

Mar 19, 2022 - 06:59 am GMT

| PDB ID       | : | 7QV3  |
|--------------|---|---|
| EMDB ID      | : | EMD-14159   |
| Title        | : | Bacillus subtilis MutS2-collided disome complex (MutS2 conf.2; Leading 70S) |
| Authors      | : | Filbeck, S.; Pfeffer, S.  |
| Deposited on | : | 2022-01-19  |
| Resolution   | : | 5.14 Å(reported)  |
|              |   |   |
|              |   |   |

This is a Full wwPDB EM 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/EMValidationReportHelp

with specific help available everywhere you see the (i) symbol.

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

| EMDB validation analysis       | : | $0.0.0.{ m dev}97$   |
|--------------------------------|---|--|
| MolProbity                     | : | 4.02b-467  |
| Percentile statistics          | : | 20191225.v01 (using entries in the PDB archive December 25th 2019) |
| Ideal geometry (proteins)      | : | Engh & Huber (2001)  |
| Ideal geometry (DNA, RNA)      | : | Parkinson et al. (1996)  |
| Validation Pipeline (wwPDB-VP) | : | 2.27   |

# 1 Overall quality at a glance (i)

The following experimental techniques were used to determine the structure:  $ELECTRON\ MICROSCOPY$ 

The reported resolution of this entry is 5.14 Å.

Percentile scores (ranging between 0-100) for global validation metrics of the entry are shown in the following graphic. The table shows the number of entries on which the scores are based.



| Metric                | $egin{array}{c} { m Whole \ archive} \ (\#{ m Entries}) \end{array}$ | ${f EM\ structures}\ (\#{ m Entries})$ |
|-----------------------|--|--|
| Ramachandran outliers | 154571   | 4023                                   |
| Sidechain outliers    | 154315   | 3826                                   |
| RNA backbone          | 4643   | 859                                    |

The table below summarises the geometric issues observed across the polymeric chains and their fit to the map. The red, orange, yellow and green segments of the 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  $\leq=5\%$  The upper red bar (where present) indicates the fraction of residues that have poor fit to the EM map (all-atom inclusion < 40%). The numeric value is given above the bar.

| Mol | Chain | Length |    | Quality of chain |     |  |  |  |  |  |  |  |  |
|-----|-------|--------|----|------------------|-----|--|--|--|--|--|--|--|--|
| 1   | 0     | 59     |    | 92%              | 8%  |  |  |  |  |  |  |  |  |
| 2   | 1     | 49     |    | 98%              | ٠   |  |  |  |  |  |  |  |  |
| 3   | 2     | 44     |    | 100%             |     |  |  |  |  |  |  |  |  |
| 4   | 3     | 66     |    | 97%              |     |  |  |  |  |  |  |  |  |
| 5   | 4     | 37     |    | 100%             |     |  |  |  |  |  |  |  |  |
| 6   | 6     | 66     | 5% | 95%              | 5%  |  |  |  |  |  |  |  |  |
| 7   | А     | 26     | 8% | 54%              | 15% |  |  |  |  |  |  |  |  |
| 8   | В     | 112    |    | 74%              | 26% |  |  |  |  |  |  |  |  |



| Conti | nued from | n previous | page             |        |
|-------|-----------|------------|------------------|--------|
| Mol   | Chain     | Length     | Quality of chain |        |
| 9     | С         | 277        | 98%              | ·      |
| 10    | D         | 209        | 98%              |        |
| 11    | Е         | 207        | 99%              |        |
| 12    | F         | 179        | 97%              | ••     |
| 13    | G         | 179        | 98%              | •      |
| 14    | Н         | 77         | 81%              | 19%    |
| 15    | Ι         | 24         | 33%              |        |
| 16    | J         | 145        | 98%              |        |
| 17    | K         | 122        | 100%             |        |
| 18    | L         | 146        | 100%             |        |
| 19    | М         | 144        | 94%              | 6%     |
| 20    | N         | 120        | 99%              |        |
| 21    | 0         | 120        | 98%              | •      |
| 22    | Р         | 115        | 100%             |        |
| 23    | Q         | 119        | 97%              | • •    |
| 24    | R         | 102        | 99%              |        |
| 25    | S         | 113        | 96%              | ·      |
| 26    | Т         | 95         | 95%              | 5%     |
| 27    | U         | 103        | 98%              | ·      |
| 28    | V         | 2928       | 75%              | 23% •• |
| 29    | W         | 94         | 87%              | 13%    |
| 30    | X         | 149        | 97%              | ·      |
| 31    | Y         | 66         | 98%              | ·      |
| 32    | Z         | 59         | 98%              | ·      |
| 33    | a         | 1533       | 83%              | 17%    |



| Mol | Chain | Length | Quality of chain |       |
|-----|-------|--------|------------------|-------|
| 34  | b     | 57     | 23%              |       |
| 35  | 0     | 218    | 17%              | 201   |
|     | C     | 210    | 94%              | 6%    |
| 36  | d     | 200    | 96%              | ••    |
| 37  | е     | 166    | 99%              |       |
| 38  | f     | 95     | 97%              | •     |
| 39  | g     | 156    | <b>•</b><br>97%  | ·     |
| 40  | h     | 132    | 99%              |       |
| 41  | i     | 130    | •                | 21%   |
| 49  | :     | 109    | •                |       |
| 42  | J     | 102    | 93%              | 7%    |
| 43  | k     | 131    | 90%              | 10%   |
| 44  | 1     | 138    | 99%              | •     |
| 45  | m     | 121    | 75%              | 24%   |
| 46  | n     | 61     | 97%              |       |
| 47  | 0     | 89     | 94%              | • •   |
| 48  | р     | 90     | 98%              | ·     |
| 40  | 1     | 07     | •                |       |
| 49  | q     | 01     | 97%              | •     |
| 50  | r     | 79     | 80%              | • 19% |
| 51  | S     | 92     | 83%              | • 16% |
| 52  | t     | 88     | 94%              | 6%    |
| 53  | u     | 62     | 94%              | 6%    |
| 54  | V     | 785    | 69%              | 30%   |
| 54  | W     | 785    | 74%              | 24%   |



# 2 Entry composition (i)

There are 54 unique types of molecules in this entry. The entry contains 149707 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 protein called 50S ribosomal protein L32.

| Mol | Chain | Residues | Atoms        |          |         |         |            | AltConf | Trace |
|-----|-------|----------|--------------|----------|---------|---------|------------|---------|-------|
| 1   | 0     | 54       | Total<br>426 | C<br>262 | N<br>86 | 0<br>71 | ${ m S} 7$ | 0       | 0     |

• Molecule 2 is a protein called 50S ribosomal protein L33 1.

| Mol | Chain | Residues | Atoms |     |    |    |   | AltConf | Trace |
|-----|-------|----------|-------|-----|----|----|---|---------|-------|
| 2   | 1     | /18      | Total | С   | Ν  | Ο  | S | 0       | 0     |
| 2   | T     | 40       | 401   | 244 | 80 | 73 | 4 | 0       | 0     |

• Molecule 3 is a protein called 50S ribosomal protein L34.

| Mol | Chain | Residues | Atoms |     |    |    |   | AltConf | Trace |
|-----|-------|----------|-------|-----|----|----|---|---------|-------|
| 3 2 | 4.4   | Total    | С     | Ν   | Ο  | S  | 0 | 0       |       |
|     | 2     | 2 44     | 367   | 222 | 89 | 54 | 2 | 0       | 0     |

• Molecule 4 is a protein called 50S ribosomal protein L35.

| Mol | Chain | Residues | Atoms        |          |          |         |   | AltConf | Trace |
|-----|-------|----------|--------------|----------|----------|---------|---|---------|-------|
| 4   | 3     | 64       | Total<br>512 | C<br>321 | N<br>107 | O<br>82 | $\begin{array}{c} \mathrm{S} \\ \mathrm{2} \end{array}$ | 0       | 0     |

• Molecule 5 is a protein called 50S ribosomal protein L36.

| Mol | Chain | Residues | Atoms        |          |         |         |            | AltConf | Trace |
|-----|-------|----------|--------------|----------|---------|---------|------------|---------|-------|
| 5   | 4     | 37       | Total<br>296 | C<br>186 | N<br>60 | O<br>45 | ${f S}{5}$ | 0       | 0     |

• Molecule 6 is a protein called 50S ribosomal protein L31.

| Mol | Chain | Residues | Atoms        |          |         |         |            | AltConf | Trace |
|-----|-------|----------|--------------|----------|---------|---------|------------|---------|-------|
| 6   | 6     | 63       | Total<br>499 | C<br>312 | N<br>91 | O<br>91 | ${f S}{5}$ | 0       | 0     |



• Molecule 7 is a RNA chain called mRNA.

| Mol | Chain | Residues |              | A        | toms     | AltConf  | Trace   |   |   |
|-----|-------|----------|--------------|----------|----------|----------|---------|---|---|
| 7   | А     | 26       | Total<br>559 | C<br>251 | N<br>106 | 0<br>176 | Р<br>26 | 0 | 0 |

• Molecule 8 is a RNA chain called 5S ribosomal RNA.

| Mol | Chain | Residues |               | A         | AltConf  | Trace    |          |   |   |
|-----|-------|----------|---------------|-----------|----------|----------|----------|---|---|
| 8   | В     | 112      | Total<br>2392 | C<br>1068 | N<br>435 | 0<br>778 | Р<br>111 | 0 | 0 |

• Molecule 9 is a protein called 50S ribosomal protein L2.

| Mol | Chain | Residues | Atoms         |           |          |          |        | AltConf | Trace |
|-----|-------|----------|---------------|-----------|----------|----------|--------|---------|-------|
| 9   | С     | 272      | Total<br>2083 | C<br>1296 | N<br>408 | O<br>373 | S<br>6 | 0       | 0     |

• Molecule 10 is a protein called 50S ribosomal protein L3.

| Mol | Chain | Residues |               | At       | oms      | AltConf  | Trace         |   |   |
|-----|-------|----------|---------------|----------|----------|----------|---------------|---|---|
| 10  | D     | 206      | Total<br>1569 | C<br>985 | N<br>289 | O<br>290 | ${S \atop 5}$ | 0 | 0 |

• Molecule 11 is a protein called 50S ribosomal protein L4.

| Mol | Chain | Residues |               | At       | oms      | AltConf  | Trace           |   |   |
|-----|-------|----------|---------------|----------|----------|----------|-----------------|---|---|
| 11  | Е     | 205      | Total<br>1561 | C<br>980 | N<br>289 | O<br>290 | ${ m S} { m 2}$ | 0 | 0 |

• Molecule 12 is a protein called 50S ribosomal protein L5.

| Mol | Chain | Residues |               | At       | oms      | AltConf  | Trace      |   |   |
|-----|-------|----------|---------------|----------|----------|----------|------------|---|---|
| 12  | F     | 176      | Total<br>1386 | C<br>882 | N<br>241 | O<br>256 | ${f S}{7}$ | 0 | 0 |

• Molecule 13 is a protein called 50S ribosomal protein L6.

| Mol | Chain | Residues |               | At       | oms      | AltConf  | Trace   |   |   |
|-----|-------|----------|---------------|----------|----------|----------|---|---|---|
| 13  | G     | 175      | Total<br>1342 | C<br>835 | N<br>248 | O<br>257 | $\begin{array}{c} \mathrm{S} \\ \mathrm{2} \end{array}$ | 0 | 0 |

• Molecule 14 is a RNA chain called P-site tRNA.



| Mol | Chain | Residues |               | $\mathbf{A}$ | AltConf  | Trace    |         |   |   |
|-----|-------|----------|---------------|--------------|----------|----------|---------|---|---|
| 14  | Н     | 77       | Total<br>1643 | С<br>731     | N<br>290 | O<br>545 | Р<br>77 | 0 | 0 |

• Molecule 15 is a protein called Nascent chain.

| Mol | Chain | Residues |              | Ator    | ns      | AltConf | Trace |   |
|-----|-------|----------|--------------|---------|---------|---------|-------|---|
| 15  | Ι     | 24       | Total<br>120 | C<br>72 | N<br>24 | O<br>24 | 0     | 0 |

• Molecule 16 is a protein called 50S ribosomal protein L13.

| Mol | Chain | Residues |               | At       | oms      | AltConf  | Trace          |   |   |
|-----|-------|----------|---------------|----------|----------|----------|----------------|---|---|
| 16  | J     | 142      | Total<br>1123 | C<br>710 | N<br>206 | O<br>202 | ${ m S}{ m 5}$ | 0 | 0 |

• Molecule 17 is a protein called 50S ribosomal protein L14.

| Mol | Chain | Residues |              | At       | oms      | AltConf  | Trace         |   |   |
|-----|-------|----------|--------------|----------|----------|----------|---------------|---|---|
| 17  | K     | 122      | Total<br>920 | C<br>571 | N<br>173 | 0<br>172 | ${S \atop 4}$ | 0 | 0 |

• Molecule 18 is a protein called 50S ribosomal protein L15.

| Mol | Chain | Residues |               | At       | oms      | AltConf  | Trace   |   |   |
|-----|-------|----------|---------------|----------|----------|----------|---|---|---|
| 18  | L     | 146      | Total<br>1081 | C<br>671 | N<br>207 | 0<br>201 | $\begin{array}{c} \mathrm{S} \\ \mathrm{2} \end{array}$ | 0 | 0 |

• Molecule 19 is a protein called 50S ribosomal protein L16.

| Mol | Chain | Residues |               | At       | oms      |          |                | AltConf | Trace |
|-----|-------|----------|---------------|----------|----------|----------|----------------|---------|-------|
| 19  | М     | 135      | Total<br>1076 | C<br>690 | N<br>205 | 0<br>176 | ${ m S}{ m 5}$ | 0       | 0     |

• Molecule 20 is a protein called 50S ribosomal protein L17.

| Mol | Chain | Residues |              | At       | oms      |          |               | AltConf | Trace |
|-----|-------|----------|--------------|----------|----------|----------|---------------|---------|-------|
| 20  | N     | 119      | Total<br>953 | C<br>583 | N<br>186 | 0<br>180 | ${S \atop 4}$ | 0       | 0     |

• Molecule 21 is a protein called 50S ribosomal protein L18.



| Mol | Chain | Residues |              | At       | oms      |          |        | AltConf | Trace |
|-----|-------|----------|--------------|----------|----------|----------|--------|---------|-------|
| 21  | 0     | 120      | Total<br>912 | C<br>564 | N<br>176 | 0<br>171 | S<br>1 | 0       | 0     |

• Molecule 22 is a protein called 50S ribosomal protein L19.

| Mol | Chain | Residues |              | At       | oms      | AltConf  | Trace  |   |   |
|-----|-------|----------|--------------|----------|----------|----------|--------|---|---|
| 22  | Р     | 115      | Total<br>944 | C<br>600 | N<br>185 | 0<br>158 | S<br>1 | 0 | 0 |

• Molecule 23 is a protein called 50S ribosomal protein L20.

| Mol | Chain | Residues |              | At       | oms      | AltConf  | Trace         |   |   |
|-----|-------|----------|--------------|----------|----------|----------|---------------|---|---|
| 23  | Q     | 117      | Total<br>940 | C<br>591 | N<br>189 | 0<br>156 | $\frac{S}{4}$ | 0 | 0 |

• Molecule 24 is a protein called 50S ribosomal protein L21.

| Mol | Chain | Residues |              | Ato      | ms       | AltConf  | Trace |   |
|-----|-------|----------|--------------|----------|----------|----------|-------|---|
| 24  | R     | 101      | Total<br>786 | C<br>501 | N<br>139 | O<br>146 | 0     | 0 |

• Molecule 25 is a protein called 50S ribosomal protein L22.

| Mol | Chain | Residues |              | At       | oms      | AltConf  | Trace           |   |   |
|-----|-------|----------|--------------|----------|----------|----------|-----------------|---|---|
| 25  | S     | 109      | Total<br>842 | C<br>525 | N<br>164 | O<br>150 | ${ m S} { m 3}$ | 0 | 0 |

• Molecule 26 is a protein called 50S ribosomal protein L23.

| Mol | Chain | Residues |              | At       | oms      |          |                 | AltConf | Trace |
|-----|-------|----------|--------------|----------|----------|----------|-----------------|---------|-------|
| 26  | Т     | 90       | Total<br>725 | C<br>452 | N<br>134 | 0<br>136 | ${ m S} { m 3}$ | 0       | 0     |

• Molecule 27 is a protein called 50S ribosomal protein L24.

| Mol | Chain | Residues |              | At       | oms      |          |               | AltConf | Trace |
|-----|-------|----------|--------------|----------|----------|----------|---------------|---------|-------|
| 27  | U     | 101      | Total<br>762 | C<br>478 | N<br>142 | 0<br>138 | ${S \atop 4}$ | 0       | 0     |

• Molecule 28 is a RNA chain called 23S ribosomal RNA.



| Mol | Chain | Residues |                |            | Atoms      |            |           | AltConf | Trace |
|-----|-------|----------|----------------|------------|------------|------------|-----------|---------|-------|
| 28  | V     | 2887     | Total<br>61998 | C<br>27661 | N<br>11460 | O<br>19993 | Р<br>2884 | 0       | 0     |

There are 7 discrepancies between the modelled and reference sequences:

| Chain | Residue | Modelled | Actual | Comment   | Reference     |
|-------|---------|----------|--------|-----------|---------------|
| V     | 243     | G        | А      | conflict  | GB 1491848961 |
| V     | 325     | А        | -      | insertion | GB 1491848961 |
| V     | 326     | А        | -      | insertion | GB 1491848961 |
| V     | 327     | G        | -      | insertion | GB 1491848961 |
| V     | 328     | G        | -      | insertion | GB 1491848961 |
| V     | 640     | U        | С      | conflict  | GB 1491848961 |
| V     | 2232    | А        | G      | conflict  | GB 1491848961 |

• Molecule 29 is a protein called 50S ribosomal protein L27.

| Mol | Chain | Residues |              | Ato      | ms       | AltConf  | Trace |   |
|-----|-------|----------|--------------|----------|----------|----------|-------|---|
| 29  | W     | 82       | Total<br>630 | C<br>390 | N<br>123 | 0<br>117 | 0     | 0 |

• Molecule 30 is a protein called 50S ribosomal protein L9.

| Mol | Chain | Residues |               | At       | oms      | AltConf  | Trace  |   |   |
|-----|-------|----------|---------------|----------|----------|----------|--------|---|---|
| 30  | Х     | 149      | Total<br>1151 | C<br>726 | N<br>205 | O<br>219 | S<br>1 | 0 | 0 |

• Molecule 31 is a protein called 50S ribosomal protein L29.

| Mol | Chain | Residues |              | Ate      | oms      | AltConf | Trace         |   |   |
|-----|-------|----------|--------------|----------|----------|---------|---------------|---|---|
| 31  | Y     | 65       | Total<br>530 | C<br>328 | N<br>102 | O<br>98 | ${S \over 2}$ | 0 | 0 |

• Molecule 32 is a protein called 50S ribosomal protein L30.

| Mol | Chain | Residues |       | Atc | $\mathbf{ms}$ | AltConf | Trace        |   |   |
|-----|-------|----------|-------|-----|---------------|---------|--------------|---|---|
| 20  | 7     | 59       | Total | С   | Ν             | Ο       | $\mathbf{S}$ | 0 | 0 |
| 52  |       | 50       | 455   | 281 | 89            | 84      | 1            |   | U |

• Molecule 33 is a RNA chain called 16S ribosomal RNA.



| Mol | Chain | Residues |                | I          | Atoms     |            |           | AltConf | Trace |
|-----|-------|----------|----------------|------------|-----------|------------|-----------|---------|-------|
| 33  | a     | 1533     | Total<br>32891 | C<br>14667 | N<br>6034 | O<br>10657 | Р<br>1533 | 0       | 0     |

• Molecule 34 is a protein called 30S ribosomal protein S21.

