



# wwPDB X-ray Structure Validation Summary Report i

Oct 10, 2014 – 01:46 PM EDT

PDB ID : 4RB9  
Title : Crystal structure of the *Thermus thermophilus* 70S ribosome in complex with pactamycin (soaked), mRNA and three deacylated tRNAs in the A, P and E sites  
Authors : Polikanov, Y.S.; Osterman, I.A.; Szal, T.; Tashlitsky, V.N.; Serebryakova, M.V.; Kusochev, P.; Bulkley, D.; Malanicheva, I.A.; Efimenko, T.A.; Efremenkova, O.V.; Konevega, A.L.; Shaw, K.J.; Bogdanov, A.A.; Rodnina, M.V.; Dontsova, O.A.; Mankin, A.S.; Steitz, T.A.; Sergiev, P.V.  
Deposited on : 2014-09-12  
Resolution : 2.55 Å(reported)

This is a wwPDB validation summary report for a publicly released PDB entry.

We welcome your comments at [validation@mail.wwpdb.org](mailto:validation@mail.wwpdb.org)

A user guide is available at <http://wwpdb.org/ValidationPDFNotes.html>

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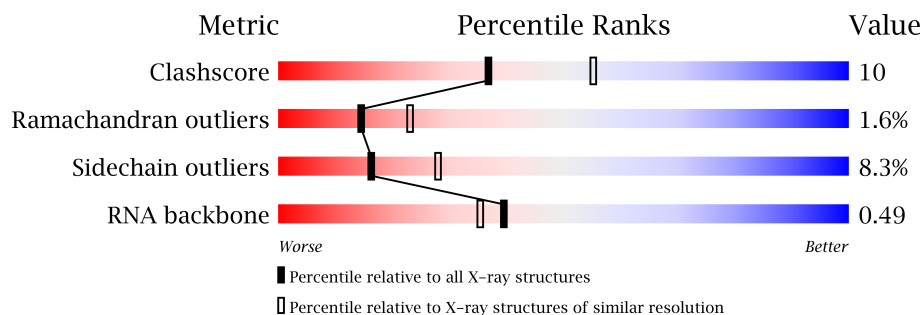
The following versions of software and data (see [references](#)) were used in the production of this report:

|                                |   |                          |
|--------------------------------|---|--------------------------|
| MolProbity                     | : | 4.02b-467                |
| Mogul                          | : | 1.16 November 2013       |
| Xtriage (Phenix)               | : | <b>NOT EXECUTED</b>      |
| EDS                            | : | <b>NOT EXECUTED</b>      |
| Percentile statistics          | : | 21963                    |
| Ideal geometry (proteins)      | : | Engh & Huber (2001)      |
| Ideal geometry (DNA, RNA)      | : | Parkinson et. al. (1996) |
| Validation Pipeline (wwPDB-VP) | : | stable23828              |

# 1 Overall quality at a glance

The reported resolution of this entry is 2.55 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<br>(#Entries) | Similar resolution<br>(#Entries, resolution range(Å)) |
|-----------------------|-----------------------------|---|
| Clashscore            | 79885                       | 4284 (2.58-2.50)                                      |
| Ramachandran outliers | 78287                       | 4193 (2.58-2.50)                                      |
| Sidechain outliers    | 78261                       | 4195 (2.58-2.50)                                      |
| RNA backbone          | 1838                        | 1058 (3.10-1.98)                                      |







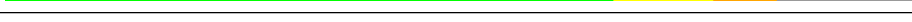

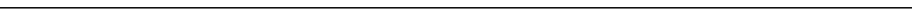


The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments on the lower bar indicate the fraction of residues that contain outliers for  $\geq 3$ , 2, 1 and 0 types of geometric quality criteria. The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density.

Note EDS was not executed.

| Mol | Chain | Length | Quality of chain |
|-----|-------|--------|------------------|
| 1   | A     | 1521   |                  |
| 2   | B     | 256    |                  |
| 3   | C     | 239    |                  |
| 4   | D     | 209    |                  |
| 5   | E     | 162    |                  |
| 6   | F     | 101    |                  |
| 7   | G     | 156    |                  |
| 8   | H     | 138    |                  |
| 9   | I     | 128    |                  |
| 10  | J     | 105    |                  |
| 11  | K     | 129    |                  |
| 12  | L     | 132    |                  |
| 13  | M     | 126    |                  |
| 14  | N     | 61     |                  |

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| Mol | Chain | Length | Quality of chain   |
|-----|-------|--------|--|
| 15  | O     | 89     |  |
| 16  | P     | 88     |  |
| 17  | Q     | 105    |  |
| 18  | R     | 88     |  |
| 19  | S     | 93     |  |
| 20  | T     | 106    |  |
| 21  | U     | 27     |  |
| 22  | V     | 24     |  |
| 23  | W     | 76     |  |
| 23  | Y     | 76     |  |
| 24  | X     | 77     |  |

## 2 Entry composition

There are 30 unique types of molecules in this entry. The entry contains 56420 atoms, of which 0 are hydrogen and 0 are deuterium.

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 Ribosomal RNA.

| Mol | Chain | Residues | Atoms |       |      |       |      | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|-------|------|-------|------|---------|---------|-------|
| 1   | A     | 1498     | Total | C     | N    | O     | P    | 0       | 0       | 0     |
|     |       |          | 32205 | 14333 | 5970 | 10404 | 1498 |         |         |       |

- Molecule 2 is a protein called 30S Ribosomal Protein S2.

| Mol | Chain | Residues | Atoms |      |     |     |   | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|------|-----|-----|---|---------|---------|-------|
| 2   | B     | 231      | Total | C    | N   | O   | S | 0       | 0       | 0     |
|     |       |          | 1846  | 1179 | 331 | 331 | 5 |         |         |       |

- Molecule 3 is a protein called 30S Ribosomal Protein S3.

| Mol | Chain | Residues | Atoms |     |     |     |   | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|---------|-------|
| 3   | C     | 206      | Total | C   | N   | O   | S | 0       | 0       | 0     |
|     |       |          | 1552  | 976 | 302 | 273 | 1 |         |         |       |

- Molecule 4 is a protein called 30S Ribosomal Protein S4.

| Mol | Chain | Residues | Atoms |      |     |     |   | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|------|-----|-----|---|---------|---------|-------|
| 4   | D     | 208      | Total | C    | N   | O   | S | 0       | 0       | 0     |
|     |       |          | 1659  | 1040 | 326 | 286 | 7 |         |         |       |

- Molecule 5 is a protein called 30S Ribosomal Protein S5.

| Mol | Chain | Residues | Atoms |     |     |     |   | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|---------|-------|
| 5   | E     | 148      | Total | C   | N   | O   | S | 0       | 0       | 0     |
|     |       |          | 1129  | 714 | 213 | 198 | 4 |         |         |       |

- Molecule 6 is a protein called 30S Ribosomal Protein S6.

| Mol | Chain | Residues | Atoms |     |     |     |   | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|---------|-------|
| 6   | F     | 100      | Total | C   | N   | O   | S | 0       | 0       | 0     |
|     |       |          | 806   | 511 | 143 | 149 | 3 |         |         |       |

- 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     |
|     |       |          | 1231  | 766 | 243 | 216 | 6 |         |         |       |

- Molecule 8 is a protein called 30S Ribosomal Protein S8.

| Mol | Chain | Residues | Atoms |     |     |     |   | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|---------|-------|
| 8   | H     | 137      | Total | C   | N   | O   | S | 0       | 0       | 0     |
|     |       |          | 1088  | 689 | 206 | 191 | 2 |         |         |       |

- 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     |
|     |       |          | 983   | 623 | 193 | 167 |         |         |       |

- Molecule 10 is a protein called 30S Ribosomal Protein S10.

