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 3.80 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.

<table>
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<tr>
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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 \( \geq 3, 2, 1 \) 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 54 unique types of molecules in this entry. The entry contains 287293 atoms, of which 0 are hydrogens and 0 are deuteriums.

In the tables below, the ZeroOcc column contains the number of atoms modelled with zero occupancy, the AltConf column contains the number of residues with at least one atom in alternate conformation and the Trace column contains the number of residues modelled with at most 2 atoms.

- Molecule 1 is a protein called 50S ribosomal protein L2.

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<th>Atoms</th>
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<tr>
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- Molecule 2 is a protein called 50S ribosomal protein L3.

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- Molecule 3 is a protein called 50S ribosomal protein L4.

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- Molecule 4 is a protein called 50S ribosomal protein L5.

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- Molecule 5 is a protein called 50S ribosomal protein L6.
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- Molecule 6 is a protein called 50S ribosomal protein L9.

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- Molecule 7 is a protein called 50S ribosomal protein L11.

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<td>692</td>
<td>191</td>
<td>199</td>
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<tr>
<td>7</td>
<td>BL11</td>
<td>147</td>
<td>Total C</td>
<td>N</td>
<td>O</td>
<td>S</td>
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<td></td>
<td>1088</td>
<td>692</td>
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<td>199</td>
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- Molecule 8 is a protein called 50S ribosomal protein L13.

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<td>707</td>
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<td>137</td>
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<td>O</td>
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- Molecule 9 is a protein called 50S ribosomal protein L14.

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<td>171</td>
<td>170</td>
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<td>122</td>
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<td>N</td>
<td>O</td>
<td>S</td>
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<td>587</td>
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- Molecule 10 is a protein called 50S ribosomal protein L15.
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- Molecule 11 is a protein called 50S ribosomal protein L16.

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- Molecule 12 is a protein called 50S ribosomal protein L17.

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<tr>
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<tr>
<td>12</td>
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<td>Total C N O</td>
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- Molecule 13 is a protein called 50S ribosomal protein L18.

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<tr>
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</tr>
<tr>
<td>13</td>
<td>BL18</td>
<td>98</td>
<td>Total C N O</td>
<td>771 486 154 131</td>
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- Molecule 14 is a protein called 50S ribosomal protein L19.

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<td>14</td>
<td>BL19</td>
<td>137</td>
<td>Total C N O S</td>
<td>1144 713 234 196 1</td>
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- Molecule 15 is a protein called 50S ribosomal protein L20.
- Molecule 16 is a protein called 50S ribosomal protein L21.

<table>
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<tr>
<td>16</td>
<td>BL21</td>
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<td>Total C N O S 779 501 142 135 1</td>
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- Molecule 17 is a protein called 50S ribosomal protein L22.

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<td>0</td>
</tr>
<tr>
<td>17</td>
<td>BL22</td>
<td>112</td>
<td>Total C N O S 891 560 175 154 2</td>
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- Molecule 18 is a protein called 50S ribosomal protein L23.

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<tr>
<td>18</td>
<td>AL23</td>
<td>92</td>
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<tr>
<td>18</td>
<td>BL23</td>
<td>92</td>
<td>Total C N O 726 471 131 124</td>
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- Molecule 19 is a protein called 50S ribosomal protein L24.

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<tr>
<td>19</td>
<td>AL24</td>
<td>100</td>
<td>Total C N O S 776 500 148 124 4</td>
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<td>0</td>
<td>0</td>
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<tr>
<td>19</td>
<td>BL24</td>
<td>100</td>
<td>Total C N O S 776 500 148 124 4</td>
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- Molecule 20 is a protein called 50S ribosomal protein L25.

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<tr>
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<td>BL25</td>
<td>187</td>
<td>Total C N O S 1483 945 264 272 2</td>
<td>0</td>
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<td>0</td>
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- Molecule 21 is a protein called 50S ribosomal protein L27.
- Molecule 22 is a protein called 50S ribosomal protein L28.

<table>
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<tr>
<td>22</td>
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<td>0</td>
<td>0</td>
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<tr>
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<td>88</td>
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- Molecule 23 is a protein called 50S ribosomal protein L29.

