52 |
| 3:A:893:MET:HE1 | 3:A:928:LEU:CD1 | 2.39 | 0.52 |
| 3:B:942:LEU:O | 3:B:950:GLN:NE2 | 2.36 | 0.52 |
| 3:A:1056:GLU:HB2 | 4:A:164:HOH:O | 2.08 | 0.52 |
| 3:A:946:PRO:HB2 | 3:A:949:GLN:NE2 | 2.25 | 0.52 |
| 3:A:830:SER:O | 3:A:834:GLU:HB2 | 2.10 | 0.52 |
| 3:A:899:ASN:O | 3:A:903:GLN:HG3 | 2.08 | 0.52 |
| 3:A:972:HIS:HE1 | 4:A:62:HOH:O | 1.93 | 0.52 |
| 2:D:16:A:C2' | 2:D:17:U:H5" | 2.39 | 0.52 |
| 3:B:1164:LEU:C | 3:B:1166:LYS:H | 2.14 | 0.52 |
| 3:A:854:MET:O | 3:A:858:GLN:HG3 | 2.10 | 0.52 |
| 3:B:874:THR:CG2 | 3:B:877:GLU:H | 2.22 | 0.52 |
| 3:B:946:PRO:HB2 | 3:B:949:GLN:NE2 | 2.25 | 0.51 |
| 3:A:954:VAL:HG21 | 3:A:981:VAL:HG21 | 1.91 | 0.51 |
| 3:B:1104:MET:HE1 | 4:B:318:HOH:O | 2.10 | 0.51 |
| 3:B:907:GLU:OE1 | 3:B:940:LYS:NZ | 2.41 | 0.51 |
| 3:B:1070:LEU:O | 3:B:1074:GLN:HG3 | 2.10 | 0.50 |
| 3:B:982:GLN:HB3 | 3:B:984:GLN:NE2 | 2.26 | 0.50 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 3:B:1010:ILE:O | 3:B:1014:LEU:HG | 2.11 | 0.50 |
| 3:B:872:ARG:H | 3:B:872:ARG:CD | 2.25 | 0.50 |
| 3:B:874:THR:HG22 | 3:B:877:GLU:HB2 | 1.94 | 0.50 |
| 3:A:831:ARG:NH1 | 4:A:452:HOH:O | 2.45 | 0.50 |
| 3:B:896:VAL:HA | 3:B:933:TYR:CE2 | 2.47 | 0.50 |
| 3:A:1165:GLU:HA | 3:A:1168:TYR:CD2 | 2.47 | 0.50 |
| 3:A:907:GLU:HG2 | 3:A:940:LYS:HD2 | 1.94 | 0.50 |
| 3:A:1046:ILE:HG23 | 3:A:1061:ILE:HD13 | 1.93 | 0.49 |
| 3:B:858:GLN:NE2 | 4:B:99:HOH:O | 2.44 | 0.49 |
| 3:B:1056:GLU:O | 3:B:1060:LYS:HG3 | 2.12 | 0.49 |
| 3:A:1153:LYS:NZ | 3:A:1153:LYS:HB2 | 2.27 | 0.49 |
| 3:B:1124:VAL:O | 3:B:1128:MET:HG3 | 2.12 | 0.49 |
| 3:B:860:GLN:HA | 3:B:897:PHE:CE2 | 2.47 | 0.49 |
| 3:A:829:ARG:HD3 | 3:A:837:ARG:HD2 | 1.95 | 0.49 |
| 3:A:869:LYS:O | 3:A:873:ALA:HB2 | 2.12 | 0.49 |
| 3:A:1165:GLU:O | 3:A:1168:TYR:HD2 | 1.96 | 0.48 |
| 3:B:1095:ALA:HA | 3:B:1136:GLN:OE1 | 2.13 | 0.48 |
| 3:A:1065:ILE:HG13 | 3:A:1085:CYS:SG | 2.52 | 0.48 |
| 3:A:831:ARG:HG2 | 3:A:831:ARG:HH11 | 1.77 | 0.48 |
| 3:B:1087:THR:HG22 | 3:B:1088:HIS:HD2 | 1.78 | 0.48 |
| 3:B:1145:ARG:HB3 | 3:B:1146:PRO:HD3 | 1.95 | 0.48 |
| 3:A:845:GLN:NE2 | 3:A:845:GLN:HA | 2.28 | 0.48 |
| 3:A:916:ALA:O | 3:A:920:ARG:HG2 | 2.14 | 0.48 |
| 3:B:1119:GLN:HG3 | 3:B:1120:TYR:CD1 | 2.49 | 0.48 |
| 3:B:1156:TYR:C | 3:B:1158:LYS:H | 2.18 | 0.48 |
| 3:B:1011:GLN:O | 3:B:1015:GLU:HG3 | 2.14 | 0.47 |
| 3:A:954:VAL:O | 3:A:957:LEU:HB2 | 2.15 | 0.47 |
| 3:B:1133:GLU:HB3 | 3:B:1134:PRO:HD2 | 1.97 | 0.47 |
| 3:B:911:LEU:HG | 3:B:915:LEU:HD22 | 1.96 | 0.47 |
