PDB ID : 2GO5
EMDB ID: : EMD-1217
Title : Structure of signal recognition particle receptor (SR) in complex with signal recognition particle (SRP) and ribosome nascent chain complex
Authors : Halic, M.; Gartmann, M.; Schlenker, O.; Mielke, T.; Pool, M.R.; Sinning, I.; Beckmann, R.
Deposited on : 2006-04-12
Resolution : 7.40 Å (reported)

This is a Full wwPDB/EMDataBank EM Map/Model Validation Report for a publicly released PDB/EMDB entry.

We welcome your comments at validation@mail.wwpdb.org
A user guide is available at http://wwpdb.org/validation/2016/EMValidationReportHelp with specific help available everywhere you see the symbol.

MolProbity : 4.02b-467
Percentile statistics : 20161228.v01 (using entries in the PDB archive December 28th 2016)
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et. al. (1996)
Validation Pipeline (wwPDB-VP) : recal29047
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

**ELECTRON MICROSCOPY**

The reported resolution of this entry is 7.40 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>
<thead>
<tr>
<th>Metric</th>
<th>Whole archive (#Entries)</th>
<th>EM structures (#Entries)</th>
</tr>
</thead>
<tbody>
<tr>
<td>Clashescore</td>
<td>125131</td>
<td>1336</td>
</tr>
<tr>
<td>Ramachandran outliers</td>
<td>121729</td>
<td>1120</td>
</tr>
<tr>
<td>Sidechain outliers</td>
<td>121581</td>
<td>1026</td>
</tr>
<tr>
<td>RNA backbone</td>
<td>3398</td>
<td>335</td>
</tr>
</tbody>
</table>

The table below summarises the geometric issues observed across the polymeric chains. The red, orange, yellow and green segments on the bar indicate the fraction of residues that contain outliers for $\geq 3$, 2, 1 and 0 types of geometric quality criteria. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions $\leq 5\%$

<table>
<thead>
<tr>
<th>Mol</th>
<th>Chain</th>
<th>Length</th>
<th>Quality of chain</th>
</tr>
</thead>
<tbody>
<tr>
<td>1</td>
<td>A</td>
<td>127</td>
<td></td>
</tr>
<tr>
<td>2</td>
<td>9</td>
<td>90</td>
<td></td>
</tr>
<tr>
<td>3</td>
<td>B</td>
<td>108</td>
<td></td>
</tr>
<tr>
<td>4</td>
<td>W</td>
<td>109</td>
<td></td>
</tr>
<tr>
<td>5</td>
<td>1</td>
<td>185</td>
<td></td>
</tr>
<tr>
<td>6</td>
<td>2</td>
<td>214</td>
<td></td>
</tr>
<tr>
<td>7</td>
<td>5</td>
<td>124</td>
<td></td>
</tr>
<tr>
<td>8</td>
<td>4</td>
<td>152</td>
<td></td>
</tr>
</tbody>
</table>

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

<table>
<thead>
<tr>
<th>Mol</th>
<th>Chain</th>
<th>Length</th>
<th>Quality of chain</th>
</tr>
</thead>
<tbody>
<tr>
<td>9</td>
<td>6</td>
<td>123</td>
<td>24% 24% 9% 9% 34%</td>
</tr>
</tbody>
</table>
2 Entry composition

There are 9 unique types of molecules in this entry. The entry contains 10724 atoms, of which 0 are hydrogens and 0 are deuteriums.

In the tables below, 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 SRP RNA.

<table>
<thead>
<tr>
<th>Mol</th>
<th>Chain</th>
<th>Residues</th>
<th>Atoms</th>
<th>AltConf</th>
<th>Trace</th>
</tr>
</thead>
<tbody>
<tr>
<td>1</td>
<td>A</td>
<td>127</td>
<td>Total C N O P</td>
<td>0</td>
<td>0</td>
</tr>
<tr>
<td></td>
<td></td>
<td></td>
<td>2728 1217 508 877 126</td>
<td></td>
<td></td>
</tr>
</tbody>
</table>

- Molecule 2 is a RNA chain called ribosomal RNA.