| Mol | Chain | Residues |              | Ato      | $\mathbf{ms}$ | AltConf | Trace  |   |   |
|-----|-------|----------|--------------|----------|---------------|---------|--------|---|---|
| 34  | b     | 57       | Total<br>476 | C<br>295 | N<br>97       | O<br>83 | S<br>1 | 0 | 0 |

There is a discrepancy between the modelled and reference sequences:

| Chain | Residue | Modelled | Actual | Comment  | Reference  |
|-------|---------|----------|--------|----------|------------|
| b     | 30      | ALA      | GLN    | conflict | UNP P21478 |

• Molecule 35 is a protein called 30S ribosomal protein S3.

| Mol | Chain | Residues |               | At        | AltConf  | Trace    |                 |   |   |
|-----|-------|----------|---------------|-----------|----------|----------|-----------------|---|---|
| 35  | С     | 206      | Total<br>1619 | C<br>1011 | N<br>304 | O<br>301 | ${ m S} { m 3}$ | 0 | 0 |

• Molecule 36 is a protein called 30S ribosomal protein S4.

| Mol | Chain | Residues |       | At  | oms |     | AltConf      | Trace |   |
|-----|-------|----------|-------|-----|-----|-----|--------------|-------|---|
| 36  | d     | 105      | Total | С   | Ν   | 0   | $\mathbf{S}$ | 0     | 0 |
| 50  | u     | 195      | 1568  | 991 | 291 | 284 | 2            | 0     | 0 |

• Molecule 37 is a protein called 30S ribosomal protein S5.

| Mol | Chain | Residues |               | At       | AltConf  | Trace    |   |   |   |
|-----|-------|----------|---------------|----------|----------|----------|---|---|---|
| 37  | е     | 164      | Total<br>1218 | C<br>767 | N<br>225 | 0<br>224 | $\begin{array}{c} \mathrm{S} \\ \mathrm{2} \end{array}$ | 0 | 0 |

• Molecule 38 is a protein called 30S ribosomal protein S6.

| Mol | Chain | Residues |              | At       | $\mathbf{oms}$ |          |        | AltConf | Trace |
|-----|-------|----------|--------------|----------|----------------|----------|--------|---------|-------|
| 38  | f     | 92       | Total<br>755 | C<br>476 | N<br>132       | 0<br>146 | S<br>1 | 0       | 0     |

• Molecule 39 is a protein called 30S ribosomal protein S7.



| Mol | Chain | Residues |               | At       | oms      |          |        | AltConf | Trace |
|-----|-------|----------|---------------|----------|----------|----------|--------|---------|-------|
| 39  | g     | 151      | Total<br>1203 | C<br>755 | N<br>224 | O<br>218 | S<br>6 | 0       | 0     |

• Molecule 40 is a protein called 30S ribosomal protein S8.

| Mol | Chain | Residues |               | At       | oms      | AltConf  | Trace           |   |   |
|-----|-------|----------|---------------|----------|----------|----------|-----------------|---|---|
| 40  | h     | 131      | Total<br>1036 | C<br>655 | N<br>191 | 0<br>187 | ${ m S} { m 3}$ | 0 | 0 |

• Molecule 41 is a protein called 30S ribosomal protein S9.

| Mol | Chain | Residues |              | Ato      | $\mathbf{ms}$ | AltConf  | Trace |   |
|-----|-------|----------|--------------|----------|---------------|----------|-------|---|
| 41  | i     | 103      | Total<br>784 | C<br>485 | N<br>151      | 0<br>148 | 0     | 0 |

• Molecule 42 is a protein called 30S ribosomal protein S10.

| Mol | Chain | Residues |              | At       | oms      |          |                 | AltConf | Trace |
|-----|-------|----------|--------------|----------|----------|----------|-----------------|---------|-------|
| 42  | j     | 95       | Total<br>761 | C<br>479 | N<br>139 | 0<br>141 | ${ m S} { m 2}$ | 0       | 0     |

• Molecule 43 is a protein called 30S ribosomal protein S11.

| Mol | Chain | Residues |              | At       | oms      |          |   | AltConf | Trace |
|-----|-------|----------|--------------|----------|----------|----------|---|---------|-------|
| 43  | k     | 118      | Total<br>871 | C<br>537 | N<br>171 | 0<br>161 | $\begin{array}{c} \mathrm{S} \\ \mathrm{2} \end{array}$ | 0       | 0     |

• Molecule 44 is a protein called 30S ribosomal protein S12.

| Mol | Chain | Residues |               | At       | oms      |          |                 | AltConf | Trace |
|-----|-------|----------|---------------|----------|----------|----------|-----------------|---------|-------|
| 44  | 1     | 136      | Total<br>1052 | C<br>653 | N<br>211 | 0<br>186 | ${ m S} { m 2}$ | 0       | 0     |

• Molecule 45 is a protein called 30S ribosomal protein S13.

| Mol | Chain | Residues |              | Ato      | ms       |          | AltConf | Trace |
|-----|-------|----------|--------------|----------|----------|----------|---------|-------|
| 45  | m     | 92       | Total<br>740 | C<br>459 | N<br>145 | O<br>136 | 0       | 0     |

• Molecule 46 is a protein called 30S ribosomal protein S14.



| Mol | Chain | Residues |              | Atc      | $\mathbf{ms}$ | AltConf | Trace          |   |   |
|-----|-------|----------|--------------|----------|---------------|---------|----------------|---|---|
| 46  | n     | 60       | Total<br>497 | C<br>317 | N<br>98       | O<br>77 | ${ m S}{ m 5}$ | 0 | 0 |

• Molecule 47 is a protein called 30S ribosomal protein S15.

| Mol | Chain | Residues |              | At       | oms      |          | AltConf | Trace |   |
|-----|-------|----------|--------------|----------|----------|----------|---------|-------|---|
| 47  | О     | 85       | Total<br>710 | C<br>436 | N<br>144 | O<br>129 | S<br>1  | 0     | 0 |

• Molecule 48 is a protein called 30S ribosomal protein S16.

| Mol | Chain | Residues |              | At       | oms      | AltConf  | Trace   |   |   |
|-----|-------|----------|--------------|----------|----------|----------|---|---|---|
| 48  | р     | 88       | Total<br>695 | C<br>441 | N<br>128 | 0<br>124 | $\begin{array}{c} \mathrm{S} \\ \mathrm{2} \end{array}$ | 0 | 0 |

• Molecule 49 is a protein called 30S ribosomal protein S17.

| Mol | Chain | Residues |              | At       | oms      | AltConf  | Trace           |   |   |
|-----|-------|----------|--------------|----------|----------|----------|-----------------|---|---|
| 49  | q     | 84       | Total<br>691 | C<br>435 | N<br>128 | 0<br>126 | ${ m S} { m 2}$ | 0 | 0 |

• Molecule 50 is a protein called 30S ribosomal protein S18.

| Mol | Chain | Residues |              | Ato      | $\mathbf{ms}$ |         |   | AltConf | Trace |
|-----|-------|----------|--------------|----------|---------------|---------|---|---------|-------|
| 50  | r     | 64       | Total<br>518 | C<br>332 | N<br>96       | 0<br>88 | $\begin{array}{c} \mathrm{S} \\ \mathrm{2} \end{array}$ | 0       | 0     |

• Molecule 51 is a protein called 30S ribosomal protein S19.

| Mol | Chain | Residues |              | At       | oms      |          |               | AltConf | Trace |
|-----|-------|----------|--------------|----------|----------|----------|---------------|---------|-------|
| 51  | S     | 77       | Total<br>624 | C<br>403 | N<br>110 | O<br>109 | ${S \over 2}$ | 0       | 0     |

• Molecule 52 is a protein called 30S ribosomal protein S20.

| Mol | Chain | Residues |              | At       | oms      |          |        | AltConf | Trace |
|-----|-------|----------|--------------|----------|----------|----------|--------|---------|-------|
| 52  | t     | 83       | Total<br>637 | C<br>390 | N<br>130 | 0<br>116 | S<br>1 | 0       | 0     |

• Molecule 53 is a protein called 50S ribosomal protein L28.



| Mol | Chain | Residues | Atoms        |          |         | AltConf | Trace           |   |   |
|-----|-------|----------|--------------|----------|---------|---------|-----------------|---|---|
| 53  | u     | 58       | Total<br>444 | C<br>275 | N<br>92 | O<br>75 | ${ m S} { m 2}$ | 0 | 0 |

• Molecule 54 is a protein called Endonuclease MutS2.

| Mol  | Chain | Residues | Atoms |      |     | AltConf | Trace        |   |   |
|------|-------|----------|-------|------|-----|---------|--------------|---|---|
| 54   | 17    | 548      | Total | С    | Ν   | 0       | $\mathbf{S}$ | 0 | 0 |
| 04 V | V     | 040      | 4289  | 2680 | 743 | 850     | 16           | 0 | 0 |
| 54   | 117   | 503      | Total | С    | Ν   | 0       | $\mathbf{S}$ | 0 | 0 |
| 54   | W     | 090      | 4644  | 2904 | 804 | 919     | 17           | U | U |



## 3 Residue-property plots (i)

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 atom inclusion in map 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 diamond above a residue indicates a poor fit to the EM map for this residue (all-atom inclusion < 40%). 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 L32

| Chain 0:                                     | 92%   | 8% |
|--|---|----|
| MET<br>A2<br>N55<br>VAL<br>LYS<br>SER<br>ASN |   |    |
| • Molecule 2                                 | 2: 50S ribosomal protein L33 1              |    |
| Chain 1:                                     | 98%   | ·  |
| M1<br>T48<br>LYS                             |   |    |
| • Molecule 3                                 | 3: 50S ribosomal protein L34                |    |
| Chain 2:                                     | 100%  |    |
| There are no                                 | o outlier residues recorded for this chain. |    |
| • Molecule 4                                 | : 50S ribosomal protein L35                 |    |
| Chain 3:                                     | 97%   | •  |
| MET<br>P2<br>LYS<br>LYS                      |   |    |
| • Molecule 5                                 | 5: 50S ribosomal protein L36                |    |
| Chain 4:                                     | 100%  |    |
| There are no                                 | o outlier residues recorded for this chain. |    |
| • Molecule 6                                 | 5: 50S ribosomal protein L31                |    |
| Chain 6: 5%                                  | 95%   | 5% |



| M1<br>M55<br>M55<br>M55<br>M55<br>M55<br>M55<br>M55<br>M55<br>M55<br>M  |
|---|
| • Molecule 7: mRNA  |
| <sup>8%</sup><br>Chain A: 31% 54% 15%   |
| A30<br>A31<br>A33<br>A33<br>A33<br>A33<br>A33<br>A33<br>A33<br>A33<br>A33   |
| • Molecule 8: 5S ribosomal RNA  |
| Chain B: 74% 26%  |
| U3<br>411<br>411<br>411<br>411<br>412<br>412<br>437<br>437<br>437<br>437<br>437<br>449<br>455<br>449<br>455<br>455<br>455<br>455<br>455<br>455<br>455 |
| $\bullet$ Molecule 9: 50S ribosomal protein L2  |
| Chain C: 98% ·  |
| MET<br>A2<br>A2<br>A108<br>ARC<br>ARC<br>ARC<br>ARC<br>ARC  |
| • Molecule 10: 50S ribosomal protein L3   |
| Chain D: 98% .  |
| MET<br>1140<br>X207<br>SER<br>ILYS  |
| • Molecule 11: 50S ribosomal protein L4   |
| Chain E: 99%  |
| MET<br>2<br>ALA<br>ALA  |
| • Molecule 12: 50S ribosomal protein L5   |
| Chain F: 97%  |
| MET<br>M2<br>E122<br>E164<br>CLNS<br>LNS  |
| • Molecule 13: 50S ribosomal protein L6   |
| Chain G: 98% ·  |

WORLDWIDE PROTEIN DATA BANK



• Molecule 14: P-site tRNA

| Chain H:  | 81%  | 19% |
|---|--|-----|
| G1<br>A9<br>U17<br>G17A<br>G17A<br>G18<br>U19<br>U20<br>A21 | C36<br>A37<br>C48<br>U47<br>C48<br>A70<br>C74<br>C73<br>C73<br>C73<br>C73<br>C75<br>C74<br>A76 |     |
| • Molecule 15:  | Nascent chain  |     |
| Chain I:  | 33%  |     |
| X66<br>X70<br>X71<br>X72<br>X72<br>X73<br>X73<br>X80        | X81<br>X82<br>X84<br>X89   |     |
| • Molecule 16:  | 50S ribosomal protein L13  |     |
| Chain J:  | 98%  |     |
| MET<br>ARG<br>THR<br>T4<br>G145                             |  |     |
| • Molecule 17:  | 50S ribosomal protein L14  |     |
| Chain K:  | 100%   |     |
| There are no c  | outlier residues recorded for this chain.  |     |
| • Molecule 18:  | 50S ribosomal protein L15  |     |
| Chain L:  | 100%   |     |
| There are no c  | outlier residues recorded for this chain.  |     |
| • Molecule 19:  | 50S ribosomal protein L16  |     |
| Chain M:  | 94%  | 6%  |
| M1<br>E135<br>GLU<br>GLU<br>GLY<br>GLY<br>SER<br>ASN<br>ASN | S S S S S S S S S S S S S S S S S S S  |     |
| • Molecule 20:  | 50S ribosomal protein L17  |     |
| Chain N:  | 99%  |     |
| MET<br>S2<br>V120   |  |     |



| • Molecule 21: 50S ribosomal protein L18                |     |
|---|-----|
| Chain O: 98%  | •   |
| R17<br>R17<br>F120                                      |     |
| • Molecule 22: 50S ribosomal protein L19                |     |
| Chain P: 100%   |     |
| There are no outlier residues recorded for this chain.  |     |
| $\bullet$ Molecule 23: 50S ribosomal protein L20        |     |
| Chain Q: 97%  | ••• |
| MET<br>P2<br>188<br>K33<br>L103<br>L103<br>L103<br>L118 |     |
| • Molecule 24: 50S ribosomal protein L21                |     |
| Chain R: 99%  |     |
| MET<br>72<br>A102                                       |     |
| • Molecule 25: 50S ribosomal protein L22                |     |
| Chain S: 96%  | •   |
| MET<br>Q2<br>K110<br>CLYS<br>CLU<br>GLY                 |     |
| • Molecule 26: 50S ribosomal protein L23                |     |
| Chain T: 95%  | 5%  |
| MET<br>R91<br>PILE<br>ALA<br>ALA                        |     |
| • Molecule 27: 50S ribosomal protein L24                |     |
| Chain U: 98%  | ·   |
| M<br>ASP<br>LIYS  |     |

