

Nov 20, 2022 - 07:26 am GMT

| PDB ID       | : | 6HA8   |
|--------------|---|--|
| EMDB ID      | : | EMD-0177   |
| Title        | : | Cryo-EM structure of the ABCF protein VmlR bound to the Bacillus subtilis    |
|              |   | ribosome   |
| Authors      | : | Crowe-McAuliffe, C.; Graf, M.; Huter, P.; Abdelshahid, M.; Novacek, J.; Wil- |
|              |   | son, D.N.  |
| Deposited on | : | 2018-08-07   |
| Resolution   | : | 3.50  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 types of validation reports are described at http://www.wwpdb.org/validation/2017/FAQs#types.

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

| EMDB validation analysis       | : | 0.0.1. dev 43  |
|--------------------------------|---|--|
| Mogul                          | : | 1.8.4, CSD as541be (2020)  |
| MolProbity                     | : | 4.02b-467  |
| buster-report                  | : | 1.1.7(2018)  |
| Percentile statistics          | : | 20191225.v01 (using entries in the PDB archive December 25th 2019) |
| MapQ                           | : | 1.9.9  |
| Ideal geometry (proteins)      | : | Engh & Huber (2001)  |
| Ideal geometry (DNA, RNA)      | : | Parkinson et al. (1996)  |
| Validation Pipeline (wwPDB-VP) | : | 2.31.2   |

### 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 3.50 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                | Whole archive<br>(#Entries) | ${f EM} {f structures} \ (\#{f Entries})$ |  |  |
|-----------------------|-----------------------------|---|--|--|
| 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 >=3, 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions <=5% The upper red bar (where present) indicates the fraction of residues that have poor fit to the EM map (all-atom inclusion < 40%). The numeric value is given above the bar.

| Mol | Chain | Length | Quality of chain |       |
|-----|-------|--------|------------------|-------|
| 1   | А     | 2928   | 61% 31%          | 6% •  |
| 2   | В     | 112    | <b>•</b> 57% 36% | 7%    |
| 3   | С     | 277    | 97%              | ••    |
| 4   | D     | 209    | 97%              |       |
| 5   | Е     | 207    | <u>6%</u><br>96% |       |
| 6   | F     | 179    | 41%              | 6% •• |
| 7   | G     | 179    | 46%              | ·     |
| 8   | J     | 145    | 5%<br>95%        | •••   |



Continued from previous page...

| Mol | Chain | Length | Quality of chain |        |
|-----|-------|--------|------------------|--------|
| 9   | K     | 122    | 7%<br>99%        | ·      |
| 10  | L     | 146    | 9%               |        |
| 11  | М     | 144    | 93%              | • 6%   |
| 12  | Ν     | 120    | 8%               | ·      |
| 13  | Ο     | 120    | 98%              | ·      |
| 14  | Р     | 115    | 97%              | •      |
| 15  | Q     | 119    | <b>9</b> 5%      | • • •  |
| 16  | R     | 102    | 93%              | • ••   |
| 17  | S     | 113    | 94%              | ••••   |
| 18  | Т     | 95     | 93%              | • 5%   |
| 19  | U     | 103    | 97%              | ••     |
| 20  | V     | 548    | 95%              | ••     |
| 21  | W     | 94     | 84%              | •• 13% |
| 22  | Х     | 62     | 87%              | 6% 6%  |
| 23  | Y     | 66     | 98%              | ·      |
| 24  | Z     | 59     | 97%              | • •    |
| 25  | 0     | 59     | 85%              | • • 8% |
| 26  | 1     | 49     | 96%              |        |
| 27  | 2     | 44     | 98%              | ·      |
| 28  | 3     | 66     | 94%              | • •    |
| 29  | 4     | 37     | 100%             |        |
| 30  | 6     | 66     | 94%              | • 5%   |
| 31  | 7     | 3      | 67%              | 33%    |
| 32  | 8     | 232    | 91%              | 9%     |
| 33  | a     | 1554   | 66% 29           | 9% • • |



| Mol         Chain         Length         Quality of chain           34         b         246 $\frac{66\%}{82\%}$ $\frac{66\%}{11\%}$ 35         c         218 $\frac{53\%}{92\%}$ $\frac{66\%}{11\%}$ 36         d         200 $\frac{53\%}{7\%}$ $\frac{66\%}{7\%}$ 37         e         166 $\frac{31\%}{7\%}$ $\frac{31\%}{1\%}$ 38         ft         95 $\frac{95\%}{95\%}$ $\frac{1}{1\%}$ 39         g         156 $\frac{55\%}{95\%}$ $\frac{1}{1\%}$ 40         h         132 $\frac{45\%}{95\%}$ $\frac{95\%}{95\%}$ $\frac{1}{1\%}$ 41         i         130 $\frac{45\%}{92\%}$ $\frac{1}{1\%}$ $\frac{1}{1\%}$ 42         j         102 $\frac{55\%}{92\%}$ $\frac{1}{1\%}$ $\frac{1}{1\%}$ 43         k         131 $\frac{55\%}{92\%}$ $\frac{1}{1\%}$ $\frac{1}{1\%}$ 44         11         138 $\frac{60\%}{93\%}$ $\frac{1}{1\%}$ $\frac{1}{1\%}$ 45         m         121 $\frac{60\%}{93\%}$ $\frac{1}{1\%}$ $\frac{1}{1\%}$ 46         m         61 $\frac{9}{$ | Conti | nued fron | n previous | page             |             |
|--|-------|-----------|------------|------------------|-------------|
| 34         b $246$ $85%$ $6%$ $11%$ $35$ c $218$ $92%$ $6%$ $11%$ $36$ d $200$ $93%$ $.6%$ $36$ d $200$ $93%$ $.6%$ $37$ e $166$ $71%$ $.6%$ $38$ f $95$ $93%$ $$ $39$ g $156$ $55%$ $94%$ $$ $40$ h $132$ $55%$ $94%$ $$ $41$ i $130$ $92%$ $$ $$ $41$ i $130$ $92%$ $$ $$ $42$ j $102$ $51%$ $92%$ $$ $44$ 1 $138$ $60%$ $$ $45$ m $121$ $85%$ $$ $45$ m $61%$ $$ $$ $47$ o $89$   | Mol   | Chain     | Length     | Quality of chain |             |
| 34         b         246         62%         6%         13%           35         c         218 $33\%$ $6\%$ $77\%$ 36         d         200 $93\%$ $$ 37         c         166 $97\%$ $$ 38         f         95 $95\%$ $$ 39         g         156 $39\%$ $$ 40         h         132 $45\%$ $$ 41         i         130 $92\%$ $$ 42         j         102 $61\%$ $92\%$ $$ 43         k         131 $85\%$ $$ 44         1         138 $57\%$ $$ 45         m         121 $85\%$ $$ 46         n         61 $93\%$ $$ 47         o         89 $92\%$ $$ 48         p         90 $92\%$ $$ 48         p         90 $66\%$ $$ <td></td> <td></td> <td></td> <td>86%</td> <td></td>  |       |           |            | 86%              |             |
| 35         c $218$ $33%$ $36$ $d$ $200$ $77%$ $37$ $e$ $166$ $93%$ $$ $37$ $e$ $166$ $97%$ $$ $38$ $f$ $95$ $95%$ $$ $39$ $g$ $156$ $95%$ $$ $40$ $h$ $132$ $95%$ $$ $41$ $i$ $130$ $92%$ $$ $41$ $i$ $130$ $92%$ $$ $42$ $j$ $102$ $92%$ $$ $43$ $k$ $131$ $85%$ $.13%$ $44$ $1$ $138$ $93%$ $$ $44$ $1$ $138$ $93%$ $$ $45$ $m$ $121$ $85%$ $$ $45$ $m$ $216$ $85%$ $$ $47$ $o$ $89$ $92%$ $$ <  | 34    | b         | 246        | 82%              | 6% 11%      |
| 35       c $218$ $94%$ $.6%$ $36$ d $200$ $31%$ $93%$ $$ $37$ e $166$ $97%$ $$ $38$ f $95$ $95%$ $$ $39$ g $156$ $94%$ $$ $40$ h $132$ $95%$ $$ $41$ i $130$ $92%$ $$ $41$ i $130$ $92%$ $$ $42$ j $102$ $92%$ $$ $43$ k $131$ $85%$ $.13%$ $44$ 1 $138$ $60%$ $$ $44$ 1 $138$ $57%$ $$ $45$ m $121$ $85%$ $$ $46$ n $61$ $93%$ $$ $47$ o $89$ $92%$ $$ $48$ p $90$ $92%$ $$ $49$ q $87$ $92%$ $$  |       |           |            | 53%              |             |
| $36$ d $200$ $31\%$ $93\%$ $\dots$ $37$ e       166 $71\%$ $97\%$ $\dots$ $38$ f       95 $95\%$ $\dots$ $39$ g       156 $39\%$ $95\%$ $\dots$ $40$ h       132 $95\%$ $\dots$ $\dots$ $41$ i       130 $45\%$ $\dots$ $\dots$ $41$ i       130 $61\%$ $\dots$ $\dots$ $42$ j       102 $92\%$ $\dots$ $\dots$ $43$ k       131 $85\%$ $13\%$ $\dots$ $44$ 1       138 $93\%$ $\dots$ $\dots$ $44$ 1       138 $60\%$ $\dots$ $\dots$ $\dots$ $44$ 1       138 $93\%$ $\dots$ $\dots$ $\dots$ $\dots$ $44$ 1       138 $93\%$ $\dots$ <   | 35    | с         | 218        | 94%              | • 6%        |
| 36       d $200$ $33%$ $37$ e       166 $31%$ $97%$ $38$ f       95 $95%$ $39$ g       156 $39%$ $94%$ $40$ h       132 $95%$ $95%$ $41$ i       130 $55%$ $95%$ $41$ i       130 $61%$ $92%$ $42$ j       102 $92%$ $7%$ $43$ k       131 $85%$ $33%$ $44$ 1       138 $60%$ $33%$ $44$ 1       138 $60%$ $33%$ $45$ m       121 $60%$ $93%$ $11%$ $46$ n       61 $93%$ $56%$ $47$ o $89$ $66%$ $92%$ $6%$ $49$ q $87$ <   |       |           |            | 77%              |             |
| 37       e       166 $31%$ 38       f       95 $95%$ $5%$ 39       g       156 $55%$ $94%$ $$ 40       h       132 $95%$ $$ 41       i       130 $65%$ $92%$ $$ 42       j       102 $65%$ $92%$ $$ 43       k       131 $85%$ $$ 44       1       138 $60%$ $$ 45       m       121 $85%$ $$ 46       n       61 $$ $$ 47       o       89 $60%$ $$ 48       p       90 $$ $$ 49       q       87 $$ $$ 51%       s       92 $$ $$ 52       t       88 $$ $$ 53       x       75 $$ $$  | 36    | d         | 200        | 93%              | • • •       |
| 37       e       100 $71%$ $71%$ $38$ f       95 $55%$ $55%$ $39$ g       156 $39%$ $95%$ $$ $40$ h       132 $95%$ $$ $41$ i       130 $61%$ $92%$ $$ $41$ i       130 $61%$ $92%$ $$ $42$ j       102 $92%$ $$ $$ $43$ k       131 $85%$ $$ $$ $44$ 1       138 $92%$ $$ $$ $44$ 1       138 $92%$ $$ $$ $44$ 1       138 $93%$ $$ $$ $45$ m       121 $55%$ $93%$ $$ $$ $46$ n       61 $93%$ $$ $$ $47$ o       89 $66%$ $$ $$ $48$ p       90 $64%$ $$ $$   | 07    |           | 1.0.0      | 31%              |             |
| 38       f       95 $39%$ $39$ g       156 $39%$ $94%$ $40$ h       132 $55%$ $95%$ $41$ i       130 $55%$ $92%$ $42$ j       102 $61%$ $92%$ $43$ k       131 $85%$ $44$ 1       138 $93%$ $44$ 1       138 $60%$ $93%$ $44$ 1       138 $60%$ $93%$ $45$ m       121 $85%$ $11%$ $46$ n       61 $93%$ $5%$ $11%$ $47$ o $89$ $60%$ $60%$ $60%$ $60%$ $49$ q $87$ $55%$ $19%$ $55%$ $19%$ $51$ s $92$ $64%$ $55%$ $19%$ $55%$ $55%$ $51$ s $92$ $55%$ $55%$  | 37    | е         | 166        | 97%              | •••         |
| 38       1       93 $39^{3}$ $39\%$ $39\%$ 39       g       156 $39\%$ $94\%$ $\cdot$ 40       h       132 $55\%$ $95\%$ $\cdot$ 41       i       130 $45\%$ $\cdot$ $\cdot$ 41       i       130 $92\%$ $\cdot$ $\cdot$ 42       j       102 $51\%$ $92\%$ $\cdot$ $\cdot$ 43       k       131 $51\%$ $92\%$ $\cdot$ $13\%$ 44       l       138 $57\%$ $93\%$ $\cdot$ $13\%$ 45       m       121 $60\%$ $33\%$ $\cdot$ $11\%$ 46       n       61 $55\%$ $51\%$ $5\%$ $5\%$ $5\%$ 47       o       89 $66\%$ $66\%$ $ -$ 48       p       90 $64\%$ $  -$ 49       q       87 $58\%$ $92\%$ $ -$ 51       s       92 $58\%$ $55\%$ $-$   | 20    | t         | 05         | /1%              |             |
| $39$ g $156$ $94\%$ $\cdot$ $40$ h $132$ $55\%$ $95\%$ $\cdot$ $41$ i $130$ $45\%$ $92\%$ $\cdot$ $42$ j $102$ $92\%$ $\cdot$ $7\%$ $43$ k $131$ $51\%$ $92\%$ $\cdot$ $7\%$ $44$ 1 $138$ $57\%$ $93\%$ $\cdot$ $13\%$ $44$ 1 $138$ $60\%$ $\cdot$ $11\%$ $45$ m $121$ $60\%$ $\cdot$ $11\%$ $46$ n $61$ $60\%$ $5\%$ $5\%$ $5\%$ $47$ $o$ $89$ $60\%$ $5\%$ $5\%$ $5\%$ $5\%$ $47$ $o$ $89$ $92\%$ $64\%$ $ 6\%$ $ 48$ $p$ $90$ $64\%$ $92\%$ $   50$ $r$ $79$ $75\%$ $58\%$ $19\%$ $    -$   | - 30  | 1         | 90         | 95%              | • •         |
| 35       g       130 $34\%$ $1.1$ 40       h       132 $55\%$ $95\%$ $$ 41       i       130 $45\%$ $$ $$ 41       i       130 $92\%$ $$ 42       j       102 $92\%$ $$ 43       k       131 $61\%$ $92\%$ $$ 44       1       138 $93\%$ $$ 45       m       121 $60\%$ $$ 46       n       61 $93\%$ $$ 47 $o$ $89$ $93\%$ $$ 48 $p$ $900$ $64\%$ $$ 49 $q$ $87$ $92\%$ $$ 50 $r$ $79$ $58\%$ $19\%$ 51 $s$ $92$ $84\%$ $$ 52 $t$ $88$ $91\%$ $$ 53 $x$ $75$ $56\%$ $32\%$ $12\%$  | 30    | ď         | 156        | 040/             |             |
| 40       h       132 $45\%$ 41       i       130 $92\%$  | - 55  | 8         | 100        | 55%              | ••          |
| $13$ $112$ $45\%$ $41$ $i$ $130$ $45\%$ $42$ $j$ $102$ $92\%$ $\cdot$ $43$ $k$ $131$ $85\%$ $\cdot$ $44$ $1$ $138$ $92\%$ $\cdot$ $44$ $1$ $138$ $60\%$ $33\%$ $\cdot$ $44$ $1$ $138$ $60\%$ $33\%$ $\cdot$ $13\%$ $44$ $1$ $138$ $60\%$ $33\%$ $\cdot$ $13\%$ $44$ $1$ $138$ $60\%$ $33\%$ $\cdot$ $13\%$ $45$ $m$ $121$ $85\%$ $0.11\%$ $0.56\%$ $0.11\%$ $46$ $n$ $61$ $56\%$ $93\%$ $5\%$ $0.5\%$ $47$ $o$ $89$ $900$ $92\%$ $$ $$ $48$ $p$ $90$ $52\%$ $5\%$ $19\%$ $$ $50$ $r$ $79$ $76\%$ $5\%$ $19\%$ $$ $51$ $s$ <th< td=""><td>40</td><td>h</td><td>132</td><td>Q5%</td><td></td></th<>  | 40    | h         | 132        | Q5%              |             |
| $ \begin{array}{c ccccccccccccccccccccccccccccccccccc$   | 10    | 11        | 102        | 45%              |             |
| 42       j       102 $61\%$ 43       k       131 $85\%$ $7\%$ 44       1       138 $93\%$ $13\%$ 44       1       138 $93\%$ $11\%$ 45       m       121 $85\%$ $11\%$ 46       n       61 $93\%$ $5\%$ 47       o       89 $92\%$ $6\%$ 48       p       90 $64\%$ $92\%$ $6\%$ 49       q       87 $92\%$ $5\%$ $19\%$ 50       r       79 $58\%$ $5\%$ $19\%$ 51       s       92 $84\%$ $15\%$ $5\%$ $19\%$ 52       t       88 $52\%$ $91\%$ $6\%$ $6\%$ 53       x       75 $56\%$ $32\%$ $12\%$   | 41    | i         | 130        | 92%              |             |
| 42       j       102 $92\%$ $7\%$ 43       k       131 $51\%$ $85\%$ $13\%$ 44       l       138 $57\%$ $93\%$ $13\%$ 44       l       138 $57\%$ $93\%$ $13\%$ 45       m       121 $60\%$ $11\%$ $11\%$ 46       n       61 $93\%$ $51\%$ $51\%$ 47 $0$ $89$ $60\%$ $56\%$ $5\%$ 48 $p$ $90$ $64\%$ $66\%$ $66\%$ $66\%$ $64\%$ $66\%$ $65\%$ $5\%$ $5\%$ $5\%$ $5\%$ 49 $q$ $87$ $58\%$ $52\%$ $55\%$ $19\%$ $55\%$ $19\%$ 50 $r$ $79$ $52\%$ $58\%$ $5\%$ $15\%$ $15\%$ $55\%$ $15\%$ 51 $s$ $92$ $84\%$ $15\%$ $15\%$ $52\%$ $55\%$ $15\%$ $55\%$ $15\%$ 52 $t$ $88$ $755$ $56\%$ $32\%$  |       |           |            | 61%              |             |
| 43       k       131 $51%$ 44       1       138 $57%$ 44       1       138 $93%$ 45       m       121 $85%$ .13%         46       n       61 $93%$ 47       o       89 $92%$ 48       p       90 $64%$ $68%$ 49       q       87 $58%$ $5%$ 50       r       79 $76%$ $5%$ 51       s       92 $64%$ $19%$ 51       s       92 $6%$ $15%$ 52       t       88 $52%$ $91%$ $$ 53       x       75 $56%$ $32%$ $12%$   | 42    | j         | 102        | 92%              | • 7%        |
| 43       k       131       85%       13%         44       1       138 $57\%$ $57\%$ 44       1       138 $93\%$ $\cdots$ 45       m       121 $60\%$ $11\%$ 46       n       61 $56\%$ $5\%$ $5\%$ 47       o       89 $92\%$ $5\%$ $5\%$ 48       p       90 $64\%$ $66\%$ $66\%$ $66\%$ $66\%$ $66\%$ $65\%$ $5\%$   |       | 0         |            | 51%              |             |
| $44$ 1 $138$ $57\%$ $45$ m $121$ $85\%$ $\cdot$ $46$ n $61$ $93\%$ $\cdot$ $46$ n $61$ $93\%$ $5\%$ $47$ o $89$ $92\%$ $\cdot$ $48$ p $90$ $64\%$ $6\%$ $49$ q $87$ $58\%$ $6\%$ $50$ r $79$ $58\%$ $5\%$ $51$ s $92$ $84\%$ $\cdot$ $15\%$ $52$ t $88$ $91\%$ $\cdot$ $6\%$ $53$ x $75$ $56\%$ $32\%$ $12\%$   | 43    | k         | 131        | 85%              | • 13%       |
| $44$ 1       138 $93\%$ $\cdots$ $45$ m       121 $60\%$ $46$ n $61$ $56\%$ $47$ o $89$ $60\%$ $47$ o $89$ $60\%$ $47$ o $89$ $60\%$ $47$ o $89$ $66\%$ $47$ o $89$ $66\%$ $47$ o $89$ $66\%$ $49$ $q$ $87$ $68\%$ $50$ $r$ $79$ $76\%$ $5\%$ $50$ $r$ $79$ $52\%$ $19\%$ $51$ $s$ $92$ $84\%$ $15\%$ $52$ $t$ $88$ $91\%$ $66\%$ $52\%$ $52\%$ $56\%$ $32\%$ $12\%$   |       |           |            | 57%              |             |
| $ \begin{array}{c ccccccccccccccccccccccccccccccccccc$   | 44    | 1         | 138        | 93%              | • ••        |
| 45       m $121$ $85%$ $11%$ $46$ n $61$ $93%$ $5%$ $47$ o $89$ $93%$ $5%$ $47$ o $89$ $92%$ $$ $48$ p $90$ $92%$ $$ $48$ p $90$ $66%$ $6%$ $49$ $q$ $87$ $79$ $76%$ $5%$ $19%$ $50$ r $79$ $76%$ $5%$ $19%$ $51$ s $92$ $84%$ $$ $15%$ $52$ t $88$ $91%$ $$ $6%$ $53$ x $75$ $56%$ $32%$ $12%$  |       |           |            | 60%              |             |
| $ \begin{array}{c ccccccccccccccccccccccccccccccccccc$   | 45    | m         | 121        | 85%              | • 11%       |
| $46$ n $61$ $601$ $93\%$ $5\%$ $47$ o $89$ $60\%$ $47$ o $89$ $92\%$ $\cdot$ $48$ p $90$ $92\%$ $6\%$ $49$ q $87$ $68\%$ $50$ r $79$ $76\%$ $5\%$ $50$ r $79$ $76\%$ $5\%$ $51$ s $92$ $84\%$ $\cdot$ $52$ t $88$ $52\%$ $53$ x $75$ $56\%$ $32\%$   | 10    |           | 01         | 56%              |             |
| $\begin{array}{c ccccccccccccccccccccccccccccccccccc$  | 46    | n         | 61         | 93%              | 5% •        |
| $\begin{array}{c ccccccccccccccccccccccccccccccccccc$  | 47    |           | 20         | 60%              |             |
| $\begin{array}{c ccccccccccccccccccccccccccccccccccc$  | 41    | 0         | - 69       | 92%              | • •         |
| $\begin{array}{c c c c c c c c c c c c c c c c c c c $   | 18    | n         | 90         | 0.20/            | <b>C</b> 0( |
| $\begin{array}{c ccccccccccccccccccccccccccccccccccc$  | 40    | P         | 30         | 68%              | 0% •        |
| $\begin{array}{c ccccccccccccccccccccccccccccccccccc$  | 49    | n         | 87         | 020/             |             |
| $ \begin{array}{c ccccccccccccccccccccccccccccccccccc$   | 10    | Ч         | 01         | 58%              |             |
| $\begin{array}{c ccccccccccccccccccccccccccccccccccc$  | 50    | r         | 79         | 76%              | 5% 19%      |
| $\begin{array}{c ccccccccccccccccccccccccccccccccccc$  |       | -         |            | 52%              |             |
| $ \begin{array}{c ccccccccccccccccccccccccccccccccccc$   | 51    | S         | 92         | 84%              | • 15%       |
| 52         t         88         91%         • 6%           53         x         75         56%         32%         12%   |       |           |            | 52%              |             |
| 53 x 75 56% 32% 12%  | 52    | t         | 88         | 91%              | • 6%        |
| 53 x 75 56% 32% 12%  |       |           |            | 41%              |             |
|  | 53    | х         | 75         | 56% 32%          | 12%         |

The following table lists non-polymeric compounds, carbohydrate monomers and non-standard residues in protein, DNA, RNA chains that are outliers for geometric or electron-density-fit criteria:

| Mol | Type | Chain | Res  | Chirality | Geometry | Clashes | Electron density |
|-----|------|-------|------|-----------|----------|---------|------------------|
| 54  | TEL  | А     | 3001 | Х         | -        | -       | -                |



### 2 Entry composition (i)

There are 55 unique types of molecules in this entry. The entry contains 146404 atoms, of which 0 are hydrogens and 0 are deuteriums.

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

• Molecule 1 is a RNA chain called 23S rRNA.

| Mol | Chain | Residues |                |            |            | AltConf    | Trace     |   |   |
|-----|-------|----------|----------------|------------|------------|------------|-----------|---|---|
| 1   | А     | 2887     | Total<br>61997 | C<br>27661 | N<br>11460 | O<br>19992 | Р<br>2884 | 0 | 0 |

• Molecule 2 is a RNA chain called 5S rRNA.

| Mol | Chain | Residues | Atoms         |           |          |          |          | AltConf | Trace |
|-----|-------|----------|---------------|-----------|----------|----------|----------|---------|-------|
| 2   | В     | 112      | Total<br>2392 | C<br>1068 | N<br>435 | 0<br>778 | Р<br>111 | 0       | 0     |

• Molecule 3 is a protein called 50S ribosomal protein L2.

| Mol | Chain | Residues | Atoms         |           |          |          |        | AltConf | Trace |
|-----|-------|----------|---------------|-----------|----------|----------|--------|---------|-------|
| 3   | С     | 272      | Total<br>2083 | C<br>1296 | N<br>408 | 0<br>373 | S<br>6 | 0       | 0     |

• Molecule 4 is a protein called 50S ribosomal protein L3.

| Mol | Chain | Residues | Atoms         |          |          |          |                | AltConf | Trace |
|-----|-------|----------|---------------|----------|----------|----------|----------------|---------|-------|
| 4   | D     | 206      | Total<br>1569 | C<br>985 | N<br>289 | O<br>290 | ${ m S}{ m 5}$ | 0       | 0     |

• Molecule 5 is a protein called 50S ribosomal protein L4.

| Mol | Chain | Residues | Atoms         |          |          |          | AltConf       | Trace |   |
|-----|-------|----------|---------------|----------|----------|----------|---------------|-------|---|
| 5   | Е     | 205      | Total<br>1561 | C<br>980 | N<br>289 | O<br>290 | $\frac{S}{2}$ | 0     | 0 |

• Molecule 6 is a protein called 50S ribosomal protein L5.

| Mol | Chain | Residues |               | Atoms    |          |          |          |   | Trace |
|-----|-------|----------|---------------|----------|----------|----------|----------|---|-------|
| 6   | F     | 176      | Total<br>1386 | C<br>882 | N<br>241 | O<br>256 | ${f S}7$ | 0 | 0     |



• Molecule 7 is a protein called 50S ribosomal protein L6.

| Mol | Chain | Residues |               | At       | oms      |          |   | AltConf | Trace |
|-----|-------|----------|---------------|----------|----------|----------|---|---------|-------|
| 7   | 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 8 is a protein called 50S ribosomal protein L13.

| Mol | Chain | Residues |       | At       | oms      |     |        | AltConf | Trace |
|-----|-------|----------|-------|----------|----------|-----|--------|---------|-------|
| 8   | J     | 142      | Total | C<br>710 | N<br>206 | 0   | S<br>5 | 0       | 0     |
|     |       |          | 1120  | 110      | 200      | 202 | 5      |         |       |

• Molecule 9 is a protein called 50S ribosomal protein L14.

| Mol | Chain | Residues |              | At       | oms      |          | Atoms  |   |   |  |  |
|-----|-------|----------|--------------|----------|----------|----------|--------|---|---|--|--|
| 9   | K     | 122      | Total<br>920 | C<br>571 | N<br>173 | 0<br>172 | S<br>4 | 0 | 0 |  |  |

• Molecule 10 is a protein called 50S ribosomal protein L15.

| Mol | Chain | Residues |               | At       | oms      |          |               | AltConf | Trace |
|-----|-------|----------|---------------|----------|----------|----------|---------------|---------|-------|
| 10  | L     | 146      | Total<br>1081 | C<br>671 | N<br>207 | O<br>201 | ${S \over 2}$ | 0       | 0     |

• Molecule 11 is a protein called 50S ribosomal protein L16.

| Mol | Chain | Residues |               | At       | oms      |          |            | AltConf | Trace |
|-----|-------|----------|---------------|----------|----------|----------|------------|---------|-------|
| 11  | М     | 135      | Total<br>1076 | C<br>690 | N<br>205 | 0<br>176 | ${f S}{5}$ | 0       | 0     |

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

| Mol | Chain | Residues |              | At       | oms      | AltConf  | Trace         |   |   |
|-----|-------|----------|--------------|----------|----------|----------|---------------|---|---|
| 12  | Ν     | 119      | Total<br>953 | C<br>583 | N<br>186 | 0<br>180 | ${S \atop 4}$ | 0 | 0 |

• Molecule 13 is a protein called 50S ribosomal protein L18.

| Mol | Chain | Residues |              | At       | oms      |          |        | AltConf | Trace |
|-----|-------|----------|--------------|----------|----------|----------|--------|---------|-------|
| 13  | О     | 120      | Total<br>912 | C<br>564 | N<br>176 | 0<br>171 | S<br>1 | 0       | 0     |

• Molecule 14 is a protein called 50S ribosomal protein L19.



| Mol | Chain | Residues |              | At       | oms      |          |        | AltConf | Trace |
|-----|-------|----------|--------------|----------|----------|----------|--------|---------|-------|
| 14  | Р     | 115      | Total<br>944 | C<br>600 | N<br>185 | 0<br>158 | S<br>1 | 0       | 0     |

• Molecule 15 is a protein called 50S ribosomal protein L20.

| Mol | Chain | Residues |              | At       | oms      | AltConf  | Trace         |   |   |
|-----|-------|----------|--------------|----------|----------|----------|---------------|---|---|
| 15  | Q     | 117      | Total<br>940 | C<br>591 | N<br>189 | 0<br>156 | ${S \atop 4}$ | 0 | 0 |

• Molecule 16 is a protein called 50S ribosomal protein L21.

| Mol | Chain | Residues |              | Ato      | ms       | AltConf  | Trace |   |
|-----|-------|----------|--------------|----------|----------|----------|-------|---|
| 16  | R     | 101      | Total<br>786 | C<br>501 | N<br>139 | O<br>146 | 0     | 0 |

• Molecule 17 is a protein called 50S ribosomal protein L22.

| Mol | Chain | Residues |              | At       | oms      |          |                 | AltConf | Trace |
|-----|-------|----------|--------------|----------|----------|----------|-----------------|---------|-------|
| 17  | S     | 109      | Total<br>842 | C<br>525 | N<br>164 | O<br>150 | ${ m S} { m 3}$ | 0       | 0     |

• Molecule 18 is a protein called 50S ribosomal protein L23.

| Mol | Chain | Residues |              | At       | AltConf  | Trace    |                 |   |   |
|-----|-------|----------|--------------|----------|----------|----------|-----------------|---|---|
| 18  | Т     | 90       | Total<br>725 | C<br>452 | N<br>134 | O<br>136 | ${ m S} { m 3}$ | 0 | 0 |

• Molecule 19 is a protein called 50S ribosomal protein L24.

| Mol | Chain | Residues |              | At       | oms      | AltConf  | Trace         |   |   |
|-----|-------|----------|--------------|----------|----------|----------|---------------|---|---|
| 19  | U     | 101      | Total<br>762 | C<br>478 | N<br>142 | 0<br>138 | $\frac{S}{4}$ | 0 | 0 |

• Molecule 20 is a protein called Nucleotide-binding protein ExpZ.

| Mol | Chain | Residues | Atoms         |           |          |          |        | AltConf | Trace |
|-----|-------|----------|---------------|-----------|----------|----------|--------|---------|-------|
| 20  | V     | 541      | Total<br>4177 | C<br>2637 | N<br>737 | 0<br>796 | S<br>7 | 0       | 0     |

There are 66 discrepancies between the modelled and reference sequences:



| Chain | Residue | Modelled | Actual | Comment               | Reference  |
|-------|---------|----------|--------|-----------------------|------------|
| V     | -5      | MET      | -      | initiating methionine | UNP P39115 |
| V     | -4      | HIS      | -      | expression tag        | UNP P39115 |
| V     | -3      | HIS      | -      | expression tag        | UNP P39115 |
| V     | -2      | HIS      | -      | expression tag        | UNP P39115 |
| V     | -1      | HIS      | -      | expression tag        | UNP P39115 |
| V     | 0       | HIS      | -      | expression tag        | UNP P39115 |
| V     | 1       | HIS      | -      | expression tag        | UNP P39115 |
| V     | 129     | GLN      | GLU    | engineered mutation   | UNP P39115 |
| V     | 432     | GLN      | GLU    | engineered mutation   | UNP P39115 |
| V     | 486     | ALA      | -      | expression tag        | UNP P39115 |
| V     | 487     | ALA      | -      | expression tag        | UNP P39115 |
| V     | 488     | ALA      | -      | expression tag        | UNP P39115 |
| V     | 489     | ALA      | -      | expression tag        | UNP P39115 |
| V     | 490     | ALA      | -      | expression tag        | UNP P39115 |
| V     | 491     | ALA      | -      | expression tag        | UNP P39115 |
| V     | 492     | ALA      | -      | expression tag        | UNP P39115 |
| V     | 493     | ALA      | -      | expression tag        | UNP P39115 |
| V     | 494     | ALA      | -      | expression tag        | UNP P39115 |
| V     | 495     | ALA      | -      | expression tag        | UNP P39115 |
| V     | 496     | ALA      | -      | expression tag        | UNP P39115 |
| V     | 497     | ALA      | -      | expression tag        | UNP P39115 |
| V     | 498     | ALA      | -      | expression tag        | UNP P39115 |
| V     | 499     | ALA      | -      | expression tag        | UNP P39115 |
| V     | 500     | ALA      | -      | expression tag        | UNP P39115 |
| V     | 501     | ALA      | -      | expression tag        | UNP P39115 |
| V     | 502     | ALA      | -      | expression tag        | UNP P39115 |
| V     | 503     | ALA      | -      | expression tag        | UNP P39115 |
| V     | 504     | ALA      | -      | expression tag        | UNP P39115 |
| V     | 505     | ALA      | -      | expression tag        | UNP P39115 |
| V     | 506     | ALA      | -      | expression tag        | UNP P39115 |
| V     | 507     | ALA      | -      | expression tag        | UNP P39115 |
| V     | 508     | ALA      | -      | expression tag        | UNP P39115 |
| V     | 509     | ALA      | -      | expression tag        | UNP P39115 |
| V     | 510     | ALA      | -      | expression tag        | UNP P39115 |
| V     | 511     | ALA      | -      | expression tag        | UNP P39115 |
| V     | 512     | ALA      | -      | expression tag        | UNP P39115 |
| V     | 513     | ALA      | -      | expression tag        | UNP P39115 |
| V     | 514     | ALA      | -      | expression tag        | UNP P39115 |
| V     | 515     | ALA      | -      | expression tag        | UNP P39115 |
| V     | 516     | ALA      | -      | expression tag        | UNP P39115 |
| V     | 517     | ALA      | -      | expression tag        | UNP P39115 |
| V     | 518     | ALA      | -      | expression tag        | UNP P39115 |
| V     | 519     | ALA      | -      | expression tag        | UNP P39115 |



| Chain | Residue | Modelled | Actual | Comment        | Reference  |
|-------|---------|----------|--------|----------------|------------|
| V     | 520     | ALA      | -      | expression tag | UNP P39115 |
| V     | 521     | ALA      | -      | expression tag | UNP P39115 |
| V     | 522     | ALA      | -      | expression tag | UNP P39115 |
| V     | 523     | ALA      | -      | expression tag | UNP P39115 |
| V     | 524     | ALA      | -      | expression tag | UNP P39115 |
| V     | 525     | ALA      | -      | expression tag | UNP P39115 |
| V     | 526     | ALA      | -      | expression tag | UNP P39115 |
| V     | 527     | ALA      | -      | expression tag | UNP P39115 |
| V     | 528     | ALA      | -      | expression tag | UNP P39115 |
| V     | 529     | ALA      | -      | expression tag | UNP P39115 |
| V     | 530     | ALA      | -      | expression tag | UNP P39115 |
| V     | 531     | ALA      | -      | expression tag | UNP P39115 |
| V     | 532     | ALA      | -      | expression tag | UNP P39115 |
| V     | 533     | ALA      | -      | expression tag | UNP P39115 |
| V     | 534     | ALA      | -      | expression tag | UNP P39115 |
| V     | 535     | ALA      | -      | expression tag | UNP P39115 |
| V     | 536     | ALA      | -      | expression tag | UNP P39115 |
| V     | 537     | ALA      | -      | expression tag | UNP P39115 |
| V     | 538     | ALA      | -      | expression tag | UNP P39115 |
| V     | 539     | ALA      | -      | expression tag | UNP P39115 |
| V     | 540     | ALA      | -      | expression tag | UNP P39115 |
| V     | 541     | ALA      | -      | expression tag | UNP P39115 |
| V     | 542     | ALA      | -      | expression tag | UNP P39115 |

Continued from previous page...