| Mol | Chain | Residues | Atoms |     |     |     | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---------|---------|-------|
| 10  | J     | 97       | Total | C   | N   | O   | 0       | 0       | 0     |
|     |       |          | 709   | 440 | 138 | 131 |         |         |       |

- Molecule 11 is a protein called 30S Ribosomal Protein S11.

| Mol | Chain | Residues | Atoms |     |     |     |   | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|---------|-------|
| 11  | K     | 114      | Total | C   | N   | O   | S | 0       | 0       | 0     |
|     |       |          | 829   | 516 | 155 | 155 | 3 |         |         |       |

- Molecule 12 is a protein called 30S Ribosomal Protein S12.

| Mol | Chain | Residues | Atoms |     |     |     |   | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|---------|-------|
| 12  | L     | 122      | Total | C   | N   | O   | S | 0       | 0       | 0     |
|     |       |          | 930   | 585 | 185 | 159 | 1 |         |         |       |

- Molecule 13 is a protein called 30S Ribosomal Protein S13.

| Mol | Chain | Residues | Atoms |     |     |     |   | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|---------|-------|
| 13  | M     | 123      | Total | C   | N   | O   | S | 0       | 0       | 0     |
|     |       |          | 958   | 592 | 198 | 166 | 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     |
|     |       |          | 728   | 456 | 144 | 126 | 2 |         |         |       |

- Molecule 16 is a protein called 30S Ribosomal Protein S16.

| Mol | Chain | Residues | Atoms |     |     |     |   | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|---------|-------|
| 16  | P     | 82       | Total | C   | N   | O   | S | 0       | 0       | 0     |
|     |       |          | 681   | 433 | 134 | 113 | 1 |         |         |       |

- Molecule 17 is a protein called 30S Ribosomal Protein S17.

| Mol | Chain | Residues | Atoms |     |     |     |   | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|---------|-------|
| 17  | Q     | 99       | Total | C   | N   | O   | S | 0       | 0       | 0     |
|     |       |          | 823   | 528 | 151 | 142 | 2 |         |         |       |

- Molecule 18 is a protein called 30S Ribosomal Protein S18.

| Mol | Chain | Residues | Atoms |     |     |    | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|----|---------|---------|-------|
| 18  | R     | 68       | Total | C   | N   | O  | 0       | 0       | 0     |
|     |       |          | 555   | 355 | 108 | 92 |         |         |       |

- Molecule 19 is a protein called 30S Ribosomal Protein S19.

| Mol | Chain | Residues | Atoms |     |     |     |   | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|---------|-------|
| 19  | S     | 83       | Total | C   | N   | O   | S | 0       | 0       | 0     |
|     |       |          | 652   | 417 | 120 | 113 | 2 |         |         |       |

- Molecule 20 is a protein called 30S Ribosomal Protein S20.

| Mol | Chain | Residues | Atoms |     |     |     |   | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|---------|-------|
| 20  | T     | 96       | Total | C   | N   | O   | S | 0       | 0       | 0     |
|     |       |          | 728   | 446 | 156 | 124 | 2 |         |         |       |

- Molecule 21 is a protein called 30S Ribosomal Protein THX.

| Mol | Chain | Residues | Atoms |     |    |    | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|-----|----|----|---------|---------|-------|
| 21  | U     | 23       | Total | C   | N  | O  | 0       | 0       | 0     |
|     |       |          | 199   | 122 | 48 | 29 |         |         |       |

- Molecule 22 is a RNA chain called mRNA.

| Mol | Chain | Residues | Atoms |     |    |    |    | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|-----|----|----|----|---------|---------|-------|
| 22  | V     | 13       | Total | C   | N  | O  | P  | 0       | 0       | 0     |
|     |       |          | 277   | 125 | 51 | 88 | 13 |         |         |       |

- Molecule 23 is a RNA chain called A/P-site tRNA.

| Mol | Chain | Residues | Atoms |     |     |     |    |   | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|----|---|---------|---------|-------|
| 23  | W     | 74       | Total | C   | N   | O   | P  | S | 0       | 0       | 0     |
|     |       |          | 1588  | 713 | 285 | 515 | 73 | 2 |         |         |       |
| 23  | Y     | 74       | Total | C   | N   | O   | P  | S | 0       | 0       | 0     |
|     |       |          | 1581  | 707 | 285 | 515 | 73 | 1 |         |         |       |

- Molecule 24 is a RNA chain called E-site tRNA.

| Mol | Chain | Residues | Atoms |     |     |     |    |   | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|----|---|---------|---------|-------|
| 24  | X     | 76       | Total | C   | N   | O   | P  | S | 0       | 0       | 0     |
|     |       |          | 1625  | 725 | 294 | 529 | 76 | 1 |         |         |       |

- Molecule 25 is MAGNESIUM ION (three-letter code: MG) (formula: Mg).

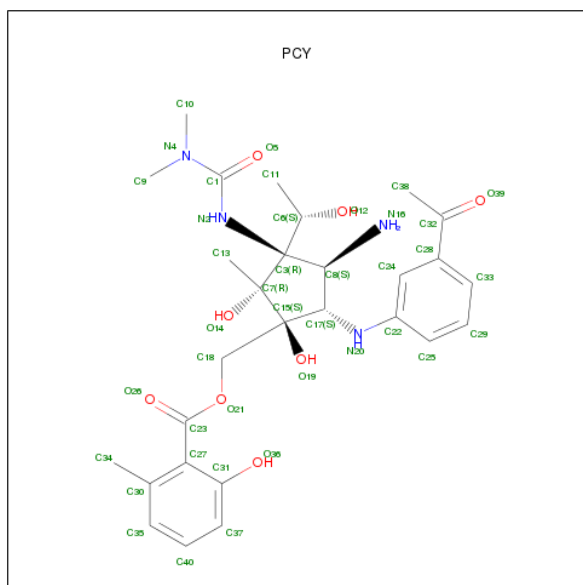
| Mol | Chain | Residues | Atoms |     | ZeroOcc | AltConf |
|-----|-------|----------|-------|-----|---------|---------|
| 25  | D     | 1        | Total | Mg  | 0       | 0       |
|     |       |          | 1     | 1   |         |         |
| 25  | K     | 2        | Total | Mg  | 0       | 0       |
|     |       |          | 2     | 2   |         |         |
| 25  | E     | 1        | Total | Mg  | 0       | 0       |
|     |       |          | 1     | 1   |         |         |
| 25  | V     | 1        | Total | Mg  | 0       | 0       |
|     |       |          | 1     | 1   |         |         |
| 25  | W     | 7        | Total | Mg  | 0       | 0       |
|     |       |          | 7     | 7   |         |         |
| 25  | A     | 230      | Total | Mg  | 0       | 0       |
|     |       |          | 230   | 230 |         |         |
| 25  | N     | 1        | Total | Mg  | 0       | 0       |
|     |       |          | 1     | 1   |         |         |
| 25  | X     | 12       | Total | Mg  | 0       | 0       |
|     |       |          | 12    | 12  |         |         |

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| Mol | Chain | Residues | Atoms |    | ZeroOcc | AltConf |
|-----|-------|----------|-------|----|---------|---------|
| 25  | Y     | 3        | Total | Mg | 0       | 0       |
|     |       |          | 3     | 3  |         |         |
| 25  | F     | 1        | Total | Mg | 0       | 0       |
|     |       |          | 1     | 1  |         |         |
| 25  | M     | 1        | Total | Mg | 0       | 0       |
|     |       |          | 1     | 1  |         |         |

