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

Feb 1, 2016 – 11:24 AM GMT

| | | |
|---|---|---|
| PDB ID | : | 3OTO |
| Title | : | Crystal Structure of the 30S ribosomal subunit from a KsgA mutant of Thermus thermophilus (HB8) |
| Authors | : | Demirci, H.; Murphy IV, F.; Belardinelli, R.; Kelley, A.C.; Ramakrishnan, V.; Gregory, S.T.; Dahlberg, A.E.; Jogl, G. |
| Deposited on | : | 2010-09-13 |
| Resolution | : | 3.69 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
http://wwpdb.org/validation/2016/XrayValidationReportHelp
with specific help available everywhere you see the (i) symbol.

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

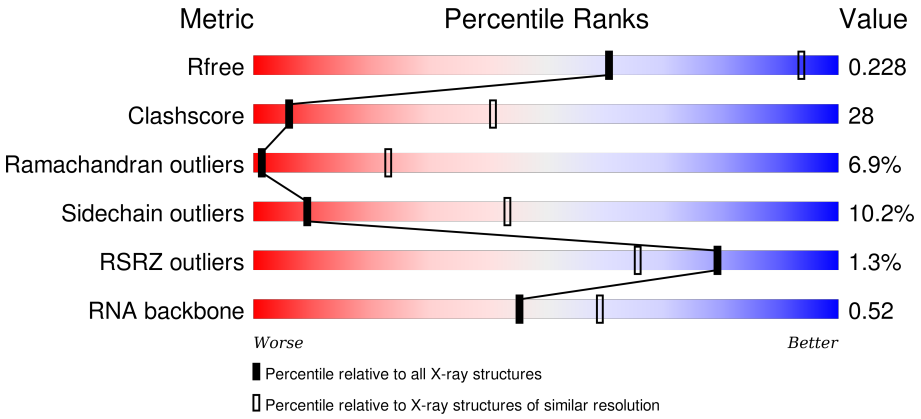
| | | |
|---|---|---|
| MolProbity | : | 4.02b-467 |
| Mogul | : | 1.7 (RC4), CSD as536be (2015) |
| Xtriage (Phenix) | : | 1.9-1692 |
| EDS | : | rb-20026688 |
| Percentile statistics | : | 20151230.v01 (using entries in the PDB archive December 30th 2015) |
| Refmac | : | 5.8.0135 |
| CCP4 | : | 6.5.0 |
| Ideal geometry (proteins) | : | Engh & Huber (2001) |
| Ideal geometry (DNA, RNA) | : | Parkinson et al. (1996) |
| Validation Pipeline (wwPDB-VP) | : | trunk26865 |

# 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 3.69 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)) |
|---|---|---|
| $R_{free}$ | 91344 | 1101 (3.90-3.50) |
| Clashscore | 102246 | 1224 (3.90-3.50) |
| Ramachandran outliers | 100387 | 1172 (3.90-3.50) |
| Sidechain outliers | 100360 | 1170 (3.90-3.50) |
| RSRZ outliers | 91569 | 1108 (3.90-3.50) |
| RNA backbone | 2183 | 1067 (4.60-2.80) |

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. 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 | 1522 | 30% 54% 14% |
| 2 | B | 256 | 38% 43% 11% 8% |
| 3 | C | 239 | 2% 36% 43% 7% 14% |
| 4 | D | 209 | 44% 49% 6% |

*Continued on next page...*

*Continued from previous page...*

| Mol | Chain | Length | Quality of chain |
|---|---|---|---|
| 5 | E | 162 | 39% 44% 9% 7% |
| 6 | F | 101 | 46% 47% 8% |
| 7 | G | 156 | % 33% 55% 12% |
| 8 | H | 138 | 48% 42% 9% |
| 9 | I | 128 | 43% 45% 12% |
| 10 | J | 105 | 7% 33% 44% 16% 7% |
| 11 | K | 129 | 2% 40% 43% 9% 8% |
| 12 | L | 135 | 36% 41% 14% 8% |
| 13 | M | 126 | % 38% 43% 10% 9% |
| 14 | N | 61 | 3% 36% 56% 7% |
| 15 | O | 89 | 42% 49% 7% |
| 16 | P | 88 | 33% 55% 6% 6% |
| 17 | Q | 105 | 4% 43% 54% |
| 18 | R | 88 | % 33% 41% 8% 17% |
| 19 | S | 93 | % 29% 44% 13% 14% |
| 20 | T | 106 | % 40% 41% 12% 7% |
| 21 | U | 27 | 15% 41% 41% 7% 11% |

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 |
|---|---|---|---|---|---|---|---|
| 23 | MG | A | 1554 | - | - | - | X |
| 23 | MG | A | 1563 | - | - | - | X |
| 23 | MG | A | 1566 | - | - | - | X |
| 23 | MG | A | 1578 | - | - | - | X |
| 23 | MG | A | 1589 | - | - | - | X |
| 23 | MG | A | 1590 | - | - | - | X |
| 23 | MG | A | 1603 | - | - | - | X |
| 23 | MG | A | 1605 | - | - | - | X |

*Continued on next page...*

*Continued from previous page...*

| Mol | Type | Chain | Res | Chirality | Geometry | Clashes | Electron density |
|---|---|---|---|---|---|---|---|
| 23 | MG | A | 1606 | - | - | - | X |
| 23 | MG | A | 1607 | - | - | - | X |
| 23 | MG | A | 1615 | - | - | - | X |
| 23 | MG | A | 1618 | - | - | - | X |
| 23 | MG | A | 1620 | - | - | - | X |
| 23 | MG | A | 1622 | - | - | - | X |
| 23 | MG | A | 1623 | - | - | - | X |
| 23 | MG | A | 1625 | - | - | - | X |
| 23 | MG | A | 1628 | - | - | - | X |
| 23 | MG | A | 1629 | - | - | - | X |
| 23 | MG | A | 94 | - | - | - | X |
| 23 | MG | B | 257 | - | - | - | X |
| 23 | MG | M | 127 | - | - | - | X |
| 24 | K | A | 1635 | - | - | - | X |
| 24 | K | A | 1636 | - | - | - | X |
| 24 | K | A | 1641 | - | - | - | X |
| 24 | K | A | 1644 | - | - | - | X |
| 24 | K | A | 1648 | - | - | - | X |
| 24 | K | A | 1651 | - | - | - | X |
| 24 | K | A | 1658 | - | - | - | X |
| 24 | K | A | 1666 | - | - | - | X |
| 24 | K | A | 1668 | - | - | - | X |
| 24 | K | A | 1669 | - | - | - | X |
| 24 | K | A | 1670 | - | - | - | X |

## 2 Entry composition

There are 24 unique types of molecules in this entry. The entry contains 51775 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 16S rRNA.

| Mol | Chain | Residues | Atoms | | | | | ZeroOcc | AltConf | Trace |
|---|---|---|---|---|---|---|---|---|---|---|
| | | | Total | C | N | O | P | | | |
| 1 | A | 1513 | 32511 | 14472 | 6016 | 10511 | 1512 | 0 | 0 | 0 |

- Molecule 2 is a protein called 30S RIBOSOMAL PROTEIN S2.

| Mol | Chain | Residues | Atoms | | | | | ZeroOcc | AltConf | Trace |
|---|---|---|---|---|---|---|---|---|---|---|
| | | | Total | C | N | O | S | | | |
| 2 | B | 235 | 1873 | 1195 | 335 | 338 | 5 | 0 | 0 | 0 |

- Molecule 3 is a protein called 30S RIBOSOMAL PROTEIN S3.

| Mol | Chain | Residues | Atoms | | | | | ZeroOcc | AltConf | Trace |
|---|---|---|---|---|---|---|---|---|---|---|
| | | | Total | C | N | O | S | | | |
| 3 | C | 206 | 1612 | 1016 | 314 | 281 | 1 | 0 | 0 | 0 |

- Molecule 4 is a protein called 30S RIBOSOMAL PROTEIN S4.

| Mol | Chain | Residues | Atoms | | | | | ZeroOcc | AltConf | Trace |
|---|---|---|---|---|---|---|---|---|---|---|
| | | | Total | C | N | O | S | | | |
| 4 | D | 208 | 1703 | 1066 | 339 | 291 | 7 | 0 | 0 | 0 |

- Molecule 5 is a protein called 30S RIBOSOMAL PROTEIN S5.

| Mol | Chain | Residues | Atoms | | | | | ZeroOcc | AltConf | Trace |
|---|---|---|---|---|---|---|---|---|---|---|
| | | | Total | C | N | O | S | | | |
| 5 | E | 150 | 1146 | 724 | 217 | 201 | 4 | 0 | 0 | 0 |

- Molecule 6 is a protein called 30S RIBOSOMAL PROTEIN S6.

| Mol | Chain | Residues | Atoms | | | | | ZeroOcc | AltConf | Trace |
|---|---|---|---|---|---|---|---|---|---|---|
| | | | Total | C | N | O | S | | | |
| 6 | F | 101 | 843 | 531 | 155 | 154 | 3 | 0 | 0 | 0 |

- Molecule 7 is a protein called 30S RIBOSOMAL PROTEIN S7.

| Mol | Chain | Residues | Atoms | | | | | ZeroOcc | AltConf | Trace |
|---|---|---|---|---|---|---|---|---|---|---|
| 7 | G | 155 | Total | C | N | O | S | 0 | 0 | 0 |
| | | | 1257 | 781 | 252 | 218 | 6 | | | |

- Molecule 8 is a protein called 30S RIBOSOMAL PROTEIN S8.

| Mol | Chain | Residues | Atoms | | | | | ZeroOcc | AltConf | Trace |
|---|---|---|---|---|---|---|---|---|---|---|
| 8 | H | 138 | Total | C | N | O | S | 0 | 0 | 0 |
| | | | 1116 | 705 | 215 | 193 | 3 | | | |

- Molecule 9 is a protein called 30S RIBOSOMAL PROTEIN S9.

