Full wwPDB X-ray Structure Validation Report

Nov 6, 2023 – 06:01 PM EST

PDB ID : 6N9E
Title : Crystal structure of the Thermus thermophilus 70S ribosome in complex with a short substrate mimic CC-Pmn and bound to mRNA and P-site tRNA at 3.7Å resolution
Authors : Melnikov, S.V.; Khabibullina, N.F.; Mairhofer, E.; Vargas-Rodriguez, O.; Reynolds, N.M.; Micura, R.; Soll, D.; Polikanov, Y.S.
Deposited on : 2018-12-03
Resolution : 3.70 Å (reported)

This is a Full wwPDB X-ray Structure Validation Report for a publicly released PDB entry.

We welcome your comments at validation@mail.wwpdb.org
A user guide is available at
with specific help available everywhere you see the ① symbol.

The types of validation reports are described at
http://www.wwpdb.org/validation/2017/FAQs#types.

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

- MolProbity : 4.02b-467
- Mogul : 1.8.5 (274361), CSD as541be (2020)
- Xtriage (Phenix) : 1.13
- EDS : 2.36
- Percentile statistics : 20191225.v01 (using entries in the PDB archive December 25th 2019)
- Refmac : 5.8.0158
- CCP4 : 7.0.044 (Gargrove)
- Ideal geometry (proteins) : Engh & Huber (2001)
- Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
- Validation Pipeline (wwPDB-VP) : 2.36
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

The reported resolution of this entry is 3.70 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.

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The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments of the lower bar indicate the fraction of residues that contain outliers for >=3, 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions <=5%. The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density. The numeric value is given above the bar.

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2 Entry composition

There are 59 unique types of molecules in this entry. The entry contains 287828 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 23S Ribosomal RNA.

<table>
<thead>
<tr>
<th>Mol</th>
<th>Chain</th>
<th>Residues</th>
<th>Atoms</th>
<th>ZeroOcc</th>
<th>AltConf</th>
<th>Trace</th>
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</thead>
<tbody>
<tr>
<td>1</td>
<td>1A</td>
<td>2871</td>
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<td>61852</td>
<td>27531</td>
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<td>60322</td>
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</table>

- Molecule 2 is a RNA chain called 5S Ribosomal RNA.

<table>
<thead>
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<th>Chain</th>
<th>Residues</th>
<th>Atoms</th>
<th>ZeroOcc</th>
<th>AltConf</th>
<th>Trace</th>
</tr>
</thead>
<tbody>
<tr>
<td>2</td>
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<td>1146</td>
<td>476</td>
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<tr>
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<td>2575</td>
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<td>476</td>
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</table>

- Molecule 3 is a protein called 50S Ribosomal Protein L2.

<table>
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<th>Chain</th>
<th>Residues</th>
<th>Atoms</th>
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<th>AltConf</th>
<th>Trace</th>
</tr>
</thead>
<tbody>
<tr>
<td>3</td>
<td>1D</td>
<td>275</td>
<td>Total C N O S</td>
<td>2136</td>
<td>1349</td>
<td>423</td>
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<tr>
<td>3</td>
<td>2D</td>
<td>275</td>
<td>Total C N O S</td>
<td>2136</td>
<td>1349</td>
<td>423</td>
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</table>

- Molecule 4 is a protein called 50S Ribosomal Protein L3.

<table>
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<th>Mol</th>
<th>Chain</th>
<th>Residues</th>
<th>Atoms</th>
<th>ZeroOcc</th>
<th>AltConf</th>
<th>Trace</th>
</tr>
</thead>
<tbody>
<tr>
<td>4</td>
<td>1E</td>
<td>204</td>
<td>Total C N O S</td>
<td>1559</td>
<td>985</td>
<td>298</td>
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<tr>
<td>4</td>
<td>2E</td>
<td>204</td>
<td>Total C N O S</td>
<td>1559</td>
<td>985</td>
<td>298</td>
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</tbody>
</table>

- Molecule 5 is a protein called 50S Ribosomal Protein L4.
- Molecule 6 is a protein called 50S Ribosomal Protein L5.

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<th>Chain</th>
<th>Residues</th>
<th>Atoms</th>
<th>ZeroOcc</th>
<th>AltConf</th>
<th>Trace</th>
</tr>
</thead>
<tbody>
<tr>
<td>6</td>
<td>1G</td>
<td>181</td>
<td>Total C N O S</td>
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<td>0</td>
<td>0</td>
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<tr>
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- Molecule 7 is a protein called 50S Ribosomal Protein L6.

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<th>Atoms</th>
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<th>AltConf</th>
<th>Trace</th>
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</thead>
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<tr>
<td>7</td>
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<td>0</td>
<td>0</td>
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<tr>
<td>7</td>
<td>2H</td>
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- Molecule 8 is a protein called 50S Ribosomal Protein L9.

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<th>Atoms</th>
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<th>AltConf</th>
<th>Trace</th>
</tr>
</thead>
<tbody>
<tr>
<td>8</td>
<td>1I</td>
<td>146</td>
<td>Total C N O S</td>
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<td>0</td>
<td>0</td>
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<tr>
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<td>2I</td>
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- Molecule 9 is a protein called 50S Ribosomal Protein L13.

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<th>Atoms</th>
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<tr>
<td>9</td>
<td>1N</td>
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<td>Total C N O S</td>
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<td>0</td>
<td>0</td>
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<tr>
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<td>2N</td>
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- Molecule 10 is a protein called 50S Ribosomal Protein L14.