| 3:B:946:PRO:O | 3:B:950:GLN:HG3 | 2.15 | 0.47 |
| 3:B:1033:THR:O | 3:B:1037:VAL:HG13 | 2.15 | 0.47 |
| 3:B:984:GLN:H | 3:B:984:GLN:CD | 2.18 | 0.47 |
| 3:B:1145:ARG:HB3 | 3:B:1146:PRO:CD | 2.45 | 0.47 |
| 3:B:922:ARG:HH22 | 3:B:952:GLU:CG | 2.28 | 0.47 |
| 3:A:879:GLN:NE2 | 3:A:883:ASN:ND2 | 2.60 | 0.46 |
| 3:B:962:LEU:HD12 | 3:B:962:LEU:N | 2.31 | 0.46 |
| 3:B:835:ASP:HB2 | 3:B:841:TYR:HE2 | 1.80 | 0.46 |
| 3:A:893:MET:CE | 3:A:921:ILE:HG12 | 2.45 | 0.46 |
| 3:A:982:GLN:HG3 | 4:A:283:HOH:O | 2.13 | 0.46 |
| 3:B:1094:ARG:HG3 | 3:B:1094:ARG:HH11 | 1.80 | 0.46 |
| 2:D:13:U:O2' | 2:D:14:G:H5' | 2.16 | 0.46 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 3:A:1086:VAL:HG12 | 3:A:1131:VAL:HG21 | 1.98 | 0.45 |
| 2:D:17:U:O4' | 3:B:1008:ARG:NH1 | 2.49 | 0.45 |
| 3:B:1050:LEU:O | 3:B:1088:HIS:ND1 | 2.47 | 0.45 |
| 3:A:978:ILE:HD13 | 3:A:1013:ILE:HG13 | 1.99 | 0.45 |
| 3:A:869:LYS:O | 3:A:873:ALA:N | 2.48 | 0.45 |
| 3:B:874:THR:HG22 | 3:B:877:GLU:CB | 2.47 | 0.45 |
| 3:A:983:PRO:HD2 | 3:A:984:GLN:OE1 | 2.16 | 0.45 |
| 3:B:896:VAL:HA | 3:B:933:TYR:CD2 | 2.52 | 0.45 |
| 3:B:896:VAL:HG13 | 3:B:897:PHE:HD1 | 1.78 | 0.45 |
| 3:A:919:GLU:OE1 | 3:A:922:ARG:NH2 | 2.48 | 0.45 |
| 3:A:1143:LYS:NZ | 3:A:1143:LYS:HB3 | 2.32 | 0.45 |
| 3:A:860:GLN:HB2 | 3:A:897:PHE:CE1 | 2.51 | 0.45 |
| 3:A:919:GLU:HB2 | 3:A:922:ARG:HH21 | 1.82 | 0.45 |
| 3:B:1122:ASN:O | 3:B:1126:GLN:HG3 | 2.17 | 0.45 |
| 3:B:829:ARG:NH1 | 3:B:837:ARG:NE | 2.65 | 0.45 |
| 3:B:844:LEU:HD11 | 3:B:849:ILE:HG23 | 1.99 | 0.45 |
| 3:A:829:ARG:HE | 3:A:837:ARG:NE | 2.15 | 0.44 |
| 3:B:1164:LEU:HD13 | 3:B:1164:LEU:O | 2.17 | 0.44 |
| 3:B:1009:VAL:O | 3:B:1013:ILE:HG12 | 2.16 | 0.44 |
| 3:B:981:VAL:CG1 | 3:B:982:GLN:N | 2.80 | 0.44 |
| 3:A:893:MET:HE3 | 3:A:937:VAL:HG11 | 1.98 | 0.44 |
| 3:B:844:LEU:HD12 | 3:B:865:PHE:CZ | 2.51 | 0.44 |
| 3:A:1152:ARG:O | 3:A:1158:LYS:HE2 | 2.18 | 0.44 |
| 3:A:874:THR:OG1 | 3:A:875:PRO:HD2 | 2.18 | 0.44 |
| 3:B:1003:HIS:ND1 | 3:B:1004:PRO:HD2 | 2.32 | 0.44 |
| 3:B:1087:THR:HG22 | 3:B:1088:HIS:CD2 | 2.53 | 0.44 |
| 3:A:951:ASN:HB3 | 3:A:955:ARG:NH2 | 2.32 | 0.44 |
| 3:B:986:LEU:HD22 | 3:B:989:ILE:HD12 | 2.00 | 0.43 |
| 3:A:1105:ASN:HA | 3:A:1110:SER:HA | 2.01 | 0.43 |
| 3:B:975:GLN:O | 3:B:979:GLU:HG2 | 2.18 | 0.43 |
| 2:D:13:U:O2 | 3:B:1156:TYR:HD1 | 2.02 | 0.43 |
| 3:A:911:LEU:CD2 | 3:A:915:LEU:HD11 | 2.48 | 0.43 |
| 3:A:910:SER:O | 3:A:914:LYS:HG3 | 2.18 | 0.43 |
| 3:B:903:GLN:HG3 | 3:B:937:VAL:HG22 | 2.01 | 0.43 |
