Full wwPDB X-ray Structure Validation Report

Sep 16, 2020 – 06:47 PM BST

PDB ID : 5NDG
Title : Crystal structure of geneticin (G418) bound to the yeast 80S ribosome
Authors : Prokhorova, I.; Djumagulov, M.; Urzhumtsev, A.; Yusupov, M.; Yusupova, G.
Deposited on : 2017-03-08
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 https://www.wwpdb.org/validation/2017/XrayValidationReportHelp
with specific help available everywhere you see the symbol.

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

- MolProbity : 4.02b-467
- Mogul : 1.8.5 (274361), CSD as541be (2020)
- Xtriage (Phenix) : 1.13
- EDS : 2.14.3.dev2
- buster-report : 1.1.7 (2018)
- 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) : 2.14.3.dev2
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 on the lower bar indicate the fraction of residues that contain outliers for ≥3, 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions <5%. The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density. The numeric value is given above the bar.

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2 Entry composition

There are 84 unique types of molecules in this entry. The entry contains 397710 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 18S ribosomal RNA.

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- Molecule 2 is a protein called 40S ribosomal protein S0-A.

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- Molecule 4 is a protein called 40S ribosomal protein S2.

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- Molecule 5 is a protein called 40S ribosomal protein S3.
Molecule 6 is a protein called 40S ribosomal protein S4-A.

Molecule 7 is a protein called 40S ribosomal protein S5.

Molecule 8 is a protein called 40S ribosomal protein S6-A.

Molecule 9 is a protein called 40S ribosomal protein S7-A.

Molecule 10 is a protein called 40S ribosomal protein S8-A.
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- Molecule 11 is a protein called 40S ribosomal protein S9-A.

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- Molecule 12 is a protein called 40S ribosomal protein S10-A.

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- Molecule 14 is a protein called 40S ribosomal protein S12.

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- Molecule 15 is a protein called 40S ribosomal protein S13.
- Molecule 16 is a protein called 40S ribosomal protein S14-A.

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- Molecule 17 is a protein called 40S ribosomal protein S15.

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<th>Residues</th>
<th>Atoms</th>
<th>ZeroOcc</th>
<th>AltConf</th>
<th>Trace</th>
</tr>
</thead>
<tbody>
<tr>
<td>17</td>
<td>C5</td>
<td>122</td>
<td>Total C N O S</td>
<td>967 616 180 164 7</td>
<td>0</td>
<td>0</td>
</tr>
<tr>
<td>17</td>
<td>c5</td>
<td>119</td>
<td>Total C N O S</td>
<td>939 595 176 161 7</td>
<td>0</td>
<td>0</td>
</tr>
</tbody>
</table>

- Molecule 18 is a protein called 40S ribosomal protein S16-A.

<table>
<thead>
<tr>
<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>C6</td>
<td>141</td>
<td>Total C N O</td>
<td>1105 708 203 194</td>
<td>0</td>
<td>0</td>
</tr>
<tr>
<td>18</td>
<td>c6</td>
<td>141</td>
<td>Total C N O</td>
<td>1105 708 203 194</td>
<td>0</td>
<td>0</td>
</tr>
</tbody>
</table>

- Molecule 19 is a protein called 40S ribosomal protein S17-A.

<table>
<thead>
<tr>
<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>19</td>
<td>C7</td>
<td>117</td>
<td>Total C N O S</td>
<td>911 568 174 167 2</td>
<td>0</td>
<td>0</td>
</tr>
<tr>
<td>19</td>
<td>c7</td>
<td>117</td>
<td>Total C N O S</td>
<td>906 563 174 167 2</td>
<td>0</td>
<td>0</td>
</tr>
</tbody>
</table>

- Molecule 20 is a protein called 40S ribosomal protein S18-A.

<table>
<thead>
<tr>
<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>20</td>
<td>C8</td>
<td>145</td>
<td>Total C N O S</td>
<td>1192 743 237 210 2</td>
<td>0</td>
<td>0</td>
</tr>
<tr>
<td>20</td>
<td>c8</td>
<td>145</td>
<td>Total C N O S</td>
<td>1192 743 237 210 2</td>
<td>0</td>
<td>0</td>
</tr>
</tbody>
</table>

- Molecule 21 is a protein called 40S ribosomal protein S19-A.
- Molecule 22 is a protein called 40S ribosomal protein S20.

<table>
<thead>
<tr>
<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>22</td>
<td>D0</td>
<td>105</td>
<td>Total C N O S</td>
<td></td>
<td></td>
<td></td>
</tr>
<tr>
<td></td>
<td></td>
<td></td>
<td>837 684 512 125 137 2</td>
<td>0</td>
<td>0</td>
<td>0</td>
</tr>
</tbody>
</table>

- Molecule 23 is a protein called 40S ribosomal protein S21-A.

<table>
<thead>
<tr>
<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>23</td>
<td>D1</td>
<td>87</td>
<td>Total C N O S</td>
<td></td>
<td></td>
<td></td>
</tr>
<tr>
<td></td>
<td></td>
<td></td>
<td>684 684 420 125 137 2</td>
<td>0</td>
<td>0</td>
<td>0</td>
</tr>
</tbody>
</table>

- Molecule 24 is a protein called 40S ribosomal protein S22-A.

<table>
<thead>
<tr>
<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>24</td>
<td>D2</td>
<td>129</td>
<td>Total C N O S</td>
<td></td>
<td></td>
<td></td>
</tr>
<tr>
<td></td>
<td></td>
<td></td>
<td>1021 1021 650 188 180 3</td>
<td>0</td>
<td>0</td>
<td>0</td>
</tr>
</tbody>
</table>

- Molecule 25 is a protein called 40S ribosomal protein S23-A.

<table>
<thead>
<tr>
<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>25</td>
<td>D3</td>
<td>144</td>
<td>Total C N O S</td>
<td></td>
<td></td>
<td></td>
</tr>
<tr>
<td></td>
<td></td>
<td></td>
<td>1121 1121 708 220 191 2</td>
<td>0</td>
<td>0</td>
<td>0</td>
</tr>
</tbody>
</table>

- Molecule 26 is a protein called 40S ribosomal protein S24-A.

<table>
<thead>
<tr>
<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>26</td>
<td>D4</td>
<td>134</td>
<td>Total C N O</td>
<td></td>
<td></td>
<td></td>
</tr>
<tr>
<td></td>
<td></td>
<td></td>
<td>1073 1073 676 208 189</td>
<td>0</td>
<td>0</td>
<td>0</td>
</tr>
</tbody>
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Continued from previous page...