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<th>Atoms</th>
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<th>Trace</th>
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<tbody>
<tr>
<td>10</td>
<td>1O</td>
<td>122</td>
<td>Total C N O S</td>
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<table>
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<th>Atoms</th>
<th>ZeroOcc</th>
<th>AltConf</th>
<th>Trace</th>
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</thead>
<tbody>
<tr>
<td>10</td>
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<td>Total C N O S</td>
<td>933 588 171 170 4</td>
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- Molecule 11 is a protein called 50S Ribosomal Protein L15.

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<tbody>
<tr>
<td>11</td>
<td>1P</td>
<td>149</td>
<td>Total C N O S</td>
<td>1135 706 230 196 3</td>
<td>0</td>
<td>0</td>
</tr>
<tr>
<td>11</td>
<td>2P</td>
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<td>Total C N O S</td>
<td>1135 706 230 196 3</td>
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- Molecule 12 is a protein called 50S Ribosomal Protein L16.

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<th>Atoms</th>
<th>ZeroOcc</th>
<th>AltConf</th>
<th>Trace</th>
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</thead>
<tbody>
<tr>
<td>12</td>
<td>1Q</td>
<td>141</td>
<td>Total C N O S</td>
<td>1122 715 212 188 7</td>
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<td>0</td>
</tr>
<tr>
<td>12</td>
<td>2Q</td>
<td>141</td>
<td>Total C N O S</td>
<td>1122 715 212 188 7</td>
<td>0</td>
<td>0</td>
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- Molecule 13 is a protein called 50S Ribosomal Protein L17.

<table>
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<th>Residues</th>
<th>Atoms</th>
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<th>AltConf</th>
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</thead>
<tbody>
<tr>
<td>13</td>
<td>1R</td>
<td>118</td>
<td>Total C N O S</td>
<td>968 604 203 160 1</td>
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<td>0</td>
</tr>
<tr>
<td>13</td>
<td>2R</td>
<td>118</td>
<td>Total C N O S</td>
<td>968 604 203 160 1</td>
<td>0</td>
<td>0</td>
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- Molecule 14 is a protein called 50S Ribosomal Protein L18.

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<th>Atoms</th>
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<th>Trace</th>
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<tr>
<td>14</td>
<td>1S</td>
<td>110</td>
<td>Total C N O S</td>
<td>873 550 174 149</td>
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<tr>
<td>14</td>
<td>2S</td>
<td>110</td>
<td>Total C N O S</td>
<td>870 549 173 148</td>
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- Molecule 15 is a protein called 50S Ribosomal Protein L19.
• Molecule 16 is a protein called 50S Ribosomal Protein L20.

<table>
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<th>Trace</th>
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</thead>
<tbody>
<tr>
<td>16</td>
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<td>116</td>
<td>Total C N O S</td>
<td>959 608 201 149 1</td>
<td>0</td>
<td>0</td>
</tr>
<tr>
<td>16</td>
<td>2U</td>
<td>116</td>
<td>Total C N O S</td>
<td>959 608 201 149 1</td>
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• Molecule 17 is a protein called 50S Ribosomal Protein L21.

<table>
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<th>Atoms</th>
<th>ZeroOcc</th>
<th>AltConf</th>
<th>Trace</th>
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</thead>
<tbody>
<tr>
<td>17</td>
<td>1V</td>
<td>101</td>
<td>Total C N O S</td>
<td>771 495 140 135 1</td>
<td>0</td>
<td>0</td>
</tr>
<tr>
<td>17</td>
<td>2V</td>
<td>101</td>
<td>Total C N O S</td>
<td>771 495 140 135 1</td>
<td>0</td>
<td>0</td>
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</table>

• Molecule 18 is a protein called 50S Ribosomal Protein L22.

<table>
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<th>Mol</th>
<th>Chain</th>
<th>Residues</th>
<th>Atoms</th>
<th>ZeroOcc</th>
<th>AltConf</th>
<th>Trace</th>
</tr>
</thead>
<tbody>
<tr>
<td>18</td>
<td>1W</td>
<td>112</td>
<td>Total C N O S</td>
<td>886 557 174 153 2</td>
<td>0</td>
<td>0</td>
</tr>
<tr>
<td>18</td>
<td>2W</td>
<td>112</td>
<td>Total C N O S</td>
<td>886 557 174 153 2</td>
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<td>0</td>
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• Molecule 19 is a protein called 50S Ribosomal Protein L23.

<table>
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<th>Chain</th>
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<th>Atoms</th>
<th>ZeroOcc</th>
<th>AltConf</th>
<th>Trace</th>
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<tbody>
<tr>
<td>19</td>
<td>1X</td>
<td>95</td>
<td>Total C N O S</td>
<td>750 488 135 126 1</td>
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<td>0</td>
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<tr>
<td>19</td>
<td>2X</td>
<td>95</td>
<td>Total C N O S</td>
<td>750 488 135 126 1</td>
<td>0</td>
<td>0</td>
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• Molecule 20 is a protein called 50S ribosomal protein L24.