| Mol | Chain | Residues | Atoms | | | | ZeroOcc | AltConf | Trace |
|---|---|---|---|---|---|---|---|---|---|
| 9 | I | 127 | Total | C | N | O | 0 | 0 | 0 |
| | | | 1011 | 639 | 198 | 174 | | | |

- Molecule 10 is a protein called 30S RIBOSOMAL PROTEIN S10.

| Mol | Chain | Residues | Atoms | | | | | ZeroOcc | AltConf | Trace |
|---|---|---|---|---|---|---|---|---|---|---|
| 10 | J | 98 | Total | C | N | O | S | 0 | 0 | 0 |
| | | | 792 | 498 | 156 | 137 | 1 | | | |

- Molecule 11 is a protein called 30S RIBOSOMAL PROTEIN S11.

| Mol | Chain | Residues | Atoms | | | | | ZeroOcc | AltConf | Trace |
|---|---|---|---|---|---|---|---|---|---|---|
| 11 | K | 119 | Total | C | N | O | S | 0 | 0 | 0 |
| | | | 885 | 549 | 168 | 165 | 3 | | | |

- Molecule 12 is a protein called 30S RIBOSOMAL PROTEIN S12.

| Mol | Chain | Residues | Atoms | | | | | ZeroOcc | AltConf | Trace |
|---|---|---|---|---|---|---|---|---|---|---|
| 12 | L | 124 | Total | C | N | O | S | 0 | 0 | 0 |
| | | | 970 | 611 | 195 | 163 | 1 | | | |

- Molecule 13 is a protein called 30S RIBOSOMAL PROTEIN S13.

| Mol | Chain | Residues | Atoms | | | | | ZeroOcc | AltConf | Trace |
|---|---|---|---|---|---|---|---|---|---|---|
| 13 | M | 115 | Total | C | N | O | S | 0 | 0 | 0 |
| | | | 921 | 569 | 190 | 160 | 2 | | | |

- Molecule 14 is a protein called 30S RIBOSOMAL PROTEIN S14.

| Mol | Chain | Residues | Atoms | | | | | ZeroOcc | AltConf | Trace |
|---|---|---|---|---|---|---|---|---|---|---|
| 14 | N | 60 | Total | C | N | O | S | 0 | 0 | 0 |
| | | | 492 | 312 | 104 | 72 | 4 | | | |

- Molecule 15 is a protein called 30S RIBOSOMAL PROTEIN S15.

| Mol | Chain | Residues | Atoms | | | | | ZeroOcc | AltConf | Trace |
|---|---|---|---|---|---|---|---|---|---|---|
| 15 | O | 88 | Total | C | N | O | S | 0 | 0 | 0 |
| | | | 734 | 459 | 147 | 126 | 2 | | | |

- Molecule 16 is a protein called 30S RIBOSOMAL PROTEIN S16.

| Mol | Chain | Residues | Atoms | | | | | ZeroOcc | AltConf | Trace |
|---|---|---|---|---|---|---|---|---|---|---|
| 16 | P | 83 | Total | C | N | O | S | 0 | 0 | 0 |
| | | | 700 | 443 | 139 | 117 | 1 | | | |

- Molecule 17 is a protein called 30S RIBOSOMAL PROTEIN S17.

| Mol | Chain | Residues | Atoms | | | | | ZeroOcc | AltConf | Trace |
|---|---|---|---|---|---|---|---|---|---|---|
| 17 | Q | 104 | Total | C | N | O | S | 0 | 0 | 0 |
| | | | 857 | 547 | 161 | 147 | 2 | | | |

- Molecule 18 is a protein called 30S RIBOSOMAL PROTEIN S18.

| Mol | Chain | Residues | Atoms | | | | ZeroOcc | AltConf | Trace |
|---|---|---|---|---|---|---|---|---|---|
| 18 | R | 73 | Total | C | N | O | 0 | 0 | 0 |
| | | | 597 | 380 | 118 | 99 | | | |

- Molecule 19 is a protein called 30S RIBOSOMAL PROTEIN S19.

| Mol | Chain | Residues | Atoms | | | | | ZeroOcc | AltConf | Trace |
|---|---|---|---|---|---|---|---|---|---|---|
| 19 | S | 80 | Total | C | N | O | S | 0 | 0 | 0 |
| | | | 647 | 414 | 119 | 112 | 2 | | | |

- Molecule 20 is a protein called 30S RIBOSOMAL PROTEIN S20.

| Mol | Chain | Residues | Atoms | | | | | ZeroOcc | AltConf | Trace |
|---|---|---|---|---|---|---|---|---|---|---|
| 20 | T | 99 | Total | C | N | O | S | 0 | 0 | 0 |
| | | | 762 | 469 | 162 | 129 | 2 | | | |

There is a discrepancy between the modelled and reference sequences:

| Chain | Residue | Modelled | Actual | Comment | Reference |
|---|---|---|---|---|---|
| T | 41 | VAL | ILE | SEE REMARK 999 | UNP P80380 |

- Molecule 21 is a protein called 30S RIBOSOMAL PROTEIN THX.

| Mol | Chain | Residues | Atoms | | | | ZeroOcc | AltConf | Trace |
|---|---|---|---|---|---|---|---|---|---|
| 21 | U | 24 | Total | C | N | O | 0 | 0 | 0 |
| | | | 208 | 128 | 50 | 30 | | | |

- Molecule 22 is ZINC ION (three-letter code: ZN) (formula: Zn).

| Mol | Chain | Residues | Atoms | | ZeroOcc | AltConf |
|---|---|---|---|---|---|---|
| 22 | D | 1 | Total | Zn | 0 | 0 |
| | | | 1 | 1 | | |
| 22 | N | 1 | Total | Zn | 0 | 0 |
| | | | 1 | 1 | | |

- Molecule 23 is MAGNESIUM ION (three-letter code: MG) (formula: Mg).

| Mol | Chain | Residues | Atoms | | ZeroOcc | AltConf |
|---|---|---|---|---|---|---|
| 23 | B | 1 | Total | Mg | 0 | 0 |
| | | | 1 | 1 | | |
| 23 | A | 91 | Total | Mg | 0 | 0 |
| | | | 91 | 91 | | |
| 23 | D | 1 | Total | Mg | 0 | 0 |
| | | | 1 | 1 | | |
| 23 | M | 1 | Total | Mg | 0 | 0 |
| | | | 1 | 1 | | |

- Molecule 24 is POTASSIUM ION (three-letter code: K) (formula: K).

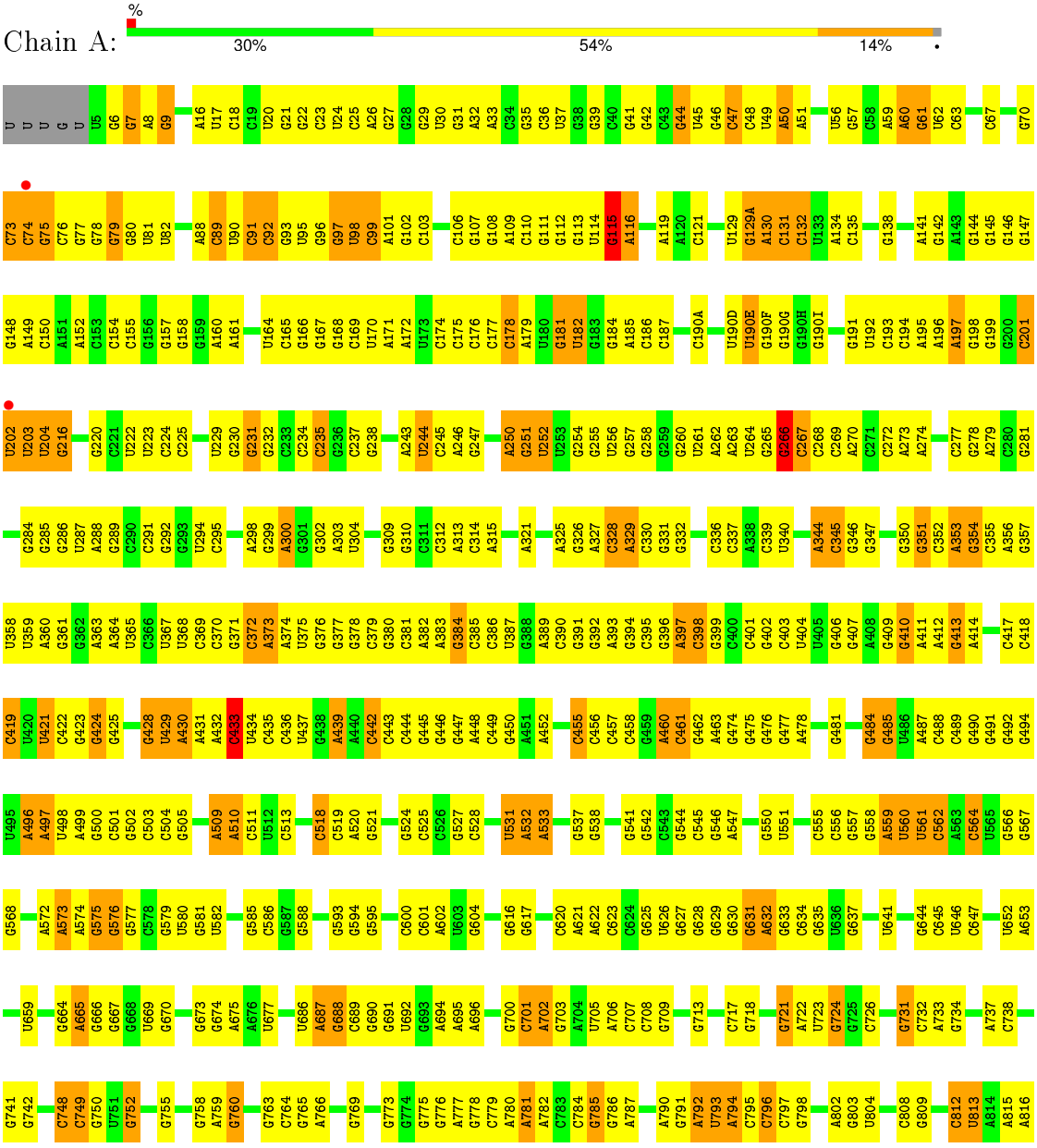
| Mol | Chain | Residues | Atoms | | ZeroOcc | AltConf |
|---|---|---|---|---|---|---|
| 24 | A | 41 | Total | K | 0 | 0 |
| | | | 41 | 41 | | |
| 24 | E | 1 | Total | K | 0 | 0 |
| | | | 1 | 1 | | |