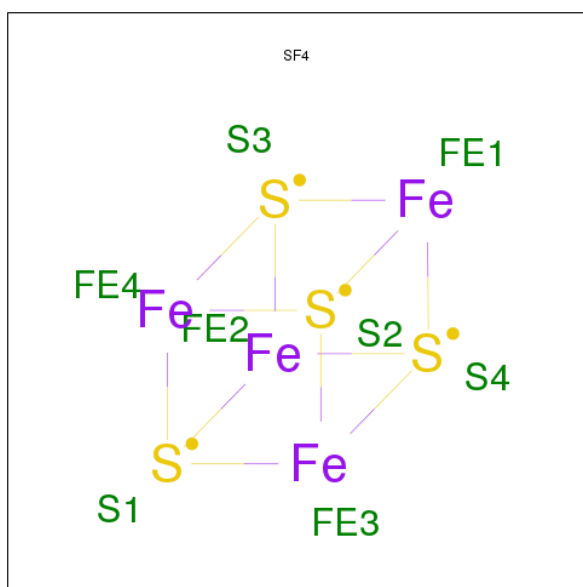
- Molecule 26 is PACTAMYCIN (three-letter code: PCY) (formula:  $C_{28}H_{38}N_4O_8$ ).



| Mol | Chain | Residues | Atoms |    |   |   | ZeroOcc | AltConf |
|-----|-------|----------|-------|----|---|---|---------|---------|
| 26  | A     | 1        | Total | C  | N | O | 0       | 0       |
|     |       |          | 40    | 28 | 4 | 8 |         |         |

- Molecule 27 is IRON/SULFUR CLUSTER (three-letter code: SF4) (formula:  $Fe_4S_4$ ).





| Mol | Chain | Residues | Atoms |    |   | ZeroOcc | AltConf |
|-----|-------|----------|-------|----|---|---------|---------|
| 27  | D     | 1        | Total | Fe | S | 0       | 0       |
|     |       |          | 8     | 4  | 4 |         |         |

- Molecule 28 is ZINC ION (three-letter code: ZN) (formula: Zn).

| Mol | Chain | Residues | Atoms |    | ZeroOcc | AltConf |
|-----|-------|----------|-------|----|---------|---------|
| 28  | N     | 1        | Total | Zn | 0       | 0       |
|     |       |          | 1     | 1  |         |         |

- Molecule 29 is POTASSIUM ION (three-letter code: K) (formula: K).

| Mol | Chain | Residues | Atoms |   | ZeroOcc | AltConf |
|-----|-------|----------|-------|---|---------|---------|
| 29  | X     | 1        | Total | K | 0       | 0       |
|     |       |          | 1     | 1 |         |         |

- Molecule 30 is water.

| Mol | Chain | Residues | Atoms |     | ZeroOcc | AltConf |
|-----|-------|----------|-------|-----|---------|---------|
| 30  | A     | 226      | Total | O   | 0       | 0       |
|     |       |          | 226   | 226 |         |         |
| 30  | E     | 3        | Total | O   | 0       | 0       |
|     |       |          | 3     | 3   |         |         |
| 30  | J     | 1        | Total | O   | 0       | 0       |
|     |       |          | 1     | 1   |         |         |
| 30  | L     | 4        | Total | O   | 0       | 0       |
|     |       |          | 4     | 4   |         |         |

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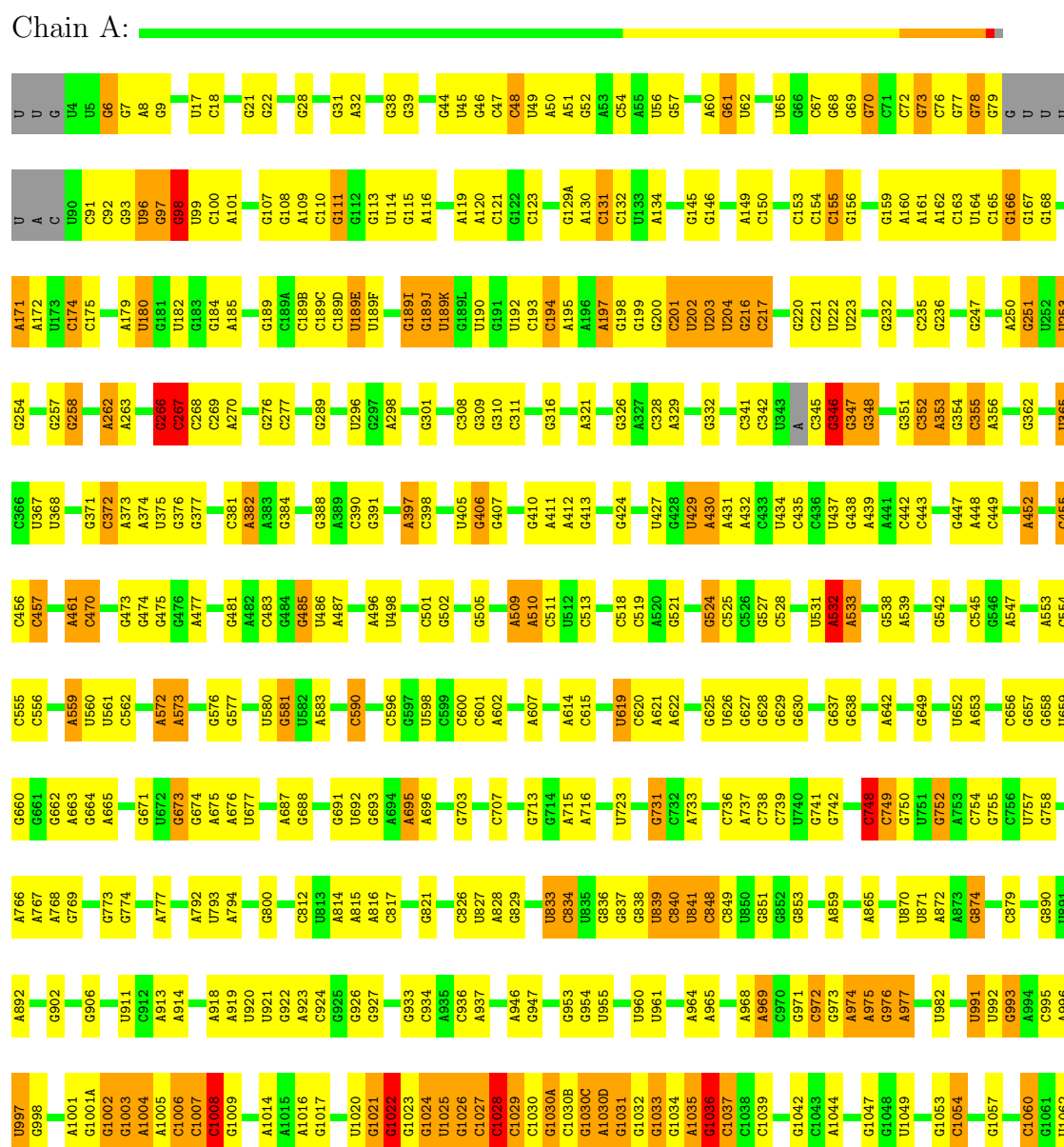
| Mol | Chain | Residues | Atoms      |        | ZeroOcc | AltConf |
|-----|-------|----------|------------|--------|---------|---------|
| 30  | M     | 1        | Total<br>1 | O<br>1 | 0       | 0       |
| 30  | V     | 4        | Total<br>4 | O<br>4 | 0       | 0       |
| 30  | W     | 6        | Total<br>6 | O<br>6 | 0       | 0       |
| 30  | X     | 8        | Total<br>8 | O<br>8 | 0       | 0       |
| 30  | Y     | 3        | Total<br>3 | O<br>3 | 0       | 0       |

### 3 Residue-property plots

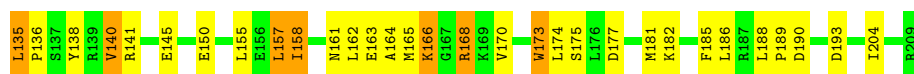
These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of errors displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. Residues are color-coded according 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.

Note EDS was not executed.