<table>
<thead>
<tr>
<th>Mol</th>
<th>Chain</th>
<th>Residues</th>
<th>Atoms</th>
<th>AltConf</th>
<th>Trace</th>
</tr>
</thead>
<tbody>
<tr>
<td>2</td>
<td>9</td>
<td>90</td>
<td>Total C N O P</td>
<td>0</td>
<td>0</td>
</tr>
<tr>
<td></td>
<td></td>
<td></td>
<td>1935 863 364 618 90</td>
<td></td>
<td></td>
</tr>
</tbody>
</table>

- Molecule 3 is a protein called Signal recognition particle 19 kDa protein (SRP19).

<table>
<thead>
<tr>
<th>Mol</th>
<th>Chain</th>
<th>Residues</th>
<th>Atoms</th>
<th>AltConf</th>
<th>Trace</th>
</tr>
</thead>
<tbody>
<tr>
<td>3</td>
<td>B</td>
<td>107</td>
<td>Total C N O S</td>
<td>0</td>
<td>0</td>
</tr>
<tr>
<td></td>
<td></td>
<td></td>
<td>870 549 159 156 6</td>
<td></td>
<td></td>
</tr>
</tbody>
</table>

- Molecule 4 is a protein called Signal recognition particle 54 kDa protein (SRP54).

<table>
<thead>
<tr>
<th>Mol</th>
<th>Chain</th>
<th>Residues</th>
<th>Atoms</th>
<th>AltConf</th>
<th>Trace</th>
</tr>
</thead>
<tbody>
<tr>
<td>4</td>
<td>W</td>
<td>109</td>
<td>Total C N O S</td>
<td>0</td>
<td>0</td>
</tr>
<tr>
<td></td>
<td></td>
<td></td>
<td>865 540 150 164 11</td>
<td></td>
<td></td>
</tr>
</tbody>
</table>

- Molecule 5 is a protein called Signal recognition particle receptor alpha subunit (SR a).

<table>
<thead>
<tr>
<th>Mol</th>
<th>Chain</th>
<th>Residues</th>
<th>Atoms</th>
<th>AltConf</th>
<th>Trace</th>
</tr>
</thead>
<tbody>
<tr>
<td>5</td>
<td>1</td>
<td>125</td>
<td>Total C N O S</td>
<td>0</td>
<td>0</td>
</tr>
<tr>
<td></td>
<td></td>
<td></td>
<td>1020 659 169 189 3</td>
<td></td>
<td></td>
</tr>
</tbody>
</table>

There are 11 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>1</td>
<td>-8</td>
<td>MET</td>
<td>-</td>
<td>CLONING ARTIFACT</td>
<td>UNP P08240</td>
</tr>
<tr>
<td>1</td>
<td>-7</td>
<td>SER</td>
<td>-</td>
<td>CLONING ARTIFACT</td>
<td>UNP P08240</td>
</tr>
<tr>
<td>1</td>
<td>-6</td>
<td>HIS</td>
<td>-</td>
<td>EXPRESSION TAG</td>
<td>UNP P08240</td>
</tr>
</tbody>
</table>

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Continued from previous page...

<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>1</td>
<td>-5</td>
<td>HIS</td>
<td>-</td>
<td>EXPRESSION TAG</td>
<td>UNP P08240</td>
</tr>
<tr>
<td>1</td>
<td>-4</td>
<td>HIS</td>
<td>-</td>
<td>EXPRESSION TAG</td>
<td>UNP P08240</td>
</tr>
<tr>
<td>1</td>
<td>-3</td>
<td>HIS</td>
<td>-</td>
<td>EXPRESSION TAG</td>
<td>UNP P08240</td>
</tr>
<tr>
<td>1</td>
<td>-2</td>
<td>HIS</td>
<td>-</td>
<td>EXPRESSION TAG</td>
<td>UNP P08240</td>
</tr>
<tr>
<td>1</td>
<td>-1</td>
<td>HIS</td>
<td>-</td>
<td>EXPRESSION TAG</td>
<td>UNP P08240</td>
</tr>
<tr>
<td>1</td>
<td>0</td>
<td>SER</td>
<td>-</td>
<td>CLONING ARTIFACT</td>
<td>UNP P08240</td>
</tr>
<tr>
<td>1</td>
<td>1</td>
<td>MET</td>
<td>-</td>
<td>CLONING ARTIFACT</td>
<td>UNP P08240</td>
</tr>
<tr>
<td>1</td>
<td>2</td>
<td>VAL</td>
<td>-</td>
<td>CLONING ARTIFACT</td>
<td>UNP P08240</td>
</tr>
</tbody>
</table>

- Molecule 6 is a protein called Signal recognition particle receptor beta subunit (SR b).

