



Full wwPDB/EMDatabank EM Map/Model Validation Report ⓘ

Jul 24, 2017 – 05:38 AM EDT

PDB ID : 5IT9
EMDB ID: : EMD-8124
Title : Structure of the yeast *Kluyveromyces lactis* small ribosomal subunit in complex with the cricket paralysis virus IRES.
Authors : Murray, J.; Savva, C.G.; Shin, B.S.; Dever, T.E.; Ramakrishnan, V.; Fernandez, I.S.
Deposited on : unknown
Resolution : 3.80 Å(reported)

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

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

MolProbity : 4.02b-467
Percentile statistics : 20161228.v01 (using entries in the PDB archive December 28th 2016)
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et. al. (1996)
Validation Pipeline (wwPDB-VP) : rb-20029824

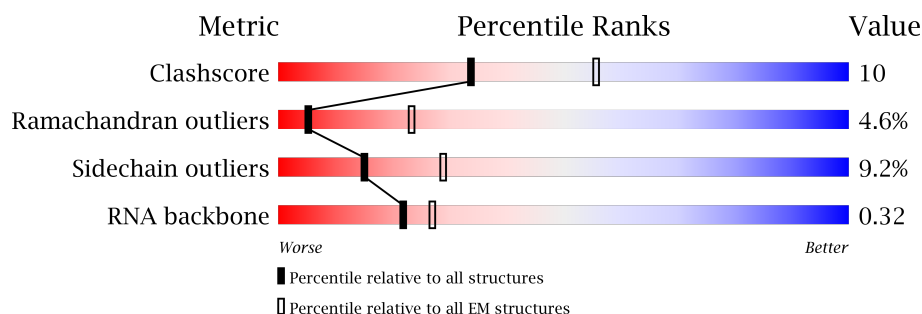
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

ELECTRON MICROSCOPY

The reported resolution of this entry is 3.80 Å.

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
























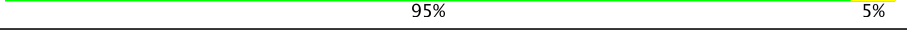



| Metric | Whole archive (#Entries) | EM structures (#Entries) |
|-----------------------|-----------------------------|-----------------------------|
| Clashscore | 125131 | 1336 |
| Ramachandran outliers | 121729 | 1120 |
| Sidechain outliers | 121581 | 1026 |
| RNA backbone | 3398 | 335 |

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

| Mol | Chain | Length | Quality of chain |
|-----|-------|--------|------------------|
| 1 | A | 206 | 76% 22% . |
| 2 | B | 214 | 89% 10% . |
| 3 | C | 217 | 83% 15% . |
| 4 | D | 223 | 87% 13% |
| 5 | E | 260 | 88% 11% . |
| 6 | F | 206 | 78% 20% . |
| 7 | G | 226 | 80% 16% . . |
| 8 | H | 184 | 82% 17% . |

Continued on next page...

Continued from previous page...

| Mol | Chain | Length | Quality of chain |
|-----|-------|--------|--|
| 9 | I | 200 |  |
| 10 | J | 182 |  |
| 11 | K | 96 |  |
| 12 | L | 155 |  |
| 13 | M | 122 |  |
| 14 | N | 150 |  |
| 15 | O | 127 |  |
| 16 | P | 123 |  |
| 17 | Q | 141 |  |
| 18 | R | 129 |  |
| 19 | S | 145 |  |
| 20 | T | 143 |  |
| 21 | U | 106 |  |
| 22 | V | 87 |  |
| 23 | W | 129 |  |
| 24 | X | 145 |  |
| 25 | Y | 134 |  |
| 26 | Z | 70 |  |
| 27 | a | 100 |  |
| 28 | b | 82 |  |
| 29 | c | 63 |  |
| 30 | d | 53 |  |
| 31 | e | 55 |  |
| 32 | f | 69 |  |
| 33 | g | 324 |  |

Continued on next page...

Continued from previous page...

| Mol | Chain | Length | Quality of chain |
|-----|-------|--------|---|
| 34 | 2 | 1780 | <div><div></div><div>36%</div><div>47%</div><div>16%</div><div></div></div> |
| 35 | i | 192 | <div><div></div><div>44%</div><div>55%</div><div></div></div> |

2 Entry composition

There are 37 unique types of molecules in this entry. The entry contains 80144 atoms, of which 0 are hydrogens and 0 are deuteriums.

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

- Molecule 1 is a protein called Ribosomal protein uS2.

| Mol | Chain | Residues | Atoms | | | | | AltConf | Trace |
|-----|-------|----------|-------|------|-----|-----|---|---------|-------|
| 1 | A | 206 | Total | C | N | O | S | 0 | 0 |
| | | | 1616 | 1035 | 285 | 294 | 2 | | |

- Molecule 2 is a protein called Ribosomal protein eS1.

| Mol | Chain | Residues | Atoms | | | | | AltConf | Trace |
|-----|-------|----------|-------|------|-----|-----|---|---------|-------|
| 2 | B | 214 | Total | C | N | O | S | 0 | 0 |
| | | | 1722 | 1089 | 313 | 317 | 3 | | |

- Molecule 3 is a protein called Ribosomal protein uS5.

| Mol | Chain | Residues | Atoms | | | | | AltConf | Trace |
|-----|-------|----------|-------|------|-----|-----|---|---------|-------|
| 3 | C | 217 | Total | C | N | O | S | 0 | 0 |
| | | | 1629 | 1041 | 287 | 297 | 4 | | |

- Molecule 4 is a protein called Ribosomal protein uS3.

| Mol | Chain | Residues | Atoms | | | | | AltConf | Trace |
|-----|-------|----------|-------|------|-----|-----|---|---------|-------|
| 4 | D | 223 | Total | C | N | O | S | 0 | 0 |
| | | | 1744 | 1108 | 313 | 318 | 5 | | |

- Molecule 5 is a protein called Ribosomal protein eS4.

| Mol | Chain | Residues | Atoms | | | | | AltConf | Trace |
|-----|-------|----------|-------|------|-----|-----|---|---------|-------|
| 5 | E | 260 | Total | C | N | O | S | 0 | 0 |
| | | | 2078 | 1322 | 393 | 359 | 4 | | |

- Molecule 6 is a protein called Ribosomal protein uS7.

| Mol | Chain | Residues | Atoms | | | | | AltConf | Trace |
|-----|-------|----------|-------|------|-----|-----|---|---------|-------|
| 6 | F | 206 | Total | C | N | O | S | 0 | 0 |
| | | | 1609 | 1008 | 298 | 300 | 3 | | |

- Molecule 7 is a protein called Ribosomal protein eS6.

| Mol | Chain | Residues | Atoms | | | | | AltConf | Trace |
|-----|-------|----------|-------|------|-----|-----|---|---------|-------|
| 7 | G | 226 | Total | C | N | O | S | 0 | 0 |
| | | | 1812 | 1134 | 348 | 326 | 4 | | |

- Molecule 8 is a protein called Ribosomal protein eS7.

| Mol | Chain | Residues | Atoms | | | | | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|-------|
| 8 | H | 184 | Total | C | N | O | S | 0 | 0 |
| | | | 1483 | 950 | 270 | 263 | | | |

- Molecule 9 is a protein called Ribosomal protein eS8.

| Mol | Chain | Residues | Atoms | | | | | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|-------|
| 9 | I | 188 | Total | C | N | O | S | 0 | 0 |
| | | | 1493 | 926 | 301 | 265 | 1 | | |

- Molecule 10 is a protein called Ribosomal protein uS4.

| Mol | Chain | Residues | Atoms | | | | | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|-------|
| 10 | J | 182 | Total | C | N | O | S | 0 | 0 |
| | | | 1471 | 929 | 287 | 254 | 1 | | |

- Molecule 11 is a protein called Ribosomal protein eS10.

| Mol | Chain | Residues | Atoms | | | | | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|-------|
| 11 | K | 96 | Total | C | N | O | S | 0 | 0 |
| | | | 809 | 533 | 129 | 146 | 1 | | |

- Molecule 12 is a protein called Ribosomal protein uS17.

| Mol | Chain | Residues | Atoms | | | | | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|-------|
| 12 | L | 155 | Total | C | N | O | S | 0 | 0 |
| | | | 1248 | 798 | 237 | 210 | 3 | | |

- Molecule 13 is a protein called Ribosomal protein eS12.

| Mol | Chain | Residues | Atoms | | | | | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|-------|
| 13 | M | 122 | Total | C | N | O | S | 0 | 0 |
| | | | 922 | 575 | 167 | 180 | | | |

- Molecule 14 is a protein called Ribosomal protein uS15.

| Mol | Chain | Residues | Atoms | | | | | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|-------|
| 14 | N | 150 | Total | C | N | O | S | 0 | 0 |
| | | | 1187 | 756 | 223 | 206 | 2 | | |

- Molecule 15 is a protein called Ribosomal protein uS14.

| Mol | Chain | Residues | Atoms | | | | | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|-------|
| 15 | O | 127 | Total | C | N | O | S | 0 | 0 |
| | | | 942 | 578 | 188 | 173 | 3 | | |

- Molecule 16 is a protein called Ribosomal protein uS19.

| Mol | Chain | Residues | Atoms | | | | | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|-------|
| 16 | P | 123 | Total | C | N | O | S | 0 | 0 |
| | | | 980 | 628 | 179 | 168 | 5 | | |

- Molecule 17 is a protein called Ribosomal protein uS9.

| Mol | Chain | Residues | Atoms | | | | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---------|-------|
| 17 | Q | 141 | Total | C | N | O | 0 | 0 |
| | | | 1105 | 709 | 204 | 192 | | |

- Molecule 18 is a protein called Ribosomal protein eS17.

| Mol | Chain | Residues | Atoms | | | | | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|-------|
| 18 | R | 129 | Total | C | N | O | S | 0 | 0 |
| | | | 1031 | 641 | 193 | 194 | 3 | | |

- Molecule 19 is a protein called Ribosomal protein uS13.

| Mol | Chain | Residues | Atoms | | | | | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|-------|
| 19 | S | 145 | Total | C | N | O | S | 0 | 0 |
| | | | 1193 | 741 | 240 | 210 | 2 | | |

- Molecule 20 is a protein called Ribosomal protein eS19.

| Mol | Chain | Residues | Atoms | | | | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---------|-------|
| 20 | T | 143 | Total | C | N | O | 0 | 0 |
| | | | 1110 | 693 | 210 | 207 | | |

- Molecule 21 is a protein called Ribosomal protein uS10.

| Mol | Chain | Residues | Atoms | | | | | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|-------|
| 21 | U | 106 | Total | C | N | O | S | 0 | 0 |
| | | | 845 | 540 | 152 | 152 | 1 | | |

- Molecule 22 is a protein called Ribosomal protein eS21.

| Mol | Chain | Residues | Atoms | | | | | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|-------|
| 22 | V | 87 | Total | C | N | O | S | 0 | 0 |
| | | | 687 | 424 | 126 | 135 | 2 | | |

- Molecule 23 is a protein called Ribosomal protein uS8.

| Mol | Chain | Residues | Atoms | | | | | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|-------|
| 23 | W | 129 | Total | C | N | O | S | 0 | 0 |
| | | | 1021 | 651 | 187 | 180 | 3 | | |

- Molecule 24 is a protein called Ribosomal protein uS21.

| Mol | Chain | Residues | Atoms | | | | | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|-------|
| 24 | X | 145 | Total | C | N | O | S | 0 | 0 |
| | | | 1127 | 713 | 219 | 192 | 3 | | |

- Molecule 25 is a protein called Ribosomal protein eS24.

| Mol | Chain | Residues | Atoms | | | | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---------|-------|
| 25 | Y | 134 | Total | C | N | O | 0 | 0 |
| | | | 1061 | 665 | 207 | 189 | | |

- Molecule 26 is a protein called Ribosomal protein eS25.

| Mol | Chain | Residues | Atoms | | | | | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|----|---|---------|-------|
| 26 | Z | 70 | Total | C | N | O | S | 0 | 0 |
| | | | 558 | 355 | 104 | 98 | 1 | | |

- Molecule 27 is a protein called Ribosomal protein eS26.

| Mol | Chain | Residues | Atoms | | | | | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|-------|
| 27 | a | 100 | Total | C | N | O | S | 0 | 0 |
| | | | 798 | 491 | 170 | 131 | 6 | | |

- Molecule 28 is a protein called Ribosomal protein eS27.

| Mol | Chain | Residues | Atoms | | | | | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|-------|
| 28 | b | 82 | Total | C | N | O | S | 0 | 0 |
| | | | 617 | 384 | 113 | 114 | 6 | | |

- Molecule 29 is a protein called Ribosomal protein eS28.

| Mol | Chain | Residues | Atoms | | | | | AltConf | Trace |
|-----|-------|----------|-------|-----|----|----|---|---------|-------|
| 29 | c | 63 | Total | C | N | O | S | 0 | 0 |
| | | | 494 | 305 | 98 | 90 | 1 | | |

- Molecule 30 is a protein called Ribosomal protein eS29.

| Mol | Chain | Residues | Atoms | | | | | AltConf | Trace |
|-----|-------|----------|-------|-----|----|----|---|---------|-------|
| 30 | d | 53 | Total | C | N | O | S | 0 | 0 |
| | | | 446 | 280 | 89 | 76 | 1 | | |

- Molecule 31 is a protein called Ribosomal protein eS30.

| Mol | Chain | Residues | Atoms | | | | | AltConf | Trace |
|-----|-------|----------|-------|-----|----|----|---|---------|-------|
| 31 | e | 55 | Total | C | N | O | S | 0 | 0 |
| | | | 443 | 276 | 90 | 76 | 1 | | |

- Molecule 32 is a protein called Ribosomal protein eS31.

| Mol | Chain | Residues | Atoms | | | | | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|----|---|---------|-------|
| 32 | f | 69 | Total | C | N | O | S | 0 | 0 |
| | | | 549 | 352 | 102 | 91 | 4 | | |

- Molecule 33 is a protein called Ribosomal protein RACK1.

| Mol | Chain | Residues | Atoms | | | | | AltConf | Trace |
|-----|-------|----------|-------|------|-----|-----|---|---------|-------|
| 33 | g | 318 | Total | C | N | O | S | 0 | 0 |
| | | | 2466 | 1561 | 430 | 470 | 5 | | |

- Molecule 34 is a RNA chain called 18S ribosomal RNA.

| Mol | Chain | Residues | Atoms | | | | | AltConf | Trace |
|-----|-------|----------|-------|-------|------|-------|------|---------|-------|
| 34 | 2 | 1780 | Total | C | N | O | P | 0 | 0 |
| | | | 37797 | 16892 | 6658 | 12467 | 1780 | | |

- Molecule 35 is a RNA chain called Cricket paralysis virus IRES RNA.

| Mol | Chain | Residues | Atoms | | | | | AltConf | Trace |
|-----|-------|----------|-------|------|-----|------|-----|---------|-------|
| 35 | i | 192 | Total | C | N | O | P | 0 | 0 |
| | | | 3968 | 1774 | 669 | 1333 | 192 | | |

There is a discrepancy between the modelled and reference sequences:

| Chain | Residue | Modelled | Actual | Comment | Reference |
|-------|---------|----------|--------|----------|------------|
| i | 6176 | C | U | conflict | GB 8895506 |

- Molecule 36 is MAGNESIUM ION (three-letter code: MG) (formula: Mg).

| Mol | Chain | Residues | Atoms | | AltConf |
|-----|-------|----------|-------|----|---------|
| 36 | X | 1 | Total | Mg | 0 |
| | | | 1 | 1 | |
| 36 | G | 1 | Total | Mg | 0 |
| | | | 1 | 1 | |
| 36 | 2 | 76 | Total | Mg | 0 |
| | | | 76 | 76 | |
| 36 | T | 1 | Total | Mg | 0 |
| | | | 1 | 1 | |
| 36 | N | 1 | Total | Mg | 0 |
| | | | 1 | 1 | |

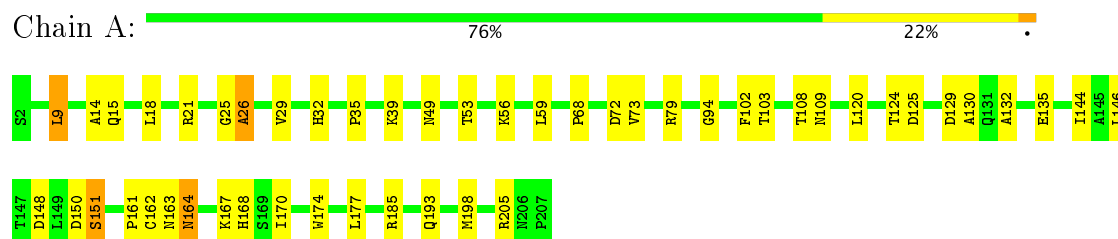
- Molecule 37 is ZINC ION (three-letter code: ZN) (formula: Zn).

| Mol | Chain | Residues | Atoms | | AltConf |
|-----|-------|----------|-------|----|---------|
| 37 | b | 1 | Total | Zn | 0 |
| | | | 1 | 1 | |
| 37 | a | 1 | Total | Zn | 0 |
| | | | 1 | 1 | |
| 37 | f | 1 | Total | Zn | 0 |
| | | | 1 | 1 | |

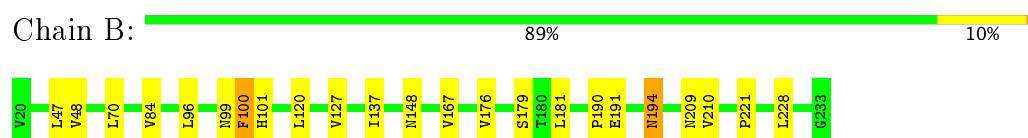
3 Residue-property plots

These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry. Residues are color-coded according to the number of geometric quality criteria for which they contain at least one outlier: green = 0, yellow = 1, orange = 2 and red = 3 or more. Stretches of 2 or more consecutive residues without any outlier are shown as a green connector. Residues present in the sample, but not in the model, are shown in grey.