• Molecule 21 is a protein called 50S ribosomal protein L27.

| Mol | Chain | Residues |              | Ato      | ms       | AltConf  | Trace |   |
|-----|-------|----------|--------------|----------|----------|----------|-------|---|
| 21  | W     | 82       | Total<br>630 | C<br>390 | N<br>123 | 0<br>117 | 0     | 0 |

• Molecule 22 is a protein called 50S ribosomal protein L28.

| Mol | Chain | Residues |              | Atc      | $\mathbf{ms}$ | AltConf | Trace                  |   |   |
|-----|-------|----------|--------------|----------|---------------|---------|------------------------|---|---|
| 22  | Х     | 58       | Total<br>444 | C<br>275 | N<br>92       | 0<br>75 | $\frac{\mathrm{S}}{2}$ | 0 | 0 |

• Molecule 23 is a protein called 50S ribosomal protein L29.

| Mol | Chain | Residues | Atoms        |          |          |         |                 | AltConf | Trace |
|-----|-------|----------|--------------|----------|----------|---------|-----------------|---------|-------|
| 23  | Y     | 65       | Total<br>530 | C<br>328 | N<br>102 | O<br>98 | ${ m S} { m 2}$ | 0       | 0     |



• Molecule 24 is a protein called 50S ribosomal protein L30.

| Mol | Chain | Residues |       | Atc | $\mathbf{ms}$ | AltConf | Trace        |   |   |
|-----|-------|----------|-------|-----|---------------|---------|--------------|---|---|
| 24  | 7     | 59       | Total | С   | Ν             | Ο       | $\mathbf{S}$ | 0 | 0 |
| 24  |       | 90       | 455   | 281 | 89            | 84      | 1            | 0 | 0 |

• Molecule 25 is a protein called 50S ribosomal protein L32.

| Mol | Chain | Residues | Atoms        |          |         |         |          | AltConf | Trace |
|-----|-------|----------|--------------|----------|---------|---------|----------|---------|-------|
| 25  | 0     | 54       | Total<br>426 | C<br>262 | N<br>86 | 0<br>71 | ${f S}7$ | 0       | 0     |

• Molecule 26 is a protein called 50S ribosomal protein L33 1.

| Mol | Chain | Residues |              | Atc      | $\mathbf{ms}$ | AltConf | Trace  |   |   |
|-----|-------|----------|--------------|----------|---------------|---------|--------|---|---|
| 26  | 1     | 48       | Total<br>401 | С<br>244 | N<br>80       | O<br>73 | S<br>4 | 0 | 0 |

• Molecule 27 is a protein called 50S ribosomal protein L34.

| Mol  | Chain | Residues |     | Ato | $\mathbf{ms}$ | AltConf | Trace |   |
|------|-------|----------|-----|-----|---------------|---------|-------|---|
| 27 2 | 4.4   | Total    | С   | Ν   | Ο             | S       | 0     | 0 |
|      | Z     | 44       | 367 | 222 | 89            | 54      | 2     | 0 |

• Molecule 28 is a protein called 50S ribosomal protein L35.

| Mol | Chain | Residues |              | At       | oms      | AltConf | Trace   |   |   |
|-----|-------|----------|--------------|----------|----------|---------|---|---|---|
| 28  | 3     | 64       | Total<br>512 | C<br>321 | N<br>107 | 0<br>82 | $\begin{array}{c} \mathrm{S} \\ \mathrm{2} \end{array}$ | 0 | 0 |

• Molecule 29 is a protein called 50S ribosomal protein L36.

| Mol | Chain | Residues |              | Atc      | $\mathbf{ms}$ | AltConf | Trace          |   |   |
|-----|-------|----------|--------------|----------|---------------|---------|----------------|---|---|
| 29  | 4     | 37       | Total<br>296 | C<br>186 | N<br>60       | O<br>45 | ${ m S}{ m 5}$ | 0 | 0 |

• Molecule 30 is a protein called 50S ribosomal protein L31.

| Mol | Chain | Residues |              | Atc      | $\mathbf{ms}$ |         | AltConf    | Trace |   |
|-----|-------|----------|--------------|----------|---------------|---------|------------|-------|---|
| 30  | 6     | 63       | Total<br>499 | C<br>312 | N<br>91       | 0<br>91 | ${f S}{5}$ | 0     | 0 |

• Molecule 31 is a RNA chain called mRNA.



| Mol | Chain | Residues |             | Atoms   |        |         |        |   | Trace |
|-----|-------|----------|-------------|---------|--------|---------|--------|---|-------|
| 31  | 7     | 3        | Total<br>60 | С<br>27 | N<br>7 | O<br>23 | Р<br>3 | 0 | 0     |

• Molecule 32 is a protein called 50S ribosomal protein L1.

| Mol | Chain | Residues |               | Atoms     |          |          |                |   | Trace |
|-----|-------|----------|---------------|-----------|----------|----------|----------------|---|-------|
| 32  | 8     | 212      | Total<br>1599 | C<br>1015 | N<br>273 | O<br>306 | ${ m S}{ m 5}$ | 0 | 0     |

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

| Mol | Chain | Residues |                | 1          | 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 S2.

| Mol | Chain | Residues |               | Ate       |          | AltConf  | Trace  |   |   |
|-----|-------|----------|---------------|-----------|----------|----------|--------|---|---|
| 34  | b     | 218      | Total<br>1757 | C<br>1119 | N<br>309 | 0<br>323 | S<br>6 | 0 | 0 |

• 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 | 0<br>301 | $\frac{S}{3}$ | 0 | 0 |

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

| Mol | Chain | Residues |               | At       | oms      |          | AltConf       | Trace |   |
|-----|-------|----------|---------------|----------|----------|----------|---------------|-------|---|
| 36  | d     | 195      | Total<br>1568 | C<br>991 | N<br>291 | 0<br>284 | ${S \over 2}$ | 0     | 0 |

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

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

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



| Mol | Chain | Residues |              | At       | 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 | Atoms         |          |          |          |        | AltConf | Trace |
|-----|-------|----------|---------------|----------|----------|----------|--------|---------|-------|
| 39  | g     | 149      | Total<br>1181 | C<br>740 | N<br>220 | 0<br>215 | 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 | $\begin{array}{c} \mathrm{C} \\ 655 \end{array}$ | 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 |              | At       | oms      |          |        | AltConf | Trace |
|-----|-------|----------|--------------|----------|----------|----------|--------|---------|-------|
| 41  | i     | 125      | Total<br>966 | C<br>599 | N<br>191 | 0<br>175 | S<br>1 | 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 | $\begin{array}{c} \mathrm{S} \\ \mathrm{2} \end{array}$ | 0 | 0 |

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

| Mol | Chain | Residues |              | At       | oms      |          |               | AltConf | Trace |
|-----|-------|----------|--------------|----------|----------|----------|---------------|---------|-------|
| 43  | k     | 114      | Total<br>838 | C<br>516 | N<br>164 | 0<br>156 | ${S \over 2}$ | 0       | 0     |

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

| Mol | Chain | Residues |               | At       | oms      | Atoms    |   |   |   |  |  |
|-----|-------|----------|---------------|----------|----------|----------|---|---|---|--|--|
| 44  | 1     | 136      | Total<br>1052 | C<br>653 | N<br>211 | 0<br>186 | $\begin{array}{c} \mathrm{S} \\ \mathrm{2} \end{array}$ | 0 | 0 |  |  |

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



| Mol | Chain | Residues |              | Ato      | ms       |          | AltConf | Trace |
|-----|-------|----------|--------------|----------|----------|----------|---------|-------|
| 45  | m     | 108      | Total<br>868 | C<br>534 | N<br>176 | 0<br>158 | 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       | 0<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  | 0     | 85       | Total<br>710 | C<br>436 | N<br>144 | 0<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 | $\frac{\mathrm{S}}{2}$ | 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 | $\begin{array}{c} \mathrm{S} \\ \mathrm{2} \end{array}$ | 0 | 0 |

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

| Mol  | Chain | Residues |       | Ato | $\mathbf{ms}$ |    |   | AltConf | Trace |
|------|-------|----------|-------|-----|---------------|----|---|---------|-------|
| 50   | r     | 64       | Total | С   | Ν             | 0  | S | 0       | 0     |
| - 50 | 1     | 04       | 518   | 332 | 96            | 88 | 2 | 0       | 0     |

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

| Mol | Chain | Residues |              | At       | oms      |          |               | AltConf | Trace |
|-----|-------|----------|--------------|----------|----------|----------|---------------|---------|-------|
| 51  | s     | 78       | Total<br>633 | C<br>409 | N<br>112 | 0<br>110 | ${S \over 2}$ | 0       | 0     |

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



| Mol | Chain | Residues |              | At       | 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 RNA chain called P-tRNA(Leu).

| Mol | Chain | Residues |               | $\mathbf{A}^{\dagger}$ | AltConf  | Trace    |         |   |   |
|-----|-------|----------|---------------|------------------------|----------|----------|---------|---|---|
| 53  | x     | 75       | Total<br>1603 | C<br>714               | N<br>284 | O<br>530 | Р<br>75 | 0 | 0 |

• Molecule 54 is TELITHROMYCIN (three-letter code: TEL) (formula:  $C_{43}H_{65}N_5O_{10}$ ).



| Mol | Chain | Residues | I           | Aton    | ns     |         | AltConf |
|-----|-------|----------|-------------|---------|--------|---------|---------|
| 54  | А     | 1        | Total<br>58 | C<br>43 | N<br>5 | O<br>10 | 0       |

• Molecule 55 is ADENOSINE-5'-TRIPHOSPHATE (three-letter code: ATP) (formula:  $C_{10}H_{16}N_5O_{13}P_3$ ).





| Mol | Chain | Residues |       | AltConf |    |    |   |   |  |
|-----|-------|----------|-------|---------|----|----|---|---|--|
| 55  | V     | 1        | Total | С       | Ν  | Ο  | Р | 0 |  |
| 55  | v     | L        | 62    | 20      | 10 | 26 | 6 | 0 |  |
| 55  | V     | 1        | Total | С       | Ν  | Ο  | Р | 0 |  |
| 55  | v     | L        | 62    | 20      | 10 | 26 | 6 | 0 |  |



### 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: 23S rRNA





| U954   | A957<br>A958             | C959            | C962<br>6963           | A964<br>A965            | 0960<br>1      | A970           | U972           | 6973<br>A974   | C975<br>U976        | 1977<br>1977   | C980           | C981           | A987           | 6992           | 0000           | 0004           | A1003          | A1006<br>61007 |                | C1011          | A1019<br>A1020     | A1076          | A1027          | A1029          | G1030<br>C1031 | C1032          | A1036<br>C1037               | C1041          | A1042          | U1045          | C1051<br>C1052 | C1053<br>A1054       |                |                |       |                    |                |                       |
|--------|--------------------------|-----------------|------------------------|-------------------------|----------------|----------------|----------------|----------------|---------------------|----------------|----------------|----------------|----------------|----------------|----------------|----------------|----------------|----------------|----------------|----------------|--------------------|----------------|----------------|----------------|----------------|----------------|------------------------------|----------------|----------------|----------------|----------------|----------------------|----------------|----------------|-------|--------------------|----------------|-----------------------|
| A1055  | U1058<br>A1059           | A 1067          | G1068<br>011069        | G1071<br>G1071          | A1072<br>A1073 | 111079         |                | U1086<br>U1087 | G1088               | C1089          | U1090          | A1092          | G1093          | A1096          | A1097          | C1098          | C1099          | G1101          | G1102          | A1103          | 01104<br>G1105     | U1106          | U1107<br>G1108 | G1109          | C1110          |                | A1113                        | A1115          | A1116          | C1118          | A1119          | C1121                | C1122          | C1124          | C1125 | U1127              | U1128<br>U1129 | A1130 + A1131 + A1131 |
| A1132  | G1133                    | G1135           | 01136<br>G1137         | C1138                   | U1140          | A1141          | A1142<br>U1143 | A1144          | G1145               | 01146<br>01147 | C1148          | A1149          | C1150          | G1152          | G1153          | U1154 C1155    | G1156          | A1157<br>G1158 | U1 159         | G1160          | C1162              | A1172          | A1173<br>A1174 | A1175<br>U1176 | G1177<br>U1178 | A1179          | C1180<br>C1181<br>C1182      |                | C1186          | A1188          | A1197          | C1198<br>C1199       | 61200<br>A1201 | 61203<br>61203 | A1210 | C1216              |                |                       |
| n<br>H | с<br>С<br>G1220          | A1221<br>A1222  | C1223                  | U1226                   | A1235<br>G1236 | C1237<br>C1237 | 01239          | A1243          | A1244<br>G1245      | G1246          | G1248<br>C1248 | U1249<br>G1250 | U1251          | 79719          | G1259<br>41260 | C1261          | A1266          | A 1769         | C1270          | 01274          | G1275<br>G1276     | A1277          | C1279<br>C1279 | C1281          | 01282          | G1290          | A1293<br>A1294               | 01295<br>G1296 | A1305          | G1306<br>U1307 | G1311          | A1312<br>A1313       |                |                |       |                    |                |                       |
| A1314  | 41323<br>A1323           | G1324<br>A1325  | A1326<br>U1327         | C1328<br>C1328<br>C1329 | C1330          | C1333          | A1335          | C1330          | A1339<br>A1340      | U1341          | G1342<br>C1343 | C1344<br>U1345 | A1346          | U1350          | U1351<br>11352 | C1353          | C1354          | 61362<br>61363 | C1364          | U1365<br>C1366 | G1367<br>U1368     | C1369          | G1371<br>G1377 | U1373          | C1374<br>A1375 | G1376          | U1379                        | C1384<br>G1385 | A1388          | C1389<br>C1390 | U1391          | G1 <mark>3</mark> 97 |                |                |       |                    |                |                       |
| A1404  | C1415<br>G1416           | A1417<br>111418 | C1422                  | A1423<br>A1424<br>A1424 | C1425<br>A1426 | 111435         | U1436          | C143/          | A1442<br>C1443      |                | 01448<br>C1449 | C1450<br>U1451 | C1452          | A1453<br>C1454 | 111457         | U1458          | 01459          |                | A1464<br>A1465 | U1466          | 6140 <i>/</i>      | G1472<br>A1473 | C1474<br>G1475 | C1476          | G1481          | U1484          | A1485<br>G1486<br>G1486      | G1488          | 01469<br>A1490 | A1499          | U1500<br>U1501 | G1502                | A1506          |                |       |                    |                |                       |
| U1507  | C1508                    |                 |                        | G1526<br>G1526<br>G1526 | U1528<br>01528 | G1530          | G1531<br>A1532 | A1533<br>A1534 | U1535               | AL DOD         | C1539<br>A1540 | A1541          | A1542<br>U1543 | C1544<br>C1545 |                | U1549<br>C1550 | C1551<br>C1552 | A1553          | U<br>A1555     | A1556<br>G1557 | G1558              | U1560          | G1561<br>A1562 | G1563<br>C1564 | U1565<br>G1566 | U1567<br>G1568 | A1569                        | G1571          | C1573          | C1577          | G A            | A<br>I               | n              |                |       |                    |                |                       |
| A      | o ≼ ೮                    | D<br>N          | <br>G1589              | C1597                   | U1602<br>U1603 | C1604          | A1606          |                | C1613               | A1614          | A1617          | C1622          |                | 01626<br>A1627 | G1628          | A1631          | G1632<br>G1633 | U1634          | C1644          | C1645          | A1653<br>A1654     | A1655          | C1657<br>C1657 |                | A1661          | G1671<br>A1672 | A1679                        | A1680          | A1691<br>U1692 | C1693<br>G1694 | A1695<br>G1696 | A1697<br>G1698       |                |                |       |                    |                |                       |
| A1699  | C1701<br>C1701<br>U1702  | C1 705          | <b>G1706</b><br>111707 | U1708<br>A1709          | G1712          | A1713<br>A1714 | C1715          | 01/16<br>C1717 | G1718<br>G1719      | C1720          | G1726          | A1727          | C1731          | U1738          | C1739<br>C1740 |                | A1745<br>A1746 | G1747<br>G1748 | G1749          | G1750<br>U1751 | G1752<br>C1753     | C1 767         | U1758          | U1759<br>A1760 | G1761<br>G1762 | C1766          | A1767<br>A1768               | G1769<br>C1770 | C1771          | A1776          | A1778          | C1780                | TOTO           |                |       |                    |                |                       |
| G1782  | C17 03<br>A1784<br>G1785 | A1789           | 01790<br>01790         | G1792<br>G1793          | C1794          | A1797          | C1800          | 41801<br>A1802 | C1803<br>U1804      | G1805          | G1810          | C1811<br>A1812 | A1813          | A1814<br>A1815 | A1816<br>C1817 |                | A1820          | G1828<br>C1829 | G1830          | A1831<br>A1832 | <mark>G1833</mark> | A1839          | G1843<br>A1844 | A1845          | G1846<br>U1847 | A1848<br>U1849 | A1858                        | C1867          | C1872          | A 1076         |                | A1882<br>A1883       | CODTW          |                |       |                    |                |                       |
| G1884  | A1000<br>G1886<br>31887  | 1895            |                        |                         | C1903          | d.1904         | C1922          | G1932          | 61 <mark>935</mark> | A1941          | A1942          | C1943          | A1945          | 01946          | 01952          | C190           | A1956<br>A1957 | G1958          | 61700          | C1963          | A1966              | 01968          | C1970          | 01972          | U1973          | A1981          | 01 <mark>984</mark><br>01985 | 21991          | C1992          | C1994          | 01996          | A1998                | A1999<br>A2000 |                |       |                    |                |                       |
| G2001  | G2004                    | G2009<br>42010  |                        | G2021<br>U2022          | C2023<br>U2024 | C2025          |                | 42033<br>A2034 | C2035               | G2050          | 02051<br>A2052 | C2053<br>C2054 | U2055          | A2059          | A2060<br>C2061 | A2062          | 02063<br>G2064 | C2065          | G2068          | U2069<br>U2070 | A2071<br>C2072     |                | G2077          | C2079          | A2080<br>G2081 | C2084          | G2085                        | A2089<br>G2090 | A2091<br>C2092 | C2093<br>C2094 | G2098          | G2101                |                |                |       |                    |                |                       |
| C2102  | U2105                    | C2114           | U2121<br>G2122         | A2123<br>A2124          | U2125<br>G2126 | U2127          | U2128<br>G2129 | G2130          | U2131               | A2132          | A2134          | G2135          | C2136          | U2138          | G2139          | U2140          | C2142          | A2143          | G2144          | G2145<br>A2146 |                    | G2149          | G2150          | A2152          | G2153          | G2154          | G2156                        | C2158          | U2159<br>U2160 | G2161          | G2162          | A2165                | C2167          | G2168          | A2170 | G2171 •<br>C2172 • | G2173<br>C2174 | c2175                 |















• Molecule 16: 50S ribosomal protein L21







• •

13%

6% 6%

### A520 A522 A522 A522 A523 A531 A531 A534 A534 A533 A534 A533 A534 A533 A534 A537 A537 A537 A537 A537 A537 A540 A541

- Molecule 21: 50S ribosomal protein L27
  Chain W: 84%
  Molecule 22: 50S ribosomal protein L28
  Chain X: 87%
- $\bullet$  Molecule 23: 50S ribosomal protein L29



• Molecule 24: 50S ribosomal protein L30





| •        |    | •   |     |     |
|----------|----|-----|-----|-----|
| TM<br>BO | Y. | R24 | T48 | LYS |

| • Molecule 27: 50S ri   | bosomal protein L34   |  |   |
|---|---|--|---|
| Chain 2:  | 98%   |  |   |
| M1<br>100<br>100<br>100<br>100<br>100<br>100<br>100<br>100<br>100<br>1  |   |  |   |
| • Molecule 28: 50S ri   | bosomal protein L35   |  |   |
| Chain 3:  | 94%   |  | -   |
| MET<br>P2<br>K15<br>K16<br>L32<br>L32<br>L62<br>L95<br>LYS  |   |  |   |
| • Molecule 29: 50S ri   | bosomal protein L36   |  |   |
| Chain 4:  | 100%  |  | •   |
| M1<br>E12<br>K15<br>E28<br>G37  |   |  |   |
| • Molecule 30: 50S ri   | bosomal protein L31   |  |   |
| Chain 6:  | 67%<br>94%  | • 5'   | %   |
| M1<br>K2<br>A3<br>G4<br>K10<br>K11<br>A12<br>A17<br>C18   | d 19<br>N20<br>F 22<br>F 22<br>E 23<br>C 23<br>K 26<br>E 29<br>V 31<br>V 31<br>V 31<br>V 33<br>V 33<br>V 33<br>E 30<br>V 31<br>V 33<br>C 39<br>C 39<br>C 39<br>C 39<br>C 39<br>C 44 | P41<br>F42<br>Y43<br>C45<br>C45<br>C45<br>C45<br>C45<br>C45<br>F49<br>F49<br>F49<br>S51<br>S51 | D53<br>G54<br>R55<br>D57<br>R56<br>F59<br>C17<br>C17<br>LEV<br>LVS  |
| • Molecule 31: mRNA   | ł   |  |   |
| Chain 7:  | 67%   | 33%  | -   |
| C25<br>U26<br>U27   |   |  |   |
| • Molecule 32: 50S ri   | bosomal protein L1  |  |   |
|   | 89%   |  |   |
| Chain 8:  | 91%   | 9%   |   |
| MET<br>ALA<br>LYS<br>LYS<br>LYS<br>GLY<br>GLV<br>VAL<br>ALA<br>ALA<br>ALA<br>ALA<br>ALA<br>ALA<br>ALA<br>ALA<br>A | R17<br>518<br>721<br>721<br>721<br>722<br>722<br>723<br>726<br>726<br>726<br>726<br>726<br>726<br>728<br>728<br>728<br>729<br>729<br>733<br>733                                     | T35<br>A36<br>K37<br>F38<br>F38<br>D39<br>A40<br>T41<br>V42<br>E43<br>E43<br>A45<br>A45        | R47<br>148<br>49<br>951<br>952<br>853<br>853<br>853<br>955<br>955<br>955<br>955<br>955<br>853<br>850                            |
|   |   |  |   |
| 661<br>A62<br>V63<br>V64<br>V64<br>P66<br>N67<br>C68<br>C68<br>C68<br>C68<br>C70<br>C70<br>C72                    | 973<br>177<br>177<br>177<br>177<br>177<br>177<br>177<br>177<br>177<br>1   | G91<br>A92<br>F94<br>F94<br>V95<br>G96<br>D97<br>T98<br>D97<br>T98<br>D99<br>Y100<br>Y100      | K103<br>1104<br>q105<br>q106<br>f107<br>K108<br>F111<br>D112<br>V113<br>V113<br>V115<br>A116<br>A116<br>P1118<br>P1118<br>P1118 |
|   |   |  |   |



























• Molecule 53: P-tRNA(Leu)





# 4 Experimental information (i)

| Property                           | Value                        | Source    |
|------------------------------------|------------------------------|-----------|
| EM reconstruction method           | SINGLE PARTICLE              | Depositor |
| Imposed symmetry                   | POINT, C1                    | Depositor |
| Number of particles used           | 28972                        | 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 $(e^-/\text{\AA}^2)$ | 1.425                        | Depositor |
| Minimum defocus (nm)               | Not provided                 |           |
| Maximum defocus (nm)               | Not provided                 |           |
| Magnification                      | Not provided                 |           |
| Image detector                     | FEI FALCON III $(4k \ge 4k)$ | Depositor |
| Maximum map value                  | 0.634                        | Depositor |
| Minimum map value                  | -0.379                       | Depositor |
| Average map value                  | 0.003                        | Depositor |
| Map value standard deviation       | 0.027                        | Depositor |
| Recommended contour level          | 0.11                         | Depositor |
| Map size (Å)                       | 381.96, 381.96, 381.96       | wwPDB     |
| Map dimensions                     | 360, 360, 360                | wwPDB     |
| Map angles (°)                     | 90.0, 90.0, 90.0             | wwPDB     |
| Pixel spacing (Å)                  | 1.061, 1.061, 1.061          | Depositor |



## 5 Model quality (i)

### 5.1 Standard geometry (i)

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

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).

| Mal  | Chain | B    | ond lengths     | Bond angles |                   |  |  |  |
|------|-------|------|-----------------|-------------|-------------------|--|--|--|
| NIOI | Chain | RMSZ | # Z  > 5        | RMSZ        | # Z  > 5          |  |  |  |
| 1    | А     | 1.05 | 17/69438~(0.0%) | 1.31        | 711/108311~(0.7%) |  |  |  |
| 2    | В     | 0.79 | 0/2675          | 1.34        | 36/4170~(0.9%)    |  |  |  |
| 3    | С     | 0.59 | 0/2120          | 0.76        | 0/2845            |  |  |  |
| 4    | D     | 0.61 | 0/1591          | 0.75        | 1/2132~(0.0%)     |  |  |  |
| 5    | Ε     | 0.54 | 0/1580          | 0.74        | 2/2132~(0.1%)     |  |  |  |
| 6    | F     | 0.44 | 0/1405          | 0.83        | 4/1887~(0.2%)     |  |  |  |
| 7    | G     | 0.40 | 0/1360          | 0.70        | 0/1832            |  |  |  |
| 8    | J     | 0.57 | 0/1146          | 0.78        | 0/1542            |  |  |  |
| 9    | Κ     | 0.60 | 0/927           | 0.79        | 1/1245~(0.1%)     |  |  |  |
| 10   | L     | 0.53 | 0/1093          | 0.77        | 2/1457~(0.1%)     |  |  |  |
| 11   | М     | 0.55 | 0/1099          | 0.76        | 0/1468            |  |  |  |
| 12   | Ν     | 0.54 | 0/960           | 0.74        | 0/1284            |  |  |  |
| 13   | 0     | 0.45 | 0/921           | 0.77        | 0/1236            |  |  |  |
| 14   | Р     | 0.55 | 0/957           | 0.77        | 0/1279            |  |  |  |
| 15   | Q     | 0.62 | 0/952           | 0.81        | 2/1266~(0.2%)     |  |  |  |
| 16   | R     | 0.62 | 0/797           | 0.87        | 4/1070~(0.4%)     |  |  |  |
| 17   | S     | 0.54 | 0/851           | 0.78        | 2/1146~(0.2%)     |  |  |  |
| 18   | Т     | 0.52 | 0/731           | 0.71        | 0/974             |  |  |  |
| 19   | U     | 0.51 | 1/772~(0.1%)    | 0.75        | 0/1032            |  |  |  |
| 20   | V     | 0.41 | 0/4247          | 0.72        | 3/5736~(0.1%)     |  |  |  |
| 21   | W     | 0.62 | 0/638           | 0.94        | 2/847~(0.2%)      |  |  |  |
| 22   | Х     | 0.46 | 0/448           | 0.77        | 1/596~(0.2%)      |  |  |  |
| 23   | Y     | 0.44 | 0/531           | 0.70        | 0/707             |  |  |  |
| 24   | Z     | 0.47 | 0/457           | 0.79        | 0/613             |  |  |  |
| 25   | 0     | 0.61 | 0/433           | 0.81        | 0/574             |  |  |  |
| 26   | 1     | 0.57 | 0/406           | 0.76        | 1/540~(0.2%)      |  |  |  |
| 27   | 2     | 0.58 | 0/370           | 0.78        | 0/483             |  |  |  |
| 28   | 3     | 0.55 | 0/519           | 0.70        | 0/680             |  |  |  |
| 29   | 4     | 0.47 | 0/299           | 0.66        | 0/393             |  |  |  |
| 30   | 6     | 0.42 | 0/509           | 0.72        | 0/678             |  |  |  |
| 31   | 7     | 0.61 | 0/65            | 1.36        | 2/98~(2.0%)       |  |  |  |
| 32   | 8     | 0.32 | 0/1624          | 0.66        | 0/2192            |  |  |  |



| Mal | Chain | В    | ond lengths      |      | Bond angles        |
|-----|-------|------|------------------|------|--------------------|
|     | Unain | RMSZ | # Z  > 5         | RMSZ | # Z  > 5           |
| 33  | a     | 0.63 | 1/36826~(0.0%)   | 1.23 | 291/57450~(0.5%)   |
| 34  | b     | 0.35 | 0/1782           | 0.71 | 3/2392~(0.1%)      |
| 35  | с     | 0.38 | 0/1641           | 0.67 | 0/2208             |
| 36  | d     | 0.36 | 0/1598           | 0.72 | 0/2147             |
| 37  | е     | 0.39 | 0/1230           | 0.75 | 1/1655~(0.1%)      |
| 38  | f     | 0.32 | 0/766            | 0.61 | 0/1031             |
| 39  | g     | 0.38 | 0/1196           | 0.75 | 0/1604             |
| 40  | h     | 0.36 | 0/1048           | 0.75 | 0/1407             |
| 41  | i     | 0.38 | 0/979            | 0.76 | 2/1315~(0.2%)      |
| 42  | j     | 0.38 | 0/773            | 0.70 | 0/1044             |
| 43  | k     | 0.35 | 0/852            | 0.70 | 1/1153~(0.1%)      |
| 44  | 1     | 0.37 | 0/1069           | 0.79 | 3/1435~(0.2%)      |
| 45  | m     | 0.36 | 0/873            | 0.76 | 1/1166~(0.1%)      |
| 46  | n     | 0.41 | 0/507            | 0.82 | 1/672~(0.1%)       |
| 47  | 0     | 0.33 | 0/718            | 0.62 | 0/960              |
| 48  | р     | 0.39 | 0/708            | 0.73 | 0/950              |
| 49  | q     | 0.40 | 0/699            | 0.79 | 1/933~(0.1%)       |
| 50  | r     | 0.33 | 0/526            | 0.67 | 0/705              |
| 51  | s     | 0.35 | 0/649            | 0.69 | 0/872              |
| 52  | t     | 0.36 | 0/639            | 0.65 | 0/852              |
| 53  | Х     | 0.65 | 0/1790           | 1.52 | 28/2787~(1.0%)     |
| All | All   | 0.81 | 19/158790~(0.0%) | 1.17 | 1106/237183~(0.5%) |

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 | <b>#Planarity outliers</b> |
|-----|-------|---------------------|----------------------------|
| 3   | С     | 0                   | 1                          |
| 4   | D     | 0                   | 1                          |
| 6   | F     | 0                   | 3                          |
| 8   | J     | 0                   | 1                          |
| 10  | L     | 0                   | 2                          |
| 13  | 0     | 0                   | 1                          |
| 15  | Q     | 0                   | 1                          |
| 16  | R     | 0                   | 2                          |
| 17  | S     | 0                   | 1                          |
| 20  | V     | 0                   | 11                         |
| 25  | 0     | 0                   | 2                          |
| 30  | 6     | 0                   | 1                          |
| 34  | b     | 0                   | 5                          |



| Mol | Chain | #Chirality outliers | #Planarity outliers |
|-----|-------|---------------------|---------------------|
| 36  | d     | 0                   | 5                   |
| 37  | е     | 0                   | 1                   |
| 38  | f     | 0                   | 1                   |
| 39  | g     | 0                   | 2                   |
| 40  | h     | 0                   | 1                   |
| 44  | 1     | 0                   | 2                   |
| 45  | m     | 0                   | 3                   |
| 47  | 0     | 0                   | 1                   |
| 49  | q     | 0                   | 1                   |
| 50  | r     | 0                   | 2                   |
| All | All   | 0                   | 51                  |

Continued from previous page...

All (19) bond length outliers are listed below:

| Mol | Chain | Res  | Type | Atoms  | Z     | Observed(Å) | $\operatorname{Ideal}(\operatorname{\AA})$ |
|-----|-------|------|------|--------|-------|-------------|--|
| 1   | А     | 631  | G    | N9-C4  | -7.63 | 1.31        | 1.38                                       |
| 1   | А     | 830  | А    | N9-C4  | -6.90 | 1.33        | 1.37                                       |
| 1   | А     | 1067 | А    | N9-C4  | -6.87 | 1.33        | 1.37                                       |
| 1   | А     | 574  | А    | N9-C4  | -6.32 | 1.34        | 1.37                                       |
| 1   | А     | 631  | G    | C2-N3  | -5.92 | 1.28        | 1.32                                       |
| 1   | А     | 776  | G    | C8-N7  | -5.80 | 1.27        | 1.30                                       |
| 1   | А     | 1812 | А    | N9-C4  | -5.80 | 1.34        | 1.37                                       |
| 1   | А     | 700  | U    | C1'-N1 | 5.70  | 1.57        | 1.48                                       |
| 1   | А     | 1188 | А    | N9-C4  | -5.57 | 1.34        | 1.37                                       |
| 1   | А     | 847  | А    | N9-C4  | -5.52 | 1.34        | 1.37                                       |
| 19  | U     | 3    | VAL  | CB-CG1 | -5.48 | 1.41        | 1.52                                       |
| 1   | А     | 1820 | А    | N9-C4  | -5.47 | 1.34        | 1.37                                       |
| 1   | А     | 776  | G    | N7-C5  | -5.47 | 1.35        | 1.39                                       |
| 33  | а     | 993  | А    | N9-C4  | 5.43  | 1.41        | 1.37                                       |
| 1   | А     | 572  | А    | N9-C4  | -5.38 | 1.34        | 1.37                                       |
| 1   | А     | 589  | G    | N9-C4  | -5.37 | 1.33        | 1.38                                       |
| 1   | A     | 1054 | A    | N9-C4  | -5.18 | 1.34        | 1.37                                       |
| 1   | А     | 374  | А    | N9-C4  | -5.00 | 1.34        | 1.37                                       |
| 1   | А     | 589  | G    | N3-C4  | -5.00 | 1.31        | 1.35                                       |

All (1106) bond angle outliers are listed below:

| Mol | Chain | Res  | Type | Atoms     | Z      | $Observed(^{o})$ | $Ideal(^{o})$ |
|-----|-------|------|------|-----------|--------|------------------|---------------|
| 33  | a     | 1502 | A    | C8-N9-C4  | -14.51 | 100.00           | 105.80        |
| 53  | Х     | 6    | G    | O5'-P-OP2 | -14.04 | 93.07            | 105.70        |
| 1   | А     | 756  | U    | N3-C2-O2  | -12.07 | 113.75           | 122.20        |
| 1   | А     | 2054 | С    | C5-C6-N1  | 12.06  | 127.03           | 121.00        |