• Molecule 28: 23S ribosomal RNA



| Chain V:  | 75%   | 23%   |
|---|---|---|
| G<br>02<br>08<br>08<br>03<br>02<br>03<br>03<br>05<br>05<br>05<br>05<br>05<br>05<br>05<br>05<br>05<br>05<br>05<br>05<br>05   | 476<br>477<br>478<br>485<br>486<br>486<br>486<br>487<br>487<br>487<br>487<br>487<br>490<br>410<br>4117<br>4117<br>4117<br>4117<br>4124  | A125<br>U138<br>A139<br>0141<br>0141<br>0141<br>0141<br>0145<br>U163  |
| 6175<br>6176<br>6177<br>6177<br>6187<br>6188<br>6188<br>6188<br>6188  | A219<br>A224<br>A225<br>A226<br>A226<br>A231<br>U232<br>C234<br>C233<br>C234<br>C233<br>C234<br>C262<br>C252<br>C255<br>C255<br>C255<br>C255<br>C255<br>C265<br>C26   | U285<br>U286<br>G287<br>C291<br>C291<br>C291<br>C297<br>C297<br>C297<br>C297<br>C297<br>C297<br>C297<br>C297  |
|   | A342<br>A345<br>A345<br>A345<br>A345<br>A346<br>A348<br>A374<br>A373<br>A373<br>A373<br>A373<br>A373<br>A373<br>A374<br>C35<br>C35<br>C35<br>C35<br>C35<br>C35<br>C35<br>C35<br>C35<br>C35  | C<br>C<br>C<br>G<br>6406<br>6410<br>6411<br>6411<br>6411<br>6417<br>6417<br>6417<br>6417<br>6417  |
| 0420<br>0421<br>421<br>421<br>433<br>433<br>433<br>433<br>6443<br>6445<br>6445<br>6445<br>644   | C491<br>1498<br>1498<br>1498<br>1498<br>1490<br>1506<br>1506<br>1506<br>1506<br>1512<br>1523<br>1537<br>1537<br>1537<br>1537<br>1537<br>1537<br>1537<br>153   | 6550<br>1954<br>0555<br>0556<br>0556<br>0556<br>0556<br>0573<br>A575<br>A575<br>0575  |
| A578<br>(579<br>(579<br>(579<br>(5894<br>(5894<br>(5896<br>(5896<br>(5896<br>(5896<br>(5896<br>(5896<br>(5896<br>(5896<br>(5896<br>(5896<br>(5896<br>(5816<br>(5816<br>(5816<br>(5816<br>(5816)<br>(5816)<br>(5816)<br>(5816)<br>(5816)<br>(5816)<br>(5816)<br>(5816)<br>(5816)<br>(5816)<br>(5816)<br>(5816)<br>(5816)<br>(5816)<br>(5816)<br>(5816)<br>(5816)<br>(5816)<br>(5816)<br>(5816)<br>(5816)<br>(5816)<br>(5816)<br>(5816)<br>(5816)<br>(5816)<br>(5816)<br>(5816)<br>(5816)<br>(5816)<br>(5816)<br>(5816)<br>(5816)<br>(5816)<br>(5816)<br>(5816)<br>(5816)<br>(5816)<br>(5816)<br>(5816)<br>(5816)<br>(5816)<br>(5816)<br>(5816)<br>(5816)<br>(5816)<br>(5816)<br>(5816)<br>(5816)<br>(5816)<br>(5816)<br>(5816)<br>(5816)<br>(5816)<br>(5816)<br>(5816)<br>(5816)<br>(5816)<br>(5816)<br>(5816)<br>(5816)<br>(5816)<br>(5816)<br>(5816)<br>(5816)<br>(5816)<br>(5816)<br>(5816)<br>(5816)<br>(5816)<br>(5816)<br>(5816)<br>(5816)<br>(5816)<br>(5816)<br>(5816)<br>(5816)<br>(5816)<br>(5816)<br>(5816)<br>(5816)<br>(5816)<br>(5816)<br>(5816)<br>(5816)<br>(5816)<br>(5816)<br>(5816)<br>(5816)<br>(5816)<br>(5816)<br>(5816)<br>(5816)<br>(5816)<br>(5816)<br>(5816)<br>(5816)<br>(5816)<br>(5816)<br>(5816)<br>(5816)<br>(5816)<br>(5816)<br>(5816)<br>(5816)<br>(5816)<br>(5816)<br>(5816)<br>(5816)<br>(5816)<br>(5816)<br>(5816)<br>(5816)<br>(5816)<br>(5816)<br>(5816)<br>(5816)<br>(5816)<br>(5816)<br>(5816)<br>(5816)<br>(5816)<br>(5816)<br>(5816)<br>(5816)<br>(5816)<br>(5816)<br>(5816)<br>(5816)<br>(5816)<br>(5816)<br>(5816)<br>(5816)<br>(5816)<br>(5816)<br>(5816)<br>(5816)<br>(5816)<br>(5816)<br>(5816)<br>(5816)<br>(5816)<br>(5816)<br>(5816)<br>(5816)<br>(5816)<br>(5816)<br>(5816)<br>(5816)<br>(5816)<br>(5816)<br>(5816)<br>(5816)<br>(5816)<br>(5816)<br>(5816)<br>(5816)<br>(5816)<br>(5816)<br>(5816)<br>(5816)<br>(5816)<br>(5816)<br>(5816)<br>(5816)<br>(5816)<br>(5816)<br>(5816)<br>(5816)<br>(5816)<br>(5816)<br>(5816)<br>(5816)<br>(5816)<br>(5816)<br>(5816)<br>(5816)<br>(5816)<br>(5816)<br>(5816)<br>(5816)<br>(5816)<br>(5816)<br>(5816)<br>(5816)<br>(5816)<br>(5816)<br>(5816)<br>(5816)<br>(5816)<br>(5816)<br>(5816)<br>(5816)<br>(5816)<br>(5816)<br>(5816)<br>(5816)<br>(5816)<br>(5816)<br>(5816)<br>(5816)<br>(5816)<br>(5816)<br>(5816)<br>(5816)<br>(5816)<br>(5816)<br>(5816)<br>(5816)<br>(5816)<br>(5816)<br>(5816)<br>(5816)<br>(5816)<br>(5816)<br>(5816)<br>(5816)<br>(5816)<br>(5816)<br>(5816)<br>(5816)<br>(5816)<br>(5816)<br>(5816)<br>(5816)<br>(5816)<br>(5816)<br>(5816)<br>(5816)<br>(5816)<br>(5816)<br>(5816)<br>(5816)<br>(5816)<br>(5816)<br>(5816)<br>(5816)<br>(5816)<br>(5816)<br>(5816)<br>(5816)<br>(5816)<br>(5816)<br>(5816)<br>(5816)<br>(5816)<br>(5816)<br>(5816)<br>(5816)<br>(5816)<br>(5816)<br>(5816)<br>(5816)<br>(5816)<br>(5816)<br>(5816)<br>(5816)<br>(5816)<br>(5816)<br>(5816)<br>(5816)<br>(5816)<br>(5816)<br>(5816)<br>(5816)<br>(5816)<br>(5816)<br>(5816)<br>(5816)<br>(5816)<br>(5816)<br>(5816)<br>(5816)<br>(5816)<br>(5816) | A658<br>A659<br>1065<br>A657<br>A673<br>A689<br>A689<br>A689<br>A689<br>A689<br>A689<br>A689<br>A689  | UT 33<br>UT 33<br>CT 64<br>AT 65<br>GT 72<br>GT 72<br>CT 77<br>CT 77<br>CT 77<br>CT 77  |
| 6789<br>7790<br>0795<br>6810<br>6810<br>6823<br>6823<br>6823<br>6823<br>6823<br>6823<br>6825<br>6845<br>6845<br>6845  | C859<br>C859<br>C874<br>C874<br>C892<br>C992<br>C914<br>A908<br>A908<br>A908<br>A908<br>C914<br>A913<br>C914<br>C931<br>C931<br>C933<br>C933<br>C933<br>C933<br>C933  | U934<br>U935<br>C9355<br>C937<br>C933<br>C933<br>C940<br>U941<br>A942<br>C9443<br>C9443   |
| A957<br>A958<br>C959<br>C956<br>C966<br>C963<br>G963<br>G963<br>G963<br>C963<br>C980<br>C980<br>A1005<br>A1005  | 41007<br>41027<br>61028<br>41028<br>41028<br>41036<br>71042<br>61053<br>71042<br>61053<br>71058<br>71055<br>71055<br>71055<br>71055<br>71055<br>71055<br>71055<br>71055<br>71055<br>71055<br>71055<br>71055<br>71055<br>71055<br>71055<br>71055<br>71055<br>71055<br>71055<br>71055<br>71055<br>71055<br>71055<br>71055<br>71055<br>71055<br>71055<br>71055<br>71055<br>71055<br>71055<br>71055<br>71055<br>71055<br>71055<br>71055<br>71055<br>71055<br>71055<br>71055<br>71055<br>71055<br>71055<br>71055<br>71055<br>71055<br>71055<br>71055<br>71055<br>71055<br>71055<br>71055<br>71055<br>71055<br>71055<br>71055<br>71055<br>71055<br>71055<br>71055<br>71055<br>71055<br>71055<br>71055<br>71055<br>71055<br>71055<br>71055<br>71055<br>71055<br>71055<br>71055<br>71055<br>71055<br>71055<br>71055<br>71055<br>71055<br>71055<br>71055<br>71055<br>71055<br>71055<br>71055<br>71055<br>71055<br>71055<br>71055<br>71055<br>71055<br>71055<br>71055<br>71055<br>71055<br>71055<br>71055<br>71055<br>71055<br>71055<br>71055<br>71055<br>71055<br>71055<br>71055<br>71055<br>71055<br>71055<br>71055<br>71055<br>71055<br>71055<br>71055<br>71055<br>71055<br>71055<br>71055<br>71055<br>71055<br>71055<br>71055<br>71055<br>71055<br>71055<br>71055<br>71055<br>71055<br>71055<br>71055<br>71055<br>71055<br>71055<br>71055<br>71055<br>71055<br>71055<br>71055<br>71055<br>71055<br>71055<br>71055<br>71055<br>71055<br>71055<br>71055<br>71055<br>71055<br>71055<br>71055<br>71055<br>71055<br>71055<br>71055<br>71055<br>71055<br>71055<br>71055<br>71055<br>71055<br>71055<br>71055<br>71055<br>71055<br>71055<br>71055<br>71055<br>71055<br>71055<br>71055<br>71055<br>71055<br>71055<br>71055<br>71055<br>71055<br>71055<br>71055<br>71055<br>71055<br>71055<br>71055<br>71055<br>71055<br>71055<br>71055<br>71055<br>71055<br>71055<br>71055<br>71055<br>71055<br>71055<br>71055<br>71055<br>71055<br>71055<br>71055<br>71055<br>71055<br>71055<br>71055<br>71055<br>71055<br>71055<br>71055<br>71055<br>71055<br>71055<br>71055<br>71055<br>71055<br>71055<br>71055<br>71055<br>71055<br>71055<br>71055<br>71055<br>71055<br>71055<br>71055<br>71055<br>71055<br>71055<br>71055<br>71055<br>71055<br>71055<br>71055<br>71055<br>71055<br>71055<br>71055<br>71055<br>71055<br>71055<br>71055<br>71055<br>71055<br>71055<br>71055<br>71055<br>71055<br>71055<br>71055<br>71055<br>71055<br>71055<br>71055<br>71055<br>71055<br>71055<br>71055<br>71055<br>71055<br>71055<br>71055<br>71055<br>71055<br>71055<br>71055<br>71055<br>71055<br>71055<br>71055<br>71055<br>71055<br>71055<br>71055<br>71055<br>71055<br>71055<br>71055<br>71055<br>71055<br>71055<br>71055<br>71055<br>71055<br>71055<br>71055<br>71055<br>71055<br>71055<br>71055<br>71055<br>71055<br>71055<br>71055<br>71055<br>71055<br>71055<br>71055<br>71055<br>71055<br>71055<br>71055<br>71055<br>71055<br>71055<br>71055<br>71055<br>71055<br>71055<br>71055<br>71055<br>71055<br>71055<br>71055<br>71055<br>71055<br>71055<br>71055<br>71055<br>71055<br>71055<br>71055<br>71055<br>71055<br>71055<br>710557<br>710557<br>710557<br>710557<br>710557<br>710557<br>710557<br>710557<br>710557<br>710   | U1079<br>1091<br>11091<br>11093<br>1093<br>1093<br>61101<br>61102<br>61102<br>11103<br>11103  |
| C1110<br>U1111<br>A1116<br>A1116<br>A11119<br>A1119<br>C1120<br>C1124<br>C1124<br>C1124<br>C1126<br>A1126<br>A1126<br>A1128<br>A1136<br>G1128<br>G1138<br>G1138   | 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| d1 259<br>A1 260<br>d1 264<br>A1 265<br>A1 265<br>d1 265<br>d1 266<br>d1 275<br>d1 275<br>d1 277<br>d1 293<br>d1 296<br>d1 306<br>d1 311  | A1312<br>A1312<br>A1315<br>A1315<br>A1323<br>A1323<br>A1323<br>A1325<br>A1325<br>A1325<br>A1325<br>C1344<br>C1342<br>C1344<br>C1342<br>C1344<br>C1342<br>C1342<br>C1342<br>C1342<br>C1362<br>C1362<br>C1362<br>C1362<br>C1362<br>C1362<br>C1362<br>C1362<br>C1362<br>C1362<br>C1362<br>C1362<br>C1362<br>C1362<br>C1362<br>C1362<br>C1362<br>C1362<br>C1362<br>C1362<br>C1362<br>C1362<br>C1362<br>C1362<br>C1362<br>C1362<br>C1362<br>C1362<br>C1362<br>C1362<br>C1362<br>C1362<br>C1362<br>C1362<br>C1362<br>C1362<br>C1362<br>C1362<br>C1362<br>C1362<br>C1362<br>C1362<br>C1362<br>C1362<br>C1362<br>C1362<br>C1362<br>C1362<br>C1362<br>C1362<br>C1362<br>C1362<br>C1362<br>C1362<br>C1362<br>C1362<br>C1362<br>C1362<br>C1362<br>C1362<br>C1362<br>C1362<br>C1362<br>C1362<br>C1362<br>C1362<br>C1362<br>C1362<br>C1362<br>C1362<br>C1362<br>C1362<br>C1362<br>C1362<br>C1362<br>C1362<br>C1362<br>C1362<br>C1362<br>C1362<br>C1362<br>C1362<br>C1362<br>C1362<br>C1362<br>C1362<br>C1362<br>C1362<br>C1362<br>C1362<br>C1362<br>C1362<br>C1362<br>C1362<br>C1362<br>C1362<br>C1362<br>C1362<br>C1362<br>C1362<br>C1362<br>C1362<br>C1362<br>C1362<br>C1362<br>C1362<br>C1362<br>C1362<br>C1362<br>C1362<br>C1362<br>C1362<br>C1362<br>C1362<br>C1362<br>C1362<br>C1362<br>C1362<br>C1362<br>C1362<br>C1362<br>C1362<br>C1362<br>C1362<br>C1362<br>C1362<br>C1362<br>C1362<br>C1362<br>C1362<br>C1362<br>C1362<br>C1362<br>C1362<br>C1362<br>C1362<br>C1362<br>C1362<br>C1362<br>C1362<br>C1362<br>C1362<br>C1362<br>C1362<br>C1362<br>C1362<br>C1362<br>C1362<br>C1362<br>C1362<br>C1362<br>C1362<br>C1362<br>C1362<br>C1362<br>C1362<br>C1362<br>C1362<br>C1362<br>C1362<br>C1362<br>C1362<br>C1362<br>C1362<br>C1362<br>C1362<br>C1362<br>C1362<br>C1362<br>C1362<br>C1362<br>C1362<br>C1362<br>C1362<br>C1362<br>C1362<br>C1362<br>C1362<br>C1362<br>C1362<br>C1362<br>C1362<br>C1362<br>C1362<br>C1362<br>C1362<br>C1362<br>C1362<br>C1362<br>C1362<br>C1362<br>C1362<br>C1362<br>C1362<br>C1362<br>C1362<br>C1362<br>C1362<br>C1362<br>C1362<br>C1362<br>C1362<br>C1362<br>C1362<br>C1362<br>C1362<br>C1362<br>C1362<br>C1362<br>C1362<br>C1362<br>C1362<br>C1362<br>C1362<br>C1362<br>C1362<br>C1362<br>C1362<br>C1362<br>C1362<br>C1362<br>C1362<br>C1362<br>C1362<br>C1362<br>C1362<br>C1362<br>C1362<br>C1362<br>C1362<br>C1362<br>C1362<br>C1362<br>C1362<br>C1362<br>C1362<br>C1362<br>C1362<br>C1362<br>C1362<br>C1362<br>C1362<br>C1362<br>C1362<br>C1362<br>C1362<br>C1362<br>C1362<br>C1362<br>C1362<br>C1362<br>C1362<br>C1362<br>C1362<br>C1362<br>C1362<br>C1362<br>C1362<br>C1362<br>C1362<br>C1362<br>C1362<br>C1362<br>C1362<br>C1362<br>C1362<br>C1362<br>C1362<br>C1362<br>C1362<br>C1362<br>C1362<br>C1362<br>C1362<br>C1362<br>C1362<br>C1362<br>C1362<br>C1362<br>C1362<br>C1362<br>C1362<br>C1362<br>C1362<br>C1362<br>C1362<br>C1362<br>C1362<br>C1362<br>C1362<br>C1362<br>C1362<br>C1362<br>C1362<br>C1362<br>C1362<br>C1362<br>C1362<br>C1362<br>C1362<br>C1362<br>C1362<br>C1362<br>C1362<br>C1362<br>C1362<br>C1362<br>C1362<br>C1362<br>C1362<br>C1362<br>C1362<br>C1362<br>C1362<br>C1362<br>C1362<br>C1362<br>C1362<br>C1362<br>C1362<br>C1362 | U1365<br>U1368<br>C1369<br>C1370<br>C1370<br>C1371<br>C1372<br>C1372<br>C1375<br>C1384  |
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C1389<br>A1404<br>A1404<br>C1415<br>C1415<br>C1415<br>G1416<br>G1418<br>G1424<br>G1424<br>G1424<br>G1424<br>G1424<br>G1425<br>G1424<br>G1425<br>G1425<br>G1425<br>G1425<br>G1425<br>G1425<br>G1426<br>G1426<br>G1426<br>G1426<br>G1426<br>G1426<br>G1426<br>G1426<br>G1426<br>G1426<br>G1426<br>G1426<br>G1426<br>G1426<br>G1426<br>G1426<br>G1426<br>G1426<br>G1426<br>G1426<br>G1426<br>G1426<br>G1426<br>G1426<br>G1426<br>G1426<br>G1426<br>G1426<br>G1426<br>G1426<br>G1426<br>G1426<br>G1426<br>G1426<br>G1426<br>G1426<br>G1426<br>G1426<br>G1426<br>G1426<br>G1426<br>G1426<br>G1426<br>G1426<br>G1426<br>G1426<br>G1426<br>G1426<br>G1426<br>G1426<br>G1426<br>G1426<br>G1426<br>G1426<br>G1426<br>G1426<br>G1426<br>G1426<br>G1426<br>G1426<br>G1426<br>G1426<br>G1426<br>G1426<br>G1426<br>G1426<br>G1426<br>G1426<br>G1426<br>G1426<br>G1426<br>G1426<br>G1426<br>G1426<br>G1426<br>G1426<br>G1426<br>G1426<br>G1426<br>G1426<br>G1426<br>G1426<br>G1426<br>G1426<br>G1426<br>G1426<br>G1426<br>G1426<br>G1426<br>G1426<br>G1426<br>G1426<br>G1426<br>G1426<br>G1426<br>G1426<br>G1426<br>G1426<br>G1426<br>G1426<br>G1426<br>G1426<br>G1426<br>G1426<br>G1426<br>G1426<br>G1426<br>G1426<br>G1426<br>G1426<br>G1426<br>G1426<br>G1426<br>G1426<br>G1426<br>G1426<br>G1426<br>G1426<br>G1426<br>G1426<br>G1426<br>G1426<br>G1426<br>G1426<br>G1426<br>G1426<br>G1426<br>G1426<br>G1426<br>G1426<br>G1426<br>G1426<br>G1426<br>G1426<br>G1426<br>G1426<br>G1426<br>G1426<br>G1426<br>G1426<br>G1426<br>G1426<br>G1426<br>G1426<br>G1426<br>G1426<br>G1426<br>G1426<br>G1426<br>G1426<br>G1426<br>G1426<br>G1426<br>G1426<br>G1426<br>G1426<br>G1426<br>G1426<br>G1426<br>G1426<br>G1426<br>G1426<br>G1426<br>G1426<br>G1426<br>G1426<br>G1426<br>G1426<br>G1426<br>G1426<br>G1426<br>G1426<br>G1426<br>G1426<br>G1426<br>G1426<br>G1426<br>G1426<br>G1426<br>G1426<br>G1426<br>G1426<br>G1426<br>G1426<br>G1426<br>G1426<br>G1426<br>G1426<br>G1426<br>G1426<br>G1426<br>G1426<br>G1426<br>G1426<br>G1426<br>G1426<br>G1426<br>G1426<br>G1426<br>G1426<br>G1426<br>G1426<br>G1426<br>G1426<br>G1426<br>G1426<br>G1426<br>G1426<br>G1426<br>G1426<br>G146<br>G146<br>G146<br>G146<br>G146<br>G146<br>G146<br>G14 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| A1499<br>U1500<br>U1500<br>G1502<br>G1502<br>C1508<br>C1508<br>C1514<br>A1516<br>A1516  |
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|   | A12<br>A12<br>A12<br>A12<br>A12<br>A12<br>A12<br>A12<br>A12<br>A12  |   |
| U1972<br>U1973<br>U1984<br>U1984<br>C1991<br>C1992<br>C1995<br>C1996<br>C1996<br>C1996<br>C1996<br>C1996<br>C1996<br>C1996<br>C2001<br>C2002<br>C2002<br>C2002<br>C2002<br>C2002  | 22025<br>42026<br>22050<br>22050<br>42055<br>42055<br>22054<br>42055<br>72054<br>42055<br>72054<br>42056<br>72054<br>72054<br>72054<br>72054<br>72054<br>72054<br>72054<br>72054<br>72054<br>72054<br>72055<br>72055<br>72055<br>72055<br>72055<br>72055<br>72055<br>72055<br>72055<br>72055<br>72055<br>72055<br>72055<br>72055<br>72055<br>72055<br>72055<br>72055<br>72055<br>72055<br>72055<br>72055<br>72055<br>72055<br>72055<br>72055<br>72055<br>72055<br>72055<br>72055<br>72055<br>72055<br>72055<br>72055<br>72055<br>72055<br>72055<br>72055<br>72055<br>72055<br>72055<br>72055<br>72055<br>72055<br>72055<br>72055<br>72055<br>72055<br>72055<br>72055<br>72055<br>72055<br>72055<br>72055<br>72055<br>72055<br>72055<br>72055<br>72055<br>72055<br>72055<br>72055<br>72055<br>72055<br>72055<br>72055<br>72055<br>72055<br>72055<br>72055<br>72055<br>72055<br>72055<br>72055<br>72055<br>72055<br>72055<br>72055<br>72055<br>72055<br>72055<br>72055<br>72055<br>72055<br>72055<br>72055<br>72055<br>72055<br>72055<br>72055<br>72055<br>72055<br>72055<br>72055<br>72055<br>72055<br>72055<br>72055<br>72055<br>72055<br>72055<br>72055<br>72055<br>72055<br>72055<br>72055<br>72055<br>72055<br>72055<br>72055<br>72055<br>72055<br>72055<br>72055<br>72055<br>72055<br>72055<br>72055<br>72055<br>72055<br>72055<br>72055<br>72055<br>72055<br>72055<br>72055<br>72055<br>72055<br>72055<br>72055<br>72055<br>72055<br>72055<br>72055<br>72055<br>72055<br>72055<br>72055<br>72055<br>72055<br>72055<br>72055<br>72055<br>72055<br>72055<br>72055<br>72055<br>72055<br>72055<br>72055<br>72055<br>72055<br>72055<br>72055<br>72055<br>72055<br>72055<br>72055<br>72055<br>72055<br>72055<br>72055<br>72055<br>72055<br>72055<br>72055<br>72055<br>72055<br>72055<br>72055<br>72055<br>72055<br>72055<br>72055<br>72055<br>72055<br>72055<br>72055<br>72055<br>72055<br>72055<br>72055<br>72055<br>72055<br>72055<br>72055<br>72055<br>72055<br>72055<br>72055<br>72055<br>72055<br>72055<br>72055<br>72055<br>72055<br>72055<br>72055<br>72055<br>72055<br>72055<br>72055<br>72055<br>72055<br>72055<br>72055<br>72055<br>72055<br>72055<br>72055<br>72055<br>72055<br>72055<br>72055<br>72055<br>72055<br>72055<br>72055<br>72055<br>72055<br>72055<br>72055<br>72055<br>72055<br>72055<br>72055<br>72055<br>72055<br>72055<br>72055<br>72055<br>72055<br>72055<br>72055<br>72055<br>72055<br>72055<br>72055<br>72055<br>72055<br>72055<br>72055<br>72055<br>72055<br>72055<br>72055<br>72055<br>72055<br>72055<br>72055<br>72055<br>72055<br>72055<br>72055<br>72055<br>72055<br>72055<br>72055<br>72055<br>72055<br>72055<br>72055<br>72055<br>72055<br>72055<br>72055<br>72055<br>72055<br>72055<br>72055<br>72055<br>72055<br>72055<br>72055<br>72055<br>72055<br>72055<br>72055<br>72055<br>72055<br>72055<br>72055<br>72055<br>72055<br>72055<br>72055<br>72055<br>72055<br>72055<br>72055<br>72055<br>72055<br>72055<br>72055<br>72055<br>72055<br>72055<br>72055<br>72055<br>72055<br>72055<br>72055<br>72055<br>72055<br>72055<br>72055<br>72055<br>72055<br>72055<br>72055<br>72055<br>72055<br>72055<br>72055<br>72055<br>72055<br>72055<br>72055<br>72055 | A2089<br>G2090<br>G2098<br>C2114<br>U2121<br>G2122<br>A2123<br>A2125<br>U2125   |