<table>
<thead>
<tr>
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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>26</td>
<td>d4</td>
<td>134</td>
<td>Total C N O</td>
<td>0</td>
<td>0</td>
<td>0</td>
</tr>
<tr>
<td></td>
<td></td>
<td></td>
<td>1073 676 208 189</td>
<td></td>
<td></td>
<td></td>
</tr>
</tbody>
</table>

- Molecule 27 is a protein called 40S ribosomal protein S25-A.

<table>
<thead>
<tr>
<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>27</td>
<td>D5</td>
<td>70</td>
<td>Total C N O</td>
<td>0</td>
<td>0</td>
<td>0</td>
</tr>
<tr>
<td></td>
<td></td>
<td></td>
<td>563 360 104 99</td>
<td></td>
<td></td>
<td></td>
</tr>
<tr>
<td>27</td>
<td>d5</td>
<td>69</td>
<td>Total C N O</td>
<td>0</td>
<td>0</td>
<td>0</td>
</tr>
<tr>
<td></td>
<td></td>
<td></td>
<td>558 357 103 98</td>
<td></td>
<td></td>
<td></td>
</tr>
</tbody>
</table>

- Molecule 28 is a protein called 40S ribosomal protein S26-B.

<table>
<thead>
<tr>
<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>28</td>
<td>D6</td>
<td>97</td>
<td>Total C N O S</td>
<td>0</td>
<td>0</td>
<td>0</td>
</tr>
<tr>
<td></td>
<td></td>
<td></td>
<td>769 475 160 129 5</td>
<td></td>
<td></td>
<td></td>
</tr>
<tr>
<td>28</td>
<td>d6</td>
<td>97</td>
<td>Total C N O S</td>
<td>0</td>
<td>0</td>
<td>0</td>
</tr>
<tr>
<td></td>
<td></td>
<td></td>
<td>769 475 160 129 5</td>
<td></td>
<td></td>
<td></td>
</tr>
</tbody>
</table>

- Molecule 29 is a protein called 40S ribosomal protein S27-A.

<table>
<thead>
<tr>
<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>29</td>
<td>D7</td>
<td>81</td>
<td>Total C N O S</td>
<td>0</td>
<td>0</td>
<td>0</td>
</tr>
<tr>
<td></td>
<td></td>
<td></td>
<td>610 382 110 113 5</td>
<td></td>
<td></td>
<td></td>
</tr>
<tr>
<td>29</td>
<td>d7</td>
<td>81</td>
<td>Total C N O S</td>
<td>0</td>
<td>0</td>
<td>0</td>
</tr>
<tr>
<td></td>
<td></td>
<td></td>
<td>610 382 110 113 5</td>
<td></td>
<td></td>
<td></td>
</tr>
</tbody>
</table>

- Molecule 30 is a protein called 40S ribosomal protein S28-A.

<table>
<thead>
<tr>
<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>30</td>
<td>D8</td>
<td>63</td>
<td>Total C N O S</td>
<td>0</td>
<td>0</td>
<td>0</td>
</tr>
<tr>
<td></td>
<td></td>
<td></td>
<td>497 306 99 91 1</td>
<td></td>
<td></td>
<td></td>
</tr>
<tr>
<td>30</td>
<td>d8</td>
<td>63</td>
<td>Total C N O S</td>
<td>0</td>
<td>0</td>
<td>0</td>
</tr>
<tr>
<td></td>
<td></td>
<td></td>
<td>497 306 99 91 1</td>
<td></td>
<td></td>
<td></td>
</tr>
</tbody>
</table>

- Molecule 31 is a protein called 40S ribosomal protein S29-A.
• Molecule 32 is a protein called 40S ribosomal protein S30-A.

<table>
<thead>
<tr>
<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>32</td>
<td>E0</td>
<td>60</td>
<td>Total C N O S 475 299 98 77 1</td>
<td>0</td>
<td>0</td>
<td>0</td>
</tr>
<tr>
<td>32</td>
<td>e0</td>
<td>60</td>
<td>Total C N O S 475 299 98 77 1</td>
<td>0</td>
<td>0</td>
<td>0</td>
</tr>
</tbody>
</table>

• Molecule 33 is a protein called Ubiquitin-40S ribosomal protein S31.

<table>
<thead>
<tr>
<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>33</td>
<td>E1</td>
<td>71</td>
<td>Total C N O S 566 362 106 94 4</td>
<td>0</td>
<td>0</td>
<td>0</td>
</tr>
<tr>
<td>33</td>
<td>e1</td>
<td>45</td>
<td>Total C N O S 352 222 66 60 4</td>
<td>0</td>
<td>0</td>
<td>0</td>
</tr>
</tbody>
</table>

• Molecule 34 is a protein called Guanine nucleotide-binding protein subunit beta-like protein.

<table>
<thead>
<tr>
<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>34</td>
<td>SR</td>
<td>318</td>
<td>Total C N O S 2437 1541 418 470 8</td>
<td>0</td>
<td>0</td>
<td>0</td>
</tr>
<tr>
<td>34</td>
<td>sR</td>
<td>313</td>
<td>Total C N O S 2403 1521 411 463 8</td>
<td>0</td>
<td>0</td>
<td>0</td>
</tr>
</tbody>
</table>

There are 2 discrepancies between the modelled and reference sequences:

<table>
<thead>
<tr>
<th>Chain</th>
<th>Residue</th>
<th>Modelled</th>
<th>Actual</th>
<th>Comment</th>
<th>Reference</th>
</tr>
</thead>
<tbody>
<tr>
<td>SR</td>
<td>161</td>
<td>ALA</td>
<td>LYS</td>
<td>conflict</td>
<td>UNP P38011</td>
</tr>
<tr>
<td>sR</td>
<td>161</td>
<td>ALA</td>
<td>LYS</td>
<td>conflict</td>
<td>UNP P38011</td>
</tr>
</tbody>
</table>

• Molecule 35 is a protein called Suppressor protein STM1.