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| Mol | Chain | Res  | Type | Atoms       | Z      | $Observed(^{o})$ | $Ideal(^{o})$ |
|-----|-------|------|------|-------------|--------|------------------|---------------|
| 1   | А     | 2243 | С    | N1-C2-O2    | 11.98  | 126.09           | 118.90        |
| 1   | А     | 2334 | U    | C5-C4-O4    | -11.91 | 118.75           | 125.90        |
| 1   | А     | 2334 | U    | O4'-C1'-N1  | 11.30  | 117.24           | 108.20        |
| 33  | a     | 1502 | A    | N7-C8-N9    | 11.27  | 119.43           | 113.80        |
| 1   | А     | 2334 | U    | C2-N1-C1'   | 11.01  | 130.92           | 117.70        |
| 53  | Х     | 8    | U    | O5'-P-OP1   | 10.86  | 123.73           | 110.70        |
| 1   | А     | 398  | U    | N3-C2-O2    | -10.81 | 114.63           | 122.20        |
| 1   | А     | 2025 | C    | N3-C2-O2    | -10.76 | 114.37           | 121.90        |
| 1   | А     | 1943 | С    | N1-C2-O2    | 10.51  | 125.21           | 118.90        |
| 1   | А     | 2243 | C    | N3-C2-O2    | -10.51 | 114.54           | 121.90        |
| 2   | В     | 24   | C    | N1-C2-O2    | 10.51  | 125.21           | 118.90        |
| 1   | А     | 92   | G    | C8-N9-C4    | 10.44  | 110.58           | 106.40        |
| 1   | А     | 589  | G    | N3-C4-N9    | -10.43 | 119.74           | 126.00        |
| 1   | А     | 631  | G    | N3-C4-C5    | 10.38  | 133.79           | 128.60        |
| 1   | А     | 2157 | C    | N1-C2-O2    | 10.38  | 125.13           | 118.90        |
| 1   | А     | 631  | G    | N3-C4-N9    | -10.30 | 119.82           | 126.00        |
| 1   | А     | 483  | С    | C5-C6-N1    | 10.07  | 126.04           | 121.00        |
| 1   | А     | 769  | А    | N1-C6-N6    | -10.07 | 112.56           | 118.60        |
| 1   | А     | 1527 | С    | C2-N1-C1'   | 10.07  | 129.87           | 118.80        |
| 1   | А     | 2335 | U    | N3-C2-O2    | -9.96  | 115.23           | 122.20        |
| 33  | a     | 1009 | С    | C2-N1-C1'   | 9.92   | 129.72           | 118.80        |
| 1   | А     | 2695 | C    | N1-C2-O2    | 9.74   | 124.74           | 118.90        |
| 1   | А     | 2334 | U    | C6-N1-C1'   | -9.58  | 107.78           | 121.20        |
| 33  | a     | 1176 | A    | O5'-P-OP1   | -9.46  | 97.19            | 105.70        |
| 1   | А     | 1366 | С    | C5-C6-N1    | 9.40   | 125.70           | 121.00        |
| 1   | А     | 631  | G    | C4-N9-C1'   | -9.31  | 114.40           | 126.50        |
| 1   | А     | 2822 | С    | C2-N1-C1'   | 9.25   | 128.98           | 118.80        |
| 33  | a     | 1009 | С    | N1-C2-O2    | 9.21   | 124.43           | 118.90        |
| 33  | a     | 1076 | С    | N1-C2-O2    | 9.07   | 124.34           | 118.90        |
| 33  | a     | 1046 | G    | O5'-P-OP1   | -9.06  | 97.54            | 105.70        |
| 1   | А     | 2025 | С    | N1-C2-O2    | 9.05   | 124.33           | 118.90        |
| 2   | В     | 62   | U    | C2-N1-C1'   | 9.04   | 128.54           | 117.70        |
| 1   | А     | 1476 | С    | C5-C6-N1    | 9.03   | 125.51           | 121.00        |
| 1   | A     | 1353 | С    | C2-N1-C1'   | 9.01   | 128.71           | 118.80        |
| 1   | А     | 442  | С    | C6-N1-C2    | -8.99  | 116.70           | 120.30        |
| 33  | a     | 60   | C    | C6-N1-C2    | -8.92  | 116.73           | 120.30        |
| 1   | A     | 2350 | G    | N3-C4-C5    | -8.86  | 124.17           | 128.60        |
| 53  | x     | 19   | U    | O5'-P-OP2   | -8.84  | 97.75            | 105.70        |
| 33  | a     | 1502 | A    | C5'-C4'-O4' | -8.71  | 98.65            | 109.10        |
| 1   | A     | 2334 | U    | N3-C4-O4    | 8.70   | 125.49           | 119.40        |
| 33  | a     | 1076 | C    | C2-N1-C1'   | 8.68   | 128.34           | 118.80        |
| 33  | a     | 1331 | C    | C2-N1-C1'   | 8.66   | 128.33           | 118.80        |



| $\alpha$ $\cdot$ $\cdot$ $\cdot$ | C    | •        |      |
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|                                  | J    | 1        | 1 5  |

| Mol | Chain | Res  | Type | Atoms                  | Z     | $Observed(^{o})$    | $Ideal(^{o})$ |
|-----|-------|------|------|------------------------|-------|---------------------|---------------|
| 1   | А     | 2695 | С    | N3-C2-O2               | -8.65 | 115.84              | 121.90        |
| 33  | a     | 101  | С    | N1-C2-O2               | 8.63  | 124.08              | 118.90        |
| 1   | А     | 442  | С    | C5-C6-N1               | 8.62  | 125.31              | 121.00        |
| 1   | А     | 1943 | С    | N3-C2-O2               | -8.61 | 115.87              | 121.90        |
| 1   | А     | 272  | С    | N1-C2-O2               | 8.54  | 124.02              | 118.90        |
| 2   | В     | 24   | С    | C2-N1-C1'              | 8.51  | 128.16              | 118.80        |
| 1   | А     | 1872 | С    | C6-N1-C2               | -8.51 | 116.90              | 120.30        |
| 33  | а     | 101  | С    | N3-C2-O2               | -8.47 | 115.97              | 121.90        |
| 33  | а     | 989  | С    | N1-C2-O2               | 8.46  | 123.98              | 118.90        |
| 1   | А     | 2918 | G    | C4-N9-C1'              | 8.45  | 137.49              | 126.50        |
| 21  | W     | 28   | ARG  | NE-CZ-NH2              | 8.44  | 124.52              | 120.30        |
| 1   | А     | 75   | G    | O4'-C1'-N9             | 8.40  | 114.92              | 108.20        |
| 1   | А     | 769  | А    | N1-C2-N3               | -8.38 | 125.11              | 129.30        |
| 1   | А     | 1872 | С    | C5-C6-N1               | 8.36  | 125.18              | 121.00        |
| 1   | А     | 631  | G    | C8-N9-C1'              | 8.34  | 137.84              | 127.00        |
| 1   | А     | 588  | С    | N1-C2-O2               | 8.32  | 123.89              | 118.90        |
| 1   | А     | 1133 | G    | O4'-C1'-N9             | 8.27  | 114.82              | 108.20        |
| 1   | А     | 442  | С    | O5'-P-OP1              | 8.26  | 120.62              | 110.70        |
| 1   | А     | 1707 | U    | N3-C2-O2               | -8.26 | 116.42              | 122.20        |
| 1   | А     | 1985 | U    | N3-C2-O2               | -8.21 | 116.45              | 122.20        |
| 1   | А     | 2054 | С    | C6-N1-C2               | -8.19 | 117.02              | 120.30        |
| 1   | А     | 1343 | С    | C2-N1-C1'              | 8.19  | 127.81              | 118.80        |
| 1   | А     | 1527 | С    | N1-C2-O2               | 8.18  | 123.81              | 118.90        |
| 1   | А     | 508  | С    | C2-N1-C1'              | 8.16  | 127.78              | 118.80        |
| 1   | А     | 442  | С    | O5'-P-OP2              | -8.16 | 98.36               | 105.70        |
| 53  | Х     | 42   | А    | P-O3'-C3'              | 8.16  | 129.49              | 119.70        |
| 1   | А     | 2335 | U    | C6-N1-C2               | -8.16 | 116.11              | 121.00        |
| 1   | А     | 398  | U    | N1-C2-O2               | 8.14  | 128.50              | 122.80        |
| 33  | a     | 1170 | С    | C6-N1-C2               | -8.13 | 117.05              | 120.30        |
| 1   | А     | 397  | U    | N1-C2-O2               | 8.09  | 128.46              | 122.80        |
| 33  | a     | 1076 | С    | C6-N1-C2               | -8.09 | 117.06              | 120.30        |
| 33  | a     | 620  | С    | N1-C2-O2               | 8.08  | 123.75              | 118.90        |
| 1   | А     | 1343 | С    | C6-N1-C2               | -8.07 | 117.07              | 120.30        |
| 1   | А     | 2105 | U    | C2-N1-C1'              | 8.05  | 127.36              | 117.70        |
| 1   | А     | 1352 | U    | C2-N1-C1'              | 8.03  | 127.33              | 117.70        |
| 1   | А     | 648  | G    | O4'-C1'-N9             | 8.02  | 114.61              | 108.20        |
| 1   | А     | 483  | С    | C6-N1-C2               | -8.01 | 117.09              | 120.30        |
| 1   | A     | 756  | U    | N1-C2-O2               | 8.01  | 128.41              | 122.80        |
| 1   | A     | 2350 | G    | C4-N9-C1'              | 8.00  | 136.90              | 126.50        |
| 1   | A     | 719  | C    | C5-C6-N1               | 8.00  | 125.00              | 121.00        |
| 1   | A     | 589  | G    | $C8-N9-\overline{C1'}$ | 8.00  | $137.4\overline{0}$ | 127.00        |
| 1   | А     | 1527 | С    | C5-C6-N1               | 7.94  | 124.97              | 121.00        |


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| Mol | Chain | Res  | Type | Atoms     | Z     | $Observed(^{o})$ | $Ideal(^{o})$ |
|-----|-------|------|------|-----------|-------|------------------|---------------|
| 33  | a     | 1331 | С    | N1-C2-O2  | 7.92  | 123.65           | 118.90        |
| 1   | А     | 1067 | А    | C5-N7-C8  | -7.92 | 99.94            | 103.90        |
| 53  | X     | 20   | А    | P-O3'-C3' | 7.91  | 129.19           | 119.70        |
| 1   | А     | 1476 | С    | C6-N1-C2  | -7.91 | 117.14           | 120.30        |
| 1   | А     | 2105 | U    | N1-C2-O2  | 7.90  | 128.33           | 122.80        |
| 1   | А     | 573  | С    | N1-C2-O2  | 7.88  | 123.63           | 118.90        |
| 1   | А     | 2296 | А    | O5'-P-OP1 | -7.88 | 98.61            | 105.70        |
| 1   | А     | 589  | G    | N9-C4-C5  | 7.86  | 108.54           | 105.40        |
| 1   | А     | 1571 | G    | O5'-P-OP2 | -7.86 | 98.63            | 105.70        |
| 33  | a     | 1439 | С    | N3-C2-O2  | -7.84 | 116.41           | 121.90        |
| 33  | a     | 1305 | С    | N3-C2-O2  | -7.83 | 116.42           | 121.90        |
| 1   | А     | 1036 | А    | C8-N9-C4  | -7.83 | 102.67           | 105.80        |
| 33  | a     | 136  | U    | N3-C2-O2  | -7.80 | 116.74           | 122.20        |
| 1   | А     | 397  | U    | N3-C2-O2  | -7.80 | 116.74           | 122.20        |
| 1   | А     | 645  | С    | C6-N1-C2  | -7.80 | 117.18           | 120.30        |
| 1   | А     | 2768 | U    | N3-C2-O2  | -7.76 | 116.77           | 122.20        |
| 1   | А     | 2114 | С    | C2-N1-C1' | 7.75  | 127.33           | 118.80        |
| 33  | a     | 1037 | С    | N1-C2-O2  | 7.75  | 123.55           | 118.90        |
| 1   | А     | 672  | С    | C6-N1-C2  | -7.75 | 117.20           | 120.30        |
| 1   | А     | 1872 | С    | C2-N1-C1' | 7.74  | 127.32           | 118.80        |
| 1   | А     | 2485 | С    | C5-C6-N1  | 7.74  | 124.87           | 121.00        |
| 1   | А     | 831  | U    | N3-C2-O2  | -7.73 | 116.79           | 122.20        |
| 1   | А     | 2388 | С    | O5'-P-OP2 | -7.73 | 98.75            | 105.70        |
| 33  | a     | 993  | A    | C2-N3-C4  | 7.71  | 114.46           | 110.60        |
| 1   | А     | 2255 | С    | N1-C2-O2  | 7.69  | 123.51           | 118.90        |
| 1   | А     | 1028 | С    | N1-C2-O2  | 7.68  | 123.51           | 118.90        |
| 33  | a     | 143  | С    | N3-C2-O2  | -7.68 | 116.52           | 121.90        |
| 1   | A     | 1343 | С    | C5-C6-N1  | 7.68  | 124.84           | 121.00        |
| 1   | A     | 272  | С    | N3-C2-O2  | -7.67 | 116.53           | 121.90        |
| 53  | x     | 21   | G    | C4-N9-C1' | 7.67  | 136.47           | 126.50        |
| 1   | А     | 1771 | С    | N1-C2-O2  | 7.66  | 123.50           | 118.90        |
| 2   | В     | 24   | С    | N3-C2-O2  | -7.66 | 116.54           | 121.90        |
| 1   | A     | 1985 | U    | N1-C2-O2  | 7.66  | 128.16           | 122.80        |
| 2   | В     | 79   | С    | N1-C2-O2  | 7.65  | 123.49           | 118.90        |
| 1   | А     | 1374 | С    | N1-C2-O2  | 7.65  | 123.49           | 118.90        |
| 1   | А     | 2356 | A    | N7-C8-N9  | 7.62  | 117.61           | 113.80        |
| 1   | A     | 92   | G    | N7-C8-N9  | -7.62 | 109.29           | 113.10        |
| 1   | A     | 1963 | C    | C6-N1-C2  | -7.62 | 117.25           | 120.30        |
| 33  | a     | 60   | C    | C5-C6-N1  | 7.61  | 124.81           | 121.00        |
| 33  | a     | 1009 | С    | N3-C2-O2  | -7.61 | 116.57           | 121.90        |
| 1   | A     | 2157 | C    | N3-C2-O2  | -7.60 | 116.58           | 121.90        |
| 1   | A     | 1817 | C    | C2-N1-C1' | 7.58  | 127.14           | 118.80        |



| $\alpha$ $\cdot$ $\cdot$ $\cdot$ | C    | •        |      |
|----------------------------------|------|----------|------|
| Continued                        | trom | previous | page |
|                                  | J    | 1        | 1 5  |

| Mol | Chain | Res  | Type | Atoms      | Z     | $Observed(^{o})$ | $Ideal(^{o})$ |
|-----|-------|------|------|------------|-------|------------------|---------------|
| 1   | А     | 2072 | С    | N1-C2-O2   | 7.57  | 123.44           | 118.90        |
| 33  | a     | 620  | С    | N3-C2-O2   | -7.57 | 116.60           | 121.90        |
| 33  | a     | 1047 | С    | C6-N1-C2   | -7.56 | 117.28           | 120.30        |
| 1   | А     | 1831 | А    | N7-C8-N9   | 7.55  | 117.57           | 113.80        |
| 1   | А     | 508  | С    | N1-C2-O2   | 7.54  | 123.42           | 118.90        |
| 2   | В     | 15   | С    | C5-C6-N1   | 7.54  | 124.77           | 121.00        |
| 1   | А     | 1122 | С    | N1-C2-O2   | 7.53  | 123.42           | 118.90        |
| 1   | А     | 589  | G    | C4-N9-C1'  | -7.51 | 116.74           | 126.50        |
| 33  | a     | 1149 | U    | C2-N1-C1'  | 7.48  | 126.68           | 117.70        |
| 33  | a     | 465  | U    | N1-C2-O2   | 7.48  | 128.03           | 122.80        |
| 1   | А     | 554  | U    | OP2-P-O3'  | 7.47  | 121.64           | 105.20        |
| 2   | В     | 59   | U    | C2-N1-C1'  | 7.46  | 126.66           | 117.70        |
| 33  | a     | 853  | С    | N1-C2-O2   | 7.46  | 123.38           | 118.90        |
| 1   | А     | 1656 | С    | N1-C2-O2   | 7.46  | 123.37           | 118.90        |
| 33  | a     | 1009 | С    | C6-N1-C1'  | -7.45 | 111.86           | 120.80        |
| 1   | А     | 1366 | С    | C6-N1-C2   | -7.45 | 117.32           | 120.30        |
| 1   | А     | 2822 | С    | C5-C6-N1   | 7.43  | 124.71           | 121.00        |
| 1   | А     | 1476 | С    | C2-N1-C1'  | 7.41  | 126.95           | 118.80        |
| 1   | А     | 2371 | С    | C6-N1-C2   | -7.41 | 117.34           | 120.30        |
| 33  | a     | 60   | С    | C2-N1-C1'  | 7.40  | 126.94           | 118.80        |
| 33  | a     | 989  | С    | N3-C2-O2   | -7.40 | 116.72           | 121.90        |
| 33  | a     | 746  | С    | C6-N1-C2   | -7.40 | 117.34           | 120.30        |
| 1   | А     | 681  | С    | C6-N1-C2   | -7.39 | 117.34           | 120.30        |
| 1   | А     | 2334 | U    | C5-C6-N1   | 7.39  | 126.39           | 122.70        |
| 1   | А     | 1067 | А    | N7-C8-N9   | 7.38  | 117.49           | 113.80        |
| 33  | a     | 1331 | С    | N3-C2-O2   | -7.36 | 116.75           | 121.90        |
| 1   | А     | 2131 | U    | C2-N1-C1'  | 7.36  | 126.53           | 117.70        |
| 53  | Х     | 19   | U    | O5'-P-OP1  | 7.35  | 119.52           | 110.70        |
| 33  | a     | 759  | С    | C6-N1-C2   | -7.35 | 117.36           | 120.30        |
| 33  | a     | 1076 | С    | N3-C2-O2   | -7.35 | 116.75           | 121.90        |
| 33  | a     | 1438 | С    | N3-C2-O2   | -7.34 | 116.76           | 121.90        |
| 6   | F     | 136  | LEU  | CB-CG-CD1  | -7.33 | 98.55            | 111.00        |
| 33  | a     | 113  | G    | O5'-P-OP1  | -7.31 | 99.12            | 105.70        |
| 1   | А     | 1942 | А    | O4'-C1'-N9 | 7.29  | 114.03           | 108.20        |
| 1   | А     | 1450 | С    | C2-N1-C1'  | 7.29  | 126.82           | 118.80        |
| 1   | А     | 1817 | С    | N1-C2-O2   | 7.28  | 123.27           | 118.90        |
| 1   | А     | 593  | А    | C2-N3-C4   | 7.27  | 114.24           | 110.60        |
| 1   | А     | 2335 | U    | C2-N1-C1'  | 7.27  | 126.43           | 117.70        |
| 1   | А     | 508  | С    | C6-N1-C2   | -7.27 | 117.39           | 120.30        |
| 33  | a     | 92   | U    | P-O3'-C3'  | 7.27  | 128.42           | 119.70        |
| 33  | a     | 136  | U    | N1-C2-O2   | 7.26  | 127.88           | 122.80        |
| 1   | А     | 1527 | С    | OP1-P-O3'  | 7.26  | 121.17           | 105.20        |



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| Mol | Chain | Res  | Type | Atoms      | Z     | $Observed(^{o})$ | $Ideal(^{o})$ |
|-----|-------|------|------|------------|-------|------------------|---------------|
| 1   | А     | 2356 | А    | C8-N9-C4   | -7.26 | 102.90           | 105.80        |
| 1   | А     | 1942 | А    | N7-C8-N9   | -7.26 | 110.17           | 113.80        |
| 33  | a     | 168  | С    | N1-C2-O2   | 7.26  | 123.25           | 118.90        |
| 1   | А     | 1415 | С    | N1-C2-O2   | 7.25  | 123.25           | 118.90        |
| 43  | k     | 80   | GLY  | N-CA-C     | 7.25  | 131.24           | 113.10        |
| 1   | А     | 576  | G    | OP2-P-O3'  | 7.25  | 121.15           | 105.20        |
| 1   | А     | 1701 | С    | C6-N1-C2   | -7.24 | 117.40           | 120.30        |
| 2   | В     | 59   | U    | N1-C2-O2   | 7.24  | 127.87           | 122.80        |
| 33  | a     | 465  | U    | C2-N1-C1'  | 7.24  | 126.39           | 117.70        |
| 33  | a     | 1439 | С    | N1-C2-O2   | 7.24  | 123.24           | 118.90        |
| 1   | А     | 2025 | С    | C2-N1-C1'  | 7.24  | 126.76           | 118.80        |
| 1   | А     | 284  | C    | N3-C2-O2   | -7.23 | 116.84           | 121.90        |
| 1   | А     | 1327 | U    | N1-C2-O2   | 7.23  | 127.86           | 122.80        |
| 33  | a     | 1076 | С    | C5-C6-N1   | 7.23  | 124.61           | 121.00        |
| 1   | А     | 1848 | A    | O5'-P-OP2  | -7.22 | 99.20            | 105.70        |
| 1   | А     | 2350 | G    | C2-N3-C4   | 7.21  | 115.50           | 111.90        |
| 1   | А     | 1527 | С    | C6-N1-C2   | -7.21 | 117.42           | 120.30        |
| 33  | a     | 362  | G    | O5'-P-OP1  | -7.20 | 99.22            | 105.70        |
| 33  | a     | 1070 | U    | C5-C6-N1   | 7.19  | 126.30           | 122.70        |
| 1   | А     | 2386 | U    | O5'-P-OP1  | -7.19 | 99.23            | 105.70        |
| 33  | a     | 1175 | G    | OP1-P-O3'  | -7.17 | 89.42            | 105.20        |
| 1   | А     | 8    | U    | C2-N1-C1'  | 7.17  | 126.30           | 117.70        |
| 1   | А     | 1941 | A    | N7-C8-N9   | 7.16  | 117.38           | 113.80        |
| 20  | V     | 393  | LEU  | CA-CB-CG   | 7.15  | 131.74           | 115.30        |
| 1   | А     | 2485 | С    | C6-N1-C2   | -7.13 | 117.45           | 120.30        |
| 1   | А     | 2323 | С    | C2-N1-C1'  | 7.13  | 126.64           | 118.80        |
| 2   | В     | 41   | С    | C5-C6-N1   | 7.13  | 124.56           | 121.00        |
| 53  | Х     | 62   | С    | P-O3'-C3'  | 7.13  | 128.25           | 119.70        |
| 10  | L     | 79   | LEU  | CA-CB-CG   | 7.12  | 131.68           | 115.30        |
| 1   | A     | 2918 | G    | C8-N9-C1'  | -7.12 | 117.75           | 127.00        |
| 1   | A     | 1369 | С    | C2-N1-C1'  | 7.11  | 126.62           | 118.80        |
| 1   | A     | 2345 | U    | C5-C6-N1   | 7.11  | 126.26           | 122.70        |
| 53  | Х     | 22   | A    | P-O3'-C3'  | 7.10  | 128.22           | 119.70        |
| 1   | А     | 831  | U    | N1-C2-O2   | 7.08  | 127.76           | 122.80        |
| 1   | A     | 1244 | A    | OP1-P-O3'  | 7.08  | 120.77           | 105.20        |
| 33  | a     | 1421 | C    | C6-N1-C2   | -7.07 | 117.47           | 120.30        |
| 1   | A     | 1244 | A    | O4'-C1'-N9 | 7.07  | 113.86           | 108.20        |
| 33  | a     | 143  | C    | N1-C2-O2   | 7.05  | 123.13           | 118.90        |
| 1   | A     | 1817 | C    | C6-N1-C2   | -7.05 | 117.48           | 120.30        |
| 1   | A     | 2094 | C    | C6-N1-C2   | -7.04 | 117.48           | 120.30        |
| 33  | a     | 271  | A    | C8-N9-C4   | -7.04 | 102.98           | 105.80        |
| 2   | В     | 28   | C    | N1-C2-O2   | 7.04  | 123.12           | 118.90        |



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|----------------------------------|------|----------|------|
| Continued                        | trom | previous | page |
|                                  | J    | 1        | 1 5  |

| Mol | Chain | Res  | Type | Atoms      | Z     | $Observed(^{o})$ | $Ideal(^{o})$ |
|-----|-------|------|------|------------|-------|------------------|---------------|
| 1   | А     | 2054 | С    | C2-N1-C1'  | 7.03  | 126.53           | 118.80        |
| 1   | А     | 2105 | U    | N3-C2-O2   | -7.03 | 117.28           | 122.20        |
| 1   | А     | 284  | С    | C6-N1-C2   | -7.02 | 117.49           | 120.30        |
| 1   | А     | 2131 | U    | C5-C6-N1   | 7.01  | 126.21           | 122.70        |
| 1   | А     | 1831 | А    | C8-N9-C4   | -7.01 | 103.00           | 105.80        |
| 2   | В     | 24   | С    | C6-N1-C2   | -6.98 | 117.51           | 120.30        |
| 33  | a     | 1287 | С    | N1-C2-O2   | 6.98  | 123.09           | 118.90        |
| 46  | n     | 3    | LYS  | CD-CE-NZ   | -6.98 | 95.65            | 111.70        |
| 53  | Х     | 69   | С    | C5-C6-N1   | 6.97  | 124.49           | 121.00        |
| 1   | А     | 422  | С    | C2-N1-C1'  | 6.97  | 126.47           | 118.80        |
| 1   | А     | 1366 | С    | C2-N1-C1'  | 6.96  | 126.46           | 118.80        |
| 1   | А     | 1559 | С    | N3-C2-O2   | -6.96 | 117.03           | 121.90        |
| 1   | А     | 1817 | С    | C5-C6-N1   | 6.95  | 124.48           | 121.00        |
| 33  | a     | 143  | С    | C6-N1-C2   | -6.95 | 117.52           | 120.30        |
| 33  | a     | 486  | С    | C2-N1-C1'  | 6.95  | 126.44           | 118.80        |
| 1   | А     | 1527 | С    | C6-N1-C1'  | -6.94 | 112.47           | 120.80        |
| 33  | a     | 1463 | А    | O5'-P-OP2  | -6.94 | 99.46            | 105.70        |
| 1   | А     | 2648 | U    | N3-C2-O2   | -6.93 | 117.35           | 122.20        |
| 2   | В     | 29   | С    | C2-N1-C1'  | 6.93  | 126.42           | 118.80        |
| 1   | А     | 1028 | С    | C2-N1-C1'  | 6.93  | 126.42           | 118.80        |
| 16  | R     | 48   | VAL  | CG1-CB-CG2 | 6.92  | 121.98           | 110.90        |
| 1   | А     | 2795 | G    | N3-C4-C5   | -6.92 | 125.14           | 128.60        |
| 33  | a     | 280  | С    | N1-C2-O2   | 6.91  | 123.04           | 118.90        |
| 33  | a     | 1305 | С    | N1-C2-O2   | 6.91  | 123.04           | 118.90        |
| 1   | А     | 2035 | С    | C6-N1-C2   | -6.90 | 117.54           | 120.30        |
| 33  | a     | 1391 | С    | N1-C2-O2   | 6.89  | 123.04           | 118.90        |
| 1   | А     | 422  | С    | C5-C6-N1   | 6.89  | 124.45           | 121.00        |
| 2   | В     | 24   | С    | C5-C6-N1   | 6.89  | 124.44           | 121.00        |
| 33  | a     | 465  | U    | N3-C2-O2   | -6.88 | 117.38           | 122.20        |
| 1   | А     | 1545 | С    | C2-N1-C1'  | 6.88  | 126.36           | 118.80        |
| 1   | А     | 8    | U    | C5-C6-N1   | 6.87  | 126.14           | 122.70        |
| 1   | А     | 2822 | С    | C6-N1-C2   | -6.86 | 117.56           | 120.30        |
| 1   | А     | 1803 | С    | C6-N1-C2   | -6.86 | 117.56           | 120.30        |
| 1   | А     | 1942 | А    | C6-C5-N7   | 6.86  | 137.10           | 132.30        |
| 1   | А     | 2157 | С    | C2-N1-C1'  | 6.86  | 126.34           | 118.80        |
| 1   | А     | 2503 | С    | C6-N1-C2   | -6.84 | 117.56           | 120.30        |
| 1   | А     | 2255 | С    | N3-C2-O2   | -6.83 | 117.12           | 121.90        |
| 2   | В     | 15   | C    | C2-N1-C1'  | 6.83  | 126.31           | 118.80        |
| 1   | A     | 1122 | C    | C6-N1-C2   | -6.82 | 117.57           | 120.30        |
| 1   | А     | 442  | C    | C2-N3-C4   | 6.81  | 123.30           | 119.90        |
| 33  | a     | 1036 | С    | C5-C6-N1   | 6.81  | 124.40           | 121.00        |
| 33  | а     | 1010 | U    | N3-C2-O2   | -6.80 | 117.44           | 122.20        |



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| Mol | Chain | Res  | Type | Atoms       | Z     | $Observed(^{o})$ | $Ideal(^{o})$ |
|-----|-------|------|------|-------------|-------|------------------|---------------|
| 1   | А     | 1942 | А    | C8-N9-C4    | 6.80  | 108.52           | 105.80        |
| 1   | А     | 924  | U    | C5-C6-N1    | 6.79  | 126.10           | 122.70        |
| 1   | А     | 914  | С    | C6-N1-C2    | -6.78 | 117.59           | 120.30        |
| 1   | А     | 2471 | С    | C6-N1-C2    | -6.77 | 117.59           | 120.30        |
| 49  | q     | 76   | ARG  | NE-CZ-NH2   | -6.75 | 116.92           | 120.30        |
| 33  | a     | 853  | С    | N3-C2-O2    | -6.73 | 117.19           | 121.90        |
| 1   | А     | 769  | A    | C5-C6-N6    | 6.73  | 129.08           | 123.70        |
| 44  | 1     | 44   | ARG  | CA-CB-CG    | 6.73  | 128.20           | 113.40        |
| 1   | А     | 2223 | U    | N3-C2-O2    | -6.72 | 117.50           | 122.20        |
| 1   | А     | 2350 | G    | N3-C4-N9    | 6.71  | 130.03           | 126.00        |
| 1   | А     | 2432 | C    | C6-N1-C2    | -6.70 | 117.62           | 120.30        |
| 1   | А     | 92   | G    | N9-C4-C5    | -6.70 | 102.72           | 105.40        |
| 1   | А     | 631  | G    | N3-C2-N2    | -6.69 | 115.22           | 119.90        |
| 1   | А     | 1941 | A    | C4-N9-C1'   | 6.68  | 138.32           | 126.30        |
| 1   | А     | 508  | С    | C5-C6-N1    | 6.67  | 124.33           | 121.00        |
| 1   | А     | 633  | U    | C5-C6-N1    | 6.67  | 126.03           | 122.70        |
| 1   | А     | 1247 | G    | O4'-C1'-N9  | 6.67  | 113.53           | 108.20        |
| 1   | А     | 1328 | С    | N1-C2-O2    | 6.67  | 122.90           | 118.90        |
| 21  | W     | 28   | ARG  | CB-CG-CD    | 6.66  | 128.93           | 111.60        |
| 1   | А     | 445  | С    | C5-C6-N1    | 6.66  | 124.33           | 121.00        |
| 1   | А     | 1963 | С    | N3-C2-O2    | -6.65 | 117.24           | 121.90        |
| 1   | А     | 830  | A    | C5-N7-C8    | -6.65 | 100.58           | 103.90        |
| 1   | А     | 1559 | C    | N1-C2-O2    | 6.64  | 122.88           | 118.90        |
| 1   | А     | 2092 | С    | N1-C2-O2    | 6.64  | 122.88           | 118.90        |
| 1   | А     | 670  | С    | C5-C6-N1    | 6.62  | 124.31           | 121.00        |
| 1   | А     | 1352 | U    | N3-C2-O2    | -6.62 | 117.57           | 122.20        |
| 2   | В     | 28   | С    | N3-C2-O2    | -6.61 | 117.27           | 121.90        |
| 1   | А     | 2316 | A    | P-O3'-C3'   | 6.61  | 127.63           | 119.70        |
| 1   | A     | 2102 | С    | C6-N1-C2    | -6.60 | 117.66           | 120.30        |
| 53  | Х     | 53   | G    | N9-C4-C5    | -6.60 | 102.76           | 105.40        |
| 53  | Х     | 69   | С    | C2-N1-C1'   | 6.60  | 126.06           | 118.80        |
| 33  | a     | 1176 | A    | O5'-C5'-C4' | 6.59  | 124.22           | 111.70        |
| 1   | А     | 1327 | U    | N3-C2-O2    | -6.58 | 117.59           | 122.20        |
| 1   | А     | 1028 | С    | N3-C2-O2    | -6.58 | 117.29           | 121.90        |
| 53  | x     | 53   | G    | C8-N9-C1'   | -6.58 | 118.45           | 127.00        |
| 1   | A     | 1757 | G    | O4'-C1'-N9  | 6.57  | 113.46           | 108.20        |
| 1   | А     | 1570 | U    | OP2-P-O3'   | 6.56  | 119.64           | 105.20        |
| 33  | a     | 1037 | C    | N3-C2-O2    | -6.56 | 117.31           | 121.90        |
| 1   | A     | 2833 | U    | N3-C2-O2    | -6.56 | 117.61           | 122.20        |
| 1   | А     | 1339 | A    | P-O3'-C3'   | 6.55  | 127.56           | 119.70        |
| 1   | A     | 430  | C    | N3-C2-O2    | -6.55 | 117.32           | 121.90        |
| 1   | А     | 554  | U    | P-O3'-C3'   | 6.54  | 127.55           | 119.70        |



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| Mol | Chain | $\mathbf{Res}$ | Type | Atoms      |       | $Observed(^{o})$ | $Ideal(^{o})$ |
|-----|-------|----------------|------|------------|-------|------------------|---------------|
| 1   | А     | 1712           | G    | C4-N9-C1'  | 6.54  | 135.00           | 126.50        |
| 1   | А     | 933            | С    | P-O3'-C3'  | 6.54  | 127.54           | 119.70        |
| 6   | F     | 136            | LEU  | CA-CB-CG   | 6.53  | 130.32           | 115.30        |
| 1   | А     | 662            | U    | C5-C6-N1   | 6.53  | 125.96           | 122.70        |
| 33  | a     | 39             | U    | N3-C2-O2   | -6.51 | 117.64           | 122.20        |
| 1   | А     | 2202           | А    | O4'-C1'-N9 | 6.50  | 113.40           | 108.20        |
| 1   | А     | 573            | С    | C2-N1-C1'  | 6.50  | 125.95           | 118.80        |
| 1   | А     | 2752           | С    | C6-N1-C2   | -6.49 | 117.70           | 120.30        |
| 33  | a     | 1525           | С    | C5-C6-N1   | 6.48  | 124.24           | 121.00        |
| 1   | А     | 62             | С    | P-O3'-C3'  | 6.48  | 127.48           | 119.70        |
| 1   | А     | 1036           | А    | N7-C8-N9   | 6.48  | 117.04           | 113.80        |
| 33  | a     | 1468           | С    | O5'-P-OP1  | -6.48 | 99.87            | 105.70        |
| 1   | А     | 2295           | А    | OP2-P-O3'  | 6.47  | 119.45           | 105.20        |
| 1   | А     | 1828           | G    | P-O3'-C3'  | 6.46  | 127.46           | 119.70        |
| 1   | А     | 2675           | С    | C5-C6-N1   | 6.46  | 124.23           | 121.00        |
| 33  | a     | 993            | А    | N3-C4-N9   | 6.46  | 132.57           | 127.40        |
| 33  | a     | 1438           | С    | N1-C2-O2   | 6.46  | 122.78           | 118.90        |
| 1   | А     | 2094           | С    | C5-C6-N1   | 6.46  | 124.23           | 121.00        |
| 33  | a     | 459            | А    | P-O3'-C3'  | 6.46  | 127.45           | 119.70        |
| 1   | А     | 1792           | G    | O5'-P-OP2  | -6.45 | 99.89            | 105.70        |
| 1   | А     | 1237           | С    | N3-C2-O2   | -6.45 | 117.38           | 121.90        |
| 1   | А     | 1527           | С    | N3-C2-O2   | -6.45 | 117.39           | 121.90        |
| 1   | А     | 719            | С    | C6-N1-C2   | -6.44 | 117.72           | 120.30        |
| 1   | А     | 1804           | U    | N3-C2-O2   | -6.44 | 117.69           | 122.20        |
| 1   | А     | 2371           | С    | C5-C6-N1   | 6.43  | 124.22           | 121.00        |
| 1   | А     | 2765           | G    | N3-C4-N9   | 6.43  | 129.86           | 126.00        |
| 1   | А     | 2254           | А    | P-O3'-C3'  | 6.43  | 127.42           | 119.70        |
| 1   | А     | 2774           | С    | C2-N1-C1'  | 6.43  | 125.87           | 118.80        |
| 1   | А     | 778            | С    | N1-C2-O2   | 6.42  | 122.75           | 118.90        |
| 2   | В     | 61             | U    | C2-N1-C1'  | 6.42  | 125.41           | 117.70        |
| 33  | a     | 1111           | А    | P-O3'-C3'  | 6.42  | 127.40           | 119.70        |
| 33  | a     | 372            | А    | OP1-P-O3'  | 6.41  | 119.30           | 105.20        |
| 15  | Q     | 103            | LEU  | CA-CB-CG   | 6.41  | 130.03           | 115.30        |
| 1   | А     | 2243           | С    | C2-N1-C1'  | 6.40  | 125.84           | 118.80        |
| 1   | А     | 2911           | G    | N7-C8-N9   | 6.39  | 116.30           | 113.10        |
| 1   | А     | 1731           | С    | N1-C2-O2   | 6.39  | 122.74           | 118.90        |
| 1   | А     | 2768           | U    | N1-C2-O2   | 6.38  | 127.27           | 122.80        |
| 33  | a     | 1158           | C    | C6-N1-C2   | -6.38 | 117.75           | 120.30        |
| 33  | a     | 271            | A    | N7-C8-N9   | 6.38  | 116.99           | 113.80        |
| 1   | А     | 482            | С    | O4'-C1'-N1 | 6.37  | 113.29           | 108.20        |
| 33  | a     | 1149           | U    | N1-C2-O2   | 6.36  | 127.25           | 122.80        |
| 1   | А     | 445            | C    | C6-N1-C2   | -6.36 | 117.76           | 120.30        |



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| Mol | Chain | Res  | Type | Atoms                  | Z                 | $Observed(^{o})$ | $Ideal(^{o})$ |
|-----|-------|------|------|------------------------|-------------------|------------------|---------------|
| 1   | А     | 2503 | С    | N3-C2-O2               | -6.36             | 117.45           | 121.90        |
| 1   | А     | 875  | U    | C2-N1-C1'              | 6.36              | 125.33           | 117.70        |
| 31  | 7     | 25   | С    | N1-C2-O2               | 6.35              | 122.71           | 118.90        |
| 1   | А     | 1771 | С    | C2-N1-C1'              | 6.35              | 125.78           | 118.80        |
| 1   | А     | 502  | С    | O5'-P-OP2              | -6.34             | 100.00           | 105.70        |
| 1   | А     | 635  | С    | C6-N1-C2               | -6.34             | 117.76           | 120.30        |
| 1   | А     | 589  | G    | C6-C5-N7               | 6.33              | 134.20           | 130.40        |
| 1   | А     | 2739 | С    | C6-N1-C2               | -6.33             | 117.77           | 120.30        |
| 1   | А     | 716  | G    | C4-N9-C1'              | 6.33              | 134.73           | 126.50        |
| 2   | В     | 15   | С    | C6-N1-C2               | -6.33             | 117.77           | 120.30        |
| 1   | А     | 2350 | G    | C8-N9-C4               | -6.33             | 103.87           | 106.40        |
| 1   | А     | 2665 | U    | N3-C2-O2               | -6.33             | 117.77           | 122.20        |
| 1   | А     | 735  | U    | C5-C4-O4               | -6.32             | 122.11           | 125.90        |
| 1   | А     | 1771 | С    | C6-N1-C2               | -6.32             | 117.77           | 120.30        |
| 33  | a     | 264  | U    | C5-C6-N1               | 6.32              | 125.86           | 122.70        |
| 1   | А     | 1476 | С    | N1-C2-O2               | 6.32              | 122.69           | 118.90        |
| 1   | А     | 716  | G    | C8-N9-C1'              | -6.31             | 118.80           | 127.00        |
| 1   | А     | 2695 | С    | C2-N1-C1'              | 6.31              | 125.74           | 118.80        |
| 33  | a     | 747  | U    | C5-C6-N1               | 6.31              | 125.85           | 122.70        |
| 33  | a     | 1460 | U    | N1-C2-O2               | 6.29              | 127.20           | 122.80        |
| 1   | А     | 1450 | С    | N1-C2-O2               | 6.29              | 122.67           | 118.90        |
| 2   | В     | 62   | U    | C6-N1-C1'              | -6.29             | 112.39           | 121.20        |
| 22  | Х     | 39   | LEU  | CA-CB-CG               | 6.29              | 129.76           | 115.30        |
| 1   | А     | 1353 | С    | N1-C2-O2               | 6.29              | 122.67           | 118.90        |
| 33  | a     | 1438 | С    | C6-N1-C2               | -6.28             | 117.79           | 120.30        |
| 1   | А     | 299  | U    | N3-C2-O2               | -6.28             | 117.80           | 122.20        |
| 53  | X     | 69   | С    | C6-N1-C2               | -6.28             | 117.79           | 120.30        |
| 1   | А     | 1296 | G    | C4-N9-C1'              | 6.28              | 134.66           | 126.50        |
| 1   | А     | 2223 | U    | N1-C2-O2               | 6.28              | 127.19           | 122.80        |
| 33  | a     | 467  | С    | C6-N1-C2               | -6.28             | 117.79           | 120.30        |
| 33  | a     | 537  | С    | C2-N1-C1'              | 6.27              | 125.69           | 118.80        |
| 1   | А     | 588  | С    | C2-N1-C1'              | 6.26              | 125.69           | 118.80        |
| 1   | А     | 1450 | С    | C6-N1-C2               | -6.26             | 117.80           | 120.30        |
| 1   | А     | 397  | U    | C2-N1-C1'              | 6.26              | 125.21           | 117.70        |
| 1   | А     | 776  | G    | C4-N9-C1'              | 6.25              | 134.63           | 126.50        |
| 33  | a     | 92   | U    | OP1-P-O3'              | 6.25              | 118.95           | 105.20        |
| 1   | A     | 2157 | С    | C5-C6-N1               | 6.25              | 124.12           | 121.00        |
| 2   | B     | 59   | U    | N3-C2-O2               | -6.25             | 117.83           | 122.20        |
| 33  | a     | 1391 | C    | $C2-N1-\overline{C1'}$ | $6.2\overline{4}$ | 125.67           | 118.80        |
| 1   | А     | 2822 | С    | C6-N1-C1'              | -6.24             | 113.31           | 120.80        |
| 33  | a     | 119  | C    | O5'-P-OP1              | -6.24             | 100.08           | 105.70        |
| 1   | А     | 1712 | G    | N9-C1'-C2'             | 6.24              | 122.11           | 114.00        |