| 3:B:872:ARG:N | 3:B:872:ARG:HD2 | 2.32 | 0.42 |
| 3:A:1038:GLN:NE2 | 4:A:382:HOH:O | 2.51 | 0.42 |
| 3:B:1117:LYS:HG3 | 4:B:147:HOH:O | 2.19 | 0.42 |
| 3:A:858:GLN:NE2 | 4:A:260:HOH:O | 2.50 | 0.42 |
| 3:B:929:ALA:O | 3:B:935:CYS:HB3 | 2.18 | 0.42 |
| 1:C:12:U:O2 | 1:C:12:U:H2' | 2.20 | 0.42 |
| 3:A:1007:CYS:O | 3:A:1011:GLN:HG3 | 2.20 | 0.42 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 3:A:1113:TYR:HD1 | 3:A:1116:MET:HE3 | 1.84 | 0.42 |
| 3:A:1145:ARG:HB3 | 3:A:1146:PRO:CD | 2.50 | 0.42 |
| 3:A:1073:SER:HB2 | 3:A:1124:VAL:HG21 | 2.01 | 0.42 |
| 3:B:1113:TYR:O | 3:B:1116:MET:HG2 | 2.20 | 0.42 |
| 3:A:1147:HIS:O | 3:A:1151:LEU:HG | 2.20 | 0.42 |
| 3:B:983:PRO:HB2 | 3:B:1018:LEU:CD2 | 2.50 | 0.41 |
| 3:B:830:SER:HB2 | 4:B:70:HOH:O | 2.20 | 0.41 |
| 3:B:983:PRO:HB2 | 3:B:1018:LEU:HD22 | 2.02 | 0.41 |
| 3:B:829:ARG:HD2 | 3:B:834:GLU:OE1 | 2.19 | 0.41 |
| 3:A:996:GLN:HA | 4:A:72:HOH:O | 2.19 | 0.41 |
| 3:A:963:LYS:NZ | 4:A:321:HOH:O | 2.51 | 0.41 |
| 3:B:1167:TYR:HD1 | 3:B:1167:TYR:O | 2.03 | 0.41 |
| 3:B:1128:MET:O | 3:B:1132:ALA:HB2 | 2.21 | 0.41 |
| 3:B:1113:TYR:HD1 | 3:B:1147:HIS:HB3 | 1.85 | 0.41 |
| 3:B:906:PHE:O | 3:B:914:LYS:HE2 | 2.21 | 0.41 |
| 3:B:933:TYR:O | 3:B:936:ARG:HB2 | 2.20 | 0.41 |
| 3:A:941:ALA:O | 3:A:945:ILE:HG12 | 2.21 | 0.41 |
| 3:B:1054:ARG:HD2 | 3:B:1056:GLU:OE1 | 2.19 | 0.41 |
| 3:B:835:ASP:HB3 | 3:B:840:ARG:HB2 | 2.02 | 0.41 |
| 3:B:890:TYR:HD2 | 3:B:890:TYR:O | 2.03 | 0.41 |
| 3:B:990:ILE:HG12 | 3:B:1021:GLN:HB3 | 2.01 | 0.41 |
| 3:A:1070:LEU:HD13 | 3:A:1111:ALA:HB1 | 2.03 | 0.41 |
| 3:A:911:LEU:HD22 | 3:A:915:LEU:HD11 | 2.02 | 0.41 |
| 3:B:1056:GLU:N | 3:B:1056:GLU:OE2 | 2.50 | 0.41 |
| 3:B:892:LEU:O | 3:B:899:ASN:N | 2.54 | 0.41 |
| 3:B:1164:LEU:O | 3:B:1166:LYS:N | 2.53 | 0.41 |
| 3:A:954:VAL:CG2 | 3:A:981:VAL:HG21 | 2.51 | 0.41 |
| 3:A:926:LEU:HD22 | 3:A:960:HIS:CD2 | 2.57 | 0.40 |
| 3:B:1021:GLN:O | 3:B:1024:PRO:HD2 | 2.22 | 0.40 |
| 3:B:1137:ARG:O | 3:B:1141:MET:HG2 | 2.21 | 0.40 |
| 3:B:922:ARG:HH22 | 3:B:952:GLU:HG2 | 1.87 | 0.40 |
| 3:B:996:GLN:O | 3:B:1000:LEU:HG | 2.21 | 0.40 |
| 3:B:1116:MET:CE | 3:B:1144:ILE:HG23 | 2.50 | 0.40 |
| 3:A:1005:TYR:O | 3:A:1008:ARG:HB2 | 2.22 | 0.40 |
| 3:B:831:ARG:HD2 | 4:B:468:HOH:O | 2.20 | 0.40 |
| 3:B:990:ILE:N | 3:B:990:ILE:HD12 | 2.36 | 0.40 |
| 3:A:978:ILE:HA | 3:A:986:LEU:CD1 | 2.51 | 0.40 |
| 3:B:1148:ILE:O | 3:B:1151:LEU:HB3 | 2.21 | 0.40 |
| 3:B:1164:LEU:C | 3:B:1166:LYS:N | 2.74 | 0.40 |