<table>
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<th>Chain</th>
<th>Residues</th>
<th>Atoms</th>
<th>ZeroOcc</th>
<th>AltConf</th>
<th>Trace</th>
</tr>
</thead>
<tbody>
<tr>
<td>20</td>
<td>1Y</td>
<td>107</td>
<td>Total C N O S</td>
<td>806 517 152 131 6</td>
<td>0</td>
<td>0</td>
</tr>
<tr>
<td>20</td>
<td>2Y</td>
<td>107</td>
<td>Total C N O S</td>
<td>806 517 152 131 6</td>
<td>0</td>
<td>0</td>
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</tbody>
</table>

• Molecule 21 is a protein called 50S ribosomal protein L25.
<table>
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<th>Atoms</th>
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<th>AltConf</th>
<th>Trace</th>
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</thead>
<tbody>
<tr>
<td>21</td>
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</tr>
<tr>
<td>21</td>
<td>2Z</td>
<td>160</td>
<td>Total C N O S</td>
<td>1271</td>
<td>814</td>
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</table>

- Molecule 22 is a protein called 50S ribosomal protein L27.

<table>
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<th>Residues</th>
<th>Atoms</th>
<th>ZeroOcc</th>
<th>AltConf</th>
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</thead>
<tbody>
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<td>10</td>
<td>83</td>
<td>Total C N O S</td>
<td>653</td>
<td>404</td>
<td>139</td>
</tr>
<tr>
<td></td>
<td></td>
<td></td>
<td></td>
<td></td>
<td>109</td>
<td>1</td>
</tr>
<tr>
<td>22</td>
<td>20</td>
<td>83</td>
<td>Total C N O S</td>
<td>653</td>
<td>404</td>
<td>139</td>
</tr>
<tr>
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</table>

- Molecule 23 is a protein called 50S ribosomal protein L28.

<table>
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<th>Residues</th>
<th>Atoms</th>
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<th>AltConf</th>
<th>Trace</th>
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<tbody>
<tr>
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<td>97</td>
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<td>475</td>
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<tr>
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- Molecule 24 is a protein called 50S ribosomal protein L29.

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<td>365</td>
<td>118</td>
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<td>588</td>
<td>365</td>
<td>118</td>
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- Molecule 25 is a protein called 50S ribosomal protein L30.

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- Molecule 26 is a protein called 50S ribosomal protein L31.

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<td>0</td>
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<td>532   339  97  91  5</td>
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- Molecule 27 is a protein called 50S ribosomal protein L32.

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<td>59</td>
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<td>0</td>
<td>0</td>
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<tr>
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- Molecule 28 is a protein called 50S ribosomal protein L33.

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- Molecule 29 is a protein called 50S ribosomal protein L34.

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<td>27</td>
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<td></td>
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<td>418   257  104 55 2</td>
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- Molecule 30 is a protein called 50S Ribosomal Protein L35.

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<td>517   331  102 82 2</td>
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<td></td>
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- Molecule 31 is a protein called 50S Ribosomal Protein L36.
• Molecule 32 is a RNA chain called 16S Ribosomal RNA.

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• Molecule 33 is a protein called 30S Ribosomal Protein S2.

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• Molecule 34 is a protein called 30S Ribosomal Protein S3.

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• Molecule 35 is a protein called 30S Ribosomal Protein S4.

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• Molecule 36 is a protein called 30S Ribosomal Protein S5.

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• Molecule 37 is a protein called 30S Ribosomal Protein S6.
- Molecule 38 is a protein called 30S Ribosomal Protein S7.

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- Molecule 39 is a protein called 30S Ribosomal Protein S8.

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- Molecule 40 is a protein called 30S ribosomal protein S9.

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<td>0</td>
<td>0</td>
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<tr>
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<td>2i</td>
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- Molecule 41 is a protein called 30S ribosomal protein S10.

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<th>Atoms</th>
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<tbody>
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<td>0</td>
<td>0</td>
</tr>
<tr>
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<td>2j</td>
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- Molecule 42 is a protein called 30S ribosomal protein S11.

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<th>Atoms</th>
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<th>AltConf</th>
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<tbody>
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<tbody>
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<td>2k</td>
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- Molecule 43 is a protein called 30S ribosomal protein S12.

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<td>932 586 185 159 2</td>
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<tr>
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<td>2l</td>
<td>122</td>
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<td>0</td>
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- Molecule 44 is a protein called 30S ribosomal protein S13.

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- Molecule 45 is a protein called 30S ribosomal protein S14 type Z.

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- Molecule 46 is a protein called 30S ribosomal protein S15.

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<td>728 456 144 126 2</td>
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- Molecule 47 is a protein called 30S ribosomal protein S16.
- Molecule 48 is a protein called 30S ribosomal protein S17.

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- Molecule 49 is a protein called 30S ribosomal protein S18.

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<tr>
<td>49</td>
<td>2r</td>
<td>68</td>
<td>Total C N O</td>
<td>555 355 108 92</td>
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- Molecule 50 is a protein called 30S Ribosomal Protein S19.

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- Molecule 51 is a protein called 30S Ribosomal Protein S20.

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- Molecule 52 is a protein called 30S ribosomal protein Thx.

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- Molecule 53 is a RNA chain called mRNA.
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- Molecule 54 is a RNA chain called CC-Pmn.

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- Molecule 55 is a RNA chain called P-site tRNA, Deacylated Initiator Methionyl-tRNA.

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<td>1625 725 294 529</td>
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- Molecule 56 is MAGNESIUM ION (three-letter code: MG) (formula: Mg).

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- Molecule 57 is ZINC ION (three-letter code: ZN) (formula: Zn).

<table>
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- Molecule 58 is IRON/SULFUR CLUSTER (three-letter code: SF4) (formula: Fe₄S₄).

![SF4](image_url)

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<td>Total Fe S</td>
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- Molecule 59 is water.