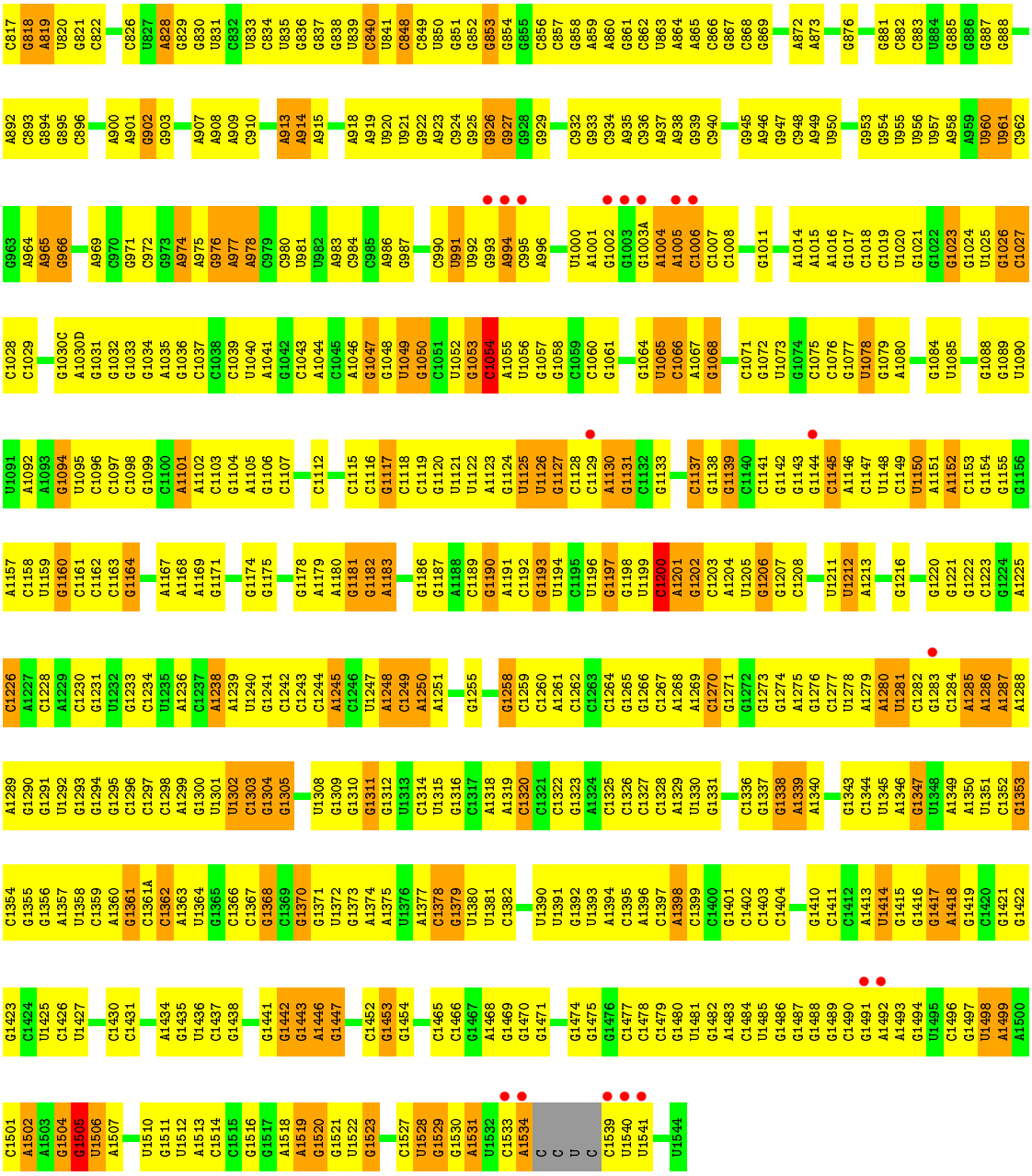
# 3 Residue-property plots (i)

These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of errors 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: 16S rRNA

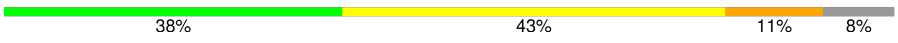
Chain A:

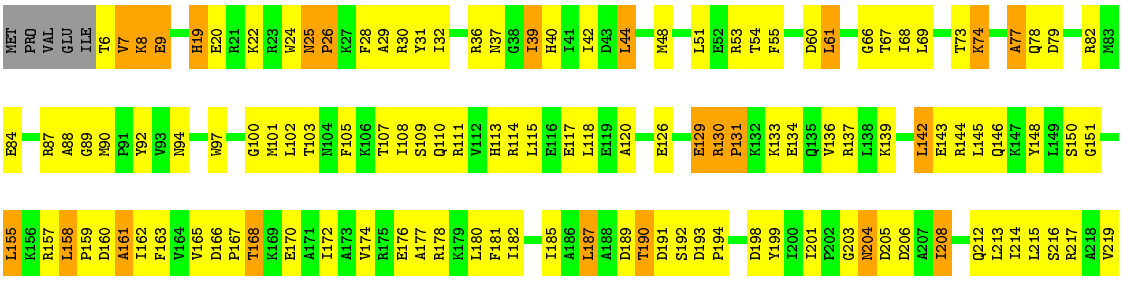


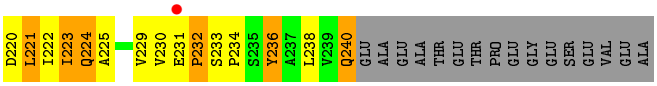


• Molecule 2: 30S RIBOSOMAL PROTEIN S2

Chain B:

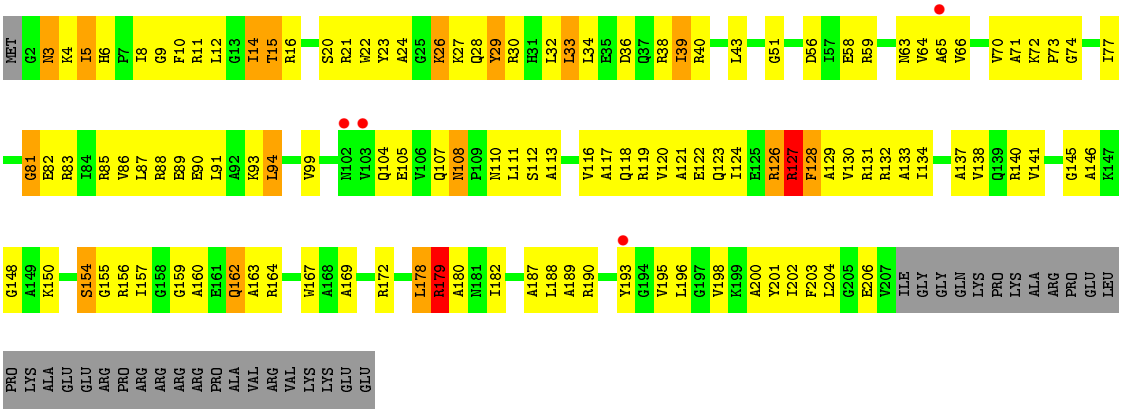




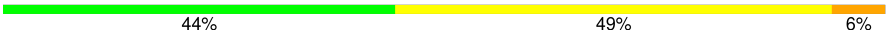
- Molecule 3: 30S RIBOSOMAL PROTEIN S3

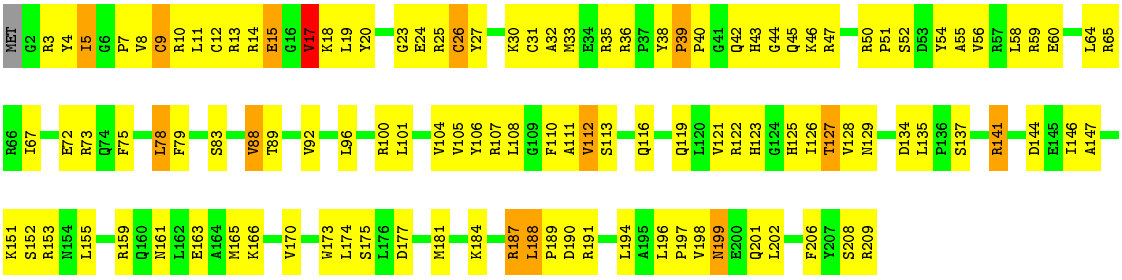
Chain C:

- Molecule 4: 30S RIBOSOMAL PROTEIN S4

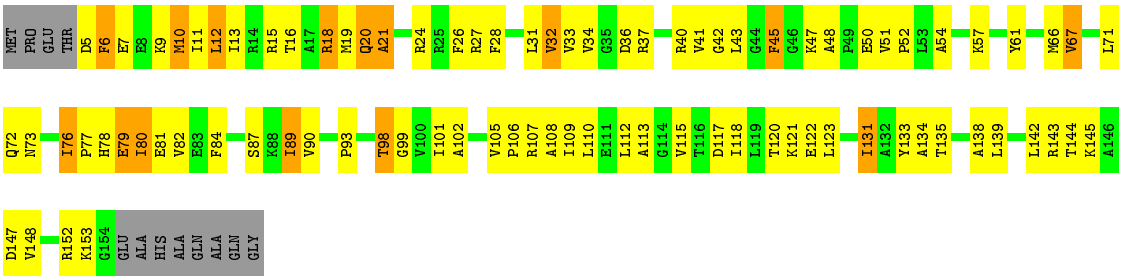
Chain D:



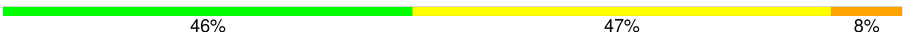
- Molecule 5: 30S RIBOSOMAL PROTEIN S5

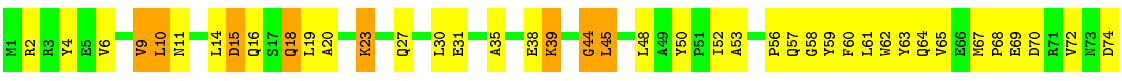
Chain E:

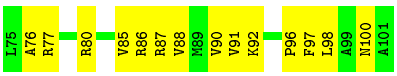



- Molecule 6: 30S RIBOSOMAL PROTEIN S6

Chain F:

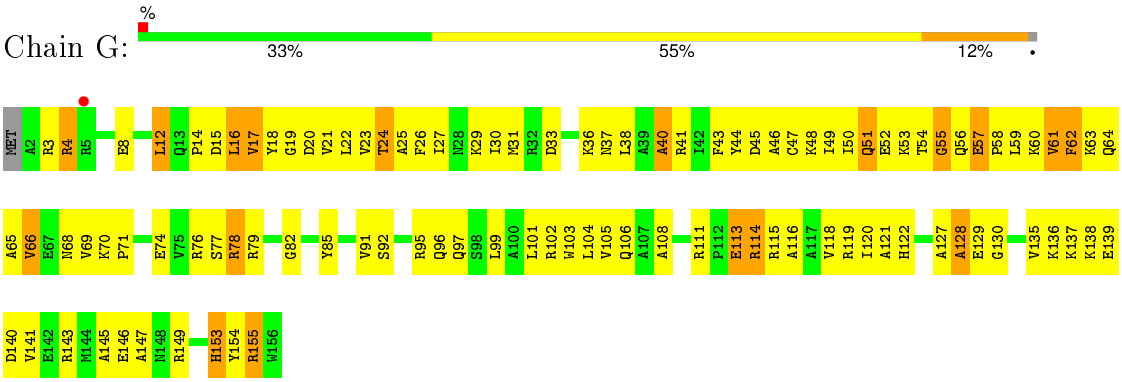




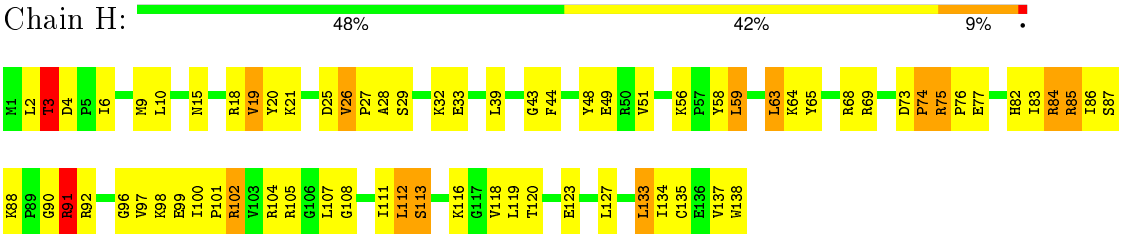

- Molecule 7: 30S RIBOSOMAL PROTEIN S7

Chain G:



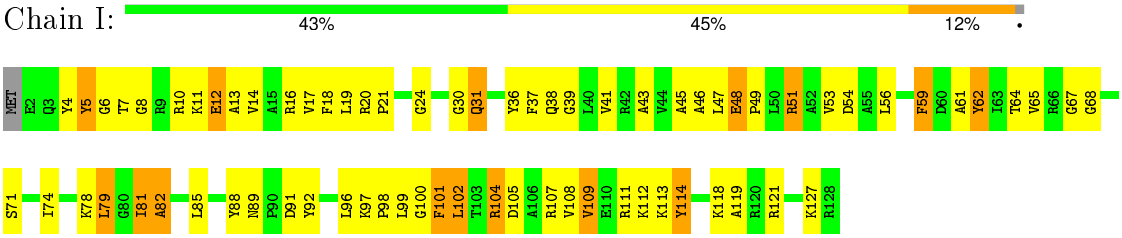

- Molecule 8: 30S RIBOSOMAL PROTEIN S8

Chain H:



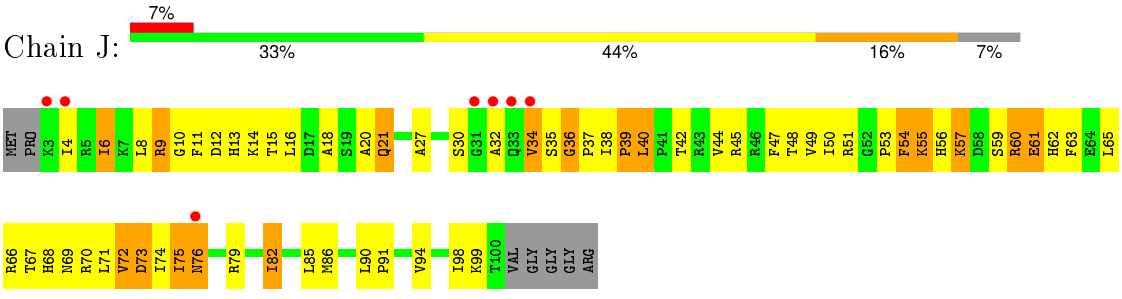

- Molecule 9: 30S RIBOSOMAL PROTEIN S9

Chain I:



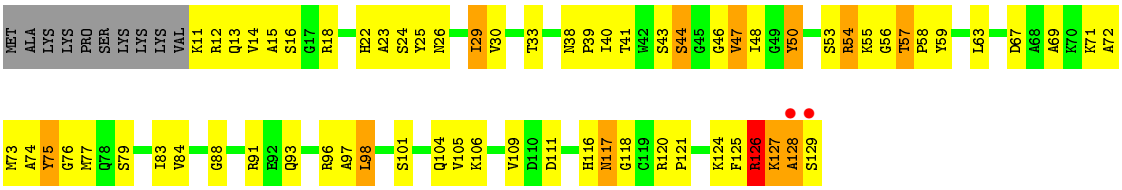

- Molecule 10: 30S RIBOSOMAL PROTEIN S10

Chain J:




- Molecule 11: 30S RIBOSOMAL PROTEIN S11

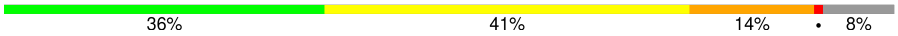
Chain K:

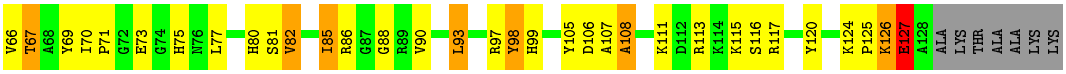




- Molecule 12: 30S RIBOSOMAL PROTEIN S12

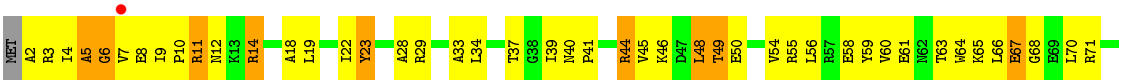
Chain L:



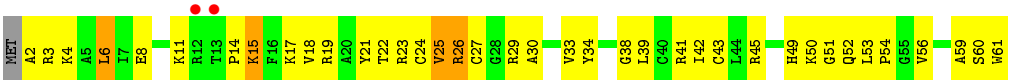
- Molecule 13: 30S RIBOSOMAL PROTEIN S13

Chain M:

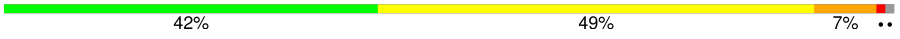
- Molecule 14: 30S RIBOSOMAL PROTEIN S14

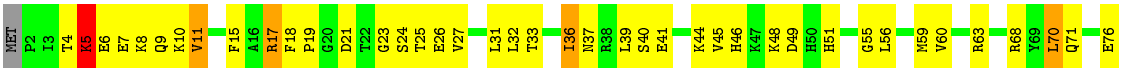
Chain N:

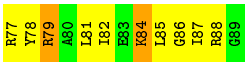



- Molecule 15: 30S RIBOSOMAL PROTEIN S15

Chain O:





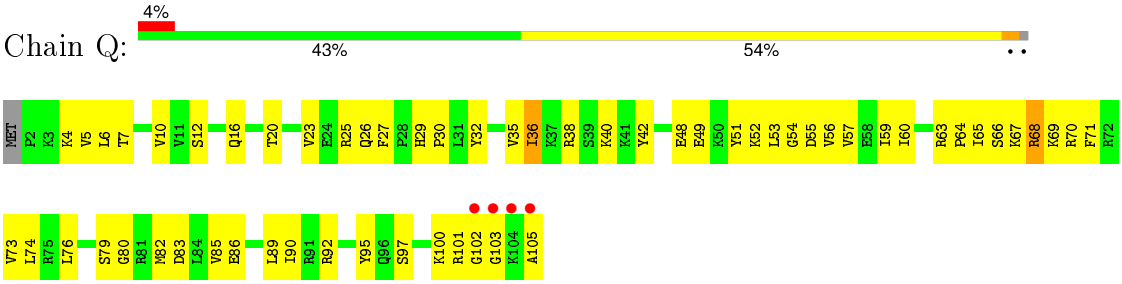
- Molecule 16: 30S RIBOSOMAL PROTEIN S16

Chain P:



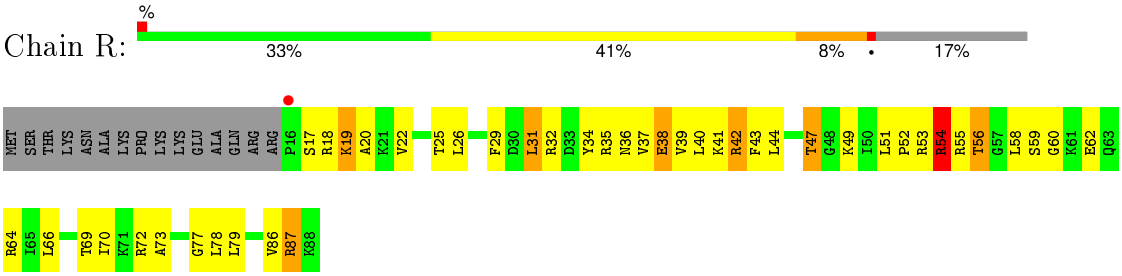

- Molecule 17: 30S RIBOSOMAL PROTEIN S17

Chain Q:



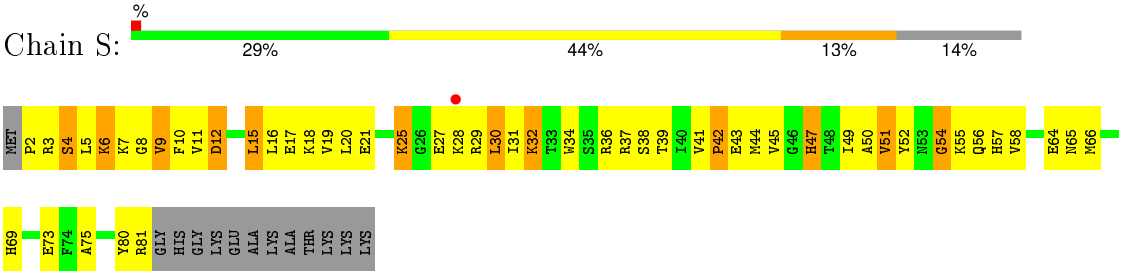

- Molecule 18: 30S RIBOSOMAL PROTEIN S18

Chain R:



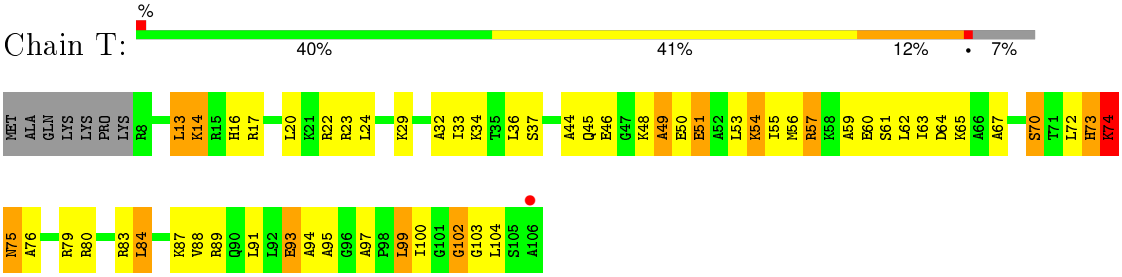

- Molecule 19: 30S RIBOSOMAL PROTEIN S19

Chain S:




- Molecule 20: 30S RIBOSOMAL PROTEIN S20

Chain T:




- Molecule 21: 30S RIBOSOMAL PROTEIN THX

Chain U:

# 4 Data and refinement statistics (i)

| Property | Value | Source |
|---|---|---|
| Space group | P 41 21 2 | Depositor |
| Cell constants<br>a, b, c, $\alpha$, $\beta$, $\gamma$ | 402.09Å 402.09Å 173.25Å<br>90.00° 90.00° 90.00° | Depositor |
| Resolution (Å) | 29.84 – 3.69<br>29.84 – 3.69 | Depositor<br>EDS |
| % Data completeness<br>(in resolution range) | 92.7 (29.84-3.69)<br>97.8 (29.84-3.69) | Depositor<br>EDS |
| $R_{merge}$ | 0.13 | Depositor |
| $R_{sym}$ | (Not available) | Depositor |
| $< I/\sigma(I) >$ [1] | 2.27 (at 3.65Å) | Xtriage |
| Refinement program | PHENIX (phenix.refine: 1.6.4_486) | Depositor |
| R, $R_{free}$ | 0.173 , 0.231<br>0.176 , 0.228 | Depositor<br>DCC |
| $R_{free}$ test set | 7456 reflections (5.31%) | DCC |
| Wilson B-factor (Å$^2$) | 112.1 | Xtriage |
| Anisotropy | 0.382 | Xtriage |
| Bulk solvent $k_{sol}$(e/Å$^3$), $B_{sol}$(Å$^2$) | 0.24 , 85.3 | EDS |
| Estimated twinning fraction | No twinning to report. | Xtriage |
| L-test for twinning[2] | $< \|L\| > = 0.46$, $< L^2 > = 0.29$ | Xtriage |
| Outliers | 0 of 148377 reflections | Xtriage |
| $F_o$,$F_c$ correlation | 0.95 | EDS |
| Total number of atoms | 51775 | wwPDB-VP |
| Average B, all atoms (Å$^2$) | 127.0 | wwPDB-VP |

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 1.71% 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, 0.375 respectively for untwinned datasets, and 0.333, 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: K, 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).

| Mol | Chain | Bond lengths | | Bond angles | |
|---|---|---|---|---|---|
| | | RMSZ | #$\|Z\|>5$ | RMSZ | #$\|Z\|>5$ |
| 1 | A | 0.45 | 0/36390 | 0.81 | 19/56793 (0.0%) |
| 2 | B | 0.32 | 0/1908 | 0.49 | 0/2577 |
| 3 | C | 0.25 | 0/1636 | 0.44 | 0/2205 |
| 4 | D | 0.31 | 0/1733 | 0.47 | 0/2318 |
| 5 | E | 0.39 | 0/1162 | 0.58 | 0/1564 |
| 6 | F | 0.29 | 0/856 | 0.47 | 0/1154 |
| 7 | G | 0.26 | 0/1276 | 0.44 | 0/1709 |
| 8 | H | 0.42 | 0/1136 | 0.59 | 0/1527 |
| 9 | I | 0.28 | 0/1029 | 0.46 | 0/1378 |
| 10 | J | 0.27 | 0/805 | 0.47 | 0/1082 |
| 11 | K | 0.32 | 0/900 | 0.50 | 0/1213 |
| 12 | L | 0.34 | 0/986 | 0.55 | 0/1320 |
| 13 | M | 0.27 | 0/931 | 0.49 | 0/1248 |
| 14 | N | 0.26 | 0/501 | 0.46 | 0/664 |
| 15 | O | 0.33 | 0/745 | 0.51 | 0/992 |
| 16 | P | 0.33 | 0/716 | 0.52 | 0/963 |
| 17 | Q | 0.39 | 0/870 | 0.59 | 0/1159 |
| 18 | R | 0.30 | 0/603 | 0.50 | 0/799 |
| 19 | S | 0.23 | 0/661 | 0.45 | 0/890 |
| 20 | T | 0.31 | 0/764 | 0.50 | 0/1006 |
| 21 | U | 0.28 | 0/212 | 0.51 | 0/277 |
| All | All | 0.41 | 0/55820 | 0.73 | 19/82838 (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 | A | 1 | 0 |

There are no bond length outliers.

The worst 5 of 19 bond angle outliers are listed below:

| Mol | Chain | Res | Type | Atoms | Z | Observed($^o$) | Ideal($^o$) |
|---|---|---|---|---|---|---|---|
| 1 | A | 1505 | G | C4-N9-C1' | 8.15 | 137.09 | 126.50 |
| 1 | A | 1505 | G | C6-C5-N7 | -6.83 | 126.30 | 130.40 |
| 1 | A | 1505 | G | C8-N9-C1' | -6.33 | 118.77 | 127.00 |
| 1 | A | 1505 | G | N7-C8-N9 | 6.30 | 116.25 | 113.10 |
| 1 | A | 235 | C | C6-N1-C2 | 5.81 | 122.62 | 120.30 |

All (1) chirality outliers are listed below:

| Mol | Chain | Res | Type | Atom |
|---|---|---|---|---|
| 1 | A | 410 | G | C3' |

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 | A | 32511 | 0 | 16413 | 1239 | 0 |
| 2 | B | 1873 | 0 | 1887 | 144 | 0 |
| 3 | C | 1612 | 0 | 1677 | 128 | 0 |
| 4 | D | 1703 | 0 | 1763 | 104 | 0 |
| 5 | E | 1146 | 0 | 1207 | 86 | 0 |
| 6 | F | 843 | 0 | 857 | 44 | 0 |
| 7 | G | 1257 | 0 | 1296 | 117 | 0 |
| 8 | H | 1116 | 0 | 1177 | 73 | 0 |
| 9 | I | 1011 | 0 | 1043 | 69 | 0 |
| 10 | J | 792 | 0 | 835 | 73 | 0 |
| 11 | K | 885 | 0 | 904 | 54 | 0 |
| 12 | L | 970 | 0 | 1057 | 95 | 0 |
| 13 | M | 921 | 0 | 978 | 65 | 0 |
| 14 | N | 492 | 0 | 530 | 48 | 0 |
| 15 | O | 734 | 0 | 771 | 59 | 0 |
| 16 | P | 700 | 0 | 720 | 47 | 0 |
| 17 | Q | 857 | 0 | 930 | 59 | 0 |
| 18 | R | 597 | 0 | 668 | 47 | 0 |

*Continued on next page...*

*Continued from previous page...*

| Mol | Chain | Non-H | H(model) | H(added) | Clashes | Symm-Clashes |
|---|---|---|---|---|---|---|
| 19 | S | 647 | 0 | 673 | 47 | 0 |
| 20 | T | 762 | 0 | 859 | 63 | 0 |
| 21 | U | 208 | 0 | 221 | 13 | 0 |
| 22 | D | 1 | 0 | 0 | 0 | 0 |
| 22 | N | 1 | 0 | 0 | 0 | 0 |
| 23 | A | 91 | 0 | 0 | 0 | 0 |
| 23 | B | 1 | 0 | 0 | 0 | 0 |
| 23 | D | 1 | 0 | 0 | 0 | 0 |
| 23 | M | 1 | 0 | 0 | 0 | 0 |
| 24 | A | 41 | 0 | 0 | 0 | 0 |
| 24 | E | 1 | 0 | 0 | 0 | 0 |
| All | All | 51775 | 0 | 36466 | 2487 | 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 28.