• Molecule 37: 30S ribosomal protein S5



• Molecule 43: 30S ribosomal protein S11



| Chain k:   | 90%   | 10%   |
|--|---|-------|
| MET<br>ALA<br>ALA<br>ALA<br>ALC<br>ACC<br>CYS<br>SER<br>ASN<br>THR<br>ASN<br>ACC | ARG<br>V14<br>N13<br>V131   |       |
| • Molecule 44:   | 30S ribosomal protein S12   |       |
| Chain l:   | 99%   |       |
| MET<br>P2<br>K136<br>A137<br>LYS   |   |       |
| • Molecule 45:   | 30S ribosomal protein S13   |       |
| Chain m:   | 75%   | • 24% |
| MET<br>ALA<br>R3<br>C94<br>C94<br>C17<br>PRO<br>G1N<br>G1N<br>G1N                | SER<br>SER<br>LYS<br>ASN<br>ASN<br>ASN<br>ARG<br>CLY<br>PRO<br>PRO<br>ARG<br>ARG<br>ARG<br>ARG<br>ARG<br>CLYS<br>LYS<br>LYS |       |
| • Molecule 46:   | 30S ribosomal protein S14   |       |
| Chain n:   | 97%   |       |
| MET<br>A2<br>332<br>153<br>W61   |   |       |
| • Molecule 47:   | 30S ribosomal protein S15   |       |
| Chain o:   | 94%   |       |
| MET<br>ALA<br>1LE<br>1LE<br>14<br>142<br>AR8<br>AR6<br>AR6                       |   |       |
| • Molecule 48:   | 30S ribosomal protein S16   |       |
| Chain p:   | 98%   |       |
| MET<br>A2<br>A47<br>E48<br>G89<br>LVS  |   |       |
| • Molecule 49:   | 30S ribosomal protein S17   |       |
| Chain q:   | 97%   | •     |
| NET<br>S2<br>V85<br>ILE<br>ILE   |   |       |



| • Molecule 50: 30S ribosoma  | al protein S18   |   |  |
|--|--|---|--|
| Chain r:   | 80%  | • 19%   |  |
| MET<br>ALA<br>GLY<br>GLY<br>GLY<br>GLY<br>GLY<br>ARG<br>ALA<br>ARG<br>K14<br>X14<br>ARG<br>K14<br>CLY<br>GLY<br>GLY<br>GLY   |  |   |  |
| • Molecule 51: 30S ribosoma  | al protein S19   |   |  |
| Chain s:   | 83%  | • 16%   |  |
| MET<br>ALA<br>ALA<br>ARG<br>ARG<br>CYS<br>CYS<br>CYS<br>CYS<br>CYS<br>ALA<br>ALA<br>ASP<br>ASP<br>ASP<br>ASP<br>ASP<br>ASP<br>ASP<br>ASP<br>ASP<br>AS  | ARG  |   |  |
| • Molecule 52: 30S ribosoma  | al protein S20   |   |  |
| Chain t:   | 94%  |   | 6%   |
| MET<br>PRO<br>14<br>14<br>Les<br>Ala   |  |   |  |
| • Molecule 53: 50S ribosoma  | al protein L28   |   |  |
| Chain u:   | 94%  |   | 6%   |
| MET<br>ALA<br>83<br>860<br>ARG<br>VAL<br>VAL   |  |   |  |
| • Molecule 54: Endonuclease  | e MutS2  |   |  |
| Chain v:   | 69%  | • 30%   |  |
| M1<br>V5<br>A8<br>A8<br>A8<br>A8<br>A8<br>A8<br>A8<br>A8<br>A8<br>A19<br>A17<br>Q17<br>Q17<br>Q17<br>Q17<br>Q17<br>Q17<br>A8<br>A8<br>A8<br>A8<br>A8<br>A8<br>A8<br>A8<br>A8<br>A8<br>A8<br>A8<br>A8   | K28<br>E29<br>M30<br>L31<br>L32<br>L32<br>E33<br>L32<br>K35<br>K35<br>S39<br>140<br>T41                                  | 143<br>143<br>145<br>147<br>147<br>147<br>148<br>148<br>148<br>148<br>148<br>148<br>148<br>151  | R58<br>L59<br>R60<br>G61<br>G61<br>G61<br>P64<br>F65<br>G66<br>G67<br>G66<br>G67<br>C66<br>G67<br>C66<br>G67<br>G67<br>G67<br>G77<br>T71<br>R72<br>G77<br>G77  |
| RT7<br>A78<br>E79<br>E79<br>G81<br>986<br>887<br>E91<br>4100<br>M100<br>M110<br>E111   | 0113<br>V114<br>1115<br>1116<br>1116<br>1116<br>1116<br>1126<br>1122<br>1122   | 8130 4<br>1131 4<br>1132 4<br>1135 4<br>1135 4<br>1135 4<br>1137 8<br>1138 4<br>1140 4<br>1141 4<br>1142 4  | H143<br>C144<br>E145<br>V146<br>U147<br>L147<br>A150<br>A150<br>S151<br>E152<br>T153<br>R155<br>R155<br>R155<br>C156<br>C156<br>C156<br>C156<br>C156<br>C156<br>C156<br>C156<br>C156<br>C156<br>C156<br>C156<br>C156<br>C156<br>C156<br>C156<br>C156<br>C156<br>C156<br>C156<br>C156<br>C156<br>C156<br>C156<br>C156<br>C156<br>C156<br>C156<br>C156<br>C156<br>C156<br>C156<br>C156<br>C156<br>C156<br>C156<br>C156<br>C156<br>C156<br>C156<br>C156<br>C156<br>C156<br>C156<br>C156<br>C156<br>C156<br>C156<br>C156<br>C156<br>C156<br>C156<br>C156<br>C156<br>C156<br>C156<br>C156<br>C156<br>C156<br>C156<br>C156<br>C156<br>C156<br>C156<br>C156<br>C156<br>C156<br>C156<br>C156<br>C156<br>C156<br>C156<br>C156<br>C156<br>C156<br>C156<br>C156<br>C156<br>C156<br>C156<br>C156<br>C156<br>C156<br>C156<br>C156<br>C156<br>C156<br>C156<br>C156<br>C156<br>C156<br>C156<br>C156<br>C156<br>C156<br>C156<br>C156<br>C156<br>C156<br>C156<br>C156<br>C156<br>C156<br>C156<br>C156<br>C156<br>C156<br>C156<br>C156<br>C156<br>C156<br>C156<br>C156<br>C156<br>C156<br>C156<br>C156<br>C156<br>C156<br>C156<br>C156<br>C156<br>C156<br>C156<br>C156<br>C156<br>C156<br>C156<br>C156<br>C156<br>C156<br>C156<br>C156<br>C156<br>C156<br>C156<br>C156<br>C156<br>C156<br>C156<br>C156<br>C156<br>C156<br>C156<br>C156<br>C156<br>C156<br>C156<br>C156<br>C156<br>C156<br>C156<br>C156<br>C156<br>C156<br>C156<br>C156<br>C156<br>C156<br>C156<br>C156<br>C156<br>C156<br>C156<br>C156<br>C156<br>C156<br>C156<br>C156<br>C156<br>C156<br>C156<br>C156<br>C156<br>C156<br>C156<br>C156<br>C156<br>C156<br>C156<br>C156<br>C156<br>C156<br>C156<br>C156<br>C156<br>C156<br>C156<br>C156<br>C156<br>C156<br>C156<br>C156<br>C156<br>C156<br>C156<br>C156<br>C156<br>C156<br>C156<br>C156<br>C156<br>C156<br>C156<br>C156<br>C156<br>C156<br>C156<br>C156<br>C156<br>C156<br>C156<br>C156<br>C156<br>C156<br>C156<br>C156<br>C156<br>C156<br>C156<br>C156<br>C156<br>C156<br>C156<br>C156<br>C156<br>C156<br>C156<br>C156<br>C156 |
| L161<br>R162<br>L164<br>E165<br>E165<br>S166<br>R165<br>R169<br>R169<br>E173<br>S174<br>M175<br>M175<br>S174<br>M175<br>S174<br>S174<br>M175<br>S174<br>S174<br>S176<br>S178<br>S176<br>S166<br>S166<br>S166<br>S166<br>S166<br>S166<br>S166<br>S166<br>S166<br>S166<br>S166<br>S166<br>S166<br>S166<br>S166<br>S166<br>S166<br>S166<br>S166<br>S166<br>S166<br>S166<br>S166<br>S166<br>S166<br>S166<br>S166<br>S166<br>S166<br>S166<br>S166<br>S166<br>S166<br>S166<br>S166<br>S166<br>S166<br>S166<br>S166<br>S166<br>S166<br>S166<br>S166<br>S166<br>S166<br>S166<br>S166<br>S166<br>S166<br>S166<br>S166<br>S166<br>S166<br>S176<br>S176<br>S176<br>S176<br>S176<br>S176<br>S176<br>S176<br>S176<br>S176<br>S176<br>S176<br>S176<br>S176<br>S176<br>S176<br>S176<br>S176<br>S176<br>S176<br>S176<br>S176<br>S176<br>S176<br>S176<br>S176<br>S176<br>S176<br>S176<br>S176<br>S176<br>S176<br>S176<br>S176<br>S176<br>S176<br>S176<br>S176<br>S176<br>S176<br>S176<br>S176<br>S176<br>S176<br>S176<br>S176<br>S176<br>S176<br>S176<br>S176<br>S177<br>S177<br>S177<br>S177<br>S177<br>S177<br>S177<br>S177<br>S177<br>S177<br>S177<br>S177<br>S177<br>S177<br>S177<br>S176<br>S176<br>S176<br>S176<br>S176<br>S176<br>S176<br>S176<br>S176<br>S176<br>S176<br>S176<br>S176<br>S176<br>S176<br>S176<br>S176<br>S176<br>S176<br>S176<br>S176<br>S176<br>S176<br>S176<br>S176<br>S176<br>S176<br>S176<br>S176<br>S176<br>S176<br>S176<br>S176<br>S176<br>S176<br>S176<br>S176<br>S176<br>S176<br>S176<br>S176<br>S176<br>S176<br>S176<br>S176<br>S176<br>S176<br>S176<br>S176<br>S176<br>S176<br>S176<br>S176<br>S176<br>S176<br>S176<br>S176<br>S176<br>S176<br>S176<br>S176<br>S176<br>S176<br>S176<br>S176<br>S176<br>S176<br>S176<br>S176<br>S176<br>S176<br>S176<br>S176 | ALA<br>ALA<br>SERA<br>SERA<br>LIYS<br>MET<br>LIVS<br>LUSU<br>LEU<br>LEU<br>THR<br>THR<br>THR<br>THR<br>THR<br>ASN<br>ASN | ARG<br>PHE<br>VAL<br>TILE<br>PRO<br>VAL<br>VAL<br>TYR<br>GLN<br>SER<br>SER<br>SER<br>SER<br>SER<br>SER<br>SER<br>SER<br>SER<br>SER  | 111<br>111E<br>VAL<br>HTS<br>ASP<br>SER<br>SER<br>SER<br>ALA<br>ALA<br>THR   |
| LEU<br>PHE<br>ILLE<br>GLU<br>GLU<br>PRO<br>GLA<br>CLA<br>CLA<br>CLA<br>CLA<br>CLA<br>CLA<br>CLA<br>CLA<br>CLA<br>C   | R241<br>Y242<br>Y242<br>E244<br>Y245<br>R245<br>R245<br>E249<br>R250<br>R250<br>R250                                     | A280<br>E261<br>E261<br>Q271<br>V272<br>T275<br>L276<br>A288  | V289<br>K290<br>N297<br>N297<br>1298<br>F301<br>F300<br>F300<br>F300<br>F300<br>F300<br>K306<br>F301<br>F308<br>F314<br>F314<br>F314   |
| A319<br>A319<br>B321<br>B321<br>E322<br>C3225<br>C3225<br>C3225<br>C3225<br>C3225<br>C3225<br>C3225<br>C3225<br>C3225<br>C3225<br>C3225<br>C3225<br>C3225<br>C3225<br>C3225<br>C3225<br>C3225<br>C3225<br>C3225<br>C3225<br>C3225<br>C3225<br>C3225<br>C3225<br>C3225<br>C3225<br>C3225<br>C3225<br>C3225<br>C3225<br>C3225<br>C3225<br>C3225<br>C3225<br>C3225<br>C3225<br>C3225<br>C3225<br>C3225<br>C3225<br>C3225<br>C3225<br>C3225<br>C3225<br>C3225<br>C3225<br>C3225<br>C3225<br>C3225<br>C3225<br>C3225<br>C3225<br>C3225<br>C3225<br>C3225<br>C3225<br>C3225<br>C3225<br>C3225<br>C325<br>C3  | L348<br>C349<br>L351<br>L351<br>L353<br>L353<br>L353<br>C366<br>C366<br>C366<br>C366<br>C366<br>C366<br>C366<br>C        | nar (<br>1379<br>1379<br>1385<br>1385<br>8384<br>9383<br>8384<br>9387<br>8384<br>9387<br>8384<br>9387<br>8384<br>9387<br>8384<br>8388<br>8384<br>9387<br>8384<br>8387<br>8389<br>8387<br>8389<br>8387<br>8389<br>8389<br>8389 | 1399       V400         V400       G401         I402       F404         E403       F403         F413       F414         F414       F413         F413       F414         F414       F414         F414       F413         F414       F414         F414       F414  |

W O R L D W I D E PROTEIN DATA BANK





# 4 Experimental information (i)

| Property                           | Value                         | Source    |
|------------------------------------|-------------------------------|-----------|
| EM reconstruction method           | SINGLE PARTICLE               | Depositor |
| Imposed symmetry                   | POINT, Not provided           |           |
| Number of particles used           | 5078                          | Depositor |
| Resolution determination method    | FSC 0.143 CUT-OFF             | Depositor |
| CTF correction method              | PHASE FLIPPING AND AMPLITUDE  | Depositor |
|                                    | CORRECTION                    |           |
| Microscope                         | FEI TITAN KRIOS               | Depositor |
| Voltage (kV)                       | 300                           | Depositor |
| Electron dose $(e^-/\text{\AA}^2)$ | 46.5                          | Depositor |
| Minimum defocus (nm)               | 750                           | Depositor |
| Maximum defocus (nm)               | 2000                          | Depositor |
| Magnification                      | Not provided                  |           |
| Image detector                     | GATAN K3 BIOQUANTUM (6k x 4k) | Depositor |
| Maximum map value                  | 0.341                         | Depositor |
| Minimum map value                  | -0.207                        | Depositor |
| Average map value                  | 0.001                         | Depositor |
| Map value standard deviation       | 0.009                         | Depositor |
| Recommended contour level          | 0.0172                        | Depositor |
| Map size (Å)                       | 590.64, 590.64, 590.64        | wwPDB     |
| Map dimensions                     | 368, 368, 368                 | wwPDB     |
| Map angles (°)                     | 90.0, 90.0, 90.0              | wwPDB     |
| Pixel spacing (Å)                  | 1.605, 1.605, 1.605           | Depositor |



# 5 Model quality (i)

## 5.1 Standard geometry (i)

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

| Mol Chain |       | Bond lengths |              | Bond angles |                     |  |
|-----------|-------|--------------|--------------|-------------|---------------------|--|
|           | Unain | RMSZ         | # Z  > 5     | RMSZ        | # Z  > 5            |  |
| 1         | 0     | 0.25         | 0/433        | 0.41        | 0/574               |  |
| 2         | 1     | 0.25         | 0/406        | 0.44        | 0/540               |  |
| 3         | 2     | 0.26         | 0/370        | 0.42        | 0/483               |  |
| 4         | 3     | 0.24         | 0/519        | 0.41        | 0/680               |  |
| 5         | 4     | 0.25         | 0/299        | 0.40        | 0/393               |  |
| 6         | 6     | 0.26         | 0/509        | 0.40        | 0/678               |  |
| 7         | А     | 0.72         | 2/627~(0.3%) | 1.17        | 8/975~(0.8%)        |  |
| 8         | В     | 0.18         | 0/2675       | 0.73        | 0/4170              |  |
| 9         | С     | 0.25         | 0/2120       | 0.43        | 0/2845              |  |
| 10        | D     | 0.25         | 0/1591       | 0.45        | 0/2132              |  |
| 11        | Ε     | 0.24         | 0/1580       | 0.41        | 0/2132              |  |
| 12        | F     | 0.39         | 0/1405       | 0.66        | 0/1887              |  |
| 13        | G     | 0.24         | 0/1360       | 0.42        | 0/1832              |  |
| 14        | Н     | 0.16         | 0/1834       | 0.72        | 0/2858              |  |
| 16        | J     | 0.24         | 0/1146       | 0.41        | 0/1542              |  |
| 17        | Κ     | 0.26         | 0/927        | 0.45        | 0/1245              |  |
| 18        | L     | 0.26         | 0/1093       | 0.44        | 0/1457              |  |
| 19        | М     | 0.25         | 0/1099       | 0.41        | 0/1468              |  |
| 20        | Ν     | 0.23         | 0/960        | 0.41        | 0/1284              |  |
| 21        | 0     | 0.30         | 0/921        | 0.55        | 2/1236~(0.2%)       |  |
| 22        | Р     | 0.25         | 0/957        | 0.43        | 0/1279              |  |
| 23        | Q     | 0.25         | 0/952        | 0.40        | 0/1266              |  |
| 24        | R     | 0.26         | 0/797        | 0.46        | 0/1070              |  |
| 25        | S     | 0.24         | 0/851        | 0.43        | 0/1146              |  |
| 26        | Т     | 0.24         | 0/731        | 0.41        | 0/974               |  |
| 27        | U     | 0.25         | 0/772        | 0.43        | 0/1032              |  |
| 28        | V     | 0.27         | 0/69444      | 0.81        | 91/108334~(0.1%)    |  |
| 29        | W     | 0.25         | 0/638        | 0.43        | 0/847               |  |
| 30        | Х     | 0.24         | 0/1162       | 0.41        | 0/1551              |  |
| 31        | Y     | 0.24         | 0/531        | 0.37        | 0/707               |  |
| 32        | Z     | 0.23         | 0/457        | 0.43        | 0/613               |  |
| 33        | a     | 0.20         | 0/36826      | 0.73        | $4/57450 \ (0.0\%)$ |  |
| 34        | b     | 0.26         | 0/480        | 0.42        | 0/628               |  |
| 35        | с     | 0.25         | 0/1641       | 0.43        | 0/2208              |  |



| Mol Chain |       | Bo   | ond lengths                    | Bond angles |                              |  |
|-----------|-------|------|--------------------------------|-------------|------------------------------|--|
|           | Unain | RMSZ | # Z  > 5                       | RMSZ        | # Z  > 5                     |  |
| 36        | d     | 0.25 | 0/1598                         | 0.40        | 0/2147                       |  |
| 37        | е     | 0.25 | 0/1230                         | 0.43        | 0/1655                       |  |
| 38        | f     | 0.24 | 0/766                          | 0.41        | 0/1031                       |  |
| 39        | g     | 0.23 | 0/1220                         | 0.38        | 0/1637                       |  |
| 40        | h     | 0.25 | 0/1048                         | 0.45        | 0/1407                       |  |
| 41        | i     | 0.23 | 0/794                          | 0.43        | 0/1074                       |  |
| 42        | j     | 0.23 | 0/773                          | 0.40        | 0/1044                       |  |
| 43        | k     | 0.25 | 0/885                          | 0.44        | 0/1196                       |  |
| 44        | 1     | 0.25 | 0/1069                         | 0.45        | 0/1435                       |  |
| 45        | m     | 0.23 | 0/744                          | 0.41        | 0/994                        |  |
| 46        | n     | 0.24 | 0/507                          | 0.40        | 0/672                        |  |
| 47        | 0     | 0.23 | 0/718                          | 0.42        | 0/960                        |  |
| 48        | р     | 0.25 | 0/708                          | 0.41        | 0/950                        |  |
| 49        | q     | 0.25 | 0/699                          | 0.42        | 0/933                        |  |
| 50        | r     | 0.24 | 0/526                          | 0.40        | 0/705                        |  |
| 51        | S     | 0.24 | 0/640                          | 0.43        | 0/861                        |  |
| 52        | t     | 0.23 | 0/639                          | 0.39        | 0/852                        |  |
| 53        | u     | 0.23 | 0/448                          | 0.46        | 0/596                        |  |
| 54        | V     | 0.52 | 0/4341                         | 0.77        | 6/5847~(0.1%)                |  |
| 54        | W     | 0.53 | 0/4703                         | 0.78        | 7/6337~(0.1%)                |  |
| All       | All   | 0.27 | $2/1\overline{62169}\ (0.0\%)$ | 0.72        | $\boxed{118/241849~(0.0\%)}$ |  |