<table>
<thead>
<tr>
<th>Mol</th>
<th>Chain</th>
<th>Residues</th>
<th>Atoms</th>
<th>AltConf</th>
<th>Trace</th>
</tr>
</thead>
<tbody>
<tr>
<td>6</td>
<td>2</td>
<td>188</td>
<td>Total C N O S</td>
<td>0</td>
<td>0</td>
</tr>
<tr>
<td></td>
<td></td>
<td></td>
<td>1479 940 256 278 5</td>
<td></td>
<td></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>2</td>
<td>56</td>
<td>MET</td>
<td>-</td>
<td>INITIATING METHIONINE</td>
<td>UNP P47758</td>
</tr>
<tr>
<td>2</td>
<td>57</td>
<td>ALA</td>
<td>-</td>
<td>CLONING ARTIFACT</td>
<td>UNP P47758</td>
</tr>
</tbody>
</table>

- Molecule 7 is a protein called ribosomal protein L35.

<table>
<thead>
<tr>
<th>Mol</th>
<th>Chain</th>
<th>Residues</th>
<th>Atoms</th>
<th>AltConf</th>
<th>Trace</th>
</tr>
</thead>
<tbody>
<tr>
<td>7</td>
<td>5</td>
<td>64</td>
<td>Total C N O</td>
<td>0</td>
<td>0</td>
</tr>
<tr>
<td></td>
<td></td>
<td></td>
<td>504 314 99 91</td>
<td></td>
<td></td>
</tr>
</tbody>
</table>

- Molecule 8 is a protein called ribosomal protein L23.

<table>
<thead>
<tr>
<th>Mol</th>
<th>Chain</th>
<th>Residues</th>
<th>Atoms</th>
<th>AltConf</th>
<th>Trace</th>
</tr>
</thead>
<tbody>
<tr>
<td>8</td>
<td>4</td>
<td>81</td>
<td>Total C N O S</td>
<td>0</td>
<td>0</td>
</tr>
<tr>
<td></td>
<td></td>
<td></td>
<td>652 423 108 119 2</td>
<td></td>
<td></td>
</tr>
</tbody>
</table>

- Molecule 9 is a protein called ribosomal protein L31.
3  Residue-property plots

These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry. 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. 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: SRP RNA

Chain A:

• Molecule 2: ribosomal RNA

Chain 9:

• Molecule 3: Signal recognition particle 19 kDa protein (SRP19)

Chain B:

• Molecule 4: Signal recognition particle 54 kDa protein (SRP54)

Chain W:

• Molecule 5: Signal recognition particle receptor alpha subunit (SR a)

Chain 1:
- Molecule 6: Signal recognition particle receptor beta subunit (SR b)

Chain 2:

- Molecule 7: ribosomal protein L35

Chain 5:

- Molecule 8: ribosomal protein L23

Chain 4:

- Molecule 9: ribosomal protein L31

Chain 6:
4 Experimental information

<table>
<thead>
<tr>
<th>Property</th>
<th>Value</th>
<th>Source</th>
</tr>
</thead>
<tbody>
<tr>
<td>Reconstruction method</td>
<td>SINGLE PARTICLE</td>
<td>Depositor</td>
</tr>
<tr>
<td>Imposed symmetry</td>
<td>POINT, Not provided</td>
<td>Depositor</td>
</tr>
<tr>
<td>Number of particles used</td>
<td>Not provided</td>
<td>Depositor</td>
</tr>
<tr>
<td>Resolution determination method</td>
<td>Not provided</td>
<td>Depositor</td>
</tr>
<tr>
<td>CTF correction method</td>
<td>Not provided</td>
<td>Depositor</td>
</tr>
<tr>
<td>Microscope</td>
<td>FEI TECNAI F30</td>
<td>Depositor</td>
</tr>
<tr>
<td>Voltage (kV)</td>
<td>300</td>
<td>Depositor</td>
</tr>
<tr>
<td>Electron dose ($e^-/Å^2$)</td>
<td>Not provided</td>
<td>Depositor</td>
</tr>
<tr>
<td>Minimum defocus (nm)</td>
<td>800</td>
<td>Depositor</td>
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<tr>
<td>Maximum defocus (nm)</td>
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<td>Depositor</td>
</tr>
<tr>
<td>Magnification</td>
<td>Not provided</td>
<td>Depositor</td>
</tr>
<tr>
<td>Image detector</td>
<td>KODAK SO163 FILM</td>
<td>Depositor</td>
</tr>
</tbody>
</table>
5 Model quality

5.1 Standard geometry

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).