The worst 5 of 2487 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) |
|---|---|---|---|
| 15:O:17:ARG:HH11 | 15:O:17:ARG:HG3 | 1.12 | 1.08 |
| 1:A:1057:G:H5" | 3:C:154:SER:HB2 | 1.32 | 1.08 |
| 1:A:559:A:H4' | 1:A:560:U:H3' | 1.35 | 1.06 |
| 11:K:15:ALA:HA | 11:K:77:MET:HA | 1.35 | 1.06 |
| 1:A:1443:G:H4' | 1:A:1446:A:O5' | 1.55 | 1.02 |

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 |
|---|---|---|---|---|---|---|
| 2 | B | 233/256 (91%) | 168 (72%) | 45 (19%) | 20 (9%) | 1 16 |

*Continued on next page...*

*Continued from previous page...*

| Mol | Chain | Analysed | Favoured | Allowed | Outliers | Percentiles |
|---|---|---|---|---|---|---|
| 3 | C | 204/239 (85%) | 152 (74%) | 37 (18%) | 15 (7%) | 1 21 |
| 4 | D | 206/209 (99%) | 168 (82%) | 32 (16%) | 6 (3%) | 6 46 |
| 5 | E | 148/162 (91%) | 119 (80%) | 26 (18%) | 3 (2%) | 9 55 |
| 6 | F | 99/101 (98%) | 80 (81%) | 17 (17%) | 2 (2%) | 9 55 |
| 7 | G | 153/156 (98%) | 105 (69%) | 34 (22%) | 14 (9%) | 1 15 |
| 8 | H | 136/138 (99%) | 115 (85%) | 15 (11%) | 6 (4%) | 3 35 |
| 9 | I | 125/128 (98%) | 86 (69%) | 28 (22%) | 11 (9%) | 1 15 |
| 10 | J | 96/105 (91%) | 60 (62%) | 22 (23%) | 14 (15%) | 0 5 |
| 11 | K | 117/129 (91%) | 85 (73%) | 22 (19%) | 10 (8%) | 1 16 |
| 12 | L | 122/135 (90%) | 87 (71%) | 22 (18%) | 13 (11%) | 0 10 |
| 13 | M | 113/126 (90%) | 91 (80%) | 16 (14%) | 6 (5%) | 2 29 |
| 14 | N | 58/61 (95%) | 40 (69%) | 13 (22%) | 5 (9%) | 1 16 |
| 15 | O | 86/89 (97%) | 70 (81%) | 13 (15%) | 3 (4%) | 4 43 |
| 16 | P | 81/88 (92%) | 63 (78%) | 11 (14%) | 7 (9%) | 1 16 |
| 17 | Q | 102/105 (97%) | 86 (84%) | 14 (14%) | 2 (2%) | 9 55 |
| 18 | R | 71/88 (81%) | 53 (75%) | 14 (20%) | 4 (6%) | 2 28 |
| 19 | S | 78/93 (84%) | 47 (60%) | 19 (24%) | 12 (15%) | 0 5 |
| 20 | T | 97/106 (92%) | 60 (62%) | 28 (29%) | 9 (9%) | 1 15 |
| 21 | U | 22/27 (82%) | 17 (77%) | 5 (23%) | 0 | 100 100 |
| All | All | 2347/2541 (92%) | 1752 (75%) | 433 (18%) | 162 (7%) | 1 23 |

5 of 162 Ramachandran outliers are listed below:

| Mol | Chain | Res | Type |
|---|---|---|---|
| 2 | B | 7 | VAL |
| 2 | B | 8 | LYS |
| 3 | C | 15 | THR |
| 3 | C | 29 | TYR |
| 3 | C | 127 | 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 sidechain conformation was analysed, and the total number of residues.

| Mol | Chain | Analysed | Rotameric | Outliers | Percentiles |
|---|---|---|---|---|---|
| 2 | B | 194/220 (88%) | 173 (89%) | 21 (11%) | 8 41 |
| 3 | C | 160/188 (85%) | 148 (92%) | 12 (8%) | 17 57 |
| 4 | D | 180/181 (99%) | 166 (92%) | 14 (8%) | 16 56 |
| 5 | E | 115/123 (94%) | 98 (85%) | 17 (15%) | 4 26 |
| 6 | F | 90/90 (100%) | 81 (90%) | 9 (10%) | 9 44 |
| 7 | G | 126/127 (99%) | 116 (92%) | 10 (8%) | 15 55 |
| 8 | H | 119/119 (100%) | 104 (87%) | 15 (13%) | 5 32 |
| 9 | I | 98/99 (99%) | 87 (89%) | 11 (11%) | 7 39 |
| 10 | J | 87/92 (95%) | 80 (92%) | 7 (8%) | 15 55 |
| 11 | K | 90/99 (91%) | 80 (89%) | 10 (11%) | 8 39 |
| 12 | L | 104/111 (94%) | 90 (86%) | 14 (14%) | 5 31 |
| 13 | M | 93/101 (92%) | 81 (87%) | 12 (13%) | 5 32 |
| 14 | N | 49/50 (98%) | 47 (96%) | 2 (4%) | 37 75 |
| 15 | O | 79/80 (99%) | 69 (87%) | 10 (13%) | 5 32 |
| 16 | P | 72/74 (97%) | 63 (88%) | 9 (12%) | 6 33 |
| 17 | Q | 96/97 (99%) | 92 (96%) | 4 (4%) | 36 75 |
| 18 | R | 64/77 (83%) | 57 (89%) | 7 (11%) | 8 40 |
| 19 | S | 71/80 (89%) | 64 (90%) | 7 (10%) | 10 45 |
| 20 | T | 76/82 (93%) | 67 (88%) | 9 (12%) | 6 36 |
| 21 | U | 19/22 (86%) | 17 (90%) | 2 (10%) | 8 42 |
| All | All | 1982/2112 (94%) | 1780 (90%) | 202 (10%) | 9 43 |

5 of 202 residues with a non-rotameric sidechain are listed below:

| Mol | Chain | Res | Type |
|---|---|---|---|
| 8 | H | 85 | ARG |
| 10 | J | 57 | LYS |
| 19 | S | 18 | LYS |
| 8 | H | 102 | ARG |
| 9 | I | 79 | LEU |

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 50 such sidechains are listed below:

| Mol | Chain | Res | Type |
|---|---|---|---|
| 7 | G | 37 | ASN |
| 8 | H | 82 | HIS |
| 19 | S | 47 | HIS |
| 7 | G | 68 | ASN |
| 7 | G | 97 | GLN |

### 5.3.3 RNA

| Mol | Chain | Analysed | Backbone Outliers | Pucker Outliers |
|---|---|---|---|---|
| 1 | A | 1511/1522 (99%) | 281 (18%) | 35 (2%) |

5 of 281 RNA backbone outliers are listed below:

| Mol | Chain | Res | Type |
|---|---|---|---|
| 1 | A | 7 | G |
| 1 | A | 9 | G |
| 1 | A | 31 | G |
| 1 | A | 32 | A |
| 1 | A | 33 | A |

5 of 35 RNA pucker outliers are listed below:

| Mol | Chain | Res | Type |
|---|---|---|---|
| 1 | A | 560 | U |
| 1 | A | 812 | C |
| 1 | A | 1504 | G |
| 1 | A | 687 | A |
| 1 | A | 701 | C |

## 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 carbohydrates in this entry.

## 5.6 Ligand geometry

Of 138 ligands modelled in this entry, 138 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

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 | 1513/1522 (99%) | -0.28 | 20 (1%) 79 66 | 50, 108, 253, 361 | 0 |
| 2 | B | 235/256 (91%) | -0.63 | 1 (0%) 93 88 | 65, 115, 197, 256 | 0 |
| 3 | C | 206/239 (86%) | -0.34 | 4 (1%) 70 55 | 116, 170, 237, 271 | 0 |
| 4 | D | 208/209 (99%) | -0.52 | 0 100 100 | 63, 111, 160, 175 | 0 |
| 5 | E | 150/162 (92%) | -0.63 | 0 100 100 | 51, 78, 114, 154 | 0 |
| 6 | F | 101/101 (100%) | -0.65 | 0 100 100 | 87, 129, 155, 177 | 0 |
| 7 | G | 155/156 (99%) | -0.46 | 1 (0%) 90 83 | 99, 152, 220, 233 | 0 |
| 8 | H | 138/138 (100%) | -0.73 | 0 100 100 | 41, 72, 104, 137 | 0 |
| 9 | I | 127/128 (99%) | -0.45 | 0 100 100 | 78, 171, 216, 224 | 0 |
| 10 | J | 98/105 (93%) | 0.08 | 7 (7%) 19 11 | 122, 178, 274, 291 | 0 |
| 11 | K | 119/129 (92%) | -0.50 | 2 (1%) 73 58 | 62, 106, 146, 183 | 0 |
| 12 | L | 124/135 (91%) | -0.49 | 0 100 100 | 48, 107, 143, 174 | 0 |
| 13 | M | 115/126 (91%) | -0.41 | 1 (0%) 85 75 | 96, 136, 170, 180 | 0 |
| 14 | N | 60/61 (98%) | -0.04 | 2 (3%) 50 35 | 125, 157, 213, 229 | 0 |
| 15 | O | 88/89 (98%) | -0.65 | 0 100 100 | 54, 95, 133, 171 | 0 |
| 16 | P | 83/88 (94%) | -0.67 | 0 100 100 | 69, 99, 137, 199 | 0 |
| 17 | Q | 104/105 (99%) | -0.46 | 4 (3%) 44 30 | 54, 83, 125, 223 | 0 |
| 18 | R | 73/88 (82%) | -0.60 | 1 (1%) 78 64 | 65, 99, 164, 209 | 0 |
| 19 | S | 80/93 (86%) | -0.07 | 1 (1%) 79 66 | 149, 183, 219, 231 | 0 |
| 20 | T | 99/106 (93%) | -0.66 | 1 (1%) 84 72 | 76, 107, 165, 190 | 0 |
| 21 | U | 24/27 (88%) | 0.51 | 4 (16%) 2 2 | 121, 141, 162, 171 | 0 |
| All | All | 3900/4063 (95%) | -0.40 | 49 (1%) 79 66 | 41, 116, 222, 361 | 0 |