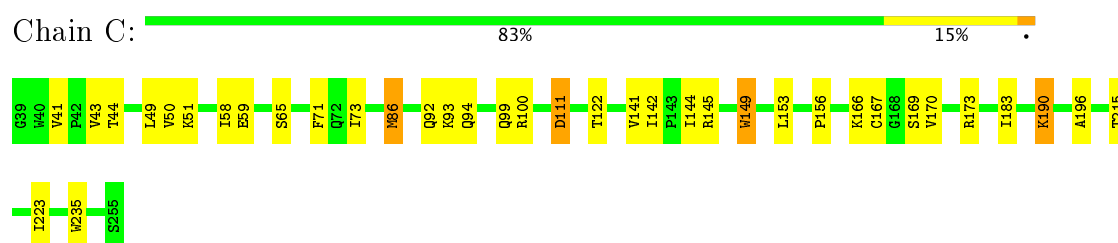
- Molecule 1: Ribosomal protein uS2



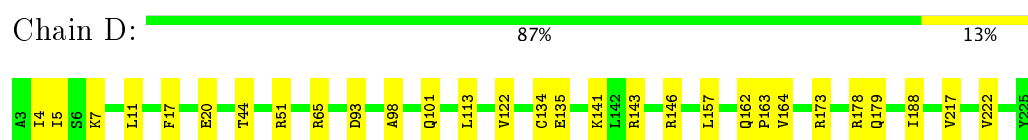
- Molecule 2: Ribosomal protein eS1



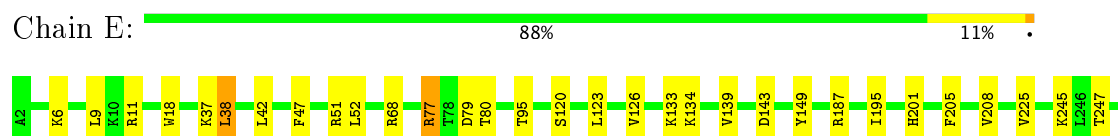
- Molecule 3: Ribosomal protein uS5



- Molecule 4: Ribosomal protein uS3


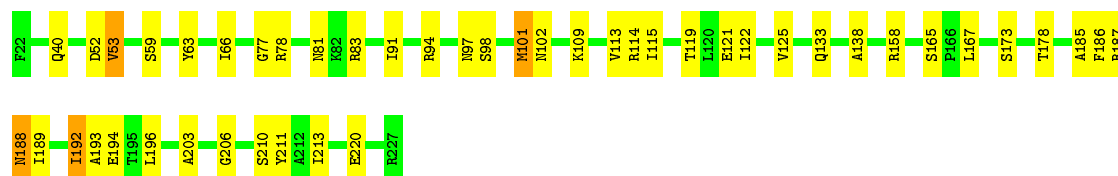


- Molecule 5: Ribosomal protein eS4


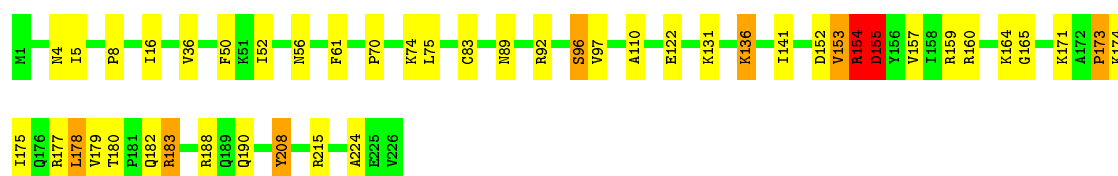


L261


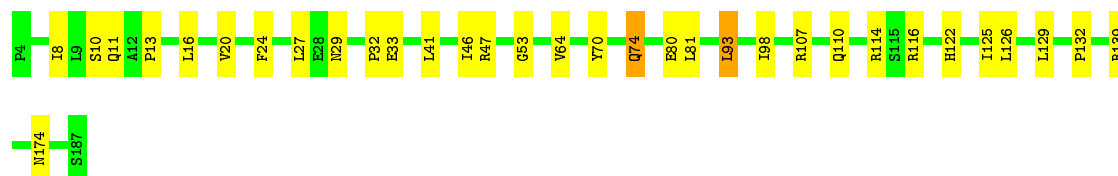
- Molecule 6: Ribosomal protein uS7

Chain F:  78% 20%

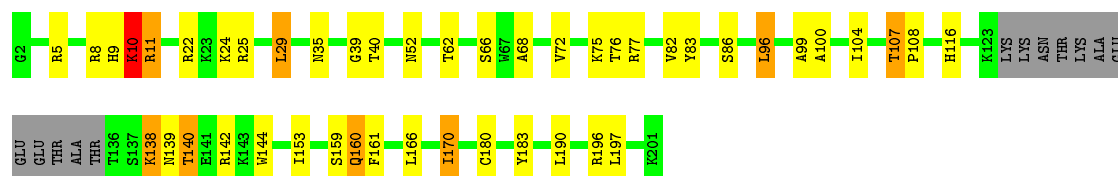
- Molecule 7: Ribosomal protein eS6

Chain G:  80% 16%

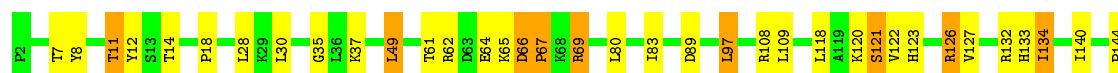
- Molecule 8: Ribosomal protein eS7

Chain H:  82% 17%

- Molecule 9: Ribosomal protein eS8

Chain I:  71% 19% 6%

- Molecule 10: Ribosomal protein uS4

Chain J:  73% 19% 8%



- Molecule 11: Ribosomal protein eS10

Chain K: 80% 20%



- Molecule 12: Ribosomal protein uS17

Chain L: 88% 10%



- Molecule 13: Ribosomal protein eS12

Chain M: 82% 16%



- Molecule 14: Ribosomal protein uS15

Chain N: 86% 13%



- Molecule 15: Ribosomal protein uS14

Chain O: 86% 13%



- Molecule 16: Ribosomal protein uS19

Chain P: 77% 19%

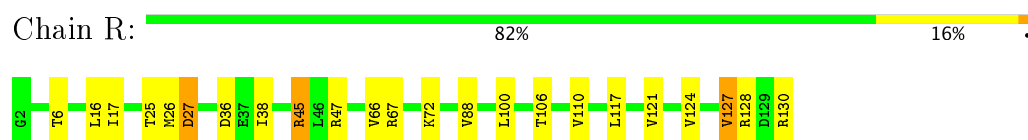


- Molecule 17: Ribosomal protein uS9

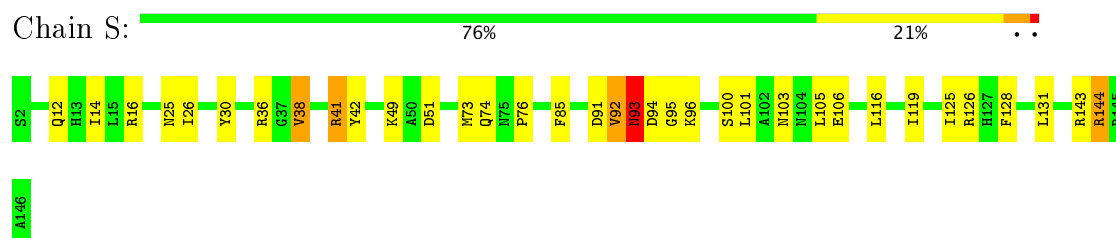
Chain Q: 84% 13%



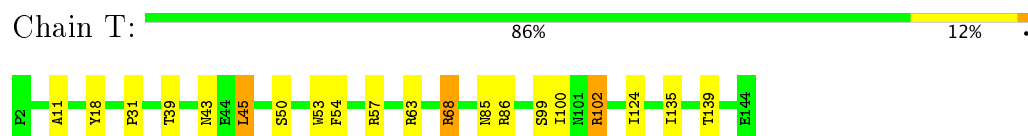
- Molecule 18: Ribosomal protein eS17



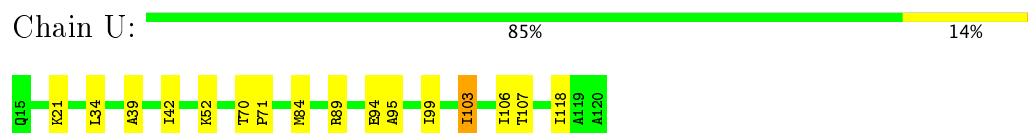
- Molecule 19: Ribosomal protein uS13



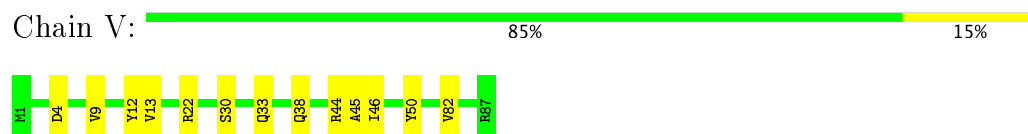
- Molecule 20: Ribosomal protein eS19



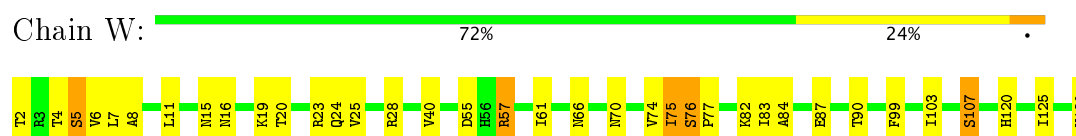
- Molecule 21: Ribosomal protein uS10



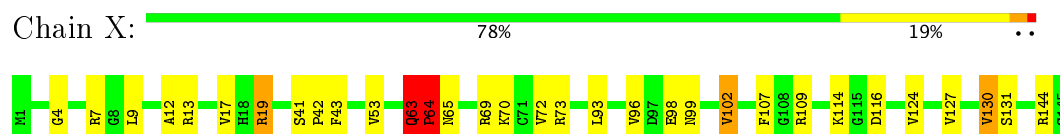
- Molecule 22: Ribosomal protein eS21



- Molecule 23: Ribosomal protein uS8

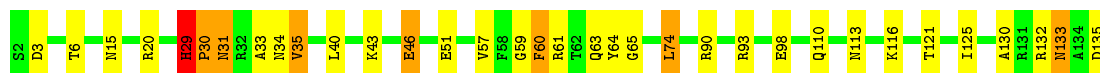


- Molecule 24: Ribosomal protein uS21



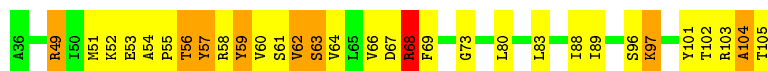
- Molecule 25: Ribosomal protein eS24

Chain Y:  75% 19% 5% .




- Molecule 26: Ribosomal protein eS25

Chain Z:  56% 31% 11% .



- Molecule 27: Ribosomal protein eS26

Chain a:  80% 16% .



- Molecule 28: Ribosomal protein eS27

Chain b:  90% 10%



- Molecule 29: Ribosomal protein eS28

Chain c:  95% 5%




- Molecule 30: Ribosomal protein eS29

Chain d:  92% 8%




- Molecule 31: Ribosomal protein eS30

Chain e:  87% 13%



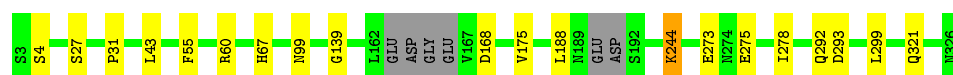
- Molecule 32: Ribosomal protein eS31

Chain f:  80% 17% .



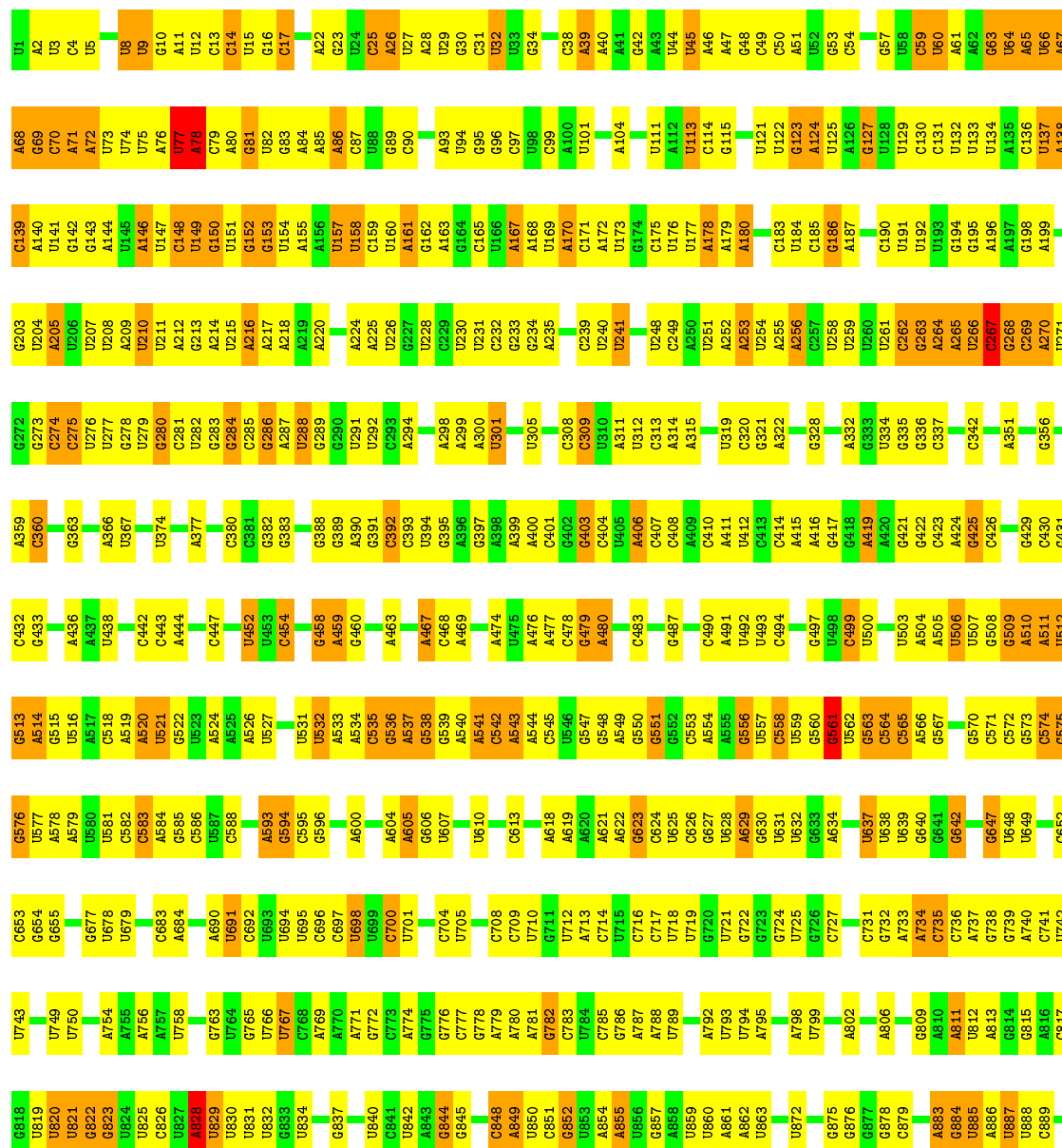
• Molecule 33: Ribosomal protein RACK1

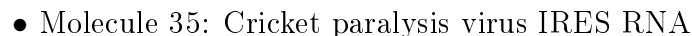
Chain g:  92% 6% .