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| Mol | Chain | Res  | Type | Atoms      | Z     | $Observed(^{o})$ | $Ideal(^{o})$ |
|-----|-------|------|------|------------|-------|------------------|---------------|
| 33  | a     | 460  | А    | C2-N3-C4   | 6.24  | 113.72           | 110.60        |
| 1   | А     | 2422 | U    | N1-C2-O2   | 6.23  | 127.16           | 122.80        |
| 1   | А     | 589  | G    | N3-C4-C5   | 6.23  | 131.71           | 128.60        |
| 1   | А     | 152  | С    | C6-N1-C2   | -6.23 | 117.81           | 120.30        |
| 1   | А     | 1352 | U    | N1-C2-O2   | 6.23  | 127.16           | 122.80        |
| 1   | А     | 233  | G    | O4'-C1'-N9 | 6.22  | 113.18           | 108.20        |
| 1   | А     | 1712 | G    | C8-N9-C1'  | -6.22 | 118.91           | 127.00        |
| 33  | a     | 476  | U    | C2-N1-C1'  | 6.22  | 125.17           | 117.70        |
| 1   | А     | 2207 | С    | C6-N1-C2   | -6.22 | 117.81           | 120.30        |
| 33  | a     | 1036 | C    | C6-N1-C2   | -6.22 | 117.81           | 120.30        |
| 1   | А     | 1353 | С    | C6-N1-C1'  | -6.21 | 113.34           | 120.80        |
| 1   | А     | 2092 | С    | C2-N1-C1'  | 6.21  | 125.64           | 118.80        |
| 1   | А     | 1448 | U    | N3-C2-O2   | -6.21 | 117.85           | 122.20        |
| 33  | a     | 970  | U    | C2-N1-C1'  | 6.21  | 125.15           | 117.70        |
| 33  | a     | 1210 | A    | OP2-P-O3'  | 6.21  | 118.85           | 105.20        |
| 1   | А     | 975  | С    | C2-N1-C1'  | 6.20  | 125.62           | 118.80        |
| 33  | a     | 1148 | G    | P-O3'-C3'  | 6.20  | 127.14           | 119.70        |
| 33  | a     | 21   | C    | C6-N1-C2   | -6.20 | 117.82           | 120.30        |
| 33  | a     | 763  | С    | C2-N1-C1'  | 6.19  | 125.61           | 118.80        |
| 1   | А     | 76   | C    | OP1-P-OP2  | -6.18 | 110.33           | 119.60        |
| 1   | А     | 2805 | A    | P-O3'-C3'  | 6.18  | 127.12           | 119.70        |
| 33  | a     | 1041 | С    | OP2-P-O3'  | 6.17  | 118.78           | 105.20        |
| 1   | А     | 2035 | C    | C5-C6-N1   | 6.17  | 124.09           | 121.00        |
| 1   | А     | 789  | С    | C6-N1-C2   | -6.17 | 117.83           | 120.30        |
| 33  | a     | 758  | А    | N7-C8-N9   | 6.17  | 116.89           | 113.80        |
| 33  | a     | 1008 | С    | C2-N1-C1'  | 6.17  | 125.59           | 118.80        |
| 2   | В     | 62   | U    | N1-C2-O2   | 6.17  | 127.12           | 122.80        |
| 1   | А     | 1567 | U    | OP1-P-O3'  | 6.17  | 118.76           | 105.20        |
| 1   | A     | 1831 | A    | O4'-C1'-N9 | 6.17  | 113.13           | 108.20        |
| 33  | a     | 1170 | С    | N3-C2-O2   | -6.17 | 117.58           | 121.90        |
| 1   | А     | 2467 | U    | OP2-P-O3'  | 6.16  | 118.76           | 105.20        |
| 1   | А     | 1671 | G    | C8-N9-C4   | -6.16 | 103.94           | 106.40        |
| 33  | a     | 319  | С    | C6-N1-C2   | -6.16 | 117.84           | 120.30        |
| 17  | S     | 38   | LEU  | C-N-CA     | 6.15  | 137.07           | 121.70        |
| 1   | А     | 1634 | U    | N1-C2-O2   | 6.14  | 127.10           | 122.80        |
| 33  | a     | 1210 | A    | P-O3'-C3'  | 6.14  | 127.07           | 119.70        |
| 1   | A     | 1656 | C    | N3-C2-O2   | -6.14 | 117.60           | 121.90        |
| 1   | A     | 872  | C    | C6-N1-C2   | -6.14 | 117.84           | 120.30        |
| 1   | A     | 1702 | U    | O5'-P-OP1  | -6.13 | 100.18           | 105.70        |
| 1   | А     | 1631 | A    | N7-C8-N9   | 6.13  | 116.86           | 113.80        |
| 1   | A     | 2065 | C    | C5-C6-N1   | 6.12  | 124.06           | 121.00        |
| 33  | a     | 336  | С    | N1-C2-O2   | 6.12  | 122.57           | 118.90        |



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| Mol | Chain | Res               | Type | Atoms     | Z     | $Observed(^{o})$ | $Ideal(^{o})$ |
|-----|-------|-------------------|------|-----------|-------|------------------|---------------|
| 1   | А     | 2092              | С    | C6-N1-C2  | -6.12 | 117.85           | 120.30        |
| 1   | А     | 1527              | С    | P-O3'-C3' | 6.11  | 127.03           | 119.70        |
| 33  | a     | 942               | С    | C6-N1-C2  | -6.11 | 117.86           | 120.30        |
| 1   | А     | 1545              | С    | C5-C6-N1  | 6.11  | 124.06           | 121.00        |
| 1   | А     | 2350              | G    | C8-N9-C1' | -6.11 | 119.06           | 127.00        |
| 1   | А     | 977               | U    | C5-C6-N1  | 6.11  | 125.75           | 122.70        |
| 1   | А     | 810               | G    | OP1-P-O3' | 6.10  | 118.63           | 105.20        |
| 1   | А     | 1707              | U    | N1-C2-O2  | 6.10  | 127.07           | 122.80        |
| 1   | А     | 885               | С    | N1-C2-O2  | 6.10  | 122.56           | 118.90        |
| 1   | А     | 2791              | U    | C5-C6-N1  | 6.10  | 125.75           | 122.70        |
| 1   | А     | 2055              | U    | C5-C6-N1  | 6.10  | 125.75           | 122.70        |
| 53  | Х     | 53                | G    | C4-C5-N7  | 6.10  | 113.24           | 110.80        |
| 1   | А     | 1045              | U    | N3-C2-O2  | -6.09 | 117.94           | 122.20        |
| 1   | А     | 62                | С    | OP2-P-O3' | 6.08  | 118.58           | 105.20        |
| 1   | А     | 885               | С    | C6-N1-C2  | -6.07 | 117.87           | 120.30        |
| 1   | А     | 936               | С    | C2-N1-C1' | 6.07  | 125.48           | 118.80        |
| 1   | А     | 2685              | U    | C2-N1-C1' | 6.07  | 124.98           | 117.70        |
| 33  | a     | 591               | С    | N1-C2-O2  | 6.07  | 122.54           | 118.90        |
| 53  | Х     | 21                | G    | N3-C4-C5  | -6.07 | 125.57           | 128.60        |
| 1   | А     | 972               | U    | C5-C6-N1  | 6.06  | 125.73           | 122.70        |
| 1   | А     | 980               | С    | C5-C6-N1  | 6.06  | 124.03           | 121.00        |
| 9   | K     | 89                | ASP  | CB-CG-OD1 | 6.05  | 123.75           | 118.30        |
| 1   | А     | 1067              | А    | C8-N9-C4  | -6.05 | 103.38           | 105.80        |
| 1   | А     | 2423              | С    | N1-C2-O2  | 6.05  | 122.53           | 118.90        |
| 33  | a     | 1331              | С    | C6-N1-C2  | -6.05 | 117.88           | 120.30        |
| 33  | a     | 1020              | С    | C6-N1-C2  | -6.05 | 117.88           | 120.30        |
| 33  | a     | 1110              | С    | C6-N1-C2  | -6.05 | 117.88           | 120.30        |
| 33  | a     | 468               | С    | C6-N1-C2  | -6.05 | 117.88           | 120.30        |
| 2   | В     | 59                | U    | C5-C6-N1  | 6.04  | 125.72           | 122.70        |
| 33  | a     | 87                | С    | N1-C2-O2  | 6.04  | 122.52           | 118.90        |
| 1   | А     | 1122              | С    | N3-C2-O2  | -6.03 | 117.68           | 121.90        |
| 1   | А     | 1307              | U    | N1-C2-O2  | 6.03  | 127.02           | 122.80        |
| 1   | А     | 1771              | С    | C5-C6-N1  | 6.03  | 124.02           | 121.00        |
| 33  | a     | 1457              | С    | C2-N1-C1' | 6.03  | 125.44           | 118.80        |
| 1   | А     | 2620              | С    | C6-N1-C2  | -6.03 | 117.89           | 120.30        |
| 33  | a     | 86                | G    | N7-C8-N9  | 6.03  | 116.12           | 113.10        |
| 33  | a     | 85                | U    | C2-N1-C1' | 6.03  | 124.94           | 117.70        |
| 33  | a     | 1439              | C    | C6-N1-C2  | -6.03 | 117.89           | 120.30        |
| 33  | a     | 167               | G    | C6-C5-N7  | -6.03 | 126.78           | 130.40        |
| 1   | A     | $2\overline{0}23$ | C    | C6-N1-C2  | -6.02 | 117.89           | 120.30        |
| 53  | х     | 53                | G    | C4-N9-C1' | 6.02  | 134.33           | 126.50        |
| 53  | х     | 21                | G    | N3-C4-N9  | 6.01  | 129.61           | 126.00        |



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| Mol | Chain | Res  | Type | Atoms     | Z     | $Observed(^{o})$ | $Ideal(^{o})$ |
|-----|-------|------|------|-----------|-------|------------------|---------------|
| 1   | А     | 2189 | G    | C8-N9-C1' | -6.01 | 119.19           | 127.00        |
| 33  | a     | 1391 | С    | C6-N1-C2  | -6.00 | 117.90           | 120.30        |
| 33  | a     | 413  | U    | C5-C6-N1  | 6.00  | 125.70           | 122.70        |
| 33  | a     | 171  | А    | C8-N9-C4  | -6.00 | 103.40           | 105.80        |
| 53  | Х     | 38   | U    | N3-C2-O2  | -5.99 | 118.00           | 122.20        |
| 53  | Х     | 53   | G    | C6-C5-N7  | -5.99 | 126.80           | 130.40        |
| 1   | А     | 2503 | С    | N1-C2-O2  | 5.99  | 122.49           | 118.90        |
| 33  | a     | 1463 | А    | P-O3'-C3' | 5.99  | 126.89           | 119.70        |
| 33  | a     | 1390 | U    | N1-C2-O2  | 5.99  | 126.99           | 122.80        |
| 1   | А     | 1067 | A    | C2-N3-C4  | -5.99 | 107.61           | 110.60        |
| 1   | А     | 442  | С    | N1-C2-O2  | 5.98  | 122.49           | 118.90        |
| 1   | А     | 2795 | G    | N3-C4-N9  | 5.98  | 129.59           | 126.00        |
| 33  | a     | 856  | С    | C6-N1-C2  | -5.98 | 117.91           | 120.30        |
| 53  | х     | 21   | G    | C8-N9-C1' | -5.97 | 119.24           | 127.00        |
| 1   | A     | 1305 | A    | P-O3'-C3' | 5.97  | 126.86           | 119.70        |
| 1   | А     | 1339 | A    | OP2-P-O3' | 5.97  | 118.33           | 105.20        |
| 33  | a     | 537  | C    | N1-C2-O2  | 5.97  | 122.48           | 118.90        |
| 1   | А     | 1353 | C    | C5-C6-N1  | 5.96  | 123.98           | 121.00        |
| 1   | А     | 2749 | U    | N3-C2-O2  | -5.96 | 118.03           | 122.20        |
| 33  | a     | 632  | С    | C5-C6-N1  | 5.96  | 123.98           | 121.00        |
| 1   | А     | 1237 | С    | N1-C2-O2  | 5.95  | 122.47           | 118.90        |
| 33  | a     | 101  | С    | C6-N1-C2  | -5.95 | 117.92           | 120.30        |
| 1   | А     | 1450 | С    | N3-C2-O2  | -5.95 | 117.73           | 121.90        |
| 20  | V     | 389  | LEU  | CA-CB-CG  | 5.95  | 128.98           | 115.30        |
| 1   | A     | 46   | С    | O5'-P-OP2 | -5.95 | 100.35           | 105.70        |
| 33  | a     | 476  | U    | N1-C2-O2  | 5.94  | 126.96           | 122.80        |
| 1   | A     | 1397 | G    | OP2-P-O3' | 5.94  | 118.27           | 105.20        |
| 1   | A     | 1631 | A    | C8-N9-C4  | -5.94 | 103.42           | 105.80        |
| 1   | А     | 2452 | U    | OP2-P-O3' | 5.94  | 118.27           | 105.20        |
| 1   | A     | 2454 | A    | OP2-P-O3' | 5.94  | 118.26           | 105.20        |
| 1   | A     | 2114 | С    | C5-C6-N1  | 5.93  | 123.97           | 121.00        |
| 1   | A     | 2604 | С    | C6-N1-C2  | -5.93 | 117.93           | 120.30        |
| 33  | a     | 1441 | G    | O5'-P-OP1 | -5.93 | 100.36           | 105.70        |
| 33  | a     | 993  | A    | N3-C4-C5  | -5.92 | 122.65           | 126.80        |
| 1   | A     | 2155 | A    | P-O3'-C3' | 5.92  | 126.80           | 119.70        |
| 33  | a     | 1024 | A    | O5'-P-OP2 | -5.91 | 100.39           | 105.70        |
| 1   | A     | 1353 | C    | C6-N1-C2  | -5.90 | 117.94           | 120.30        |
| 33  | a     | 537  | C    | C6-N1-C2  | -5.90 | 117.94           | 120.30        |
| 53  | X     | 38   | U    | N1-C2-O2  | 5.90  | 126.93           | 122.80        |
| 1   | A     | 186  | C    | O5'-P-OP1 | -5.90 | 100.39           | 105.70        |
| 1   | A     | 1307 | U    | N3-C2-O2  | -5.89 | 118.07           | 122.20        |
| 1   | A     | 1781 | C    | C5-C6-N1  | 5.89  | 123.95           | 121.00        |



| $\alpha$ $\cdot$ $\cdot$ $\cdot$ | C    | •        |      |
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| Mol | Chain | Res  | Type | Atoms      | Z     | $Observed(^{o})$ | $Ideal(^{o})$ |
|-----|-------|------|------|------------|-------|------------------|---------------|
| 1   | А     | 2712 | С    | N1-C2-O2   | 5.89  | 122.44           | 118.90        |
| 1   | А     | 783  | С    | C5-C6-N1   | 5.88  | 123.94           | 121.00        |
| 1   | А     | 936  | С    | N1-C2-O2   | 5.88  | 122.43           | 118.90        |
| 33  | a     | 136  | U    | C2-N1-C1'  | 5.88  | 124.75           | 117.70        |
| 33  | a     | 168  | С    | N3-C2-O2   | -5.87 | 117.79           | 121.90        |
| 1   | А     | 1963 | С    | N1-C2-O2   | 5.87  | 122.42           | 118.90        |
| 1   | А     | 2749 | U    | N1-C2-O2   | 5.87  | 126.91           | 122.80        |
| 33  | a     | 1237 | С    | N1-C2-O2   | 5.87  | 122.42           | 118.90        |
| 1   | А     | 588  | С    | N3-C2-O2   | -5.87 | 117.79           | 121.90        |
| 1   | А     | 1507 | U    | OP2-P-O3'  | 5.87  | 118.11           | 105.20        |
| 1   | А     | 430  | С    | N1-C2-O2   | 5.87  | 122.42           | 118.90        |
| 1   | А     | 2092 | С    | N3-C2-O2   | -5.86 | 117.80           | 121.90        |
| 1   | А     | 1883 | А    | C8-N9-C4   | -5.86 | 103.46           | 105.80        |
| 1   | А     | 1631 | А    | P-O3'-C3'  | 5.86  | 126.73           | 119.70        |
| 1   | А     | 2388 | С    | C6-N1-C2   | -5.86 | 117.96           | 120.30        |
| 33  | a     | 411  | С    | C6-N1-C2   | -5.86 | 117.96           | 120.30        |
| 33  | a     | 1331 | С    | C6-N1-C1'  | -5.85 | 113.78           | 120.80        |
| 1   | А     | 2833 | U    | N1-C2-O2   | 5.85  | 126.89           | 122.80        |
| 1   | А     | 2459 | А    | O4'-C1'-N9 | 5.85  | 112.88           | 108.20        |
| 1   | А     | 1626 | U    | N3-C2-O2   | -5.84 | 118.11           | 122.20        |
| 1   | А     | 2685 | U    | N3-C2-O2   | -5.84 | 118.11           | 122.20        |
| 2   | В     | 58   | С    | C6-N1-C2   | -5.84 | 117.96           | 120.30        |
| 1   | А     | 573  | С    | N3-C2-O2   | -5.84 | 117.81           | 121.90        |
| 5   | Е     | 38   | LEU  | CB-CG-CD1  | -5.84 | 101.08           | 111.00        |
| 1   | А     | 2605 | G    | C4-N9-C1'  | 5.84  | 134.09           | 126.50        |
| 1   | А     | 2665 | U    | N1-C2-O2   | 5.84  | 126.89           | 122.80        |
| 1   | А     | 940  | G    | N7-C8-N9   | 5.83  | 116.02           | 113.10        |
| 33  | a     | 591  | C    | N3-C2-O2   | -5.83 | 117.82           | 121.90        |
| 1   | А     | 1454 | С    | N3-C2-O2   | -5.83 | 117.82           | 121.90        |
| 1   | А     | 406  | G    | N3-C4-N9   | -5.83 | 122.50           | 126.00        |
| 1   | А     | 1560 | U    | C2-N1-C1'  | 5.83  | 124.69           | 117.70        |
| 1   | А     | 975  | С    | C5-C6-N1   | 5.82  | 123.91           | 121.00        |
| 1   | А     | 309  | U    | OP1-P-O3'  | 5.82  | 118.00           | 105.20        |
| 1   | А     | 954  | U    | C5-C6-N1   | 5.82  | 125.61           | 122.70        |
| 33  | a     | 260  | U    | N3-C2-O2   | -5.82 | 118.13           | 122.20        |
| 33  | a     | 1363 | С    | C6-N1-C2   | -5.82 | 117.97           | 120.30        |
| 1   | A     | 1942 | A    | C4-C5-C6   | -5.82 | 114.09           | 117.00        |
| 1   | A     | 1981 | A    | N7-C8-N9   | 5.81  | 116.71           | 113.80        |
| 1   | A     | 2911 | G    | C8-N9-C4   | -5.81 | 104.08           | 106.40        |
| 1   | A     | 113  | U    | C2-N1-C1'  | 5.81  | 124.67           | 117.70        |
| 1   | A     | 2054 | C    | C4-C5-C6   | -5.80 | 114.50           | 117.40        |
| 1   | A     | 1800 | C    | C6-N1-C2   | -5.80 | 117.98           | 120.30        |



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| Mol | Chain | Res  | Type | Atoms      | Z     | $Observed(^{o})$ | $Ideal(^{o})$ |
|-----|-------|------|------|------------|-------|------------------|---------------|
| 33  | a     | 523  | С    | C5-C6-N1   | 5.80  | 123.90           | 121.00        |
| 1   | А     | 980  | С    | N1-C2-O2   | 5.80  | 122.38           | 118.90        |
| 33  | a     | 1416 | С    | N1-C2-O2   | 5.80  | 122.38           | 118.90        |
| 1   | А     | 810  | G    | C4-N9-C1'  | 5.80  | 134.04           | 126.50        |
| 1   | А     | 2114 | С    | C6-N1-C2   | -5.80 | 117.98           | 120.30        |
| 1   | А     | 2685 | U    | C5-C6-N1   | 5.79  | 125.60           | 122.70        |
| 1   | А     | 2840 | С    | C6-N1-C2   | -5.79 | 117.98           | 120.30        |
| 1   | А     | 2813 | U    | C5-C6-N1   | 5.79  | 125.59           | 122.70        |
| 33  | a     | 1150 | U    | C2-N1-C1'  | 5.78  | 124.64           | 117.70        |
| 10  | L     | 18   | ARG  | CA-CB-CG   | 5.78  | 126.12           | 113.40        |
| 33  | a     | 130  | С    | C5-C6-N1   | 5.78  | 123.89           | 121.00        |
| 33  | a     | 1305 | С    | C6-N1-C2   | -5.78 | 117.99           | 120.30        |
| 1   | А     | 2665 | U    | C2-N1-C1'  | 5.77  | 124.63           | 117.70        |
| 1   | А     | 885  | С    | N3-C2-O2   | -5.77 | 117.86           | 121.90        |
| 1   | А     | 2591 | U    | N3-C2-O2   | -5.77 | 118.16           | 122.20        |
| 1   | А     | 2295 | А    | P-O3'-C3'  | 5.76  | 126.62           | 119.70        |
| 33  | a     | 280  | С    | N3-C2-O2   | -5.76 | 117.86           | 121.90        |
| 1   | А     | 2072 | С    | C5-C6-N1   | 5.76  | 123.88           | 121.00        |
| 33  | a     | 859  | С    | N3-C2-O2   | -5.76 | 117.87           | 121.90        |
| 1   | А     | 860  | U    | N3-C2-O2   | -5.75 | 118.17           | 122.20        |
| 33  | a     | 1391 | С    | C5-C6-N1   | 5.75  | 123.88           | 121.00        |
| 1   | А     | 1781 | С    | C6-N1-C2   | -5.75 | 118.00           | 120.30        |
| 1   | А     | 2105 | U    | C6-N1-C1'  | -5.75 | 113.15           | 121.20        |
| 1   | А     | 2192 | U    | N1-C2-O2   | 5.75  | 126.83           | 122.80        |
| 1   | А     | 2785 | U    | O4'-C1'-N1 | 5.75  | 112.80           | 108.20        |
| 33  | a     | 448  | U    | N1-C2-O2   | 5.75  | 126.83           | 122.80        |
| 1   | А     | 1156 | G    | C8-N9-C4   | -5.75 | 104.10           | 106.40        |
| 1   | А     | 1351 | U    | P-O3'-C3'  | 5.75  | 126.60           | 119.70        |
| 1   | А     | 631  | G    | N1-C2-N2   | 5.75  | 121.37           | 116.20        |
| 33  | a     | 970  | U    | N1-C2-O2   | 5.75  | 126.82           | 122.80        |
| 1   | А     | 1770 | С    | C6-N1-C2   | -5.74 | 118.00           | 120.30        |
| 1   | А     | 576  | G    | P-O3'-C3'  | 5.74  | 126.59           | 119.70        |
| 44  | 1     | 44   | ARG  | N-CA-CB    | 5.74  | 120.93           | 110.60        |
| 1   | A     | 1941 | A    | C8-N9-C1'  | -5.74 | 117.37           | 127.70        |
| 1   | А     | 1942 | А    | C4-N9-C1'  | -5.74 | 115.97           | 126.30        |
| 1   | A     | 2445 | C    | C5-C6-N1   | 5.74  | 123.87           | 121.00        |
| 33  | a     | 467  | С    | C2-N1-C1'  | 5.73  | 125.11           | 118.80        |
| 33  | a     | 746  | С    | C5-C6-N1   | 5.73  | 123.87           | 121.00        |
| 1   | A     | 211  | C    | C5-C6-N1   | 5.73  | 123.86           | 121.00        |
| 1   | A     | 508  | С    | N3-C2-O2   | -5.73 | 117.89           | 121.90        |
| 33  | a     | 86   | G    | C8-N9-C4   | -5.72 | 104.11           | 106.40        |
| 1   | A     | 2605 | G    | C8-N9-C1'  | -5.72 | 119.56           | 127.00        |



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| Mol | Chain | Res  | Type | Atoms      | Z     | $Observed(^{o})$ | $Ideal(^{o})$ |
|-----|-------|------|------|------------|-------|------------------|---------------|
| 33  | a     | 1416 | С    | N3-C2-O2   | -5.72 | 117.90           | 121.90        |
| 1   | А     | 1883 | А    | N7-C8-N9   | 5.71  | 116.66           | 113.80        |
| 33  | a     | 1421 | С    | C5-C6-N1   | 5.71  | 123.85           | 121.00        |
| 53  | Х     | 61   | С    | C5-C6-N1   | 5.71  | 123.85           | 121.00        |
| 1   | А     | 2203 | С    | N1-C2-O2   | 5.71  | 122.32           | 118.90        |
| 1   | А     | 2733 | С    | C6-N1-C2   | -5.71 | 118.02           | 120.30        |
| 2   | В     | 79   | С    | N3-C2-O2   | -5.70 | 117.91           | 121.90        |
| 33  | a     | 856  | С    | C5-C6-N1   | 5.70  | 123.85           | 121.00        |
| 1   | А     | 86   | С    | O4'-C1'-N1 | 5.69  | 112.75           | 108.20        |
| 1   | А     | 2126 | G    | C4-N9-C1'  | 5.69  | 133.90           | 126.50        |
| 1   | А     | 842  | С    | C5-C6-N1   | 5.69  | 123.84           | 121.00        |
| 1   | А     | 252  | С    | OP2-P-O3'  | 5.68  | 117.71           | 105.20        |
| 1   | А     | 2765 | G    | C4-C5-N7   | 5.68  | 113.07           | 110.80        |
| 2   | В     | 28   | С    | C6-N1-C2   | -5.68 | 118.03           | 120.30        |
| 33  | a     | 1398 | С    | C5-C6-N1   | 5.68  | 123.84           | 121.00        |
| 33  | a     | 1502 | А    | N3-C4-C5   | -5.68 | 122.82           | 126.80        |
| 1   | А     | 966  | U    | N1-C2-O2   | 5.68  | 126.78           | 122.80        |
| 1   | А     | 1415 | С    | N3-C2-O2   | -5.68 | 117.92           | 121.90        |
| 1   | А     | 924  | U    | C6-N1-C2   | -5.67 | 117.59           | 121.00        |
| 1   | А     | 212  | С    | N1-C2-O2   | 5.67  | 122.30           | 118.90        |
| 1   | А     | 1339 | А    | O4'-C1'-N9 | -5.67 | 103.66           | 108.20        |
| 1   | А     | 308  | С    | C2-N1-C1'  | 5.67  | 125.04           | 118.80        |
| 33  | a     | 675  | G    | O5'-P-OP2  | -5.67 | 100.60           | 105.70        |
| 1   | А     | 1052 | С    | C6-N1-C2   | -5.66 | 118.03           | 120.30        |
| 1   | А     | 2335 | U    | N1-C2-O2   | 5.66  | 126.76           | 122.80        |
| 33  | a     | 86   | G    | C6-C5-N7   | -5.66 | 127.00           | 130.40        |
| 1   | А     | 2349 | А    | C2-N3-C4   | 5.66  | 113.43           | 110.60        |
| 1   | А     | 246  | U    | N1-C2-O2   | 5.66  | 126.76           | 122.80        |
| 1   | А     | 716  | G    | C4-C5-N7   | 5.66  | 113.06           | 110.80        |
| 33  | a     | 1045 | G    | P-O3'-C3'  | -5.66 | 112.91           | 119.70        |
| 1   | А     | 549  | А    | OP2-P-O3'  | 5.65  | 117.64           | 105.20        |
| 1   | А     | 1137 | G    | C4-N9-C1'  | 5.65  | 133.85           | 126.50        |
| 1   | А     | 1631 | А    | OP1-P-O3'  | 5.65  | 117.63           | 105.20        |
| 1   | А     | 1369 | С    | C6-N1-C2   | -5.65 | 118.04           | 120.30        |
| 1   | А     | 574  | А    | C5-N7-C8   | -5.65 | 101.08           | 103.90        |
| 1   | А     | 1634 | U    | N3-C2-O2   | -5.64 | 118.25           | 122.20        |
| 1   | А     | 221  | G    | N3-C2-N2   | -5.64 | 115.95           | 119.90        |
| 1   | А     | 284  | С    | C2-N1-C1'  | 5.64  | 125.00           | 118.80        |
| 33  | a     | 1237 | C    | N3-C2-O2   | -5.64 | 117.95           | 121.90        |
| 1   | А     | 1122 | С    | C5-C6-N1   | 5.63  | 123.82           | 121.00        |
| 1   | А     | 1329 | С    | C5-C6-N1   | 5.63  | 123.82           | 121.00        |
| 1   | А     | 586  | С    | N3-C2-O2   | -5.63 | 117.96           | 121.90        |



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| Mol | Chain | Res  | Type | Atoms      | Z     | $Observed(^{o})$ | $Ideal(^{o})$ |
|-----|-------|------|------|------------|-------|------------------|---------------|
| 1   | А     | 1771 | С    | N3-C2-O2   | -5.63 | 117.96           | 121.90        |
| 1   | А     | 2711 | G    | O5'-P-OP2  | -5.63 | 100.64           | 105.70        |
| 1   | А     | 4    | U    | C5-C6-N1   | 5.62  | 125.51           | 122.70        |
| 1   | А     | 914  | С    | N3-C2-O2   | -5.62 | 117.96           | 121.90        |
| 1   | А     | 1507 | U    | P-O3'-C3'  | 5.62  | 126.45           | 119.70        |
| 1   | А     | 2801 | С    | N3-C2-O2   | -5.62 | 117.97           | 121.90        |
| 33  | a     | 1003 | G    | N3-C4-N9   | 5.62  | 129.37           | 126.00        |
| 53  | Х     | 21   | G    | N7-C8-N9   | 5.62  | 115.91           | 113.10        |
| 1   | А     | 506  | U    | N1-C2-O2   | 5.61  | 126.73           | 122.80        |
| 1   | А     | 2791 | U    | C2-N1-C1'  | 5.61  | 124.43           | 117.70        |
| 1   | А     | 977  | U    | C6-N1-C2   | -5.61 | 117.64           | 121.00        |
| 1   | А     | 1333 | С    | C2-N1-C1'  | 5.60  | 124.96           | 118.80        |
| 1   | А     | 104  | С    | N3-C2-O2   | -5.60 | 117.98           | 121.90        |
| 1   | А     | 2904 | А    | OP2-P-O3'  | 5.60  | 117.52           | 105.20        |
| 33  | a     | 641  | G    | C8-N9-C4   | -5.60 | 104.16           | 106.40        |
| 1   | А     | 776  | G    | C8-N9-C1'  | -5.59 | 119.73           | 127.00        |
| 1   | А     | 1613 | С    | C6-N1-C2   | -5.59 | 118.06           | 120.30        |
| 1   | А     | 2422 | U    | N3-C2-O2   | -5.59 | 118.29           | 122.20        |
| 1   | А     | 422  | С    | C6-N1-C2   | -5.59 | 118.06           | 120.30        |
| 1   | А     | 2189 | G    | C4-N9-C1'  | 5.59  | 133.77           | 126.50        |
| 1   | А     | 2225 | С    | N1-C2-O2   | 5.59  | 122.25           | 118.90        |
| 1   | А     | 686  | С    | C5-C6-N1   | 5.59  | 123.79           | 121.00        |
| 41  | i     | 122  | ARG  | CB-CG-CD   | 5.59  | 126.13           | 111.60        |
| 1   | А     | 895  | G    | N3-C4-C5   | -5.58 | 125.81           | 128.60        |
| 1   | А     | 966  | U    | N3-C2-O2   | -5.58 | 118.29           | 122.20        |
| 33  | a     | 735  | С    | C6-N1-C2   | -5.58 | 118.07           | 120.30        |
| 33  | a     | 1032 | С    | P-O3'-C3'  | 5.58  | 126.40           | 119.70        |
| 1   | А     | 556  | С    | N1-C2-O2   | 5.58  | 122.25           | 118.90        |
| 1   | А     | 1942 | А    | N1-C6-N6   | -5.58 | 115.25           | 118.60        |
| 33  | a     | 274  | G    | O4'-C1'-N9 | -5.58 | 103.74           | 108.20        |
| 1   | А     | 1695 | A    | C8-N9-C4   | 5.58  | 108.03           | 105.80        |
| 33  | a     | 56   | С    | N1-C2-O2   | 5.58  | 122.25           | 118.90        |
| 1   | А     | 1365 | U    | N1-C1'-C2' | -5.57 | 105.87           | 112.00        |
| 33  | a     | 472  | С    | C6-N1-C2   | -5.57 | 118.07           | 120.30        |
| 33  | a     | 1460 | U    | N3-C2-O2   | -5.57 | 118.30           | 122.20        |
| 1   | А     | 88   | G    | P-O3'-C3'  | 5.57  | 126.38           | 119.70        |
| 33  | a     | 829  | U    | OP2-P-O3'  | 5.57  | 117.45           | 105.20        |
| 1   | А     | 63   | G    | OP1-P-OP2  | -5.57 | 111.25           | 119.60        |
| 1   | A     | 1753 | С    | C6-N1-C2   | -5.57 | 118.07           | 120.30        |
| 1   | A     | 1296 | G    | C8-N9-C1'  | -5.56 | 119.77           | 127.00        |
| 33  | a     | 465  | U    | C5-C6-N1   | 5.56  | 125.48           | 122.70        |
| 1   | A     | 1374 | С    | N3-C2-O2   | -5.56 | 118.01           | 121.90        |