The worst 5 of 49 RSRZ outliers are listed below:

| Mol | Chain | Res | Type | RSRZ |
|---|---|---|---|---|
| 11 | K | 128 | ALA | 8.5 |
| 17 | Q | 103 | GLY | 6.9 |
| 1 | A | 1541 | U | 6.8 |
| 17 | Q | 104 | LYS | 6.5 |
| 10 | J | 33 | GLN | 5.7 |

## 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)

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. LLDF column lists the quality of electron density of the group with respect to its neighbouring residues in protein, DNA or RNA chains. 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 | LLDF | B-factors(Å$^2$) | Q<0.9 |
|---|---|---|---|---|---|---|---|---|---|
| 24 | K | A | 1658 | 1/1 | 0.91 | 0.62 | 60.18 | 107,107,107,107 | 0 |
| 24 | K | A | 1666 | 1/1 | 0.74 | 0.55 | 42.77 | 74,74,74,74 | 0 |
| 24 | K | A | 1641 | 1/1 | 0.91 | 0.69 | 35.75 | 97,97,97,97 | 0 |
| 23 | MG | A | 1554 | 1/1 | 0.95 | 0.59 | 33.58 | 59,59,59,59 | 0 |
| 23 | MG | A | 1620 | 1/1 | 0.61 | 0.94 | 25.06 | 92,92,92,92 | 0 |
| 24 | K | A | 1668 | 1/1 | 0.90 | 0.43 | 20.26 | 95,95,95,95 | 0 |
| 23 | MG | A | 1605 | 1/1 | 0.94 | 1.19 | 19.49 | 56,56,56,56 | 0 |
| 24 | K | A | 1636 | 1/1 | 0.94 | 0.79 | 16.23 | 116,116,116,116 | 0 |
| 23 | MG | A | 1628 | 1/1 | 0.72 | 0.42 | 16.19 | 65,65,65,65 | 0 |
| 24 | K | A | 1644 | 1/1 | 0.96 | 0.49 | 13.94 | 55,55,55,55 | 0 |
| 23 | MG | A | 1603 | 1/1 | 0.70 | 0.49 | 12.15 | 100,100,100,100 | 0 |
| 23 | MG | A | 1606 | 1/1 | 0.84 | 0.42 | 11.86 | 65,65,65,65 | 0 |
| 24 | K | A | 1635 | 1/1 | 0.51 | 0.63 | 9.20 | 149,149,149,149 | 0 |
| 23 | MG | A | 1607 | 1/1 | 0.98 | 0.60 | 9.02 | 65,65,65,65 | 0 |
| 24 | K | A | 1651 | 1/1 | 0.92 | 0.48 | 8.85 | 138,138,138,138 | 0 |
| 23 | MG | A | 1590 | 1/1 | 0.96 | 0.33 | 7.99 | 39,39,39,39 | 0 |
| 23 | MG | A | 1622 | 1/1 | 0.86 | 0.55 | 7.97 | 87,87,87,87 | 0 |

*Continued on next page...*

*Continued from previous page...*

| Mol | Type | Chain | Res | Atoms | RSCC | RSR | LLDF | B-factors(Å$^2$) | Q<0.9 |
|---|---|---|---|---|---|---|---|---|---|
| 23 | MG | A | 1618 | 1/1 | 0.93 | 0.49 | 7.56 | 64,64,64,64 | 0 |
| 24 | K | A | 1670 | 1/1 | 0.94 | 0.32 | 6.72 | 107,107,107,107 | 0 |
| 23 | MG | A | 1623 | 1/1 | 0.85 | 0.37 | 6.69 | 77,77,77,77 | 0 |
| 24 | K | A | 1669 | 1/1 | 0.95 | 0.46 | 5.99 | 98,98,98,98 | 0 |
| 23 | MG | M | 127 | 1/1 | 0.96 | 0.42 | 5.78 | 76,76,76,76 | 0 |
| 23 | MG | A | 1625 | 1/1 | 0.88 | 0.24 | 4.41 | 93,93,93,93 | 0 |
| 24 | K | A | 1648 | 1/1 | 0.97 | 0.25 | 4.40 | 63,63,63,63 | 0 |
| 23 | MG | B | 257 | 1/1 | 0.69 | 0.38 | 3.82 | 77,77,77,77 | 0 |
| 23 | MG | A | 1589 | 1/1 | 0.95 | 0.23 | 3.75 | 79,79,79,79 | 0 |
| 23 | MG | A | 94 | 1/1 | 0.94 | 0.23 | 3.73 | 66,66,66,66 | 0 |
| 23 | MG | A | 1629 | 1/1 | 0.97 | 0.41 | 3.13 | 61,61,61,61 | 0 |
| 23 | MG | A | 1563 | 1/1 | 0.95 | 0.26 | 2.86 | 20,20,20,20 | 0 |
| 23 | MG | A | 1566 | 1/1 | 0.90 | 0.37 | 2.51 | 90,90,90,90 | 0 |
| 23 | MG | A | 1578 | 1/1 | 0.80 | 0.51 | 2.41 | 50,50,50,50 | 0 |
| 23 | MG | A | 1615 | 1/1 | 0.97 | 0.18 | 2.39 | 55,55,55,55 | 0 |
| 23 | MG | A | 86 | 1/1 | 0.93 | 0.22 | 1.89 | 59,59,59,59 | 0 |
| 23 | MG | A | 1613 | 1/1 | 0.99 | 0.18 | 1.58 | 39,39,39,39 | 0 |
| 23 | MG | A | 1567 | 1/1 | 0.98 | 0.24 | 1.35 | 70,70,70,70 | 0 |
| 23 | MG | A | 1579 | 1/1 | 0.98 | 0.21 | 1.22 | 29,29,29,29 | 0 |
| 23 | MG | A | 1611 | 1/1 | 0.95 | 0.18 | 1.03 | 56,56,56,56 | 0 |
| 23 | MG | A | 1585 | 1/1 | 0.98 | 0.26 | 0.98 | 78,78,78,78 | 0 |
| 23 | MG | A | 1594 | 1/1 | 0.96 | 0.14 | 0.70 | 46,46,46,46 | 0 |
| 22 | ZN | D | 210 | 1/1 | 0.99 | 0.32 | 0.30 | 85,85,85,85 | 0 |
| 23 | MG | A | 1595 | 1/1 | 0.96 | 0.18 | 0.01 | 33,33,33,33 | 0 |
| 23 | MG | A | 1604 | 1/1 | 0.92 | 0.18 | -0.41 | 52,52,52,52 | 0 |
| 23 | MG | D | 211 | 1/1 | 0.93 | 0.14 | -0.71 | 73,73,73,73 | 0 |
| 22 | ZN | N | 141 | 1/1 | 0.99 | 0.07 | -1.41 | 150,150,150,150 | 0 |
| 24 | K | A | 1650 | 1/1 | 0.97 | 0.11 | -1.64 | 86,86,86,86 | 0 |
| 23 | MG | A | 1624 | 1/1 | 0.90 | 0.11 | -1.77 | 38,38,38,38 | 0 |
| 23 | MG | A | 1621 | 1/1 | 0.98 | 0.11 | -2.57 | 58,58,58,58 | 0 |
| 24 | K | A | 1647 | 1/1 | 0.93 | 0.17 | - | 85,85,85,85 | 0 |
| 24 | K | A | 1649 | 1/1 | 0.98 | 0.26 | - | 75,75,75,75 | 0 |
| 23 | MG | A | 1609 | 1/1 | 0.86 | 0.77 | - | 96,96,96,96 | 0 |
| 23 | MG | A | 1545 | 1/1 | 0.93 | 0.22 | - | 75,75,75,75 | 0 |
| 23 | MG | A | 1582 | 1/1 | 0.91 | 0.76 | - | 83,83,83,83 | 0 |
| 23 | MG | A | 1601 | 1/1 | 0.88 | 0.22 | - | 78,78,78,78 | 0 |
| 23 | MG | A | 1569 | 1/1 | 0.97 | 0.21 | - | 59,59,59,59 | 0 |
| 24 | K | A | 1632 | 1/1 | 0.93 | 0.16 | - | 102,102,102,102 | 0 |
| 23 | MG | A | 1556 | 1/1 | 0.89 | 0.49 | - | 93,93,93,93 | 0 |
| 24 | K | E | 163 | 1/1 | 0.93 | 0.29 | - | 115,115,115,115 | 0 |
| 23 | MG | A | 1565 | 1/1 | 0.90 | 0.40 | - | 87,87,87,87 | 0 |
| 23 | MG | A | 1597 | 1/1 | 0.89 | 0.26 | - | 47,47,47,47 | 0 |