<table>
<thead>
<tr>
<th>Mol</th>
<th>Chain</th>
<th>Bond lengths</th>
<th>Bond angles</th>
</tr>
</thead>
<tbody>
<tr>
<td></td>
<td></td>
<td>RMSZ</td>
<td>#</td>
</tr>
<tr>
<td>1</td>
<td>A</td>
<td>0.45</td>
<td>0/3053</td>
</tr>
<tr>
<td>2</td>
<td>9</td>
<td>0.42</td>
<td>0/2167</td>
</tr>
<tr>
<td>3</td>
<td>B</td>
<td>0.46</td>
<td>0/884</td>
</tr>
<tr>
<td>4</td>
<td>W</td>
<td>0.95</td>
<td>2/876 (0.2%)</td>
</tr>
<tr>
<td>5</td>
<td>1</td>
<td>0.60</td>
<td>0/1035</td>
</tr>
<tr>
<td>6</td>
<td>2</td>
<td>0.53</td>
<td>0/1496</td>
</tr>
<tr>
<td>7</td>
<td>5</td>
<td>1.48</td>
<td>4/506 (0.8%)</td>
</tr>
<tr>
<td>8</td>
<td>4</td>
<td>1.43</td>
<td>10/660 (1.5%)</td>
</tr>
<tr>
<td>9</td>
<td>6</td>
<td>1.35</td>
<td>3/680 (0.4%)</td>
</tr>
<tr>
<td>All</td>
<td>All</td>
<td>0.76</td>
<td>19/11357 (0.2%)</td>
</tr>
</tbody>
</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>
<th>Chain</th>
<th>#Chirality outliers</th>
<th>#Planarity outliers</th>
</tr>
</thead>
<tbody>
<tr>
<td>1</td>
<td>A</td>
<td>0</td>
<td>3</td>
</tr>
<tr>
<td>2</td>
<td>9</td>
<td>0</td>
<td>2</td>
</tr>
<tr>
<td>4</td>
<td>W</td>
<td>0</td>
<td>5</td>
</tr>
<tr>
<td>7</td>
<td>5</td>
<td>2</td>
<td>2</td>
</tr>
<tr>
<td>8</td>
<td>4</td>
<td>3</td>
<td>7</td>
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<tr>
<td>9</td>
<td>6</td>
<td>0</td>
<td>11</td>
</tr>
<tr>
<td>All</td>
<td>All</td>
<td>5</td>
<td>30</td>
</tr>
</tbody>
</table>

All (19) bond length outliers are listed below:

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<tr>
<th>Mol</th>
<th>Chain</th>
<th>Res</th>
<th>Type</th>
<th>Atoms</th>
<th>Z</th>
<th>Observed(Å)</th>
<th>Ideal(Å)</th>
</tr>
</thead>
<tbody>
<tr>
<td>4</td>
<td>W</td>
<td>345</td>
<td>PHE</td>
<td>C-N</td>
<td>-18.40</td>
<td>0.91</td>
<td>1.34</td>
</tr>
<tr>
<td>4</td>
<td>W</td>
<td>362</td>
<td>LYS</td>
<td>C-N</td>
<td>17.62</td>
<td>1.64</td>
<td>1.33</td>
</tr>
<tr>
<td>7</td>
<td>5</td>
<td>38</td>
<td>VAL</td>
<td>C-N</td>
<td>11.88</td>
<td>1.61</td>
<td>1.34</td>
</tr>
<tr>
<td>7</td>
<td>5</td>
<td>39</td>
<td>ALA</td>
<td>N-CA</td>
<td>-11.08</td>
<td>1.24</td>
<td>1.46</td>
</tr>
<tr>
<td>7</td>
<td>5</td>
<td>38</td>
<td>VAL</td>
<td>CA-C</td>
<td>10.76</td>
<td>1.80</td>
<td>1.52</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>
<th>Z</th>
<th>Observed(Å)</th>
<th>Ideal(Å)</th>
</tr>
</thead>
<tbody>
<tr>
<td>8</td>
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<td>97</td>
<td>ASP</td>
<td>N-CA</td>
<td>-9.12</td>
<td>1.28</td>
<td>1.46</td>
</tr>
<tr>
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<td>4</td>
<td>125</td>
<td>ARG</td>
<td>CZ-NH2</td>
<td>9.02</td>
<td>1.44</td>
<td>1.33</td>
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<td>4</td>
<td>131</td>
<td>LYS</td>
<td>CD-CE</td>
<td>8.06</td>
<td>1.71</td>
<td>1.51</td>
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<tr>
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<td>CE2-CZ</td>
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<td>4</td>
<td>135</td>
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<td>CD-CE</td>
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<td>1.68</td>
<td>1.51</td>
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<td>5</td>
<td>34</td>
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<td>CB-CG</td>
<td>6.08</td>
<td>1.64</td>
<td>1.51</td>
</tr>
<tr>
<td>8</td>
<td>4</td>
<td>131</td>
<td>LYS</td>
<td>CE-NZ</td>
<td>6.01</td>
<td>1.40</td>
<td>1.33</td>
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<td>85</td>
<td>ARG</td>
<td>CZ-NH1</td>
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<td>1.40</td>
<td>1.33</td>
</tr>
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</tr>
<tr>
<td>2</td>
<td>9</td>
<td>2842</td>
<td>G</td>
<td>Sidechain</td>
</tr>
<tr>
<td>2</td>
<td>9</td>
<td>2866</td>
<td>U</td>
<td>Sidechain</td>
</tr>
<tr>
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<td>A</td>
<td>197</td>
<td>G</td>
<td>Sidechain</td>
</tr>
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<td>A</td>
<td>201</td>
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<td>208</td>
<td>A</td>
<td>Sidechain</td>
</tr>
<tr>
<td>4</td>
<td>W</td>
<td>344</td>
<td>PRO</td>
<td>Mainchain,Peptide</td>
</tr>
<tr>
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<td>W</td>
<td>361</td>
<td>SER</td>
<td>Mainchain,Peptide</td>
</tr>
<tr>
<td>4</td>
<td>W</td>
<td>362</td>
<td>LYS</td>
<td>Peptide</td>
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</tbody>
</table>

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.

<table>
<thead>
<tr>
<th>Mol</th>
<th>Chain</th>
<th>Non-H</th>
<th>H(model)</th>
<th>H(added)</th>
<th>Clashes</th>
<th>Symm-Clashes</th>
</tr>
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<tbody>
<tr>
<td>1</td>
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<td>186</td>
<td>0</td>
</tr>
<tr>
<td>2</td>
<td>9</td>
<td>1935</td>
<td>0</td>
<td>977</td>
<td>103</td>
<td>0</td>
</tr>
<tr>
<td>3</td>
<td>B</td>
<td>870</td>
<td>0</td>
<td>901</td>
<td>79</td>
<td>0</td>
</tr>
<tr>
<td>4</td>
<td>W</td>
<td>865</td>
<td>0</td>
<td>871</td>
<td>34</td>
<td>0</td>
</tr>
<tr>
<td>5</td>
<td>1</td>
<td>1020</td>
<td>0</td>
<td>1019</td>
<td>53</td>
<td>0</td>
</tr>
<tr>
<td>6</td>
<td>2</td>
<td>1479</td>
<td>0</td>
<td>1533</td>
<td>31</td>
<td>0</td>
</tr>
<tr>
<td>7</td>
<td>5</td>
<td>504</td>
<td>0</td>
<td>553</td>
<td>58</td>
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</tr>
<tr>
<td>8</td>
<td>4</td>
<td>652</td>
<td>0</td>
<td>708</td>
<td>85</td>
<td>0</td>
</tr>
<tr>
<td>9</td>
<td>6</td>
<td>671</td>
<td>0</td>
<td>705</td>
<td>90</td>
<td>0</td>
</tr>
<tr>
<td>All</td>
<td>All</td>
<td>10724</td>
<td>0</td>
<td>8633</td>
<td>627</td>
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</table>

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 33.