There are no symmetry-related clashes.

## 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 | |
|---|---|---|---|---|---|---|---|
| 3 | A | 339/349 (97%) | 328 (97%) | 9 (3%) | 2 (1%) | 25 | 26 |
| 3 | B | 339/349 (97%) | 314 (93%) | 21 (6%) | 4 (1%) | 13 | 10 |
| All | All | 678/698 (97%) | 642 (95%) | 30 (4%) | 6 (1%) | 17 | 16 |

All (6) Ramachandran outliers are listed below:

| Mol | Chain | Res | Type |
|---|---|---|---|
| 3 | B | 830 | SER |
| 3 | B | 1149 | ALA |
| 3 | B | 839 | ASN |
| 3 | B | 1165 | GLU |
| 3 | A | 838 | ASN |
| 3 | A | 1108 | PRO |

### 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 | |
|---|---|---|---|---|---|---|
| 3 | A | 304/310 (98%) | 298 (98%) | 6 (2%) | 55 | 69 |
| 3 | B | 304/310 (98%) | 299 (98%) | 5 (2%) | 62 | 76 |
| All | All | 608/620 (98%) | 597 (98%) | 11 (2%) | 59 | 72 |

All (11) residues with a non-rotameric sidechain are listed below:

| Mol | Chain | Res | Type |
|---|---|---|---|
| 3 | A | 831 | ARG |
| 3 | A | 837 | ARG |
| 3 | A | 919 | GLU |
| 3 | A | 957 | LEU |
| 3 | A | 1082 | VAL |
| 3 | A | 1168 | TYR |
| 3 | B | 872 | ARG |
| 3 | B | 890 | TYR |
| 3 | B | 915 | LEU |
| 3 | B | 957 | LEU |
| 3 | B | 984 | GLN |