*Continued on next page...*

*Continued from previous page...*

| Mol | Type | Chain | Res | Atoms | RSCC | RSR | LLDF | B-factors(Å$^2$) | Q<0.9 |
|---|---|---|---|---|---|---|---|---|---|
| 23 | MG | A | 1559 | 1/1 | 0.85 | 0.90 | - | 53,53,53,53 | 0 |
| 23 | MG | A | 1576 | 1/1 | 0.81 | 0.53 | - | 78,78,78,78 | 0 |
| 24 | K | A | 1657 | 1/1 | 0.96 | 0.56 | - | 83,83,83,83 | 0 |
| 23 | MG | A | 1564 | 1/1 | 0.93 | 0.33 | - | 59,59,59,59 | 0 |
| 24 | K | A | 1653 | 1/1 | 0.98 | 0.15 | - | 98,98,98,98 | 0 |
| 24 | K | A | 1662 | 1/1 | 0.93 | 0.28 | - | 92,92,92,92 | 0 |
| 23 | MG | A | 1573 | 1/1 | 0.81 | 0.36 | - | 70,70,70,70 | 0 |
| 23 | MG | A | 1627 | 1/1 | 0.95 | 0.54 | - | 39,39,39,39 | 0 |
| 23 | MG | A | 1547 | 1/1 | 0.52 | 0.52 | - | 86,86,86,86 | 0 |
| 24 | K | A | 1645 | 1/1 | 0.96 | 0.37 | - | 75,75,75,75 | 0 |
| 24 | K | A | 1665 | 1/1 | 0.95 | 0.35 | - | 79,79,79,79 | 0 |
| 23 | MG | A | 1581 | 1/1 | 0.75 | 0.46 | - | 68,68,68,68 | 0 |
| 23 | MG | A | 1599 | 1/1 | 0.79 | 0.57 | - | 65,65,65,65 | 0 |
| 23 | MG | A | 1552 | 1/1 | 0.96 | 0.21 | - | 80,80,80,80 | 0 |
| 23 | MG | A | 1586 | 1/1 | 0.92 | 0.33 | - | 48,48,48,48 | 0 |
| 24 | K | A | 1661 | 1/1 | 0.93 | 0.14 | - | 79,79,79,79 | 0 |
| 23 | MG | A | 1555 | 1/1 | 0.84 | 0.26 | - | 95,95,95,95 | 0 |
| 24 | K | A | 1638 | 1/1 | 0.82 | 0.33 | - | 143,143,143,143 | 0 |
| 24 | K | A | 1633 | 1/1 | 0.95 | 0.19 | - | 135,135,135,135 | 0 |
| 23 | MG | A | 1560 | 1/1 | 0.77 | 0.52 | - | 89,89,89,89 | 0 |
| 23 | MG | A | 1614 | 1/1 | 0.98 | 0.14 | - | 56,56,56,56 | 0 |
| 23 | MG | A | 1553 | 1/1 | 0.92 | 0.70 | - | 94,94,94,94 | 0 |
| 23 | MG | A | 1574 | 1/1 | 0.64 | 0.93 | - | 68,68,68,68 | 0 |
| 24 | K | A | 1667 | 1/1 | 0.95 | 0.39 | - | 80,80,80,80 | 0 |
| 23 | MG | A | 1617 | 1/1 | 0.98 | 0.32 | - | 78,78,78,78 | 0 |
| 23 | MG | A | 1608 | 1/1 | 0.89 | 0.33 | - | 72,72,72,72 | 0 |
| 24 | K | A | 1654 | 1/1 | 0.91 | 0.34 | - | 85,85,85,85 | 0 |
| 23 | MG | A | 1551 | 1/1 | 0.79 | 0.55 | - | 50,50,50,50 | 0 |
| 23 | MG | A | 1602 | 1/1 | 0.94 | 0.44 | - | 63,63,63,63 | 0 |
| 23 | MG | A | 1558 | 1/1 | 0.57 | 0.43 | - | 81,81,81,81 | 0 |
| 23 | MG | A | 1588 | 1/1 | 0.84 | 0.22 | - | 59,59,59,59 | 0 |
| 24 | K | A | 1656 | 1/1 | 0.78 | 0.42 | - | 105,105,105,105 | 0 |
| 23 | MG | A | 85 | 1/1 | 0.97 | 0.38 | - | 35,35,35,35 | 0 |
| 23 | MG | A | 1570 | 1/1 | 0.90 | 0.69 | - | 34,34,34,34 | 0 |
| 24 | K | A | 1639 | 1/1 | 0.98 | 0.64 | - | 81,81,81,81 | 0 |
| 23 | MG | A | 1593 | 1/1 | 0.58 | 0.57 | - | 87,87,87,87 | 0 |
| 23 | MG | A | 1610 | 1/1 | 0.94 | 0.28 | - | 47,47,47,47 | 0 |
| 23 | MG | A | 1549 | 1/1 | 0.77 | 0.48 | - | 59,59,59,59 | 0 |
| 23 | MG | A | 1557 | 1/1 | 0.75 | 0.84 | - | 90,90,90,90 | 0 |
| 24 | K | A | 1659 | 1/1 | 0.97 | 0.30 | - | 76,76,76,76 | 0 |
| 23 | MG | A | 1562 | 1/1 | 0.92 | 0.73 | - | 54,54,54,54 | 0 |
| 24 | K | A | 1642 | 1/1 | 0.97 | 0.49 | - | 94,94,94,94 | 0 |

*Continued on next page...*

*Continued from previous page...*

| Mol | Type | Chain | Res | Atoms | RSCC | RSR | LLDF | B-factors(Å$^2$) | Q<0.9 |
|---|---|---|---|---|---|---|---|---|---|
| 23 | MG | A | 1630 | 1/1 | 0.97 | 0.31 | - | 41,41,41,41 | 0 |
| 23 | MG | A | 1584 | 1/1 | 0.95 | 0.56 | - | 52,52,52,52 | 0 |
| 23 | MG | A | 1561 | 1/1 | 0.93 | 0.13 | - | 59,59,59,59 | 0 |
| 23 | MG | A | 1587 | 1/1 | 0.91 | 0.42 | - | 37,37,37,37 | 0 |
| 23 | MG | A | 1571 | 1/1 | 0.85 | 0.46 | - | 67,67,67,67 | 0 |
| 24 | K | A | 1663 | 1/1 | 0.94 | 0.55 | - | 99,99,99,99 | 0 |
| 23 | MG | A | 1546 | 1/1 | 0.90 | 0.75 | - | 76,76,76,76 | 0 |
| 23 | MG | A | 1575 | 1/1 | 0.95 | 0.59 | - | 32,32,32,32 | 0 |
| 24 | K | A | 1646 | 1/1 | 0.97 | 0.54 | - | 82,82,82,82 | 0 |
| 23 | MG | A | 1612 | 1/1 | 0.82 | 0.25 | - | 81,81,81,81 | 0 |
| 23 | MG | A | 100 | 1/1 | 0.99 | 0.20 | - | 126,126,126,126 | 0 |
| 23 | MG | A | 1548 | 1/1 | 0.75 | 0.94 | - | 81,81,81,81 | 0 |
| 23 | MG | A | 1577 | 1/1 | 0.88 | 0.59 | - | 63,63,63,63 | 0 |
| 23 | MG | A | 1580 | 1/1 | 0.96 | 0.43 | - | 79,79,79,79 | 0 |
| 23 | MG | A | 1583 | 1/1 | 0.72 | 0.39 | - | 67,67,67,67 | 0 |
| 23 | MG | A | 1626 | 1/1 | 0.96 | 0.16 | - | 62,62,62,62 | 0 |
| 24 | K | A | 1634 | 1/1 | 0.92 | 0.20 | - | 134,134,134,134 | 0 |
| 23 | MG | A | 1550 | 1/1 | 0.93 | 0.21 | - | 52,52,52,52 | 0 |
| 24 | K | A | 1652 | 1/1 | 0.88 | 0.23 | - | 100,100,100,100 | 0 |
| 23 | MG | A | 1596 | 1/1 | 0.69 | 1.22 | - | 54,54,54,54 | 0 |
| 23 | MG | A | 1619 | 1/1 | 0.77 | 0.47 | - | 91,91,91,91 | 0 |
| 24 | K | A | 1631 | 1/1 | 0.86 | 0.35 | - | 110,110,110,110 | 0 |
| 24 | K | A | 1664 | 1/1 | 0.86 | 0.23 | - | 111,111,111,111 | 0 |
| 23 | MG | A | 1591 | 1/1 | 0.84 | 0.34 | - | 82,82,82,82 | 0 |
| 24 | K | A | 1660 | 1/1 | 0.91 | 0.19 | - | 126,126,126,126 | 0 |
| 23 | MG | A | 1568 | 1/1 | 0.97 | 0.11 | - | 17,17,17,17 | 0 |
| 23 | MG | A | 1616 | 1/1 | 0.94 | 0.41 | - | 49,49,49,49 | 0 |
| 23 | MG | A | 71 | 1/1 | 0.85 | 0.81 | - | 74,74,74,74 | 0 |
| 24 | K | A | 1671 | 1/1 | 0.89 | 0.50 | - | 79,79,79,79 | 0 |
| 24 | K | A | 1643 | 1/1 | 0.96 | 0.27 | - | 122,122,122,122 | 0 |
| 23 | MG | A | 1572 | 1/1 | 0.96 | 0.40 | - | 35,35,35,35 | 0 |
| 24 | K | A | 1655 | 1/1 | 0.69 | 0.45 | - | 102,102,102,102 | 0 |
| 23 | MG | A | 1600 | 1/1 | 0.92 | 0.58 | - | 72,72,72,72 | 0 |
| 24 | K | A | 1640 | 1/1 | 0.93 | 0.53 | - | 108,108,108,108 | 0 |
| 24 | K | A | 1637 | 1/1 | 0.97 | 0.39 | - | 129,129,129,129 | 0 |
| 23 | MG | A | 1592 | 1/1 | 0.94 | 0.36 | - | 63,63,63,63 | 0 |
| 23 | MG | A | 1598 | 1/1 | 0.78 | 0.67 | - | 73,73,73,73 | 0 |

## 6.5 Other polymers (i)

There are no such residues in this entry.