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<td>0</td>
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<tr>
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<td>2a</td>
<td>19</td>
<td>Total O</td>
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</table>
3  Residue-property plots

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

- Molecule 1: 23S Ribosomal RNA

Chain 1A:
Chain 2A:

Molecule 1: 23S Ribosomal RNA

Chain 2A:
• Molecule 2: 5S Ribosomal RNA

Chain 1B:

• Molecule 2: 5S Ribosomal RNA
• Molecule 3: 50S Ribosomal Protein L2

• Molecule 3: 50S Ribosomal Protein L2

• Molecule 4: 50S Ribosomal Protein L3

• Molecule 4: 50S Ribosomal Protein L3

• Molecule 5: 50S Ribosomal Protein L4

• Molecule 5: 50S Ribosomal Protein L4
• Molecule 6: 50S Ribosomal Protein L5
  Chain 1G:

• Molecule 6: 50S Ribosomal Protein L5
  Chain 2G:

• Molecule 7: 50S Ribosomal Protein L6
  Chain 1H:

• Molecule 7: 50S Ribosomal Protein L6
  Chain 2H:

• Molecule 8: 50S Ribosomal Protein L9
  Chain 1I:

• Molecule 8: 50S Ribosomal Protein L9
  Chain 2I:
• Molecule 9: 50S Ribosomal Protein L13

Chain 1N: 9%

• Molecule 9: 50S Ribosomal Protein L13

Chain 2N: 19%

• Molecule 10: 50S Ribosomal Protein L14

Chain 1O: 32%

• Molecule 10: 50S Ribosomal Protein L14

Chain 2O: 20%

• Molecule 11: 50S Ribosomal Protein L15

Chain 1P: 4%

• Molecule 11: 50S Ribosomal Protein L15

Chain 2P: 21%

• Molecule 12: 50S Ribosomal Protein L16

Chain 1Q: 33%
• Molecule 12: 50S Ribosomal Protein L16

Chain 2Q:

• Molecule 13: 50S Ribosomal Protein L17

Chain 1R:

• Molecule 13: 50S Ribosomal Protein L17

Chain 2R:

• Molecule 14: 50S Ribosomal Protein L18

Chain 1S:

• Molecule 14: 50S Ribosomal Protein L18

Chain 2S:

• Molecule 15: 50S Ribosomal Protein L19

Chain 1T:

• Molecule 15: 50S Ribosomal Protein L19

Chain 2T:
• Molecule 16: 50S Ribosomal Protein L20

Chain 1U:

12% 98%

• Molecule 16: 50S Ribosomal Protein L20

Chain 2U:

13% 98%

• Molecule 17: 50S Ribosomal Protein L21

Chain 1V:

% 96%

• Molecule 17: 50S Ribosomal Protein L21

Chain 2V:

4% 97%

• Molecule 18: 50S Ribosomal Protein L22

Chain 1W:

9% 98%

• Molecule 18: 50S Ribosomal Protein L22

Chain 2W:

9% 98%

• Molecule 19: 50S Ribosomal Protein L23
Chain 1X:

- Molecule 19: 50S Ribosomal Protein L23

Chain 2X:

- Molecule 20: 50S ribosomal protein L24

Chain 1Y:

- Molecule 20: 50S ribosomal protein L24

Chain 2Y:

- Molecule 21: 50S ribosomal protein L25

Chain 1Z:

- Molecule 21: 50S ribosomal protein L25

Chain 2Z:

- Molecule 22: 50S ribosomal protein L27

Chain 10:
• Molecule 22: 50S ribosomal protein L27
  Chain 20:
  
• Molecule 23: 50S ribosomal protein L28
  Chain 11:
  
• Molecule 23: 50S ribosomal protein L28
  Chain 21:
  
• Molecule 24: 50S ribosomal protein L29
  Chain 12:
  
• Molecule 24: 50S ribosomal protein L29
  Chain 22:
  
• Molecule 25: 50S ribosomal protein L30
  Chain 13:
  
• Molecule 25: 50S ribosomal protein L30
Chain 23:

- Molecule 26: 50S ribosomal protein L31

Chain 14:

- Molecule 26: 50S ribosomal protein L31

Chain 24:

- Molecule 27: 50S ribosomal protein L32

Chain 15:

- Molecule 27: 50S ribosomal protein L32

Chain 25:

- Molecule 28: 50S ribosomal protein L33

Chain 16:

- Molecule 28: 50S ribosomal protein L33

Chain 26:

- Molecule 29: 50S ribosomal protein L34
Chain 17:

- Molecule 29: 50S ribosomal protein L34

Chain 27:

- Molecule 30: 50S Ribosomal Protein L35

Chain 18:

- Molecule 30: 50S Ribosomal Protein L35

Chain 28:

- Molecule 31: 50S Ribosomal Protein L36

Chain 19:

- Molecule 31: 50S Ribosomal Protein L36

Chain 29:

- Molecule 32: 16S Ribosomal RNA

Chain 1a:
Molecule 32: 16S Ribosomal RNA

Chain 2a:
• Molecule 33: 30S Ribosomal Protein S2

Chain 1b:

• Molecule 33: 30S Ribosomal Protein S2

Chain 2b:

• Molecule 34: 30S Ribosomal Protein S3

Chain 1c:

• Molecule 34: 30S Ribosomal Protein S3

Chain 2c:

• Molecule 35: 30S Ribosomal Protein S4
Chain 1d:

- Molecule 35: 30S Ribosomal Protein S4

Chain 2d:

- Molecule 36: 30S Ribosomal Protein S5

Chain 1e:

- Molecule 36: 30S Ribosomal Protein S5

Chain 2e:

- Molecule 37: 30S Ribosomal Protein S6

Chain 1f:

- Molecule 37: 30S Ribosomal Protein S6

Chain 2f:

- Molecule 38: 30S Ribosomal Protein S7

Chain 1g:
• Molecule 38: 30S Ribosomal Protein S7
Chain 2g:

• Molecule 39: 30S Ribosomal Protein S8
Chain 1h:

• Molecule 39: 30S Ribosomal Protein S8
Chain 2h:

• Molecule 40: 30S ribosomal protein S9
Chain 1i:

• Molecule 40: 30S ribosomal protein S9
Chain 2i:

• Molecule 41: 30S ribosomal protein S10
Chain 1j:

• Molecule 41: 30S ribosomal protein S10
Chain 2j:

- Molecule 42: 30S ribosomal protein S11

Chain 1k:

- Molecule 42: 30S ribosomal protein S11

Chain 2k:

- Molecule 43: 30S ribosomal protein S12

Chain 1l:

- Molecule 43: 30S ribosomal protein S12

Chain 2l:

- Molecule 44: 30S ribosomal protein S13

Chain 1m:

- Molecule 44: 30S ribosomal protein S13
Chain 2m:

- Molecule 45: 30S ribosomal protein S14 type Z

Chain 1n:

- Molecule 45: 30S ribosomal protein S14 type Z

Chain 2n:

- Molecule 46: 30S ribosomal protein S15

Chain 1o:

- Molecule 46: 30S ribosomal protein S15

Chain 2o:

- Molecule 47: 30S ribosomal protein S16

Chain 1p:

- Molecule 47: 30S ribosomal protein S16

Chain 2p:

- Molecule 47: 30S ribosomal protein S16
• Molecule 48: 30S ribosomal protein S17

Chain 1q:

• Molecule 48: 30S ribosomal protein S17

Chain 2q:

• Molecule 49: 30S ribosomal protein S18

Chain 1r:

• Molecule 49: 30S ribosomal protein S18

Chain 2r:

• Molecule 50: 30S Ribosomal Protein S19

Chain 1s:

• Molecule 50: 30S Ribosomal Protein S19

Chain 2s:

• Molecule 51: 30S Ribosomal Protein S20

Chain 1t:
• Molecule 51: 30S Ribosomal Protein S20

Chain 2t:

• Molecule 52: 30S ribosomal protein Thx

Chain 1u:

• Molecule 52: 30S ribosomal protein Thx

Chain 2u:

• Molecule 53: mRNA

Chain 1v:

• Molecule 53: mRNA

Chain 2v:

• Molecule 54: CC-Pmn

Chain 1w:

• Molecule 54: CC-Pmn

Chain 2w:
- Molecule 55: P-site tRNA, Deacylated Initiator Methionyl-tRNA

Chain 1x:

- Molecule 55: P-site tRNA, Deacylated Initiator Methionyl-tRNA

Chain 2x:
4 Data and refinement statistics

<table>
<thead>
<tr>
<th>Property</th>
<th>Value</th>
<th>Source</th>
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<td>Space group</td>
<td>P 21 21 21</td>
<td>Depositor</td>
</tr>
<tr>
<td>Cell constants</td>
<td>a, b, c, α, β, γ</td>
<td>Depositor</td>
</tr>
<tr>
<td>Resolution (Å)</td>
<td>146.71 – 3.70</td>
<td>EDS</td>
</tr>
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<td>% Data completeness (in resolution range)</td>
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<td>Depositor</td>
</tr>
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<td>Wilson B-factor (Å²)</td>
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<td>L</td>
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<td>Average B, all atoms (Å²)</td>
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Xtriage’s analysis on translational NCS is as follows: The largest off-origin peak in the Patterson function is 2.03% of the height of the origin peak. No significant pseudotranslation is detected.

---

^1Intensities estimated from amplitudes.

^2Theoretical values of < |L| >, < L² > for acentric reflections are 0.5, 0.333 respectively for untwinned datasets, and 0.375, 0.2 for perfectly twinned datasets.
5 Model quality

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: 7MG, 4OC, 2MG, 5MU, M2G, 2MA, 2MU, OMG, MA6, SF4, 0TD, PPU, 5MC, ZN, 4SU, UR3, PSU, MG

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).

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<th>Bond lengths</th>
<th>RMSZ</th>
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<td>0/1143</td>
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<td>0/1527</td>
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<td>0/1312</td>
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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.
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All (69) bond angle outliers are listed below:

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5.2 Too-close contacts

Due to software issues we are unable to calculate clashes - this section is therefore empty.

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.

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**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.

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5.3.3 RNA
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All (1392) RNA backbone outliers are listed below:

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

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

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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).

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<td>1a</td>
<td>1519</td>
<td>MA6</td>
<td>C10-N6-C9</td>
<td>-2.00</td>
<td>109.67</td>
<td>116.12</td>
</tr>
</tbody>
</table>

There are no chirality outliers.