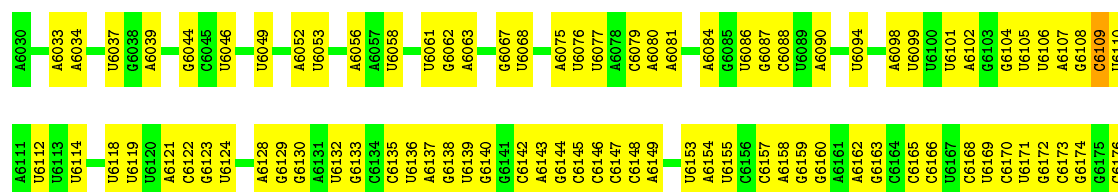
• Molecule 34: 18S ribosomal RNA

Chain 2:  36% 47% 16% .





| Response | Percentage |
|--|------------|
| U.S. should take more action to address climate change | 44% |
| U.S. should not take more action to address climate change | 55% |



| | | | | | | | | | | | | | | | | | | | | | | | | | |
|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|
| U6177 | U6178 | U6179 | U6180 | U6181 | A6182 | G6183 | A6184 | U6185 | U6186 | A6187 | G6192 | A6197 | A6198 | A6199 | A6200 | C6201 | C6202 | U6210 | U6211 | U6212 | A6213 | C6218 | U6219 | A6220 | C6221 |
|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|

4 Experimental information

| Property | Value | Source |
|--------------------------------------|-------------------------|-----------|
| Reconstruction method | SINGLE PARTICLE | Depositor |
| Imposed symmetry | POINT, Not provided | Depositor |
| Number of particles used | 54481 | Depositor |
| Resolution determination method | FSC 0.143 CUT-OFF | Depositor |
| CTF correction method | PHASE FLIPPING ONLY | Depositor |
| Microscope | FEI TITAN KRIOS | Depositor |
| Voltage (kV) | 300 | Depositor |
| Electron dose ($e^-/\text{\AA}^2$) | 25 | Depositor |
| Minimum defocus (nm) | Not provided | Depositor |
| Maximum defocus (nm) | Not provided | Depositor |
| Magnification | Not provided | Depositor |
| Image detector | FEI FALCON II (4k x 4k) | Depositor |

5 Model quality ⓘ

5.1 Standard geometry ⓘ

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

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

| Mol | Chain | Bond lengths | | Bond angles | |
|-----|-------|--------------|-----------------|-------------|-----------------|
| | | RMSZ | $\# Z > 2$ | RMSZ | $\# Z > 2$ |
| 1 | A | 0.39 | 0/1656 | 0.77 | 0/2264 |
| 10 | J | 0.44 | 1/1495 (0.1%) | 0.90 | 3/2001 (0.1%) |
| 11 | K | 0.40 | 0/831 | 0.68 | 0/1123 |
| 12 | L | 0.36 | 0/1276 | 0.67 | 0/1718 |
| 13 | M | 0.40 | 0/929 | 0.76 | 0/1255 |
| 14 | N | 0.40 | 0/1210 | 0.84 | 0/1628 |
| 15 | O | 0.40 | 0/953 | 0.77 | 0/1279 |
| 16 | P | 0.53 | 1/1000 (0.1%) | 0.80 | 1/1343 (0.1%) |
| 17 | Q | 0.38 | 0/1125 | 0.75 | 1/1510 (0.1%) |
| 18 | R | 0.40 | 0/1042 | 0.84 | 0/1399 |
| 19 | S | 0.45 | 1/1212 (0.1%) | 0.81 | 2/1629 (0.1%) |
| 2 | B | 0.38 | 0/1747 | 0.71 | 0/2353 |
| 20 | T | 0.36 | 0/1129 | 0.75 | 0/1520 |
| 21 | U | 0.35 | 0/857 | 0.69 | 0/1158 |
| 22 | V | 0.37 | 0/696 | 0.69 | 0/938 |
| 23 | W | 0.40 | 0/1039 | 0.81 | 0/1399 |
| 24 | X | 0.39 | 0/1145 | 0.81 | 1/1526 (0.1%) |
| 25 | Y | 0.39 | 0/1075 | 0.77 | 0/1433 |
| 26 | Z | 0.42 | 0/567 | 0.81 | 1/762 (0.1%) |
| 27 | a | 0.40 | 0/810 | 0.82 | 0/1084 |
| 28 | b | 0.34 | 0/627 | 0.67 | 0/847 |
| 29 | c | 0.37 | 0/496 | 0.73 | 0/666 |
| 3 | C | 0.37 | 0/1659 | 0.71 | 0/2252 |
| 30 | d | 0.38 | 0/457 | 0.64 | 0/607 |
| 31 | e | 0.36 | 0/450 | 0.68 | 0/599 |
| 32 | f | 0.42 | 0/562 | 0.67 | 0/751 |
| 33 | g | 0.35 | 0/2521 | 0.58 | 0/3431 |
| 34 | 2 | 0.34 | 14/42269 (0.0%) | 0.78 | 26/65862 (0.0%) |
| 35 | i | 0.34 | 1/4425 (0.0%) | 0.72 | 1/6875 (0.0%) |
| 4 | D | 0.36 | 0/1769 | 0.70 | 0/2378 |
| 5 | E | 0.36 | 0/2122 | 0.67 | 0/2861 |
| 6 | F | 0.38 | 0/1628 | 0.79 | 0/2198 |

| Mol | Chain | Bond lengths | | Bond angles | |
|-----|-------|--------------|-----------------|-------------|------------------|
| | | RMSZ | # Z >2 | RMSZ | # Z >2 |
| 7 | G | 0.46 | 2/1835 (0.1%) | 0.80 | 2/2451 (0.1%) |
| 8 | H | 0.38 | 0/1507 | 0.73 | 0/2028 |
| 9 | I | 0.40 | 0/1519 | 0.79 | 0/2033 |
| All | All | 0.37 | 20/85640 (0.0%) | 0.76 | 38/125161 (0.0%) |

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

| Mol | Chain | #Chirality outliers | #Planarity outliers |
|-----|-------|---------------------|---------------------|
| 1 | A | 0 | 2 |
| 10 | J | 0 | 1 |
| 15 | O | 0 | 1 |
| 17 | Q | 0 | 2 |
| 22 | V | 0 | 1 |
| 23 | W | 0 | 1 |
| 26 | Z | 0 | 1 |
| 27 | a | 0 | 1 |
| 34 | 2 | 0 | 7 |
| 7 | G | 0 | 1 |
| All | All | 0 | 18 |

All (20) bond length outliers are listed below:

| Mol | Chain | Res | Type | Atoms | Z | Observed(Å) | Ideal(Å) |
|-----|-------|------|------|-------|--------|-------------|----------|
| 34 | 2 | 1073 | G | C2-N2 | -13.62 | 1.21 | 1.34 |
| 34 | 2 | 1074 | C | C4-N4 | 11.59 | 1.44 | 1.33 |
| 34 | 2 | 1072 | G | C2-N2 | 10.69 | 1.45 | 1.34 |
| 34 | 2 | 1073 | G | N1-C2 | -10.45 | 1.29 | 1.37 |
| 34 | 2 | 1073 | G | C6-O6 | -10.32 | 1.14 | 1.24 |
| 34 | 2 | 934 | U | O3'-P | -10.18 | 1.49 | 1.61 |
| 35 | i | 6109 | C | O3'-P | -9.66 | 1.49 | 1.61 |
| 34 | 2 | 1044 | C | C2-O2 | 7.30 | 1.31 | 1.24 |
| 7 | G | 154 | ARG | CA-C | 7.19 | 1.71 | 1.52 |
| 34 | 2 | 1073 | G | C6-N1 | -7.07 | 1.34 | 1.39 |
| 34 | 2 | 8 | U | O3'-P | -7.04 | 1.52 | 1.61 |
| 34 | 2 | 520 | A | O3'-P | -6.29 | 1.53 | 1.61 |
| 34 | 2 | 77 | U | O3'-P | 6.25 | 1.68 | 1.61 |
| 34 | 2 | 1069 | C | O3'-P | -6.04 | 1.53 | 1.61 |
| 16 | P | 19 | GLY | N-CA | 5.95 | 1.54 | 1.46 |
| 7 | G | 154 | ARG | N-CA | 5.81 | 1.57 | 1.46 |

Continued on next page...

Continued from previous page...

| Mol | Chain | Res | Type | Atoms | Z | Observed(Å) | Ideal(Å) |
|-----|-------|------|------|-------|-------|-------------|----------|
| 34 | 2 | 883 | A | O3'-P | -5.39 | 1.54 | 1.61 |
| 34 | 2 | 1044 | C | N1-C2 | 5.21 | 1.45 | 1.40 |
| 10 | J | 170 | GLY | CA-C | 5.07 | 1.59 | 1.51 |
| 19 | S | 93 | ASN | N-CA | 5.00 | 1.56 | 1.46 |

All (38) bond angle outliers are listed below:

| Mol | Chain | Res | Type | Atoms | Z | Observed(°) | Ideal(°) |
|-----|-------|------|------|-------------|--------|-------------|----------|
| 34 | 2 | 1073 | G | N1-C2-N2 | -16.67 | 101.20 | 116.20 |
| 34 | 2 | 1074 | C | C2'-C3'-O3' | 11.15 | 134.03 | 109.50 |
| 34 | 2 | 1074 | C | N1-C1'-C2' | -9.84 | 101.17 | 112.00 |
| 26 | Z | 68 | ARG | N-CA-C | -8.17 | 88.93 | 111.00 |
| 34 | 2 | 78 | A | C4'-C3'-O3' | 7.94 | 128.88 | 113.00 |
| 34 | 2 | 1044 | C | N1-C2-O2 | 7.40 | 123.34 | 118.90 |
| 34 | 2 | 1044 | C | C2-N1-C1' | 7.22 | 126.74 | 118.80 |
| 34 | 2 | 78 | A | C5'-C4'-C3' | 7.09 | 127.34 | 116.00 |
| 34 | 2 | 1073 | G | N1-C6-O6 | -7.08 | 115.65 | 119.90 |
| 34 | 2 | 1082 | G | P-O3'-C3' | -6.52 | 111.88 | 119.70 |
| 34 | 2 | 911 | U | N1-C1'-C2' | 6.41 | 122.34 | 114.00 |
| 34 | 2 | 1076 | C | N1-C1'-C2' | -6.38 | 104.98 | 112.00 |
| 34 | 2 | 1074 | C | C3'-C2'-C1' | 6.34 | 106.58 | 101.50 |
| 34 | 2 | 1044 | C | C6-N1-C1' | -6.13 | 113.44 | 120.80 |
| 34 | 2 | 511 | A | O5'-P-OP1 | 6.07 | 117.98 | 110.70 |
| 34 | 2 | 1534 | G | C2'-C3'-O3' | 6.04 | 123.36 | 113.70 |
| 34 | 2 | 78 | A | P-O5'-C5' | 6.00 | 130.51 | 120.90 |
| 34 | 2 | 1083 | A | O5'-P-OP2 | -5.93 | 100.37 | 105.70 |
| 24 | X | 64 | PRO | CA-N-CD | -5.82 | 103.36 | 111.50 |
| 34 | 2 | 267 | C | N1-C1'-C2' | -5.81 | 105.61 | 112.00 |
| 34 | 2 | 113 | U | C2'-C3'-O3' | 5.76 | 122.92 | 113.70 |
| 7 | G | 155 | ASP | CB-CA-C | -5.71 | 98.99 | 110.40 |
| 35 | i | 6212 | U | N1-C1'-C2' | -5.47 | 105.98 | 112.00 |
| 34 | 2 | 930 | C | O4'-C1'-N1 | 5.46 | 112.57 | 108.20 |
| 19 | S | 30 | TYR | CB-CA-C | 5.43 | 121.26 | 110.40 |
| 17 | Q | 52 | LEU | CA-CB-CG | 5.35 | 127.61 | 115.30 |
| 34 | 2 | 828 | A | C2'-C3'-O3' | 5.29 | 122.17 | 113.70 |
| 19 | S | 93 | ASN | N-CA-C | 5.20 | 125.04 | 111.00 |
| 10 | J | 176 | ARG | N-CA-CB | 5.18 | 119.92 | 110.60 |
| 34 | 2 | 78 | A | O4'-C4'-C3' | -5.12 | 98.88 | 104.00 |
| 10 | J | 170 | GLY | N-CA-C | 5.09 | 125.81 | 113.10 |
| 10 | J | 49 | LEU | CA-CB-CG | 5.08 | 126.98 | 115.30 |
| 34 | 2 | 1628 | U | C4'-C3'-O3' | 5.08 | 123.16 | 113.00 |
| 34 | 2 | 963 | U | C2'-C3'-O3' | 5.07 | 121.82 | 113.70 |

Continued on next page...

Continued from previous page...

| Mol | Chain | Res | Type | Atoms | Z | Observed(°) | Ideal(°) |
|-----|-------|------|------|-----------|-------|-------------|----------|
| 16 | P | 20 | VAL | N-CA-C | 5.05 | 124.63 | 111.00 |
| 34 | 2 | 1073 | G | N3-C2-N2 | 5.05 | 123.43 | 119.90 |
| 34 | 2 | 511 | A | P-O5'-C5' | 5.02 | 128.93 | 120.90 |
| 7 | G | 208 | TYR | CA-CB-CG | -5.01 | 103.87 | 113.40 |

There are no chirality outliers.

All (18) planarity outliers are listed below:

| Mol | Chain | Res | Type | Group |
|-----|-------|------|------|-----------|
| 34 | 2 | 1044 | C | Sidechain |
| 34 | 2 | 1073 | G | Sidechain |
| 34 | 2 | 1074 | C | Sidechain |
| 34 | 2 | 1269 | G | Sidechain |
| 34 | 2 | 1439 | C | Sidechain |
| 34 | 2 | 561 | G | Sidechain |
| 34 | 2 | 583 | C | Sidechain |
| 1 | A | 164 | ASN | Peptide |
| 1 | A | 168 | HIS | Peptide |
| 7 | G | 155 | ASP | Peptide |
| 10 | J | 66 | ASP | Peptide |
| 15 | O | 122 | PRO | Peptide |
| 17 | Q | 40 | GLN | Peptide |
| 17 | Q | 49 | TYR | Peptide |
| 22 | V | 13 | VAL | Peptide |
| 23 | W | 75 | ILE | Peptide |
| 26 | Z | 68 | ARG | Sidechain |
| 27 | a | 83 | ILE | Peptide |

5.2 Too-close contacts

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

| Mol | Chain | Non-H | H(model) | H(added) | Clashes | Symm-Clashes |
|-----|-------|-------|----------|----------|---------|--------------|
| 1 | A | 1616 | 0 | 1636 | 18 | 0 |
| 2 | B | 1722 | 0 | 1795 | 3 | 0 |
| 3 | C | 1629 | 0 | 1710 | 8 | 0 |
| 4 | D | 1744 | 0 | 1825 | 2 | 0 |
| 5 | E | 2078 | 0 | 2157 | 4 | 0 |

Continued on next page...

Continued from previous page...

| Mol | Chain | Non-H | H(model) | H(added) | Clashes | Symm-Clashes |
|-----|-------|-------|----------|----------|---------|--------------|
| 6 | F | 1609 | 0 | 1679 | 25 | 0 |
| 7 | G | 1812 | 0 | 1911 | 56 | 0 |
| 8 | H | 1483 | 0 | 1579 | 6 | 0 |
| 9 | I | 1493 | 0 | 1515 | 19 | 0 |
| 10 | J | 1471 | 0 | 1554 | 37 | 0 |
| 11 | K | 809 | 0 | 810 | 4 | 0 |
| 12 | L | 1248 | 0 | 1311 | 5 | 0 |
| 13 | M | 922 | 0 | 953 | 7 | 0 |
| 14 | N | 1187 | 0 | 1251 | 5 | 0 |
| 15 | O | 942 | 0 | 979 | 8 | 0 |
| 16 | P | 980 | 0 | 1026 | 22 | 0 |
| 17 | Q | 1105 | 0 | 1170 | 6 | 0 |
| 18 | R | 1031 | 0 | 1082 | 6 | 0 |
| 19 | S | 1193 | 0 | 1217 | 21 | 0 |
| 20 | T | 1110 | 0 | 1124 | 4 | 0 |
| 21 | U | 845 | 0 | 913 | 5 | 0 |
| 22 | V | 687 | 0 | 682 | 2 | 0 |
| 23 | W | 1021 | 0 | 1056 | 12 | 0 |
| 24 | X | 1127 | 0 | 1210 | 22 | 0 |
| 25 | Y | 1061 | 0 | 1111 | 14 | 0 |
| 26 | Z | 558 | 0 | 585 | 74 | 0 |
| 27 | a | 798 | 0 | 855 | 0 | 0 |
| 28 | b | 617 | 0 | 642 | 0 | 0 |
| 29 | c | 494 | 0 | 534 | 0 | 0 |
| 30 | d | 446 | 0 | 436 | 0 | 0 |
| 31 | e | 443 | 0 | 481 | 0 | 0 |
| 32 | f | 549 | 0 | 564 | 0 | 0 |
| 33 | g | 2466 | 0 | 2406 | 0 | 0 |
| 34 | 2 | 37797 | 0 | 19010 | 942 | 0 |
| 35 | i | 3968 | 0 | 1986 | 0 | 0 |
| 36 | 2 | 76 | 0 | 0 | 0 | 0 |
| 36 | G | 1 | 0 | 0 | 0 | 0 |
| 36 | N | 1 | 0 | 0 | 0 | 0 |
| 36 | T | 1 | 0 | 0 | 0 | 0 |
| 36 | X | 1 | 0 | 0 | 0 | 0 |
| 37 | a | 1 | 0 | 0 | 0 | 0 |
| 37 | b | 1 | 0 | 0 | 0 | 0 |
| 37 | f | 1 | 0 | 0 | 0 | 0 |
| All | All | 80144 | 0 | 60755 | 1189 | 0 |

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 10.