<table>
<thead>
<tr>
<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>35</td>
<td>SM</td>
<td>135</td>
<td>Total C N O 985 581 197 207</td>
<td>0</td>
<td>0</td>
<td>0</td>
</tr>
<tr>
<td>35</td>
<td>sM</td>
<td>115</td>
<td>Total C N O 874 514 177 183</td>
<td>0</td>
<td>0</td>
<td>0</td>
</tr>
</tbody>
</table>

• Molecule 36 is a RNA chain called 25S 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>
</tr>
</thead>
<tbody>
<tr>
<td>36</td>
<td>1</td>
<td>3078</td>
<td>Total C N O P 65838 29408 11870 21482 3078</td>
<td>0</td>
<td>0</td>
<td>0</td>
</tr>
</tbody>
</table>

Continued on next page...
### Molecule 37

Molecule 37 is a RNA chain called 5S 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>
</tr>
</thead>
<tbody>
<tr>
<td>37</td>
<td>3</td>
<td>121</td>
<td>Total C N O P</td>
<td>0</td>
<td>0</td>
<td>0</td>
</tr>
<tr>
<td>37</td>
<td>7</td>
<td>121</td>
<td>Total C N O P</td>
<td>0</td>
<td>0</td>
<td>0</td>
</tr>
</tbody>
</table>

### Molecule 38

Molecule 38 is a RNA chain called 5.8S 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>
</tr>
</thead>
<tbody>
<tr>
<td>38</td>
<td>4</td>
<td>158</td>
<td>Total C N O P</td>
<td>0</td>
<td>0</td>
<td>0</td>
</tr>
<tr>
<td>38</td>
<td>8</td>
<td>157</td>
<td>Total C N O P</td>
<td>0</td>
<td>0</td>
<td>0</td>
</tr>
</tbody>
</table>

### Molecule 39

Molecule 39 is a protein called 60S ribosomal protein L2-A.

<table>
<thead>
<tr>
<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>39</td>
<td>L2</td>
<td>252</td>
<td>Total C N O S</td>
<td>0</td>
<td>0</td>
<td>0</td>
</tr>
<tr>
<td>39</td>
<td>l2</td>
<td>252</td>
<td>Total C N O S</td>
<td>0</td>
<td>0</td>
<td>0</td>
</tr>
</tbody>
</table>

### Molecule 40

Molecule 40 is a protein called 60S ribosomal protein L3.

<table>
<thead>
<tr>
<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>40</td>
<td>L3</td>
<td>386</td>
<td>Total C N O S</td>
<td>0</td>
<td>0</td>
<td>0</td>
</tr>
<tr>
<td>40</td>
<td>l3</td>
<td>386</td>
<td>Total C N O S</td>
<td>0</td>
<td>0</td>
<td>0</td>
</tr>
</tbody>
</table>

### Molecule 41

Molecule 41 is a protein called 60S ribosomal protein L4-A.

<table>
<thead>
<tr>
<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>41</td>
<td>L4</td>
<td>361</td>
<td>Total C N O S</td>
<td>0</td>
<td>0</td>
<td>0</td>
</tr>
<tr>
<td>41</td>
<td>l4</td>
<td>361</td>
<td>Total C N O S</td>
<td>0</td>
<td>0</td>
<td>0</td>
</tr>
</tbody>
</table>
- Molecule 42 is a protein called 60S ribosomal protein L5.

<table>
<thead>
<tr>
<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>42</td>
<td>L5</td>
<td>294</td>
<td>Total C N O S 2357 1491 410 454 2</td>
<td>0</td>
<td>0</td>
<td>0</td>
</tr>
<tr>
<td>42</td>
<td>L5</td>
<td>294</td>
<td>Total C N O S 2359 1489 412 456 2</td>
<td>0</td>
<td>0</td>
<td>0</td>
</tr>
</tbody>
</table>

- Molecule 43 is a protein called 60S ribosomal protein L6-A.

<table>
<thead>
<tr>
<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>43</td>
<td>L6</td>
<td>156</td>
<td>Total C N O S 1239 800 222 216 1</td>
<td>0</td>
<td>0</td>
<td>0</td>
</tr>
<tr>
<td>43</td>
<td>L6</td>
<td>157</td>
<td>Total C N O S 1248 806 224 217 1</td>
<td>0</td>
<td>0</td>
<td>0</td>
</tr>
</tbody>
</table>

- Molecule 44 is a protein called 60S ribosomal protein L7-A.

<table>
<thead>
<tr>
<th>Mol</th>
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<tbody>
<tr>
<td>44</td>
<td>L7</td>
<td>222</td>
<td>Total C N O S 1784 1151 324 308 1</td>
<td>0</td>
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<tr>
<td>44</td>
<td>L7</td>
<td>223</td>
<td>Total C N O S 1791 1155 325 310 1</td>
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- Molecule 45 is a protein called 60S ribosomal protein L8-A.

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<tbody>
<tr>
<td>45</td>
<td>L8</td>
<td>233</td>
<td>Total C N O S 1804 1151 323 327 3</td>
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<td>0</td>
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<tr>
<td>45</td>
<td>L8</td>
<td>231</td>
<td>Total C N O S 1763 1130 316 314 3</td>
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- Molecule 46 is a protein called 60S ribosomal protein L9-A.

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<tbody>
<tr>
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<td>L9</td>
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<td>0</td>
</tr>
<tr>
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<td>L9</td>
<td>190</td>
<td>Total C N O S 1510 957 273 276 4</td>
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- Molecule 47 is a protein called 60S ribosomal protein L10.
Molecule 48 is a protein called 60S ribosomal protein L11-A.

Molecule 49 is a protein called 60S ribosomal protein L13-A.

Molecule 50 is a protein called 60S ribosomal protein L14-A.

Molecule 51 is a protein called 60S ribosomal protein L15-A.

Molecule 52 is a protein called 60S ribosomal protein L16-A.

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<td></td>
<td>1555 1003 289 262</td>
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- Molecule 53 is a protein called 60S ribosomal protein L17-A.

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<tr>
<td></td>
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<td>1420 882 281 257</td>
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<td></td>
<td>1378 856 273 249</td>
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- Molecule 54 is a protein called 60S ribosomal protein L18-A.

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<tr>
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<td>1441 908 290 241</td>
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</tr>
<tr>
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<td>m8</td>
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<td>0</td>
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<td></td>
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<td>1441 908 290 241</td>
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- Molecule 55 is a protein called 60S ribosomal protein L19-A.

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<td>m9</td>
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<td></td>
<td></td>
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<td>1482 911 320 251</td>
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- Molecule 56 is a protein called 60S ribosomal protein L20-A.

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<tbody>
<tr>
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<td></td>
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<td>1445 930 267 244</td>
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- Molecule 57 is a protein called 60S ribosomal protein L21-A.