Chiral center outliers are detected by calculating the chiral volume of a chiral center and verifying if the center is modelled as a planar moiety or with the opposite hand. A planarity outlier is detected by checking planarity of atoms in a peptide group, atoms in a mainchain group or atoms of a sidechain that are expected to be planar.

| Mol | Chain | #Chirality outliers | #Planarity outliers |
|-----|-------|---------------------|---------------------|
| 28  | V     | 0                   | 16                  |
| 54  | W     | 0                   | 2                   |
| All | All   | 0                   | 18                  |

All (2) bond length outliers are listed below:

| Mol | Chain | Res | Type | Atoms  | Z    | Observed(Å) | Ideal(Å) |
|-----|-------|-----|------|--------|------|-------------|----------|
| 7   | А     | 41  | С    | C1'-N1 | 5.26 | 1.56        | 1.48     |
| 7   | А     | 50  | С    | C1'-N1 | 5.02 | 1.56        | 1.48     |

All (118) bond angle outliers are listed below:

| Mol | Chain | Res | Type | Atoms     | Z      | $Observed(^{o})$ | $Ideal(^{o})$ |
|-----|-------|-----|------|-----------|--------|------------------|---------------|
| 28  | V     | 138 | U    | OP1-P-O3' | -39.33 | 18.68            | 105.20        |



| Mol | Chain | Res  | Type | Atoms       | Z      | $Observed(^{o})$ | $Ideal(^{o})$ |
|-----|-------|------|------|-------------|--------|------------------|---------------|
| 28  | V     | 139  | А    | OP1-P-OP2   | -12.74 | 100.50           | 119.60        |
| 28  | V     | 2340 | А    | N1-C6-N6    | -11.09 | 111.95           | 118.60        |
| 28  | V     | 2362 | A    | N1-C6-N6    | -11.09 | 111.95           | 118.60        |
| 28  | V     | 2364 | А    | N1-C6-N6    | -9.31  | 113.01           | 118.60        |
| 28  | V     | 2328 | G    | O4'-C1'-N9  | 9.20   | 115.56           | 108.20        |
| 7   | А     | 32   | U    | P-O3'-C3'   | -9.19  | 108.67           | 119.70        |
| 28  | V     | 2349 | А    | C1'-O4'-C4' | -8.73  | 102.92           | 109.90        |
| 28  | V     | 2351 | A    | N1-C6-N6    | -8.41  | 113.55           | 118.60        |
| 28  | V     | 2339 | A    | N1-C6-N6    | -8.41  | 113.56           | 118.60        |
| 54  | W     | 544  | ARG  | NE-CZ-NH1   | 8.30   | 124.45           | 120.30        |
| 28  | V     | 1449 | С    | P-O3'-C3'   | -8.30  | 109.74           | 119.70        |
| 7   | А     | 37   | G    | P-O3'-C3'   | -8.23  | 109.82           | 119.70        |
| 28  | V     | 1450 | С    | P-O3'-C3'   | -8.17  | 109.89           | 119.70        |
| 7   | А     | 38   | А    | P-O3'-C3'   | -8.14  | 109.93           | 119.70        |
| 28  | V     | 1447 | С    | P-O3'-C3'   | -7.96  | 110.15           | 119.70        |
| 54  | W     | 308  | ARG  | NE-CZ-NH1   | 7.89   | 124.25           | 120.30        |
| 28  | V     | 2327 | A    | N1-C6-N6    | -7.84  | 113.90           | 118.60        |
| 28  | V     | 2123 | A    | P-O3'-C3'   | -7.79  | 110.35           | 119.70        |
| 28  | V     | 2351 | А    | C5-C6-N1    | 7.79   | 121.59           | 117.70        |
| 28  | V     | 2346 | С    | N3-C2-O2    | -7.74  | 116.48           | 121.90        |
| 28  | V     | 2349 | А    | N1-C6-N6    | -7.70  | 113.98           | 118.60        |
| 28  | V     | 2329 | А    | C5-C6-N1    | 7.69   | 121.54           | 117.70        |
| 28  | V     | 2323 | С    | N3-C2-O2    | -7.62  | 116.57           | 121.90        |
| 28  | V     | 2330 | А    | C5-C6-N1    | 7.51   | 121.46           | 117.70        |
| 28  | V     | 2340 | A    | C5-C6-N1    | 7.51   | 121.46           | 117.70        |
| 28  | V     | 2342 | С    | N3-C2-O2    | -7.51  | 116.64           | 121.90        |
| 28  | V     | 2330 | A    | C5'-C4'-O4' | 7.43   | 118.02           | 109.10        |
| 28  | V     | 2324 | С    | N3-C2-O2    | -7.39  | 116.73           | 121.90        |
| 28  | V     | 2362 | А    | C5-C6-N1    | 7.06   | 121.23           | 117.70        |
| 54  | V     | 326  | ARG  | NE-CZ-NH1   | 7.04   | 123.82           | 120.30        |
| 28  | V     | 2343 | A    | N1-C6-N6    | -6.98  | 114.41           | 118.60        |
| 28  | V     | 2349 | A    | C5-C6-N1    | 6.97   | 121.18           | 117.70        |
| 54  | V     | 308  | ARG  | NE-CZ-NH1   | 6.92   | 123.76           | 120.30        |
| 28  | V     | 2339 | А    | C5-C6-N1    | 6.90   | 121.15           | 117.70        |
| 28  | V     | 925  | A    | N1-C6-N6    | -6.89  | 114.46           | 118.60        |
| 28  | V     | 2323 | С    | N1-C2-O2    | 6.89   | 123.03           | 118.90        |
| 28  | V     | 2328 | G    | N9-C1'-C2'  | -6.78  | 104.55           | 112.00        |
| 28  | V     | 2350 | G    | N1-C6-O6    | -6.75  | 115.85           | 119.90        |
| 7   | А     | 35   | A    | P-O3'-C3'   | -6.74  | 111.62           | 119.70        |
| 28  | V     | 2327 | A    | C5-C6-N1    | 6.70   | 121.05           | 117.70        |
| 28  | V     | 2343 | A    | C5-C6-N1    | 6.66   | 121.03           | 117.70        |
| 28  | V     | 2335 | U    | O4'-C1'-N1  | 6.64   | 113.51           | 108.20        |



| Mol | Chain | Res  | Type | Atoms       | Z     | $Observed(^{o})$ | $Ideal(^{o})$ |
|-----|-------|------|------|-------------|-------|------------------|---------------|
| 28  | V     | 2349 | А    | C5'-C4'-O4' | 6.58  | 116.99           | 109.10        |
| 28  | V     | 2343 | А    | C4-C5-C6    | -6.51 | 113.74           | 117.00        |
| 54  | W     | 439  | ARG  | NE-CZ-NH1   | 6.51  | 123.56           | 120.30        |
| 28  | V     | 2333 | G    | N3-C2-N2    | -6.49 | 115.35           | 119.90        |
| 28  | V     | 2122 | G    | P-O3'-C3'   | -6.46 | 111.95           | 119.70        |
| 28  | V     | 2340 | А    | C4-C5-C6    | -6.43 | 113.78           | 117.00        |
| 28  | V     | 2334 | U    | N3-C2-O2    | -6.38 | 117.73           | 122.20        |
| 54  | W     | 58   | ARG  | NE-CZ-NH2   | 6.37  | 123.49           | 120.30        |
| 28  | V     | 924  | U    | O4'-C1'-N1  | 6.31  | 113.25           | 108.20        |
| 28  | V     | 2342 | С    | C5'-C4'-C3' | -6.27 | 105.97           | 116.00        |
| 54  | W     | 443  | ARG  | NE-CZ-NH1   | 6.26  | 123.43           | 120.30        |
| 28  | V     | 2324 | С    | N1-C2-O2    | 6.25  | 122.65           | 118.90        |
| 28  | V     | 2323 | С    | O4'-C1'-N1  | 6.23  | 113.18           | 108.20        |
| 33  | a     | 1149 | U    | C2-N1-C1'   | 6.18  | 125.11           | 117.70        |
| 28  | V     | 2341 | U    | O4'-C1'-N1  | 6.17  | 113.14           | 108.20        |
| 28  | V     | 2226 | U    | P-O3'-C3'   | -6.10 | 112.38           | 119.70        |
| 28  | V     | 925  | А    | C5-C6-N1    | 6.09  | 120.75           | 117.70        |
| 28  | V     | 509  | С    | N3-C2-O2    | -6.08 | 117.64           | 121.90        |
| 28  | V     | 1452 | С    | P-O3'-C3'   | -6.07 | 112.41           | 119.70        |
| 28  | V     | 2364 | А    | C5-C6-N1    | 6.07  | 120.74           | 117.70        |
| 21  | 0     | 17   | ARG  | NE-CZ-NH1   | 6.05  | 123.32           | 120.30        |
| 28  | V     | 2330 | А    | N1-C6-N6    | -6.03 | 114.98           | 118.60        |
| 7   | А     | 31   | А    | P-O3'-C3'   | -6.01 | 112.48           | 119.70        |
| 28  | V     | 2362 | А    | C4-C5-C6    | -6.01 | 114.00           | 117.00        |
| 54  | v     | 443  | ARG  | NE-CZ-NH1   | 5.98  | 123.29           | 120.30        |
| 21  | 0     | 14   | ARG  | NE-CZ-NH1   | 5.98  | 123.29           | 120.30        |
| 28  | V     | 420  | U    | P-O3'-C3'   | -5.98 | 112.53           | 119.70        |
| 28  | V     | 2331 | U    | C5'-C4'-C3' | -5.97 | 106.45           | 116.00        |
| 28  | V     | 2335 | U    | C3'-C2'-C1' | 5.95  | 106.26           | 101.50        |
| 28  | V     | 2342 | С    | C5'-C4'-O4' | 5.94  | 116.23           | 109.10        |
| 28  | V     | 2348 | С    | N3-C2-O2    | -5.89 | 117.77           | 121.90        |
| 28  | V     | 2351 | А    | C4-C5-C6    | -5.83 | 114.08           | 117.00        |
| 28  | V     | 2331 | U    | C5'-C4'-O4' | 5.80  | 116.06           | 109.10        |
| 28  | V     | 2167 | С    | N3-C2-O2    | -5.79 | 117.84           | 121.90        |
| 28  | V     | 2339 | А    | C4-C5-C6    | -5.78 | 114.11           | 117.00        |
| 28  | V     | 2336 | G    | C3'-C2'-C1' | 5.71  | 106.07           | 101.50        |
| 54  | V     | 303  | ARG  | NE-CZ-NH1   | 5.71  | 123.15           | 120.30        |
| 28  | V     | 2334 | U    | 04'-C1'-N1  | 5.71  | 112.77           | 108.20        |
| 28  | V     | 417  | G    | P-O3'-C3'   | -5.64 | 112.93           | 119.70        |
| 28  | V     | 138  | U    | OP2-P-O3'   | 5.62  | 117.58           | 105.20        |
| 28  | V     | 1693 | С    | C2-N1-C1'   | -5.57 | 112.67           | 118.80        |
| 28  | V     | 1693 | С    | C6-N1-C1'   | 5.55  | 127.46           | 120.80        |



| Mol | Chain | Res  | Type | Atoms       | Z     | $Observed(^{o})$ | $Ideal(^{o})$ |
|-----|-------|------|------|-------------|-------|------------------|---------------|
| 28  | V     | 1451 | U    | P-O3'-C3'   | -5.50 | 113.10           | 119.70        |
| 28  | V     | 2364 | A    | O4'-C1'-N9  | 5.50  | 112.60           | 108.20        |
| 28  | V     | 2346 | С    | N1-C2-O2    | 5.49  | 122.19           | 118.90        |
| 28  | V     | 2347 | G    | C5'-C4'-O4' | 5.47  | 115.67           | 109.10        |
| 33  | a     | 489  | U    | C2-N1-C1'   | 5.43  | 124.22           | 117.70        |
| 7   | А     | 30   | A    | P-O3'-C3'   | -5.40 | 113.22           | 119.70        |
| 28  | V     | 2349 | A    | N9-C1'-C2'  | 5.40  | 121.03           | 114.00        |
| 28  | V     | 419  | G    | P-O3'-C3'   | -5.40 | 113.22           | 119.70        |
| 54  | W     | 439  | ARG  | NE-CZ-NH2   | -5.38 | 117.61           | 120.30        |
| 28  | V     | 2037 | С    | N3-C2-O2    | -5.38 | 118.13           | 121.90        |
| 54  | v     | 308  | ARG  | NH1-CZ-NH2  | -5.37 | 113.49           | 119.40        |
| 28  | V     | 2333 | G    | C5'-C4'-C3' | -5.37 | 107.41           | 116.00        |
| 33  | a     | 1323 | С    | N1-C2-O2    | 5.37  | 122.12           | 118.90        |
| 28  | V     | 2329 | А    | C4-C5-C6    | -5.31 | 114.34           | 117.00        |
| 28  | V     | 2364 | А    | C4-C5-C6    | -5.28 | 114.36           | 117.00        |
| 28  | V     | 2329 | А    | N1-C6-N6    | -5.25 | 115.45           | 118.60        |
| 33  | a     | 763  | С    | C2-N1-C1'   | 5.23  | 124.56           | 118.80        |
| 28  | V     | 2342 | С    | N1-C2-O2    | 5.20  | 122.02           | 118.90        |
| 28  | V     | 2332 | G    | N1-C6-O6    | -5.19 | 116.78           | 119.90        |
| 54  | W     | 196  | ARG  | NE-CZ-NH2   | 5.19  | 122.89           | 120.30        |
| 7   | А     | 36   | U    | P-O3'-C3'   | -5.19 | 113.48           | 119.70        |
| 28  | V     | 2327 | A    | C4-C5-C6    | -5.17 | 114.42           | 117.00        |
| 28  | V     | 2336 | G    | N3-C4-C5    | -5.14 | 126.03           | 128.60        |
| 54  | V     | 497  | ARG  | NE-CZ-NH1   | 5.13  | 122.87           | 120.30        |
| 28  | V     | 2326 | С    | N3-C2-O2    | -5.09 | 118.34           | 121.90        |
| 28  | V     | 2346 | С    | N3-C4-N4    | -5.07 | 114.45           | 118.00        |
| 28  | V     | 2330 | A    | C4-C5-C6    | -5.07 | 114.46           | 117.00        |
| 28  | V     | 2352 | G    | N1-C6-O6    | -5.06 | 116.86           | 119.90        |
| 28  | V     | 2350 | G    | C5-C6-N1    | 5.06  | 114.03           | 111.50        |
| 28  | V     | 949  | U    | O4'-C1'-N1  | 5.06  | 112.25           | 108.20        |
| 28  | V     | 2350 | G    | C5'-C4'-C3' | -5.06 | 107.91           | 116.00        |
| 7   | А     | 39   | U    | OP2-P-O3'   | 5.01  | 116.22           | 105.20        |
| 28  | V     | 2347 | G    | C5'-C4'-C3' | -5.01 | 107.99           | 116.00        |

There are no chirality outliers.