All (1189) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|-------------------|--------------------------|-------------------|
| 26:Z:52:LYS:HA | 26:Z:53:GLU:CG | 1.47 | 1.43 |
| 34:2:513:G:H1 | 34:2:542:C:N4 | 1.27 | 1.31 |
| 24:X:63:GLN:NE2 | 34:2:1753:A:OP1 | 1.64 | 1.29 |
| 34:2:480:A:N1 | 34:2:506:U:C4 | 2.04 | 1.26 |
| 26:Z:51:MET:O | 26:Z:53:GLU:HA | 1.13 | 1.26 |
| 34:2:1072:G:N2 | 34:2:1073:G:N7 | 1.84 | 1.24 |
| 34:2:480:A:N1 | 34:2:506:U:O4 | 1.72 | 1.22 |
| 26:Z:58:ARG:NH1 | 26:Z:103:ARG:HH22 | 1.40 | 1.20 |
| 10:J:170:GLY:O | 34:2:511:A:H5' | 1.39 | 1.18 |
| 34:2:1044:C:N3 | 34:2:1072:G:N2 | 1.90 | 1.18 |
| 34:2:1292:U:O4 | 34:2:1321:A:N1 | 1.77 | 1.17 |
| 34:2:1044:C:N4 | 34:2:1072:G:H1 | 1.44 | 1.15 |
| 10:J:170:GLY:O | 34:2:511:A:P | 2.05 | 1.15 |
| 10:J:170:GLY:O | 34:2:511:A:C5' | 1.93 | 1.14 |
| 34:2:1221:C:O2 | 34:2:1261:U:O2 | 1.67 | 1.13 |
| 7:G:155:ASP:N | 34:2:78:A:O5' | 1.83 | 1.11 |
| 26:Z:53:GLU:HB3 | 26:Z:55:PRO:HD2 | 1.34 | 1.10 |
| 26:Z:51:MET:O | 26:Z:53:GLU:CA | 2.02 | 1.08 |
| 7:G:136:LYS:NZ | 34:2:65:A:OP1 | 1.87 | 1.08 |
| 34:2:955:C:O2' | 34:2:1046:G:O2' | 1.71 | 1.08 |
| 26:Z:52:LYS:HA | 26:Z:53:GLU:HG3 | 1.08 | 1.07 |
| 24:X:63:GLN:HE21 | 34:2:1753:A:P | 1.77 | 1.07 |
| 7:G:154:ARG:N | 34:2:78:A:O5' | 1.87 | 1.07 |
| 10:J:170:GLY:HA3 | 34:2:511:A:H5' | 1.36 | 1.07 |
| 7:G:155:ASP:H | 34:2:78:A:C5' | 1.68 | 1.07 |
| 26:Z:63:SER:O | 26:Z:66:VAL:O | 1.70 | 1.06 |
| 26:Z:58:ARG:NH1 | 26:Z:103:ARG:NH2 | 2.02 | 1.06 |
| 34:2:1292:U:C4 | 34:2:1321:A:N1 | 2.23 | 1.06 |
| 26:Z:52:LYS:CA | 26:Z:53:GLU:HG3 | 1.87 | 1.05 |
| 26:Z:54:ALA:HB2 | 26:Z:83:LEU:HD22 | 1.39 | 1.05 |
| 10:J:170:GLY:C | 34:2:511:A:P | 2.36 | 1.04 |
| 26:Z:52:LYS:HA | 26:Z:53:GLU:HG2 | 1.37 | 1.04 |
| 34:2:138:A:N7 | 34:2:265:A:H2 | 1.55 | 1.03 |
| 34:2:1072:G:C2 | 34:2:1073:G:N7 | 2.24 | 1.03 |
| 34:2:511:A:H2' | 34:2:512:U:H5' | 1.42 | 1.01 |
| 34:2:513:G:N2 | 34:2:542:C:C5 | 2.28 | 1.01 |
| 34:2:883:A:H2' | 34:2:884:G:H5' | 1.41 | 1.01 |
| 26:Z:58:ARG:O | 26:Z:102:THR:HG23 | 1.60 | 1.01 |
| 10:J:170:GLY:HA3 | 34:2:511:A:C5' | 1.91 | 0.99 |
| 34:2:935:G:OP2 | 34:2:1074:C:N3 | 1.96 | 0.98 |

Continued on next page...

Continued from previous page...

| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 26:Z:51:MET:C | 26:Z:53:GLU:HA | 1.83 | 0.98 |
| 10:J:170:GLY:C | 34:2:511:A:OP1 | 2.03 | 0.97 |
| 34:2:537:A:C8 | 34:2:542:C:N3 | 2.33 | 0.96 |
| 26:Z:60:VAL:HG12 | 26:Z:80:LEU:HD21 | 1.44 | 0.96 |
| 34:2:513:G:C2 | 34:2:542:C:H5 | 1.82 | 0.96 |
| 34:2:1084:G:N2 | 34:2:1088:U:C2 | 2.34 | 0.96 |
| 34:2:1044:C:N4 | 34:2:1072:G:N1 | 2.14 | 0.95 |
| 26:Z:52:LYS:CA | 26:Z:53:GLU:CG | 2.42 | 0.95 |
| 34:2:1218:A:N6 | 34:2:1263:G:O2' | 2.00 | 0.94 |
| 34:2:264:A:N1 | 34:2:288:U:O4 | 1.98 | 0.94 |
| 34:2:1082:G:O2' | 34:2:1093:G:O2' | 1.84 | 0.94 |
| 34:2:1082:G:H2' | 34:2:1083:A:H5'' | 1.49 | 0.94 |
| 26:Z:49:ARG:HG2 | 26:Z:49:ARG:HH11 | 1.32 | 0.92 |
| 34:2:1012:A:H2' | 34:2:1013:G:O4' | 1.70 | 0.92 |
| 34:2:513:G:N2 | 34:2:542:C:H5 | 1.68 | 0.91 |
| 34:2:1040:G:C2 | 34:2:1076:C:N3 | 2.39 | 0.91 |
| 34:2:480:A:C2 | 34:2:506:U:O4 | 2.25 | 0.90 |
| 10:J:170:GLY:CA | 34:2:511:A:H5' | 2.02 | 0.90 |
| 34:2:143:G:O6 | 34:2:170:A:N6 | 2.05 | 0.90 |
| 26:Z:104:ALA:HB1 | 26:Z:105:THR:HA | 1.52 | 0.90 |
| 34:2:267:C:N4 | 34:2:286:G:H1 | 1.69 | 0.89 |
| 7:G:154:ARG:CA | 34:2:78:A:O5' | 2.19 | 0.89 |
| 34:2:1072:G:N2 | 34:2:1073:G:C5 | 2.39 | 0.89 |
| 34:2:269:C:H2' | 34:2:270:A:H8 | 1.35 | 0.89 |
| 34:2:1258:U:C5 | 34:2:1259:U:O4 | 2.25 | 0.89 |
| 34:2:1040:G:C6 | 34:2:1076:C:N4 | 2.41 | 0.88 |
| 34:2:935:G:OP1 | 34:2:1044:C:C1' | 2.21 | 0.88 |
| 34:2:884:G:H8 | 34:2:884:G:H5' | 1.36 | 0.88 |
| 7:G:154:ARG:HA | 34:2:78:A:H3' | 1.56 | 0.88 |
| 34:2:511:A:C2' | 34:2:512:U:H5' | 2.04 | 0.87 |
| 34:2:1229:A:N3 | 34:2:1257:U:C5 | 2.43 | 0.86 |
| 34:2:560:G:HO2' | 34:2:561:G:H8 | 1.23 | 0.86 |
| 34:2:1258:U:O2' | 34:2:1259:U:C5 | 2.29 | 0.86 |
| 7:G:155:ASP:N | 34:2:78:A:C5' | 2.39 | 0.85 |
| 34:2:1044:C:C2 | 34:2:1072:G:N2 | 2.35 | 0.85 |
| 34:2:1040:G:C2 | 34:2:1076:C:C4 | 2.63 | 0.85 |
| 34:2:1229:A:C2 | 34:2:1257:U:C6 | 2.64 | 0.85 |
| 34:2:1292:U:O4 | 34:2:1321:A:C6 | 2.29 | 0.85 |
| 34:2:513:G:C2 | 34:2:542:C:C5 | 2.64 | 0.85 |
| 34:2:1042:A:N1 | 34:2:1075:A:C2 | 2.44 | 0.85 |
| 10:J:170:GLY:CA | 34:2:511:A:OP1 | 2.25 | 0.85 |

Continued on next page...

Continued from previous page...

| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 34:2:1292:U:O4 | 34:2:1321:A:C2 | 2.30 | 0.84 |
| 34:2:513:G:N1 | 34:2:542:C:N4 | 2.07 | 0.84 |
| 7:G:171:LYS:HE3 | 34:2:71:A:H61 | 1.41 | 0.84 |
| 34:2:1082:G:C2' | 34:2:1083:A:H5'' | 2.07 | 0.83 |
| 10:J:170:GLY:C | 34:2:511:A:C5' | 2.46 | 0.83 |
| 34:2:884:G:C8 | 34:2:884:G:H5' | 2.13 | 0.83 |
| 34:2:8:U:C3' | 34:2:9:U:H5' | 2.09 | 0.83 |
| 7:G:155:ASP:H | 34:2:78:A:P | 2.02 | 0.83 |
| 34:2:1222:A:C6 | 34:2:1260:G:C6 | 2.67 | 0.82 |
| 34:2:1258:U:O2' | 34:2:1259:U:C6 | 2.32 | 0.82 |
| 34:2:566:A:H2' | 34:2:567:G:O4' | 1.80 | 0.82 |
| 34:2:1292:U:C4 | 34:2:1321:A:C2 | 2.68 | 0.82 |
| 34:2:65:A:H2' | 34:2:83:G:H1 | 1.45 | 0.82 |
| 34:2:1040:G:N2 | 34:2:1076:C:C2 | 2.48 | 0.81 |
| 34:2:513:G:H1 | 34:2:542:C:H41 | 0.85 | 0.81 |
| 26:Z:54:ALA:HB3 | 26:Z:88:ILE:CG2 | 2.10 | 0.81 |
| 34:2:883:A:C2' | 34:2:884:G:H5' | 2.09 | 0.81 |
| 10:J:170:GLY:CA | 34:2:511:A:C5' | 2.57 | 0.81 |
| 7:G:155:ASP:N | 34:2:78:A:P | 2.53 | 0.81 |
| 34:2:935:G:OP1 | 34:2:1044:C:H1' | 1.80 | 0.80 |
| 34:2:480:A:C6 | 34:2:506:U:O4 | 2.33 | 0.80 |
| 26:Z:54:ALA:CB | 26:Z:83:LEU:HD22 | 2.10 | 0.80 |
| 34:2:1230:U:O3' | 34:2:1257:U:O2' | 1.99 | 0.80 |
| 34:2:1040:G:N1 | 34:2:1076:C:C4 | 2.50 | 0.80 |
| 26:Z:54:ALA:HB2 | 26:Z:83:LEU:CD2 | 2.11 | 0.80 |
| 34:2:560:G:C2' | 34:2:561:G:H8 | 1.95 | 0.80 |
| 34:2:511:A:H2' | 34:2:512:U:C5' | 2.13 | 0.79 |
| 34:2:513:G:N1 | 34:2:542:C:C5 | 2.50 | 0.79 |
| 34:2:138:A:N7 | 34:2:265:A:C2 | 2.46 | 0.79 |
| 34:2:537:A:H4' | 34:2:538:G:OP1 | 1.80 | 0.79 |
| 34:2:8:U:O4 | 34:2:15:U:O4 | 2.01 | 0.79 |
| 34:2:264:A:C2 | 34:2:287:A:N6 | 2.50 | 0.78 |
| 6:F:125:VAL:HG11 | 26:Z:59:TYR:HB3 | 1.65 | 0.78 |
| 34:2:1258:U:C2' | 34:2:1259:U:C5 | 2.66 | 0.78 |
| 34:2:564:C:H2' | 34:2:576:G:N2 | 1.98 | 0.78 |
| 34:2:1258:U:C6 | 34:2:1259:U:O4 | 2.36 | 0.78 |
| 34:2:883:A:H2' | 34:2:884:G:C5' | 2.12 | 0.78 |
| 34:2:267:C:H42 | 34:2:286:G:H1 | 1.29 | 0.77 |
| 34:2:565:C:H2' | 34:2:566:A:C8 | 2.19 | 0.77 |
| 34:2:1173:C:N3 | 34:2:1464:G:C2 | 2.53 | 0.77 |
| 34:2:883:A:C2' | 34:2:884:G:C5' | 2.62 | 0.77 |

Continued on next page...

Continued from previous page...

| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|-------------------|--------------------------|-------------------|
| 34:2:1258:U:H2' | 34:2:1259:U:H5 | 1.49 | 0.77 |
| 34:2:1229:A:H2 | 34:2:1257:U:H6 | 1.33 | 0.77 |
| 10:J:14:THR:HG21 | 34:2:23:G:OP1 | 1.83 | 0.77 |
| 34:2:1082:G:C3' | 34:2:1083:A:H5'' | 2.14 | 0.77 |
| 34:2:1229:A:C2 | 34:2:1257:U:H6 | 2.02 | 0.77 |
| 34:2:70:C:H2' | 34:2:71:A:O4' | 1.85 | 0.77 |
| 10:J:170:GLY:N | 34:2:511:A:OP1 | 2.19 | 0.76 |
| 34:2:935:G:OP2 | 34:2:1073:G:N2 | 2.18 | 0.76 |
| 34:2:888:U:H2' | 34:2:889:C:C6 | 2.21 | 0.76 |
| 16:P:18:LYS:O | 19:S:95:GLY:N | 2.18 | 0.76 |
| 26:Z:58:ARG:HH12 | 26:Z:103:ARG:HH22 | 1.29 | 0.76 |
| 34:2:1070:U:H5'' | 34:2:1071:C:OP1 | 1.86 | 0.76 |
| 8:H:70:TYR:O | 8:H:74:GLN:N | 2.19 | 0.76 |
| 34:2:1229:A:N3 | 34:2:1257:U:C6 | 2.54 | 0.76 |
| 34:2:1590:A:H2' | 34:2:1591:A:C8 | 2.21 | 0.76 |
| 26:Z:53:GLU:HB3 | 26:Z:55:PRO:CD | 2.15 | 0.76 |
| 34:2:208:U:C4 | 34:2:209:A:N7 | 2.54 | 0.75 |
| 34:2:65:A:H2' | 34:2:83:G:N1 | 2.01 | 0.75 |
| 26:Z:52:LYS:HD2 | 26:Z:53:GLU:HG3 | 1.67 | 0.75 |
| 34:2:884:G:C2' | 34:2:885:U:H4' | 2.16 | 0.75 |
| 26:Z:58:ARG:CZ | 26:Z:103:ARG:HH22 | 1.99 | 0.75 |
| 26:Z:104:ALA:HB1 | 26:Z:105:THR:CA | 2.16 | 0.75 |
| 34:2:556:G:C6 | 34:2:558:C:N4 | 2.55 | 0.74 |
| 7:G:154:ARG:C | 34:2:78:A:O5' | 2.24 | 0.74 |
| 26:Z:60:VAL:HG12 | 26:Z:80:LEU:CD2 | 2.16 | 0.74 |
| 34:2:70:C:N4 | 34:2:71:A:N1 | 2.36 | 0.74 |
| 34:2:1255:A:N3 | 34:2:1257:U:O4 | 2.20 | 0.74 |
| 34:2:267:C:N3 | 34:2:286:G:N2 | 2.35 | 0.73 |
| 34:2:8:U:O2' | 34:2:9:U:H5' | 1.89 | 0.73 |
| 34:2:264:A:H2 | 34:2:288:U:H3 | 1.37 | 0.73 |
| 10:J:170:GLY:O | 34:2:511:A:OP2 | 2.07 | 0.73 |
| 34:2:558:C:H2' | 34:2:559:U:C6 | 2.24 | 0.72 |
| 34:2:560:G:H2' | 34:2:561:G:H8 | 1.54 | 0.72 |
| 24:X:63:GLN:NE2 | 34:2:1753:A:H5' | 2.05 | 0.72 |
| 34:2:560:G:H2' | 34:2:561:G:C8 | 2.23 | 0.72 |
| 34:2:1221:C:O2 | 34:2:1261:U:C2 | 2.43 | 0.72 |
| 10:J:170:GLY:O | 34:2:511:A:O5' | 2.07 | 0.72 |
| 34:2:884:G:H2' | 34:2:885:U:H4' | 1.71 | 0.72 |
| 34:2:884:G:C5' | 34:2:884:G:H8 | 2.03 | 0.71 |
| 9:I:160:GLN:HB3 | 9:I:166:LEU:HA | 1.73 | 0.71 |
| 34:2:150:G:O6 | 34:2:162:G:O6 | 2.08 | 0.71 |

Continued on next page...