All (45) torsion outliers are listed below:

<table>
<thead>
<tr>
<th>Mol</th>
<th>Chain</th>
<th>Res</th>
<th>Type</th>
<th>Atoms</th>
</tr>
</thead>
<tbody>
<tr>
<td>43</td>
<td>2l</td>
<td>92</td>
<td>0TD</td>
<td>O-C-CA-CB</td>
</tr>
<tr>
<td>32</td>
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<td>516</td>
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<td>C2'-C1'-C5-C4</td>
</tr>
<tr>
<td>32</td>
<td>1a</td>
<td>516</td>
<td>PSU</td>
<td>C2'-C1'-C5-C6</td>
</tr>
<tr>
<td>32</td>
<td>2a</td>
<td>966</td>
<td>M2G</td>
<td>N1-C2-N2-CM2</td>
</tr>
<tr>
<td>32</td>
<td>2a</td>
<td>966</td>
<td>M2G</td>
<td>N3-C2-N2-CM1</td>
</tr>
<tr>
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<td>2a</td>
<td>966</td>
<td>M2G</td>
<td>N3-C2-N2-CM2</td>
</tr>
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<td>967</td>
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</tr>
<tr>
<td>32</td>
<td>2a</td>
<td>1400</td>
<td>5MC</td>
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</tr>
<tr>
<td>32</td>
<td>1a</td>
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</tr>
<tr>
<td>32</td>
<td>2a</td>
<td>1519</td>
<td>MA6</td>
<td>O4'-C4'-C5'-O5'</td>
</tr>
<tr>
<td>32</td>
<td>2a</td>
<td>1519</td>
<td>MA6</td>
<td>C3'-C4'-C5'-O5'</td>
</tr>
<tr>
<td>54</td>
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<td>76</td>
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<td>C3'-C4'-C5'-O5'</td>
</tr>
<tr>
<td>32</td>
<td>1a</td>
<td>967</td>
<td>5MC</td>
<td>C3'-C4'-C5'-O5'</td>
</tr>
<tr>
<td>32</td>
<td>2a</td>
<td>1400</td>
<td>5MC</td>
<td>C3'-C4'-C5'-O5'</td>
</tr>
<tr>
<td>32</td>
<td>1a</td>
<td>1519</td>
<td>MA6</td>
<td>C3'-C4'-C5'-O5'</td>
</tr>
</tbody>
</table>

Continued on next page...
Continued from previous page...

<table>
<thead>
<tr>
<th>Mol</th>
<th>Chain</th>
<th>Res</th>
<th>Type</th>
<th>Atoms</th>
</tr>
</thead>
<tbody>
<tr>
<td>54</td>
<td>1w</td>
<td>76</td>
<td>PPU</td>
<td>O4'-C4'-C5'-O5'</td>
</tr>
<tr>
<td>54</td>
<td>2w</td>
<td>76</td>
<td>PPU</td>
<td>C3'-C4'-C5'-O5'</td>
</tr>
<tr>
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<td>1a</td>
<td>1400</td>
<td>5MC</td>
<td>O4'-C4'-C5'-O5'</td>
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<td>1518</td>
<td>MA6</td>
<td>C5-C6-N6-C10</td>
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<td>2a</td>
<td>1518</td>
<td>MA6</td>
<td>C5-C6-N6-C10</td>
</tr>
<tr>
<td>54</td>
<td>2w</td>
<td>76</td>
<td>PPU</td>
<td>O4'-C4'-C5'-O5'</td>
</tr>
<tr>
<td>32</td>
<td>2a</td>
<td>966</td>
<td>M2G</td>
<td>N1-C2-N2-CM1</td>
</tr>
<tr>
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<td>2a</td>
<td>1519</td>
<td>MA6</td>
<td>C4'-C5'-O5'-P</td>
</tr>
<tr>
<td>43</td>
<td>2l</td>
<td>92</td>
<td>0TD</td>
<td>SB-CB-CG-OD1</td>
</tr>
<tr>
<td>32</td>
<td>1a</td>
<td>1519</td>
<td>MA6</td>
<td>C5-C6-N6-C10</td>
</tr>
<tr>
<td>32</td>
<td>1a</td>
<td>1519</td>
<td>MA6</td>
<td>C5-C6-N6-C10</td>
</tr>
<tr>
<td>54</td>
<td>1w</td>
<td>76</td>
<td>PPU</td>
<td>N-CA-CB-CG</td>
</tr>
<tr>
<td>54</td>
<td>1w</td>
<td>76</td>
<td>PPU</td>
<td>C5-C6-N6-C10</td>
</tr>
<tr>
<td>54</td>
<td>2w</td>
<td>76</td>
<td>PPU</td>
<td>N-CA-CB-CG</td>
</tr>
<tr>
<td>54</td>
<td>2w</td>
<td>76</td>
<td>PPU</td>
<td>C5-C6-N6-C10</td>
</tr>
<tr>
<td>32</td>
<td>1a</td>
<td>1400</td>
<td>5MC</td>
<td>C3'-C4'-C5'-O5'</td>
</tr>
<tr>
<td>32</td>
<td>1a</td>
<td>1518</td>
<td>MA6</td>
<td>N1-C6-N6-C9</td>
</tr>
<tr>
<td>32</td>
<td>1a</td>
<td>1519</td>
<td>MA6</td>
<td>C4'-C5'-O5'-P</td>
</tr>
<tr>
<td>54</td>
<td>1w</td>
<td>76</td>
<td>PPU</td>
<td>C-CA-CB-CG</td>
</tr>
<tr>
<td>54</td>
<td>2w</td>
<td>76</td>
<td>PPU</td>
<td>C-CA-CB-CG</td>
</tr>
<tr>
<td>43</td>
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<td>92</td>
<td>0TD</td>
<td>CG-CB-SB-CSB</td>
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<tr>
<td>43</td>
<td>2l</td>
<td>92</td>
<td>0TD</td>
<td>CG-CB-SB-CSB</td>
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<tr>
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<td>2A</td>
<td>2503</td>
<td>2MA</td>
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<td>1A</td>
<td>1942</td>
<td>4OC</td>
<td>C2'-C1'-N1-C2</td>
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<tr>
<td>1</td>
<td>1A</td>
<td>2515</td>
<td>2MA</td>
<td>O4'-C4'-C5'-O5'</td>
</tr>
</tbody>
</table>

There are no ring outliers.