All (627) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

<table>
<thead>
<tr>
<th>Atom-1</th>
<th>Atom-2</th>
<th>Interatomic distance (Å)</th>
<th>Clash overlap (Å)</th>
</tr>
</thead>
<tbody>
<tr>
<td>7:5:38:VAL:C</td>
<td>7:5:38:VAL:HA</td>
<td>1.20</td>
<td>1.49</td>
</tr>
<tr>
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<td>7:5:38:VAL:CA</td>
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<td>1.47</td>
</tr>
<tr>
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<td>1:A:224:G:N2</td>
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<td>1.41</td>
</tr>
<tr>
<td>1:A:173:A:H1'</td>
<td>1:A:224:G:C4'</td>
<td>0.94</td>
<td>1.39</td>
</tr>
<tr>
<td>5:1:0:SER:C</td>
<td>5:1:29:VAL:HG23</td>
<td>1.10</td>
<td>1.38</td>
</tr>
<tr>
<td>1:A:172:A:N6</td>
<td>1:A:225:C:O4'</td>
<td>1.64</td>
<td>1.29</td>
</tr>
<tr>
<td>1:A:172:A:C5</td>
<td>1:A:224:G:O2'</td>
<td>1.74</td>
<td>1.27</td>
</tr>
</tbody>
</table>

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

<table>
<thead>
<tr>
<th>Atom-1</th>
<th>Atom-2</th>
<th>Interatomic distance (Å)</th>
<th>Clash overlap (Å)</th>
</tr>
</thead>
<tbody>
<tr>
<td>5:1:0:SER:C</td>
<td>5:1:29:VAL:CG2</td>
<td>2.04</td>
<td>1.25</td>
</tr>
<tr>
<td>7:5:34:ARG:O</td>
<td>8:4:75:TYR:CD1</td>
<td>1.94</td>
<td>1.21</td>
</tr>
<tr>
<td>5:1:-1:HIS:HB2</td>
<td>5:1:4:PHE:CD2</td>
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<td>1.16</td>
</tr>
<tr>
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<td>5:1:4:PHE:CD2</td>
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<td>1.07</td>
</tr>
<tr>
<td>7:5:34:ARG:O</td>
<td>8:4:75:TYR:CE1</td>
<td>2.08</td>
<td>1.05</td>
</tr>
<tr>
<td>1:A:125:G:O2'</td>
<td>1:A:227:G:C8</td>
<td>2.08</td>
<td>1.05</td>
</tr>
<tr>
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<td>1:A:225:C:N3</td>
<td>2.05</td>
<td>1.04</td>
</tr>
<tr>
<td>7:5:38:VAL:O</td>
<td>7:5:38:VAL:HA</td>
<td>1.56</td>
<td>1.03</td>
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<tr>
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<td>5:1:49:HIS:CA</td>
<td>2.08</td>
<td>1.02</td>
</tr>
<tr>
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<td>1.01</td>
</tr>
<tr>
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<td>5:1:29:VAL:HG23</td>
<td>1.59</td>
<td>1.01</td>
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<td>1:A:125:G:O2'</td>
<td>1:A:227:G:N9</td>
<td>1.56</td>
<td>1.01</td>
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<tr>
<td>7:5:38:VAL:CG2</td>
<td>8:4:76:PRO:O</td>
<td>2.10</td>
<td>1.00</td>
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<tr>
<td>1:A:126:C:O2'</td>
<td>1:A:226:U:O4'</td>
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</tr>
<tr>
<td>5:1:-1:HIS:HB2</td>
<td>5:1:4:PHE:HD2</td>
<td>1.09</td>
<td>0.98</td>
</tr>
<tr>
<td>8:4:136:LEU:HD13</td>
<td>8:4:140:TYR:CE2</td>
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</tr>
<tr>
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</table>
### Interatomic distances and clash overlap