Continued from previous page...

| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|-----------------|------------------|--------------------------|-------------------|
| 34:2:884:G:C3' | 34:2:885:U:H4' | 2.20 | 0.71 |
| 34:2:1082:G:O6 | 34:2:1083:A:C6 | 2.44 | 0.71 |
| 10:J:170:GLY:CA | 34:2:511:A:P | 2.78 | 0.71 |
| 26:Z:54:ALA:HB3 | 26:Z:88:ILE:HG21 | 1.72 | 0.71 |
| 34:2:1043:U:N3 | 34:2:1044:C:N4 | 2.38 | 0.71 |
| 34:2:214:A:N7 | 34:2:241:U:H2' | 2.06 | 0.70 |
| 7:G:155:ASP:N | 34:2:77:U:O3' | 2.24 | 0.70 |
| 7:G:154:ARG:CA | 34:2:78:A:H3' | 2.21 | 0.70 |
| 34:2:1083:A:N1 | 34:2:1089:C:C4 | 2.59 | 0.70 |
| 26:Z:60:VAL:CG1 | 26:Z:80:LEU:HD21 | 2.21 | 0.70 |
| 26:Z:49:ARG:HG2 | 26:Z:49:ARG:NH1 | 1.96 | 0.70 |
| 34:2:564:C:H2' | 34:2:576:G:C2 | 2.25 | 0.70 |
| 34:2:1363:G:N2 | 34:2:1364:C:C2 | 2.60 | 0.69 |
| 34:2:264:A:N1 | 34:2:287:A:N6 | 2.40 | 0.69 |
| 34:2:1082:G:C6 | 34:2:1083:A:C5 | 2.80 | 0.69 |
| 34:2:537:A:C8 | 34:2:542:C:C4 | 2.80 | 0.69 |
| 34:2:515:G:C6 | 34:2:536:G:N2 | 2.61 | 0.69 |
| 16:P:19:GLY:N | 19:S:93:ASN:N | 2.41 | 0.69 |
| 34:2:1229:A:C2 | 34:2:1257:U:C5 | 2.82 | 0.68 |
| 34:2:542:C:O2' | 34:2:543:A:P | 2.50 | 0.68 |
| 26:Z:61:SER:O | 26:Z:64:VAL:N | 2.25 | 0.68 |
| 34:2:148:C:H2' | 34:2:149:U:C6 | 2.28 | 0.68 |
| 34:2:1499:C:C2 | 34:2:1505:G:N2 | 2.62 | 0.68 |
| 34:2:261:U:C4 | 34:2:262:C:N4 | 2.61 | 0.68 |
| 34:2:559:U:H2' | 34:2:560:G:H8 | 1.58 | 0.68 |
| 34:2:884:G:H2' | 34:2:885:U:C4' | 2.23 | 0.68 |
| 34:2:1258:U:H2' | 34:2:1259:U:C5 | 2.28 | 0.68 |
| 34:2:628:U:N3 | 34:2:969:A:N6 | 2.41 | 0.68 |
| 9:I:82:VAL:HG12 | 9:I:197:LEU:HD21 | 1.76 | 0.68 |
| 34:2:1042:A:N1 | 34:2:1075:A:N1 | 2.42 | 0.68 |
| 34:2:511:A:C3' | 34:2:512:U:H5' | 2.23 | 0.68 |
| 26:Z:53:GLU:CB | 26:Z:55:PRO:HD2 | 2.20 | 0.68 |
| 34:2:537:A:N7 | 34:2:542:C:N4 | 2.42 | 0.67 |
| 34:2:261:U:C4 | 34:2:262:C:C4 | 2.82 | 0.67 |
| 34:2:299:A:H2' | 34:2:300:A:C8 | 2.30 | 0.67 |
| 26:Z:61:SER:HB3 | 26:Z:64:VAL:HG23 | 1.75 | 0.67 |
| 34:2:406:A:O2' | 34:2:1669:A:N3 | 2.26 | 0.67 |
| 34:2:269:C:H2' | 34:2:270:A:C8 | 2.25 | 0.67 |
| 34:2:144:A:C2 | 34:2:170:A:C2 | 2.83 | 0.66 |
| 34:2:1082:G:O6 | 34:2:1083:A:C5 | 2.48 | 0.66 |
| 34:2:883:A:C3' | 34:2:884:G:C5' | 2.73 | 0.66 |

Continued on next page...

Continued from previous page...

| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 34:2:1218:A:N6 | 34:2:1263:G:C2' | 2.58 | 0.66 |
| 34:2:1215:C:O2' | 34:2:1442:A:N6 | 2.28 | 0.66 |
| 34:2:1223:A:N6 | 34:2:1224:U:C4 | 2.64 | 0.66 |
| 34:2:139:C:H42 | 34:2:280:G:P | 2.19 | 0.66 |
| 34:2:1084:G:N2 | 34:2:1088:U:N3 | 2.44 | 0.66 |
| 34:2:1074:C:O2 | 34:2:1074:C:C2' | 2.42 | 0.65 |
| 34:2:1215:C:HO2' | 34:2:1442:A:N6 | 1.93 | 0.65 |
| 10:J:170:GLY:HA3 | 34:2:511:A:O5' | 1.96 | 0.65 |
| 16:P:17:TYR:N | 19:S:92:VAL:O | 2.29 | 0.65 |
| 34:2:1183:A:C2 | 34:2:1453:G:O4' | 2.48 | 0.65 |
| 34:2:537:A:N7 | 34:2:542:C:C4 | 2.65 | 0.65 |
| 34:2:264:A:N1 | 34:2:288:U:C4 | 2.63 | 0.65 |
| 34:2:1417:G:C6 | 34:2:1418:C:N3 | 2.64 | 0.65 |
| 34:2:560:G:N3 | 34:2:561:G:C8 | 2.64 | 0.65 |
| 26:Z:60:VAL:CG1 | 26:Z:80:LEU:CD2 | 2.75 | 0.65 |
| 34:2:1223:A:C6 | 34:2:1224:U:C4 | 2.85 | 0.65 |
| 34:2:556:G:C2 | 34:2:558:C:C4 | 2.84 | 0.65 |
| 34:2:1044:C:C4 | 34:2:1072:G:N1 | 2.56 | 0.65 |
| 34:2:935:G:P | 34:2:1074:C:N4 | 2.70 | 0.65 |
| 34:2:1040:G:N1 | 34:2:1076:C:N4 | 2.42 | 0.65 |
| 34:2:480:A:C2 | 34:2:506:U:C4 | 2.82 | 0.65 |
| 34:2:883:A:C6 | 34:2:884:G:C6 | 2.84 | 0.65 |
| 34:2:8:U:C2' | 34:2:9:U:H5' | 2.27 | 0.65 |
| 34:2:360:C:C2 | 34:2:383:G:N2 | 2.65 | 0.65 |
| 34:2:535:C:H2' | 34:2:536:G:O4' | 1.96 | 0.65 |
| 34:2:1601:U:H2' | 34:2:1602:U:C6 | 2.32 | 0.64 |
| 34:2:1040:G:N2 | 34:2:1076:C:N3 | 2.44 | 0.64 |
| 26:Z:54:ALA:CB | 26:Z:88:ILE:CG2 | 2.75 | 0.64 |
| 26:Z:55:PRO:O | 26:Z:56:THR:OG1 | 2.12 | 0.64 |
| 34:2:1217:G:C8 | 34:2:1442:A:C5 | 2.85 | 0.64 |
| 34:2:1082:G:H3' | 34:2:1083:A:C5' | 2.27 | 0.64 |
| 26:Z:67:ASP:C | 26:Z:69:PHE:H | 1.82 | 0.64 |
| 34:2:560:G:O2' | 34:2:561:G:H8 | 1.80 | 0.64 |
| 34:2:1464:G:N2 | 34:2:1465:C:C2 | 2.66 | 0.63 |
| 34:2:67:A:OP2 | 34:2:83:G:N2 | 2.31 | 0.63 |
| 34:2:152:G:C6 | 34:2:161:A:C6 | 2.87 | 0.63 |
| 34:2:363:G:N2 | 34:2:380:C:C2 | 2.67 | 0.63 |
| 34:2:151:U:N3 | 34:2:162:G:N7 | 2.47 | 0.63 |
| 34:2:537:A:C8 | 34:2:542:C:N4 | 2.67 | 0.63 |
| 34:2:883:A:C2' | 34:2:884:G:H5'' | 2.28 | 0.63 |
| 26:Z:58:ARG:CZ | 26:Z:103:ARG:NH2 | 2.60 | 0.63 |

Continued on next page...

Continued from previous page...

| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 34:2:559:U:H2' | 34:2:560:G:C8 | 2.34 | 0.63 |
| 7:G:174:LYS:HA | 34:2:79:C:O2' | 1.99 | 0.63 |
| 34:2:264:A:H2 | 34:2:288:U:N3 | 1.96 | 0.62 |
| 34:2:264:A:C2 | 34:2:288:U:N3 | 2.67 | 0.62 |
| 34:2:70:C:C5 | 34:2:71:A:C5 | 2.87 | 0.62 |
| 34:2:363:G:C2 | 34:2:380:C:C2 | 2.88 | 0.62 |
| 34:2:1220:A:N1 | 34:2:1261:U:N3 | 2.48 | 0.62 |
| 34:2:168:A:C4 | 34:2:170:A:C8 | 2.87 | 0.62 |
| 34:2:823:G:N2 | 34:2:848:C:C2 | 2.67 | 0.62 |
| 7:G:154:ARG:HB3 | 34:2:77:U:H4' | 1.80 | 0.62 |
| 24:X:102:VAL:HG22 | 24:X:124:VAL:HG13 | 1.81 | 0.62 |
| 7:G:155:ASP:H | 34:2:78:A:H5'' | 1.60 | 0.62 |
| 7:G:188:ARG:NH1 | 34:2:283:G:O6 | 2.32 | 0.62 |
| 34:2:207:U:H2' | 34:2:208:U:C6 | 2.35 | 0.61 |
| 34:2:1220:A:C6 | 34:2:1262:G:C6 | 2.88 | 0.61 |
| 34:2:1222:A:C4 | 34:2:1260:G:C2 | 2.88 | 0.61 |
| 34:2:1222:A:C5 | 34:2:1260:G:N1 | 2.68 | 0.61 |
| 34:2:171:C:O2' | 34:2:172:A:O4' | 2.15 | 0.61 |
| 34:2:1223:A:C6 | 34:2:1259:U:N3 | 2.68 | 0.61 |
| 6:F:53:VAL:HG13 | 6:F:133:GLN:HA | 1.81 | 0.61 |
| 34:2:1229:A:H2 | 34:2:1257:U:C6 | 2.08 | 0.61 |
| 16:P:19:GLY:H | 19:S:93:ASN:N | 1.99 | 0.61 |
| 34:2:1378:U:O2' | 34:2:1514:A:N1 | 2.32 | 0.61 |
| 34:2:480:A:C6 | 34:2:506:U:C4 | 2.86 | 0.61 |
| 16:P:17:TYR:C | 19:S:92:VAL:O | 2.39 | 0.61 |
| 34:2:1082:G:C3' | 34:2:1083:A:C5' | 2.78 | 0.60 |
| 6:F:188:ASN:HA | 34:2:1533:U:C6 | 2.36 | 0.60 |
| 34:2:209:A:C2' | 34:2:210:U:H5' | 2.31 | 0.60 |
| 34:2:513:G:N7 | 34:2:536:G:N2 | 2.49 | 0.60 |
| 34:2:65:A:N1 | 34:2:83:G:H2' | 2.16 | 0.60 |
| 24:X:96:VAL:HA | 24:X:127:VAL:HG11 | 1.82 | 0.60 |
| 26:Z:54:ALA:N | 26:Z:55:PRO:HD2 | 2.16 | 0.60 |
| 7:G:154:ARG:H | 34:2:78:A:C4' | 2.14 | 0.60 |
| 34:2:267:C:O2' | 34:2:268:G:H5' | 2.02 | 0.60 |
| 34:2:65:A:C2' | 34:2:83:G:H1 | 2.10 | 0.60 |
| 7:G:154:ARG:N | 34:2:78:A:C5' | 2.64 | 0.60 |
| 20:T:68:ARG:NH1 | 34:2:1519:G:O6 | 2.33 | 0.60 |
| 26:Z:61:SER:O | 26:Z:62:VAL:C | 2.40 | 0.60 |
| 34:2:1130:A:H2' | 34:2:1131:A:O4' | 2.01 | 0.60 |
| 34:2:560:G:C4 | 34:2:561:G:N7 | 2.69 | 0.60 |
| 34:2:69:G:C6 | 34:2:70:C:C4 | 2.88 | 0.60 |

Continued on next page...

Continued from previous page...

| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 34:2:1044:C:C4 | 34:2:1072:G:N2 | 2.61 | 0.60 |
| 34:2:811:A:O4' | 34:2:857:G:N2 | 2.34 | 0.60 |
| 34:2:1219:C:N3 | 34:2:1262:G:O6 | 2.35 | 0.60 |
| 34:2:987:A:H2' | 34:2:988:U:C6 | 2.36 | 0.60 |
| 7:G:154:ARG:CB | 34:2:77:U:H4' | 2.32 | 0.60 |
| 34:2:1220:A:C5 | 34:2:1262:G:C6 | 2.90 | 0.59 |
| 34:2:1230:U:H5' | 34:2:1258:U:H4' | 1.83 | 0.59 |
| 34:2:561:G:H2' | 34:2:562:U:H6 | 1.67 | 0.59 |
| 34:2:969:A:N6 | 34:2:970:A:C4 | 2.70 | 0.59 |
| 34:2:12:U:H2' | 34:2:13:C:C6 | 2.37 | 0.59 |
| 34:2:1024:A:O2' | 34:2:1771:C:O2' | 2.20 | 0.59 |
| 34:2:70:C:H42 | 34:2:81:G:H1 | 1.50 | 0.59 |
| 34:2:65:A:C2' | 34:2:83:G:N1 | 2.66 | 0.59 |
| 9:I:107:THR:N | 9:I:108:PRO:HD2 | 2.17 | 0.59 |
| 26:Z:59:TYR:CZ | 26:Z:64:VAL:CG2 | 2.85 | 0.59 |
| 34:2:70:C:N4 | 34:2:71:A:C6 | 2.70 | 0.59 |
| 34:2:1464:G:N1 | 34:2:1465:C:C4 | 2.71 | 0.59 |
| 26:Z:59:TYR:CZ | 26:Z:64:VAL:HG21 | 2.37 | 0.59 |
| 34:2:1231:U:OP1 | 34:2:1257:U:O3' | 2.21 | 0.59 |
| 34:2:157:U:C4 | 34:2:419:A:H4' | 2.38 | 0.59 |
| 7:G:154:ARG:H | 34:2:78:A:C5' | 2.16 | 0.59 |
| 10:J:173:ALA:HA | 34:2:510:A:OP2 | 2.03 | 0.59 |
| 34:2:1671:G:C6 | 34:2:1672:C:N4 | 2.70 | 0.59 |
| 34:2:886:A:H2' | 34:2:887:U:O4' | 2.02 | 0.59 |
| 34:2:1217:G:O6 | 34:2:1442:A:H5'' | 2.03 | 0.59 |
| 34:2:1462:G:N2 | 34:2:1463:C:C2 | 2.71 | 0.59 |
| 34:2:266:U:O2 | 34:2:287:A:C2 | 2.56 | 0.59 |
| 24:X:41:SER:O | 24:X:43:PHE:N | 2.36 | 0.59 |
| 26:Z:54:ALA:HB1 | 26:Z:89:ILE:HD11 | 1.83 | 0.59 |
| 34:2:1218:A:H62 | 34:2:1263:G:H2' | 1.68 | 0.58 |
| 34:2:749:U:H2' | 34:2:750:U:C6 | 2.37 | 0.58 |
| 17:Q:36:ILE:HD11 | 17:Q:48:VAL:HG12 | 1.85 | 0.58 |
| 34:2:1082:G:C6 | 34:2:1083:A:N7 | 2.71 | 0.58 |
| 3:C:50:VAL:HG21 | 3:C:73:ILE:HG23 | 1.85 | 0.58 |
| 34:2:958:U:H2' | 34:2:958:U:O2 | 2.03 | 0.58 |
| 9:I:83:TYR:CZ | 9:I:196:ARG:HG2 | 2.37 | 0.58 |
| 34:2:1215:C:H2' | 34:2:1442:A:N1 | 2.19 | 0.58 |
| 34:2:1103:U:H2' | 34:2:1104:C:O4' | 2.04 | 0.58 |
| 34:2:1120:C:C2 | 34:2:1126:G:C2 | 2.92 | 0.58 |
| 34:2:1349:G:C2 | 34:2:1374:C:O2 | 2.57 | 0.58 |
| 34:2:1462:G:N1 | 34:2:1463:C:C4 | 2.72 | 0.58 |

Continued on next page...

Continued from previous page...

| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 24:X:63:GLN:HG3 | 24:X:64:PRO:HD2 | 1.84 | 0.58 |
| 26:Z:105:THR:O | 26:Z:105:THR:HG22 | 2.01 | 0.58 |
| 34:2:291:U:H2' | 34:2:292:U:C6 | 2.39 | 0.58 |
| 7:G:171:LYS:CE | 34:2:71:A:H61 | 2.12 | 0.58 |
| 34:2:1086:A:H2' | 34:2:1087:A:C8 | 2.38 | 0.58 |
| 34:2:561:G:C2 | 34:2:583:C:C2 | 2.93 | 0.57 |
| 34:2:561:G:C2 | 34:2:583:C:O2 | 2.57 | 0.57 |
| 34:2:1223:A:N6 | 34:2:1224:U:O4 | 2.37 | 0.57 |
| 34:2:1222:A:N1 | 34:2:1260:G:C5 | 2.73 | 0.57 |
| 34:2:1256:U:C6 | 34:2:1257:U:H1' | 2.40 | 0.57 |
| 15:O:81:ILE:HB | 15:O:115:ILE:HG22 | 1.87 | 0.57 |
| 34:2:70:C:C4 | 34:2:71:A:C6 | 2.93 | 0.57 |
| 1:A:120:LEU:HD11 | 1:A:144:ILE:HD12 | 1.87 | 0.57 |
| 34:2:556:G:N2 | 34:2:558:C:C2 | 2.73 | 0.57 |
| 34:2:1757:C:H2' | 34:2:1758:G:O4' | 2.05 | 0.57 |
| 9:I:76:THR:HG21 | 9:I:104:ILE:HG23 | 1.86 | 0.57 |
| 26:Z:54:ALA:CB | 26:Z:88:ILE:HG21 | 2.32 | 0.57 |
| 34:2:1215:C:O2' | 34:2:1442:A:C6 | 2.58 | 0.57 |
| 34:2:1793:U:O3' | 34:2:1795:A:N1 | 2.38 | 0.57 |
| 34:2:513:G:N7 | 34:2:536:G:C2 | 2.73 | 0.57 |
| 1:A:129:ASP:O | 1:A:132:ALA:N | 2.35 | 0.56 |
| 34:2:1349:G:C6 | 34:2:1374:C:N3 | 2.73 | 0.56 |
| 1:A:18:LEU:HD22 | 18:R:106:THR:HG23 | 1.86 | 0.56 |
| 25:Y:40:LEU:HD13 | 25:Y:60:PHE:CZ | 2.39 | 0.56 |
| 34:2:137:U:N3 | 34:2:138:A:N6 | 2.53 | 0.56 |
| 9:I:99:ALA:N | 9:I:170:ILE:O | 2.36 | 0.56 |
| 12:L:99:ARG:HB2 | 24:X:12:ALA:HB2 | 1.87 | 0.56 |
| 34:2:1671:G:C2 | 34:2:1672:C:C2 | 2.94 | 0.56 |
| 16:P:121:ILE:HD11 | 19:S:125:ILE:HD13 | 1.88 | 0.56 |
| 34:2:1182:A:N3 | 34:2:1209:C:O2' | 2.26 | 0.56 |
| 34:2:1218:A:N6 | 34:2:1263:G:H2' | 2.19 | 0.56 |
| 24:X:69:ARG:NH1 | 24:X:116:ASP:OD2 | 2.38 | 0.56 |
| 34:2:1012:A:H2' | 34:2:1013:G:C1' | 2.36 | 0.56 |
| 34:2:908:U:H2' | 34:2:909:C:C5 | 2.40 | 0.56 |
| 34:2:1218:A:N7 | 34:2:1264:G:H1' | 2.20 | 0.56 |
| 34:2:884:G:H2' | 34:2:885:U:O2' | 2.06 | 0.56 |
| 3:C:170:VAL:HG11 | 3:C:215:THR:HA | 1.87 | 0.56 |
| 23:W:40:VAL:HG11 | 23:W:103:ILE:HD12 | 1.86 | 0.56 |
| 34:2:556:G:C2 | 34:2:558:C:N3 | 2.74 | 0.56 |
| 34:2:564:C:O2' | 34:2:565:C:OP2 | 2.22 | 0.56 |
| 34:2:823:G:C2 | 34:2:848:C:N3 | 2.74 | 0.56 |

Continued on next page...