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| Mol | Chain | Res  | Type | Atoms       | Z     | $Observed(^{o})$ | $Ideal(^{o})$ |
|-----|-------|------|------|-------------|-------|------------------|---------------|
| 1   | А     | 236  | А    | C3'-C2'-C1' | 5.56  | 105.94           | 101.50        |
| 1   | А     | 464  | С    | C5-C6-N1    | 5.56  | 123.78           | 121.00        |
| 33  | a     | 130  | С    | N1-C2-O2    | 5.55  | 122.23           | 118.90        |
| 33  | a     | 167  | G    | C4-N9-C1'   | 5.55  | 133.72           | 126.50        |
| 1   | А     | 1622 | С    | C5-C6-N1    | 5.55  | 123.78           | 121.00        |
| 1   | А     | 2840 | С    | C5-C6-N1    | 5.55  | 123.77           | 121.00        |
| 1   | А     | 1953 | С    | C2-N1-C1'   | 5.54  | 124.90           | 118.80        |
| 1   | А     | 681  | С    | C5-C6-N1    | 5.54  | 123.77           | 121.00        |
| 1   | А     | 2177 | G    | C8-N9-C4    | -5.54 | 104.18           | 106.40        |
| 33  | a     | 60   | С    | N1-C2-O2    | 5.54  | 122.23           | 118.90        |
| 33  | a     | 1032 | С    | C6-N1-C2    | -5.54 | 118.08           | 120.30        |
| 33  | a     | 901  | U    | N1-C2-O2    | 5.54  | 126.68           | 122.80        |
| 33  | a     | 182  | U    | N1-C2-O2    | 5.54  | 126.68           | 122.80        |
| 33  | a     | 1167 | С    | C2-N1-C1'   | 5.54  | 124.89           | 118.80        |
| 53  | Х     | 43   | G    | N1-C6-O6    | -5.54 | 116.58           | 119.90        |
| 1   | А     | 2323 | С    | C5-C6-N1    | 5.53  | 123.77           | 121.00        |
| 33  | a     | 481  | С    | C6-N1-C2    | -5.53 | 118.09           | 120.30        |
| 1   | А     | 2821 | U    | N3-C2-O2    | -5.53 | 118.33           | 122.20        |
| 33  | a     | 1123 | С    | C6-N1-C2    | -5.53 | 118.09           | 120.30        |
| 1   | А     | 308  | С    | C6-N1-C2    | -5.53 | 118.09           | 120.30        |
| 1   | А     | 483  | С    | C2-N1-C1'   | 5.53  | 124.88           | 118.80        |
| 1   | А     | 533  | С    | C6-N1-C2    | -5.53 | 118.09           | 120.30        |
| 33  | a     | 1041 | С    | P-O3'-C3'   | 5.53  | 126.33           | 119.70        |
| 1   | А     | 1369 | С    | N1-C2-O2    | 5.53  | 122.22           | 118.90        |
| 20  | V     | 428  | LEU  | CA-CB-CG    | 5.52  | 128.00           | 115.30        |
| 1   | А     | 1567 | U    | P-O3'-C3'   | 5.52  | 126.32           | 119.70        |
| 5   | Е     | 126  | LEU  | CB-CG-CD1   | -5.52 | 101.62           | 111.00        |
| 33  | a     | 1016 | А    | P-O3'-C3'   | 5.52  | 126.32           | 119.70        |
| 2   | В     | 72   | U    | N3-C2-O2    | -5.51 | 118.34           | 122.20        |
| 33  | a     | 143  | C    | C2-N1-C1'   | 5.51  | 124.87           | 118.80        |
| 1   | А     | 66   | С    | N1-C2-O2    | 5.51  | 122.21           | 118.90        |
| 1   | А     | 1352 | U    | C6-N1-C1'   | -5.51 | 113.48           | 121.20        |
| 1   | А     | 1545 | С    | C6-N1-C2    | -5.51 | 118.09           | 120.30        |
| 1   | А     | 1328 | C    | N3-C2-O2    | -5.51 | 118.04           | 121.90        |
| 1   | А     | 1522 | U    | N1-C2-O2    | 5.51  | 126.66           | 122.80        |
| 1   | A     | 211  | С    | C6-N1-C2    | -5.51 | 118.10           | 120.30        |
| 1   | А     | 1245 | G    | OP1-P-OP2   | -5.51 | 111.34           | 119.60        |
| 1   | A     | 1052 | C    | C5-C6-N1    | 5.51  | 123.75           | 121.00        |
| 1   | A     | 187  | C    | O4'-C1'-N1  | 5.50  | 112.60           | 108.20        |
| 1   | А     | 2255 | C    | C6-N1-C2    | -5.50 | 118.10           | 120.30        |
| 1   | A     | 1476 | C    | N3-C2-O2    | -5.50 | 118.05           | 121.90        |
| 1   | А     | 1379 | U    | N3-C2-O2    | -5.50 | 118.35           | 122.20        |



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| Mol | Chain | Res  | Type | Atoms      | Z     | $Observed(^{o})$    | $Ideal(^{o})$ |
|-----|-------|------|------|------------|-------|---------------------|---------------|
| 1   | А     | 1946 | U    | C5-C6-N1   | 5.50  | 125.45              | 122.70        |
| 34  | b     | 18   | HIS  | C-N-CA     | 5.50  | 135.44              | 121.70        |
| 1   | А     | 1813 | А    | P-O3'-C3'  | 5.50  | 126.30              | 119.70        |
| 1   | А     | 1577 | С    | N1-C2-O2   | 5.49  | 122.19              | 118.90        |
| 1   | А     | 2025 | С    | C6-N1-C2   | -5.49 | 118.11              | 120.30        |
| 1   | А     | 2155 | А    | OP2-P-O3'  | 5.49  | 117.27              | 105.20        |
| 1   | А     | 1573 | С    | N1-C2-O2   | 5.48  | 122.19              | 118.90        |
| 33  | a     | 248  | С    | O4'-C1'-N1 | 5.48  | 112.58              | 108.20        |
| 1   | А     | 940  | G    | C8-N9-C4   | -5.47 | 104.21              | 106.40        |
| 1   | А     | 843  | С    | N1-C2-O2   | 5.47  | 122.18              | 118.90        |
| 1   | А     | 2273 | U    | N3-C4-O4   | 5.47  | 123.23              | 119.40        |
| 53  | Х     | 6    | G    | O5'-P-OP1  | 5.47  | 117.26              | 110.70        |
| 33  | a     | 1398 | С    | C2-N1-C1'  | 5.47  | 124.81              | 118.80        |
| 1   | А     | 252  | С    | P-O3'-C3'  | 5.46  | 126.26              | 119.70        |
| 1   | А     | 1325 | А    | C4-C5-C6   | -5.46 | 114.27              | 117.00        |
| 33  | a     | 989  | С    | C6-N1-C2   | -5.46 | 118.11              | 120.30        |
| 1   | А     | 2203 | С    | C5-C6-N1   | 5.46  | 123.73              | 121.00        |
| 2   | В     | 61   | U    | N1-C2-O2   | 5.46  | 126.62              | 122.80        |
| 33  | a     | 1287 | С    | N3-C2-O2   | -5.46 | 118.08              | 121.90        |
| 1   | А     | 2423 | С    | N3-C2-O2   | -5.46 | 118.08              | 121.90        |
| 1   | А     | 2345 | U    | C2-N1-C1'  | 5.46  | 124.25              | 117.70        |
| 1   | А     | 2795 | G    | C8-N9-C4   | -5.46 | 104.22              | 106.40        |
| 33  | a     | 670  | G    | N3-C4-N9   | 5.46  | 129.28              | 126.00        |
| 1   | А     | 1306 | G    | O5'-P-OP1  | -5.46 | 100.79              | 105.70        |
| 1   | А     | 1943 | С    | C6-N1-C2   | -5.46 | 118.12              | 120.30        |
| 2   | В     | 24   | С    | C6-N1-C1'  | -5.45 | 114.26              | 120.80        |
| 1   | А     | 2685 | U    | N1-C2-O2   | 5.45  | 126.61              | 122.80        |
| 1   | А     | 1485 | А    | O4'-C1'-N9 | 5.45  | 112.56              | 108.20        |
| 1   | А     | 2765 | G    | C6-C5-N7   | -5.45 | 127.13              | 130.40        |
| 33  | a     | 1051 | G    | N3-C4-N9   | 5.44  | 129.26              | 126.00        |
| 33  | a     | 1323 | С    | C6-N1-C2   | -5.44 | 118.12              | 120.30        |
| 1   | А     | 1817 | С    | N3-C2-O2   | -5.44 | 118.09              | 121.90        |
| 33  | a     | 1438 | С    | C2-N1-C1'  | 5.44  | 124.78              | 118.80        |
| 1   | А     | 270  | С    | C6-N1-C2   | -5.43 | 118.13              | 120.30        |
| 1   | А     | 1269 | А    | P-O3'-C3'  | 5.43  | 126.22              | 119.70        |
| 1   | А     | 789  | С    | C5-C6-N1   | 5.43  | 123.72              | 121.00        |
| 16  | R     | 75   | ARG  | NE-CZ-NH1  | -5.42 | 117.59              | 120.30        |
| 1   | А     | 2283 | С    | N1-C2-O2   | 5.42  | 122.15              | 118.90        |
| 15  | Q     | 92   | ARG  | CA-CB-CG   | 5.42  | 125.33              | 113.40        |
| 1   | А     | 614  | G    | N3-C4-C5   | -5.42 | 125.89              | 128.60        |
| 1   | А     | 1803 | С    | N3-C2-O2   | -5.42 | 118.11              | 121.90        |
| 1   | А     | 2487 | U    | N1-C2-O2   | 5.42  | $1\overline{26.59}$ | 122.80        |



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| Mol | Chain | Res  | Type | Atoms     | Z     | $Observed(^{o})$ | $Ideal(^{o})$ |
|-----|-------|------|------|-----------|-------|------------------|---------------|
| 1   | А     | 2915 | G    | C5-C6-O6  | -5.42 | 125.35           | 128.60        |
| 33  | a     | 633  | С    | C6-N1-C2  | -5.42 | 118.13           | 120.30        |
| 33  | a     | 1123 | С    | N1-C2-O2  | 5.42  | 122.15           | 118.90        |
| 31  | 7     | 25   | С    | N3-C2-O2  | -5.41 | 118.11           | 121.90        |
| 33  | a     | 994  | С    | C6-N1-C2  | -5.41 | 118.14           | 120.30        |
| 1   | А     | 2289 | С    | C6-N1-C2  | -5.41 | 118.14           | 120.30        |
| 1   | А     | 1327 | U    | C2-N1-C1' | 5.41  | 124.19           | 117.70        |
| 1   | А     | 2825 | С    | N1-C2-O2  | 5.41  | 122.14           | 118.90        |
| 33  | a     | 1123 | С    | C5-C6-N1  | 5.40  | 123.70           | 121.00        |
| 1   | А     | 1872 | С    | N1-C2-O2  | 5.40  | 122.14           | 118.90        |
| 1   | А     | 1137 | G    | C8-N9-C1' | -5.40 | 119.98           | 127.00        |
| 1   | А     | 1981 | А    | C5-N7-C8  | -5.40 | 101.20           | 103.90        |
| 33  | a     | 1018 | U    | C5-C6-N1  | 5.40  | 125.40           | 122.70        |
| 1   | А     | 648  | G    | N9-C4-C5  | -5.40 | 103.24           | 105.40        |
| 33  | a     | 970  | U    | N3-C2-O2  | -5.40 | 118.42           | 122.20        |
| 1   | А     | 2904 | А    | P-O3'-C3' | 5.39  | 126.17           | 119.70        |
| 1   | А     | 2333 | G    | C4-N9-C1' | 5.39  | 133.51           | 126.50        |
| 33  | a     | 563  | U    | C5-C6-N1  | 5.39  | 125.39           | 122.70        |
| 1   | А     | 1844 | А    | OP1-P-O3' | 5.38  | 117.05           | 105.20        |
| 33  | a     | 1308 | А    | C4-N9-C1' | 5.38  | 135.99           | 126.30        |
| 33  | a     | 437  | U    | OP1-P-O3' | 5.38  | 117.04           | 105.20        |
| 1   | А     | 1274 | U    | N1-C2-O2  | 5.38  | 126.57           | 122.80        |
| 1   | А     | 2823 | С    | O5'-P-OP2 | -5.38 | 100.86           | 105.70        |
| 33  | a     | 691  | С    | C5-C6-N1  | 5.38  | 123.69           | 121.00        |
| 33  | a     | 1391 | С    | N3-C2-O2  | -5.38 | 118.14           | 121.90        |
| 1   | А     | 1172 | А    | P-O3'-C3' | 5.38  | 126.15           | 119.70        |
| 1   | А     | 2910 | С    | C6-N1-C2  | -5.38 | 118.15           | 120.30        |
| 1   | А     | 1516 | А    | C8-N9-C4  | -5.37 | 103.65           | 105.80        |
| 1   | А     | 2326 | С    | C5-C6-N1  | 5.37  | 123.69           | 121.00        |
| 1   | А     | 575  | A    | OP2-P-O3' | 5.37  | 117.01           | 105.20        |
| 1   | А     | 1011 | С    | C5-C6-N1  | 5.37  | 123.69           | 121.00        |
| 1   | А     | 2159 | U    | C5-C6-N1  | 5.37  | 125.38           | 122.70        |
| 1   | А     | 2920 | С    | C6-N1-C2  | -5.37 | 118.15           | 120.30        |
| 1   | А     | 284  | С    | N1-C2-O2  | 5.36  | 122.12           | 118.90        |
| 33  | a     | 787  | G    | N7-C8-N9  | 5.36  | 115.78           | 113.10        |
| 34  | b     | 137  | LEU  | CA-CB-CG  | 5.36  | 127.64           | 115.30        |
| 1   | A     | 1351 | U    | OP2-P-O3' | 5.36  | 116.99           | 105.20        |
| 1   | А     | 941  | U    | C2-N1-C1' | 5.36  | 124.13           | 117.70        |
| 1   | A     | 1484 | U    | N3-C2-O2  | -5.36 | 118.45           | 122.20        |
| 33  | a     | 1525 | С    | C6-N1-C2  | -5.36 | 118.16           | 120.30        |
| 1   | А     | 1714 | А    | C4-N9-C1' | 5.35  | 135.93           | 126.30        |
| 1   | A     | 2296 | A    | OP1-P-OP2 | -5.35 | 111.57           | 119.60        |



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| Mol | Chain | Res  | Type | Atoms       | Z                 | $Observed(^{o})$ | $Ideal(^{o})$ |
|-----|-------|------|------|-------------|-------------------|------------------|---------------|
| 33  | a     | 848  | G    | P-O3'-C3'   | 5.35              | 126.12           | 119.70        |
| 33  | a     | 950  | С    | C6-N1-C2    | -5.35             | 118.16           | 120.30        |
| 33  | a     | 90   | С    | C6-N1-C2    | -5.35             | 118.16           | 120.30        |
| 33  | a     | 1308 | А    | C2-N3-C4    | 5.35              | 113.28           | 110.60        |
| 1   | А     | 562  | С    | C5-C6-N1    | 5.35              | 123.67           | 121.00        |
| 1   | А     | 1559 | С    | C6-N1-C2    | -5.35             | 118.16           | 120.30        |
| 33  | a     | 787  | G    | C8-N9-C4    | -5.35             | 104.26           | 106.40        |
| 1   | А     | 2432 | С    | N3-C2-O2    | -5.34             | 118.16           | 121.90        |
| 1   | А     | 1343 | С    | N1-C2-O2    | 5.34              | 122.11           | 118.90        |
| 1   | А     | 1454 | С    | N1-C2-O2    | 5.34              | 122.11           | 118.90        |
| 16  | R     | 22   | ILE  | CG1-CB-CG2  | -5.34             | 99.65            | 111.40        |
| 33  | a     | 1070 | U    | C6-N1-C2    | -5.34             | 117.80           | 121.00        |
| 1   | А     | 2503 | С    | C2-N1-C1'   | 5.34              | 124.67           | 118.80        |
| 16  | R     | 75   | ARG  | NE-CZ-NH2   | 5.34              | 122.97           | 120.30        |
| 1   | А     | 1334 | С    | C6-N1-C2    | -5.34             | 118.17           | 120.30        |
| 1   | А     | 670  | С    | C6-N1-C2    | -5.33             | 118.17           | 120.30        |
| 1   | А     | 1350 | U    | N3-C2-O2    | -5.33             | 118.47           | 122.20        |
| 33  | a     | 486  | С    | C6-N1-C1'   | -5.33             | 114.40           | 120.80        |
| 1   | А     | 1344 | С    | C6-N1-C2    | -5.33             | 118.17           | 120.30        |
| 1   | А     | 1614 | А    | N7-C8-N9    | 5.33              | 116.47           | 113.80        |
| 1   | А     | 2093 | С    | C6-N1-C2    | -5.33             | 118.17           | 120.30        |
| 33  | a     | 1170 | С    | O4'-C1'-N1  | 5.33              | 112.46           | 108.20        |
| 1   | А     | 778  | С    | N3-C2-O2    | -5.33             | 118.17           | 121.90        |
| 1   | А     | 1577 | С    | C6-N1-C2    | -5.33             | 118.17           | 120.30        |
| 1   | А     | 1941 | А    | C5-N7-C8    | -5.33             | 101.24           | 103.90        |
| 1   | А     | 2092 | С    | C5-C6-N1    | 5.33              | 123.67           | 121.00        |
| 1   | А     | 1846 | G    | C8-N9-C4    | -5.33             | 104.27           | 106.40        |
| 1   | А     | 113  | U    | N1-C2-O2    | 5.32              | 126.53           | 122.80        |
| 1   | А     | 1813 | А    | OP2-P-O3'   | 5.32              | 116.90           | 105.20        |
| 1   | А     | 2157 | С    | C6-N1-C2    | -5.32             | 118.17           | 120.30        |
| 1   | А     | 645  | С    | C5-C6-N1    | 5.32              | 123.66           | 121.00        |
| 33  | a     | 1076 | С    | C6-N1-C1'   | -5.32             | 114.42           | 120.80        |
| 1   | А     | 980  | С    | C6-N1-C2    | -5.31             | 118.17           | 120.30        |
| 1   | А     | 1336 | С    | N3-C2-O2    | -5.31             | 118.18           | 121.90        |
| 1   | А     | 1953 | С    | C5-C6-N1    | 5.31              | 123.66           | 121.00        |
| 1   | A     | 777  | C    | C5-C6-N1    | $5.3\overline{1}$ | 123.66           | 121.00        |
| 1   | A     | 716  | G    | C6-C5-N7    | -5.31             | 127.22           | 130.40        |
| 1   | A     | 2287 | С    | OP2-P-O3'   | 5.31              | 116.87           | 105.20        |
| 1   | A     | 2356 | A    | C3'-C2'-C1' | 5.31              | 105.74           | 101.50        |
| 45  | m     | 80   | LEU  | CA-CB-CG    | 5.31              | 127.50           | 115.30        |
| 1   | А     | 1752 | G    | N3-C4-N9    | 5.30              | 129.18           | 126.00        |
| 1   | A     | 2244 | G    | O4'-C1'-N9  | 5.30              | 112.44           | 108.20        |



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| Mol | Chain | Res  | Type | Atoms      | Z     | $Observed(^{o})$ | $Ideal(^{o})$ |
|-----|-------|------|------|------------|-------|------------------|---------------|
| 2   | В     | 14   | G    | N3-C4-N9   | 5.30  | 129.18           | 126.00        |
| 1   | А     | 2273 | U    | C5-C6-N1   | 5.30  | 125.35           | 122.70        |
| 1   | А     | 937  | С    | C6-N1-C2   | -5.30 | 118.18           | 120.30        |
| 1   | А     | 2795 | G    | C2-N3-C4   | 5.30  | 114.55           | 111.90        |
| 1   | А     | 2323 | С    | C6-N1-C2   | -5.29 | 118.18           | 120.30        |
| 33  | a     | 226  | С    | C6-N1-C2   | -5.29 | 118.18           | 120.30        |
| 1   | А     | 894  | А    | C5-N7-C8   | -5.29 | 101.25           | 103.90        |
| 33  | a     | 155  | С    | C2-N1-C1'  | 5.29  | 124.62           | 118.80        |
| 34  | b     | 17   | GLY  | N-CA-C     | 5.29  | 126.33           | 113.10        |
| 33  | a     | 1149 | U    | C6-N1-C1'  | -5.29 | 113.80           | 121.20        |
| 1   | А     | 1705 | С    | C5-C6-N1   | 5.29  | 123.64           | 121.00        |
| 1   | А     | 563  | С    | C6-N1-C2   | -5.28 | 118.19           | 120.30        |
| 1   | А     | 574  | А    | C2-N3-C4   | -5.28 | 107.96           | 110.60        |
| 1   | А     | 2348 | С    | C2-N1-C1'  | 5.28  | 124.61           | 118.80        |
| 2   | В     | 58   | С    | C5-C6-N1   | 5.28  | 123.64           | 121.00        |
| 33  | a     | 469  | G    | N7-C8-N9   | 5.28  | 115.74           | 113.10        |
| 1   | А     | 163  | U    | P-O3'-C3'  | 5.28  | 126.03           | 119.70        |
| 1   | А     | 2283 | С    | N3-C2-O2   | -5.28 | 118.21           | 121.90        |
| 1   | А     | 2820 | U    | C2-N1-C1'  | 5.28  | 124.03           | 117.70        |
| 1   | А     | 271  | С    | C6-N1-C2   | -5.28 | 118.19           | 120.30        |
| 1   | А     | 421  | А    | N7-C8-N9   | 5.28  | 116.44           | 113.80        |
| 33  | a     | 819  | С    | C2-N1-C1'  | 5.28  | 124.60           | 118.80        |
| 1   | А     | 2765 | G    | C4-N9-C1'  | 5.27  | 133.35           | 126.50        |
| 1   | А     | 556  | С    | C2-N1-C1'  | 5.27  | 124.60           | 118.80        |
| 1   | A     | 1699 | А    | O4'-C1'-N9 | 5.27  | 112.42           | 108.20        |
| 1   | A     | 2065 | С    | C6-N1-C2   | -5.27 | 118.19           | 120.30        |
| 33  | a     | 1175 | G    | OP2-P-O3'  | 5.27  | 116.79           | 105.20        |
| 1   | A     | 2189 | G    | N9-C4-C5   | -5.27 | 103.29           | 105.40        |
| 33  | a     | 1357 | U    | C2-N1-C1'  | 5.27  | 124.02           | 117.70        |
| 53  | x     | 21   | G    | C8-N9-C4   | -5.27 | 104.29           | 106.40        |
| 2   | В     | 37   | A    | P-O3'-C3'  | 5.26  | 126.02           | 119.70        |
| 1   | A     | 1379 | U    | N1-C2-O2   | 5.26  | 126.48           | 122.80        |
| 1   | A     | 2131 | U    | C6-N1-C2   | -5.26 | 117.84           | 121.00        |
| 1   | A     | 1942 | A    | C5-N7-C8   | 5.26  | 106.53           | 103.90        |
| 1   | A     | 2190 | С    | C6-N1-C2   | -5.26 | 118.20           | 120.30        |
| 1   | A     | 1467 | G    | C6-C5-N7   | -5.26 | 127.25           | 130.40        |
| 1   | A     | 1604 | С    | N3-C2-O2   | -5.26 | 118.22           | 121.90        |
| 33  | a     | 523  | C    | C6-N1-C2   | -5.26 | 118.20           | 120.30        |
| 33  | a     | 1494 | U    | C5-C6-N1   | 5.26  | 125.33           | 122.70        |
| 1   | А     | 732  | А    | P-O3'-C3'  | 5.25  | 126.01           | 119.70        |
| 1   | A     | 445  | С    | N1-C2-O2   | 5.25  | 122.05           | 118.90        |
| 1   | A     | 2093 | C    | C5-C6-N1   | 5.25  | 123.63           | 121.00        |



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В

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1448

2189

545

309

901

1804

1437

944

2114

476

49

773

686

С

U

G

С

U

U

U

С

С

С

U

G

С

С

N3-C2-O2

P-O3'-C3'

C6-C5-N7

N1-C2-O2

N3-C2-O2

N3-C2-O2

N1-C2-O2

C6-N1-C2

O4'-C1'-N1

C6-N1-C1'

N3-C2-O2

P-O3'-C3'

C5-C6-N1

C2-N1-C1'

-5.22

5.22

-5.22

5.22

-5.21

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5.21

5.20

5.20

118.25

125.96

127.27

122.03

118.55

118.55

126.45

118.22

104.03

114.55

118.55

125.95

123.60

124.52

Ideal(°)

115.30

105.20

113.80

117.70

126.50

121.00

118.80

122.70

118.90

122.20

106.40

119.70

118.90

121.00

119.70

120.30

122.80

118.90

121.00

118.80

128.60

122.70

126.00

113.30

118.90

119.70

121.00

118.90

121.90

119.70

130.40

118.90

122.20

122.20

122.80

120.30

108.20

120.80

122.20

119.70

121.00

118.80

| Mol | Chain | Res  | Type | Atoms     | Z     | Observed( <sup>o</sup> ) |
|-----|-------|------|------|-----------|-------|--------------------------|
| 37  | е     | 36   | LEU  | CA-CB-CG  | 5.25  | 127.38                   |
| 1   | А     | 1448 | U    | OP1-P-O3' | 5.25  | 116.75                   |
| 33  | a     | 171  | А    | N7-C8-N9  | 5.25  | 116.43                   |
| 33  | a     | 1460 | U    | C2-N1-C1' | 5.25  | 124.00                   |
| 33  | a     | 384  | G    | C4-N9-C1' | 5.25  | 133.32                   |
| 1   | А     | 1753 | С    | C5-C6-N1  | 5.25  | 123.62                   |
| 1   | А     | 1374 | С    | C2-N1-C1' | 5.25  | 124.57                   |
| 33  | a     | 1149 | U    | C5-C6-N1  | 5.25  | 125.32                   |
| 33  | a     | 155  | С    | N1-C2-O2  | 5.24  | 122.05                   |
| 33  | a     | 1357 | U    | N3-C2-O2  | -5.24 | 118.53                   |
| 2   | В     | 52   | G    | C8-N9-C4  | -5.24 | 104.30                   |
| 33  | a     | 455  | G    | P-O3'-C3' | 5.24  | 125.99                   |
| 1   | А     | 2166 | С    | N1-C2-O2  | 5.24  | 122.04                   |
| 33  | a     | 537  | С    | C5-C6-N1  | 5.24  | 123.62                   |
| 1   | А     | 458  | G    | P-O3'-C3' | 5.24  | 125.98                   |
| 1   | А     | 2277 | С    | C6-N1-C2  | -5.24 | 118.20                   |
| 1   | А     | 2591 | U    | N1-C2-O2  | 5.24  | 126.46                   |
| 1   | А     | 1336 | С    | N1-C2-O2  | 5.23  | 122.04                   |
| 1   | А     | 1701 | С    | C5-C6-N1  | 5.23  | 123.62                   |
| 1   | А     | 1559 | С    | C2-N1-C1' | 5.23  | 124.56                   |
| 1   | А     | 1671 | G    | N3-C4-C5  | -5.23 | 125.98                   |
| 33  | a     | 1460 | U    | C5-C6-N1  | 5.23  | 125.31                   |
| 53  | X     | 53   | G    | N3-C4-N9  | 5.23  | 129.14                   |
| 4   | D     | 12   | MET  | CA-CB-CG  | 5.23  | 122.19                   |
| 1   | А     | 1970 | С    | N1-C2-O2  | 5.22  | 122.03                   |
| 33  | a     | 1462 | U    | P-O3'-C3' | 5.22  | 125.97                   |
| 1   | A     | 1223 | С    | C5-C6-N1  | 5.22  | 123.61                   |
| 1   | A     | 2114 | C    | N1-C2-O2  | 5.22  | 122.03                   |

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| Mol | Chain | Res  | Type | Atoms      | Z                 | $Observed(^{o})$ | $Ideal(^{o})$ |
|-----|-------|------|------|------------|-------------------|------------------|---------------|
| 1   | А     | 179  | А    | O4'-C1'-N9 | -5.20             | 104.04           | 108.20        |
| 2   | В     | 15   | С    | N1-C2-O2   | 5.20              | 122.02           | 118.90        |
| 1   | А     | 1344 | С    | N3-C2-O2   | -5.20             | 118.26           | 121.90        |
| 1   | А     | 1922 | С    | N1-C2-O2   | 5.20              | 122.02           | 118.90        |
| 2   | В     | 62   | U    | N3-C2-O2   | -5.20             | 118.56           | 122.20        |
| 33  | a     | 113  | G    | P-O3'-C3'  | 5.20              | 125.94           | 119.70        |
| 1   | А     | 501  | А    | OP2-P-O3'  | 5.20              | 116.63           | 105.20        |
| 1   | А     | 895  | G    | N3-C4-N9   | 5.20              | 129.12           | 126.00        |
| 1   | А     | 914  | С    | N1-C2-O2   | 5.20              | 122.02           | 118.90        |
| 1   | А     | 83   | G    | N3-C4-N9   | -5.19             | 122.88           | 126.00        |
| 1   | А     | 1422 | С    | C6-N1-C2   | -5.19             | 118.22           | 120.30        |
| 33  | a     | 332  | G    | N3-C4-C5   | -5.19             | 126.00           | 128.60        |
| 1   | А     | 1343 | С    | C6-N1-C1'  | -5.19             | 114.57           | 120.80        |
| 33  | a     | 746  | С    | N1-C2-O2   | 5.19              | 122.01           | 118.90        |
| 1   | А     | 830  | А    | C4-C5-N7   | 5.19              | 113.30           | 110.70        |
| 1   | А     | 1794 | С    | C6-N1-C2   | -5.19             | 118.22           | 120.30        |
| 1   | А     | 769  | А    | C6-N1-C2   | 5.19              | 121.71           | 118.60        |
| 1   | А     | 2348 | С    | N1-C2-O2   | 5.19              | 122.01           | 118.90        |
| 33  | a     | 445  | U    | C5-C6-N1   | 5.19              | 125.29           | 122.70        |
| 1   | А     | 2254 | А    | OP2-P-O3'  | 5.19              | 116.61           | 105.20        |
| 1   | А     | 3    | U    | C5-C6-N1   | 5.18              | 125.29           | 122.70        |
| 1   | А     | 93   | С    | C6-N1-C1'  | 5.18              | 127.02           | 120.80        |
| 1   | А     | 2333 | G    | C8-N9-C1'  | -5.18             | 120.27           | 127.00        |
| 1   | А     | 2712 | С    | N3-C2-O2   | -5.18             | 118.28           | 121.90        |
| 33  | a     | 989  | С    | C2-N1-C1'  | 5.18              | 124.50           | 118.80        |
| 1   | А     | 284  | С    | OP2-P-O3'  | 5.18              | 116.59           | 105.20        |
| 1   | А     | 1671 | G    | P-O3'-C3'  | 5.18              | 125.91           | 119.70        |
| 1   | А     | 442  | С    | C2-N1-C1'  | 5.17              | 124.49           | 118.80        |
| 1   | А     | 2839 | С    | N1-C2-O2   | 5.17              | 122.00           | 118.90        |
| 33  | a     | 563  | U    | P-O3'-C3'  | 5.17              | 125.91           | 119.70        |
| 33  | a     | 966  | U    | C5-C6-N1   | 5.17              | 125.29           | 122.70        |
| 33  | a     | 981  | G    | O4'-C1'-N9 | 5.17              | 112.34           | 108.20        |
| 1   | А     | 1067 | А    | C4-C5-N7   | 5.17              | 113.28           | 110.70        |
| 1   | А     | 2445 | С    | C6-N1-C2   | -5.17             | 118.23           | 120.30        |
| 33  | a     | 467  | С    | C5-C6-N1   | 5.17              | 123.58           | 121.00        |
| 2   | В     | 29   | С    | C6-N1-C1'  | -5.17             | 114.60           | 120.80        |
| 33  | a     | 155  | С    | C5-C6-N1   | 5.17              | 123.58           | 121.00        |
| 33  | a     | 563  | U    | OP1-P-O3'  | 5.17              | 116.56           | 105.20        |
| 1   | A     | 1117 | G    | N3-C4-C5   | -5.16             | 126.02           | 128.60        |
| 1   | A     | 1156 | G    | N7-C8-N9   | 5.16              | 115.68           | 113.10        |
| 1   | A     | 2454 | A    | P-O3'-C3'  | $5.1\overline{6}$ | 125.89           | 119.70        |
| 44  | 1     | 94   | LEU  | CA-CB-CG   | 5.16              | 127.17           | 115.30        |



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| Mol | Chain | Res  | Type | Atoms      | Z     | $Observed(^{o})$ | $Ideal(^{o})$ |
|-----|-------|------|------|------------|-------|------------------|---------------|
| 1   | А     | 2509 | С    | C6-N1-C2   | -5.16 | 118.24           | 120.30        |
| 33  | a     | 1018 | U    | P-O3'-C3'  | 5.16  | 125.89           | 119.70        |
| 1   | А     | 2620 | C    | C5-C6-N1   | 5.16  | 123.58           | 121.00        |
| 1   | А     | 195  | С    | C5-C6-N1   | 5.15  | 123.58           | 121.00        |
| 1   | А     | 1759 | U    | O4'-C1'-N1 | 5.15  | 112.32           | 108.20        |
| 33  | a     | 1110 | С    | N1-C2-O2   | 5.15  | 121.99           | 118.90        |
| 33  | a     | 1392 | С    | C6-N1-C2   | -5.15 | 118.24           | 120.30        |
| 33  | a     | 1469 | С    | C6-N1-C2   | -5.15 | 118.24           | 120.30        |
| 1   | А     | 177  | G    | O5'-P-OP2  | -5.15 | 101.06           | 105.70        |
| 33  | a     | 130  | C    | C6-N1-C2   | -5.15 | 118.24           | 120.30        |
| 1   | А     | 2277 | С    | C2-N1-C1'  | 5.15  | 124.46           | 118.80        |
| 1   | А     | 2675 | С    | C6-N1-C2   | -5.15 | 118.24           | 120.30        |
| 6   | F     | 79   | LEU  | CA-CB-CG   | 5.15  | 127.14           | 115.30        |
| 1   | А     | 2840 | С    | C2-N3-C4   | 5.15  | 122.47           | 119.90        |
| 1   | А     | 211  | С    | C2-N3-C4   | 5.14  | 122.47           | 119.90        |
| 1   | А     | 2604 | С    | C5-C6-N1   | 5.14  | 123.57           | 121.00        |
| 1   | А     | 1028 | С    | C6-N1-C2   | -5.14 | 118.24           | 120.30        |
| 1   | А     | 1557 | G    | N3-C4-C5   | -5.14 | 126.03           | 128.60        |
| 1   | А     | 2523 | G    | C2-N3-C4   | 5.14  | 114.47           | 111.90        |
| 33  | a     | 859  | C    | N1-C2-O2   | 5.14  | 121.98           | 118.90        |
| 33  | a     | 1420 | С    | N3-C2-O2   | -5.14 | 118.30           | 121.90        |
| 1   | А     | 2827 | A    | N1-C6-N6   | 5.13  | 121.68           | 118.60        |
| 1   | А     | 2920 | С    | C5-C6-N1   | 5.13  | 123.57           | 121.00        |
| 1   | А     | 2323 | С    | N1-C2-O2   | 5.13  | 121.98           | 118.90        |
| 33  | a     | 1398 | C    | C6-N1-C2   | -5.13 | 118.25           | 120.30        |
| 1   | А     | 1613 | С    | C2-N1-C1'  | 5.13  | 124.44           | 118.80        |
| 33  | a     | 1010 | U    | N1-C2-O2   | 5.13  | 126.39           | 122.80        |
| 1   | А     | 393  | U    | N1-C2-O2   | 5.13  | 126.39           | 122.80        |
| 1   | А     | 1246 | G    | O4'-C1'-N9 | 5.13  | 112.30           | 108.20        |
| 1   | А     | 1831 | А    | C5-N7-C8   | -5.13 | 101.34           | 103.90        |
| 33  | a     | 167  | G    | N3-C4-N9   | 5.13  | 129.08           | 126.00        |
| 33  | a     | 174  | C    | N1-C2-O2   | 5.13  | 121.98           | 118.90        |
| 33  | a     | 982  | С    | C6-N1-C2   | -5.13 | 118.25           | 120.30        |
| 33  | a     | 1502 | A    | C5-N7-C8   | -5.13 | 101.34           | 103.90        |
| 33  | a     | 21   | С    | C2-N1-C1'  | 5.12  | 124.43           | 118.80        |
| 33  | a     | 1390 | U    | N3-C2-O2   | -5.12 | 118.61           | 122.20        |
| 33  | a     | 439  | A    | C2-N3-C4   | 5.12  | 113.16           | 110.60        |
| 1   | A     | 2126 | G    | N7-C8-N9   | 5.11  | 115.66           | 113.10        |
| 33  | a     | 746  | C    | N3-C2-O2   | -5.11 | 118.32           | 121.90        |
| 1   | А     | 113  | U    | N3-C2-O2   | -5.11 | 118.62           | 122.20        |
| 1   | A     | 299  | U    | N1-C2-N3   | 5.11  | 117.97           | 114.90        |
| 33  | a     | 466  | G    | N1-C6-O6   | -5.11 | 116.83           | 119.90        |