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</thead>
<tbody>
<tr>
<td>57</td>
<td>N1</td>
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<td>0</td>
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<tr>
<td></td>
<td></td>
<td></td>
<td>1276 805 246 221</td>
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<td></td>
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<tr>
<td>57</td>
<td>n1</td>
<td>159</td>
<td>Total C N O S</td>
<td>0</td>
<td>0</td>
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</tr>
<tr>
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<td></td>
<td></td>
<td>1276 805 246 221</td>
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• Molecule 58 is a protein called 60S ribosomal protein L22-A.

<table>
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</thead>
<tbody>
<tr>
<td>58</td>
<td>N2</td>
<td>98</td>
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<td>778 505 127 146</td>
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<td>0</td>
</tr>
<tr>
<td>58</td>
<td>n2</td>
<td>98</td>
<td>Total C N O</td>
<td>778 505 127 146</td>
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<td>0</td>
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• Molecule 59 is a protein called 60S ribosomal protein L23-A.

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<tbody>
<tr>
<td>59</td>
<td>N3</td>
<td>135</td>
<td>Total C N O S</td>
<td>997 625 188 177 7</td>
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<td>0</td>
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<tr>
<td>59</td>
<td>n3</td>
<td>134</td>
<td>Total C N O S</td>
<td>993 623 187 176 7</td>
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• Molecule 60 is a protein called 60S ribosomal protein L24-A.

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<tbody>
<tr>
<td>60</td>
<td>N4</td>
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<td>Total C N O S</td>
<td>925 582 184 158 1</td>
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<tr>
<td>60</td>
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<td>118</td>
<td>Total C N O S</td>
<td>946 597 188 160 1</td>
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• Molecule 61 is a protein called 60S ribosomal protein L25.

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<th>Trace</th>
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<tbody>
<tr>
<td>61</td>
<td>N5</td>
<td>121</td>
<td>Total C N O S</td>
<td>964 620 169 173 2</td>
<td>0</td>
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<td>959 617 168 172 2</td>
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• Molecule 62 is a protein called 60S ribosomal protein L26-A.

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<th>Trace</th>
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<tbody>
<tr>
<td>62</td>
<td>N6</td>
<td>126</td>
<td>Total C N O</td>
<td>993 625 192 176</td>
<td>0</td>
<td>0</td>
</tr>
<tr>
<td>62</td>
<td>n6</td>
<td>124</td>
<td>Total C N O</td>
<td>976 614 190 172</td>
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• Molecule 63 is a protein called 60S ribosomal protein L27-A.
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<th>Trace</th>
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</thead>
<tbody>
<tr>
<td>63</td>
<td>N7</td>
<td>135</td>
<td>Total C 1092 N 710 O 202</td>
<td>0</td>
<td>0</td>
<td>0</td>
</tr>
<tr>
<td>63</td>
<td>n7</td>
<td>135</td>
<td>Total C 1092 N 710 O 202</td>
<td>0</td>
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- Molecule 64 is a protein called 60S ribosomal protein L28.

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<th>Trace</th>
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</thead>
<tbody>
<tr>
<td>64</td>
<td>N8</td>
<td>148</td>
<td>Total C 1173 N 749 O 231</td>
<td>0</td>
<td>0</td>
<td>0</td>
</tr>
<tr>
<td>64</td>
<td>n8</td>
<td>148</td>
<td>Total C 1173 N 749 O 231</td>
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- Molecule 65 is a protein called 60S ribosomal protein L29.

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<th>Trace</th>
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<tbody>
<tr>
<td>65</td>
<td>N9</td>
<td>58</td>
<td>Total C 462 N 289 O 100</td>
<td>0</td>
<td>0</td>
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<td>n9</td>
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<td>Total C 462 N 289 O 100</td>
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- Molecule 66 is a protein called 60S ribosomal protein L30.

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<tbody>
<tr>
<td>66</td>
<td>O0</td>
<td>97</td>
<td>Total C 743 N 479 O 124</td>
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<td>Total C 767 N 492 O 128</td>
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- Molecule 67 is a protein called 60S ribosomal protein L31-A.

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<tr>
<td>67</td>
<td>O1</td>
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<td>0</td>
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<tr>
<td>67</td>
<td>o1</td>
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- Molecule 68 is a protein called 60S ribosomal protein L32.

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<tr>
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<td>Total C 1020 N 647 O 205</td>
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<tbody>
<tr>
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<td>127</td>
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<td>0</td>
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<tr>
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<td></td>
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<td>1020 647 205 167 1</td>
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- Molecule 69 is a protein called 60S ribosomal protein L33-A.

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<tbody>
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<td>850 540 165 144 1</td>
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<tbody>
<tr>
<td>69</td>
<td>o3</td>
<td>106</td>
<td>Total C N O S</td>
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<td>0</td>
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- Molecule 70 is a protein called 60S ribosomal protein L34-A.

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</thead>
<tbody>
<tr>
<td>70</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>
<td></td>
<td></td>
<td></td>
<td>880 545 179 152 4</td>
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<table>
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<tr>
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<th>Residues</th>
<th>Atoms</th>
<th>ZeroOcc</th>
<th>AltConf</th>
<th>Trace</th>
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</thead>
<tbody>
<tr>
<td>70</td>
<td>o4</td>
<td>112</td>
<td>Total C N O S</td>
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<td>0</td>
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<tr>
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<td></td>
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<td>880 545 179 152 4</td>
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- Molecule 71 is a protein called 60S ribosomal protein L35-A.

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</thead>
<tbody>
<tr>
<td>71</td>
<td>O5</td>
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<tr>
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<table>
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<th>Atoms</th>
<th>ZeroOcc</th>
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<th>Trace</th>
</tr>
</thead>
<tbody>
<tr>
<td>71</td>
<td>o5</td>
<td>119</td>
<td>Total C N O S</td>
<td>0</td>
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- Molecule 72 is a protein called 60S ribosomal protein L36-A.

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- Molecule 73 is a protein called 60S ribosomal protein L37-A.

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Molecule 74 is a protein called 60S ribosomal protein L38.

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Molecule 75 is a protein called 60S ribosomal protein L39.

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Molecule 76 is a protein called Ubiquitin-60S ribosomal protein L40.

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Molecule 77 is a protein called 60S ribosomal protein L41-A.

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Molecule 78 is a protein called 60S ribosomal protein L42-A.