Continued from previous page...

| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 7:G:153:VAL:HG21 | 7:G:178:LEU:HD11 | 1.87 | 0.56 |
| 23:W:82:LYS:O | 23:W:84:ALA:N | 2.37 | 0.56 |
| 34:2:1154:G:C2 | 34:2:1622:C:C2 | 2.94 | 0.56 |
| 34:2:1277:G:C2 | 34:2:1278:C:C2 | 2.95 | 0.55 |
| 34:2:511:A:C2' | 34:2:512:U:C5' | 2.76 | 0.55 |
| 34:2:1042:A:C6 | 34:2:1043:U:C4 | 2.93 | 0.55 |
| 7:G:136:LYS:HZ2 | 34:2:65:A:P | 2.20 | 0.55 |
| 34:2:1239:U:O2' | 34:2:1241:A:C8 | 2.59 | 0.55 |
| 34:2:1230:U:C5' | 34:2:1258:U:H4' | 2.35 | 0.55 |
| 34:2:1173:C:N4 | 34:2:1464:G:C6 | 2.75 | 0.55 |
| 34:2:1586:G:N1 | 34:2:1587:C:C2 | 2.73 | 0.55 |
| 34:2:209:A:C6 | 34:2:210:U:C4 | 2.94 | 0.55 |
| 1:A:14:ALA:O | 1:A:18:LEU:HG | 2.06 | 0.55 |
| 16:P:19:GLY:HA3 | 19:S:94:ASP:C | 2.26 | 0.55 |
| 34:2:150:G:C2 | 34:2:163:A:C5 | 2.95 | 0.55 |
| 34:2:50:C:O2 | 34:2:429:G:C2 | 2.60 | 0.55 |
| 23:W:55:ASP:O | 23:W:57:ARG:N | 2.39 | 0.55 |
| 34:2:1042:A:C2 | 34:2:1043:U:C2 | 2.95 | 0.55 |
| 34:2:1173:C:C2 | 34:2:1464:G:C2 | 2.94 | 0.55 |
| 34:2:1223:A:C4 | 34:2:1259:U:O2 | 2.59 | 0.55 |
| 6:F:185:ALA:HB2 | 6:F:192:ILE:HG23 | 1.89 | 0.55 |
| 34:2:1081:C:O2' | 34:2:1082:G:H5'' | 2.06 | 0.55 |
| 34:2:1292:U:O4 | 34:2:1293:G:C4 | 2.60 | 0.55 |
| 34:2:976:A:H2' | 34:2:977:A:O4' | 2.07 | 0.55 |
| 11:K:46:LEU:HD13 | 11:K:66:TYR:CE2 | 2.42 | 0.55 |
| 34:2:884:G:C3' | 34:2:885:U:C4' | 2.85 | 0.55 |
| 34:2:990:G:O2' | 34:2:1012:A:N6 | 2.39 | 0.55 |
| 34:2:1042:A:C6 | 34:2:1043:U:N3 | 2.75 | 0.55 |
| 34:2:1257:U:H2' | 34:2:1258:U:O4' | 2.06 | 0.55 |
| 34:2:884:G:H3' | 34:2:885:U:C4' | 2.37 | 0.55 |
| 26:Z:58:ARG:NH1 | 26:Z:103:ARG:CZ | 2.68 | 0.55 |
| 34:2:69:G:C2 | 34:2:70:C:C2 | 2.95 | 0.54 |
| 34:2:1183:A:C2 | 34:2:1452:G:N3 | 2.74 | 0.54 |
| 34:2:1343:A:H2' | 34:2:1344:A:C8 | 2.42 | 0.54 |
| 25:Y:121:THR:OG1 | 34:2:148:C:OP1 | 2.20 | 0.54 |
| 34:2:1778:G:HO2' | 34:2:1779:A:H8 | 1.53 | 0.54 |
| 34:2:262:C:O2' | 34:2:263:G:O4' | 2.25 | 0.54 |
| 34:2:161:A:C6 | 34:2:162:G:C6 | 2.95 | 0.54 |
| 34:2:65:A:HO2' | 34:2:83:G:N2 | 2.06 | 0.54 |
| 1:A:49:ASN:O | 1:A:53:THR:HG23 | 2.08 | 0.54 |
| 34:2:562:U:H2' | 34:2:563:G:C8 | 2.43 | 0.54 |

Continued on next page...

Continued from previous page...

| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 7:G:131:LYS:HB3 | 34:2:165:C:O2' | 2.07 | 0.54 |
| 34:2:594:G:C6 | 34:2:595:C:N4 | 2.76 | 0.54 |
| 10:J:170:GLY:CA | 34:2:511:A:O5' | 2.56 | 0.54 |
| 34:2:1072:G:N2 | 34:2:1073:G:C6 | 2.75 | 0.54 |
| 34:2:1220:A:H2' | 34:2:1221:C:C6 | 2.43 | 0.54 |
| 34:2:147:U:H2' | 34:2:148:C:O4' | 2.08 | 0.54 |
| 24:X:63:GLN:NE2 | 34:2:1753:A:P | 2.54 | 0.54 |
| 34:2:1043:U:H3 | 34:2:1044:C:N4 | 2.05 | 0.54 |
| 34:2:1726:U:H2' | 34:2:1727:C:C6 | 2.43 | 0.54 |
| 34:2:268:G:C6 | 34:2:269:C:C4 | 2.96 | 0.54 |
| 34:2:168:A:C5 | 34:2:170:A:C8 | 2.95 | 0.54 |
| 34:2:65:A:H2' | 34:2:83:G:C6 | 2.43 | 0.54 |
| 3:C:173:ARG:NH1 | 34:2:1096:U:O3' | 2.41 | 0.54 |
| 34:2:1219:C:O2 | 34:2:1262:G:N1 | 2.41 | 0.54 |
| 34:2:1333:U:H2' | 34:2:1334:U:O4' | 2.08 | 0.54 |
| 34:2:1499:C:C2 | 34:2:1505:G:C2 | 2.95 | 0.54 |
| 34:2:922:A:N1 | 34:2:923:A:C6 | 2.76 | 0.54 |
| 34:2:1222:A:C2 | 34:2:1260:G:C4 | 2.96 | 0.53 |
| 34:2:1378:U:H2' | 34:2:1379:U:C6 | 2.44 | 0.53 |
| 7:G:155:ASP:HB2 | 34:2:78:A:OP2 | 2.08 | 0.53 |
| 26:Z:52:LYS:HD2 | 26:Z:53:GLU:CG | 2.37 | 0.53 |
| 34:2:121:U:H2' | 34:2:122:U:C6 | 2.43 | 0.53 |
| 34:2:1772:G:H2' | 34:2:1773:U:O4' | 2.08 | 0.53 |
| 7:G:171:LYS:HE3 | 34:2:71:A:N6 | 2.18 | 0.53 |
| 34:2:150:G:C6 | 34:2:163:A:C6 | 2.96 | 0.53 |
| 23:W:75:ILE:HD11 | 23:W:125:ILE:HB | 1.90 | 0.53 |
| 6:F:53:VAL:HG12 | 6:F:53:VAL:O | 2.08 | 0.53 |
| 23:W:16:ASN:O | 23:W:20:THR:HG23 | 2.08 | 0.53 |
| 34:2:1363:G:N1 | 34:2:1364:C:C4 | 2.77 | 0.53 |
| 34:2:1794:C:O2 | 34:2:1794:C:O4' | 2.25 | 0.53 |
| 34:2:394:U:H2' | 34:2:395:G:O4' | 2.08 | 0.53 |
| 34:2:70:C:N4 | 34:2:71:A:C2 | 2.77 | 0.53 |
| 9:I:82:VAL:HG12 | 9:I:197:LEU:CD2 | 2.37 | 0.53 |
| 34:2:1671:G:C5 | 34:2:1672:C:C4 | 2.97 | 0.53 |
| 34:2:1671:G:C6 | 34:2:1672:C:C4 | 2.97 | 0.53 |
| 34:2:143:G:C6 | 34:2:170:A:N6 | 2.68 | 0.53 |
| 26:Z:104:ALA:CB | 26:Z:105:THR:HA | 2.21 | 0.53 |
| 6:F:97:ASN:HB3 | 34:2:1609:A:O2' | 2.09 | 0.53 |
| 34:2:170:A:H2' | 34:2:171:C:C6 | 2.44 | 0.53 |
| 34:2:1653:A:N6 | 34:2:1743:G:O2' | 2.42 | 0.53 |
| 34:2:22:A:C2 | 34:2:23:G:C8 | 2.97 | 0.53 |

Continued on next page...

Continued from previous page...

| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|-----------------|------------------|--------------------------|-------------------|
| 34:2:1494:U:O2 | 34:2:1509:G:O6 | 2.27 | 0.53 |
| 34:2:1231:U:C4 | 34:2:1253:U:C6 | 2.97 | 0.52 |
| 34:2:406:A:H2' | 34:2:407:C:C6 | 2.44 | 0.52 |
| 34:2:478:C:H2' | 34:2:479:G:O4' | 2.09 | 0.52 |
| 7:G:155:ASP:O | 7:G:157:VAL:HB | 2.08 | 0.52 |
| 10:J:121:SER:O | 10:J:123:HIS:N | 2.41 | 0.52 |
| 34:2:1277:G:C6 | 34:2:1278:C:C4 | 2.97 | 0.52 |
| 34:2:150:G:N1 | 34:2:162:G:N7 | 2.57 | 0.52 |
| 7:G:190:GLN:NE2 | 34:2:266:U:O4 | 2.42 | 0.52 |
| 34:2:582:C:O2 | 34:2:582:C:H2' | 2.08 | 0.52 |
| 34:2:1146:A:H2' | 34:2:1147:C:O4' | 2.09 | 0.52 |
| 34:2:467:A:N1 | 34:2:593:A:O2' | 2.38 | 0.52 |
| 34:2:565:C:H2' | 34:2:566:A:H8 | 1.74 | 0.52 |
| 34:2:700:C:C2 | 34:2:739:G:N1 | 2.77 | 0.52 |
| 34:2:886:A:C5 | 34:2:887:U:C4 | 2.98 | 0.52 |
| 6:F:115:ILE:O | 6:F:119:THR:HG23 | 2.08 | 0.52 |
| 34:2:1338:C:O2' | 34:2:1340:A:N7 | 2.29 | 0.52 |
| 34:2:150:G:C6 | 34:2:163:A:N6 | 2.77 | 0.52 |
| 34:2:25:C:O4' | 34:2:25:C:O2 | 2.26 | 0.52 |
| 34:2:268:G:C2 | 34:2:269:C:C2 | 2.97 | 0.52 |
| 34:2:628:U:C2 | 34:2:969:A:N6 | 2.77 | 0.52 |
| 34:2:86:A:H2' | 34:2:87:C:C6 | 2.45 | 0.52 |
| 5:E:149:TYR:HB3 | 7:G:208:TYR:CD1 | 2.44 | 0.52 |
| 26:Z:56:THR:O | 26:Z:57:TYR:HB2 | 2.10 | 0.52 |
| 34:2:266:U:O2 | 34:2:267:C:C5 | 2.63 | 0.52 |
| 34:2:1771:C:C2 | 34:2:1787:G:C2 | 2.97 | 0.52 |
| 34:2:519:A:N1 | 34:2:532:U:C2 | 2.77 | 0.52 |
| 34:2:700:C:N3 | 34:2:739:G:C6 | 2.78 | 0.52 |
| 34:2:884:G:C4 | 34:2:885:U:H1' | 2.44 | 0.52 |
| 9:I:142:ARG:NH2 | 34:2:196:A:N1 | 2.57 | 0.52 |
| 34:2:1137:A:H2' | 34:2:1138:A:C8 | 2.44 | 0.52 |
| 34:2:1671:G:H2' | 34:2:1672:C:C6 | 2.45 | 0.52 |
| 34:2:360:C:C2 | 34:2:383:G:C2 | 2.97 | 0.52 |
| 26:Z:54:ALA:N | 26:Z:55:PRO:CD | 2.73 | 0.52 |
| 34:2:1041:G:H2' | 34:2:1042:A:O4' | 2.10 | 0.52 |
| 34:2:255:A:H2' | 34:2:256:A:C8 | 2.45 | 0.52 |
| 34:2:560:G:O6 | 34:2:584:A:C6 | 2.63 | 0.52 |
| 34:2:508:G:H2' | 34:2:509:G:O4' | 2.09 | 0.52 |
| 34:2:1014:U:C6 | 34:2:1015:C:N3 | 2.78 | 0.52 |
| 34:2:1586:G:C6 | 34:2:1587:C:C4 | 2.97 | 0.52 |
| 34:2:214:A:C5 | 34:2:241:U:C6 | 2.97 | 0.52 |

Continued on next page...

Continued from previous page...

| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 34:2:431:G:C6 | 34:2:432:C:N3 | 2.78 | 0.52 |
| 34:2:509:G:C6 | 34:2:510:A:N7 | 2.78 | 0.52 |
| 34:2:309:C:C2 | 34:2:356:G:C2 | 2.98 | 0.51 |
| 34:2:624:C:H2' | 34:2:625:U:C6 | 2.45 | 0.51 |
| 15:O:123:SER:O | 34:2:884:G:N2 | 2.41 | 0.51 |
| 26:Z:103:ARG:O | 26:Z:104:ALA:O | 2.28 | 0.51 |
| 34:2:1137:A:C4 | 34:2:1138:A:N7 | 2.78 | 0.51 |
| 34:2:1651:C:C2 | 34:2:1746:G:C2 | 2.98 | 0.51 |
| 34:2:820:U:H2' | 34:2:821:U:C6 | 2.45 | 0.51 |
| 8:H:93:LEU:HD21 | 8:H:125:ILE:HG23 | 1.92 | 0.51 |
| 12:L:101:GLU:OE2 | 24:X:13:ARG:N | 2.43 | 0.51 |
| 14:N:94:LYS:O | 14:N:98:VAL:HG23 | 2.09 | 0.51 |
| 34:2:1012:A:C2' | 34:2:1013:G:O4' | 2.53 | 0.51 |
| 7:G:174:LYS:HD3 | 34:2:65:A:H5' | 1.93 | 0.51 |
| 7:G:83:CYS:N | 34:2:161:A:OP1 | 2.43 | 0.51 |
| 9:I:68:ALA:HB1 | 12:L:20:PHE:CZ | 2.46 | 0.51 |
| 34:2:1266:G:O2' | 34:2:1446:G:O2' | 2.27 | 0.51 |
| 34:2:520:A:C2 | 34:2:531:U:N3 | 2.78 | 0.51 |
| 2:B:99:ASN:O | 2:B:101:HIS:N | 2.43 | 0.51 |
| 34:2:1349:G:N1 | 34:2:1374:C:C2 | 2.78 | 0.51 |
| 34:2:28:A:H2' | 34:2:29:U:O4' | 2.10 | 0.51 |
| 34:2:849:A:C2 | 34:2:850:U:C2 | 2.98 | 0.51 |
| 34:2:1070:U:H5'' | 34:2:1071:C:P | 2.50 | 0.51 |
| 34:2:214:A:C5 | 34:2:215:U:C5 | 2.98 | 0.51 |
| 34:2:776:G:N2 | 34:2:777:C:C2 | 2.79 | 0.51 |
| 34:2:928:A:P | 34:2:930:C:N4 | 2.84 | 0.51 |
| 34:2:150:G:N2 | 34:2:163:A:C4 | 2.79 | 0.51 |
| 34:2:480:A:N1 | 34:2:506:U:C5 | 2.76 | 0.51 |
| 15:O:123:SER:HB3 | 34:2:884:G:H1' | 1.92 | 0.51 |
| 34:2:1020:C:C4 | 34:2:1021:C:C4 | 2.99 | 0.51 |
| 34:2:1120:C:O2 | 34:2:1126:G:C2 | 2.63 | 0.51 |
| 34:2:1353:G:C6 | 34:2:1354:C:C4 | 2.99 | 0.51 |
| 34:2:273:G:C6 | 34:2:274:C:N4 | 2.79 | 0.51 |
| 34:2:425:G:N2 | 34:2:426:C:C2 | 2.79 | 0.51 |
| 34:2:885:U:H2' | 34:2:886:A:O4' | 2.10 | 0.51 |
| 34:2:1558:U:O2 | 34:2:1558:U:O4' | 2.28 | 0.51 |
| 34:2:541:A:H2' | 34:2:542:C:H3' | 1.93 | 0.51 |
| 34:2:642:G:C2 | 34:2:692:C:O2 | 2.63 | 0.51 |
| 8:H:107:ARG:HD3 | 34:2:698:U:H1' | 1.93 | 0.51 |
| 3:C:86:MET:HA | 3:C:86:MET:HE3 | 1.92 | 0.51 |
| 34:2:85:A:O2' | 34:2:147:U:O3' | 2.22 | 0.51 |

Continued on next page...