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| Mol | Chain | Res  | Type | Atoms      | Z     | $Observed(^{o})$ | $Ideal(^{o})$ |
|-----|-------|------|------|------------|-------|------------------|---------------|
| 33  | a     | 1022 | A    | C2-N3-C4   | 5.11  | 113.16           | 110.60        |
| 41  | i     | 87   | LEU  | CB-CG-CD2  | -5.11 | 102.31           | 111.00        |
| 1   | А     | 1805 | G    | C4-N9-C1'  | 5.11  | 133.14           | 126.50        |
| 2   | В     | 49   | G    | OP1-P-O3'  | 5.11  | 116.44           | 105.20        |
| 33  | a     | 967  | U    | C2-N1-C1'  | 5.11  | 123.83           | 117.70        |
| 1   | А     | 1671 | G    | C6-C5-N7   | -5.11 | 127.34           | 130.40        |
| 1   | А     | 2822 | С    | N1-C2-O2   | 5.11  | 121.96           | 118.90        |
| 33  | a     | 223  | С    | O4'-C1'-N1 | 5.11  | 112.28           | 108.20        |
| 33  | a     | 361  | A    | OP2-P-O3'  | 5.11  | 116.43           | 105.20        |
| 33  | a     | 521  | U    | C5-C6-N1   | 5.11  | 125.25           | 122.70        |
| 1   | А     | 185  | А    | P-O5'-C5'  | 5.10  | 129.06           | 120.90        |
| 1   | А     | 1644 | С    | N1-C2-O2   | 5.10  | 121.96           | 118.90        |
| 1   | А     | 2617 | G    | C4-C5-N7   | 5.10  | 112.84           | 110.80        |
| 1   | А     | 203  | U    | N1-C2-O2   | 5.10  | 126.37           | 122.80        |
| 1   | А     | 104  | С    | N1-C2-O2   | 5.10  | 121.96           | 118.90        |
| 1   | А     | 1626 | U    | N1-C2-O2   | 5.10  | 126.37           | 122.80        |
| 1   | А     | 1307 | U    | C2-N1-C1'  | 5.10  | 123.82           | 117.70        |
| 1   | А     | 309  | U    | N1-C2-O2   | 5.09  | 126.37           | 122.80        |
| 33  | a     | 363  | С    | C6-N1-C2   | -5.09 | 118.26           | 120.30        |
| 1   | А     | 136  | С    | C5-C6-N1   | 5.09  | 123.55           | 121.00        |
| 1   | А     | 1597 | С    | C5-C6-N1   | 5.09  | 123.55           | 121.00        |
| 33  | a     | 572  | А    | O4'-C1'-N9 | 5.09  | 112.28           | 108.20        |
| 33  | a     | 934  | С    | C5-C6-N1   | 5.09  | 123.55           | 121.00        |
| 1   | А     | 549  | А    | P-O3'-C3'  | 5.09  | 125.81           | 119.70        |
| 1   | А     | 2072 | С    | C2-N3-C4   | 5.09  | 122.44           | 119.90        |
| 33  | a     | 1420 | С    | C6-N1-C2   | -5.09 | 118.26           | 120.30        |
| 1   | А     | 136  | C    | C6-N1-C2   | -5.09 | 118.27           | 120.30        |
| 1   | А     | 1199 | C    | N1-C2-O2   | 5.09  | 121.95           | 118.90        |
| 1   | А     | 2203 | C    | C2-N1-C1'  | 5.09  | 124.40           | 118.80        |
| 1   | А     | 2452 | U    | N3-C2-O2   | -5.09 | 118.64           | 122.20        |
| 1   | А     | 2711 | G    | N3-C4-N9   | 5.09  | 129.05           | 126.00        |
| 1   | A     | 1779 | G    | C8-N9-C1'  | -5.08 | 120.39           | 127.00        |
| 1   | A     | 1223 | С    | C6-N1-C2   | -5.08 | 118.27           | 120.30        |
| 1   | A     | 2774 | С    | N1-C2-O2   | 5.08  | 121.95           | 118.90        |
| 33  | a     | 1501 | G    | N3-C4-N9   | -5.08 | 122.95           | 126.00        |
| 1   | А     | 8    | U    | N3-C4-O4   | 5.08  | 122.96           | 119.40        |
| 1   | A     | 2468 | A    | P-O3'-C3'  | 5.08  | 125.80           | 119.70        |
| 33  | a     | 338  | C    | N1-C2-O2   | 5.08  | 121.95           | 118.90        |
| 1   | A     | 1452 | C    | C6-N1-C2   | -5.08 | 118.27           | 120.30        |
| 1   | A     | 237  | U    | C2-N1-C1'  | 5.08  | 123.79           | 117.70        |
| 1   | A     | 393  | U    | N3-C2-O2   | -5.08 | 118.65           | 122.20        |
| 1   | А     | 1534 | А    | C8-N9-C4   | -5.07 | 103.77           | 105.80        |



| Mol | Chain | Res               | Type | Atoms      | Z     | $Observed(^{o})$ | $Ideal(^{o})$ |
|-----|-------|-------------------|------|------------|-------|------------------|---------------|
| 26  | 1     | 2                 | ARG  | NE-CZ-NH1  | -5.07 | 117.76           | 120.30        |
| 33  | a     | 963               | G    | C4-N9-C1'  | 5.07  | 133.09           | 126.50        |
| 33  | a     | 1021              | U    | C5-C6-N1   | 5.07  | 125.23           | 122.70        |
| 33  | a     | 1457              | С    | C5-C6-N1   | 5.07  | 123.53           | 121.00        |
| 1   | А     | 1037              | С    | C5-C6-N1   | 5.07  | 123.53           | 121.00        |
| 33  | a     | 820               | С    | C2-N1-C1'  | 5.07  | 124.37           | 118.80        |
| 33  | a     | 855               | G    | P-O3'-C3'  | 5.06  | 125.78           | 119.70        |
| 1   | А     | 2077              | G    | C4-N9-C1'  | 5.06  | 133.08           | 126.50        |
| 1   | А     | 2648              | U    | N1-C2-O2   | 5.06  | 126.34           | 122.80        |
| 1   | А     | 1998              | А    | OP1-P-O3'  | 5.06  | 116.33           | 105.20        |
| 1   | А     | 981               | С    | C6-N1-C2   | -5.06 | 118.28           | 120.30        |
| 33  | a     | 369               | G    | C6-C5-N7   | -5.06 | 127.37           | 130.40        |
| 33  | a     | 854               | С    | N1-C2-O2   | 5.06  | 121.93           | 118.90        |
| 1   | А     | 2076              | С    | C6-N1-C2   | -5.05 | 118.28           | 120.30        |
| 33  | a     | 1499              | G    | P-O3'-C3'  | 5.05  | 125.76           | 119.70        |
| 1   | А     | 1715              | С    | C5-C6-N1   | 5.05  | 123.52           | 121.00        |
| 1   | А     | 2365              | А    | N1-C6-N6   | 5.04  | 121.63           | 118.60        |
| 1   | А     | 529               | С    | C5-C6-N1   | 5.04  | 123.52           | 121.00        |
| 33  | a     | 336               | С    | N3-C2-O2   | -5.04 | 118.37           | 121.90        |
| 1   | А     | 624               | С    | N1-C2-O2   | 5.04  | 121.92           | 118.90        |
| 6   | F     | 112               | ARG  | CA-CB-CG   | 5.04  | 124.49           | 113.40        |
| 33  | a     | 982               | С    | N3-C2-O2   | -5.04 | 118.37           | 121.90        |
| 1   | А     | 508               | С    | C6-N1-C1'  | -5.04 | 114.75           | 120.80        |
| 1   | А     | 1565              | U    | P-O3'-C3'  | 5.04  | 125.74           | 119.70        |
| 33  | a     | 982               | С    | N1-C2-O2   | 5.04  | 121.92           | 118.90        |
| 1   | А     | 309               | U    | P-O3'-C3'  | 5.03  | 125.74           | 119.70        |
| 33  | a     | 589               | С    | C6-N1-C2   | -5.03 | 118.29           | 120.30        |
| 1   | А     | 2420              | G    | O5'-P-OP2  | -5.03 | 101.17           | 105.70        |
| 33  | a     | 1293              | С    | C6-N1-C2   | -5.03 | 118.29           | 120.30        |
| 1   | А     | 18                | C    | C5-C6-N1   | 5.03  | 123.51           | 121.00        |
| 1   | А     | 1727              | A    | O5'-P-OP1  | -5.03 | 101.17           | 105.70        |
| 1   | А     | 2733              | С    | C5-C6-N1   | 5.03  | 123.51           | 121.00        |
| 1   | А     | 698               | C    | O4'-C1'-N1 | 5.02  | 112.22           | 108.20        |
| 17  | S     | 40                | PRO  | N-CA-C     | 5.02  | 125.16           | 112.10        |
| 33  | а     | 481               | C    | C5-C6-N1   | 5.02  | 123.51           | 121.00        |
| 1   | А     | 506               | U    | N3-C2-O2   | -5.02 | 118.69           | 122.20        |
| 1   | A     | 946               | G    | C4-N9-C1'  | 5.02  | 133.02           | 126.50        |
| 33  | a     | 319               | C    | N3-C2-O2   | -5.02 | 118.39           | 121.90        |
| 1   | A     | $11\overline{75}$ | A    | OP2-P-O3'  | 5.02  | 116.24           | 105.20        |
| 1   | A     | 1250              | G    | P-O3'-C3'  | 5.02  | 125.72           | 119.70        |
| 1   | A     | 1803              | C    | C5-C6-N1   | 5.02  | 123.51           | 121.00        |
| 1   | А     | 1117              | G    | C4-N9-C1'  | 5.01  | 133.02           | 126.50        |



| Mol | Chain | $\operatorname{Res}$ | Type | Atoms       | $\mathbf{Z}$ | $Observed(^{o})$ | $Ideal(^{o})$ |
|-----|-------|----------------------|------|-------------|--------------|------------------|---------------|
| 1   | А     | 1529                 | G    | P-O3'-C3'   | 5.01         | 125.72           | 119.70        |
| 1   | А     | 2313                 | С    | N1-C2-O2    | 5.01         | 121.91           | 118.90        |
| 33  | a     | 1078                 | G    | N3-C4-N9    | 5.01         | 129.01           | 126.00        |
| 1   | А     | 2296                 | А    | O5'-P-OP2   | 5.01         | 116.71           | 110.70        |
| 1   | А     | 648                  | G    | C5'-C4'-C3' | -5.00        | 107.99           | 116.00        |
| 1   | А     | 1160                 | G    | O4'-C1'-N9  | 5.00         | 112.20           | 108.20        |
| 1   | А     | 1333                 | С    | C6-N1-C2    | -5.00        | 118.30           | 120.30        |
| 33  | a     | 1078                 | G    | C6-C5-N7    | -5.00        | 127.40           | 130.40        |
| 1   | А     | 1239                 | U    | C2-N1-C1'   | 5.00         | 123.70           | 117.70        |
| 33  | a     | 182                  | Ū    | C2-N1-C1'   | 5.00         | 123.70           | 117.70        |

There are no chirality outliers.

All (51) planarity outliers are listed below:

| Mol | Chain | Res | Type | Group   |
|-----|-------|-----|------|---------|
| 25  | 0     | 50  | ASN  | Peptide |
| 25  | 0     | 51  | GLY  | Peptide |
| 30  | 6     | 59  | PHE  | Peptide |
| 3   | С     | 153 | GLN  | Peptide |
| 4   | D     | 53  | PHE  | Peptide |
| 6   | F     | 117 | VAL  | Peptide |
| 6   | F     | 138 | PHE  | Peptide |
| 6   | F     | 53  | ALA  | Peptide |
| 8   | J     | 132 | PRO  | Peptide |
| 10  | L     | 18  | ARG  | Peptide |
| 10  | L     | 35  | HIS  | Peptide |
| 13  | 0     | 1   | MET  | Peptide |
| 15  | Q     | 102 | ASP  | Peptide |
| 16  | R     | 50  | ASN  | Peptide |
| 16  | R     | 51  | PRO  | Peptide |
| 17  | S     | 39  | THR  | Peptide |
| 20  | V     | 15  | LYS  | Peptide |
| 20  | V     | 19  | VAL  | Peptide |
| 20  | V     | 278 | ARG  | Peptide |
| 20  | V     | 279 | PHE  | Peptide |
| 20  | V     | 281 | ILE  | Peptide |
| 20  | V     | 342 | THR  | Peptide |
| 20  | V     | 405 | LYS  | Peptide |
| 20  | V     | 412 | ARG  | Peptide |
| 20  | V     | 521 | ALA  | Peptide |
| 20  | V     | 75  | THR  | Peptide |
| 20  | V     | 98  | LEU  | Peptide |



| Mol | Chain | Res | Type | Group   |
|-----|-------|-----|------|---------|
| 34  | b     | 148 | LEU  | Peptide |
| 34  | b     | 16  | PHE  | Peptide |
| 34  | b     | 18  | HIS  | Peptide |
| 34  | b     | 65  | GLY  | Peptide |
| 34  | b     | 66  | LYS  | Peptide |
| 36  | d     | 117 | GLY  | Peptide |
| 36  | d     | 192 | ALA  | Peptide |
| 36  | d     | 31  | TYR  | Peptide |
| 36  | d     | 32  | ALA  | Peptide |
| 36  | d     | 33  | PRO  | Peptide |
| 37  | е     | 20  | ARG  | Peptide |
| 38  | f     | 33  | ASN  | Peptide |
| 39  | g     | 114 | LYS  | Peptide |
| 39  | g     | 129 | ASN  | Peptide |
| 40  | h     | 98  | LEU  | Peptide |
| 44  | 1     | 34  | GLU  | Peptide |
| 44  | 1     | 57  | LYS  | Peptide |
| 45  | m     | 104 | ASN  | Peptide |
| 45  | m     | 3   | ARG  | Peptide |
| 45  | m     | 65  | VAL  | Peptide |
| 47  | 0     | 24  | SER  | Peptide |
| 49  | q     | 30  | TYR  | Peptide |
| 50  | r     | 24  | THR  | Peptide |
| 50  | r     | 25  | HIS  | Peptide |

Continued from previous page...

# 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 |
|-----|-------|---------------|-----------|----------|----------|-------|---------|
| Mol | Chain | Analysed      | Favoured  | Allowed  | Outliers | Perce | entiles |
| 3   | С     | 270/277 (98%) | 253 (94%) | 17 (6%)  | 0        | 100   | 100     |
| 4   | D     | 204/209~(98%) | 195 (96%) | 9 (4%)   | 0        | 100   | 100     |
| 5   | Е     | 203/207 (98%) | 187 (92%) | 16 (8%)  | 0        | 100   | 100     |
| 6   | F     | 174/179~(97%) | 159 (91%) | 15 (9%)  | 0        | 100   | 100     |
| 7   | G     | 173/179~(97%) | 153 (88%) | 20 (12%) | 0        | 100   | 100     |
| 8   | J     | 140/145~(97%) | 129 (92%) | 9 (6%)   | 2 (1%)   | 11    | 46      |
| 9   | K     | 120/122 (98%) | 110 (92%) | 10 (8%)  | 0        | 100   | 100     |
| 10  | L     | 144/146~(99%) | 137 (95%) | 7 (5%)   | 0        | 100   | 100     |
| 11  | М     | 133/144 (92%) | 125 (94%) | 8 (6%)   | 0        | 100   | 100     |
| 12  | N     | 117/120 (98%) | 108 (92%) | 9 (8%)   | 0        | 100   | 100     |
| 13  | Ο     | 118/120~(98%) | 107 (91%) | 11 (9%)  | 0        | 100   | 100     |
| 14  | Р     | 113/115 (98%) | 105 (93%) | 8 (7%)   | 0        | 100   | 100     |
| 15  | Q     | 115/119~(97%) | 107 (93%) | 6 (5%)   | 2 (2%)   | 9     | 42      |
| 16  | R     | 99/102~(97%)  | 83 (84%)  | 15 (15%) | 1 (1%)   | 15    | 54      |
| 17  | S     | 107/113~(95%) | 92 (86%)  | 13 (12%) | 2 (2%)   | 8     | 40      |
| 18  | Т     | 88/95~(93%)   | 84 (96%)  | 4 (4%)   | 0        | 100   | 100     |
| 19  | U     | 99/103~(96%)  | 86 (87%)  | 13 (13%) | 0        | 100   | 100     |
| 20  | V     | 539/548~(98%) | 464 (86%) | 73 (14%) | 2 (0%)   | 34    | 72      |
| 21  | W     | 80/94~(85%)   | 71 (89%)  | 9 (11%)  | 0        | 100   | 100     |
| 22  | Х     | 56/62~(90%)   | 46 (82%)  | 10 (18%) | 0        | 100   | 100     |
| 23  | Y     | 63/66~(96%)   | 60 (95%)  | 3 (5%)   | 0        | 100   | 100     |
| 24  | Z     | 56/59~(95%)   | 54 (96%)  | 2 (4%)   | 0        | 100   | 100     |
| 25  | 0     | 52/59~(88%)   | 49 (94%)  | 2 (4%)   | 1 (2%)   | 8     | 40      |
| 26  | 1     | 46/49~(94%)   | 43 (94%)  | 3 (6%)   | 0        | 100   | 100     |
| 27  | 2     | 42/44~(96%)   | 41 (98%)  | 1 (2%)   | 0        | 100   | 100     |
| 28  | 3     | 62/66~(94%)   | 60 (97%)  | 2 (3%)   | 0        | 100   | 100     |
| 29  | 4     | 35/37~(95%)   | 32 (91%)  | 3 (9%)   | 0        | 100   | 100     |
| 30  | 6     | 61/66~(92%)   | 53 (87%)  | 8 (13%)  | 0        | 100   | 100     |
| 32  | 8     | 210/232~(90%) | 192 (91%) | 18 (9%)  | 0        | 100   | 100     |
| 34  | b     | 216/246~(88%) | 188 (87%) | 24 (11%) | 4 (2%)   | 8     | 40      |



| Mol | Chain | Analysed        | Favoured   | Allowed  | Outliers | Perce | entiles |
|-----|-------|-----------------|------------|----------|----------|-------|---------|
| 35  | с     | 204/218~(94%)   | 185 (91%)  | 19 (9%)  | 0        | 100   | 100     |
| 36  | d     | 193/200~(96%)   | 173 (90%)  | 18 (9%)  | 2(1%)    | 15    | 54      |
| 37  | е     | 162/166~(98%)   | 150 (93%)  | 12 (7%)  | 0        | 100   | 100     |
| 38  | f     | 90/95~(95%)     | 83 (92%)   | 7 (8%)   | 0        | 100   | 100     |
| 39  | g     | 147/156~(94%)   | 136 (92%)  | 11 (8%)  | 0        | 100   | 100     |
| 40  | h     | 129/132~(98%)   | 107 (83%)  | 20 (16%) | 2(2%)    | 9     | 43      |
| 41  | i     | 123/130~(95%)   | 104 (85%)  | 18 (15%) | 1 (1%)   | 19    | 58      |
| 42  | j     | 93/102~(91%)    | 83 (89%)   | 9 (10%)  | 1 (1%)   | 14    | 52      |
| 43  | k     | 112/131~(86%)   | 100 (89%)  | 12 (11%) | 0        | 100   | 100     |
| 44  | 1     | 134/138~(97%)   | 117 (87%)  | 16 (12%) | 1 (1%)   | 22    | 61      |
| 45  | m     | 106/121~(88%)   | 94 (89%)   | 11 (10%) | 1 (1%)   | 17    | 56      |
| 46  | n     | 58/61~(95%)     | 46 (79%)   | 11 (19%) | 1 (2%)   | 9     | 42      |
| 47  | О     | 83/89~(93%)     | 79~(95%)   | 3~(4%)   | 1 (1%)   | 13    | 50      |
| 48  | р     | 86/90~(96%)     | 76~(88%)   | 7 (8%)   | 3~(4%)   | 3     | 27      |
| 49  | q     | 82/87~(94%)     | 77 (94%)   | 5~(6%)   | 0        | 100   | 100     |
| 50  | r     | 62/79~(78%)     | 57 (92%)   | 5 (8%)   | 0        | 100   | 100     |
| 51  | S     | 76/92~(83%)     | 66 (87%)   | 10 (13%) | 0        | 100   | 100     |
| 52  | t     | 81/88~(92%)     | 76 (94%)   | 3 (4%)   | 2(2%)    | 5     | 34      |
| All | All   | 5956/6298~(95%) | 5382 (90%) | 545 (9%) | 29 (0%)  | 32    | 68      |

All (29) Ramachandran outliers are listed below:

| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 8   | J     | 133 | HIS  |
| 15  | Q     | 93  | LYS  |
| 17  | S     | 40  | PRO  |
| 20  | V     | 280 | SER  |
| 34  | b     | 18  | HIS  |
| 34  | b     | 19  | GLN  |
| 36  | d     | 32  | ALA  |
| 40  | h     | 99  | ASN  |
| 48  | р     | 47  | ALA  |
| 52  | t     | 69  | LYS  |
| 8   | J     | 132 | PRO  |
| 15  | Q     | 92  | ARG  |
| 34  | b     | 67  | ILE  |



| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 36  | d     | 33  | PRO  |
| 40  | h     | 4   | THR  |
| 46  | n     | 32  | SER  |
| 34  | b     | 66  | LYS  |
| 45  | m     | 105 | ASN  |
| 17  | S     | 39  | THR  |
| 25  | 0     | 51  | GLY  |
| 44  | 1     | 135 | PRO  |
| 48  | р     | 48  | GLU  |
| 52  | t     | 68  | HIS  |
| 16  | R     | 50  | ASN  |
| 41  | i     | 125 | PRO  |
| 48  | р     | 46  | PRO  |
| 20  | V     | 281 | ILE  |
| 42  | j     | 79  | PRO  |
| 47  | 0     | 25  | PRO  |

#### 5.3.2 Protein sidechains (i)

In the following table, the Percentiles column shows the percent sidechain outliers of the chain as a percentile score with respect to all PDB entries followed by that with respect to all EM entries.

The Analysed column shows the number of residues for which the sidechain conformation was analysed, and the total number of residues.

| Mol | Chain | Analysed       | Rotameric  | Outliers | Percentiles |
|-----|-------|----------------|------------|----------|-------------|
| 3   | С     | 220/225~(98%)  | 218~(99%)  | 2(1%)    | 78 90       |
| 4   | D     | 167/170~(98%)  | 166~(99%)  | 1 (1%)   | 86 94       |
| 5   | Е     | 169/170~(99%)  | 164~(97%)  | 5(3%)    | 41 71       |
| 6   | F     | 151/154~(98%)  | 144~(95%)  | 7~(5%)   | 27 61       |
| 7   | G     | 148/151~(98%)  | 148 (100%) | 0        | 100 100     |
| 8   | J     | 120/123~(98%)  | 118~(98%)  | 2(2%)    | 60 82       |
| 9   | Κ     | 101/101~(100%) | 101 (100%) | 0        | 100 100     |
| 10  | L     | 110/110~(100%) | 108~(98%)  | 2(2%)    | 59 81       |
| 11  | М     | 109/116~(94%)  | 108~(99%)  | 1 (1%)   | 78 90       |
| 12  | Ν     | 99/100~(99%)   | 99 (100%)  | 0        | 100 100     |
| 13  | Ο     | 93/93~(100%)   | 91~(98%)   | 2(2%)    | 52 78       |



| Mol | Chain | Analysed       | Rotameric     | Outliers | Perce | $\mathbf{ntiles}$ |
|-----|-------|----------------|---------------|----------|-------|-------------------|
| 14  | Р     | 100/100~(100%) | 97~(97%)      | 3~(3%)   | 41    | 71                |
| 15  | Q     | 96/98~(98%)    | 96 (100%)     | 0        | 100   | 100               |
| 16  | R     | 83/84~(99%)    | 81 (98%)      | 2(2%)    | 49    | 76                |
| 17  | S     | 90/93~(97%)    | 90 (100%)     | 0        | 100   | 100               |
| 18  | Т     | 81/85~(95%)    | 79~(98%)      | 2(2%)    | 47    | 75                |
| 19  | U     | 85/87~(98%)    | 85 (100%)     | 0        | 100   | 100               |
| 20  | V     | 424/431~(98%)  | 417 (98%)     | 7 (2%)   | 60    | 82                |
| 21  | W     | 64/74~(86%)    | 61~(95%)      | 3~(5%)   | 26    | 60                |
| 22  | Х     | 47/50~(94%)    | 44 (94%)      | 3~(6%)   | 17    | 50                |
| 23  | Υ     | 56/57~(98%)    | 56 (100%)     | 0        | 100   | 100               |
| 24  | Ζ     | 52/53~(98%)    | 51 (98%)      | 1 (2%)   | 57    | 80                |
| 25  | 0     | 48/53~(91%)    | 45 (94%)      | 3~(6%)   | 18    | 51                |
| 26  | 1     | 46/47~(98%)    | 46 (100%)     | 0        | 100   | 100               |
| 27  | 2     | 39/39~(100%)   | 38~(97%)      | 1 (3%)   | 46    | 74                |
| 28  | 3     | 54/56~(96%)    | 52 (96%)      | 2(4%)    | 34    | 65                |
| 29  | 4     | 35/35~(100%)   | 35~(100%)     | 0        | 100   | 100               |
| 30  | 6     | 53/55~(96%)    | 53~(100%)     | 0        | 100   | 100               |
| 32  | 8     | 169/185~(91%)  | 168 (99%)     | 1 (1%)   | 86    | 94                |
| 34  | b     | 189/212~(89%)  | 182~(96%)     | 7~(4%)   | 34    | 65                |
| 35  | с     | 168/178~(94%)  | 166 (99%)     | 2(1%)    | 71    | 87                |
| 36  | d     | 169/173~(98%)  | 165~(98%)     | 4 (2%)   | 49    | 76                |
| 37  | е     | 128/130~(98%)  | 126~(98%)     | 2(2%)    | 62    | 83                |
| 38  | f     | 81/84~(96%)    | 80~(99%)      | 1 (1%)   | 71    | 87                |
| 39  | g     | 125/132~(95%)  | 124 (99%)     | 1 (1%)   | 81    | 91                |
| 40  | h     | 111/112~(99%)  | 109~(98%)     | 2(2%)    | 59    | 81                |
| 41  | i     | 98/102~(96%)   | 96~(98%)      | 2(2%)    | 55    | 79                |
| 42  | j     | 86/92~(94%)    | 86 (100%)     | 0        | 100   | 100               |
| 43  | k     | 86/100~(86%)   | $85 \ (99\%)$ | 1 (1%)   | 71    | 87                |
| 44  | 1     | 114/116~(98%)  | 111 (97%)     | 3~(3%)   | 46    | 74                |
| 45  | m     | 94/104~(90%)   | 94 (100%)     | 0        | 100   | 100               |
| 46  | n     | 53/54 (98%)    | 52 (98%)      | 1 (2%)   | 57    | 80                |



| Mol | Chain | Analysed        | Rotameric  | Outliers | Percentiles |
|-----|-------|-----------------|------------|----------|-------------|
| 47  | О     | 80/83~(96%)     | 79~(99%)   | 1 (1%)   | 69 86       |
| 48  | р     | 74/76~(97%)     | 72~(97%)   | 2(3%)    | 44 73       |
| 49  | q     | 77/80~(96%)     | 74 (96%)   | 3~(4%)   | 32 64       |
| 50  | r     | 56/64~(88%)     | 54 (96%)   | 2(4%)    | 35 66       |
| 51  | S     | 70/81~(86%)     | 69~(99%)   | 1 (1%)   | 67 85       |
| 52  | t     | 66/70~(94%)     | 65~(98%)   | 1 (2%)   | 65 84       |
| All | All   | 5034/5238~(96%) | 4948 (98%) | 86 (2%)  | 62 82       |

All (86) residues with a non-rotameric sidechain are listed below:

| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 3   | С     | 221 | ARG  |
| 3   | С     | 273 | ARG  |
| 4   | D     | 199 | LEU  |
| 5   | Е     | 10  | ASN  |
| 5   | Е     | 29  | ASN  |
| 5   | Е     | 188 | ASN  |
| 5   | Е     | 192 | LEU  |
| 5   | Е     | 194 | ILE  |
| 6   | F     | 3   | ARG  |
| 6   | F     | 4   | LEU  |
| 6   | F     | 78  | ARG  |
| 6   | F     | 119 | LYS  |
| 6   | F     | 133 | LYS  |
| 6   | F     | 136 | LEU  |
| 6   | F     | 165 | GLU  |
| 8   | J     | 26  | LEU  |
| 8   | J     | 123 | LEU  |
| 10  | L     | 18  | ARG  |
| 10  | L     | 47  | ARG  |
| 11  | М     | 124 | LYS  |
| 13  | 0     | 4   | LYS  |
| 13  | 0     | 61  | LYS  |
| 14  | Р     | 36  | ASN  |
| 14  | Р     | 39  | ARG  |
| 14  | Р     | 51  | ARG  |
| 16  | R     | 47  | LYS  |
| 16  | R     | 48  | VAL  |
| 18  | Т     | 65  | ARG  |
| 18  | Т     | 68  | ARG  |



| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 20  | V     | 14  | VAL  |
| 20  | V     | 63  | ARG  |
| 20  | V     | 160 | ARG  |
| 20  | V     | 182 | LYS  |
| 20  | V     | 309 | ASN  |
| 20  | V     | 380 | PHE  |
| 20  | V     | 388 | ASN  |
| 21  | W     | 22  | ARG  |
| 21  | W     | 28  | ARG  |
| 21  | W     | 79  | ARG  |
| 22  | Х     | 4   | LYS  |
| 22  | Х     | 17  | ASN  |
| 22  | Х     | 27  | ARG  |
| 24  | Z     | 9   | LYS  |
| 25  | 0     | 22  | LEU  |
| 25  | 0     | 38  | LEU  |
| 25  | 0     | 50  | ASN  |
| 27  | 2     | 28  | ARG  |
| 28  | 3     | 32  | LEU  |
| 28  | 3     | 62  | LEU  |
| 32  | 8     | 121 | MET  |
| 34  | b     | 24  | ASN  |
| 34  | b     | 36  | ASN  |
| 34  | b     | 113 | ARG  |
| 34  | b     | 123 | ASN  |
| 34  | b     | 154 | MET  |
| 34  | b     | 179 | LEU  |
| 34  | b     | 203 | ASN  |
| 35  | с     | 71  | LYS  |
| 35  | с     | 163 | ARG  |
| 36  | d     | 54  | LYS  |
| 36  | d     | 147 | ASN  |
| 36  | d     | 172 | LEU  |
| 36  | d     | 182 | ARG  |
| 37  | е     | 36  | LEU  |
| 37  | е     | 95  | LEU  |
| 38  | f     | 77  | ARG  |
| 39  | g     | 9   | LYS  |
| 40  | h     | 57  | GLN  |
| 40  | h     | 96  | ARG  |
| 41  | i     | 12  | ARG  |
| 41  | i     | 106 | ARG  |



| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 43  | k     | 95  | ARG  |
| 44  | 1     | 44  | ARG  |
| 44  | l     | 56  | LYS  |
| 44  | l     | 96  | ARG  |
| 46  | n     | 29  | ARG  |
| 47  | 0     | 54  | ARG  |
| 48  | р     | 32  | ARG  |
| 48  | р     | 71  | ARG  |
| 49  | q     | 32  | LYS  |
| 49  | q     | 67  | ARG  |
| 49  | q     | 76  | ARG  |
| 50  | r     | 29  | LYS  |
| 50  | r     | 48  | ARG  |
| 51  | s     | 5   | LEU  |
| 52  | t     | 78  | ARG  |

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (78) such sidechains are listed below:

| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 3   | С     | 86  | ASN  |
| 3   | С     | 177 | ASN  |
| 3   | С     | 230 | HIS  |
| 3   | С     | 232 | HIS  |
| 4   | D     | 33  | ASN  |
| 5   | Е     | 10  | ASN  |
| 5   | Е     | 29  | ASN  |
| 5   | Е     | 188 | ASN  |
| 6   | F     | 45  | GLN  |
| 7   | G     | 148 | ASN  |
| 10  | L     | 126 | ASN  |
| 12  | Ν     | 27  | ASN  |
| 12  | N     | 61  | GLN  |
| 12  | Ν     | 68  | ASN  |
| 13  | 0     | 15  | HIS  |
| 14  | Р     | 36  | ASN  |
| 15  | Q     | 29  | HIS  |
| 15  | Q     | 37  | GLN  |
| 15  | Q     | 66  | ASN  |
| 16  | R     | 83  | HIS  |
| 17  | S     | 102 | HIS  |
| 19  | U     | 64  | HIS  |
| 20  | V     | 73  | GLN  |



| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 20  | V     | 158 | HIS  |
| 20  | V     | 207 | GLN  |
| 20  | V     | 218 | ASN  |
| 20  | V     | 296 | ASN  |
| 20  | V     | 309 | ASN  |
| 20  | V     | 335 | ASN  |
| 20  | V     | 360 | GLN  |
| 20  | V     | 388 | ASN  |
| 20  | V     | 406 | HIS  |
| 20  | V     | 435 | ASN  |
| 20  | V     | 461 | HIS  |
| 21  | W     | 37  | GLN  |
| 22  | Х     | 17  | ASN  |
| 22  | Х     | 23  | ASN  |
| 25  | 0     | 40  | HIS  |
| 25  | 0     | 50  | ASN  |
| 26  | 1     | 22  | ASN  |
| 26  | 1     | 26  | ASN  |
| 28  | 3     | 60  | GLN  |
| 32  | 8     | 67  | ASN  |
| 32  | 8     | 106 | GLN  |
| 32  | 8     | 188 | ASN  |
| 34  | b     | 18  | HIS  |
| 34  | b     | 24  | ASN  |
| 34  | b     | 36  | ASN  |
| 34  | b     | 123 | ASN  |
| 34  | b     | 203 | ASN  |
| 35  | с     | 136 | GLN  |
| 36  | d     | 96  | ASN  |
| 36  | d     | 112 | GLN  |
| 36  | d     | 118 | HIS  |
| 36  | d     | 147 | ASN  |
| 37  | e     | 83  | HIS  |
| 38  | f     | 33  | ASN  |
| 38  | f     | 61  | GLN  |
| 39  | g     | 84  | ASN  |
| 39  | g     | 142 | HIS  |
| 40  | h     | 57  | GLN  |
| 41  | i     | 81  | HIS  |
| 41  | i     | 126 | GLN  |
| 44  | 1     | 59  | ASN  |
| 44  | 1     | 85  | HIS  |



| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 44  | 1     | 90  | HIS  |
| 44  | l     | 109 | HIS  |
| 45  | m     | 76  | ASN  |
| 46  | n     | 10  | GLN  |
| 47  | 0     | 28  | GLN  |
| 47  | 0     | 37  | ASN  |
| 47  | 0     | 42  | HIS  |
| 47  | 0     | 46  | HIS  |
| 47  | 0     | 51  | HIS  |
| 47  | 0     | 83  | ASN  |
| 49  | q     | 49  | HIS  |
| 52  | t     | 70  | ASN  |
| 52  | t     | 84  | ASN  |

### 5.3.3 RNA (i)

| Mol | Chain | Analysed        | Backbone Outliers | Pucker Outliers |
|-----|-------|-----------------|-------------------|-----------------|
| 1   | А     | 2876/2928~(98%) | 857~(29%)         | 90~(3%)         |
| 2   | В     | 111/112~(99%)   | 40 (36%)          | 3~(2%)          |
| 31  | 7     | 2/3~(66%)       | 0                 | 0               |
| 33  | a     | 1532/1554~(98%) | 411 (26%)         | 0               |
| 53  | Х     | 73/75~(97%)     | 29~(39%)          | 0               |
| All | All   | 4594/4672~(98%) | 1337~(29%)        | 93~(2%)         |