- Molecule 1: 16S Ribosomal RNA

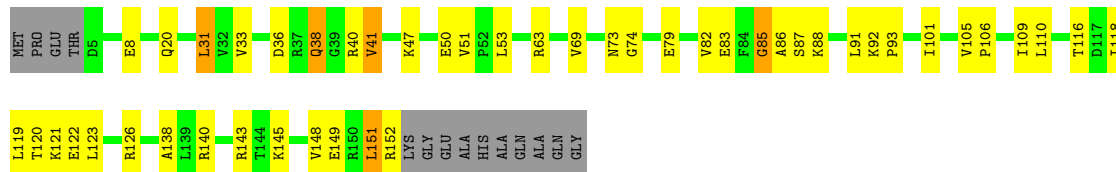






• Molecule 5: 30S Ribosomal Protein S5

Chain E:



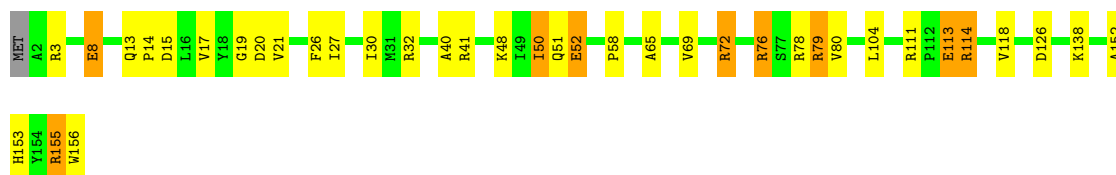
• Molecule 6: 30S Ribosomal Protein S6

Chain F:



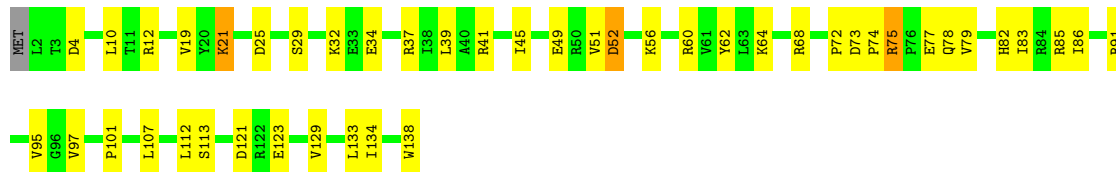
• Molecule 7: 30S Ribosomal Protein S7

Chain G:



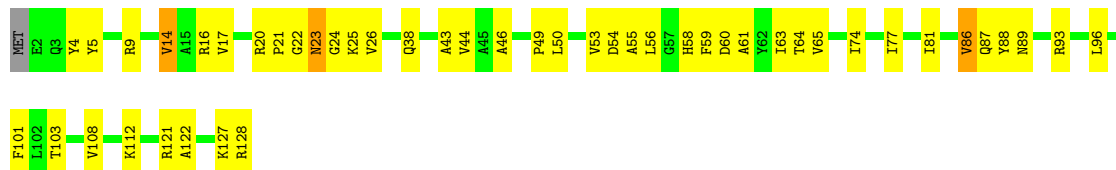
• Molecule 8: 30S Ribosomal Protein S8

Chain H:



• Molecule 9: 30S Ribosomal Protein S9

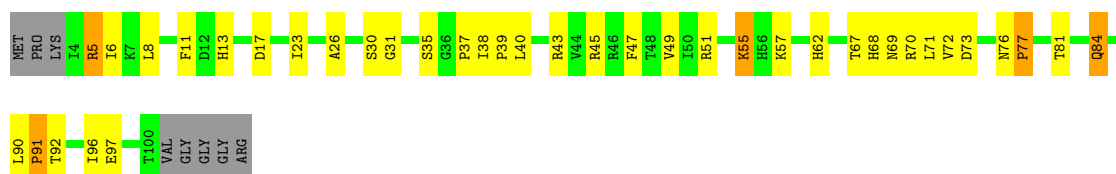
Chain I:



• Molecule 10: 30S Ribosomal Protein S10

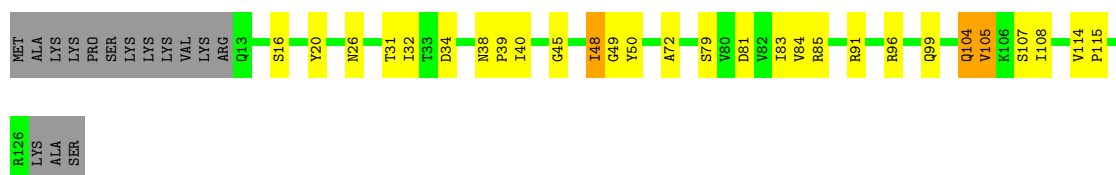
Chain J:





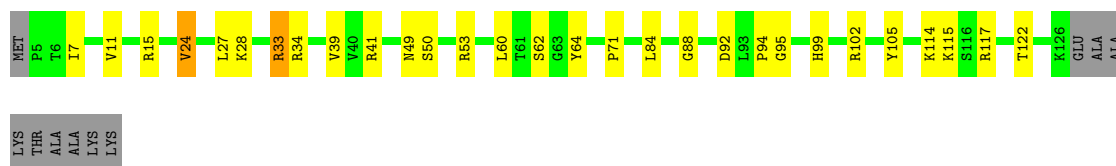
• Molecule 11: 30S Ribosomal Protein S11

Chain K:



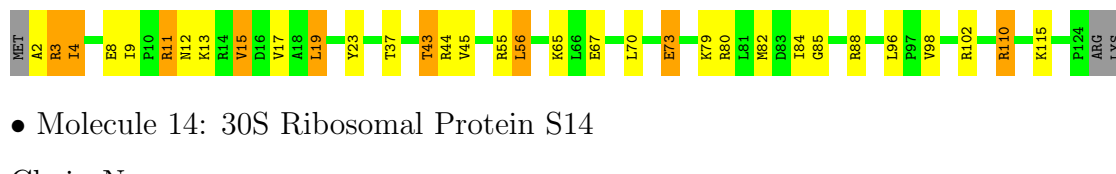
• Molecule 12: 30S Ribosomal Protein S12

Chain L:



• Molecule 13: 30S Ribosomal Protein S13

Chain M:



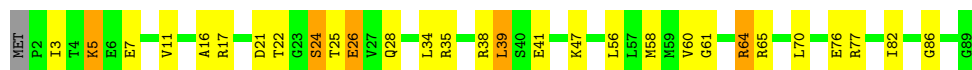
• Molecule 14: 30S Ribosomal Protein S14

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: 



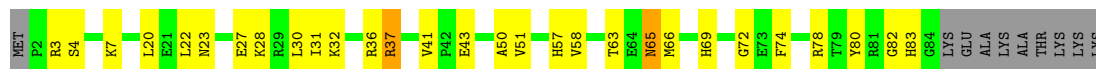
- Molecule 18: 30S Ribosomal Protein S18

Chain R: 



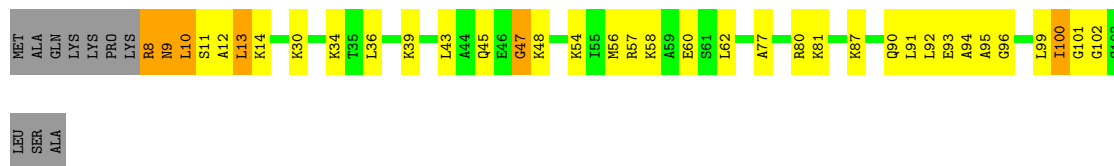
- Molecule 19: 30S Ribosomal Protein S19

Chain S: 



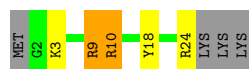
- Molecule 20: 30S Ribosomal Protein S20

Chain T: 



- Molecule 21: 30S Ribosomal Protein THX

Chain U: 