Continued from previous page...

| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 34:2:1611:U:C5 | 34:2:1612:A:C2 | 2.98 | 0.51 |
| 34:2:70:C:C4 | 34:2:71:A:C5 | 2.98 | 0.51 |
| 16:P:34:VAL:HG21 | 16:P:45:PHE:CG | 2.45 | 0.51 |
| 24:X:63:GLN:HB3 | 24:X:64:PRO:HD2 | 1.93 | 0.51 |
| 34:2:1137:A:H2' | 34:2:1138:A:H8 | 1.76 | 0.50 |
| 34:2:1363:G:C2 | 34:2:1364:C:C4 | 2.99 | 0.50 |
| 1:A:148:ASP:OD1 | 1:A:151:SER:N | 2.44 | 0.50 |
| 26:Z:54:ALA:CB | 26:Z:88:ILE:HG22 | 2.41 | 0.50 |
| 34:2:980:U:O2' | 34:2:1122:C:N3 | 2.45 | 0.50 |
| 34:2:72:A:H2' | 34:2:72:A:N3 | 2.26 | 0.50 |
| 24:X:65:ASN:HB3 | 34:2:574:C:H41 | 1.76 | 0.50 |
| 34:2:887:U:O4 | 34:2:888:U:O4 | 2.28 | 0.50 |
| 34:2:89:G:C6 | 34:2:90:C:C4 | 3.00 | 0.50 |
| 34:2:1173:C:C2 | 34:2:1464:G:N2 | 2.79 | 0.50 |
| 24:X:63:GLN:HG3 | 24:X:64:PRO:CD | 2.41 | 0.50 |
| 26:Z:104:ALA:HB1 | 26:Z:105:THR:OG1 | 2.12 | 0.50 |
| 34:2:1353:G:C2 | 34:2:1354:C:C2 | 2.99 | 0.50 |
| 34:2:281:C:H2' | 34:2:282:U:O4' | 2.12 | 0.50 |
| 34:2:65:A:C5 | 34:2:83:G:C5 | 3.00 | 0.50 |
| 6:F:192:ILE:HD11 | 34:2:1471:U:H5' | 1.94 | 0.50 |
| 15:O:129:LYS:HA | 34:2:989:C:H4' | 1.94 | 0.50 |
| 23:W:87:GLU:O | 23:W:90:THR:HG22 | 2.12 | 0.50 |
| 34:2:137:U:C2 | 34:2:138:A:C6 | 2.99 | 0.50 |
| 34:2:150:G:N1 | 34:2:163:A:C6 | 2.80 | 0.50 |
| 34:2:1666:G:H2' | 34:2:1667:U:O4' | 2.11 | 0.50 |
| 1:A:18:LEU:HD22 | 18:R:106:THR:CG2 | 2.41 | 0.50 |
| 21:U:34:LEU:HD11 | 21:U:89:ARG:HG3 | 1.94 | 0.50 |
| 34:2:1471:U:O2 | 34:2:1471:U:C2' | 2.59 | 0.50 |
| 34:2:261:U:N3 | 34:2:262:C:C4 | 2.80 | 0.50 |
| 34:2:508:G:H2' | 34:2:509:G:C8 | 2.47 | 0.50 |
| 34:2:542:C:HO2' | 34:2:543:A:P | 2.33 | 0.50 |
| 34:2:883:A:C3' | 34:2:884:G:H5' | 2.40 | 0.50 |
| 7:G:155:ASP:N | 34:2:78:A:H5'' | 2.23 | 0.50 |
| 34:2:515:G:O6 | 34:2:536:G:N2 | 2.45 | 0.50 |
| 34:2:700:C:O2 | 34:2:739:G:C2 | 2.65 | 0.50 |
| 7:G:154:ARG:C | 34:2:78:A:H3' | 2.32 | 0.50 |
| 17:Q:50:GLU:N | 17:Q:51:PRO:CD | 2.74 | 0.50 |
| 6:F:194:GLU:OE2 | 26:Z:59:TYR:HE2 | 1.95 | 0.50 |
| 34:2:1238:U:H1' | 34:2:1247:C:N4 | 2.27 | 0.49 |
| 7:G:173:PRO:HA | 34:2:66:U:O4' | 2.11 | 0.49 |
| 34:2:1005:C:C6 | 34:2:1006:C:C5 | 3.00 | 0.49 |

Continued on next page...

Continued from previous page...

| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 34:2:1417:G:C2 | 34:2:1418:C:O2 | 2.65 | 0.49 |
| 34:2:1661:G:C6 | 34:2:1662:C:C4 | 3.00 | 0.49 |
| 34:2:564:C:C4 | 34:2:575:G:C8 | 3.00 | 0.49 |
| 34:2:150:G:C2 | 34:2:163:A:C4 | 3.00 | 0.49 |
| 34:2:1611:U:O2 | 34:2:1611:U:O4' | 2.27 | 0.49 |
| 34:2:266:U:H3 | 34:2:267:C:H41 | 1.60 | 0.49 |
| 34:2:38:C:O2 | 34:2:469:A:N1 | 2.44 | 0.49 |
| 1:A:73:VAL:HG13 | 1:A:120:LEU:HD12 | 1.94 | 0.49 |
| 13:M:56:VAL:HG22 | 13:M:85:ALA:HB2 | 1.94 | 0.49 |
| 34:2:1015:C:O4' | 34:2:1015:C:O2 | 2.29 | 0.49 |
| 34:2:39:A:O2' | 34:2:468:C:N4 | 2.46 | 0.49 |
| 34:2:782:G:N2 | 34:2:783:C:C2 | 2.81 | 0.49 |
| 34:2:921:G:C6 | 34:2:922:A:C6 | 3.00 | 0.49 |
| 34:2:1292:U:C5 | 34:2:1321:A:C2 | 3.01 | 0.49 |
| 34:2:1396:U:H3' | 34:2:1397:C:H5' | 1.95 | 0.49 |
| 34:2:1527:C:H2' | 34:2:1528:C:C6 | 2.46 | 0.49 |
| 6:F:189:ILE:HG23 | 34:2:1533:U:O2 | 2.12 | 0.49 |
| 34:2:561:G:H2' | 34:2:562:U:C6 | 2.46 | 0.49 |
| 10:J:62:ARG:HB2 | 10:J:69:ARG:HG2 | 1.95 | 0.49 |
| 17:Q:52:LEU:HD22 | 17:Q:60:PHE:CZ | 2.47 | 0.49 |
| 34:2:1183:A:H2 | 34:2:1453:G:O4' | 1.95 | 0.49 |
| 34:2:70:C:C5 | 34:2:71:A:C6 | 3.00 | 0.49 |
| 15:O:123:SER:HA | 34:2:928:A:C5 | 2.47 | 0.49 |
| 34:2:932:A:N7 | 34:2:934:U:H1' | 2.26 | 0.49 |
| 34:2:1083:A:H2' | 34:2:1084:G:O4' | 2.13 | 0.49 |
| 34:2:1346:U:O2 | 34:2:1514:A:H5' | 2.13 | 0.49 |
| 16:P:115:TYR:OH | 34:2:1554:A:OP1 | 2.29 | 0.49 |
| 34:2:30:G:H2' | 34:2:31:C:O4' | 2.13 | 0.49 |
| 34:2:922:A:C2 | 34:2:923:A:C6 | 3.01 | 0.49 |
| 34:2:1222:A:N6 | 34:2:1260:G:O6 | 2.46 | 0.49 |
| 34:2:1571:A:O4' | 34:2:1572:G:C2 | 2.65 | 0.49 |
| 34:2:1671:G:C5 | 34:2:1672:C:N4 | 2.80 | 0.49 |
| 34:2:560:G:N3 | 34:2:561:G:N7 | 2.60 | 0.49 |
| 7:G:171:LYS:CE | 34:2:71:A:N6 | 2.75 | 0.49 |
| 34:2:886:A:C6 | 34:2:887:U:C4 | 3.01 | 0.49 |
| 13:M:24:VAL:HG22 | 13:M:124:ARG:HD3 | 1.94 | 0.49 |
| 34:2:925:A:H4' | 34:2:1015:C:O2' | 2.13 | 0.49 |
| 34:2:1255:A:H1' | 34:2:1257:U:O4 | 2.12 | 0.49 |
| 34:2:767:U:O4' | 34:2:767:U:O2 | 2.30 | 0.49 |
| 34:2:94:U:H2' | 34:2:95:G:O4' | 2.13 | 0.49 |
| 34:2:1131:A:C2 | 34:2:1132:A:C4 | 3.01 | 0.49 |

Continued on next page...

Continued from previous page...

| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|-------------------|--------------------------|-------------------|
| 34:2:390:A:O2' | 34:2:1728:A:O2' | 2.31 | 0.49 |
| 34:2:334:U:H2' | 34:2:335:G:O4' | 2.12 | 0.49 |
| 34:2:261:U:O4 | 34:2:262:C:N4 | 2.46 | 0.48 |
| 20:T:31:PRO:HG3 | 20:T:54:PHE:CZ | 2.48 | 0.48 |
| 34:2:1501:A:O2' | 34:2:1502:G:OP1 | 2.26 | 0.48 |
| 34:2:1637:C:H2' | 34:2:1638:C:O4' | 2.13 | 0.48 |
| 34:2:975:G:H1 | 34:2:1022:A:HO2' | 1.59 | 0.48 |
| 34:2:1046:G:N1 | 34:2:1071:C:C2 | 2.81 | 0.48 |
| 34:2:522:G:H8 | 34:2:522:G:O5' | 1.97 | 0.48 |
| 34:2:89:G:C2 | 34:2:90:C:C2 | 3.01 | 0.48 |
| 25:Y:132:ARG:O | 25:Y:135:ASP:N | 2.46 | 0.48 |
| 34:2:1175:G:C2 | 34:2:1176:C:C2 | 3.02 | 0.48 |
| 34:2:150:G:N1 | 34:2:163:A:C5 | 2.81 | 0.48 |
| 34:2:1032:C:N4 | 34:2:1033:C:N4 | 2.61 | 0.48 |
| 34:2:1306:U:O2 | 34:2:1306:U:O4' | 2.31 | 0.48 |
| 7:G:136:LYS:HB3 | 34:2:167:A:H4' | 1.96 | 0.48 |
| 34:2:888:U:O4' | 34:2:987:A:H4' | 2.14 | 0.48 |
| 14:N:35:GLU:HA | 14:N:38:ILE:HG12 | 1.95 | 0.48 |
| 19:S:143:ARG:NH1 | 34:2:1460:G:N7 | 2.62 | 0.48 |
| 34:2:1222:A:C6 | 34:2:1260:G:N1 | 2.82 | 0.48 |
| 34:2:1400:G:C6 | 34:2:1401:C:C4 | 3.02 | 0.48 |
| 34:2:14:C:C2 | 34:2:1140:G:C2 | 3.02 | 0.48 |
| 34:2:487:G:C2 | 34:2:499:C:C2 | 3.02 | 0.48 |
| 34:2:594:G:C2 | 34:2:595:C:N3 | 2.81 | 0.48 |
| 34:2:637:U:O4' | 34:2:637:U:O2 | 2.31 | 0.48 |
| 34:2:763:G:O6 | 34:2:772:G:O6 | 2.30 | 0.48 |
| 6:F:203:ALA:HA | 6:F:213:ILE:HD11 | 1.96 | 0.48 |
| 34:2:9:U:H2' | 34:2:11:A:OP2 | 2.13 | 0.48 |
| 34:2:1220:A:C5 | 34:2:1221:C:C4 | 3.02 | 0.48 |
| 34:2:1786:G:H2' | 34:2:1787:G:O4' | 2.14 | 0.48 |
| 34:2:388:G:C2 | 34:2:408:C:C2 | 3.02 | 0.48 |
| 34:2:963:U:O4' | 34:2:964:U:C5 | 2.66 | 0.48 |
| 10:J:80:LEU:O | 10:J:83:ILE:HG22 | 2.13 | 0.48 |
| 34:2:1255:A:O4' | 34:2:1257:U:C5 | 2.67 | 0.48 |
| 34:2:1499:C:N3 | 34:2:1505:G:C2 | 2.82 | 0.48 |
| 34:2:1661:G:C2 | 34:2:1662:C:C2 | 3.02 | 0.48 |
| 25:Y:43:LYS:O | 25:Y:46:GLU:HG3 | 2.14 | 0.48 |
| 34:2:511:A:C6 | 34:2:512:U:C4 | 3.02 | 0.48 |
| 19:S:42:TYR:CE1 | 19:S:101:LEU:HD11 | 2.49 | 0.48 |
| 34:2:151:U:O2 | 34:2:162:G:C8 | 2.67 | 0.47 |
| 34:2:152:G:H2' | 34:2:153:G:C8 | 2.49 | 0.47 |

Continued on next page...

Continued from previous page...

| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 34:2:1620:G:C2 | 34:2:1621:C:C2 | 3.02 | 0.47 |
| 24:X:65:ASN:CB | 34:2:574:C:H41 | 2.27 | 0.47 |
| 24:X:19:ARG:HA | 24:X:19:ARG:HD2 | 1.57 | 0.47 |
| 34:2:1138:A:H2' | 34:2:1139:G:O4' | 2.14 | 0.47 |
| 34:2:1586:G:C2 | 34:2:1587:C:C2 | 3.02 | 0.47 |
| 34:2:1670:G:C2 | 34:2:1671:G:C5 | 3.03 | 0.47 |
| 34:2:30:G:C6 | 34:2:31:C:C4 | 3.02 | 0.47 |
| 34:2:84:A:H2' | 34:2:85:A:O4' | 2.14 | 0.47 |
| 34:2:921:G:H2' | 34:2:922:A:C8 | 2.49 | 0.47 |
| 18:R:25:THR:O | 18:R:27:ASP:N | 2.47 | 0.47 |
| 34:2:1262:G:C2 | 34:2:1263:G:H1' | 2.49 | 0.47 |
| 13:M:55:LEU:HD22 | 13:M:79:LEU:HD22 | 1.96 | 0.47 |
| 34:2:1044:C:C4 | 34:2:1072:G:C2 | 3.02 | 0.47 |
| 34:2:204:U:C2 | 34:2:205:A:C8 | 3.03 | 0.47 |
| 34:2:1083:A:N6 | 34:2:1089:C:N4 | 2.62 | 0.47 |
| 34:2:1497:G:C6 | 34:2:1498:C:C4 | 3.02 | 0.47 |
| 34:2:1533:U:O2 | 34:2:1533:U:O4' | 2.31 | 0.47 |
| 34:2:212:A:C6 | 34:2:252:A:C6 | 3.03 | 0.47 |
| 34:2:560:G:C2' | 34:2:561:G:C8 | 2.82 | 0.47 |
| 34:2:96:G:C6 | 34:2:97:C:C4 | 3.03 | 0.47 |
| 34:2:1042:A:C5 | 34:2:1043:U:C4 | 3.02 | 0.47 |
| 34:2:1240:G:H2' | 34:2:1241:A:O5' | 2.15 | 0.47 |
| 34:2:1220:A:N6 | 34:2:1261:U:O4 | 2.47 | 0.47 |
| 34:2:207:U:O2 | 34:2:208:U:C2 | 2.67 | 0.47 |
| 34:2:360:C:N3 | 34:2:383:G:C2 | 2.82 | 0.47 |
| 34:2:565:C:O2' | 34:2:566:A:O4' | 2.25 | 0.47 |
| 9:I:10:LYS:O | 9:I:11:ARG:C | 2.52 | 0.47 |
| 26:Z:52:LYS:CD | 26:Z:53:GLU:HG3 | 2.41 | 0.47 |
| 34:2:935:G:OP1 | 34:2:1044:C:O4' | 2.33 | 0.47 |
| 34:2:1218:A:C5 | 34:2:1264:G:H1' | 2.49 | 0.47 |
| 7:G:179:VAL:HG11 | 34:2:139:C:H1' | 1.97 | 0.47 |
| 34:2:1231:U:C2 | 34:2:1253:U:H1' | 2.50 | 0.47 |
| 34:2:1437:C:H2' | 34:2:1438:C:C6 | 2.49 | 0.47 |
| 34:2:567:G:C6 | 34:2:575:G:C2 | 3.03 | 0.47 |
| 34:2:988:U:C4 | 34:2:989:C:N4 | 2.83 | 0.47 |
| 26:Z:104:ALA:CB | 26:Z:105:THR:CA | 2.85 | 0.47 |
| 26:Z:52:LYS:HG3 | 26:Z:52:LYS:O | 2.14 | 0.47 |
| 34:2:1038:A:N6 | 34:2:1077:C:H42 | 2.12 | 0.47 |
| 6:F:91:ILE:HG12 | 34:2:1443:G:C5 | 90.86 | 0.47 |
| 34:2:1444:A:N7 | 34:2:1446:G:C5 | 2.82 | 0.47 |
| 34:2:1454:C:O2 | 34:2:1454:C:O4' | 2.33 | 0.47 |

Continued on next page...