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<tbody>
<tr>
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<td>Total C N O</td>
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<td>0</td>
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<td>BL29</td>
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<td>Total C N O</td>
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- Molecule 24 is a protein called 50S ribosomal protein L30.

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<td>Total C N O</td>
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- Molecule 25 is a protein called 50S ribosomal protein L32.

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<tbody>
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- Molecule 26 is a protein called 50S ribosomal protein L33.

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<tbody>
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<td>0</td>
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<td>381 235 77 65 4</td>
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- Molecule 27 is a protein called 50S ribosomal protein L34.

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<td>419 257 104 56 2</td>
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- Molecule 28 is a protein called 50S ribosomal protein L35.

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<td>508 326 101 79 2</td>
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- Molecule 29 is a protein called 30S ribosomal protein S2.

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<tbody>
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<td>1901 1213 341 342 5</td>
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- Molecule 30 is a protein called 30S ribosomal protein S3.

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<td>0</td>
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</tr>
<tr>
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<td></td>
<td></td>
<td>1613 1016 314 282 1</td>
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- Molecule 31 is a protein called 30S ribosomal protein S4.
- Molecule 32 is a protein called 30S ribosomal protein S5.

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<td></td>
<td></td>
<td></td>
<td>O 4</td>
<td>0</td>
<td>0</td>
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</tr>
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<td></td>
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- Molecule 33 is a protein called 30S ribosomal protein S6.

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<th>Atoms</th>
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<tbody>
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- Molecule 34 is a protein called 30S ribosomal protein S7.

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- Molecule 35 is a protein called 30S ribosomal protein S8.

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<td>BS08</td>
<td>138</td>
<td>C 193</td>
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- Molecule 36 is a protein called 30S ribosomal protein S9.

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<td></td>
<td></td>
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<td></td>
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- Molecule 37 is a protein called 30S ribosomal protein S10.
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</thead>
<tbody>
<tr>
<td>37</td>
<td>AS10</td>
<td>98</td>
<td>Total C N O S &lt;br&gt;795 499 156 139 1</td>
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<td>0</td>
<td>0</td>
</tr>
<tr>
<td>37</td>
<td>BS10</td>
<td>98</td>
<td>Total C N O S &lt;br&gt;795 499 156 139 1</td>
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- Molecule 38 is a protein called 30S ribosomal protein S11.

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<tr>
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<td>0</td>
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<tr>
<td>38</td>
<td>BS11</td>
<td>114</td>
<td>Total C N O S &lt;br&gt;843 522 159 159 3</td>
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- Molecule 39 is a protein called 30S ribosomal protein S12.

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<th>Atoms</th>
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<tbody>
<tr>
<td>39</td>
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<td>122</td>
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<td>0</td>
<td>0</td>
</tr>
<tr>
<td>39</td>
<td>BS12</td>
<td>122</td>
<td>Total C N O S &lt;br&gt;957 603 193 160 1</td>
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- Molecule 40 is a protein called 30S ribosomal protein S13.

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<tr>
<td>40</td>
<td>AS13</td>
<td>117</td>
<td>Total C N O S &lt;br&gt;934 577 192 163 2</td>
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<td>0</td>
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</tr>
<tr>
<td>40</td>
<td>BS13</td>
<td>117</td>
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- Molecule 41 is a protein called 30S ribosomal protein S14.

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<tr>
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<tr>
<td>41</td>
<td>BS14</td>
<td>60</td>
<td>Total C N O S &lt;br&gt;492 312 104 72 4</td>
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- Molecule 42 is a protein called 30S ribosomal protein S15.

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Continued from previous page...

<table>
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<tr>
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- Molecule 43 is a protein called 30S ribosomal protein S16.

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<td>701</td>
<td>443</td>
<td>139</td>
<td>118</td>
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<tr>
<td>43</td>
<td>BS16</td>
<td>83</td>
<td>Total C,N,O,S</td>
<td>0</td>
<td>0</td>
<td>0</td>
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<tr>
<td>701</td>
<td>443</td>
<td>139</td>
<td>118</td>
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- Molecule 44 is a protein called 30S ribosomal protein S17.