No monomer is involved in short contacts.

5.5 Carbohydrates

There are no monosaccharides in this entry.

5.6 Ligand geometry

Of 1170 ligands modelled in this entry, 1168 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).

<table>
<thead>
<tr>
<th>Mol</th>
<th>Type</th>
<th>Chain</th>
<th>Res</th>
<th>Link</th>
<th>Bond lengths</th>
<th>Bond angles</th>
</tr>
</thead>
<tbody>
<tr>
<td></td>
<td></td>
<td></td>
<td></td>
<td></td>
<td>Counts</td>
<td>RMSZ</td>
</tr>
<tr>
<td>58</td>
<td>SF4</td>
<td>1d</td>
<td>302</td>
<td>35</td>
<td>0,12,12</td>
<td>-</td>
</tr>
<tr>
<td>58</td>
<td>SF4</td>
<td>2d</td>
<td>302</td>
<td>35</td>
<td>0,12,12</td>
<td>-</td>
</tr>
</tbody>
</table>

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.

<table>
<thead>
<tr>
<th>Mol</th>
<th>Type</th>
<th>Chain</th>
<th>Res</th>
<th>Link</th>
<th>Chirals</th>
<th>Torsions</th>
<th>Rings</th>
</tr>
</thead>
<tbody>
<tr>
<td>58</td>
<td>SF4</td>
<td>1d</td>
<td>302</td>
<td>35</td>
<td>-</td>
<td>0/6/5/5</td>
<td></td>
</tr>
<tr>
<td>58</td>
<td>SF4</td>
<td>2d</td>
<td>302</td>
<td>35</td>
<td>-</td>
<td>0/6/5/5</td>
<td></td>
</tr>
</tbody>
</table>

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

The following chains have linkage breaks:

<table>
<thead>
<tr>
<th>Mol</th>
<th>Chain</th>
<th>Number of breaks</th>
</tr>
</thead>
<tbody>
<tr>
<td>3</td>
<td>2D</td>
<td>1</td>
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</tbody>
</table>

All chain breaks are listed below:

<table>
<thead>
<tr>
<th>Model</th>
<th>Chain</th>
<th>Residue-1</th>
<th>Atom-1</th>
<th>Residue-2</th>
<th>Atom-2</th>
<th>Distance (Å)</th>
</tr>
</thead>
<tbody>
<tr>
<td>1</td>
<td>2D</td>
<td>7:LYS</td>
<td>C</td>
<td>8:PRO</td>
<td>N</td>
<td>1.17</td>
</tr>
</tbody>
</table>
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, 95th 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.