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (18) such sidechains are listed below:

| Mol | Chain | Res | Type |
|---|---|---|---|
| 3 | A | 845 | GLN |
| 3 | A | 852 | HIS |
| 3 | A | 858 | GLN |
| 3 | A | 883 | ASN |
| 3 | A | 891 | GLN |
| 3 | A | 949 | GLN |
| 3 | A | 951 | ASN |
| 3 | A | 972 | HIS |
| 3 | A | 1105 | ASN |
| 3 | A | 1119 | GLN |
| 3 | B | 845 | GLN |
| 3 | B | 883 | ASN |
| 3 | B | 891 | GLN |
| 3 | B | 949 | GLN |
| 3 | B | 951 | ASN |
| 3 | B | 1031 | GLN |
| 3 | B | 1119 | GLN |
| 3 | B | 1147 | HIS |

### 5.3.3 RNA

| Mol | Chain | Analysed | Backbone Outliers | Pucker Outliers |
|---|---|---|---|---|
| 1 | C | 7/8 (87%) | 0 | 0 |
| 2 | D | 6/7 (85%) | 1 (16%) | 0 |
| All | All | 13/15 (86%) | 1 (7%) | 0 |

All (1) RNA backbone outliers are listed below:

| Mol | Chain | Res | Type |
|---|---|---|---|
| 2 | D | 17 | U |

There are no RNA pucker outliers to report.

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

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

## 5.5 Carbohydrates (i)

There are no carbohydrates in this entry.

## 5.6 Ligand geometry (i)

There are no ligands in this entry.

## 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

## 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 | C | 8/8 (100%) | 0.49 | 1 (12%) 3 3 | 32, 49, 66, 103 | 0 |
| 2 | D | 7/7 (100%) | 0.35 | 0 100 100 | 46, 67, 83, 85 | 0 |
| 3 | A | 341/349 (97%) | 0.14 | 9 (2%) 56 53 | 19, 34, 71, 87 | 0 |
| 3 | B | 341/349 (97%) | 0.39 | 24 (7%) 16 15 | 28, 51, 97, 110 | 0 |
| All | All | 697/713 (97%) | 0.27 | 34 (4%) 29 28 | 19, 43, 80, 110 | 0 |

All (34) RSRZ outliers are listed below:

| Mol | Chain | Res | Type | RSRZ |
|---|---|---|---|---|
| 3 | B | 1156 | TYR | 8.6 |
| 3 | B | 1157 | GLY | 6.4 |
| 3 | A | 828 | GLY | 5.1 |
| 3 | A | 868 | LEU | 4.8 |
| 3 | B | 1168 | TYR | 4.8 |
| 3 | B | 1155 | THR | 4.7 |
| 3 | B | 1160 | ILE | 4.5 |
| 3 | A | 872 | ARG | 4.0 |
| 3 | B | 1158 | LYS | 3.5 |
| 3 | B | 1164 | LEU | 3.4 |
| 3 | A | 1104 | MET | 3.3 |
| 3 | A | 1168 | TYR | 3.2 |
| 1 | C | 12 | U | 3.2 |
| 3 | B | 840 | ARG | 3.1 |
| 3 | B | 1147 | HIS | 3.1 |
| 3 | B | 1152 | ARG | 3.1 |
| 3 | B | 1150 | THR | 3.0 |
| 3 | B | 1167 | TYR | 2.9 |
| 3 | B | 1159 | HIS | 2.7 |
| 3 | B | 1153 | LYS | 2.6 |
| 3 | B | 1146 | PRO | 2.5 |

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| Mol | Chain | Res | Type | RSRZ |
|---|---|---|---|---|
| 3 | B | 1163 | LYS | 2.4 |
| 3 | A | 847 | ARG | 2.4 |
| 3 | B | 839 | ASN | 2.3 |
| 3 | B | 1142 | HIS | 2.3 |
| 3 | B | 995 | GLY | 2.2 |
| 3 | B | 874 | THR | 2.2 |
| 3 | A | 842 | PRO | 2.2 |
| 3 | B | 1161 | LEU | 2.1 |
| 3 | A | 861 | HIS | 2.1 |
| 3 | A | 908 | PHE | 2.1 |
| 3 | B | 1166 | LYS | 2.0 |
| 3 | B | 1113 | TYR | 2.0 |
| 3 | B | 1148 | ILE | 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 carbohydrates 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.