All (18) planarity outliers are listed below:

| Mol | Chain | Res  | Type | Group     |
|-----|-------|------|------|-----------|
| 28  | V     | 2323 | С    | Sidechain |
| 28  | V     | 2326 | С    | Sidechain |
| 28  | V     | 2327 | А    | Sidechain |
| 28  | V     | 2329 | А    | Sidechain |



| Mol             | Chain | Res  | Type | Group     |
|-----------------|-------|------|------|-----------|
| 28              | V     | 2333 | G    | Sidechain |
| 28              | V     | 2334 | U    | Sidechain |
| 28              | V     | 2335 | U    | Sidechain |
| 28              | V     | 2337 | G    | Sidechain |
| 28              | V     | 2340 | А    | Sidechain |
| 28              | V     | 2342 | С    | Sidechain |
| 28              | V     | 2343 | А    | Sidechain |
| 28              | V     | 2344 | U    | Sidechain |
| 28              | V     | 2346 | С    | Sidechain |
| 28              | V     | 2362 | А    | Sidechain |
| 28              | V     | 2364 | А    | Sidechain |
| 28              | V     | 924  | U    | Sidechain |
| 54              | W     | 308  | ARG  | Sidechain |
| $\overline{54}$ | W     | 456  | TYR  | Sidechain |

## 5.2 Too-close contacts (i)

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

## 5.3 Torsion angles (i)

#### 5.3.1 Protein backbone (i)

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.

| Mol | Chain | Analysed      | Favoured  | Allowed | Outliers | Perce | entiles |
|-----|-------|---------------|-----------|---------|----------|-------|---------|
| 1   | 0     | 52/59~(88%)   | 50 (96%)  | 2(4%)   | 0        | 100   | 100     |
| 2   | 1     | 46/49~(94%)   | 44 (96%)  | 2(4%)   | 0        | 100   | 100     |
| 3   | 2     | 42/44~(96%)   | 42 (100%) | 0       | 0        | 100   | 100     |
| 4   | 3     | 62/66~(94%)   | 60 (97%)  | 2(3%)   | 0        | 100   | 100     |
| 5   | 4     | 35/37~(95%)   | 33 (94%)  | 2(6%)   | 0        | 100   | 100     |
| 6   | 6     | 61/66~(92%)   | 60~(98%)  | 1 (2%)  | 0        | 100   | 100     |
| 9   | С     | 270/277~(98%) | 260 (96%) | 10 (4%) | 0        | 100   | 100     |
| 10  | D     | 204/209~(98%) | 193 (95%) | 11 (5%) | 0        | 100   | 100     |



| Continued | from | previous | page |
|-----------|------|----------|------|

| Mol | Chain | Analysed      | Favoured  | Allowed  | Outliers | Perce | ntiles |
|-----|-------|---------------|-----------|----------|----------|-------|--------|
| 11  | Е     | 203/207~(98%) | 193~(95%) | 10~(5%)  | 0        | 100   | 100    |
| 12  | F     | 174/179~(97%) | 161 (92%) | 13 (8%)  | 0        | 100   | 100    |
| 13  | G     | 173/179~(97%) | 165~(95%) | 8 (5%)   | 0        | 100   | 100    |
| 16  | J     | 140/145~(97%) | 133 (95%) | 7 (5%)   | 0        | 100   | 100    |
| 17  | K     | 120/122~(98%) | 117 (98%) | 3 (2%)   | 0        | 100   | 100    |
| 18  | L     | 144/146~(99%) | 139 (96%) | 5 (4%)   | 0        | 100   | 100    |
| 19  | М     | 133/144 (92%) | 132 (99%) | 1 (1%)   | 0        | 100   | 100    |
| 20  | N     | 117/120~(98%) | 113 (97%) | 4 (3%)   | 0        | 100   | 100    |
| 21  | Ο     | 118/120 (98%) | 113 (96%) | 5 (4%)   | 0        | 100   | 100    |
| 22  | Р     | 113/115 (98%) | 108 (96%) | 5 (4%)   | 0        | 100   | 100    |
| 23  | Q     | 115/119~(97%) | 107 (93%) | 6 (5%)   | 2(2%)    | 9     | 43     |
| 24  | R     | 99/102~(97%)  | 88 (89%)  | 11 (11%) | 0        | 100   | 100    |
| 25  | S     | 107/113~(95%) | 102 (95%) | 5 (5%)   | 0        | 100   | 100    |
| 26  | Т     | 88/95~(93%)   | 87 (99%)  | 1 (1%)   | 0        | 100   | 100    |
| 27  | U     | 99/103~(96%)  | 92 (93%)  | 7 (7%)   | 0        | 100   | 100    |
| 29  | W     | 80/94~(85%)   | 76 (95%)  | 4 (5%)   | 0        | 100   | 100    |
| 30  | Х     | 147/149~(99%) | 135 (92%) | 12 (8%)  | 0        | 100   | 100    |
| 31  | Y     | 63/66~(96%)   | 62 (98%)  | 1 (2%)   | 0        | 100   | 100    |
| 32  | Z     | 56/59~(95%)   | 53 (95%)  | 3 (5%)   | 0        | 100   | 100    |
| 34  | b     | 55/57~(96%)   | 53 (96%)  | 2 (4%)   | 0        | 100   | 100    |
| 35  | с     | 204/218~(94%) | 194 (95%) | 10 (5%)  | 0        | 100   | 100    |
| 36  | d     | 193/200~(96%) | 176 (91%) | 17 (9%)  | 0        | 100   | 100    |
| 37  | е     | 162/166~(98%) | 155 (96%) | 7 (4%)   | 0        | 100   | 100    |
| 38  | f     | 90/95~(95%)   | 87 (97%)  | 3 (3%)   | 0        | 100   | 100    |
| 39  | g     | 149/156~(96%) | 144 (97%) | 5 (3%)   | 0        | 100   | 100    |
| 40  | h     | 129/132~(98%) | 116 (90%) | 13 (10%) | 0        | 100   | 100    |
| 41  | i     | 101/130~(78%) | 95 (94%)  | 6 (6%)   | 0        | 100   | 100    |
| 42  | j     | 93/102~(91%)  | 87 (94%)  | 6 (6%)   | 0        | 100   | 100    |
| 43  | k     | 116/131~(88%) | 110 (95%) | 6 (5%)   | 0        | 100   | 100    |
| 44  | 1     | 134/138~(97%) | 124 (92%) | 10 (8%)  | 0        | 100   | 100    |
| 45  | m     | 90/121~(74%)  | 85 (94%)  | 5 (6%)   | 0        | 100   | 100    |



| Mol | Chain | Analysed        | Favoured   | Allowed  | Outliers | Perce | $\mathbf{entiles}$ |
|-----|-------|-----------------|------------|----------|----------|-------|--------------------|
| 46  | n     | 58/61~(95%)     | 52 (90%)   | 5 (9%)   | 1 (2%)   | 9     | 43                 |
| 47  | О     | 83/89~(93%)     | 79~(95%)   | 4 (5%)   | 0        | 100   | 100                |
| 48  | р     | 86/90~(96%)     | 81 (94%)   | 5 (6%)   | 0        | 100   | 100                |
| 49  | q     | 82/87~(94%)     | 76~(93%)   | 6 (7%)   | 0        | 100   | 100                |
| 50  | r     | 62/79~(78%)     | 56~(90%)   | 5 (8%)   | 1 (2%)   | 9     | 44                 |
| 51  | S     | 75/92~(82%)     | 69~(92%)   | 6 (8%)   | 0        | 100   | 100                |
| 52  | t     | 81/88~(92%)     | 79~(98%)   | 2 (2%)   | 0        | 100   | 100                |
| 53  | u     | 56/62~(90%)     | 54 (96%)   | 2 (4%)   | 0        | 100   | 100                |
| 54  | v     | 544/785~(69%)   | 527~(97%)  | 15 (3%)  | 2~(0%)   | 34    | 72                 |
| 54  | W     | 589/785~(75%)   | 569(97%)   | 16 (3%)  | 4 (1%)   | 22    | 62                 |
| All | All   | 6293/7048~(89%) | 5986 (95%) | 297 (5%) | 10 (0%)  | 50    | 81                 |

All (10) Ramachandran outliers are listed below:

| Mol | Chain | $\mathbf{Res}$ | Type |
|-----|-------|----------------|------|
| 54  | V     | 384            | SER  |
| 54  | W     | 384            | SER  |
| 23  | Q     | 103            | LEU  |
| 50  | r     | 28             | TYR  |
| 54  | W     | 382            | GLU  |
| 54  | W     | 114            | VAL  |
| 54  | W     | 337            | ASN  |
| 46  | n     | 32             | SER  |
| 54  | V     | 114            | VAL  |
| 23  | Q     | 93             | LYS  |

#### 5.3.2 Protein sidechains (i)

In the following table, the Percentiles column shows the percent side chain 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.

| Mol | Chain | Analysed    | Rotameric | Outliers | Perce | ntiles |
|-----|-------|-------------|-----------|----------|-------|--------|
| 1   | 0     | 48/53~(91%) | 48 (100%) | 0        | 100   | 100    |
| 2   | 1     | 46/47~(98%) | 46 (100%) | 0        | 100   | 100    |



| Mol | Chain | Analysed       | Rotameric  | Outliers | Perce | ntiles |
|-----|-------|----------------|------------|----------|-------|--------|
| 3   | 2     | 39/39~(100%)   | 39~(100%)  | 0        | 100   | 100    |
| 4   | 3     | 54/56~(96%)    | 54 (100%)  | 0        | 100   | 100    |
| 5   | 4     | 35/35~(100%)   | 35~(100%)  | 0        | 100   | 100    |
| 6   | 6     | 53/55~(96%)    | 53~(100%)  | 0        | 100   | 100    |
| 9   | С     | 220/225~(98%)  | 219 (100%) | 1 (0%)   | 88    | 93     |
| 10  | D     | 167/170~(98%)  | 166 (99%)  | 1 (1%)   | 86    | 91     |
| 11  | Е     | 169/170~(99%)  | 169 (100%) | 0        | 100   | 100    |
| 12  | F     | 151/154~(98%)  | 149 (99%)  | 2 (1%)   | 69    | 82     |
| 13  | G     | 148/151 (98%)  | 148 (100%) | 0        | 100   | 100    |
| 16  | J     | 120/123~(98%)  | 120 (100%) | 0        | 100   | 100    |
| 17  | Κ     | 101/101 (100%) | 101 (100%) | 0        | 100   | 100    |
| 18  | L     | 110/110 (100%) | 110 (100%) | 0        | 100   | 100    |
| 19  | М     | 109/116~(94%)  | 109 (100%) | 0        | 100   | 100    |
| 20  | Ν     | 99/100~(99%)   | 99 (100%)  | 0        | 100   | 100    |
| 21  | О     | 93/93~(100%)   | 93 (100%)  | 0        | 100   | 100    |
| 22  | Р     | 100/100~(100%) | 100 (100%) | 0        | 100   | 100    |
| 23  | Q     | 96/98~(98%)    | 96 (100%)  | 0        | 100   | 100    |
| 24  | R     | 83/84~(99%)    | 83 (100%)  | 0        | 100   | 100    |
| 25  | S     | 90/93~(97%)    | 90 (100%)  | 0        | 100   | 100    |
| 26  | Т     | 81/85~(95%)    | 81 (100%)  | 0        | 100   | 100    |
| 27  | U     | 85/87~(98%)    | 85 (100%)  | 0        | 100   | 100    |
| 29  | W     | 64/74~(86%)    | 64 (100%)  | 0        | 100   | 100    |
| 30  | Х     | 124/124~(100%) | 119 (96%)  | 5 (4%)   | 31    | 56     |
| 31  | Y     | 56/57~(98%)    | 56 (100%)  | 0        | 100   | 100    |
| 32  | Ζ     | 52/53~(98%)    | 52 (100%)  | 0        | 100   | 100    |
| 34  | b     | 51/51~(100%)   | 51 (100%)  | 0        | 100   | 100    |
| 35  | с     | 168/178~(94%)  | 168 (100%) | 0        | 100   | 100    |
| 36  | d     | 169/173~(98%)  | 167 (99%)  | 2 (1%)   | 71    | 84     |
| 37  | е     | 128/130~(98%)  | 128 (100%) | 0        | 100   | 100    |
| 38  | f     | 81/84 (96%)    | 81 (100%)  | 0        | 100   | 100    |
| 39  | g     | 127/132~(96%)  | 127 (100%) | 0        | 100   | 100    |



| Mol | Chain | Analysed                      | Rotameric                | Outliers | Perc | centile | es |
|-----|-------|-------------------------------|--------------------------|----------|------|---------|----|
| 40  | h     | 111/112~(99%)                 | 111 (100%)               | 0        | 100  | 100     | )  |
| 41  | i     | 81/102~(79%)                  | 81 (100%)                | 0        | 100  | 100     | )  |
| 42  | j     | 86/92~(94%)                   | 86 (100%)                | 0        | 100  | 100     | )  |
| 43  | k     | 90/100~(90%)                  | 90 (100%)                | 0        | 100  | 100     | )  |
| 44  | 1     | 114/116~(98%)                 | 114 (100%)               | 0        | 100  | 100     | )  |
| 45  | m     | 80/104~(77%)                  | 79~(99%)                 | 1 (1%)   | 69   | 82      |    |
| 46  | n     | 53/54~(98%)                   | 53~(100%)                | 0        | 100  | 100     | )  |
| 47  | О     | 80/83~(96%)                   | 79~(99%)                 | 1 (1%)   | 69   | 82      |    |
| 48  | р     | 74/76~(97%)                   | 74 (100%)                | 0        | 100  | 100     | )  |
| 49  | q     | 77/80~(96%)                   | 77~(100%)                | 0        | 100  | 100     | )  |
| 50  | r     | 56/64~(88%)                   | 56~(100%)                | 0        | 100  | 100     | )  |
| 51  | S     | 69/81~(85%)                   | 68~(99%)                 | 1 (1%)   | 67   | 81      |    |
| 52  | t     | 66/70~(94%)                   | 66 (100%)                | 0        | 100  | 100     | )  |
| 53  | u     | 47/50~(94%)                   | 47 (100%)                | 0        | 100  | 100     | )  |
| 54  | v     | 472/674~(70%)                 | 470 (100%)               | 2 (0%)   | 91   | 94      |    |
| 54  | W     | $51\overline{3}/674~(76\%)$   | $5\overline{10}\ (99\%)$ | 3 (1%)   | 86   | 91      |    |
| All | All   | $538\overline{6}/5933~(91\%)$ | 5367 (100%)              | 19 (0%)  | 91   | 94      |    |

All (19) residues with a non-rotameric side chain are listed below:

| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 9   | С     | 108 | LYS  |
| 10  | D     | 140 | HIS  |
| 12  | F     | 122 | PHE  |
| 12  | F     | 164 | GLU  |
| 30  | Х     | 15  | LYS  |
| 30  | Х     | 25  | TYR  |
| 30  | Х     | 30  | LEU  |
| 30  | Х     | 68  | LEU  |
| 30  | Х     | 75  | LEU  |
| 36  | d     | 54  | LYS  |
| 36  | d     | 176 | PHE  |
| 45  | m     | 3   | ARG  |
| 47  | 0     | 42  | HIS  |
| 51  | s     | 25  | THR  |
| 54  | V     | 338 | THR  |



Continued from previous page...

| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 54  | V     | 554 | LEU  |
| 54  | W     | 196 | ARG  |
| 54  | W     | 205 | TYR  |
| 54  | W     | 592 | HIS  |

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (10) such sidechains are listed below:

| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 36  | d     | 137 | GLN  |
| 38  | f     | 27  | ASN  |
| 42  | j     | 78  | ASN  |
| 48  | р     | 72  | ASN  |
| 54  | V     | 143 | HIS  |
| 54  | V     | 235 | ASN  |
| 54  | W     | 46  | GLN  |
| 54  | W     | 125 | GLN  |
| 54  | W     | 239 | GLN  |
| 54  | W     | 551 | HIS  |

#### 5.3.3 RNA (i)

| Mol | Chain | Analysed        | Backbone Outliers | Pucker Outliers |
|-----|-------|-----------------|-------------------|-----------------|
| 14  | Н     | 76/77~(98%)     | 14 (18%)          | 2(2%)           |
| 28  | V     | 2881/2928~(98%) | 634 (22%)         | 64 (2%)         |
| 33  | a     | 1532/1533~(99%) | 266 (17%)         | 0               |
| 7   | А     | 25/26~(96%)     | 12 (48%)          | 5~(20%)         |
| 8   | В     | 111/112~(99%)   | 28 (25%)          | 4(3%)           |
| All | All   | 4625/4676 (98%) | 954 (20%)         | 75 (1%)         |

All (954) RNA backbone outliers are listed below:

| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 7   | А     | 33  | А    |
| 7   | А     | 34  | А    |
| 7   | А     | 35  | А    |
| 7   | А     | 37  | G    |
| 7   | А     | 38  | А    |
| 7   | А     | 39  | U    |
| 7   | А     | 40  | G    |
| 7   | А     | 43  | G    |



| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 7   | А     | 45  | С    |
| 7   | А     | 46  | А    |
| 7   | А     | 47  | G    |
| 7   | А     | 49  | А    |
| 8   | В     | 10  | G    |
| 8   | В     | 11  | А    |
| 8   | В     | 12  | U    |
| 8   | В     | 22  | G    |
| 8   | В     | 23  | U    |
| 8   | В     | 31  | G    |
| 8   | В     | 32  | U    |
| 8   | В     | 33  | U    |
| 8   | В     | 38  | U    |
| 8   | В     | 39  | A    |
| 8   | В     | 41  | С    |
| 8   | В     | 48  | G    |
| 8   | В     | 49  | G    |
| 8   | В     | 50  | А    |
| 8   | В     | 53  | U    |
| 8   | В     | 54  | U    |
| 8   | В     | 55  | А    |
| 8   | В     | 59  | U    |
| 8   | В     | 60  | С    |
| 8   | В     | 62  | U    |
| 8   | В     | 66  | С    |
| 8   | В     | 86  | U    |
| 8   | В     | 87  | U    |
| 8   | В     | 97  | A    |
| 8   | В     | 101 | U    |
| 8   | В     | 107 | G    |
| 8   | В     | 108 | C    |
| 8   | В     | 110 | G    |
| 14  | Н     | 9   | A    |
| 14  | Н     | 17  | U    |
| 14  | Н     | 18  | G    |
| 14  | Н     | 19  | U    |
| 14  | Н     | 21  | A    |
| 14  | Н     | 36  | C    |
| 14  | Н     | 37  | A    |
| 14  | Н     | 48  | С    |
| 14  | Н     | 55  | U    |
| 14  | Н     | 56  | С    |



| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 14  | Н     | 70  | А    |
| 14  | Н     | 72  | С    |
| 14  | Н     | 74  | С    |
| 14  | Н     | 76  | А    |
| 28  | V     | 8   | U    |
| 28  | V     | 13  | А    |
| 28  | V     | 23  | G    |
| 28  | V     | 26  | G    |
| 28  | V     | 34  | U    |
| 28  | V     | 46  | С    |
| 28  | V     | 51  | G    |
| 28  | V     | 60  | G    |
| 28  | V     | 71  | А    |
| 28  | V     | 74  | U    |
| 28  | V     | 75  | G    |
| 28  | V     | 76  | С    |
| 28  | V     | 77  | U    |
| 28  | V     | 78  | U    |
| 28  | V     | 79  | С    |
| 28  | V     | 85  | G    |
| 28  | V     | 86  | С    |
| 28  | V     | 87  | U    |
| 28  | V     | 89  | U    |
| 28  | V     | 90  | А    |
| 28  | V     | 92  | G    |
| 28  | V     | 93  | С    |
| 28  | V     | 99  | U    |
| 28  | V     | 100 | U    |
| 28  | V     | 101 | G    |
| 28  | V     | 117 | А    |
| 28  | V     | 119 | U    |
| 28  | V     | 124 | А    |
| 28  | V     | 125 | A    |
| 28  | V     | 141 | U    |
| 28  | V     | 145 | G    |
| 28  | V     | 162 | A    |
| 28  | V     | 164 | U    |
| 28  | V     | 175 | G    |
| 28  | V     | 176 | А    |
| 28  | V     | 177 | G    |
| 28  | V     | 178 | A    |
| 28  | V     | 179 | А    |



| Mol             | Chain | Res | Type |
|-----------------|-------|-----|------|
| 28              | V     | 182 | С    |
| 28              | V     | 184 | G    |
| 28              | V     | 186 | С    |
| 28              | V     | 187 | С    |
| 28              | V     | 188 | С    |
| 28              | V     | 199 | А    |
| 28              | V     | 200 | А    |
| 28              | V     | 202 | А    |
| 28              | V     | 207 | А    |
| 28              | V     | 215 | G    |
| 28              | V     | 216 | А    |
| 28              | V     | 219 | А    |
| 28              | V     | 224 | A    |
| 28              | V     | 225 | A    |
| 28              | V     | 226 | А    |
| 28              | V     | 231 | A    |
| 28              | V     | 232 | U    |
| 28              | V     | 233 | G    |
| 28              | V     | 234 | С    |
| 28              | V     | 242 | U    |
| 28              | V     | 251 | G    |
| 28              | V     | 252 | С    |
| 28              | V     | 253 | G    |
| 28              | V     | 258 | А    |
| 28              | V     | 269 | G    |
| 28              | V     | 283 | G    |
| 28              | V     | 284 | С    |
| 28              | V     | 286 | U    |
| 28              | V     | 287 | G    |
| 28              | V     | 291 | С    |
| 28              | V     | 296 | G    |
| 28              | V     | 297 | G    |
| 28              | V     | 301 | U    |
| 28              | V     | 302 | A    |
| 28              | V     | 307 | A    |
| 28              | V     | 308 | С    |
| 28              | V     | 310 | С    |
| 28              | V     | 329 | A    |
| 28              | V     | 342 | A    |
| 28              | V     | 344 | G    |
| $\overline{28}$ | V     | 345 | A    |
| 28              | V     | 346 | G    |



| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 28  | V     | 348 | U    |
| 28  | V     | 352 | G    |
| 28  | V     | 361 | G    |
| 28  | V     | 367 | G    |
| 28  | V     | 373 | А    |
| 28  | V     | 374 | А    |
| 28  | V     | 375 | С    |
| 28  | V     | 382 | G    |
| 28  | V     | 407 | А    |
| 28  | V     | 410 | G    |
| 28  | V     | 411 | G    |
| 28  | V     | 412 | А    |
| 28  | V     | 418 | A    |
| 28  | V     | 419 | G    |
| 28  | V     | 420 | U    |
| 28  | V     | 421 | A    |
| 28  | V     | 432 | С    |
| 28  | V     | 433 | G    |
| 28  | V     | 434 | U    |
| 28  | V     | 442 | С    |
| 28  | V     | 444 | U    |
| 28  | V     | 445 | С    |
| 28  | V     | 458 | G    |
| 28  | V     | 459 | А    |
| 28  | V     | 471 | G    |
| 28  | V     | 476 | А    |
| 28  | V     | 477 | А    |
| 28  | V     | 482 | С    |
| 28  | V     | 483 | С    |
| 28  | V     | 491 | С    |
| 28  | V     | 498 | U    |
| 28  | V     | 502 | С    |
| 28  | V     | 504 | A    |
| 28  | V     | 506 | U    |
| 28  | V     | 512 | G    |
| 28  | V     | 527 | A    |
| 28  | V     | 528 | G    |
| 28  | V     | 530 | A    |
| 28  | V     | 537 | A    |
| 28  | V     | 548 | A    |
| 28  | V     | 550 | G    |
| 28  | V     | 554 | U    |



| Mol             | Chain | Res | Type |
|-----------------|-------|-----|------|
| 28              | V     | 555 | С    |
| 28              | V     | 556 | С    |
| 28              | V     | 568 | G    |
| 28              | V     | 573 | С    |
| 28              | V     | 575 | А    |
| 28              | V     | 577 | U    |
| 28              | V     | 578 | А    |
| 28              | V     | 579 | G    |
| 28              | V     | 592 | А    |
| 28              | V     | 593 | А    |
| 28              | V     | 595 | G    |
| 28              | V     | 598 | U    |
| 28              | V     | 599 | G    |
| 28              | V     | 607 | G    |
| 28              | V     | 616 | A    |
| 28              | V     | 617 | G    |
| 28              | V     | 619 | А    |
| 28              | V     | 632 | U    |
| 28              | V     | 647 | А    |
| 28              | V     | 648 | G    |
| 28              | V     | 649 | G    |
| 28              | V     | 658 | А    |
| 28              | V     | 659 | А    |
| 28              | V     | 662 | U    |
| 28              | V     | 667 | А    |
| 28              | V     | 673 | А    |
| 28              | V     | 683 | А    |
| 28              | V     | 690 | А    |
| 28              | V     | 691 | U    |
| 28              | V     | 692 | А    |
| 28              | V     | 699 | A    |
| 28              | V     | 700 | U    |
| 28              | V     | 701 | G    |
| 28              | V     | 702 | A    |
| 28              | V     | 718 | С    |
| 28              | V     | 719 | С    |
| 28              | V     | 733 | U    |
| 28              | V     | 764 | С    |
| 28              | V     | 765 | A    |
| 28              | V     | 773 | G    |
| 28              | V     | 777 | С    |
| $\overline{28}$ | V     | 787 | С    |



| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 28  | V     | 788 | G    |
| 28  | V     | 790 | А    |
| 28  | V     | 794 | U    |
| 28  | V     | 795 | G    |
| 28  | V     | 810 | G    |
| 28  | V     | 811 | А    |
| 28  | V     | 822 | G    |
| 28  | V     | 823 | G    |
| 28  | V     | 829 | А    |
| 28  | V     | 831 | U    |
| 28  | V     | 832 | G    |
| 28  | V     | 837 | U    |
| 28  | V     | 845 | G    |
| 28  | V     | 852 | G    |
| 28  | V     | 859 | С    |
| 28  | V     | 866 | A    |
| 28  | V     | 874 | U    |
| 28  | V     | 892 | U    |
| 28  | V     | 906 | G    |
| 28  | V     | 908 | А    |
| 28  | V     | 913 | А    |
| 28  | V     | 914 | С    |
| 28  | V     | 929 | G    |
| 28  | V     | 931 | С    |
| 28  | V     | 933 | С    |
| 28  | V     | 934 | U    |
| 28  | V     | 935 | А    |
| 28  | V     | 936 | С    |
| 28  | V     | 937 | С    |
| 28  | V     | 939 | G    |
| 28  | V     | 940 | G    |
| 28  | V     | 941 | U    |
| 28  | V     | 942 | U    |
| 28  | V     | 943 | А    |
| 28  | V     | 944 | C    |
| 28  | V     | 957 | A    |
| 28  | V     | 959 | С    |
| 28  | V     | 961 | С    |
| 28  | V     | 962 | С    |
| 28  | V     | 964 | A    |
| 28  | V     | 973 | G    |
| 28  | V     | 980 | C    |



| Mol | Chain | Res               | Type |
|-----|-------|-------------------|------|
| 28  | V     | 987               | А    |
| 28  | V     | 991               | A    |
| 28  | V     | 992               | G    |
| 28  | V     | 999               | А    |
| 28  | V     | 1005              | А    |
| 28  | V     | 1007              | G    |
| 28  | V     | 1020              | А    |
| 28  | V     | 1027              | А    |
| 28  | V     | 1029              | А    |
| 28  | V     | 1036              | А    |
| 28  | V     | 1042              | А    |
| 28  | V     | 1051              | С    |
| 28  | V     | 1053              | С    |
| 28  | V     | 1054              | A    |
| 28  | V     | 1055              | А    |
| 28  | V     | 1058              | U    |
| 28  | V     | 1059              | А    |
| 28  | V     | 1068              | G    |
| 28  | V     | 1073              | А    |
| 28  | V     | 1079              | U    |
| 28  | V     | 1091              | U    |
| 28  | V     | 1094              | А    |
| 28  | V     | 1101              | G    |
| 28  | V     | 1102              | G    |
| 28  | V     | 1103              | А    |
| 28  | V     | 1106              | U    |
| 28  | V     | 1110              | С    |
| 28  | V     | 1111              | U    |
| 28  | V     | 1116              | А    |
| 28  | V     | 1117              | G    |
| 28  | V     | 1118              | С    |
| 28  | V     | 1119              | А    |
| 28  | V     | 1121              | С    |
| 28  | V     | 1124              | С    |
| 28  | V     | 1125              | С    |
| 28  | V     | 1126              | A    |
| 28  | V     | 1127              | U    |
| 28  | V     | 1128              | U    |
| 28  | V     | 1134              | A    |
| 28  | V     | $1\overline{139}$ | G    |
| 28  | V     | 1148              | С    |
| 28  | V     | 1158              | G    |



| Mol             | Chain | Res  | Type |
|-----------------|-------|------|------|
| 28              | V     | 1159 | U    |
| 28              | V     | 1160 | G    |
| 28              | V     | 1161 | А    |
| 28              | V     | 1173 | А    |
| 28              | V     | 1178 | U    |
| 28              | V     | 1179 | А    |
| 28              | V     | 1180 | С    |
| 28              | V     | 1181 | С    |
| 28              | V     | 1182 | G    |
| 28              | V     | 1185 | G    |
| 28              | V     | 1187 | U    |
| 28              | V     | 1188 | А    |
| 28              | V     | 1243 | А    |
| 28              | V     | 1244 | A    |
| 28              | V     | 1245 | G    |
| 28              | V     | 1248 | С    |
| 28              | V     | 1249 | U    |
| 28              | V     | 1251 | U    |
| 28              | V     | 1259 | G    |
| 28              | V     | 1260 | А    |
| 28              | V     | 1264 | G    |
| 28              | V     | 1265 | А    |
| 28              | V     | 1270 | С    |
| 28              | V     | 1275 | G    |
| 28              | V     | 1276 | G    |
| 28              | V     | 1278 | G    |
| 28              | V     | 1293 | А    |
| 28              | V     | 1296 | G    |
| 28              | V     | 1306 | G    |
| 28              | V     | 1311 | G    |
| 28              | V     | 1312 | A    |
| $\overline{28}$ | V     | 1313 | A    |
| 28              | V     | 1315 | G    |
| 28              | V     | 1323 | A    |
| 28              | V     | 1325 | A    |
| 28              | V     | 1326 | A    |
| 28              | V     | 1327 | U    |
| 28              | V     | 1339 | A    |
| 28              | V     | 1340 | A    |
| 28              | V     | 1341 | U    |
| 28              | V     | 1343 | С    |
| 28              | V     | 1344 | С    |



| Mol             | Chain | Res  | Type |
|-----------------|-------|------|------|
| 28              | V     | 1351 | U    |
| 28              | V     | 1352 | U    |
| 28              | V     | 1362 | G    |
| 28              | V     | 1364 | С    |
| 28              | V     | 1365 | U    |
| 28              | V     | 1368 | U    |
| 28              | V     | 1369 | С    |
| 28              | V     | 1370 | С    |
| 28              | V     | 1371 | G    |
| 28              | V     | 1372 | С    |
| 28              | V     | 1375 | А    |
| 28              | V     | 1384 | С    |
| 28              | V     | 1385 | G    |
| 28              | V     | 1389 | С    |
| 28              | V     | 1404 | A    |
| 28              | V     | 1415 | С    |
| 28              | V     | 1417 | А    |
| 28              | V     | 1418 | U    |
| 28              | V     | 1422 | С    |
| 28              | V     | 1423 | А    |
| 28              | V     | 1425 | С    |
| 28              | V     | 1426 | А    |
| 28              | V     | 1427 | G    |
| 28              | V     | 1431 | G    |
| 28              | V     | 1434 | А    |
| 28              | V     | 1435 | U    |
| 28              | V     | 1436 | U    |
| 28              | V     | 1442 | А    |
| 28              | V     | 1449 | С    |
| 28              | V     | 1450 | С    |
| $\overline{28}$ | V     | 1457 | U    |
| 28              | V     | 1459 | U    |
| 28              | V     | 1460 | G    |
| 28              | V     | 1465 | A    |
| 28              | V     | 1466 | U    |
| $\overline{28}$ | V     | 1472 | G    |
| 28              | V     | 1473 | A    |
| 28              | V     | 1475 | G    |
| 28              | V     | 1476 | С    |
| 28              | V     | 1489 | U    |
| 28              | V     | 1490 | A    |
| $\overline{28}$ | V     | 1499 | А    |



| Mol             | Chain | Res  | Type |
|-----------------|-------|------|------|
| 28              | V     | 1500 | U    |
| 28              | V     | 1501 | U    |
| 28              | V     | 1502 | G    |
| 28              | V     | 1506 | А    |
| 28              | V     | 1507 | U    |
| 28              | V     | 1508 | С    |
| 28              | V     | 1514 | С    |
| 28              | V     | 1516 | А    |
| 28              | V     | 1525 | G    |
| 28              | V     | 1526 | G    |
| 28              | V     | 1527 | С    |
| 28              | V     | 1528 | U    |
| 28              | V     | 1529 | G    |
| 28              | V     | 1530 | G    |
| 28              | V     | 1531 | G    |
| 28              | V     | 1532 | A    |
| 28              | V     | 1536 | А    |
| 28              | V     | 1539 | С    |
| 28              | V     | 1540 | А    |
| 28              | V     | 1542 | А    |
| 28              | V     | 1543 | U    |
| 28              | V     | 1547 | U    |
| 28              | V     | 1553 | А    |
| 28              | V     | 1557 | G    |
| 28              | V     | 1558 | G    |
| 28              | V     | 1559 | С    |
| 28              | V     | 1560 | U    |
| 28              | V     | 1566 | G    |
| 28              | V     | 1568 | G    |
| 28              | V     | 1570 | U    |
| $\overline{28}$ | V     | 1571 | G    |
| $\overline{28}$ | V     | 1573 | С    |
| $\overline{28}$ | V     | 1614 | A    |
| 28              | V     | 1617 | A    |
| 28              | V     | 1626 | U    |
| 28              | V     | 1632 | G    |
| 28              | V     | 1634 | U    |
| 28              | V     | 1638 | A    |
| $\overline{28}$ | V     | 1653 | A    |
| 28              | V     | 1655 | A    |
| $\overline{28}$ | V     | 1661 | A    |
| 28              | V     | 1679 | А    |



| Mol | Chain | Res  | Type |
|-----|-------|------|------|
| 28  | V     | 1691 | А    |
| 28  | V     | 1692 | U    |
| 28  | V     | 1693 | С    |
| 28  | V     | 1696 | G    |
| 28  | V     | 1697 | А    |
| 28  | V     | 1699 | А    |
| 28  | V     | 1700 | А    |
| 28  | V     | 1708 | U    |
| 28  | V     | 1719 | G    |
| 28  | V     | 1727 | А    |
| 28  | V     | 1738 | U    |
| 28  | V     | 1745 | А    |
| 28  | V     | 1757 | G    |
| 28  | V     | 1758 | U    |
| 28  | V     | 1759 | U    |
| 28  | V     | 1760 | А    |
| 28  | V     | 1761 | G    |
| 28  | V     | 1775 | G    |
| 28  | V     | 1776 | А    |
| 28  | V     | 1778 | А    |
| 28  | V     | 1779 | G    |
| 28  | V     | 1780 | С    |
| 28  | V     | 1781 | С    |
| 28  | V     | 1782 | G    |
| 28  | V     | 1785 | G    |
| 28  | V     | 1791 | А    |
| 28  | V     | 1792 | G    |
| 28  | V     | 1793 | G    |
| 28  | V     | 1802 | А    |
| 28  | V     | 1810 | G    |
| 28  | V     | 1811 | С    |
| 28  | V     | 1813 | A    |
| 28  | V     | 1829 | С    |
| 28  | V     | 1830 | G    |
| 28  | V     | 1837 | U    |
| 28  | V     | 1838 | A    |
| 28  | V     | 1843 | G    |
| 28  | V     | 1845 | A    |
| 28  | V     | 1846 | G    |
| 28  | V     | 1850 | A    |
| 28  | V     | 1858 | A    |
| 28  | V     | 1862 | С    |



| Mol | Chain | Res  | Type |
|-----|-------|------|------|
| 28  | V     | 1864 | G    |
| 28  | V     | 1877 | А    |
| 28  | V     | 1883 | А    |
| 28  | V     | 1885 | А    |
| 28  | V     | 1887 | G    |
| 28  | V     | 1891 | G    |
| 28  | V     | 1895 | А    |
| 28  | V     | 1899 | U    |
| 28  | V     | 1904 | G    |
| 28  | V     | 1915 | U    |
| 28  | V     | 1935 | G    |
| 28  | V     | 1943 | С    |
| 28  | V     | 1948 | А    |
| 28  | V     | 1958 | G    |
| 28  | V     | 1959 | G    |
| 28  | V     | 1965 | A    |
| 28  | V     | 1966 | А    |
| 28  | V     | 1967 | А    |
| 28  | V     | 1968 | U    |
| 28  | V     | 1969 | U    |
| 28  | V     | 1973 | U    |
| 28  | V     | 1984 | U    |
| 28  | V     | 1992 | С    |
| 28  | V     | 1993 | G    |
| 28  | V     | 1996 | С    |
| 28  | V     | 1999 | А    |
| 28  | V     | 2000 | А    |
| 28  | V     | 2001 | G    |
| 28  | V     | 2010 | А    |
| 28  | V     | 2020 | U    |
| 28  | V     | 2022 | U    |
| 28  | V     | 2023 | С    |
| 28  | V     | 2025 | С    |
| 28  | V     | 2026 | A    |
| 28  | V     | 2050 | G    |
| 28  | V     | 2051 | U    |
| 28  | V     | 2052 | A    |
| 28  | V     | 2054 | C    |
| 28  | V     | 2059 | A    |
| 28  | V     | 2060 | A    |
| 28  | V     | 2061 | G    |
| 28  | V     | 2062 | А    |



| Mol | Chain | Res  | Type |
|-----|-------|------|------|
| 28  | V     | 2064 | G    |
| 28  | V     | 2072 | С    |
| 28  | V     | 2079 | С    |
| 28  | V     | 2084 | С    |
| 28  | V     | 2085 | G    |
| 28  | V     | 2089 | А    |
| 28  | V     | 2090 | G    |
| 28  | V     | 2098 | G    |
| 28  | V     | 2114 | С    |
| 28  | V     | 2121 | U    |
| 28  | V     | 2122 | G    |
| 28  | V     | 2123 | А    |
| 28  | V     | 2125 | U    |
| 28  | V     | 2128 | U    |
| 28  | V     | 2131 | U    |
| 28  | V     | 2134 | A    |
| 28  | V     | 2135 | G    |
| 28  | V     | 2136 | С    |
| 28  | V     | 2145 | G    |
| 28  | V     | 2146 | А    |
| 28  | V     | 2147 | U    |
| 28  | V     | 2148 | А    |
| 28  | V     | 2149 | G    |
| 28  | V     | 2154 | G    |
| 28  | V     | 2156 | G    |
| 28  | V     | 2161 | G    |
| 28  | V     | 2162 | G    |
| 28  | V     | 2167 | С    |
| 28  | V     | 2174 | С    |
| 28  | V     | 2177 | G    |
| 28  | V     | 2182 | G    |
| 28  | V     | 2184 | U    |
| 28  | V     | 2185 | G    |
| 28  | V     | 2187 | A    |
| 28  | V     | 2188 | G    |
| 28  | V     | 2189 | G    |
| 28  | V     | 2197 | G    |
| 28  | V     | 2199 | G    |
| 28  | V     | 2200 | A    |
| 28  | V     | 2201 | U    |
| 28  | V     | 2203 | С    |
| 28  | V     | 2204 | U    |
|     |       |      | ]    |



| Mol | Chain | Res  | Type |
|-----|-------|------|------|
| 28  | V     | 2205 | А    |
| 28  | V     | 2206 | С    |
| 28  | V     | 2208 | С    |
| 28  | V     | 2219 | G    |
| 28  | V     | 2226 | U    |
| 28  | V     | 2227 | А    |
| 28  | V     | 2228 | А    |
| 28  | V     | 2229 | С    |
| 28  | V     | 2230 | С    |
| 28  | V     | 2231 | С    |
| 28  | V     | 2232 | А    |
| 28  | V     | 2233 | С    |
| 28  | V     | 2234 | С    |
| 28  | V     | 2245 | G    |
| 28  | V     | 2246 | G    |
| 28  | V     | 2252 | A    |
| 28  | V     | 2254 | A    |
| 28  | V     | 2255 | С    |
| 28  | V     | 2267 | G    |
| 28  | V     | 2268 | G    |
| 28  | V     | 2280 | G    |
| 28  | V     | 2296 | А    |
| 28  | V     | 2307 | А    |
| 28  | V     | 2312 | С    |
| 28  | V     | 2316 | А    |
| 28  | V     | 2317 | А    |
| 28  | V     | 2328 | G    |
| 28  | V     | 2330 | А    |
| 28  | V     | 2334 | U    |
| 28  | V     | 2335 | U    |
| 28  | V     | 2336 | G    |
| 28  | V     | 2337 | G    |
| 28  | V     | 2338 | A    |
| 28  | V     | 2341 | U    |
| 28  | V     | 2347 | G    |
| 28  | V     | 2348 | С    |
| 28  | V     | 2350 | G    |
| 28  | V     | 2351 | А    |
| 28  | V     | 2356 | А    |
| 28  | V     | 2362 | А    |
| 28  | V     | 2363 | С    |
| 28  | V     | 2364 | А    |



| Mol | Chain | Res  | Type |
|-----|-------|------|------|
| 28  | V     | 2368 | G    |
| 28  | V     | 2376 | С    |
| 28  | V     | 2378 | G    |
| 28  | V     | 2379 | С    |
| 28  | V     | 2401 | G    |
| 28  | V     | 2412 | G    |
| 28  | V     | 2414 | С    |
| 28  | V     | 2431 | U    |
| 28  | V     | 2432 | С    |
| 28  | V     | 2435 | С    |
| 28  | V     | 2452 | U    |
| 28  | V     | 2453 | С    |
| 28  | V     | 2454 | А    |
| 28  | V     | 2455 | А    |
| 28  | V     | 2457 | G    |
| 28  | V     | 2458 | G    |
| 28  | V     | 2459 | А    |
| 28  | V     | 2460 | U    |
| 28  | V     | 2469 | С    |
| 28  | V     | 2470 | С    |
| 28  | V     | 2477 | А    |
| 28  | V     | 2488 | А    |
| 28  | V     | 2504 | С    |
| 28  | V     | 2505 | А    |
| 28  | V     | 2507 | А    |
| 28  | V     | 2511 | А    |
| 28  | V     | 2523 | G    |
| 28  | V     | 2525 | С    |
| 28  | V     | 2527 | С    |
| 28  | V     | 2531 | G    |
| 28  | V     | 2532 | А    |
| 28  | V     | 2534 | G    |
| 28  | V     | 2535 | U    |
| 28  | V     | 2547 | А    |
| 28  | V     | 2549 | С    |
| 28  | V     | 2558 | G    |
| 28  | V     | 2564 | G    |
| 28  | V     | 2583 | U    |
| 28  | V     | 2584 | U    |
| 28  | V     | 2593 | A    |
| 28  | V     | 2596 | G    |
| 28  | V     | 2601 | A    |