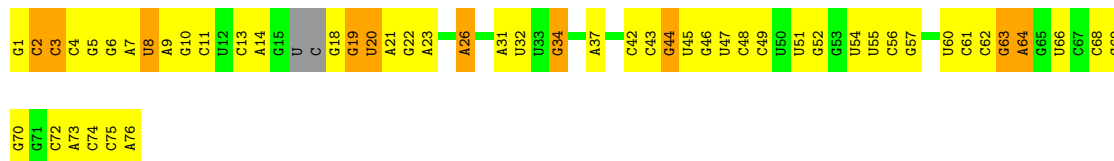
- Molecule 22: mRNA

Chain V: 



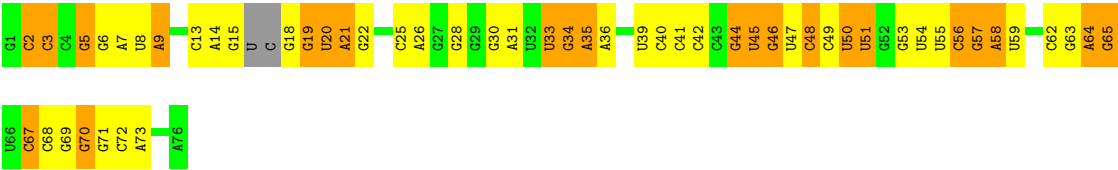
- Molecule 23: A/P-site tRNA

Chain W: 



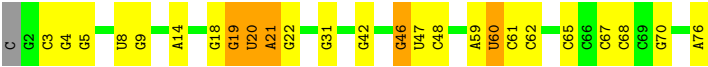
- Molecule 23: A/P-site tRNA

Chain Y: 



● Molecule 24: E-site tRNA

Chain X:





## 4 Data and refinement statistics

Xtriage (Phenix) and EDS were not executed - this section will therefore be incomplete.

| Property   | Value   | Source    |
|--|---|-----------|
| Space group  | P 21 21 21                                      | Depositor |
| Cell constants<br>a, b, c, $\alpha$ , $\beta$ , $\gamma$ | 209.35Å 449.01Å 621.98Å<br>90.00° 90.00° 90.00° | Depositor |
| Resolution (Å)   | 145.52 – 2.55                                   | Depositor |
| % Data completeness<br>(in resolution range)             | 99.0 (145.52-2.55)                              | Depositor |
| $R_{merge}$  | 0.14  | Depositor |
| $R_{sym}$  | (Not available)                                 | Depositor |
| Refinement program                                       | PHENIX (phenix.refine: 1.8.2_1309)              | Depositor |
| R, $R_{free}$  | 0.225 , 0.273                                   | Depositor |
| Estimated twinning fraction                              | No twinning to report.                          | Xtriage   |
| Total number of atoms                                    | 56420   | wwPDB-VP  |
| Average B, all atoms (Å <sup>2</sup> )                   | 69.0  | wwPDB-VP  |

## 5 Model quality ⓘ

### 5.1 Standard geometry ⓘ

Bond lengths and bond angles in the following residue types are not validated in this section: 5MU, ZN, PCY, MIA, SF4, MG, 5MC, 4SU, 7MG, K, PSU

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     | 0.43         | 0/36049        | 0.93        | 45/56261 (0.1%) |
| 2   | B     | 0.31         | 0/1881         | 0.62        | 1/2542 (0.0%)   |
| 3   | C     | 0.30         | 0/1576         | 0.52        | 0/2130          |
| 4   | D     | 0.32         | 0/1689         | 0.53        | 0/2267          |
| 5   | E     | 0.31         | 0/1145         | 0.54        | 0/1543          |
| 6   | F     | 0.32         | 0/819          | 0.53        | 0/1111          |
| 7   | G     | 0.30         | 0/1250         | 0.49        | 0/1679          |
| 8   | H     | 0.30         | 0/1108         | 0.51        | 0/1494          |
| 9   | I     | 0.32         | 0/1002         | 0.56        | 0/1346          |
| 10  | J     | 0.30         | 0/722          | 0.56        | 0/982           |
| 11  | K     | 0.31         | 0/844          | 0.54        | 0/1145          |
| 12  | L     | 0.33         | 0/946          | 0.53        | 0/1274          |
| 13  | M     | 0.30         | 0/969          | 0.57        | 0/1302          |
| 14  | N     | 0.34         | 0/501          | 0.50        | 0/664           |
| 15  | O     | 0.30         | 0/739          | 0.56        | 0/985           |
| 16  | P     | 0.32         | 0/697          | 0.53        | 0/939           |
| 17  | Q     | 0.31         | 0/836          | 0.49        | 0/1117          |
| 18  | R     | 0.32         | 0/560          | 0.55        | 0/746           |
| 19  | S     | 0.30         | 0/667          | 0.54        | 0/900           |
| 20  | T     | 0.29         | 0/730          | 0.57        | 0/965           |
| 21  | U     | 0.33         | 0/203          | 0.50        | 0/266           |
| 22  | V     | 0.48         | 0/310          | 1.00        | 0/480           |
| 23  | W     | 0.48         | 0/1602         | 1.06        | 0/2493          |
| 23  | Y     | 0.52         | 0/1602         | 1.16        | 4/2493 (0.2%)   |
| 24  | X     | 0.55         | 2/1725 (0.1%)  | 1.16        | 12/2689 (0.4%)  |
| All | All   | 0.41         | 2/60172 (0.0%) | 0.86        | 62/89813 (0.1%) |

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 |
|-----|-------|---------------------|---------------------|
| 2   | B     | 0                   | 1                   |
| 7   | G     | 0                   | 1                   |
| All | All   | 0                   | 2                   |

All (2) bond length outliers are listed below:

| Mol | Chain | Res | Type | Atoms | Z     | Observed(Å) | Ideal(Å) |
|-----|-------|-----|------|-------|-------|-------------|----------|
| 24  | X     | 14  | A    | N7-C5 | -6.24 | 1.35        | 1.39     |
| 24  | X     | 14  | A    | C8-N7 | -6.01 | 1.27        | 1.31     |

The worst 5 of 62 bond angle outliers are listed below:

| Mol | Chain | Res | Type | Atoms    | Z     | Observed(°) | Ideal(°) |
|-----|-------|-----|------|----------|-------|-------------|----------|
| 24  | X     | 14  | A    | C4-C5-C6 | 10.08 | 122.04      | 117.00   |
| 24  | X     | 46  | G    | C6-N1-C2 | -9.82 | 119.21      | 125.10   |
| 24  | X     | 14  | A    | C5-N7-C8 | 9.60  | 108.70      | 103.90   |
| 23  | Y     | 64  | A    | C5-C6-N6 | 8.55  | 130.54      | 123.70   |
| 24  | X     | 14  | A    | C5-C6-N1 | -8.12 | 113.64      | 117.70   |

There are no chirality outliers.