All (1337) RNA backbone outliers are listed below:

| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1   | А     | 7   | G    |
| 1   | А     | 8   | U    |
| 1   | А     | 10  | А    |
| 1   | А     | 13  | А    |
| 1   | А     | 18  | С    |
| 1   | А     | 26  | G    |
| 1   | А     | 34  | U    |
| 1   | А     | 35  | G    |
| 1   | А     | 36  | G    |
| 1   | А     | 45  | G    |
| 1   | А     | 46  | С    |
| 1   | А     | 55  | G    |
| 1   | А     | 60  | G    |
| 1   | А     | 61  | А    |



| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1   | А     | 62  | С    |
| 1   | А     | 63  | G    |
| 1   | А     | 64  | А    |
| 1   | А     | 65  | А    |
| 1   | А     | 66  | С    |
| 1   | А     | 71  | A    |
| 1   | А     | 74  | U    |
| 1   | А     | 75  | G    |
| 1   | А     | 76  | С    |
| 1   | А     | 77  | U    |
| 1   | А     | 78  | U    |
| 1   | А     | 79  | С    |
| 1   | А     | 83  | G    |
| 1   | A     | 84  | A    |
| 1   | А     | 85  | G    |
| 1   | A     | 86  | С    |
| 1   | А     | 87  | U    |
| 1   | А     | 89  | U    |
| 1   | А     | 90  | А    |
| 1   | А     | 92  | G    |
| 1   | А     | 93  | С    |
| 1   | А     | 96  | G    |
| 1   | А     | 99  | U    |
| 1   | А     | 100 | U    |
| 1   | А     | 101 | G    |
| 1   | А     | 117 | А    |
| 1   | А     | 118 | А    |
| 1   | А     | 119 | U    |
| 1   | А     | 124 | А    |
| 1   | А     | 125 | A    |
| 1   | A     | 126 | A    |
| 1   | A     | 127 | С    |
| 1   | A     | 134 | С    |
| 1   | A     | 141 | U    |
| 1   | A     | 156 | A    |
| 1   | A     | 162 | A    |
| 1   | A     | 163 | U    |
| 1   | A     | 164 | U    |
| 1   | A     | 167 | U    |
| 1   | A     | 174 | U    |
| 1   | A     | 175 | G    |
| 1   | A     | 176 | A    |


| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1   | А     | 177 | G    |
| 1   | А     | 178 | А    |
| 1   | А     | 179 | A    |
| 1   | А     | 182 | С    |
| 1   | А     | 187 | С    |
| 1   | А     | 188 | С    |
| 1   | А     | 196 | U    |
| 1   | А     | 199 | A    |
| 1   | А     | 202 | A    |
| 1   | А     | 207 | A    |
| 1   | А     | 216 | A    |
| 1   | А     | 218 | G    |
| 1   | А     | 219 | A    |
| 1   | А     | 225 | A    |
| 1   | А     | 226 | А    |
| 1   | А     | 227 | G    |
| 1   | А     | 229 | A    |
| 1   | А     | 231 | A    |
| 1   | А     | 232 | U    |
| 1   | А     | 233 | G    |
| 1   | А     | 234 | С    |
| 1   | А     | 236 | А    |
| 1   | А     | 237 | U    |
| 1   | А     | 244 | А    |
| 1   | А     | 247 | А    |
| 1   | А     | 248 | G    |
| 1   | А     | 251 | G    |
| 1   | А     | 252 | С    |
| 1   | А     | 253 | G    |
| 1   | A     | 255 | G    |
| 1   | A     | 258 | A    |
| 1   | A     | 266 | U    |
| 1   | А     | 267 | С    |
| 1   | A     | 268 | A    |
| 1   | А     | 269 | G    |
| 1   | A     | 270 | C    |
| 1   | A     | 272 | С    |
| 1   | A     | 275 | A    |
| 1   | A     | 282 | G    |
| 1   | A     | 283 | G    |
| 1   | A     | 284 | С    |
| 1   | А     | 285 | U    |
|     | ~     | -   |      |



| 1       A       286       U         1       A       290       U         1       A       291       C         1       A       298       U         1       A       299       U         1       A       301       U         1       A       302       A         1       A       302       A         1       A       302       A         1       A       302       A         1       A       309       U         1       A       345       A         1       A       348       U         1       A       352       G         1       A       366       A         1       A       366       A         1       A       367       G         1       A       389       A </th <th>Mol</th> <th>Chain</th> <th>Res</th> <th>Type</th> | Mol | Chain | Res | Type |
|---|-----|-------|-----|------|
| 1       A       290       U         1       A       291       C         1       A       298       U         1       A       299       U         1       A       301       U         1       A       302       A         1       A       309       U         1       A       309       U         1       A       310       C         1       A       345       A         1       A       345       A         1       A       349       C         1       A       352       G         1       A       366       A         1       A       367       G         1       A       373       A         1       A       389       A </td <td>1</td> <td>А</td> <td>286</td> <td>U</td>          | 1   | А     | 286 | U    |
| 1       A       291       C         1       A       298       U         1       A       299       U         1       A       301       U         1       A       302       A         1       A       309       U         1       A       309       U         1       A       309       U         1       A       309       U         1       A       345       A         1       A       345       A         1       A       346       G         1       A       352       G         1       A       366       A         1       A       366       A         1       A       367       G         1       A       373       A         1       A       389       A </td <td>1</td> <td>А</td> <td>290</td> <td>U</td>          | 1   | А     | 290 | U    |
| 1       A       298       U         1       A       301       U         1       A       302       A         1       A       309       U         1       A       310       C         1       A       345       A         1       A       345       A         1       A       346       G         1       A       346       G         1       A       346       G         1       A       352       G         1       A       366       A         1       A       367       G         1       A       373       A         1       A       375       C         1       A       398       U         1       A       409       U </td <td>1</td> <td>А</td> <td>291</td> <td>С</td>          | 1   | А     | 291 | С    |
| 1       A       299       U         1       A       301       U         1       A       302       A         1       A       308       C         1       A       309       U         1       A       309       U         1       A       310       C         1       A       310       C         1       A       345       A         1       A       345       A         1       A       346       G         1       A       348       U         1       A       348       U         1       A       346       G         1       A       352       G         1       A       360       C         1       A       366       A         1       A       367       G         1       A       373       A         1       A       375       C         1       A       398       A         1       A       398       U         1       A       410       G </td <td>1</td> <td>А</td> <td>298</td> <td>U</td>          | 1   | А     | 298 | U    |
| 1       A       301       U         1       A       302       A         1       A       308       C         1       A       309       U         1       A       309       U         1       A       310       C         1       A       337       A         1       A       345       A         1       A       345       A         1       A       346       G         1       A       348       U         1       A       346       G         1       A       349       C         1       A       352       G         1       A       360       C         1       A       366       A         1       A       366       A         1       A       367       G         1       A       373       A         1       A       375       C         1       A       398       U         1       A       398       U         1       A       410       G </td <td>1</td> <td>А</td> <td>299</td> <td>U</td>          | 1   | А     | 299 | U    |
| 1       A $302$ A         1       A $308$ C         1       A $309$ U         1       A $310$ C         1       A $310$ C         1       A $345$ A         1       A $345$ A         1       A $346$ G         1       A $344$ U         1       A $346$ G         1       A $345$ A         1       A $346$ G         1       A $346$ G         1       A $352$ G         1       A $366$ A         1       A $366$ A         1       A $367$ G         1       A $373$ A         1       A $375$ C         1       A $398$ U         1       A $398$ U         1       A $4109$ U         1  | 1   | А     | 301 | U    |
| 1       A       308       C         1       A       309       U         1       A       310       C         1       A       337       A         1       A       345       A         1       A       346       G         1       A       348       U         1       A       348       U         1       A       346       G         1       A       352       G         1       A       360       C         1       A       366       A         1       A       367       G         1       A       373       A         1       A       375       C         1       A       395       C         1       A       398       U         1       A       409       U         1       A       410       G </td <td>1</td> <td>А</td> <td>302</td> <td>A</td>          | 1   | А     | 302 | A    |
| 1       A $309$ U         1       A $310$ C         1       A $337$ A         1       A $345$ A         1       A $346$ G         1       A $352$ G         1       A $366$ A         1       A $366$ A         1       A $367$ G         1       A $373$ A         1       A $375$ C         1       A $389$ A         1       A $396$ G         1       A $409$ U         1       A $410$ G         1   | 1   | А     | 308 | С    |
| 1       A       310       C         1       A       337       A         1       A       345       A         1       A       345       A         1       A       346       G         1       A       348       U         1       A       349       C         1       A       352       G         1       A       354       A         1       A       360       C         1       A       366       A         1       A       366       A         1       A       366       A         1       A       367       G         1       A       373       A         1       A       375       C         1       A       395       C         1       A       398       U         1       A       409       U         1       A       410       G         1       A       412       A         1       A       420       U         1       A       433       G </td <td>1</td> <td>А</td> <td>309</td> <td>U</td>          | 1   | А     | 309 | U    |
| 1       A       337       A         1       A       345       A         1       A       346       G         1       A       348       U         1       A       349       C         1       A       352       G         1       A       354       A         1       A       360       C         1       A       366       A         1       A       367       G         1       A       367       G         1       A       373       A         1       A       375       C         1       A       389       A         1       A       395       C         1       A       398       U         1       A       410       U         1       A       412       A         1       A       412       A         1       A       419       G         1       A       420       U         1       A       433       G         1       A       434       U </td <td>1</td> <td>А</td> <td>310</td> <td>С</td>          | 1   | А     | 310 | С    |
| 1       A $345$ A         1       A $346$ G         1       A $348$ U         1       A $349$ C         1       A $352$ G         1       A $352$ G         1       A $354$ A         1       A $360$ C         1       A $366$ A         1       A $366$ A         1       A $367$ G         1       A $373$ A         1       A $375$ C         1       A $375$ C         1       A $395$ C         1       A $396$ G         1       A $409$ U         1       A $411$ G         1       A $412$ A         1       A $412$ A         1       A $419$ G         1       A $433$ G         1   | 1   | А     | 337 | A    |
| 1       A       346       G         1       A       348       U         1       A       349       C         1       A       352       G         1       A       354       A         1       A       360       C         1       A       361       G         1       A       366       A         1       A       367       G         1       A       367       G         1       A       373       A         1       A       375       C         1       A       382       G         1       A       395       C         1       A       398       U         1       A       409       U         1       A       412       A         1       A       413       G         1       A       412       A         1       A       419       G         1       A       420       U         1       A       433       G         1       A       436       A </td <td>1</td> <td>А</td> <td>345</td> <td>A</td>          | 1   | А     | 345 | A    |
| $\begin{array}{c ccccccccccccccccccccccccccccccccccc$   | 1   | А     | 346 | G    |
| $\begin{array}{c ccccccccccccccccccccccccccccccccccc$   | 1   | А     | 348 | U    |
| $\begin{array}{c ccccccccccccccccccccccccccccccccccc$   | 1   | А     | 349 | C    |
| $\begin{array}{c ccccccccccccccccccccccccccccccccccc$   | 1   | А     | 352 | G    |
| $\begin{array}{c ccccccccccccccccccccccccccccccccccc$   | 1   | А     | 354 | А    |
| $\begin{array}{c ccccccccccccccccccccccccccccccccccc$   | 1   | А     | 360 | С    |
| $\begin{array}{c ccccccccccccccccccccccccccccccccccc$   | 1   | А     | 361 | G    |
| $\begin{array}{c ccccccccccccccccccccccccccccccccccc$   | 1   | А     | 366 | А    |
| $\begin{array}{c ccccccccccccccccccccccccccccccccccc$   | 1   | А     | 367 | G    |
| $\begin{array}{c ccccccccccccccccccccccccccccccccccc$   | 1   | А     | 373 | А    |
| $\begin{array}{c ccccccccccccccccccccccccccccccccccc$   | 1   | А     | 374 | А    |
| $\begin{array}{c ccccccccccccccccccccccccccccccccccc$   | 1   | А     | 375 | С    |
| $\begin{array}{c ccccccccccccccccccccccccccccccccccc$   | 1   | А     | 382 | G    |
| $\begin{array}{c ccccccccccccccccccccccccccccccccccc$   | 1   | А     | 389 | А    |
| $\begin{array}{c ccccccccccccccccccccccccccccccccccc$   | 1   | А     | 395 | С    |
| $\begin{array}{c ccccccccccccccccccccccccccccccccccc$   | 1   | А     | 396 | G    |
| $\begin{array}{c ccccccccccccccccccccccccccccccccccc$   | 1   | А     | 398 | U    |
| $\begin{array}{c ccccccccccccccccccccccccccccccccccc$   | 1   | A     | 409 | U    |
| $\begin{array}{c ccccccccccccccccccccccccccccccccccc$   | 1   | A     | 411 | G    |
| $\begin{array}{c c c c c c c c c c c c c c c c c c c $  | 1   | A     | 412 | A    |
| $\begin{array}{c ccccccccccccccccccccccccccccccccccc$   | 1   | А     | 418 | А    |
| $\begin{array}{c ccccccccccccccccccccccccccccccccccc$   | 1   | A     | 419 | G    |
| $\begin{array}{c ccccccccccccccccccccccccccccccccccc$   | 1   | A     | 420 | U    |
| $\begin{array}{c ccccccccccccccccccccccccccccccccccc$   | 1   | A     | 421 | A    |
| $ \begin{array}{c ccccccccccccccccccccccccccccccccccc$  | 1   | A     | 430 | С    |
| $ \begin{array}{c ccccccccccccccccccccccccccccccccccc$  | 1   | A     | 433 | G    |
| $ \begin{array}{c ccccccccccccccccccccccccccccccccccc$  | 1   | A     | 434 | U    |
| $\begin{array}{c c c c c c c c c c c c c c c c c c c $  | 1   | A     | 436 | A    |
| 1 A 444 Ū   | 1   | A     | 442 | C    |
|   | 1   | А     | 444 | U    |



| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1   | А     | 445 | С    |
| 1   | А     | 453 | G    |
| 1   | А     | 458 | G    |
| 1   | А     | 459 | А    |
| 1   | А     | 469 | А    |
| 1   | А     | 471 | G    |
| 1   | А     | 482 | С    |
| 1   | А     | 483 | С    |
| 1   | А     | 489 | G    |
| 1   | А     | 490 | А    |
| 1   | А     | 494 | A    |
| 1   | А     | 498 | U    |
| 1   | А     | 502 | С    |
| 1   | А     | 503 | С    |
| 1   | А     | 504 | A    |
| 1   | А     | 506 | U    |
| 1   | А     | 508 | С    |
| 1   | А     | 511 | U    |
| 1   | А     | 524 | А    |
| 1   | А     | 526 | А    |
| 1   | А     | 527 | А    |
| 1   | А     | 528 | G    |
| 1   | А     | 529 | С    |
| 1   | А     | 548 | А    |
| 1   | А     | 550 | G    |
| 1   | А     | 551 | А    |
| 1   | А     | 552 | G    |
| 1   | А     | 554 | U    |
| 1   | А     | 555 | С    |
| 1   | А     | 556 | С    |
| 1   | A     | 558 | G    |
| 1   | A     | 568 | G    |
| 1   | A     | 573 | С    |
| 1   | A     | 575 | A    |
| 1   | A     | 577 | U    |
| 1   | A     | 578 | A    |
| 1   | A     | 583 | G    |
| 1   | A     | 584 | A    |
| 1   | A     | 590 | U    |
| 1   | А     | 591 | U    |
| 1   | A     | 592 | A    |
| 1   | А     | 593 | A    |



| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1   | А     | 594 | С    |
| 1   | А     | 595 | G    |
| 1   | А     | 599 | G    |
| 1   | А     | 607 | G    |
| 1   | А     | 613 | U    |
| 1   | А     | 617 | G    |
| 1   | А     | 618 | А    |
| 1   | А     | 619 | А    |
| 1   | А     | 622 | А    |
| 1   | А     | 630 | А    |
| 1   | А     | 632 | U    |
| 1   | А     | 646 | А    |
| 1   | А     | 647 | A    |
| 1   | A     | 648 | G    |
| 1   | А     | 649 | G    |
| 1   | A     | 655 | С    |
| 1   | А     | 658 | А    |
| 1   | А     | 659 | А    |
| 1   | А     | 662 | U    |
| 1   | А     | 667 | А    |
| 1   | А     | 668 | G    |
| 1   | А     | 673 | А    |
| 1   | А     | 680 | G    |
| 1   | А     | 683 | А    |
| 1   | А     | 686 | С    |
| 1   | А     | 689 | А    |
| 1   | А     | 690 | А    |
| 1   | А     | 691 | U    |
| 1   | А     | 698 | С    |
| 1   | А     | 699 | А    |
| 1   | A     | 700 | U    |
| 1   | А     | 701 | G    |
| 1   | A     | 703 | G    |
| 1   | А     | 715 | А    |
| 1   | A     | 716 | G    |
| 1   | А     | 717 | А    |
| 1   | А     | 718 | C    |
| 1   | A     | 733 | U    |
| 1   | А     | 741 | U    |
| 1   | А     | 749 | G    |
| 1   | А     | 764 | С    |
| 1   | А     | 765 | A    |



| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1   | А     | 766 | С    |
| 1   | А     | 777 | С    |
| 1   | А     | 787 | С    |
| 1   | А     | 788 | G    |
| 1   | А     | 790 | А    |
| 1   | А     | 794 | U    |
| 1   | А     | 804 | G    |
| 1   | А     | 810 | G    |
| 1   | А     | 811 | А    |
| 1   | А     | 812 | G    |
| 1   | А     | 822 | G    |
| 1   | А     | 823 | G    |
| 1   | А     | 824 | G    |
| 1   | A     | 829 | A    |
| 1   | А     | 830 | А    |
| 1   | A     | 831 | U    |
| 1   | А     | 832 | G    |
| 1   | А     | 837 | U    |
| 1   | А     | 839 | G    |
| 1   | А     | 847 | А    |
| 1   | А     | 852 | G    |
| 1   | А     | 853 | С    |
| 1   | А     | 858 | U    |
| 1   | А     | 859 | С    |
| 1   | А     | 866 | А    |
| 1   | А     | 874 | U    |
| 1   | А     | 875 | U    |
| 1   | А     | 878 | G    |
| 1   | А     | 890 | G    |
| 1   | A     | 891 | G    |
| 1   | A     | 892 | U    |
| 1   | A     | 893 | A    |
| 1   | А     | 906 | G    |
| 1   | A     | 908 | A    |
| 1   | А     | 913 | А    |
| 1   | A     | 914 | С    |
| 1   | A     | 916 | G    |
| 1   | А     | 919 | U    |
| 1   | A     | 923 | С    |
| 1   | А     | 928 | G    |
| 1   | A     | 929 | G    |
| 1   | А     | 931 | С    |



| Mol | Chain | Res  | Type |
|-----|-------|------|------|
| 1   | А     | 933  | С    |
| 1   | А     | 934  | U    |
| 1   | А     | 935  | А    |
| 1   | А     | 936  | С    |
| 1   | А     | 937  | С    |
| 1   | А     | 939  | G    |
| 1   | А     | 940  | G    |
| 1   | А     | 941  | U    |
| 1   | А     | 942  | U    |
| 1   | А     | 943  | А    |
| 1   | А     | 944  | С    |
| 1   | А     | 948  | А    |
| 1   | А     | 953  | G    |
| 1   | А     | 954  | U    |
| 1   | А     | 957  | А    |
| 1   | А     | 958  | А    |
| 1   | А     | 959  | С    |
| 1   | А     | 962  | С    |
| 1   | А     | 964  | А    |
| 1   | А     | 970  | А    |
| 1   | А     | 973  | G    |
| 1   | А     | 975  | С    |
| 1   | А     | 977  | U    |
| 1   | А     | 980  | С    |
| 1   | А     | 987  | А    |
| 1   | А     | 992  | G    |
| 1   | А     | 999  | А    |
| 1   | А     | 1003 | А    |
| 1   | А     | 1006 | А    |
| 1   | A     | 1007 | G    |
| 1   | A     | 1019 | A    |
| 1   | A     | 1020 | A    |
| 1   | A     | 1026 | А    |
| 1   | A     | 1029 | А    |
| 1   | A     | 1031 | С    |
| 1   | A     | 1036 | A    |
| 1   | A     | 1037 | С    |
| 1   | A     | 1042 | A    |
| 1   | A     | 1051 | C    |
| 1   | A     | 1054 | A    |
| 1   | A     | 1055 | А    |
| 1   | A     | 1058 | U    |



| Mol | Chain | Res  | Type |
|-----|-------|------|------|
| 1   | А     | 1059 | А    |
| 1   | А     | 1067 | А    |
| 1   | А     | 1068 | G    |
| 1   | А     | 1069 | U    |
| 1   | А     | 1070 | G    |
| 1   | А     | 1071 | G    |
| 1   | А     | 1072 | А    |
| 1   | А     | 1073 | А    |
| 1   | А     | 1079 | U    |
| 1   | A     | 1086 | U    |
| 1   | A     | 1091 | U    |
| 1   | A     | 1101 | G    |
| 1   | А     | 1102 | G    |
| 1   | A     | 1103 | A    |
| 1   | А     | 1106 | U    |
| 1   | A     | 1110 | С    |
| 1   | A     | 1111 | U    |
| 1   | А     | 1116 | A    |
| 1   | A     | 1117 | G    |
| 1   | A     | 1118 | С    |
| 1   | A     | 1119 | A    |
| 1   | A     | 1120 | G    |
| 1   | A     | 1121 | C    |
| 1   | A     | 1122 | С    |
| 1   | A     | 1123 | A    |
| 1   | A     | 1124 | С    |
| 1   | A     | 1125 | С    |
| 1   | A     | 1127 | U    |
| 1   | A     | 1128 | U    |
| 1   | A     | 1134 | A    |
| 1   | A     | 1142 | A    |
| 1   | A     | 1143 | U    |
| 1   | A     | 1145 | G    |
| 1   | A     | 1146 | C    |
| 1   | A     | 1157 | A    |
| 1   | A     | 1158 | G    |
| 1   | A     | 1159 | U    |
| 1   | A     | 1160 | G    |
| 1   | A     | 1161 | A    |
| 1   | A     | 1173 | A    |
| 1   | A     | 1174 | A    |
| 1   | A     | 1176 | U    |



| Mol | Chain | Res  | Type |
|-----|-------|------|------|
| 1   | А     | 1178 | U    |
| 1   | А     | 1179 | А    |
| 1   | А     | 1180 | С    |
| 1   | А     | 1181 | С    |
| 1   | А     | 1182 | G    |
| 1   | А     | 1185 | G    |
| 1   | А     | 1188 | А    |
| 1   | А     | 1197 | А    |
| 1   | А     | 1201 | А    |
| 1   | А     | 1203 | G    |
| 1   | А     | 1210 | А    |
| 1   | А     | 1221 | А    |
| 1   | А     | 1235 | А    |
| 1   | A     | 1236 | G    |
| 1   | A     | 1244 | A    |
| 1   | A     | 1245 | G    |
| 1   | А     | 1248 | С    |
| 1   | А     | 1249 | U    |
| 1   | А     | 1250 | G    |
| 1   | А     | 1251 | U    |
| 1   | А     | 1252 | G    |
| 1   | А     | 1259 | G    |
| 1   | А     | 1260 | А    |
| 1   | A     | 1261 | С    |
| 1   | А     | 1270 | С    |
| 1   | А     | 1276 | G    |
| 1   | А     | 1278 | G    |
| 1   | А     | 1280 | G    |
| 1   | A     | 1281 | C    |
| 1   | A     | 1282 | U    |
| 1   | А     | 1290 | G    |
| 1   | A     | 1293 | A    |
| 1   | A     | 1294 | A    |
| 1   | A     | 1295 | U    |
| 1   | A     | 1296 | G    |
| 1   | A     | 1306 | G    |
| 1   | A     | 1307 | U    |
| 1   | A     | 1311 | G    |
| 1   | A     | 1312 | A    |
| 1   | A     | 1313 | A    |
| 1   | A     | 1314 | A    |
| 1   | A     | 1315 | G    |



| Mol | Chain | Res  | Type |
|-----|-------|------|------|
| 1   | А     | 1323 | А    |
| 1   | А     | 1325 | А    |
| 1   | А     | 1330 | С    |
| 1   | А     | 1333 | С    |
| 1   | А     | 1339 | А    |
| 1   | А     | 1340 | А    |
| 1   | А     | 1341 | U    |
| 1   | А     | 1343 | С    |
| 1   | А     | 1344 | С    |
| 1   | А     | 1346 | А    |
| 1   | А     | 1351 | U    |
| 1   | А     | 1352 | U    |
| 1   | А     | 1354 | С    |
| 1   | A     | 1362 | G    |
| 1   | А     | 1363 | G    |
| 1   | А     | 1364 | С    |
| 1   | А     | 1365 | U    |
| 1   | А     | 1366 | С    |
| 1   | А     | 1368 | U    |
| 1   | А     | 1369 | С    |
| 1   | А     | 1370 | С    |
| 1   | А     | 1371 | G    |
| 1   | А     | 1372 | С    |
| 1   | А     | 1375 | А    |
| 1   | А     | 1376 | G    |
| 1   | А     | 1384 | С    |
| 1   | А     | 1385 | G    |
| 1   | А     | 1388 | А    |
| 1   | А     | 1389 | С    |
| 1   | А     | 1391 | U    |
| 1   | A     | 1404 | A    |
| 1   | A     | 1417 | A    |
| 1   | A     | 1418 | U    |
| 1   | A     | 1422 | C    |
| 1   | A     | 1423 | A    |
| 1   | A     | 1424 | A    |
| 1   | А     | 1425 | С    |
| 1   | A     | 1426 | A    |
| 1   | A     | 1435 | U    |
| 1   | A     | 1436 | U    |
| 1   | A     | 1442 | A    |
| 1   | А     | 1443 | С    |



| Mol | Chain | Res  | Type |
|-----|-------|------|------|
| 1   | А     | 1448 | U    |
| 1   | А     | 1449 | С    |
| 1   | А     | 1451 | U    |
| 1   | А     | 1457 | U    |
| 1   | А     | 1459 | U    |
| 1   | А     | 1460 | G    |
| 1   | А     | 1465 | A    |
| 1   | А     | 1467 | G    |
| 1   | А     | 1472 | G    |
| 1   | А     | 1473 | А    |
| 1   | А     | 1475 | G    |
| 1   | А     | 1481 | G    |
| 1   | А     | 1487 | G    |
| 1   | A     | 1489 | U    |
| 1   | А     | 1490 | A    |
| 1   | A     | 1499 | A    |
| 1   | А     | 1500 | U    |
| 1   | А     | 1502 | G    |
| 1   | А     | 1506 | А    |
| 1   | А     | 1507 | U    |
| 1   | А     | 1508 | С    |
| 1   | А     | 1516 | A    |
| 1   | А     | 1522 | U    |
| 1   | А     | 1525 | G    |
| 1   | А     | 1526 | G    |
| 1   | А     | 1527 | С    |
| 1   | А     | 1528 | U    |
| 1   | А     | 1529 | G    |
| 1   | А     | 1530 | G    |
| 1   | А     | 1531 | G    |
| 1   | A     | 1532 | A    |
| 1   | A     | 1536 | A    |
| 1   | А     | 1539 | С    |
| 1   | A     | 1540 | A    |
| 1   | А     | 1542 | A    |
| 1   | A     | 1543 | U    |
| 1   | A     | 1544 | C    |
| 1   | A     | 1545 | С    |
| 1   | A     | 1549 | U    |
| 1   | A     | 1550 | С    |
| 1   | A     | 1551 | С    |
| 1   | A     | 1553 | A    |



| Mol | Chain | Res  | Type |
|-----|-------|------|------|
| 1   | А     | 1556 | А    |
| 1   | А     | 1557 | G    |
| 1   | А     | 1558 | G    |
| 1   | А     | 1559 | С    |
| 1   | А     | 1560 | U    |
| 1   | А     | 1561 | G    |
| 1   | А     | 1562 | А    |
| 1   | А     | 1563 | G    |
| 1   | А     | 1566 | G    |
| 1   | А     | 1568 | G    |
| 1   | А     | 1569 | А    |
| 1   | А     | 1570 | U    |
| 1   | A     | 1571 | G    |
| 1   | A     | 1573 | С    |
| 1   | A     | 1602 | U    |
| 1   | A     | 1606 | A    |
| 1   | А     | 1607 | С    |
| 1   | А     | 1608 | А    |
| 1   | А     | 1613 | С    |
| 1   | А     | 1617 | А    |
| 1   | А     | 1626 | U    |
| 1   | А     | 1628 | G    |
| 1   | А     | 1631 | А    |
| 1   | А     | 1632 | G    |
| 1   | А     | 1645 | С    |
| 1   | А     | 1653 | А    |
| 1   | А     | 1655 | А    |
| 1   | A     | 1657 | С    |
| 1   | A     | 1658 | G    |
| 1   | A     | 1661 | A    |
| 1   | A     | 1672 | A    |
| 1   | А     | 1679 | A    |
| 1   | A     | 1680 | A    |
| 1   | А     | 1691 | A    |
| 1   | A     | 1692 | U    |
| 1   | A     | 1693 | С    |
| 1   | А     | 1694 | G    |
| 1   | А     | 1696 | G    |
| 1   | А     | 1697 | A    |
| 1   | А     | 1699 | A    |
| 1   | А     | 1700 | A    |
| 1   | A     | 1708 | U    |



| main Res | Type |
|----------|------|
| 1 A 1709 | А    |
| 1 A 1712 | G    |
| 1 A 1717 | С    |
| 1 A 1719 | G    |
| 1 A 1720 | С    |
| 1 A 1727 | А    |
| 1 A 1738 | U    |
| 1 A 1740 | G    |
| 1 A 1745 | А    |
| 1 A 1746 | А    |
| 1 A 1748 | G    |
| 1 A 1750 | G    |
| 1 A 1752 | G    |
| 1 A 1753 | С    |
| 1 A 1757 | G    |
| 1 A 1758 | U    |
| 1 A 1759 | U    |
| 1 A 1760 | А    |
| 1 A 1762 | G    |
| 1 A 1766 | С    |
| 1 A 1768 | А    |
| 1 A 1771 | С    |
| 1 A 1776 | А    |
| 1 A 1777 | G    |
| 1 A 1778 | А    |
| 1 A 1779 | G    |
| 1 A 1781 | С    |
| 1 A 1782 | G    |
| 1 A 1783 | С    |
| 1 A 1785 | G    |
| 1 A 1789 | А    |
| 1 A 1790 | U    |
| 1 A 1792 | G    |
| 1 A 1793 | G    |
| 1 A 1797 | А    |
| 1 A 1802 | A    |
| 1 A 1810 | G    |
| 1 A 1811 | С    |
| 1 A 1812 | A    |
| 1 A 1813 | A    |
| 1 A 1814 | А    |
| 1 A 1815 | A    |



| Mol | Chain | Res  | Type |
|-----|-------|------|------|
| 1   | А     | 1829 | С    |
| 1   | А     | 1830 | G    |
| 1   | А     | 1831 | А    |
| 1   | А     | 1833 | G    |
| 1   | А     | 1839 | А    |
| 1   | А     | 1843 | G    |
| 1   | А     | 1845 | А    |
| 1   | А     | 1846 | G    |
| 1   | А     | 1849 | U    |
| 1   | А     | 1858 | А    |
| 1   | А     | 1867 | С    |
| 1   | А     | 1872 | С    |
| 1   | А     | 1877 | А    |
| 1   | A     | 1882 | А    |
| 1   | A     | 1883 | А    |
| 1   | А     | 1884 | G    |
| 1   | А     | 1885 | А    |
| 1   | А     | 1887 | G    |
| 1   | А     | 1895 | А    |
| 1   | А     | 1899 | U    |
| 1   | А     | 1902 | G    |
| 1   | А     | 1904 | G    |
| 1   | А     | 1932 | G    |
| 1   | А     | 1935 | G    |
| 1   | А     | 1941 | А    |
| 1   | А     | 1942 | А    |
| 1   | А     | 1943 | С    |
| 1   | А     | 1944 | U    |
| 1   | А     | 1946 | U    |
| 1   | А     | 1952 | U    |
| 1   | А     | 1956 | А    |
| 1   | A     | 1958 | G    |
| 1   | А     | 1959 | G    |
| 1   | A     | 1966 | A    |
| 1   | А     | 1967 | А    |
| 1   | A     | 1968 | U    |
| 1   | A     | 1969 | U    |
| 1   | А     | 1970 | С    |
| 1   | A     | 1972 | U    |
| 1   | А     | 1973 | U    |
| 1   | A     | 1984 | U    |
| 1   | А     | 1992 | С    |



| Mol | Chain | Res  | Type |
|-----|-------|------|------|
| 1   | А     | 1993 | G    |
| 1   | А     | 1995 | А    |
| 1   | А     | 1996 | С    |
| 1   | А     | 1999 | А    |
| 1   | А     | 2000 | А    |
| 1   | А     | 2001 | G    |
| 1   | А     | 2004 | G    |
| 1   | А     | 2010 | А    |
| 1   | А     | 2020 | U    |
| 1   | А     | 2022 | U    |
| 1   | А     | 2025 | С    |
| 1   | А     | 2026 | А    |
| 1   | А     | 2033 | G    |
| 1   | A     | 2050 | G    |
| 1   | А     | 2051 | U    |
| 1   | A     | 2052 | A    |
| 1   | А     | 2053 | С    |
| 1   | А     | 2059 | А    |
| 1   | А     | 2060 | А    |
| 1   | А     | 2061 | G    |
| 1   | А     | 2062 | А    |
| 1   | А     | 2064 | G    |
| 1   | А     | 2065 | С    |
| 1   | А     | 2068 | G    |
| 1   | А     | 2070 | U    |
| 1   | А     | 2072 | С    |
| 1   | А     | 2079 | С    |
| 1   | А     | 2080 | А    |
| 1   | А     | 2081 | G    |
| 1   | А     | 2084 | С    |
| 1   | A     | 2085 | G    |
| 1   | A     | 2089 | А    |
| 1   | A     | 2090 | G    |
| 1   | A     | 2098 | G    |
| 1   | A     | 2101 | G    |
| 1   | A     | 2121 | U    |
| 1   | A     | 2123 | А    |
| 1   | A     | 2125 | U    |
| 1   | А     | 2128 | U    |
| 1   | А     | 2131 | U    |
| 1   | A     | 2134 | A    |
| 1   | A     | 2135 | G    |



| Mol | Chain | Res  | Type |
|-----|-------|------|------|
| 1   | А     | 2136 | С    |
| 1   | А     | 2139 | G    |
| 1   | А     | 2140 | U    |
| 1   | А     | 2145 | G    |
| 1   | А     | 2146 | А    |
| 1   | А     | 2147 | U    |
| 1   | А     | 2149 | G    |
| 1   | А     | 2156 | G    |
| 1   | А     | 2160 | U    |
| 1   | А     | 2161 | G    |
| 1   | А     | 2162 | G    |
| 1   | А     | 2166 | С    |
| 1   | А     | 2174 | С    |
| 1   | А     | 2175 | С    |
| 1   | А     | 2176 | A    |
| 1   | А     | 2177 | G    |
| 1   | А     | 2185 | G    |
| 1   | А     | 2187 | A    |
| 1   | А     | 2198 | G    |
| 1   | А     | 2200 | А    |
| 1   | А     | 2201 | U    |
| 1   | А     | 2202 | А    |
| 1   | А     | 2203 | С    |
| 1   | А     | 2205 | А    |
| 1   | А     | 2206 | С    |
| 1   | А     | 2208 | С    |
| 1   | А     | 2210 | G    |
| 1   | А     | 2212 | С    |
| 1   | А     | 2213 | U    |
| 1   | А     | 2217 | U    |
| 1   | А     | 2219 | G    |
| 1   | А     | 2228 | A    |
| 1   | А     | 2232 | G    |
| 1   | А     | 2233 | С    |
| 1   | А     | 2240 | U    |
| 1   | А     | 2241 | А    |
| 1   | А     | 2242 | U    |
| 1   | А     | 2244 | G    |
| 1   | А     | 2245 | G    |
| 1   | А     | 2246 | G    |
| 1   | А     | 2249 | G    |
| 1   | А     | 2252 | A    |
|     | ~     | -    |      |



| Mol | Chain | Res  | Type |
|-----|-------|------|------|
| 1   | А     | 2254 | А    |
| 1   | А     | 2255 | С    |
| 1   | А     | 2260 | U    |
| 1   | А     | 2267 | G    |
| 1   | А     | 2268 | G    |
| 1   | А     | 2295 | А    |
| 1   | А     | 2296 | А    |
| 1   | А     | 2307 | A    |
| 1   | А     | 2308 | G    |
| 1   | А     | 2311 | G    |
| 1   | А     | 2312 | С    |
| 1   | А     | 2316 | А    |
| 1   | А     | 2317 | А    |
| 1   | A     | 2323 | С    |
| 1   | А     | 2324 | С    |
| 1   | A     | 2325 | U    |
| 1   | А     | 2327 | А    |
| 1   | А     | 2331 | U    |
| 1   | А     | 2332 | G    |
| 1   | А     | 2333 | G    |
| 1   | А     | 2334 | U    |
| 1   | А     | 2335 | U    |
| 1   | А     | 2336 | G    |
| 1   | А     | 2338 | А    |
| 1   | А     | 2340 | А    |
| 1   | А     | 2341 | U    |
| 1   | А     | 2342 | С    |
| 1   | А     | 2343 | A    |
| 1   | А     | 2344 | U    |
| 1   | A     | 2345 | U    |
| 1   | А     | 2348 | С    |
| 1   | A     | 2349 | A    |
| 1   | А     | 2350 | G    |
| 1   | A     | 2354 | G    |
| 1   | А     | 2356 | А    |
| 1   | A     | 2357 | A    |
| 1   | А     | 2363 | С    |
| 1   | A     | 2364 | A    |
| 1   | А     | 2368 | G    |
| 1   | A     | 2374 | G    |
| 1   | A     | 2376 | С    |
| 1   | А     | 2379 | С    |



| Mol | Chain | Res  | Type |
|-----|-------|------|------|
| 1   | А     | 2381 | А    |
| 1   | А     | 2387 | А    |
| 1   | А     | 2390 | А    |
| 1   | А     | 2401 | G    |
| 1   | А     | 2406 | А    |
| 1   | А     | 2408 | G    |
| 1   | А     | 2412 | G    |
| 1   | А     | 2413 | G    |
| 1   | А     | 2414 | С    |
| 1   | А     | 2418 | G    |
| 1   | А     | 2420 | G    |
| 1   | А     | 2431 | U    |
| 1   | А     | 2432 | С    |
| 1   | A     | 2435 | С    |
| 1   | А     | 2448 | U    |
| 1   | A     | 2451 | С    |
| 1   | А     | 2452 | U    |
| 1   | А     | 2453 | С    |
| 1   | А     | 2454 | А    |
| 1   | А     | 2455 | А    |
| 1   | А     | 2458 | G    |
| 1   | А     | 2459 | А    |
| 1   | А     | 2460 | U    |
| 1   | А     | 2464 | А    |
| 1   | А     | 2468 | А    |
| 1   | А     | 2469 | С    |
| 1   | А     | 2470 | С    |
| 1   | А     | 2476 | G    |
| 1   | А     | 2477 | А    |
| 1   | А     | 2488 | А    |
| 1   | A     | 2497 | A    |
| 1   | A     | 2503 | C    |
| 1   | А     | 2505 | А    |
| 1   | A     | 2506 | C    |
| 1   | А     | 2507 | А    |
| 1   | A     | 2511 | A    |
| 1   | A     | 2523 | G    |
| 1   | А     | 2524 | G    |
| 1   | A     | 2525 | С    |
| 1   | А     | 2527 | С    |
| 1   | А     | 2531 | G    |
| 1   | A     | 2532 | A    |



| Mol | Chain | Res               | Type |
|-----|-------|-------------------|------|
| 1   | А     | 2533              | U    |
| 1   | А     | 2534              | G    |
| 1   | А     | 2547              | А    |
| 1   | А     | 2554              | G    |
| 1   | А     | 2558              | G    |
| 1   | А     | 2563              | С    |
| 1   | А     | 2564              | G    |
| 1   | А     | 2570              | А    |
| 1   | А     | 2583              | U    |
| 1   | А     | 2593              | А    |
| 1   | А     | 2595              | А    |
| 1   | А     | 2596              | G    |
| 1   | Α     | 2598              | G    |
| 1   | A     | $2\overline{601}$ | A    |
| 1   | А     | 2602              | С    |
| 1   | A     | 2607              | G    |
| 1   | А     | 2612              | G    |
| 1   | А     | 2613              | U    |
| 1   | А     | 2614              | U    |
| 1   | А     | 2615              | С    |
| 1   | А     | 2630              | С    |
| 1   | А     | 2631              | А    |
| 1   | А     | 2638              | U    |
| 1   | А     | 2642              | U    |
| 1   | А     | 2644              | U    |
| 1   | А     | 2654              | G    |
| 1   | А     | 2659              | G    |
| 1   | А     | 2660              | G    |
| 1   | А     | 2667              | G    |
| 1   | А     | 2674              | G    |
| 1   | A     | $2\overline{675}$ | C    |
| 1   | А     | 2689              | A    |
| 1   | A     | 2692              | G    |
| 1   | A     | 2696              | С    |
| 1   | A     | 2702              | G    |
| 1   | A     | 2711              | G    |
| 1   | А     | 2714              | G    |
| 1   | A     | 2718              | U    |
| 1   | A     | 2720              | С    |
| 1   | A     | 2743              | G    |
| 1   | A     | 2747              | G    |
| 1   | А     | 2753              | U    |