<table>
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<th>Interatomic distance (Å)</th>
<th>Clash overlap (Å)</th>
</tr>
</thead>
<tbody>
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<td>1:A:221:C:H5''</td>
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<td>0.96</td>
</tr>
<tr>
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<td>7;5:48:ILE:HG23</td>
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</tr>
<tr>
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<td>5;1:4:PHE:CE2</td>
<td>2.01</td>
<td>0.95</td>
</tr>
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<td>8;4:135:LYS:HZ3</td>
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</tr>
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<td>0.95</td>
</tr>
<tr>
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</tr>
<tr>
<td>Atom-1</td>
<td>Atom-2</td>
<td>Interatomic distance (Å)</td>
<td>Clash overlap (Å)</td>
</tr>
<tr>
<td>--------</td>
<td>--------</td>
<td>--------------------------</td>
<td>-------------------</td>
</tr>
<tr>
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<tr>
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<tr>
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<td>1.81</td>
<td>0.79</td>
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<td>0.79</td>
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</tr>
<tr>
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<td>3:B:93:LEU:N</td>
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<td>3:B:111:MET:HG2</td>
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</tr>
<tr>
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<td>0.41</td>
</tr>
<tr>
<td>3:B:18:Ile:HD12</td>
<td>3:B:105:MET:HG2</td>
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</tr>
<tr>
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<td>8:4:125:ARG:HH22</td>
<td>8:4:131:LYS:CE</td>
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<td>0.41</td>
</tr>
<tr>
<td>7:5:36:GLN:O</td>
<td>7:5:41:SER:HA</td>
<td>2.20</td>
<td>0.41</td>
</tr>
<tr>
<td>2:9:2858:U:H2'</td>
<td>2:9:2859:C:H6</td>
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<td>1:A:127:A:O4'</td>
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<td>0.41</td>
</tr>
<tr>
<td>6:2:103:VAL:HG21</td>
<td>6:2:269:ALA:HB2</td>
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<td>0.41</td>
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<th>Atom-2</th>
<th>Interatomic distance (Å)</th>
<th>Clash overlap (Å)</th>
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<td>7:5:6:VAL:HG23</td>
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<td>2:9:2894:C:O5'</td>
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<td>0.41</td>
</tr>
<tr>
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<td>3:B:77:GLN:H</td>
<td>2.34</td>
<td>0.41</td>
</tr>
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<td>3:B:89:GLU:C</td>
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<td>0.41</td>
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<tr>
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<td>9:6:26:LYS:CE</td>
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<td>2:9:2826:G:C5</td>
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<td>0.41</td>
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<td>1:A:194:G:O4'</td>
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<td>0.41</td>
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<tr>
<td>2:9:2906:A:P</td>
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<td>1:A:208:A:H5'</td>
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<td>0.41</td>
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<td>6:2:75:LYS:HD3</td>
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<td>0.40</td>
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<tr>
<td>8:4:119:LYS:HE2</td>
<td>8:4:135:LYS:CB</td>
<td>2.52</td>
<td>0.40</td>
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<td>6:2:246:ALA:HB1</td>
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</tr>
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<td>2:9:2881:C:O4'</td>
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<td>2.03</td>
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<td>8:4:109:VAL:HG12</td>
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</table>

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 PDB entries followed by that with respect to all EM entries.
The Analysed column shows the number of residues for which the backbone conformation was analysed, and the total number of residues.

<table>
<thead>
<tr>
<th>Mol</th>
<th>Chain</th>
<th>Analysed</th>
<th>Favoured</th>
<th>Allowed</th>
<th>Outliers</th>
<th>Percentiles</th>
</tr>
</thead>
<tbody>
<tr>
<td>3</td>
<td>B</td>
<td>105/108 (97%)</td>
<td>87 (83%)</td>
<td>11 (10%)</td>
<td>7 (7%)</td>
<td>1/21</td>
</tr>
<tr>
<td>4</td>
<td>W</td>
<td>107/109 (98%)</td>
<td>100 (94%)</td>
<td>2 (2%)</td>
<td>5 (5%)</td>
<td>3/28</td>
</tr>
<tr>
<td>5</td>
<td>1</td>
<td>115/185 (62%)</td>
<td>107 (93%)</td>
<td>7 (6%)</td>
<td>1 (1%)</td>
<td>20/63</td>
</tr>
<tr>
<td>6</td>
<td>2</td>
<td>182/214 (85%)</td>
<td>177 (97%)</td>
<td>5 (3%)</td>
<td>0</td>
<td>100/100</td>
</tr>
<tr>
<td>7</td>
<td>5</td>
<td>62/124 (50%)</td>
<td>55 (89%)</td>
<td>2 (3%)</td>
<td>5 (8%)</td>
<td>1/16</td>
</tr>
<tr>
<td>8</td>
<td>4</td>
<td>79/152 (52%)</td>
<td>71 (90%)</td>
<td>4 (5%)</td>
<td>4 (5%)</td>
<td>2/26</td>
</tr>
<tr>
<td>9</td>
<td>6</td>
<td>79/123 (64%)</td>
<td>66 (84%)</td>
<td>10 (13%)</td>
<td>3 (4%)</td>
<td>4/32</td>
</tr>
<tr>
<td>All</td>
<td>All</td>
<td>729/1015 (72%)</td>
<td>663 (91%)</td>
<td>41 (6%)</td>
<td>25 (3%)</td>
<td>7/35</td>
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</tbody>
</table>