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Molecule 79 is a protein called 60S ribosomal protein L43-A.
Molecule 80 is a protein called 60S acidic ribosomal protein P0.

Molecule 81 is MAGNESIUM ION (three-letter code: MG) (formula: Mg).

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- Molecule 82 is GENETICIN (three-letter code: GET) (formula: C$_{20}$H$_{40}$N$_4$O$_{10}$).

![GENETICIN Structure](image)

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- Molecule 83 is ZINC ION (three-letter code: ZN) (formula: Zn).
**Molecule 84 is water.**

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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: 18S ribosomal RNA

Chain 2:
• Molecule 1: 18S ribosomal RNA

Chain 6:
Chain S0:

Molecule 2: 40S ribosomal protein S0-A

Chain s0:

Molecule 2: 40S ribosomal protein S0-A
- Molecule 3: 40S ribosomal protein S1-A

Chain S1:

- Molecule 3: 40S ribosomal protein S1-A

Chain s1:

- Molecule 4: 40S ribosomal protein S2

Chain S2:

- Molecule 4: 40S ribosomal protein S2

Chain s2:
• Molecule 5: 40S ribosomal protein S3

Chain S3:

• Molecule 5: 40S ribosomal protein S3

Chain s3:

• Molecule 6: 40S ribosomal protein S4-A

Chain S4:

• Molecule 6: 40S ribosomal protein S4-A

Chain S4:

• Molecule 7: 40S ribosomal protein S5

Chain S5:
• Molecule 7: 40S ribosomal protein S5

Chain S5:

• Molecule 8: 40S ribosomal protein S6-A

Chain S6:

• Molecule 8: 40S ribosomal protein S6-A

Chain S6:

• Molecule 9: 40S ribosomal protein S7-A

Chain S7:
- Molecule 9: 40S ribosomal protein S7-A

Chain s7:

- Molecule 10: 40S ribosomal protein S8-A

Chain S8:

- Molecule 10: 40S ribosomal protein S8-A

Chain s8:

- Molecule 11: 40S ribosomal protein S9-A

Chain S9:
- Molecule 11: 40S ribosomal protein S9-A
  Chain s9:

- Molecule 12: 40S ribosomal protein S10-A
  Chain C0:

- Molecule 12: 40S ribosomal protein S10-A
  Chain c0:

- Molecule 13: 40S ribosomal protein S11-A
  Chain C1:

- Molecule 13: 40S ribosomal protein S11-A
  Chain c1:
• Molecule 14: 40S ribosomal protein S12

Chain C2:

• Molecule 14: 40S ribosomal protein S12

Chain c2:

• Molecule 15: 40S ribosomal protein S13

Chain C3:

• Molecule 15: 40S ribosomal protein S13

Chain c3:

• Molecule 16: 40S ribosomal protein S14-A

Chain C4:

• Molecule 16: 40S ribosomal protein S14-A
Chain C7:

- Molecule 19: 40S ribosomal protein S17-A

Chain C8:

- Molecule 20: 40S ribosomal protein S18-A

Chain C9:

- Molecule 21: 40S ribosomal protein S19-A
• Molecule 21: 40S ribosomal protein S19-A

Chain c9:

• Molecule 22: 40S ribosomal protein S20

Chain D0:

• Molecule 22: 40S ribosomal protein S20

Chain d0:

• Molecule 23: 40S ribosomal protein S21-A

Chain D1:

• Molecule 23: 40S ribosomal protein S21-A

Chain d1:

• Molecule 24: 40S ribosomal protein S22-A

Chain D2:
• Molecule 24: 40S ribosomal protein S22-A

Chain d2:

• Molecule 25: 40S ribosomal protein S23-A

Chain D3:

• Molecule 25: 40S ribosomal protein S23-A

Chain d3:

• Molecule 26: 40S ribosomal protein S24-A

Chain D4:

• Molecule 26: 40S ribosomal protein S24-A

Chain d4:

• Molecule 27: 40S ribosomal protein S25-A

Chain D5:
- Molecule 27: 40S ribosomal protein S25-A
  Chain d5:

- Molecule 28: 40S ribosomal protein S26-B
  Chain D6:

- Molecule 28: 40S ribosomal protein S26-B
  Chain d6:

- Molecule 29: 40S ribosomal protein S27-A
  Chain D7:

- Molecule 29: 40S ribosomal protein S27-A
  Chain d7:

- Molecule 30: 40S ribosomal protein S28-A
  Chain D8:

- Molecule 30: 40S ribosomal protein S28-A
Chain d8:

- Molecule 31: 40S ribosomal protein S29-A

Chain D9:

- Molecule 31: 40S ribosomal protein S29-A

Chain d9:

- Molecule 32: 40S ribosomal protein S30-A

Chain E0:

- Molecule 32: 40S ribosomal protein S30-A

Chain e0:

- Molecule 33: Ubiquitin-40S ribosomal protein S31

Chain E1:

- Molecule 33: Ubiquitin-40S ribosomal protein S31
• Molecule 34: Guanine nucleotide-binding protein subunit beta-like protein

• Molecule 34: Guanine nucleotide-binding protein subunit beta-like protein

• Molecule 35: Suppressor protein STM1
• Molecule 35: Suppressor protein STM1

Chain sM:

• Molecule 36: 25S ribosomal RNA

Chain 1:
### Chain 5:

- **Molecule 36: 25S ribosomal RNA**

- **61%**
- **26%**
- **5%**
- **8%**
• Molecule 37: 5S ribosomal RNA

Chain 3:

• Molecule 37: 5S ribosomal RNA

Chain 7:

• Molecule 38: 5.8S ribosomal RNA

Chain 4:

• Molecule 38: 5.8S ribosomal RNA

Chain 8:

• Molecule 39: 60S ribosomal protein L2-A

Chain L2:
Chain L2:

- Molecule 40: 60S ribosomal protein L3

Chain L3:

- Molecule 40: 60S ribosomal protein L3

Chain L3:

- Molecule 40: 60S ribosomal protein L3

Chain L4:

- Molecule 41: 60S ribosomal protein L4-A

- Molecule 41: 60S ribosomal protein L4-A
• Molecule 42: 60S ribosomal protein L5

• Molecule 43: 60S ribosomal protein L6-A
• Molecule 43: 60S ribosomal protein L6-A

Chain 16:

• Molecule 44: 60S ribosomal protein L7-A

Chain L7:

• Molecule 45: 60S ribosomal protein L8-A

Chain L8:

• Molecule 45: 60S ribosomal protein L8-A

Chain 18:
• Molecule 46: 60S ribosomal protein L9-A

Chain L9:

• Molecule 46: 60S ribosomal protein L9-A

Chain l9:

• Molecule 47: 60S ribosomal protein L10

Chain M0:

• Molecule 47: 60S ribosomal protein L10

Chain m0:

• Molecule 48: 60S ribosomal protein L11-A

Chain M1:
- Molecule 48: 60S ribosomal protein L11-A

Chain m1:

- Molecule 49: 60S ribosomal protein L13-A

Chain M3:

- Molecule 49: 60S ribosomal protein L13-A

Chain m3:

- Molecule 50: 60S ribosomal protein L14-A

Chain M4:

- Molecule 50: 60S ribosomal protein L14-A

Chain m4:
• Molecule 51: 60S ribosomal protein L15-A

Chain M5:

• Molecule 51: 60S ribosomal protein L15-A

Chain m5:

• Molecule 52: 60S ribosomal protein L16-A

Chain M6:

• Molecule 52: 60S ribosomal protein L16-A

Chain m6:

• Molecule 53: 60S ribosomal protein L17-A

Chain M7:
• Molecule 53: 60S ribosomal protein L17-A

Chain m7:

• Molecule 54: 60S ribosomal protein L18-A

Chain M8:

• Molecule 54: 60S ribosomal protein L18-A

Chain m8:

• Molecule 55: 60S ribosomal protein L19-A

Chain M9:

• Molecule 55: 60S ribosomal protein L19-A

Chain m9:
• Molecule 56: 60S ribosomal protein L20-A

Chain N0:

• Molecule 56: 60S ribosomal protein L20-A

Chain n0:

• Molecule 57: 60S ribosomal protein L21-A

Chain N1:

• Molecule 57: 60S ribosomal protein L21-A

Chain n1:

• Molecule 58: 60S ribosomal protein L22-A

Chain N2:

• Molecule 58: 60S ribosomal protein L22-A

Chain n2:
• Molecule 59: 60S ribosomal protein L23-A

Chain N3:

• Molecule 59: 60S ribosomal protein L23-A

Chain n3:

• Molecule 60: 60S ribosomal protein L24-A

Chain N4:

• Molecule 60: 60S ribosomal protein L24-A

Chain n4:

• Molecule 61: 60S ribosomal protein L25

Chain N5:

• Molecule 61: 60S ribosomal protein L25

Chain n5:

• Molecule 62: 60S ribosomal protein L26-A
Chain N6:

- Molecule 62: 60S ribosomal protein L26-A

Chain n6:

- Molecule 63: 60S ribosomal protein L27-A

Chain N7:

- Molecule 63: 60S ribosomal protein L27-A

Chain n7:

- Molecule 64: 60S ribosomal protein L28

Chain N8:

- Molecule 64: 60S ribosomal protein L28
- Molecule 68: 60S ribosomal protein L32

Chain O2:

- Molecule 68: 60S ribosomal protein L32

Chain o2:

- Molecule 69: 60S ribosomal protein L33-A

Chain O3:

- Molecule 69: 60S ribosomal protein L33-A

Chain o3:

- Molecule 70: 60S ribosomal protein L34-A

Chain O4:

- Molecule 70: 60S ribosomal protein L34-A

Chain o4:

- Molecule 71: 60S ribosomal protein L35-A
Chain O5:

- Molecule 71: 60S ribosomal protein L35-A

Chain O5:

- Molecule 72: 60S ribosomal protein L36-A

Chain O6:

- Molecule 72: 60S ribosomal protein L36-A

Chain O6:

- Molecule 73: 60S ribosomal protein L37-A

Chain O7:

- Molecule 73: 60S ribosomal protein L37-A

Chain O7:

- Molecule 74: 60S ribosomal protein L38

Chain O8:

- Molecule 74: 60S ribosomal protein L38
Chain o8:

- Molecule 75: 60S ribosomal protein L39

Chain O9:

- Molecule 75: 60S ribosomal protein L39

Chain o9:

- Molecule 76: Ubiquitin-60S ribosomal protein L40

Chain Q0:

- Molecule 76: Ubiquitin-60S ribosomal protein L40

Chain q0:

- Molecule 77: 60S ribosomal protein L41-A

Chain Q1:

- Molecule 77: 60S ribosomal protein L41-A

Chain q1:
• Molecule 78: 60S ribosomal protein L42-A

Chain Q2:

• Molecule 78: 60S ribosomal protein L42-A

Chain q2:

• Molecule 79: 60S ribosomal protein L43-A

Chain Q3:

• Molecule 79: 60S ribosomal protein L43-A

Chain q3:

• Molecule 80: 60S acidic ribosomal protein P0

Chain p0:
| VAL | SER | THR | ILE | ALA | SER | ILE | SER | LEU | ALA | ILE | GLY | TYR | PRO | THR | LEU | PRO | SER | VAL | GLY | HIS | THR | LEU | ILE | ASN | ASN | TYR | LYS | ASP | LEU | LEU | ALA | VAL | ALA | ILE | ALA | ALA | SER | TYR | TYR | PRO | GLU | ILE | GLU | ASP | ARG | ILE | GLU |
|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|

| ASN | PRO | GLU | LYS | TYR | ALA | ALA | ALA | ALA | PRO | ALA | ALA | THR | SER | ALA | ALA | SER | GLY | ASP | ALA | ALA | PRO | GLU | GLU | GLU | GLU | GLU | SER | ASP | ASP | ASP | MET | GLY | PHE | GLY | LEU | PHE | ASP |
## 4 Data and refinement statistics

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<tr>
<td>&lt;I/σ(I)&gt;&lt;sup&gt;1&lt;/sup&gt;</td>
<td>0.77 (at 3.67Å)</td>
<td>Xtriage</td>
</tr>
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<td>16296 reflections (2.00%)</td>
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<tr>
<td>Wilson B-factor (Å&lt;sup&gt;2&lt;/sup&gt;)</td>
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<td>Bulk solvent k&lt;sub&gt;sol&lt;/sub&gt;(e/Å&lt;sup&gt;3&lt;/sup&gt;) , B&lt;sub&gt;sol&lt;/sub&gt;(Å&lt;sup&gt;2&lt;/sup&gt;)</td>
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<td>Average B, all atoms (Å&lt;sup&gt;2&lt;/sup&gt;)</td>
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Xtriage’s analysis on translational NCS is as follows: The largest off-origin peak in the Patterson function is 1.61% of the height of the origin peak. No significant pseudotranslation is detected.