All (2) planarity outliers are listed below:

| Mol | Chain | Res | Type | Group   |
|-----|-------|-----|------|---------|
| 2   | B     | 231 | GLU  | Peptide |
| 7   | G     | 78  | ARG  | Peptide |

## 5.2 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 hydrogens added by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, and the number in parentheses is this value normalized per 1000 atoms of the molecule in the chain. The Symm-Clashes column gives symmetry related clashes, in the same way as for the Clashes column.

| Mol | Chain | Non-H | H(model) | H(added) | Clashes | Symm-Clashes |
|-----|-------|-------|----------|----------|---------|--------------|
| 1   | A     | 32205 | 0        | 16255    | 428     | 0            |
| 2   | B     | 1846  | 0        | 1867     | 70      | 0            |
| 3   | C     | 1552  | 0        | 1546     | 45      | 0            |
| 4   | D     | 1659  | 0        | 1676     | 53      | 0            |
| 5   | E     | 1129  | 0        | 1185     | 33      | 0            |
| 6   | F     | 806   | 0        | 793      | 17      | 0            |

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| Mol | Chain | Non-H | H(model) | H(added) | Clashes | Symm-Clashes |
|-----|-------|-------|----------|----------|---------|--------------|
| 7   | G     | 1231  | 0        | 1238     | 22      | 0            |
| 8   | H     | 1088  | 0        | 1126     | 32      | 0            |
| 9   | I     | 983   | 0        | 986      | 28      | 0            |
| 10  | J     | 709   | 0        | 650      | 32      | 0            |
| 11  | K     | 829   | 0        | 825      | 15      | 0            |
| 12  | L     | 930   | 0        | 980      | 18      | 0            |
| 13  | M     | 958   | 0        | 1002     | 24      | 0            |
| 14  | N     | 492   | 0        | 529      | 20      | 0            |
| 15  | O     | 728   | 0        | 760      | 18      | 0            |
| 16  | P     | 681   | 0        | 697      | 21      | 0            |
| 17  | Q     | 823   | 0        | 891      | 16      | 0            |
| 18  | R     | 555   | 0        | 618      | 12      | 0            |
| 19  | S     | 652   | 0        | 662      | 30      | 0            |
| 20  | T     | 728   | 0        | 798      | 19      | 0            |
| 21  | U     | 199   | 0        | 208      | 5       | 0            |
| 22  | V     | 277   | 0        | 140      | 2       | 0            |
| 23  | W     | 1588  | 0        | 820      | 29      | 0            |
| 23  | Y     | 1581  | 0        | 805      | 56      | 0            |
| 24  | X     | 1625  | 0        | 828      | 9       | 0            |
| 25  | A     | 230   | 0        | 0        | 0       | 0            |
| 25  | D     | 1     | 0        | 0        | 0       | 0            |
| 25  | E     | 1     | 0        | 0        | 0       | 0            |
| 25  | F     | 1     | 0        | 0        | 0       | 0            |
| 25  | K     | 2     | 0        | 0        | 0       | 0            |
| 25  | M     | 1     | 0        | 0        | 0       | 0            |
| 25  | N     | 1     | 0        | 0        | 0       | 0            |
| 25  | V     | 1     | 0        | 0        | 0       | 0            |
| 25  | W     | 7     | 0        | 0        | 0       | 0            |
| 25  | X     | 12    | 0        | 0        | 0       | 0            |
| 25  | Y     | 3     | 0        | 0        | 0       | 0            |
| 26  | A     | 40    | 0        | 37       | 7       | 0            |
| 27  | D     | 8     | 0        | 0        | 0       | 0            |
| 28  | N     | 1     | 0        | 0        | 0       | 0            |
| 29  | X     | 1     | 0        | 0        | 0       | 0            |
| 30  | A     | 226   | 0        | 0        | 17      | 0            |
| 30  | E     | 3     | 0        | 0        | 0       | 0            |
| 30  | J     | 1     | 0        | 0        | 0       | 0            |
| 30  | L     | 4     | 0        | 0        | 1       | 0            |
| 30  | M     | 1     | 0        | 0        | 0       | 0            |
| 30  | V     | 4     | 0        | 0        | 0       | 0            |
| 30  | W     | 6     | 0        | 0        | 0       | 0            |
| 30  | X     | 8     | 0        | 0        | 0       | 0            |

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| Mol | Chain | Non-H | H(model) | H(added) | Clashes | Symm-Clashes |
|-----|-------|-------|----------|----------|---------|--------------|
| 30  | Y     | 3     | 0        | 0        | 0       | 0            |
| All | All   | 56420 | 0        | 37922    | 934     | 0            |

Clashscore is defined as the number of clashes calculated for the entry per 1000 atoms (including hydrogens) of the entry. The overall clashscore for this entry is 10.

The worst 5 of 934 close contacts within the same asymmetric unit are listed below.

| Atom-1        | Atom-2        | Distance(Å) | Clash(Å) |
|---------------|---------------|-------------|----------|
| 1:A:1025:U:O2 | 1:A:1036:G:O6 | 1.82        | 0.98     |
| 23:Y:2:C:H42  | 23:Y:71:G:H1  | 1.15        | 0.94     |
| 23:Y:51:U:H3  | 23:Y:63:G:H1  | 0.97        | 0.93     |
| 23:Y:19:G:N2  | 23:Y:56:C:N3  | 2.20        | 0.90     |
| 23:Y:26:A:H61 | 23:Y:44:G:H1  | 0.96        | 0.89     |

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 |     |
|-----|-------|---------------|-----------|---------|----------|-------------|-----|
| 2   | B     | 229/256 (90%) | 200 (87%) | 19 (8%) | 10 (4%)  | 4           | 4   |
| 3   | C     | 204/239 (85%) | 184 (90%) | 17 (8%) | 3 (2%)   | 15          | 25  |
| 4   | D     | 206/209 (99%) | 192 (93%) | 12 (6%) | 2 (1%)   | 22          | 37  |
| 5   | E     | 146/162 (90%) | 134 (92%) | 9 (6%)  | 3 (2%)   | 11          | 16  |
| 6   | F     | 98/101 (97%)  | 97 (99%)  | 1 (1%)  | 0        | 100         | 100 |
| 7   | G     | 153/156 (98%) | 143 (94%) | 8 (5%)  | 2 (1%)   | 18          | 29  |
| 8   | H     | 135/138 (98%) | 129 (96%) | 6 (4%)  | 0        | 100         | 100 |
| 9   | I     | 125/128 (98%) | 111 (89%) | 11 (9%) | 3 (2%)   | 9           | 13  |
| 10  | J     | 95/105 (90%)  | 83 (87%)  | 9 (10%) | 3 (3%)   | 6           | 7   |
| 11  | K     | 112/129 (87%) | 106 (95%) | 4 (4%)  | 2 (2%)   | 13          | 20  |

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| Mol | Chain | Analysed        | Favoured   | Allowed  | Outliers | Percentiles |     |
|-----|-------|-----------------|------------|----------|----------|-------------|-----|
| 12  | L     | 120/132 (91%)   | 115 (96%)  | 5 (4%)   | 0        | 100         | 100 |
| 13  | M     | 121/126 (96%)   | 110 (91%)  | 9 (7%)   | 2 (2%)   | 14          | 21  |
| 14  | N     | 58/61 (95%)     | 54 (93%)   | 4 (7%)   | 0        | 100         | 100 |
| 15  | O     | 86/89 (97%)     | 83 (96%)   | 3 (4%)   | 0        | 100         | 100 |
| 16  | P     | 80/88 (91%)     | 78 (98%)   | 2 (2%)   | 0        | 100         | 100 |
| 17  | Q     | 97/105 (92%)    | 90 (93%)   | 7 (7%)   | 0        | 100         | 100 |
| 18  | R     | 66/88 (75%)     | 64 (97%)   | 2 (3%)   | 0        | 100         | 100 |
| 19  | S     | 81/93 (87%)     | 72 (89%)   | 9 (11%)  | 0        | 100         | 100 |
| 20  | T     | 94/106 (89%)    | 84 (89%)   | 3 (3%)   | 7 (7%)   | 2           | 1   |
| 21  | U     | 21/27 (78%)     | 18 (86%)   | 3 (14%)  | 0        | 100         | 100 |
| All | All   | 2327/2538 (92%) | 2147 (92%) | 143 (6%) | 37 (2%)  | 14          | 23  |

5 of 37 Ramachandran outliers are listed below:

| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 2   | B     | 9   | GLU  |
| 2   | B     | 15  | VAL  |
| 2   | B     | 16  | HIS  |
| 2   | B     | 17  | PHE  |
| 2   | B     | 126 | GLU  |