<table>
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<th>Atoms</th>
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<td>BS17</td>
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<td>Total C,N,O,S</td>
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<tr>
<td>824</td>
<td>528</td>
<td>152</td>
<td>142</td>
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- Molecule 45 is a protein called 30S ribosomal protein S18.

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<td>112</td>
<td>95</td>
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<td></td>
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<tr>
<td>45</td>
<td>BS18</td>
<td>70</td>
<td>Total C,N,O</td>
<td>0</td>
<td>0</td>
<td>0</td>
</tr>
<tr>
<td>574</td>
<td>367</td>
<td>112</td>
<td>95</td>
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- Molecule 46 is a protein called 30S ribosomal protein S19.

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<th>Trace</th>
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<tbody>
<tr>
<td>46</td>
<td>AS19</td>
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<td>0</td>
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<tr>
<td>630</td>
<td>403</td>
<td>114</td>
<td>111</td>
<td>2</td>
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</tr>
<tr>
<td>46</td>
<td>BS19</td>
<td>78</td>
<td>Total C,N,O,S</td>
<td>0</td>
<td>0</td>
<td>0</td>
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<tr>
<td>630</td>
<td>403</td>
<td>114</td>
<td>111</td>
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- Molecule 47 is a protein called 30S ribosomal protein S20.
• Molecule 48 is a protein called 30S ribosomal protein Thx.

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<tr>
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• Molecule 49 is a protein called 50S ribosomal protein L31.

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<th>Atoms</th>
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<tbody>
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<td>BL31</td>
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<td>Total C N O S</td>
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• Molecule 50 is a RNA chain called 16S ribosomal RNA.

<table>
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<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>50</td>
<td>A16S</td>
<td>1504</td>
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<tr>
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<td>B16S</td>
<td>1504</td>
<td>Total C N O P</td>
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• Molecule 51 is a RNA chain called 23S ribosomal RNA.

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<th>Atoms</th>
<th>ZeroOcc</th>
<th>AltConf</th>
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</thead>
<tbody>
<tr>
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<td>0</td>
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<tr>
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There are 4 discrepancies between the modelled and reference sequences:

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<th>Modelled</th>
<th>Actual</th>
<th>Comment</th>
<th>Reference</th>
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<tbody>
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<td>U</td>
<td>C</td>
<td>conflict</td>
<td>GB 46197919</td>
</tr>
<tr>
<td>A23S</td>
<td>2825</td>
<td>U</td>
<td>G</td>
<td>conflict</td>
<td>GB 46197919</td>
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<td>B23S</td>
<td>1141A</td>
<td>U</td>
<td>C</td>
<td>conflict</td>
<td>GB 46197919</td>
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<tr>
<td>B23S</td>
<td>2825</td>
<td>U</td>
<td>G</td>
<td>conflict</td>
<td>GB 46197919</td>
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• Molecule 52 is a RNA chain called 5S ribosomal RNA.
<table>
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<th>Atoms</th>
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<tbody>
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<tr>
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- Molecule 53 is a RNA chain called IRES RNA.

<table>
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<th>Atoms</th>
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- Molecule 54 is ZINC ION (three-letter code: ZN) (formula: Zn).

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<th>Atoms</th>
<th>ZeroOcc</th>
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<td>0</td>
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<tr>
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<td>BS14</td>
<td>1</td>
<td>Total Zn</td>
<td>0</td>
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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: 50S ribosomal protein L2

Chain AL02:

- Molecule 1: 50S ribosomal protein L2

Chain BL02:

- Molecule 2: 50S ribosomal protein L3

Chain AL03:

- Molecule 2: 50S ribosomal protein L3

Chain BL03:
• Molecule 3: 50S ribosomal protein L4

Chain AL04:

• Molecule 3: 50S ribosomal protein L4

Chain BL04:

• Molecule 4: 50S ribosomal protein L5

Chain AL05:

• Molecule 4: 50S ribosomal protein L5

Chain BL05:

• Molecule 5: 50S ribosomal protein L6

Chain AL06:
• Molecule 5: 50S ribosomal protein L6

Chain BL06:

• Molecule 6: 50S ribosomal protein L9

Chain AL09:

• Molecule 6: 50S ribosomal protein L9

Chain BL09:

• Molecule 7: 50S ribosomal protein L11

Chain AL11:
• Molecule 7: 50S ribosomal protein L11

Chain BL11:

• Molecule 8: 50S ribosomal protein L13

Chain AL13:

• Molecule 8: 50S ribosomal protein L13

Chain BL13:

• Molecule 9: 50S ribosomal protein L14

Chain AL14:

• Molecule 9: 50S ribosomal protein L14

Chain BL14:

• Molecule 10: 50S ribosomal protein L15
Chain AL15:

- Molecule 10: 50S ribosomal protein L15

Chain BL15:

- Molecule 11: 50S ribosomal protein L16

Chain AL16:

- Molecule 11: 50S ribosomal protein L16

Chain BL16:

- Molecule 12: 50S ribosomal protein L17

Chain AL17:

- Molecule 12: 50S ribosomal protein L17

Chain BL17:
• Molecule 13: 50S ribosomal protein L18

Chain AL18:

Chain BL18:

• Molecule 13: 50S ribosomal protein L18

Chain AL19:

Chain BL19:

• Molecule 14: 50S ribosomal protein L19

Chain AL20:

Chain BL20:
• Molecule 16: 50S ribosomal protein L21

Chain AL21:

• Molecule 16: 50S ribosomal protein L21

Chain BL21:

• Molecule 17: 50S ribosomal protein L22

Chain AL22:

• Molecule 17: 50S ribosomal protein L22

Chain BL22:

• Molecule 18: 50S ribosomal protein L23

Chain AL23:

• Molecule 18: 50S ribosomal protein L23

Chain BL23:

• Molecule 19: 50S ribosomal protein L24

Chain AL24:
- Molecule 19: 50S ribosomal protein L24

Chain BL24:

- Molecule 20: 50S ribosomal protein L25

Chain AL25:

- Molecule 20: 50S ribosomal protein L25

Chain BL25:

- Molecule 21: 50S ribosomal protein L27

Chain AL27:

- Molecule 21: 50S ribosomal protein L27

Chain BL27:

- Molecule 22: 50S ribosomal protein L28
Chain AL28:

- Molecule 22: 50S ribosomal protein L28

Chain BL28:

- Molecule 23: 50S ribosomal protein L29

Chain AL29:

- Molecule 23: 50S ribosomal protein L29

Chain BL29:

- Molecule 24: 50S ribosomal protein L30

Chain AL30:

- Molecule 24: 50S ribosomal protein L30

Chain BL30:

- Molecule 25: 50S ribosomal protein L32

Chain AL32:
• Molecule 25: 50S ribosomal protein L32
  Chain BL32:

• Molecule 26: 50S ribosomal protein L33
  Chain AL33:

• Molecule 26: 50S ribosomal protein L33
  Chain BL33:

• Molecule 27: 50S ribosomal protein L34
  Chain AL34:

• Molecule 27: 50S ribosomal protein L34
  Chain BL34:

• Molecule 28: 50S ribosomal protein L35
  Chain AL35:

• Molecule 28: 50S ribosomal protein L35
  Chain BL35: 
• Molecule 29: 30S ribosomal protein S2

Chain AS02:

• Molecule 29: 30S ribosomal protein S2

Chain BS02:

• Molecule 30: 30S ribosomal protein S3

Chain AS03:

• Molecule 30: 30S ribosomal protein S3

Chain BS03:

• Molecule 31: 30S ribosomal protein S4

Chain AS04:
- Molecule 31: 30S ribosomal protein S4

Chain BS04:

- Molecule 32: 30S ribosomal protein S5

Chain AS05:

- Molecule 32: 30S ribosomal protein S5

Chain BS05:

- Molecule 33: 30S ribosomal protein S6

Chain AS06:

- Molecule 33: 30S ribosomal protein S6

Chain BS06:

- Molecule 34: 30S ribosomal protein S7

Chain AS07:
• Molecule 34: 30S ribosomal protein S7

Chain BS07:

• Molecule 35: 30S ribosomal protein S8

Chain AS08:

• Molecule 35: 30S ribosomal protein S8

Chain BS08:

• Molecule 36: 30S ribosomal protein S9

Chain AS09:

• Molecule 36: 30S ribosomal protein S9

Chain BS09:

• Molecule 37: 30S ribosomal protein S10

Chain AS10:
- Molecule 37: 30S ribosomal protein S10
  Chain BS10:

- Molecule 38: 30S ribosomal protein S11
  Chain AS11:

- Molecule 38: 30S ribosomal protein S11
  Chain BS11:

- Molecule 39: 30S ribosomal protein S12
  Chain AS12:

- Molecule 39: 30S ribosomal protein S12
  Chain BS12:

- Molecule 40: 30S ribosomal protein S13
  Chain AS13:
• Molecule 40: 30S ribosomal protein S13

Chain BS13:

• Molecule 41: 30S ribosomal protein S14

Chain AS14:

• Molecule 41: 30S ribosomal protein S14

Chain BS14:

• Molecule 42: 30S ribosomal protein S15

Chain AS15:

• Molecule 42: 30S ribosomal protein S15

Chain BS15:

• Molecule 43: 30S ribosomal protein S16

Chain AS16:

• Molecule 43: 30S ribosomal protein S16
Chain BS16:

- Molecule 44: 30S ribosomal protein S17

Chain AS17:

- Molecule 44: 30S ribosomal protein S17

Chain BS17:

- Molecule 45: 30S ribosomal protein S18

Chain AS18:

- Molecule 45: 30S ribosomal protein S18

Chain BS18:

- Molecule 46: 30S ribosomal protein S19

Chain AS19:

- Molecule 46: 30S ribosomal protein S19
• Molecule 47: 30S ribosomal protein S20

Chain AS20:

• Molecule 47: 30S ribosomal protein S20

Chain BS20:

• Molecule 48: 30S ribosomal protein Thx

Chain ATHX:

• Molecule 48: 30S ribosomal protein Thx

Chain BTHX:

• Molecule 49: 50S ribosomal protein L31

Chain AL31:

• Molecule 49: 50S ribosomal protein L31

Chain BL31:

• Molecule 50: 16S ribosomal RNA

Chain A16S:
Molecule 50: 16S ribosomal RNA

Chain B16S:
• Molecule 51: 23S ribosomal RNA

Chain A23S:
• Molecule 51: 23S ribosomal RNA

Chain B23S:
- Molecule 52: 5S ribosomal RNA

Chain A5S:

- Molecule 52: 5S ribosomal RNA

Chain B5S:

- Molecule 53: IRES RNA

Chain AIRe:

- Molecule 53: IRES RNA

Chain BIRE:
4 Data and refinement statistics

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<tr>
<th>Property</th>
<th>Value</th>
<th>Source</th>
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<td>Depositor</td>
</tr>
<tr>
<td>Cell constants</td>
<td>a, b, c, α, β, γ</td>
<td></td>
</tr>
<tr>
<td>Resolution (Å)</td>
<td>60.00 – 3.80</td>
<td>Depositor</td>
</tr>
<tr>
<td>% Data completeness</td>
<td>99.9 (60.00-3.80)</td>
<td>Depositor</td>
</tr>
<tr>
<td>Refinement program</td>
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<td>Rsym</td>
<td>(Not available)</td>
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<tr>
<td>( &lt;I/\sigma(I) &gt; ^1 )</td>
<td>1.45 (at 3.77Å)</td>
<td>Xtriage</td>
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<td>Wilson B-factor (Å²)</td>
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<td>Bulk solvent ( k_{sol} e/Å³ ), ( B_{sol} Å² )</td>
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<td>EDS</td>
</tr>
<tr>
<td>L-test for twinning</td>
<td>(&lt;</td>
<td>L</td>
</tr>
<tr>
<td>Estimated twinning fraction</td>
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<td>Xtriage</td>
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<td>( F_o,F_c ) correlation</td>
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<tr>
<td>Average B, all atoms (Å²)</td>
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<td>wwPDB-VP</td>
</tr>
</tbody>
</table>

Xtriage’s analysis on translational NCS is as follows: The largest off-origin peak in the Patterson function is 1.66% of the height of the origin peak. No significant pseudotranslation is detected.