| Mol | Chain | Res               | Type |
|-----|-------|-------------------|------|
| 28  | V     | 2602              | С    |
| 28  | V     | 2605              | G    |
| 28  | V     | 2611              | G    |
| 28  | V     | 2613              | U    |
| 28  | V     | 2614              | U    |
| 28  | V     | 2631              | А    |
| 28  | V     | 2632              | G    |
| 28  | V     | 2638              | U    |
| 28  | V     | 2639              | С    |
| 28  | V     | 2642              | U    |
| 28  | V     | 2644              | U    |
| 28  | V     | 2659              | G    |
| 28  | V     | 2675              | С    |
| 28  | V     | 2690              | G    |
| 28  | V     | 2711              | G    |
| 28  | V     | 2718              | U    |
| 28  | V     | 2720              | С    |
| 28  | V     | 2743              | G    |
| 28  | V     | 2755              | U    |
| 28  | V     | 2762              | А    |
| 28  | V     | 2763              | С    |
| 28  | V     | 2764              | G    |
| 28  | V     | 2765              | G    |
| 28  | V     | 2773              | G    |
| 28  | V     | 2777              | A    |
| 28  | V     | 2784              | С    |
| 28  | V     | 2785              | U    |
| 28  | V     | 2794              | А    |
| 28  | V     | 2806              | G    |
| 28  | V     | 2807              | A    |
| 28  | V     | 2808              | U    |
| 28  | V     | 2818              | С    |
| 28  | V     | $2\overline{823}$ | С    |
| 28  | V     | 2824              | G    |
| 28  | V     | 2826              | A    |
| 28  | V     | 2831              | A    |
| 28  | V     | 2845              | А    |
| 28  | V     | 2859              | G    |
| 28  | V     | 2860              | A    |
| 28  | V     | 2867              | U    |
| 28  | V     | 2868              | G    |
| 28  | V     | 2884              | G    |



| Mol | Chain | Res  | Type |
|-----|-------|------|------|
| 28  | V     | 2892 | G    |
| 28  | V     | 2897 | G    |
| 28  | V     | 2899 | С    |
| 28  | V     | 2900 | А    |
| 28  | V     | 2901 | G    |
| 28  | V     | 2905 | С    |
| 28  | V     | 2916 | А    |
| 28  | V     | 2918 | G    |
| 33  | a     | 10   | А    |
| 33  | a     | 11   | G    |
| 33  | a     | 31   | А    |
| 33  | a     | 32   | С    |
| 33  | a     | 33   | G    |
| 33  | a     | 34   | A    |
| 33  | a     | 41   | G    |
| 33  | a     | 49   | С    |
| 33  | a     | 50   | С    |
| 33  | a     | 53   | А    |
| 33  | a     | 75   | G    |
| 33  | a     | 77   | U    |
| 33  | a     | 78   | G    |
| 33  | a     | 84   | U    |
| 33  | a     | 85   | U    |
| 33  | a     | 86   | G    |
| 33  | a     | 87   | С    |
| 33  | a     | 89   | С    |
| 33  | a     | 90   | С    |
| 33  | a     | 93   | G    |
| 33  | a     | 99   | А    |
| 33  | a     | 114  | А    |
| 33  | a     | 119  | С    |
| 33  | a     | 120  | A    |
| 33  | a     | 128  | A    |
| 33  | a     | 129  | A    |
| 33  | a     | 130  | С    |
| 33  | a     | 136  | U    |
| 33  | a     | 142  | A    |
| 33  | a     | 143  | C    |
| 33  | a     | 153  | U    |
| 33  | a     | 154  | С    |
| 33  | a     | 158  | G    |
| 33  | a     | 162  | С    |



| $\mathbf{Mol}$ | Chain | Res | Type |
|----------------|-------|-----|------|
| 33             | а     | 172 | U    |
| 33             | a     | 177 | G    |
| 33             | a     | 181 | G    |
| 33             | а     | 182 | U    |
| 33             | a     | 189 | А    |
| 33             | a     | 197 | G    |
| 33             | а     | 208 | А    |
| 33             | а     | 209 | А    |
| 33             | а     | 211 | А    |
| 33             | a     | 218 | U    |
| 33             | a     | 219 | U    |
| 33             | a     | 221 | G    |
| 33             | a     | 249 | G    |
| 33             | a     | 253 | U    |
| 33             | a     | 255 | G    |
| 33             | a     | 258 | А    |
| 33             | a     | 259 | G    |
| 33             | a     | 274 | G    |
| 33             | a     | 275 | С    |
| 33             | a     | 287 | А    |
| 33             | a     | 297 | G    |
| 33             | a     | 314 | А    |
| 33             | a     | 336 | С    |
| 33             | a     | 337 | А    |
| 33             | a     | 338 | С    |
| 33             | a     | 340 | G    |
| 33             | a     | 352 | А    |
| 33             | a     | 354 | G    |
| 33             | a     | 360 | С    |
| 33             | a     | 362 | G    |
| 33             | a     | 373 | U    |
| 33             | a     | 375 | U    |
| 33             | a     | 380 | С    |
| 33             | a     | 381 | А    |
| 33             | a     | 385 | G    |
| 33             | a     | 392 | G    |
| 33             | a     | 396 | G    |
| 33             | a     | 405 | А    |
| 33             | a     | 414 | G    |
| 33             | a     | 419 | А    |
| 33             | a     | 420 | U    |
| 33             | a     | 421 | G    |



| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 33  | a     | 429 | U    |
| 33  | a     | 430 | С    |
| 33  | a     | 435 | С    |
| 33  | a     | 436 | G    |
| 33  | a     | 437 | U    |
| 33  | a     | 448 | U    |
| 33  | a     | 456 | А    |
| 33  | a     | 460 | А    |
| 33  | a     | 461 | С    |
| 33  | a     | 466 | G    |
| 33  | a     | 474 | А    |
| 33  | a     | 475 | А    |
| 33  | a     | 476 | U    |
| 33  | a     | 477 | A    |
| 33  | a     | 478 | G    |
| 33  | a     | 481 | С    |
| 33  | a     | 485 | A    |
| 33  | a     | 487 | С    |
| 33  | a     | 488 | U    |
| 33  | a     | 489 | U    |
| 33  | a     | 490 | G    |
| 33  | a     | 491 | А    |
| 33  | a     | 494 | G    |
| 33  | a     | 502 | С    |
| 33  | a     | 504 | А    |
| 33  | a     | 506 | А    |
| 33  | a     | 508 | А    |
| 33  | a     | 518 | А    |
| 33  | a     | 520 | С    |
| 33  | a     | 526 | G    |
| 33  | a     | 527 | C    |
| 33  | a     | 530 | G    |
| 33  | a     | 536 | G    |
| 33  | a     | 541 | А    |
| 33  | a     | 542 | А    |
| 33  | a     | 556 | A    |
| 33  | a     | 564 | С    |
| 33  | a     | 568 | A    |
| 33  | a     | 571 | U    |
| 33  | a     | 573 | U    |
| 33  | a     | 582 | A    |
| 33  | a     | 585 | G    |



| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 33  | a     | 586 | G    |
| 33  | a     | 590 | G    |
| 33  | a     | 597 | G    |
| 33  | a     | 605 | А    |
| 33  | a     | 641 | G    |
| 33  | a     | 642 | U    |
| 33  | a     | 643 | С    |
| 33  | a     | 651 | А    |
| 33  | a     | 662 | U    |
| 33  | a     | 696 | А    |
| 33  | a     | 732 | U    |
| 33  | a     | 733 | G    |
| 33  | a     | 756 | U    |
| 33  | a     | 757 | A    |
| 33  | a     | 758 | A    |
| 33  | a     | 764 | G    |
| 33  | a     | 787 | G    |
| 33  | a     | 802 | U    |
| 33  | a     | 803 | А    |
| 33  | a     | 824 | A    |
| 33  | a     | 826 | С    |
| 33  | a     | 841 | G    |
| 33  | a     | 849 | G    |
| 33  | a     | 853 | С    |
| 33  | a     | 855 | G    |
| 33  | a     | 856 | С    |
| 33  | a     | 882 | A    |
| 33  | a     | 883 | A    |
| 33  | a     | 885 | С    |
| 33  | a     | 924 | A    |
| 33  | a     | 943 | G    |
| 33  | a     | 944 | С    |
| 33  | a     | 945 | A    |
| 33  | a     | 950 | С    |
| 33  | a     | 963 | G    |
| 33  | a     | 964 | G    |
| 33  | a     | 966 | U    |
| 33  | a     | 968 | A    |
| 33  | a     | 969 | A    |
| 33  | a     | 970 | U    |
| 33  | a     | 979 | A    |
| 33  | a     | 981 | G    |



| Mol | Chain | Res  | Type |
|-----|-------|------|------|
| 33  | a     | 985  | А    |
| 33  | a     | 986  | G    |
| 33  | a     | 987  | А    |
| 33  | a     | 993  | А    |
| 33  | a     | 999  | U    |
| 33  | a     | 1002 | U    |
| 33  | a     | 1003 | G    |
| 33  | a     | 1007 | U    |
| 33  | a     | 1008 | С    |
| 33  | a     | 1009 | С    |
| 33  | a     | 1010 | U    |
| 33  | a     | 1011 | С    |
| 33  | a     | 1012 | U    |
| 33  | a     | 1014 | А    |
| 33  | a     | 1015 | С    |
| 33  | a     | 1017 | А    |
| 33  | a     | 1019 | С    |
| 33  | a     | 1023 | G    |
| 33  | a     | 1024 | A    |
| 33  | a     | 1028 | А    |
| 33  | a     | 1030 | G    |
| 33  | a     | 1033 | G    |
| 33  | a     | 1035 | С    |
| 33  | a     | 1036 | С    |
| 33  | a     | 1039 | U    |
| 33  | a     | 1041 | С    |
| 33  | a     | 1042 | G    |
| 33  | a     | 1046 | G    |
| 33  | a     | 1047 | С    |
| 33  | a     | 1050 | А    |
| 33  | a     | 1053 | G    |
| 33  | a     | 1058 | G    |
| 33  | a     | 1064 | С    |
| 33  | a     | 1075 | U    |
| 33  | a     | 1088 | U    |
| 33  | a     | 1089 | G    |
| 33  | a     | 1095 | U    |
| 33  | a     | 1104 | G    |
| 33  | a     | 1105 | U    |
| 33  | a     | 1111 | A    |
| 33  | a     | 1112 | A    |
| 33  | a     | 1118 | G    |



| Mol | Chain | Res  | Type |
|-----|-------|------|------|
| 33  | a     | 1122 | С    |
| 33  | a     | 1134 | G    |
| 33  | a     | 1135 | U    |
| 33  | a     | 1136 | U    |
| 33  | a     | 1140 | А    |
| 33  | a     | 1142 | С    |
| 33  | a     | 1145 | U    |
| 33  | a     | 1148 | G    |
| 33  | a     | 1149 | U    |
| 33  | a     | 1153 | G    |
| 33  | a     | 1161 | А    |
| 33  | a     | 1166 | А    |
| 33  | a     | 1168 | U    |
| 33  | a     | 1176 | A    |
| 33  | a     | 1178 | A    |
| 33  | a     | 1190 | G    |
| 33  | a     | 1192 | U    |
| 33  | a     | 1193 | G    |
| 33  | a     | 1205 | A    |
| 33  | a     | 1206 | А    |
| 33  | a     | 1211 | U    |
| 33  | a     | 1221 | U    |
| 33  | a     | 1222 | А    |
| 33  | a     | 1223 | U    |
| 33  | a     | 1237 | С    |
| 33  | a     | 1259 | А    |
| 33  | a     | 1261 | A    |
| 33  | a     | 1267 | G    |
| 33  | a     | 1278 | А    |
| 33  | a     | 1279 | G    |
| 33  | a     | 1289 | A    |
| 33  | a     | 1294 | A    |
| 33  | a     | 1295 | С    |
| 33  | a     | 1296 | A    |
| 33  | a     | 1308 | A    |
| 33  | a     | 1314 | G    |
| 33  | a     | 1326 | С    |
| 33  | a     | 1329 | С    |
| 33  | a     | 1330 | U    |
| 33  | a     | 1331 | С    |
| 33  | a     | 1341 | A    |
| 33  | a     | 1347 | G    |



| Mol | Chain | Res  | Type |
|-----|-------|------|------|
| 33  | a     | 1355 | А    |
| 33  | a     | 1366 | А    |
| 33  | a     | 1370 | G    |
| 33  | a     | 1372 | А    |
| 33  | a     | 1373 | U    |
| 33  | a     | 1377 | G    |
| 33  | a     | 1387 | С    |
| 33  | a     | 1407 | А    |
| 33  | a     | 1451 | А    |
| 33  | a     | 1455 | А    |
| 33  | a     | 1460 | U    |
| 33  | a     | 1462 | U    |
| 33  | a     | 1463 | А    |
| 33  | a     | 1464 | G    |
| 33  | a     | 1490 | А    |
| 33  | a     | 1500 | U    |
| 33  | a     | 1502 | А    |
| 33  | a     | 1503 | А    |
| 33  | a     | 1516 | U    |
| 33  | a     | 1527 | G    |
| 33  | a     | 1539 | G    |
| 33  | a     | 1540 | G    |

All (75) RNA pucker outliers are listed below:

| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 7   | А     | 33  | А    |
| 7   | А     | 34  | А    |
| 7   | А     | 38  | А    |
| 7   | А     | 39  | U    |
| 7   | А     | 45  | С    |
| 8   | В     | 31  | G    |
| 8   | В     | 37  | А    |
| 8   | В     | 48  | G    |
| 8   | В     | 49  | G    |
| 14  | Н     | 47  | U    |
| 14  | Н     | 55  | U    |
| 28  | V     | 88  | G    |
| 28  | V     | 183 | А    |
| 28  | V     | 252 | С    |
| 28  | V     | 347 | G    |
| 28  | V     | 411 | G    |



| Mol | Chain | Res  | Type |
|-----|-------|------|------|
| 28  | V     | 441  | С    |
| 28  | V     | 444  | U    |
| 28  | V     | 549  | А    |
| 28  | V     | 554  | U    |
| 28  | V     | 689  | А    |
| 28  | V     | 772  | G    |
| 28  | V     | 810  | G    |
| 28  | V     | 905  | G    |
| 28  | V     | 1093 | G    |
| 28  | V     | 1172 | А    |
| 28  | V     | 1243 | А    |
| 28  | V     | 1244 | А    |
| 28  | V     | 1250 | G    |
| 28  | V     | 1264 | G    |
| 28  | V     | 1269 | А    |
| 28  | V     | 1275 | G    |
| 28  | V     | 1305 | А    |
| 28  | V     | 1351 | U    |
| 28  | V     | 1435 | U    |
| 28  | V     | 1448 | U    |
| 28  | V     | 1507 | U    |
| 28  | V     | 1525 | G    |
| 28  | V     | 1527 | С    |
| 28  | V     | 1529 | G    |
| 28  | V     | 1530 | G    |
| 28  | V     | 1535 | U    |
| 28  | V     | 1565 | U    |
| 28  | V     | 1567 | U    |
| 28  | V     | 1570 | U    |
| 28  | V     | 1631 | А    |
| 28  | V     | 1726 | G    |
| 28  | V     | 1757 | G    |
| 28  | V     | 1784 | A    |
| 28  | V     | 1828 | G    |
| 28  | V     | 1882 | A    |
| 28  | V     | 1914 | A    |
| 28  | V     | 1972 | U    |
| 28  | V     | 1991 | С    |
| 28  | V     | 2009 | G    |
| 28  | V     | 2022 | U    |
| 28  | V     | 2127 | U    |
| 28  | V     | 2155 | А    |



| Mol | Chain | Res  | Type |
|-----|-------|------|------|
| 28  | V     | 2205 | А    |
| 28  | V     | 2254 | А    |
| 28  | V     | 2316 | А    |
| 28  | V     | 2335 | U    |
| 28  | V     | 2336 | G    |
| 28  | V     | 2349 | А    |
| 28  | V     | 2364 | А    |
| 28  | V     | 2452 | U    |
| 28  | V     | 2454 | А    |
| 28  | V     | 2468 | А    |
| 28  | V     | 2510 | G    |
| 28  | V     | 2534 | G    |
| 28  | V     | 2631 | А    |
| 28  | V     | 2710 | С    |
| 28  | V     | 2805 | A    |
| 28  | V     | 2883 | С    |
| 28  | V     | 2904 | A    |

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

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

## 5.5 Carbohydrates (i)

There are no monosaccharides in this entry.

## 5.6 Ligand geometry (i)

There are no ligands in this entry.

#### 5.7 Other polymers (i)

There are no such residues in this entry.

#### 5.8 Polymer linkage issues (i)

There are no chain breaks in this entry.



# 6 Map visualisation (i)

This section contains visualisations of the EMDB entry EMD-14159. These allow visual inspection of the internal detail of the map and identification of artifacts.

No raw map or half-maps were deposited for this entry and therefore no images, graphs, etc. pertaining to the raw map can be shown.

## 6.1 Orthogonal projections (i)

#### 6.1.1 Primary map



The images above show the map projected in three orthogonal directions.

## 6.2 Central slices (i)

#### 6.2.1 Primary map



X Index: 184



Y Index: 184



Z Index: 184

The images above show central slices of the map in three orthogonal directions.

## 6.3 Largest variance slices (i)

#### 6.3.1 Primary map



X Index: 254

Y Index: 196

Z Index: 169

The images above show the largest variance slices of the map in three orthogonal directions.

## 6.4 Orthogonal surface views (i)

#### 6.4.1 Primary map



The images above show the 3D surface view of the map at the recommended contour level 0.0172. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.



## 6.5 Mask visualisation (i)

This section was not generated. No masks/segmentation were deposited.



## 7 Map analysis (i)

This section contains the results of statistical analysis of the map.

## 7.1 Map-value distribution (i)



The map-value distribution is plotted in 128 intervals along the x-axis. The y-axis is logarithmic. A spike in this graph at zero usually indicates that the volume has been masked.



## 7.2 Volume estimate (i)



The volume at the recommended contour level is 6043  $\rm nm^3;$  this corresponds to an approximate mass of 5459 kDa.

The volume estimate graph shows how the enclosed volume varies with the contour level. The recommended contour level is shown as a vertical line and the intersection between the line and the curve gives the volume of the enclosed surface at the given level.



## 7.3 Rotationally averaged power spectrum (i)



\*Reported resolution corresponds to spatial frequency of 0.195  ${\rm \AA^{-1}}$ 



# 8 Fourier-Shell correlation (i)

This section was not generated. No FSC curve or half-maps provided.



## 9 Map-model fit (i)

This section contains information regarding the fit between EMDB map EMD-14159 and PDB model 7QV3. Per-residue inclusion information can be found in section 3 on page 14.

## 9.1 Map-model overlay (i)



The images above show the 3D surface view of the map at the recommended contour level 0.0172 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.



## 9.2 Atom inclusion (i)



At the recommended contour level, 96% of all backbone atoms, 93% of all non-hydrogen atoms, are inside the map.