### 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 |    |
|-----|-------|---------------|-----------|----------|-------------|----|
| 2   | B     | 192/220 (87%) | 169 (88%) | 23 (12%) | 7           | 12 |
| 3   | C     | 143/188 (76%) | 132 (92%) | 11 (8%)  | 18          | 32 |
| 4   | D     | 170/181 (94%) | 155 (91%) | 15 (9%)  | 14          | 25 |
| 5   | E     | 113/123 (92%) | 106 (94%) | 7 (6%)   | 26          | 43 |
| 6   | F     | 83/90 (92%)   | 77 (93%)  | 6 (7%)   | 21          | 35 |
| 7   | G     | 119/127 (94%) | 106 (89%) | 13 (11%) | 9           | 15 |
| 8   | H     | 114/119 (96%) | 107 (94%) | 7 (6%)   | 26          | 44 |

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| Mol | Chain | Analysed        | Rotameric  | Outliers | Percentiles |    |
|-----|-------|-----------------|------------|----------|-------------|----|
| 9   | I     | 90/99 (91%)     | 82 (91%)   | 8 (9%)   | 14          | 25 |
| 10  | J     | 66/92 (72%)     | 62 (94%)   | 4 (6%)   | 26          | 44 |
| 11  | K     | 82/99 (83%)     | 76 (93%)   | 6 (7%)   | 20          | 35 |
| 12  | L     | 97/109 (89%)    | 93 (96%)   | 4 (4%)   | 41          | 66 |
| 13  | M     | 93/101 (92%)    | 83 (89%)   | 10 (11%) | 9           | 16 |
| 14  | N     | 49/50 (98%)     | 43 (88%)   | 6 (12%)  | 7           | 12 |
| 15  | O     | 78/80 (98%)     | 67 (86%)   | 11 (14%) | 5           | 8  |
| 16  | P     | 69/74 (93%)     | 62 (90%)   | 7 (10%)  | 11          | 19 |
| 17  | Q     | 94/97 (97%)     | 91 (97%)   | 3 (3%)   | 51          | 77 |
| 18  | R     | 59/77 (77%)     | 56 (95%)   | 3 (5%)   | 33          | 55 |
| 19  | S     | 69/80 (86%)     | 66 (96%)   | 3 (4%)   | 40          | 64 |
| 20  | T     | 70/82 (85%)     | 64 (91%)   | 6 (9%)   | 15          | 26 |
| 21  | U     | 18/22 (82%)     | 16 (89%)   | 2 (11%)  | 9           | 15 |
| All | All   | 1868/2110 (88%) | 1713 (92%) | 155 (8%) | 16          | 28 |

5 of 155 residues with a non-rotameric sidechain are listed below:

| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 7   | G     | 104 | LEU  |
| 9   | I     | 89  | ASN  |
| 18  | R     | 76  | LEU  |
| 7   | G     | 114 | ARG  |
| 8   | H     | 78  | GLN  |

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 38 such sidechains are listed below:

| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 5   | E     | 38  | GLN  |
| 7   | G     | 97  | GLN  |
| 19  | S     | 83  | HIS  |
| 6   | F     | 100 | ASN  |
| 9   | I     | 23  | ASN  |

### 5.3.3 RNA ⓘ

| Mol | Chain | Analysed        | Backbone Outliers | Pucker Outliers |
|-----|-------|-----------------|-------------------|-----------------|
| 1   | A     | 1495/1521 (98%) | 306 (20%)         | 21 (1%)         |
| 22  | V     | 12/24 (50%)     | 3 (25%)           | 0               |
| 23  | W     | 71/76 (93%)     | 30 (42%)          | 2 (2%)          |
| 23  | Y     | 71/76 (93%)     | 33 (46%)          | 1 (1%)          |
| 24  | X     | 75/77 (97%)     | 18 (24%)          | 1 (1%)          |
| All | All   | 1724/1774 (97%) | 390 (22%)         | 25 (1%)         |

5 of 390 RNA backbone outliers are listed below:

| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1   | A     | 6   | G    |
| 1   | A     | 9   | G    |
| 1   | A     | 22  | G    |
| 1   | A     | 32  | A    |
| 1   | A     | 39  | G    |

5 of 25 RNA pucker outliers are listed below:

| Mol | Chain | Res  | Type |
|-----|-------|------|------|
| 1   | A     | 991  | U    |
| 1   | A     | 1065 | U    |
| 24  | X     | 47   | U    |
| 1   | A     | 1036 | G    |
| 1   | A     | 1067 | A    |

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

18 non-standard protein/DNA/RNA residues are modelled in this entry.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the chemical component dictionary. The Link column lists molecule types, if any, to which the group is linked. The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with  $|Z| > 2$  is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

| Mol | Type | Chain | Res | Link  | Bond lengths |      |             | Bond angles |      |             |
|-----|------|-------|-----|-------|--------------|------|-------------|-------------|------|-------------|
|     |      |       |     |       | Counts       | RMSZ | $\# Z  > 2$ | Counts      | RMSZ | $\# Z  > 2$ |
| 23  | PSU  | W     | 32  | 25,23 | 19,21,22     | 1.85 | 5 (26%)     | 23,30,33    | 1.18 | 1 (4%)      |
| 23  | MIA  | W     | 37  | 23    | 29,31,32     | 1.88 | 4 (13%)     | 41,44,47    | 1.81 | 8 (19%)     |
| 23  | PSU  | W     | 39  | 23    | 19,21,22     | 1.81 | 5 (26%)     | 23,30,33    | 0.96 | 2 (8%)      |
| 23  | 7MG  | W     | 46  | 23    | 24,26,27     | 2.04 | 6 (25%)     | 34,39,42    | 2.45 | 10 (29%)    |



| Mol | Type | Chain | Res | Link  | Bond lengths |      |          | Bond angles |       |          |
|-----|------|-------|-----|-------|--------------|------|----------|-------------|-------|----------|
|     |      |       |     |       | Counts       | RMSZ | # Z  > 2 | Counts      | RMSZ  | # Z  > 2 |
| 23  | 5MU  | W     | 54  | 23    | 20,22,23     | 1.69 | 5 (25%)  | 25,32,35    | 2.07  | 3 (12%)  |
| 23  | PSU  | W     | 55  | 23    | 19,21,22     | 1.79 | 4 (21%)  | 23,30,33    | 1.58  | 2 (8%)   |
| 23  | 4SU  | W     | 8   | 23    | 19,21,22     | 1.82 | 4 (21%)  | 23,30,33    | 8.03  | 4 (17%)  |
| 24  | 5MC  | X     | 32  | 24    | 20,22,23     | 1.70 | 4 (20%)  | 26,32,35    | 1.59  | 4 (15%)  |
| 24  | 5MU  | X     | 54  | 24,25 | 20,22,23     | 1.67 | 5 (25%)  | 25,32,35    | 1.71  | 4 (16%)  |
| 24  | PSU  | X     | 55  | 24    | 19,21,22     | 1.97 | 4 (21%)  | 23,30,33    | 1.04  | 2 (8%)   |
| 24  | 4SU  | X     | 8   | 24    | 19,21,22     | 1.76 | 3 (15%)  | 23,30,33    | 37.45 | 2 (8%)   |
| 23  | PSU  | Y     | 32  | 23    | 19,21,22     | 1.86 | 4 (21%)  | 23,30,33    | 1.30  | 2 (8%)   |
| 23  | MIA  | Y     | 37  | 23    | 20,24,32     | 1.79 | 5 (25%)  | 27,35,47    | 1.82  | 4 (14%)  |
| 23  | PSU  | Y     | 39  | 23    | 19,21,22     | 1.86 | 6 (31%)  | 23,30,33    | 1.14  | 1 (4%)   |
| 23  | 7MG  | Y     | 46  | 23    | 24,26,27     | 2.06 | 7 (29%)  | 34,39,42    | 2.60  | 10 (29%) |
| 23  | 5MU  | Y     | 54  | 23    | 20,22,23     | 1.80 | 5 (25%)  | 25,32,35    | 1.79  | 3 (12%)  |
| 23  | PSU  | Y     | 55  | 23    | 19,21,22     | 1.83 | 4 (21%)  | 23,30,33    | 1.06  | 2 (8%)   |
| 23  | 4SU  | Y     | 8   | 23    | 19,21,22     | 1.82 | 4 (21%)  | 23,30,33    | 11.54 | 3 (13%)  |