<table>
<thead>
<tr>
<th>Mol</th>
<th>Chain</th>
<th>Analysed</th>
<th>&lt;RSRZ&gt;</th>
<th>#RSRZ&gt;2</th>
<th>OWAB(Å²)</th>
<th>Q&lt;0.9</th>
</tr>
</thead>
<tbody>
<tr>
<td>1</td>
<td>1A</td>
<td>2860/2915</td>
<td>0.24</td>
<td>80 (2%)</td>
<td>53 40</td>
<td>82 102 143 157</td>
</tr>
<tr>
<td>1</td>
<td>2A</td>
<td>2789/2915</td>
<td>0.12</td>
<td>95 (3%)</td>
<td>45 34</td>
<td>88 107 136 157</td>
</tr>
<tr>
<td>2</td>
<td>1B</td>
<td>120/121</td>
<td>-0.38</td>
<td>0 100</td>
<td>100</td>
<td>104 121 132 134</td>
</tr>
<tr>
<td>2</td>
<td>2B</td>
<td>120/121</td>
<td>-0.57</td>
<td>0 100</td>
<td>100</td>
<td>111 125 135 152</td>
</tr>
<tr>
<td>3</td>
<td>1D</td>
<td>275/276</td>
<td>0.88</td>
<td>27 (9%)</td>
<td>7 6</td>
<td>84 95 108 127</td>
</tr>
<tr>
<td>3</td>
<td>2D</td>
<td>275/276</td>
<td>1.15</td>
<td>53 (19%)</td>
<td>1 1</td>
<td>88 104 114 123</td>
</tr>
<tr>
<td>4</td>
<td>1E</td>
<td>204/206</td>
<td>0.63</td>
<td>41 (20%)</td>
<td>1 0</td>
<td>86 108 122 131</td>
</tr>
<tr>
<td>4</td>
<td>2E</td>
<td>204/206</td>
<td>0.31</td>
<td>26 (12%)</td>
<td>3 4</td>
<td>88 105 119 129</td>
</tr>
<tr>
<td>5</td>
<td>1F</td>
<td>203/210</td>
<td>0.23</td>
<td>14 (6%)</td>
<td>16 11</td>
<td>79 102 120 137</td>
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<tr>
<td>5</td>
<td>2F</td>
<td>203/210</td>
<td>0.64</td>
<td>38 (18%)</td>
<td>1 1</td>
<td>90 108 122 130</td>
</tr>
<tr>
<td>6</td>
<td>1G</td>
<td>181/182</td>
<td>-0.27</td>
<td>2 (1%)</td>
<td>80 71</td>
<td>112 122 131 139</td>
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<tr>
<td>6</td>
<td>2G</td>
<td>181/182</td>
<td>0.72</td>
<td>30 (16%)</td>
<td>1 1</td>
<td>113 126 136 149</td>
</tr>
<tr>
<td>7</td>
<td>1H</td>
<td>174/180</td>
<td>0.20</td>
<td>4 (2%)</td>
<td>60 48</td>
<td>96 113 124 131</td>
</tr>
<tr>
<td>7</td>
<td>2H</td>
<td>174/180</td>
<td>0.49</td>
<td>15 (8%)</td>
<td>10 8</td>
<td>105 125 134 142</td>
</tr>
<tr>
<td>8</td>
<td>1I</td>
<td>146/148</td>
<td>-0.32</td>
<td>3 (2%)</td>
<td>63 52</td>
<td>102 115 124 134</td>
</tr>
<tr>
<td>8</td>
<td>2I</td>
<td>146/148</td>
<td>0.30</td>
<td>18 (12%)</td>
<td>4 4</td>
<td>109 124 138 143</td>
</tr>
<tr>
<td>9</td>
<td>1N</td>
<td>140/140</td>
<td>0.72</td>
<td>13 (9%)</td>
<td>8 6</td>
<td>93 106 119 122</td>
</tr>
<tr>
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<td>39 (31%)</td>
<td>0 0</td>
<td>90 108 122 128</td>
</tr>
<tr>
<td>10</td>
<td>2O</td>
<td>122/122</td>
<td>1.19</td>
<td>25 (20%)</td>
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<td>87 102 113 118</td>
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<tr>
<td>11</td>
<td>1P</td>
<td>149/150</td>
<td>0.40</td>
<td>6 (4%)</td>
<td>38 28</td>
<td>85 109 124 130</td>
</tr>
<tr>
<td>11</td>
<td>2P</td>
<td>149/150</td>
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<td>32 (21%)</td>
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<tr>
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<td>1Q</td>
<td>141/141</td>
<td>1.58</td>
<td>47 (33%)</td>
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<td>89 108 119 127</td>
</tr>
<tr>
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<td>2Q</td>
<td>141/141</td>
<td>0.22</td>
<td>10 (7%)</td>
<td>16 11</td>
<td>96 110 122 130</td>
</tr>
</tbody>
</table>
Continued from previous page...

<table>
<thead>
<tr>
<th>Mol</th>
<th>Chain</th>
<th>Analysed</th>
<th>&lt;RSRZ&gt;</th>
<th>#&lt;RSRZ&gt;2</th>
<th>OWAB(Å²)</th>
<th>Q&lt;0.9</th>
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<tbody>
<tr>
<td>13</td>
<td>1R</td>
<td>118/118 (100%)</td>
<td>0.35</td>
<td>1 (0%)</td>
<td>86, 78</td>
<td>94, 104, 116, 125</td>
</tr>
<tr>
<td>13</td>
<td>2R</td>
<td>118/118 (100%)</td>
<td>0.63</td>
<td>13 (11%)</td>
<td>5, 4</td>
<td>89, 103, 111, 118</td>
</tr>
<tr>
<td>14</td>
<td>1S</td>
<td>110/112 (98%)</td>
<td>-0.42</td>
<td>0</td>
<td>100</td>
<td>106, 116, 125, 131</td>
</tr>
<tr>
<td>14</td>
<td>2S</td>
<td>110/112 (98%)</td>
<td>-0.16</td>
<td>1 (0%)</td>
<td>84, 76</td>
<td>106, 119, 127, 130</td>
</tr>
<tr>
<td>15</td>
<td>1T</td>
<td>131/146 (89%)</td>
<td>0.46</td>
<td>15 (11%)</td>
<td>4, 4</td>
<td>95, 110, 123, 138</td>
</tr>
<tr>
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<td>2T</td>
<td>131/146 (89%)</td>
<td>0.86</td>
<td>26 (19%)</td>
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<td>92, 106, 121, 129</td>
</tr>
<tr>
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<td>1U</td>
<td>116/118 (98%)</td>
<td>0.55</td>
<td>14 (12%)</td>
<td>3, 3</td>
<td>86, 105, 119, 134</td>
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<td>2U</td>
<td>116/118 (98%)</td>
<td>0.81</td>
<td>15 (12%)</td>
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<td>94, 109, 121, 125</td>
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<td>1V</td>
<td>101/101 (100%)</td>
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<td>1 (0%)</td>
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<td>88, 106, 120, 127</td>
</tr>
<tr>
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<td>2V</td>
<td>101/101 (100%)</td>
<td>0.21</td>
<td>4 (3%)</td>
<td>38, 28</td>
<td>93, 114, 127, 136</td>
</tr>
<tr>
<td>18</td>
<td>1W</td>
<td>112/113 (99%)</td>
<td>0.84</td>
<td>10 (8%)</td>
<td>9, 7</td>
<td>88, 101, 120, 131</td>
</tr>
<tr>
<td>18</td>
<td>2W</td>
<td>112/113 (99%)</td>
<td>0.47</td>
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6.2 Non-standard residues in protein, DNA, RNA chains

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6.3 Carbohydrates

There are no monosaccharides in this entry.

6.4 Ligands

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th 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.
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### 6.5 Other polymers

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