---

<sup>1</sup>Intensities estimated from amplitudes.

<sup>2</sup>Theoretical values of < |L| >, < L<sup>2</sup> > 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, MG, GET

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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36 | 1 | 1179 | A | O5'-P-OP1 | -5.97 | 100.33 | 105.70
36 | 1 | 1581 | C | C6-N1-C2 | -5.97 | 117.91 | 120.30
36 | 1 | 3021 | A | C8-N9-C4 | 5.97 | 108.19 | 105.80
1 | 2 | 1059 | U | N3-C2-O2 | -5.96 | 118.03 | 122.20
36 | 1 | 2613 | U | O5'-P-OP2 | -5.96 | 100.33 | 105.70
36 | 5 | 2206 | G | P-O3'-C3' | 5.96 | 126.86 | 119.70
36 | 5 | 3209 | A | N1-C6-N6 | 5.96 | 122.18 | 118.60
36 | 5 | 1152 | G | N9-C4-C5 | 5.96 | 107.78 | 105.40
36 | 1 | 34 | A | O5'-P-OP2 | -5.96 | 100.34 | 105.70
1 | 2 | 187 | G | P-O3'-C3' | 5.96 | 126.85 | 119.70
36 | 1 | 360 | G | C8-N9-C4 | -5.96 | 104.02 | 106.40
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36 | 5 | 186 | U | O5'-P-OP1 | -5.95 | 100.34 | 105.70
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36 | 5 | 1331 | U | C6-N1-C2 | 5.94 | 124.57 | 121.00
1 | 2 | 1504 | G | N3-C4-C5 | -5.94 | 125.63 | 128.60
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36 | 1 | 2145 | A | C5-C6-N6 | -5.94 | 118.95 | 123.70
36 | 5 | 2353 | G | N3-C4-C5 | -5.94 | 125.63 | 128.60
36 | 1 | 688 | G | N7-C8-N9 | 5.94 | 116.07 | 113.10
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36 | 5 | 348 | A | N1-C6-N6 | 5.21 | 121.72 | 118.60
36 | 5 | 2610 | G | C4-N9-C1' | -5.21 | 119.73 | 126.50
36 | 5 | 339 | C | N3-C4-C5 | 5.21 | 123.98 | 121.90
1 | 2 | 1430 | U | N3-C4-C5' | -5.20 | 111.48 | 114.60
36 | 1 | 2922 | G | C6-C5-N7 | -5.20 | 127.28 | 130.40
36 | 1 | 1635 | G | C4-N9-C1' | -5.20 | 119.74 | 126.50
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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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### Mol Chain Analysed Favoured Allowed Outliers Percentiles

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### Mol | Chain | Analysed | Favoured | Allowed | Outliers | Percentiles
---|---|---|---|---|---|---
52 | m6 | 195/197 (99%) | 185 (95%) | 10 (5%) | 0 | 100 100
53 | M7 | 181/184 (98%) | 168 (93%) | 11 (6%) | 2 (1%) | 14 50
53 | m7 | 171/184 (93%) | 159 (93%) | 12 (7%) | 0 | 100 100
54 | M8 | 183/185 (99%) | 171 (93%) | 11 (6%) | 1 (0%) | 29 66
54 | m8 | 183/185 (99%) | 171 (93%) | 12 (7%) | 0 | 100 100
55 | M9 | 186/188 (99%) | 174 (94%) | 10 (5%) | 2 (1%) | 14 50
55 | m9 | 181/188 (96%) | 171 (94%) | 9 (5%) | 1 (1%) | 25 62
56 | N0 | 168/172 (98%) | 154 (92%) | 12 (7%) | 2 (1%) | 13 48
56 | n0 | 170/172 (99%) | 165 (97%) | 5 (3%) | 0 | 100 100
57 | N1 | 157/159 (99%) | 143 (91%) | 13 (8%) | 1 (1%) | 25 62
57 | n1 | 157/159 (99%) | 151 (96%) | 5 (3%) | 1 (1%) | 25 62
58 | N2 | 96/98 (98%) | 86 (90%) | 10 (10%) | 0 | 100 100
58 | n2 | 96/98 (98%) | 91 (95%) | 4 (4%) | 1 (1%) | 15 51
59 | N3 | 133/135 (98%) | 128 (96%) | 5 (4%) | 0 | 100 100
59 | n3 | 132/135 (98%) | 128 (97%) | 3 (2%) | 1 (1%) | 19 56
60 | N4 | 118/155 (76%) | 110 (93%) | 8 (7%) | 0 | 100 100
60 | n4 | 114/155 (74%) | 106 (93%) | 8 (7%) | 0 | 100 100
61 | N5 | 119/121 (98%) | 109 (92%) | 10 (8%) | 0 | 100 100
61 | n5 | 118/121 (98%) | 102 (86%) | 15 (13%) | 1 (1%) | 19 56
62 | N6 | 124/126 (98%) | 116 (94%) | 8 (6%) | 0 | 100 100
62 | n6 | 122/126 (97%) | 116 (95%) | 4 (3%) | 2 (2%) | 9 43
63 | N7 | 133/135 (98%) | 120 (90%) | 11 (8%) | 2 (2%) | 10 44
63 | n7 | 133/135 (98%) | 117 (88%) | 14 (10%) | 2 (2%) | 10 44
64 | N8 | 146/148 (99%) | 125 (86%) | 16 (11%) | 5 (3%) | 3 30
64 | n8 | 146/148 (99%) | 128 (88%) | 16 (11%) | 2 (1%) | 11 45
65 | N9 | 56/58 (97%) | 50 (89%) | 6 (11%) | 0 | 100 100
65 | n9 | 56/58 (97%) | 46 (82%) | 8 (14%) | 2 (4%) | 3 29
66 | O0 | 95/100 (95%) | 93 (98%) | 2 (2%) | 0 | 100 100
66 | o0 | 98/100 (98%) | 93 (95%) | 5 (5%) | 0 | 100 100
67 | O1 | 107/109 (98%) | 97 (91%) | 7 (6%) | 3 (3%) | 5 33
67 | o1 | 107/109 (98%) | 98 (92%) | 7 (6%) | 2 (2%) | 8 40

*Continued on next page...*
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All (297) Ramachandran outliers are listed below:

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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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5.4 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 1260 ligands modelled in this entry, 1239 are monoatomic - leaving 21 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).