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral centers analysed, the number of these observed in the model and the number defined in the chemical component dictionary. Similar counts are reported in the Torsion and Rings columns. '-' means no outliers of that kind were identified.

| Mol | Type | Chain | Res | Link  | Chirals | Torsions   | Rings   |
|-----|------|-------|-----|-------|---------|------------|---------|
| 23  | PSU  | W     | 32  | 25,23 | -       | 0/8/25/26  | 0/2/2/2 |
| 23  | MIA  | W     | 37  | 23    | -       | 0/16/33/34 | 0/3/3/3 |
| 23  | PSU  | W     | 39  | 23    | -       | 0/8/25/26  | 0/2/2/2 |
| 23  | 7MG  | W     | 46  | 23    | -       | 0/8/37/38  | 0/3/3/3 |
| 23  | 5MU  | W     | 54  | 23    | -       | 0/6/25/26  | 0/2/2/2 |
| 23  | PSU  | W     | 55  | 23    | -       | 0/8/25/26  | 0/2/2/2 |
| 23  | 4SU  | W     | 8   | 23    | -       | 0/6/25/26  | 0/2/2/2 |
| 24  | 5MC  | X     | 32  | 24    | -       | 0/6/25/26  | 0/2/2/2 |
| 24  | 5MU  | X     | 54  | 24,25 | -       | 0/6/25/26  | 0/2/2/2 |
| 24  | PSU  | X     | 55  | 24    | -       | 0/8/25/26  | 0/2/2/2 |
| 24  | 4SU  | X     | 8   | 24    | -       | 0/6/25/26  | 0/2/2/2 |
| 23  | PSU  | Y     | 32  | 23    | -       | 0/8/25/26  | 0/2/2/2 |
| 23  | MIA  | Y     | 37  | 23    | -       | 0/8/25/34  | 0/3/3/3 |
| 23  | PSU  | Y     | 39  | 23    | -       | 0/8/25/26  | 0/2/2/2 |
| 23  | 7MG  | Y     | 46  | 23    | -       | 0/8/37/38  | 0/3/3/3 |
| 23  | 5MU  | Y     | 54  | 23    | -       | 0/6/25/26  | 0/2/2/2 |
| 23  | PSU  | Y     | 55  | 23    | -       | 0/8/25/26  | 0/2/2/2 |
| 23  | 4SU  | Y     | 8   | 23    | -       | 0/6/25/26  | 0/2/2/2 |

The worst 5 of 84 bond length outliers are listed below:

| Mol | Chain | Res | Type | Atoms  | Z     | Observed(Å) | Ideal(Å) |
|-----|-------|-----|------|--------|-------|-------------|----------|
| 23  | W     | 37  | MIA  | C2-S10 | -7.30 | 1.69        | 1.75     |
| 23  | W     | 46  | 7MG  | C6-C5  | 5.50  | 1.48        | 1.41     |
| 23  | Y     | 46  | 7MG  | C6-C5  | 5.46  | 1.48        | 1.41     |
| 24  | X     | 55  | PSU  | C5-C1' | -4.82 | 1.48        | 1.52     |
| 23  | W     | 46  | 7MG  | P-OP1  | 4.66  | 1.52        | 1.46     |

The worst 5 of 67 bond angle outliers are listed below:

| Mol | Chain | Res | Type | Atoms    | Z      | Observed(°) | Ideal(°) |
|-----|-------|-----|------|----------|--------|-------------|----------|
| 24  | X     | 8   | 4SU  | C4-N3-C2 | 179.47 | 129.28      | 121.60   |
| 23  | Y     | 8   | 4SU  | C4-N3-C2 | 54.70  | 123.94      | 121.60   |
| 23  | W     | 8   | 4SU  | C4-N3-C2 | 37.68  | 123.21      | 121.60   |
| 23  | Y     | 46  | 7MG  | N3-C4-N9 | 7.78   | 139.09      | 126.80   |
| 23  | W     | 46  | 7MG  | N3-C4-N9 | 7.69   | 138.96      | 126.80   |

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

## 5.5 Carbohydrates ⓘ

There are no carbohydrates in this entry.

## 5.6 Ligand geometry ⓘ

Of 264 ligands modelled in this entry, 262 are monoatomic - leaving 2 for Mogul analysis.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the chemical component dictionary. The Link column lists molecule types, if any, to which the group is linked. The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with  $|Z| > 2$  is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

| Mol | Type | Chain | Res  | Link | Bond lengths |       |           | Bond angles |      |          |
|-----|------|-------|------|------|--------------|-------|-----------|-------------|------|----------|
|     |      |       |      |      | Counts       | RMSZ  | # Z  > 2  | Counts      | RMSZ | # Z  > 2 |
| 26  | PCY  | A     | 3231 | -    | 42,42,42     | 1.62  | 6 (14%)   | 65,65,65    | 1.76 | 13 (20%) |
| 27  | SF4  | D     | 501  | 4    | 12,12,12     | 22.91 | 12 (100%) | 0,24,24     | 0.00 | -        |

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral centers analysed, the number of these observed in the model and the number defined in the chemical component dictionary. Similar counts are reported in the Torsion and Rings columns. '-' means no outliers of that kind were identified.

| Mol | Type | Chain | Res  | Link | Chirals | Torsions   | Rings   |
|-----|------|-------|------|------|---------|------------|---------|
| 26  | PCY  | A     | 3231 | -    | -       | 0/33/67/67 | 0/3/3/3 |
| 27  | SF4  | D     | 501  | 4    | -       | 0/0/48/48  | 0/6/5/5 |

The worst 5 of 18 bond length outliers are listed below:

| Mol | Chain | Res | Type | Atoms  | Z      | Observed(Å) | Ideal(Å) |
|-----|-------|-----|------|--------|--------|-------------|----------|
| 27  | D     | 501 | SF4  | S3-FE2 | -24.24 | 2.16        | 2.33     |
| 27  | D     | 501 | SF4  | S4-FE2 | -23.51 | 2.17        | 2.33     |
| 27  | D     | 501 | SF4  | S1-FE3 | -23.49 | 2.17        | 2.33     |
| 27  | D     | 501 | SF4  | S1-FE2 | -23.30 | 2.17        | 2.33     |
| 27  | D     | 501 | SF4  | S2-FE1 | -23.16 | 2.17        | 2.33     |

The worst 5 of 13 bond angle outliers are listed below:

| Mol | Chain | Res  | Type | Atoms       | Z     | Observed(°) | Ideal(°) |
|-----|-------|------|------|-------------|-------|-------------|----------|
| 26  | A     | 3231 | PCY  | C6-C3-N2    | 7.74  | 114.08      | 107.39   |
| 26  | A     | 3231 | PCY  | C7-C3-C8    | -4.43 | 94.46       | 102.92   |
| 26  | A     | 3231 | PCY  | C18-O21-C23 | -4.38 | 107.00      | 116.57   |
| 26  | A     | 3231 | PCY  | C8-C17-N20  | -2.95 | 107.50      | 112.80   |
| 26  | A     | 3231 | PCY  | O21-C23-C27 | 2.91  | 119.12      | 112.32   |

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

## 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 ⓘ

EDS was not executed - this section will therefore be empty.

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

EDS was not executed - this section will therefore be empty.

### 6.3 Carbohydrates ⓘ

EDS was not executed - this section will therefore be empty.

### 6.4 Ligands ⓘ

EDS was not executed - this section will therefore be empty.

### 6.5 Other polymers ⓘ

EDS was not executed - this section will therefore be empty.