---

1 Intensities estimated from amplitudes.
2 Theoretical values of \(<|L|>, <L^2>\) for acentric reflections are 0.5, 0.333 respectively for untwinned datasets, and 0.375, 0.2 for perfectly twinned datasets.
5  Model quality

5.1  Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: ZN

The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 5$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

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<th>Chain</th>
<th>bond lengths</th>
<th>Bond angles</th>
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</tr>
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<td>0.39</td>
<td>0/745</td>
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<td>42</td>
<td>BS15</td>
<td>0.38</td>
<td>0/745</td>
</tr>
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<td>43</td>
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<td>0.31</td>
<td>0/717</td>
</tr>
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<td>BS16</td>
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<td>0/579</td>
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<td>BTHX</td>
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<td>BL31</td>
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<td>0/229</td>
</tr>
<tr>
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<td>A23S</td>
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<td>2/69356 (0.0%)</td>
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<td>B23S</td>
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<td>B5S</td>
<td>0.24</td>
<td>0/2853</td>
</tr>
<tr>
<td>53</td>
<td>AIRE</td>
<td>0.25</td>
<td>0/748</td>
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<tr>
<td>53</td>
<td>BIRE</td>
<td>0.27</td>
<td>0/748</td>
</tr>
<tr>
<td>All</td>
<td>All</td>
<td>0.34</td>
<td>12/312170 (0.0%)</td>
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</table>

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.

<table>
<thead>
<tr>
<th>Mol</th>
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<th>#Chirality outliers</th>
<th>#Planarity outliers</th>
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<td>19</td>
<td>AL24</td>
<td>0</td>
<td>1</td>
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Continued on next page...
Continued from previous page...

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<th>#Chirality outliers</th>
<th>#Planarity outliers</th>
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All (12) bond length outliers are listed below:

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<th>Z</th>
<th>Observed(Å)</th>
<th>Ideal(Å)</th>
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<td>HIS</td>
<td>CA-C</td>
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<td>1.69</td>
<td>1.52</td>
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<td>VAL</td>
<td>C-O</td>
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All (54) bond angle outliers are listed below:

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<td>CG-ND1-CE1</td>
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<td>6</td>
<td>HIS</td>
<td>CG-CD2-NE2</td>
<td>-17.32</td>
<td>76.28</td>
<td>109.20</td>
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<td>69</td>
<td>HIS</td>
<td>N-CA-CB</td>
<td>17.00</td>
<td>141.21</td>
<td>110.60</td>
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<td>A23S</td>
<td>253</td>
<td>C</td>
<td>N3-C4-N4</td>
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<td>253</td>
<td>C</td>
<td>C5-C4-N4</td>
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<td>G</td>
<td>OP1-P-O3'</td>
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<td>139.34</td>
<td>105.20</td>
</tr>
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<td>A23S</td>
<td>1444</td>
<td>G</td>
<td>OP2-P-O3'</td>
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<td>AL24</td>
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<td>CA-C-N</td>
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<td>CA-C-O</td>
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There are no chirality outliers.

All (5) planarity outliers are listed below:

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<th>Type</th>
<th>Group</th>
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### 5.2 Too-close contacts

In the following table, the Non-H and H(model) columns list the number of non-hydrogen atoms and hydrogen atoms in the chain respectively. The H(added) column lists the number of hydrogen atoms added and optimized by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, whereas Symm-Clashes lists symmetry-related clashes.

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<th>H(model)</th>
<th>H(added)</th>
<th>Clashes</th>
<th>Symm-Clashes</th>
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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.

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<tr>
<th>Mol</th>
<th>Chain</th>
<th>Analysed</th>
<th>Favoured</th>
<th>Allowed</th>
<th>Outliers</th>
<th>Percentiles</th>
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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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5.4 Non-standard residues in protein, DNA, RNA chains

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

5.5 Carbohydrates

There are no monosaccharides in this entry.

5.6 Ligand geometry

Of 4 ligands modelled in this entry, 4 are monoatomic - leaving 0 for Mogul analysis.

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

No monomer is involved in short contacts.

5.7 Other polymers

There are no such residues in this entry.

5.8 Polymer linkage issues

There are no chain breaks in this entry.
6 Fit of model and data

6.1 Protein, DNA and RNA chains

In the following table, the column labelled ‘#RSRZ> 2’ contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 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.

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

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

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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