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### Full wwPDB X-ray Structure Validation Report

5NDG

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No monomer is involved in short contacts.

The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. For torsion angles, if less then 5% of the Mogul distribution of torsion angles is within 10 degrees of the torsion angle in question, then that torsion angle is considered an outlier. Any bond that is central to one or more torsion angles identified as an outlier by Mogul will be highlighted in the graph. For rings, the root-mean-square deviation (RMSD) between the ring in question and similar rings identified by Mogul is calculated over all ring torsion angles. If the average RMSD is greater than 60 degrees and the minimal RMSD between the ring in question and any Mogul-identified rings is also greater than 60 degrees, then that ring is considered an outlier. The outliers are highlighted in purple. The color gray indicates Mogul did not find sufficient equivalents in the CSD to analyse the geometry.
Page 324  Full wwPDB X-ray Structure Validation Report  5NDG

Ligand GET 53848

Bond lengths

Bond angles

Torsions

Rings

Ligand GET 53847

Bond lengths

Bond angles

Torsions

Rings
Ligand GET 1 3809

Bond lengths

Bond angles

Torsions

Rings

Ligand GET 1 3808

Bond lengths

Bond angles

Torsions

Rings
5.7 Other polymers

There are no such residues in this entry.

5.8 Polymer linkage issues

The following chains have linkage breaks:

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<th>Residue-2</th>
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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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All (2661) RSRZ outliers are listed below:

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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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| 81 | MG N8 | 201 | 1/1 | 0.97 | 0.18 | 119,119,119,119 | 0 |
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| 81 | MG mO | 301 | 1/1 | 0.97 | 0.20 | 107,107,107,107 | 0 |
| 81 | MG 6 | 1 | 1920 | 1/1 | 0.97 | 0.32 | 134,134,134,134 | 0 |
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### Full wwPDB X-ray Structure Validation Report

5NDG

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Continued on next page...
The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation to approximate a three-dimensional view.
**Electron density around GET 6 2015:**

\[2mF_o - DF_c\text{ (at 0.7 rmsd) in gray}\]
\[mF_o - DF_c\text{ (at 3 rmsd) in purple (negative) and green (positive)}\]

**Electron density around GET 1 3809:**

\[2mF_o - DF_c\text{ (at 0.7 rmsd) in gray}\]
\[mF_o - DF_c\text{ (at 3 rmsd) in purple (negative) and green (positive)}\]
Electron density around GET n6 201:

\[ 2mF_o - DF_c \text{ (at 0.7 rmsd) in gray} \]
\[ mF_o - DF_c \text{ (at 3 rmsd) in purple (negative) and green (positive)} \]

Electron density around GET 6 2014:

\[ 2mF_o - DF_c \text{ (at 0.7 rmsd) in gray} \]
\[ mF_o - DF_c \text{ (at 3 rmsd) in purple (negative) and green (positive)} \]
Electron density around GET 5 3851:

\[ 2mF_o - DF_c \text{ (at 0.7 rmsd) in gray} \]
\[ mF_o - DF_c \text{ (at 3 rmsd) in purple (negative) and green (positive)} \]

Electron density around GET 2 2012:

\[ 2mF_o - DF_c \text{ (at 0.7 rmsd) in gray} \]
\[ mF_o - DF_c \text{ (at 3 rmsd) in purple (negative) and green (positive)} \]
**Electron density around GET 5 3846:**

$2mF_o - DF_c$ (at 0.7 rmsd) in gray
$mF_o - DF_c$ (at 3 rmsd) in purple (negative)
and green (positive)

---

**Electron density around GET 1 3813:**

$2mF_o - DF_c$ (at 0.7 rmsd) in gray
$mF_o - DF_c$ (at 3 rmsd) in purple (negative)
and green (positive)
Electron density around GET 1 3812:

\[2mF_o - DF_c\] (at 0.7 rmsd) in gray
\[mF_o - DF_c\] (at 3 rmsd) in purple (negative)
and green (positive)

Electron density around GET 1 3811:

\[2mF_o - DF_c\] (at 0.7 rmsd) in gray
\[mF_o - DF_c\] (at 3 rmsd) in purple (negative)
and green (positive)
Electron density around GET 1 3810:

$2mF_o - DF_c$ (at 0.7 rmsd) in gray
$mF_o - DF_c$ (at 3 rmsd) in purple (negative) and green (positive)

Electron density around GET 2 2013:

$2mF_o - DF_c$ (at 0.7 rmsd) in gray
$mF_o - DF_c$ (at 3 rmsd) in purple (negative) and green (positive)
Electron density around GET 5 3850:

$2mF_o - DF_c$ (at 0.7 rmsd) in gray
$mF_o - DF_c$ (at 3 rmsd) in purple (negative) and green (positive)

Electron density around GET 5 3845:

$2mF_o - DF_c$ (at 0.7 rmsd) in gray
$mF_o - DF_c$ (at 3 rmsd) in purple (negative) and green (positive)
Electron density around GET 5 3849:

$2mF_o - DF_c$ (at 0.7 rmsd) in gray
$mF_o - DF_c$ (at 3 rmsd) in purple (negative) and green (positive)

Electron density around GET 2 2014:

$2mF_o - DF_c$ (at 0.7 rmsd) in gray
$mF_o - DF_c$ (at 3 rmsd) in purple (negative) and green (positive)
Electron density around GET 5 3848:

\[ 2mF - DF \] (at 0.7 rmsd) in gray
\[ mF - DF \] (at 3 rmsd) in purple (negative) and green (positive)

Electron density around GET 5 3844:

\[ 2mF - DF \] (at 0.7 rmsd) in gray
\[ mF - DF \] (at 3 rmsd) in purple (negative) and green (positive)
Electron density around GET 5 3847:

$2mF_o - DF_c$ (at 0.7 rmsd) in gray
$mF_o - DF_c$ (at 3 rmsd) in purple (negative) and green (positive)

Electron density around GET 1 3808:

$2mF_o - DF_c$ (at 0.7 rmsd) in gray
$mF_o - DF_c$ (at 3 rmsd) in purple (negative) and green (positive)
Electron density around GET 6 2013:

2mFo-DFc (at 0.7 rmsd) in gray
mFo-DFc (at 3 rmsd) in purple (negative)
and green (positive)

6.5 Other polymers

There are no such residues in this entry.