All (25) Ramachandran outliers are listed below:

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<td>W</td>
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<td>4</td>
<td>W</td>
<td>345</td>
<td>PHE</td>
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<td>4</td>
<td>W</td>
<td>362</td>
<td>LYS</td>
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<td>5</td>
<td>39</td>
<td>ALA</td>
</tr>
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<td>5</td>
<td>45</td>
<td>LEU</td>
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<td>4</td>
<td>101</td>
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<td>4</td>
<td>125</td>
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<td>W</td>
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<td>SER</td>
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<td>66</td>
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<tr>
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<td>B</td>
<td>96</td>
<td>VAL</td>
</tr>
</tbody>
</table>
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 PDB entries followed by that with respect to all EM entries.

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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<th>Mol</th>
<th>Chain</th>
<th>Analysed</th>
<th>Rotameric</th>
<th>Outliers</th>
<th>Percentiles</th>
</tr>
</thead>
<tbody>
<tr>
<td>3</td>
<td>B</td>
<td>96/97 (99%)</td>
<td>92 (96%)</td>
<td>4 (4%)</td>
<td>34 64</td>
</tr>
<tr>
<td>4</td>
<td>W</td>
<td>96/96 (100%)</td>
<td>91 (95%)</td>
<td>5 (5%)</td>
<td>27 59</td>
</tr>
<tr>
<td>5</td>
<td>1</td>
<td>115/166 (69%)</td>
<td>111 (96%)</td>
<td>4 (4%)</td>
<td>41 69</td>
</tr>
<tr>
<td>6</td>
<td>2</td>
<td>164/182 (90%)</td>
<td>163 (99%)</td>
<td>1 (1%)</td>
<td>89 94</td>
</tr>
<tr>
<td>7</td>
<td>5</td>
<td>55/109 (50%)</td>
<td>44 (80%)</td>
<td>11 (20%)</td>
<td>1 9</td>
</tr>
<tr>
<td>8</td>
<td>4</td>
<td>72/128 (56%)</td>
<td>53 (74%)</td>
<td>19 (26%)</td>
<td>0 4</td>
</tr>
<tr>
<td>9</td>
<td>6</td>
<td>72/108 (67%)</td>
<td>51 (71%)</td>
<td>21 (29%)</td>
<td>0 3</td>
</tr>
<tr>
<td>All</td>
<td>All</td>
<td>670/886 (76%)</td>
<td>605 (90%)</td>
<td>65 (10%)</td>
<td>14 35</td>
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All (65) residues with a non-rotameric sidechain are listed below:

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<th>Type</th>
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Continued on next page...
Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (21) such sidechains are listed below:

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5.3.3 RNA

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<th>Mol</th>
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<th>Backbone Outliers</th>
<th>Pucker Outliers</th>
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<td>22 (17%)</td>
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</tr>
<tr>
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<td>9</td>
<td>89/90 (98%)</td>
<td>10 (11%)</td>
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<tr>
<td>All</td>
<td>All</td>
<td>213/217 (98%)</td>
<td>32 (15%)</td>
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All (32) RNA backbone outliers are listed below:

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There are no RNA pucker outliers to report.

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

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

5.5 Carbohydrates

There are no carbohydrates in this entry.
5.6  Ligand geometry

There are no ligands in this entry.

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.