| Mol | Chain | Res  | Type |
|-----|-------|------|------|
| 1   | А     | 2755 | U    |
| 1   | А     | 2760 | G    |
| 1   | А     | 2762 | А    |
| 1   | А     | 2764 | G    |
| 1   | А     | 2765 | G    |
| 1   | А     | 2766 | G    |
| 1   | А     | 2773 | G    |
| 1   | А     | 2777 | А    |
| 1   | А     | 2784 | С    |
| 1   | А     | 2785 | U    |
| 1   | А     | 2786 | А    |
| 1   | А     | 2789 | С    |
| 1   | А     | 2794 | A    |
| 1   | А     | 2795 | G    |
| 1   | А     | 2806 | G    |
| 1   | А     | 2807 | A    |
| 1   | А     | 2808 | U    |
| 1   | А     | 2818 | С    |
| 1   | А     | 2821 | U    |
| 1   | А     | 2822 | С    |
| 1   | А     | 2823 | С    |
| 1   | А     | 2824 | G    |
| 1   | А     | 2826 | A    |
| 1   | А     | 2828 | G    |
| 1   | А     | 2831 | А    |
| 1   | А     | 2832 | G    |
| 1   | А     | 2833 | U    |
| 1   | А     | 2843 | G    |
| 1   | А     | 2855 | G    |
| 1   | А     | 2859 | G    |
| 1   | A     | 2860 | A    |
| 1   | А     | 2862 | А    |
| 1   | A     | 2866 | C    |
| 1   | A     | 2868 | G    |
| 1   | A     | 2874 | G    |
| 1   | A     | 2886 | C    |
| 1   | A     | 2891 | G    |
| 1   | A     | 2892 | G    |
| 1   | A     | 2897 | G    |
| 1   | A     | 2900 | A    |
| 1   | A     | 2901 | G    |
| 1   | А     | 2905 | С    |



| Mol | Chain | Res  | Type |
|-----|-------|------|------|
| 1   | А     | 2908 | А    |
| 1   | А     | 2916 | А    |
| 1   | А     | 2917 | G    |
| 2   | В     | 10   | G    |
| 2   | В     | 12   | U    |
| 2   | В     | 15   | С    |
| 2   | В     | 22   | G    |
| 2   | В     | 23   | U    |
| 2   | В     | 28   | С    |
| 2   | В     | 31   | G    |
| 2   | В     | 32   | U    |
| 2   | В     | 33   | U    |
| 2   | В     | 34   | С    |
| 2   | В     | 38   | U    |
| 2   | В     | 39   | A    |
| 2   | В     | 40   | С    |
| 2   | В     | 41   | С    |
| 2   | В     | 42   | G    |
| 2   | В     | 47   | С    |
| 2   | В     | 48   | G    |
| 2   | В     | 49   | G    |
| 2   | В     | 50   | А    |
| 2   | В     | 52   | G    |
| 2   | В     | 53   | U    |
| 2   | В     | 54   | U    |
| 2   | В     | 55   | А    |
| 2   | В     | 59   | U    |
| 2   | В     | 60   | С    |
| 2   | В     | 62   | U    |
| 2   | В     | 63   | С    |
| 2   | В     | 64   | A    |
| 2   | В     | 65   | G    |
| 2   | В     | 66   | С    |
| 2   | В     | 85   | U    |
| 2   | В     | 86   | U    |
| 2   | В     | 87   | U    |
| 2   | В     | 88   | С    |
| 2   | В     | 97   | A    |
| 2   | В     | 101  | U    |
| 2   | В     | 106  | C    |
| 2   | В     | 107  | G    |
| 2   | В     | 110  | G    |



| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 2   | В     | 114 | А    |
| 33  | a     | 9   | G    |
| 33  | a     | 10  | А    |
| 33  | a     | 11  | G    |
| 33  | a     | 24  | G    |
| 33  | a     | 32  | С    |
| 33  | a     | 33  | G    |
| 33  | а     | 34  | А    |
| 33  | a     | 41  | G    |
| 33  | a     | 46  | G    |
| 33  | a     | 49  | С    |
| 33  | a     | 50  | С    |
| 33  | a     | 51  | U    |
| 33  | a     | 52  | A    |
| 33  | a     | 53  | A    |
| 33  | a     | 60  | С    |
| 33  | a     | 65  | С    |
| 33  | a     | 66  | G    |
| 33  | a     | 72  | А    |
| 33  | a     | 75  | G    |
| 33  | a     | 77  | U    |
| 33  | a     | 80  | G    |
| 33  | a     | 84  | U    |
| 33  | a     | 85  | U    |
| 33  | a     | 86  | G    |
| 33  | a     | 87  | С    |
| 33  | а     | 88  | U    |
| 33  | a     | 89  | С    |
| 33  | a     | 90  | С    |
| 33  | a     | 92  | U    |
| 33  | a     | 93  | G    |
| 33  | a     | 99  | A    |
| 33  | a     | 114 | A    |
| 33  | a     | 117 | A    |
| 33  | a     | 118 | A    |
| 33  | a     | 119 | C    |
| 33  | a     | 120 | A    |
| 33  | a     | 128 | A    |
| 33  | a     | 129 | A    |
| 33  | a     | 130 | C    |
| 33  | a     | 136 | U    |
| 33  | a     | 137 | G    |



| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 33  | a     | 140 | А    |
| 33  | a     | 141 | G    |
| 33  | a     | 142 | А    |
| 33  | a     | 144 | U    |
| 33  | a     | 153 | U    |
| 33  | a     | 154 | С    |
| 33  | a     | 158 | G    |
| 33  | a     | 162 | С    |
| 33  | a     | 167 | G    |
| 33  | a     | 172 | U    |
| 33  | a     | 176 | G    |
| 33  | a     | 181 | G    |
| 33  | a     | 182 | U    |
| 33  | a     | 189 | A    |
| 33  | a     | 190 | A    |
| 33  | a     | 193 | G    |
| 33  | a     | 194 | С    |
| 33  | a     | 197 | G    |
| 33  | a     | 207 | U    |
| 33  | a     | 208 | А    |
| 33  | a     | 209 | А    |
| 33  | a     | 211 | А    |
| 33  | a     | 218 | U    |
| 33  | a     | 219 | U    |
| 33  | a     | 220 | С    |
| 33  | a     | 221 | G    |
| 33  | a     | 222 | G    |
| 33  | a     | 249 | G    |
| 33  | a     | 253 | U    |
| 33  | a     | 255 | G    |
| 33  | a     | 259 | G    |
| 33  | a     | 262 | G    |
| 33  | a     | 274 | G    |
| 33  | a     | 275 | С    |
| 33  | a     | 277 | С    |
| 33  | a     | 280 | C    |
| 33  | a     | 287 | А    |
| 33  | a     | 288 | C    |
| 33  | a     | 297 | G    |
| 33  | a     | 306 | A    |
| 33  | a     | 314 | А    |
| 33  | a     | 316 | С    |



| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 33  | a     | 321 | А    |
| 33  | a     | 329 | А    |
| 33  | a     | 336 | С    |
| 33  | a     | 337 | А    |
| 33  | a     | 338 | С    |
| 33  | a     | 340 | G    |
| 33  | a     | 352 | А    |
| 33  | a     | 353 | С    |
| 33  | a     | 355 | G    |
| 33  | a     | 357 | А    |
| 33  | a     | 359 | G    |
| 33  | a     | 360 | С    |
| 33  | a     | 362 | G    |
| 33  | a     | 371 | А    |
| 33  | a     | 373 | U    |
| 33  | a     | 375 | U    |
| 33  | a     | 380 | С    |
| 33  | a     | 383 | U    |
| 33  | a     | 385 | G    |
| 33  | a     | 390 | А    |
| 33  | a     | 392 | G    |
| 33  | a     | 396 | G    |
| 33  | a     | 400 | G    |
| 33  | a     | 405 | А    |
| 33  | a     | 406 | С    |
| 33  | a     | 414 | G    |
| 33  | a     | 419 | А    |
| 33  | a     | 420 | U    |
| 33  | a     | 421 | G    |
| 33  | a     | 426 | U    |
| 33  | a     | 429 | U    |
| 33  | a     | 430 | С    |
| 33  | a     | 432 | G    |
| 33  | a     | 436 | G    |
| 33  | a     | 437 | U    |
| 33  | a     | 438 | A    |
| 33  | a     | 439 | А    |
| 33  | a     | 442 | С    |
| 33  | a     | 447 | U    |
| 33  | a     | 456 | A    |
| 33  | a     | 457 | A    |
| 33  | a     | 459 | A    |



| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 33  | a     | 460 | А    |
| 33  | a     | 461 | С    |
| 33  | a     | 465 | U    |
| 33  | a     | 466 | G    |
| 33  | a     | 467 | С    |
| 33  | a     | 473 | G    |
| 33  | a     | 474 | А    |
| 33  | a     | 476 | U    |
| 33  | a     | 477 | А    |
| 33  | a     | 478 | G    |
| 33  | a     | 480 | G    |
| 33  | a     | 483 | G    |
| 33  | a     | 484 | U    |
| 33  | a     | 485 | А    |
| 33  | a     | 487 | С    |
| 33  | a     | 488 | U    |
| 33  | a     | 490 | G    |
| 33  | a     | 491 | А    |
| 33  | a     | 494 | G    |
| 33  | a     | 506 | А    |
| 33  | a     | 508 | А    |
| 33  | a     | 518 | А    |
| 33  | a     | 519 | А    |
| 33  | a     | 520 | С    |
| 33  | a     | 526 | G    |
| 33  | a     | 527 | С    |
| 33  | a     | 530 | G    |
| 33  | a     | 533 | G    |
| 33  | a     | 536 | G    |
| 33  | a     | 539 | G    |
| 33  | a     | 540 | U    |
| 33  | a     | 541 | A    |
| 33  | a     | 542 | A    |
| 33  | a     | 553 | G    |
| 33  | a     | 554 | С    |
| 33  | a     | 556 | A    |
| 33  | a     | 563 | U    |
| 33  | a     | 564 | С    |
| 33  | a     | 568 | A    |
| 33  | a     | 571 | U    |
| 33  | a     | 573 | U    |
| 33  | a     | 581 | А    |



| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 33  | a     | 582 | А    |
| 33  | a     | 585 | G    |
| 33  | a     | 586 | G    |
| 33  | a     | 588 | U    |
| 33  | a     | 591 | С    |
| 33  | a     | 597 | G    |
| 33  | a     | 616 | А    |
| 33  | a     | 627 | С    |
| 33  | a     | 628 | U    |
| 33  | a     | 629 | С    |
| 33  | a     | 641 | G    |
| 33  | a     | 642 | U    |
| 33  | a     | 643 | C    |
| 33  | a     | 648 | G    |
| 33  | a     | 650 | A    |
| 33  | a     | 661 | U    |
| 33  | a     | 662 | U    |
| 33  | a     | 670 | G    |
| 33  | a     | 674 | А    |
| 33  | a     | 694 | G    |
| 33  | a     | 696 | А    |
| 33  | a     | 704 | А    |
| 33  | a     | 727 | А    |
| 33  | a     | 732 | U    |
| 33  | a     | 733 | G    |
| 33  | a     | 740 | G    |
| 33  | a     | 742 | G    |
| 33  | a     | 745 | U    |
| 33  | a     | 756 | U    |
| 33  | a     | 757 | A    |
| 33  | a     | 758 | A    |
| 33  | a     | 762 | A    |
| 33  | a     | 764 | G    |
| 33  | a     | 768 | A    |
| 33  | a     | 787 | G    |
| 33  | a     | 802 | U    |
| 33  | a     | 803 | A    |
| 33  | a     | 806 | С    |
| 33  | a     | 815 | С    |
| 33  | a     | 821 | G    |
| 33  | a     | 824 | А    |
| 33  | a     | 826 | С    |



| 33         a         828         A           33         a         829         U |  |
|---|--|
| 33 a 829 U  |  |
|   |  |
| 33   a   841   G  |  |
| 33 a 845 G  |  |
| 33 a 849 G  |  |
| 33 a 853 C  |  |
| 33 a 855 G  |  |
| 33 a 856 C  |  |
| 33 a 861 U  |  |
| 33 a 880 U  |  |
| 33 a 884 G  |  |
| 33 a 885 C  |  |
| 33 a 895 G  |  |
| 33 a 899 A  |  |
| 33 a 909 C  |  |
| 33 a 924 A  |  |
| 33 a 932 G  |  |
| 33 a 936 G  |  |
| 33 a 944 C  |  |
| 33 a 945 A  |  |
| 33 a 952 G  |  |
| 33 a 964 G  |  |
| 33 a 966 U  |  |
| 33 a 967 U  |  |
| 33 a 968 A  |  |
| 33 a 970 U  |  |
| 33 a 975 A  |  |
| 33 a 976 G  |  |
| 33 a 978 A  |  |
| 33 a 979 A  |  |
| 33 a 981 G  |  |
| 33 a 984 A  |  |
| 33 a 985 A  |  |
| 33 a 986 G  |  |
| 33 a 987 A  |  |
| 33 a 992 U  |  |
| 33 a 993 A  |  |
| 33 a 999 U  |  |
| 33 a 1000 C   |  |
| 33 a 1002 U   |  |
| 33 a 1003 G   |  |
| 33 a 1006 A   |  |



| Mol | Chain | Res  | Type |
|-----|-------|------|------|
| 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     | 1020 | С    |
| 33  | a     | 1023 | G    |
| 33  | a     | 1024 | А    |
| 33  | a     | 1027 | U    |
| 33  | a     | 1028 | A    |
| 33  | a     | 1030 | G    |
| 33  | a     | 1031 | A    |
| 33  | a     | 1033 | G    |
| 33  | a     | 1035 | С    |
| 33  | a     | 1036 | С    |
| 33  | a     | 1039 | U    |
| 33  | a     | 1040 | U    |
| 33  | a     | 1041 | С    |
| 33  | a     | 1042 | G    |
| 33  | a     | 1043 | G    |
| 33  | a     | 1046 | G    |
| 33  | a     | 1047 | С    |
| 33  | a     | 1050 | А    |
| 33  | a     | 1051 | G    |
| 33  | a     | 1052 | U    |
| 33  | a     | 1053 | G    |
| 33  | a     | 1056 | A    |
| 33  | a     | 1058 | G    |
| 33  | a     | 1060 | G    |
| 33  | a     | 1064 | C    |
| 33  | a     | 1071 | G    |
| 33  | a     | 1074 | G    |
| 33  | a     | 1075 | U    |
| 33  | a     | 1095 | U    |
| 33  | a     | 1102 | A    |
| 33  | a     | 1104 | G    |
| 33  | a     | 1105 | U    |
| 33  | a     | 1110 | С    |



| Mol | Chain | Res  | Type |
|-----|-------|------|------|
| 33  | a     | 1111 | А    |
| 33  | a     | 1112 | А    |
| 33  | a     | 1114 | G    |
| 33  | a     | 1118 | G    |
| 33  | a     | 1124 | С    |
| 33  | a     | 1128 | А    |
| 33  | a     | 1134 | G    |
| 33  | a     | 1136 | U    |
| 33  | a     | 1140 | А    |
| 33  | a     | 1141 | G    |
| 33  | a     | 1142 | С    |
| 33  | a     | 1143 | А    |
| 33  | a     | 1145 | U    |
| 33  | a     | 1148 | G    |
| 33  | a     | 1149 | U    |
| 33  | a     | 1150 | U    |
| 33  | a     | 1151 | G    |
| 33  | a     | 1153 | G    |
| 33  | a     | 1155 | А    |
| 33  | a     | 1163 | G    |
| 33  | a     | 1166 | А    |
| 33  | a     | 1167 | С    |
| 33  | a     | 1168 | U    |
| 33  | a     | 1169 | G    |
| 33  | a     | 1170 | С    |
| 33  | a     | 1176 | А    |
| 33  | a     | 1177 | С    |
| 33  | a     | 1178 | А    |
| 33  | a     | 1180 | А    |
| 33  | a     | 1190 | G    |
| 33  | a     | 1192 | U    |
| 33  | a     | 1193 | G    |
| 33  | a     | 1205 | A    |
| 33  | a     | 1206 | А    |
| 33  | a     | 1209 | С    |
| 33  | a     | 1211 | U    |
| 33  | a     | 1214 | U    |
| 33  | a     | 1221 | U    |
| 33  | a     | 1222 | А    |
| 33  | a     | 1224 | G    |
| 33  | a     | 1233 | U    |
| 33  | a     | 1235 | С    |



| Mol | Chain | Res  | Type |
|-----|-------|------|------|
| 33  | a     | 1236 | А    |
| 33  | a     | 1237 | С    |
| 33  | a     | 1238 | А    |
| 33  | a     | 1239 | С    |
| 33  | a     | 1245 | А    |
| 33  | a     | 1247 | А    |
| 33  | a     | 1258 | С    |
| 33  | a     | 1259 | А    |
| 33  | a     | 1265 | С    |
| 33  | a     | 1266 | А    |
| 33  | a     | 1267 | G    |
| 33  | a     | 1269 | G    |
| 33  | a     | 1279 | G    |
| 33  | a     | 1288 | А    |
| 33  | a     | 1289 | А    |
| 33  | a     | 1291 | С    |
| 33  | a     | 1294 | А    |
| 33  | a     | 1295 | С    |
| 33  | a     | 1296 | А    |
| 33  | a     | 1299 | U    |
| 33  | a     | 1307 | С    |
| 33  | a     | 1308 | А    |
| 33  | a     | 1309 | G    |
| 33  | a     | 1311 | U    |
| 33  | a     | 1312 | С    |
| 33  | a     | 1313 | G    |
| 33  | a     | 1314 | G    |
| 33  | a     | 1323 | С    |
| 33  | a     | 1326 | С    |
| 33  | a     | 1329 | С    |
| 33  | a     | 1331 | С    |
| 33  | a     | 1332 | G    |
| 33  | a     | 1336 | G    |
| 33  | a     | 1340 | G    |
| 33  | a     | 1345 | U    |
| 33  | a     | 1347 | G    |
| 33  | a     | 1349 | A    |
| 33  | a     | 1354 | U    |
| 33  | a     | 1355 | A    |
| 33  | a     | 1362 | G    |
| 33  | a     | 1366 | A    |
| 33  | a     | 1371 | С    |



| Mol | Chain | Res   | Type |
|-----|-------|-------|------|
| 33  | a     | 1372  | А    |
| 33  | a     | 1373  | U    |
| 33  | a     | 1377  | G    |
| 33  | a     | 1379  | G    |
| 33  | a     | 1387  | С    |
| 33  | a     | 1403  | А    |
| 33  | a     | 1406  | С    |
| 33  | a     | 1407  | А    |
| 33  | a     | 1413  | С    |
| 33  | a     | 1428  | G    |
| 33  | a     | 1435  | А    |
| 33  | a     | 1451  | А    |
| 33  | a     | 1452  | G    |
| 33  | a     | 1455  | А    |
| 33  | a     | 1461  | U    |
| 33  | a     | 1462  | U    |
| 33  | a     | 1463  | А    |
| 33  | a     | 1464  | G    |
| 33  | a     | 1478  | А    |
| 33  | a     | 1494  | U    |
| 33  | a     | 1496  | G    |
| 33  | a     | 1497  | G    |
| 33  | a     | 1500  | U    |
| 33  | a     | 1502  | А    |
| 33  | a     | 1503  | А    |
| 33  | a     | 1507  | G    |
| 33  | a     | 1513  | А    |
| 33  | a     | 1515  | G    |
| 33  | a     | 1516  | U    |
| 33  | a     | 1517  | А    |
| 33  | a     | 1527  | G    |
| 33  | a     | 1529  | А    |
| 33  | a     | 1539  | G    |
| 33  | a     | 1540  | G    |
| 53  | х     | 6     | G    |
| 53  | x     | 8     | U    |
| 53  | X     | 9     | G    |
| 53  | X     | 13    | G    |
| 53  | X     | 16    | U    |
| 53  | X     | 17    | U    |
| 53  | X     | 17(A) | G    |
| 53  | x     | 18    | G    |



|                | v     | 1 10           |      |  |
|----------------|-------|----------------|------|--|
| $\mathbf{Mol}$ | Chain | $\mathbf{Res}$ | Type |  |
| 53             | Х     | 19             | U    |  |
| 53             | Х     | 20             | А    |  |
| 53             | Х     | 21             | G    |  |
| 53             | Х     | 22             | А    |  |
| 53             | Х     | 23             | С    |  |
| 53             | Х     | 25             | С    |  |
| 53             | Х     | 26             | G    |  |
| 53             | Х     | 36             | G    |  |
| 53             | Х     | 41             | U    |  |
| 53             | Х     | 43             | G    |  |
| 53             | Х     | 44             | U    |  |
| 53             | Х     | 51             | G    |  |
| 53             | Х     | 52             | G    |  |
| 53             | Х     | 53             | G    |  |
| 53             | Х     | 56             | С    |  |
| 53             | Х     | 60             | U    |  |
| 53             | Х     | 61             | С    |  |
| 53             | Х     | 63             | С    |  |
| 53             | Х     | 70             | G    |  |
| 53             | Х     | 75             | С    |  |
| 53             | Х     | 76             | А    |  |

All (93) RNA pucker outliers are listed below:

| Mol | Chain  | Res | Type |
|-----|--------|-----|------|
| 1   | А      | 62  | С    |
| 1   | А      | 88  | G    |
| 1   | А      | 92  | G    |
| 1   | А      | 118 | А    |
| 1   | А      | 163 | U    |
| 1   | А      | 181 | G    |
| 1   | А      | 199 | А    |
| 1   | А      | 236 | А    |
| 1   | А      | 252 | С    |
| 1   | 1 A 34 |     | G    |
| 1   | А      | 410 | G    |
| 1   | А      | 411 | G    |
| 1   | А      | 441 | С    |
| 1   | А      | 455 | G    |
| 1   | А      | 458 | G    |
| 1   | А      | 459 | А    |
| 1   | А      | 482 | С    |



| Mol | Chain | Res  | Type |
|-----|-------|------|------|
| 1   | А     | 525  | А    |
| 1   | А     | 549  | А    |
| 1   | А     | 554  | U    |
| 1   | А     | 576  | G    |
| 1   | А     | 594  | С    |
| 1   | А     | 666  | G    |
| 1   | А     | 689  | A    |
| 1   | А     | 702  | A    |
| 1   | А     | 732  | А    |
| 1   | А     | 756  | U    |
| 1   | А     | 810  | G    |
| 1   | А     | 831  | U    |
| 1   | А     | 848  | G    |
| 1   | A     | 855  | G    |
| 1   | A     | 933  | С    |
| 1   | A     | 1028 | С    |
| 1   | А     | 1032 | С    |
| 1   | А     | 1036 | А    |
| 1   | А     | 1041 | С    |
| 1   | А     | 1172 | А    |
| 1   | А     | 1176 | U    |
| 1   | А     | 1187 | U    |
| 1   | А     | 1210 | А    |
| 1   | А     | 1226 | U    |
| 1   | А     | 1243 | А    |
| 1   | А     | 1250 | G    |
| 1   | А     | 1260 | А    |
| 1   | А     | 1266 | A    |
| 1   | А     | 1269 | A    |
| 1   | A     | 1294 | А    |
| 1   | A     | 1305 | A    |
| 1   | А     | 1325 | A    |
| 1   | A     | 1339 | A    |
| 1   | A     | 1351 | U    |
| 1   | A     | 1365 | U    |
| 1   | A     | 1448 | U    |
| 1   | А     | 1464 | А    |
| 1   | A     | 1507 | U    |
| 1   | A     | 1525 | G    |
| 1   | A     | 1529 | G    |
| 1   | A     | 1530 | G    |
| 1   | А     | 1535 | U    |



| Mol | Chain | Res  | Type |
|-----|-------|------|------|
| 1   | А     | 1543 | U    |
| 1   | А     | 1565 | U    |
| 1   | А     | 1570 | U    |
| 1   | А     | 1631 | А    |
| 1   | А     | 1671 | G    |
| 1   | А     | 1726 | G    |
| 1   | А     | 1751 | U    |
| 1   | А     | 1784 | А    |
| 1   | А     | 1813 | А    |
| 1   | А     | 1828 | G    |
| 1   | А     | 1844 | А    |
| 1   | А     | 1882 | А    |
| 1   | А     | 1883 | А    |
| 1   | А     | 1886 | G    |
| 1   | А     | 1991 | С    |
| 1   | А     | 2009 | G    |
| 1   | А     | 2127 | U    |
| 1   | А     | 2139 | G    |
| 1   | А     | 2155 | А    |
| 1   | А     | 2254 | А    |
| 1   | А     | 2295 | А    |
| 1   | А     | 2316 | А    |
| 1   | А     | 2356 | А    |
| 1   | А     | 2454 | А    |
| 1   | А     | 2456 | С    |
| 1   | А     | 2468 | А    |
| 1   | А     | 2531 | G    |
| 1   | А     | 2630 | С    |
| 1   | А     | 2710 | С    |
| 1   | А     | 2805 | А    |
| 1   | А     | 2904 | А    |
| 2   | В     | 37   | А    |
| 2   | В     | 48   | G    |
| 2   | В     | 49   | G    |

Continued from previous page...

## 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)

3 ligands are modelled in this entry.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the Chemical Component Dictionary. The Link column lists molecule types, if any, to which the group is linked. The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with |Z| > 2 is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

| Mal | I Tuno Chain Bog |       | Tiple | Bond lengths |          |      | Bond angles |          |      |          |
|-----|------------------|-------|-------|--------------|----------|------|-------------|----------|------|----------|
|     | туре             | Unain | nes   |              | Counts   | RMSZ | # Z  > 2    | Counts   | RMSZ | # Z >2   |
| 54  | TEL              | А     | 3001  | -            | 59,62,62 | 1.29 | 4 (6%)      | 77,92,92 | 1.97 | 13 (16%) |
| 55  | ATP              | V     | 900   | 20           | 26,33,33 | 0.91 | 1 (3%)      | 31,52,52 | 1.66 | 6 (19%)  |
| 55  | ATP              | V     | 901   | -            | 26,33,33 | 0.98 | 1 (3%)      | 31,52,52 | 1.83 | 4 (12%)  |

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral centers analysed, the number of these observed in the model and the number defined in the Chemical Component Dictionary. Similar counts are reported in the Torsion and Rings columns. '-' means no outliers of that kind were identified.

| Mol | Type | Chain | Res  | Link | Chirals   | Torsions      | Rings   |
|-----|------|-------|------|------|-----------|---------------|---------|
| 54  | TEL  | А     | 3001 | -    | 1/1/19/19 | 14/73/108/108 | 0/4/5/5 |
| 55  | ATP  | V     | 900  | 20   | -         | 3/18/38/38    | 0/3/3/3 |
| 55  | ATP  | V     | 901  | -    | -         | 4/18/38/38    | 0/3/3/3 |

All (6) bond length outliers are listed below:

| Mol | Chain | Res  | Type | Atoms   | Z     | Observed(Å) | Ideal(Å) |
|-----|-------|------|------|---------|-------|-------------|----------|
| 54  | А     | 3001 | TEL  | O5-C10  | 5.85  | 1.45        | 1.35     |
| 54  | А     | 3001 | TEL  | O9-C15  | 4.91  | 1.45        | 1.34     |
| 54  | А     | 3001 | TEL  | C36-N31 | -2.79 | 1.34        | 1.38     |
| 54  | А     | 3001 | TEL  | O5-C2   | -2.74 | 1.43        | 1.47     |
| 55  | V     | 901  | ATP  | C5-C4   | 2.38  | 1.47        | 1.40     |
| 55  | V     | 900  | ATP  | C5-C4   | 2.13  | 1.46        | 1.40     |

All (23) bond angle outliers are listed below:



| Mol | Chain | Res  | Type | Atoms       | Ζ     | $Observed(^{o})$ | $Ideal(^{o})$ |
|-----|-------|------|------|-------------|-------|------------------|---------------|
| 54  | А     | 3001 | TEL  | O9-C15-C21  | 9.27  | 120.30           | 110.88        |
| 54  | А     | 3001 | TEL  | C11-N6-C10  | 6.88  | 130.94           | 122.25        |
| 55  | V     | 901  | ATP  | PB-O3B-PG   | -6.13 | 111.78           | 132.83        |
| 54  | А     | 3001 | TEL  | C17-C11-N6  | -5.42 | 104.94           | 113.31        |
| 55  | V     | 901  | ATP  | PA-O3A-PB   | -5.15 | 115.17           | 132.83        |
| 55  | V     | 900  | ATP  | PA-O3A-PB   | -4.69 | 116.72           | 132.83        |
| 54  | А     | 3001 | TEL  | C1-C2-C3    | -4.60 | 111.15           | 116.69        |
| 54  | А     | 3001 | TEL  | C4-O9-C15   | -3.65 | 111.69           | 118.18        |
| 55  | V     | 900  | ATP  | N3-C2-N1    | -3.41 | 123.35           | 128.68        |
| 54  | А     | 3001 | TEL  | O20-C15-C21 | -3.21 | 120.55           | 124.77        |
| 55  | V     | 901  | ATP  | N3-C2-N1    | -3.19 | 123.69           | 128.68        |
| 54  | А     | 3001 | TEL  | C8-C4-C2    | -3.10 | 110.96           | 115.23        |
| 54  | А     | 3001 | TEL  | C28-C24-C19 | -2.97 | 111.07           | 116.11        |
| 55  | V     | 900  | ATP  | PB-O3B-PG   | -2.97 | 122.65           | 132.83        |
| 55  | V     | 900  | ATP  | C4-C5-N7    | -2.75 | 106.54           | 109.40        |
| 54  | А     | 3001 | TEL  | O9-C15-O20  | -2.56 | 119.15           | 123.94        |
| 54  | А     | 3001 | TEL  | C56-N52-C47 | 2.50  | 121.17           | 116.85        |
| 54  | А     | 3001 | TEL  | C42-O39-C34 | -2.39 | 112.10           | 116.25        |
| 54  | А     | 3001 | TEL  | C24-C19-C13 | -2.29 | 109.38           | 113.32        |
| 55  | V     | 901  | ATP  | C4-C5-N7    | -2.26 | 107.05           | 109.40        |
| 54  | А     | 3001 | TEL  | C54-C49-N53 | -2.19 | 109.48           | 115.67        |
| 55  | V     | 900  | ATP  | O2A-PA-O1A  | 2.07  | 122.50           | 112.24        |
| 55  | V     | 900  | ATP  | O3G-PG-O2G  | 2.06  | 115.51           | 107.64        |

All (1) chirality outliers are listed below:

| Mol | Chain | Res  | Type | Atom |
|-----|-------|------|------|------|
| 54  | А     | 3001 | TEL  | C21  |

All (21) torsion outliers are listed below:

| Mol | Chain | Res  | Type | Atoms           |
|-----|-------|------|------|-----------------|
| 54  | А     | 3001 | TEL  | C15-C21-C26-O29 |
| 54  | А     | 3001 | TEL  | C15-C21-C26-C30 |
| 55  | V     | 900  | ATP  | C5'-O5'-PA-O1A  |
| 55  | V     | 901  | ATP  | C5'-O5'-PA-O1A  |
| 54  | А     | 3001 | TEL  | C21-C15-O9-C4   |
| 54  | А     | 3001 | TEL  | O20-C15-O9-C4   |
| 54  | А     | 3001 | TEL  | O9-C4-C8-C14    |
| 54  | А     | 3001 | TEL  | N6-C3-C7-C12    |
| 54  | А     | 3001 | TEL  | C17-C22-C27-N31 |
| 54  | А     | 3001 | TEL  | C17-C11-N6-C10  |
| 54  | А     | 3001 | TEL  | O20-C15-C21-C25 |



|     |       | 1              | 1 0  |                 |
|-----|-------|----------------|------|-----------------|
| Mol | Chain | $\mathbf{Res}$ | Type | Atoms           |
| 54  | А     | 3001           | TEL  | O9-C15-C21-C25  |
| 55  | V     | 900            | ATP  | C5'-O5'-PA-O3A  |
| 55  | V     | 901            | ATP  | C5'-O5'-PA-O3A  |
| 55  | V     | 900            | ATP  | C5'-O5'-PA-O2A  |
| 55  | V     | 901            | ATP  | C5'-O5'-PA-O2A  |
| 54  | А     | 3001           | TEL  | C35-C30-C34-C28 |
| 54  | А     | 3001           | TEL  | C2-C4-C8-C14    |
| 55  | V     | 901            | ATP  | PB-O3A-PA-O1A   |
| 54  | А     | 3001           | TEL  | O20-C15-C21-C26 |
| 54  | А     | 3001           | TEL  | C26-C30-C34-C28 |

There are no ring outliers.

No monomer is involved in short contacts.

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










## 5.7 Other polymers (i)

There are no such residues in this entry.

## 5.8 Polymer linkage issues (i)

The following chains have linkage breaks:

| Mol | Chain | Number of breaks |
|-----|-------|------------------|
| 1   | А     | 5                |
| 53  | Х     | 1                |

All chain breaks are listed below:

| Model | Chain | Residue-1 | Atom-1 | Residue-2 | Atom-2 | Distance (Å) |
|-------|-------|-----------|--------|-----------|--------|--------------|
| 1     | Х     | 44:U      | O3'    | 47:U      | Р      | 14.81        |
| 1     | A     | 182:C     | O3'    | 183:A     | Р      | 6.43         |
| 1     | А     | 1449:C    | O3'    | 1450:C    | Р      | 4.34         |
| 1     | A     | 1451:U    | O3'    | 1452:C    | Р      | 3.29         |

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| Continueu from previous page |       |           |        |           |        |              |
|------------------------------|-------|-----------|--------|-----------|--------|--------------|
| Model                        | Chain | Residue-1 | Atom-1 | Residue-2 | Atom-2 | Distance (Å) |
| 1                            | А     | 1452:C    | O3'    | 1453:A    | Р      | 3.25         |
| 1                            | A     | 183:A     | O3'    | 184:G     | Р      | 3.12         |

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### Map visualisation (i) 6

This section contains visualisations of the EMDB entry EMD-0177. 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.

#### Orthogonal projections (i) 6.1

#### 6.1.1Primary map



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

#### Central slices (i) 6.2

#### 6.2.1Primary map



X Index: 180



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: 177

Y Index: 199

Z Index: 189

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 0.11. 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  $793 \text{ nm}^3$ ; this corresponds to an approximate mass of 716 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 0.286  $\mathrm{\AA^{-1}}$ 



# 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-0177 and PDB model 6HA8. Per-residue inclusion information can be found in section 3 on page 16.

## 9.1 Map-model overlay (i)



The images above show the 3D surface view of the map at the recommended contour level 0.11 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 Q-score mapped to coordinate model (i)



The images above show the model with each residue coloured according its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions at which atoms can be resolved. Low Q-score values may therefore be expected for many entries.

### 9.3 Atom inclusion mapped to coordinate model (i)



The images above show the model with each residue coloured according to its atom inclusion. This shows to what extent they are inside the map at the recommended contour level (0.11).



## 9.4 Atom inclusion (i)



At the recommended contour level, 71% of all backbone atoms, 66% of all non-hydrogen atoms, are inside the map.



1.0

0.0 <0.0

## 9.5 Map-model fit summary (i)

The table lists the average atom inclusion at the recommended contour level (0.11) and Q-score for the entire model and for each chain.

| $\mathbf{Chain}$ | Atom inclusion | $\mathbf{Q}	extsf{-score}$ |
|------------------|----------------|----------------------------|
| All              | 0.6582         | 0.3890                     |
| 0                | 0.7191         | 0.4870                     |
| 1                | 0.6744         | 0.4410                     |
| 2                | 0.7362         | 0.5030                     |
| 3                | 0.7255         | 0.5080                     |
| 4                | 0.6138         | 0.4620                     |
| 6                | 0.2945         | 0.2640                     |
| 7                | 0.6667         | 0.4050                     |
| 8                | 0.0760         | 0.1430                     |
| А                | 0.7959         | 0.4370                     |
| В                | 0.7847         | 0.4020                     |
| С                | 0.6757         | 0.4800                     |
| D                | 0.6958         | 0.4810                     |
| Ε                | 0.6819         | 0.4500                     |
| F                | 0.4591         | 0.3260                     |
| G                | 0.4146         | 0.3170                     |
| J                | 0.7095         | 0.4720                     |
| Κ                | 0.6455         | 0.4620                     |
| L                | 0.6629         | 0.4490                     |
| М                | 0.6353         | 0.4500                     |
| Ν                | 0.6838         | 0.4640                     |
| О                | 0.5468         | 0.3630                     |
| Р                | 0.6325         | 0.4500                     |
| Q                | 0.7074         | 0.4500                     |
| R                | 0.6894         | 0.4530                     |
| S                | 0.7033         | 0.4810                     |
| Т                | 0.6136         | 0.4430                     |
| U                | 0.6146         | 0.4040                     |
| V                | 0.4241         | 0.3890                     |
| W                | 0.6486         | 0.4500                     |
| Х                | 0.5231         | 0.4500                     |
| Y                | 0.5875         | 0.3610                     |
| Z                | 0.6360         | 0.4400                     |
| a                | 0.6450         | 0.3360                     |
| b                | 0.1212         | 0.1970                     |

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| Chain | Atom inclusion | Q-score |
|-------|----------------|---------|
| с     | 0.3994         | 0.3340  |
| d     | 0.2454         | 0.2270  |
| е     | 0.4966         | 0.3750  |
| f     | 0.2840         | 0.2490  |
| g     | 0.4504         | 0.3240  |
| h     | 0.3958         | 0.2870  |
| i     | 0.4339         | 0.3220  |
| j     | 0.3405         | 0.3210  |
| k     | 0.3794         | 0.2970  |
| 1     | 0.3722         | 0.3080  |
| m     | 0.3810         | 0.2880  |
| n     | 0.3812         | 0.3480  |
| 0     | 0.3852         | 0.2490  |
| р     | 0.3260         | 0.2690  |
| q     | 0.2853         | 0.2390  |
| r     | 0.3406         | 0.2730  |
| S     | 0.3457         | 0.2600  |
| t     | 0.3714         | 0.2630  |
| X     | 0.4336         | 0.3210  |