Continued from previous page...

| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 34:2:564:C:H2' | 34:2:576:G:H21 | 1.75 | 0.47 |
| 34:2:71:A:C2 | 34:2:72:A:C6 | 3.02 | 0.47 |
| 34:2:925:A:H3' | 34:2:926:C:C6 | 2.50 | 0.47 |
| 7:G:136:LYS:NZ | 34:2:65:A:P | 2.84 | 0.47 |
| 7:G:173:PRO:HB2 | 7:G:175:ILE:HD12 | 1.95 | 0.47 |
| 34:2:1040:G:H2' | 34:2:1041:G:C8 | 2.50 | 0.47 |
| 34:2:1222:A:N6 | 34:2:1260:G:C6 | 2.82 | 0.47 |
| 34:2:1400:G:C2 | 34:2:1401:C:C2 | 3.03 | 0.47 |
| 34:2:1588:G:C2 | 34:2:1589:C:C2 | 3.03 | 0.47 |
| 9:I:100:ALA:O | 9:I:170:ILE:HD12 | 2.14 | 0.47 |
| 10:J:148:VAL:HG11 | 10:J:156:ILE:HD11 | 1.96 | 0.47 |
| 34:2:1183:A:C2 | 34:2:1452:G:N2 | 2.82 | 0.47 |
| 1:A:164:ASN:HA | 1:A:170:ILE:HD11 | 1.96 | 0.47 |
| 26:Z:104:ALA:HB1 | 26:Z:105:THR:CB | 2.45 | 0.47 |
| 34:2:1081:C:O2' | 34:2:1082:G:C5' | 2.62 | 0.46 |
| 34:2:1239:U:O4' | 34:2:1245:C:N4 | 2.48 | 0.46 |
| 34:2:1560:G:C6 | 34:2:1561:C:C4 | 3.03 | 0.46 |
| 34:2:214:A:C5 | 34:2:241:U:C5 | 3.03 | 0.46 |
| 34:2:967:U:H5'' | 34:2:1032:C:O2' | 2.16 | 0.46 |
| 34:2:1598:A:H1' | 34:2:1599:G:H5' | 1.98 | 0.46 |
| 10:J:172:VAL:N | 34:2:511:A:OP2 | 2.48 | 0.46 |
| 10:J:66:ASP:HB3 | 10:J:67:PRO:CD | 2.45 | 0.46 |
| 20:T:18:TYR:CD2 | 20:T:135:ILE:HD13 | 2.50 | 0.46 |
| 34:2:1175:G:C6 | 34:2:1176:C:C4 | 3.04 | 0.46 |
| 34:2:142:G:H2' | 34:2:143:G:C8 | 2.50 | 0.46 |
| 34:2:1578:C:H2' | 34:2:1579:C:O4' | 2.15 | 0.46 |
| 34:2:274:C:N4 | 34:2:275:C:N4 | 2.64 | 0.46 |
| 34:2:585:G:C6 | 34:2:586:C:C4 | 3.03 | 0.46 |
| 34:2:980:U:H2' | 34:2:981:U:C6 | 2.50 | 0.46 |
| 3:C:169:SER:OG | 3:C:169:SER:O | 2.34 | 0.46 |
| 34:2:1222:A:N3 | 34:2:1260:G:C2 | 2.84 | 0.46 |
| 34:2:1363:G:C6 | 34:2:1364:C:N4 | 2.83 | 0.46 |
| 34:2:1620:G:C6 | 34:2:1621:C:C4 | 3.04 | 0.46 |
| 34:2:1670:G:H2' | 34:2:1671:G:C8 | 2.50 | 0.46 |
| 34:2:254:U:C4 | 34:2:255:A:N7 | 2.84 | 0.46 |
| 34:2:585:G:C2 | 34:2:586:C:C2 | 3.03 | 0.46 |
| 7:G:160:ARG:NE | 34:2:68:A:C8 | 2.83 | 0.46 |
| 34:2:884:G:C8 | 34:2:884:G:C5' | 2.85 | 0.46 |
| 34:2:935:G:C6 | 34:2:936:C:C4 | 3.03 | 0.46 |
| 7:G:175:ILE:HG22 | 34:2:78:A:N3 | 2.31 | 0.46 |
| 9:I:68:ALA:HB2 | 9:I:183:TYR:OH | 2.14 | 0.46 |

Continued on next page...

Continued from previous page...

| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|------------------|--------------------------|-------------------|
| 25:Y:33:ALA:CB | 34:2:532:U:H4' | 2.46 | 0.46 |
| 34:2:1203:A:H2' | 34:2:1203:A:N3 | 2.31 | 0.46 |
| 34:2:1290:G:H2' | 34:2:1291:G:H8 | 1.81 | 0.46 |
| 34:2:149:U:O2' | 34:2:150:G:O4' | 2.23 | 0.46 |
| 34:2:284:G:N2 | 34:2:285:C:C2 | 2.84 | 0.46 |
| 34:2:266:U:O2 | 34:2:287:A:N1 | 2.48 | 0.46 |
| 34:2:887:U:C4 | 34:2:888:U:C4 | 3.04 | 0.46 |
| 16:P:79:HIS:O | 16:P:81:ARG:N | 2.49 | 0.46 |
| 25:Y:90:ARG:HA | 25:Y:93:ARG:HD3 | 1.98 | 0.46 |
| 24:X:7:ARG:NH2 | 34:2:1099:G:O4' | 2.48 | 0.46 |
| 34:2:210:U:H2' | 34:2:211:U:C6 | 2.51 | 0.46 |
| 34:2:268:G:O6 | 34:2:285:C:N3 | 2.49 | 0.46 |
| 34:2:30:G:C2 | 34:2:31:C:C2 | 3.04 | 0.46 |
| 34:2:458:G:H3' | 34:2:459:A:C5' | 2.45 | 0.46 |
| 34:2:642:G:N1 | 34:2:692:C:C2 | 2.84 | 0.46 |
| 7:G:155:ASP:HB2 | 34:2:78:A:P | 2.55 | 0.46 |
| 21:U:95:ALA:HB1 | 21:U:99:ILE:HG21 | 1.96 | 0.46 |
| 16:P:122:THR:HG21 | 34:2:1452:G:H4' | 1.98 | 0.46 |
| 34:2:1643:G:N2 | 34:2:1644:C:C2 | 2.84 | 0.46 |
| 34:2:266:U:C2 | 34:2:287:A:N1 | 2.83 | 0.46 |
| 34:2:89:G:N1 | 34:2:90:C:C2 | 2.84 | 0.46 |
| 9:I:139:ASN:HB2 | 34:2:186:G:H2' | 1.98 | 0.46 |
| 24:X:63:GLN:CB | 24:X:64:PRO:HD2 | 2.46 | 0.46 |
| 26:Z:54:ALA:HB1 | 26:Z:89:ILE:CD1 | 2.46 | 0.46 |
| 34:2:1289:U:H2' | 34:2:1290:G:C8 | 2.51 | 0.46 |
| 7:G:74:LYS:HA | 7:G:96:SER:HA | 1.97 | 0.46 |
| 14:N:98:VAL:CG1 | 14:N:115:LEU:HB2 | 2.46 | 0.46 |
| 25:Y:59:GLY:O | 25:Y:60:PHE:HB2 | 2.16 | 0.46 |
| 34:2:1589:C:C2 | 34:2:1590:A:C8 | 3.04 | 0.46 |
| 34:2:209:A:O2' | 34:2:210:U:H5' | 2.15 | 0.46 |
| 34:2:214:A:C4 | 34:2:241:U:C5 | 3.04 | 0.46 |
| 34:2:988:U:H2' | 34:2:989:C:C2 | 2.51 | 0.46 |
| 7:G:4:ASN:HB3 | 7:G:110:ALA:HA | 1.98 | 0.46 |
| 34:2:1082:G:O6 | 34:2:1083:A:N6 | 2.49 | 0.46 |
| 34:2:1083:A:H2' | 34:2:1084:G:C8 | 2.51 | 0.46 |
| 34:2:1603:G:C6 | 34:2:1604:C:C4 | 3.03 | 0.46 |
| 34:2:1778:G:O2' | 34:2:1779:A:H8 | 1.98 | 0.46 |
| 7:G:153:VAL:HA | 34:2:78:A:H5' | 1.98 | 0.46 |
| 34:2:987:A:C2 | 34:2:988:U:C2 | 3.04 | 0.46 |
| 34:2:935:G:OP1 | 34:2:1074:C:N4 | 2.49 | 0.45 |
| 19:S:41:ARG:HD2 | 34:2:1563:C:H5" | 1.97 | 0.45 |

Continued on next page...

Continued from previous page...

| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|-------------------|--------------------------|-------------------|
| 34:2:1074:C:O2 | 34:2:1074:C:H2' | 2.10 | 0.45 |
| 34:2:1647:G:H2' | 34:2:1648:U:C6 | 2.51 | 0.45 |
| 34:2:1733:U:H2' | 34:2:1734:G:O4' | 2.16 | 0.45 |
| 34:2:991:A:H4' | 34:2:1783:U:O2' | 2.16 | 0.45 |
| 6:F:119:THR:HG22 | 6:F:193:ALA:O | 2.16 | 0.45 |
| 21:U:103:ILE:O | 21:U:106:ILE:O | 2.34 | 0.45 |
| 34:2:1042:A:N1 | 34:2:1043:U:C2 | 2.84 | 0.45 |
| 34:2:1223:A:C6 | 34:2:1259:U:C2 | 3.04 | 0.45 |
| 34:2:1439:C:H2' | 34:2:1440:U:O4' | 2.16 | 0.45 |
| 34:2:85:A:N3 | 34:2:147:U:H1' | 2.31 | 0.45 |
| 34:2:623:G:C2 | 34:2:624:C:C2 | 3.04 | 0.45 |
| 8:H:116:ARG:NH2 | 34:2:855:A:O2' | 2.49 | 0.45 |
| 34:2:89:G:C6 | 34:2:90:C:N3 | 2.84 | 0.45 |
| 15:O:41:ARG:NH2 | 34:2:915:U:O2 | 2.49 | 0.45 |
| 34:2:123:G:C5 | 34:2:124:A:C8 | 3.04 | 0.45 |
| 34:2:1730:A:H2' | 34:2:1731:C:C6 | 2.51 | 0.45 |
| 34:2:403:G:C2 | 34:2:404:C:C2 | 3.05 | 0.45 |
| 10:J:62:ARG:HB2 | 10:J:69:ARG:CG | 2.46 | 0.45 |
| 34:2:1220:A:C2 | 34:2:1262:G:C4 | 3.05 | 0.45 |
| 34:2:1598:A:H1' | 34:2:1599:G:C5' | 2.47 | 0.45 |
| 34:2:1783:U:H2' | 34:2:1784:G:C8 | 2.52 | 0.45 |
| 34:2:626:C:H2' | 34:2:627:G:O4' | 2.16 | 0.45 |
| 6:F:63:TYR:CE1 | 6:F:167:LEU:HD11 | 2.52 | 0.45 |
| 12:L:94:VAL:CG2 | 24:X:12:ALA:HB1 | 2.47 | 0.45 |
| 19:S:116:LEU:HA | 19:S:119:ILE:HG12 | 1.97 | 0.45 |
| 25:Y:130:ALA:O | 25:Y:133:ASN:HB2 | 2.16 | 0.45 |
| 34:2:1185:U:C4 | 34:2:1207:A:N6 | 2.84 | 0.45 |
| 34:2:1217:G:C4 | 34:2:1442:A:C8 | 3.04 | 0.45 |
| 34:2:266:U:C2 | 34:2:267:C:C5 | 3.04 | 0.45 |
| 34:2:96:G:C2 | 34:2:97:C:C2 | 3.05 | 0.45 |
| 3:C:183:ILE:HG21 | 3:C:190:LYS:HA | 1.98 | 0.45 |
| 25:Y:29:HIS:CD2 | 25:Y:35:VAL:HG13 | 2.51 | 0.45 |
| 34:2:1007:G:H2' | 34:2:1008:U:C6 | 2.51 | 0.45 |
| 34:2:1220:A:N1 | 34:2:1261:U:C4 | 2.85 | 0.45 |
| 34:2:1269:G:C2 | 34:2:1439:C:O2 | 2.70 | 0.45 |
| 34:2:137:U:O2 | 34:2:137:U:C2' | 2.64 | 0.45 |
| 7:G:183:ARG:NH1 | 34:2:266:U:OP1 | 2.50 | 0.45 |
| 34:2:269:C:C2' | 34:2:270:A:H8 | 2.17 | 0.45 |
| 34:2:45:U:O2' | 34:2:46:A:H2' | 2.17 | 0.45 |
| 34:2:1170:A:H2' | 34:2:1171:G:C8 | 2.52 | 0.45 |
| 34:2:1560:G:C2 | 34:2:1561:C:C2 | 3.05 | 0.45 |

Continued on next page...

Continued from previous page...

| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 2:B:194:ASN:N | 2:B:194:ASN:OD1 | 2.48 | 0.45 |
| 16:P:79:HIS:CE1 | 16:P:97:TYR:CD2 | 3.04 | 0.45 |
| 26:Z:54:ALA:HB1 | 26:Z:89:ILE:CG1 | 2.47 | 0.45 |
| 34:2:1447:U:H2' | 34:2:1448:U:O4' | 2.17 | 0.45 |
| 34:2:1497:G:C2 | 34:2:1498:C:C2 | 3.05 | 0.45 |
| 34:2:48:G:C2 | 34:2:49:C:C2 | 3.05 | 0.45 |
| 34:2:48:G:C6 | 34:2:49:C:C4 | 3.05 | 0.45 |
| 34:2:782:G:C2 | 34:2:783:C:C2 | 3.05 | 0.45 |
| 5:E:134:LYS:N | 34:2:252:A:OP1 | 2.50 | 0.45 |
| 9:I:76:THR:HG23 | 9:I:108:PRO:HG2 | 1.99 | 0.45 |
| 10:J:108:ARG:NH2 | 10:J:145:SER:OG | 2.50 | 0.45 |
| 23:W:99:PHE:HB3 | 23:W:130:TYR:CE1 | 2.52 | 0.45 |
| 34:2:1223:A:N6 | 34:2:1259:U:H3 | 2.14 | 0.44 |
| 34:2:1442:A:N3 | 34:2:1442:A:H2' | 2.32 | 0.44 |
| 34:2:1781:C:H2' | 34:2:1782:C:C6 | 2.51 | 0.44 |
| 34:2:208:U:N3 | 34:2:209:A:N7 | 2.65 | 0.44 |
| 34:2:520:A:C2' | 34:2:521:U:O5' | 2.65 | 0.44 |
| 34:2:70:C:N4 | 34:2:81:G:H1 | 2.14 | 0.44 |
| 34:2:932:A:C6 | 34:2:934:U:C2 | 3.05 | 0.44 |
| 34:2:991:A:C5' | 34:2:991:A:N3 | 2.80 | 0.44 |
| 4:D:98:ALA:HA | 4:D:188:ILE:HD13 | 1.98 | 0.44 |
| 34:2:1126:G:C6 | 34:2:1127:C:C4 | 3.05 | 0.44 |
| 34:2:1269:G:C2 | 34:2:1439:C:C2 | 3.06 | 0.44 |
| 26:Z:97:LYS:NZ | 34:2:1471:U:OP2 | 2.49 | 0.44 |
| 9:I:140:THR:CG2 | 34:2:185:C:H3' | 2.47 | 0.44 |
| 7:G:155:ASP:OD2 | 34:2:77:U:O2' | 2.34 | 0.44 |
| 1:A:124:THR:OG1 | 1:A:125:ASP:N | 2.51 | 0.44 |
| 34:2:1307:G:C2 | 34:2:1308:C:C2 | 3.05 | 0.44 |
| 34:2:1584:A:C2 | 34:2:1609:A:N7 | 2.86 | 0.44 |
| 34:2:798:A:C2 | 34:2:799:U:C2 | 3.05 | 0.44 |
| 34:2:878:G:C2 | 34:2:879:C:C2 | 3.05 | 0.44 |
| 26:Z:51:MET:O | 26:Z:53:GLU:CB | 2.64 | 0.44 |
| 34:2:1603:G:C2 | 34:2:1604:C:C2 | 3.05 | 0.44 |
| 34:2:515:G:O6 | 34:2:536:G:C2 | 2.70 | 0.44 |
| 34:2:560:G:C6 | 34:2:584:A:C6 | 3.06 | 0.44 |
| 34:2:883:A:N6 | 34:2:884:G:C6 | 2.84 | 0.44 |
| 34:2:935:G:C2 | 34:2:936:C:C2 | 3.05 | 0.44 |
| 6:F:109:LYS:HB2 | 34:2:1608:G:C5' | 2.48 | 0.44 |
| 26:Z:103:ARG:C | 26:Z:104:ALA:O | 2.54 | 0.44 |
| 26:Z:59:TYR:HA | 26:Z:101:TYR:O | 2.17 | 0.44 |
| 34:2:1031:G:C6 | 34:2:1032:C:C4 | 3.05 | 0.44 |

Continued on next page...

Continued from previous page...

| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|------------------|--------------------------|-------------------|
| 34:2:1042:A:C6 | 34:2:1075:A:N1 | 2.85 | 0.44 |
| 16:P:43:ARG:NH2 | 34:2:1550:U:OP2 | 2.50 | 0.44 |
| 34:2:269:C:H42 | 34:2:284:G:H1 | 1.64 | 0.44 |
| 34:2:567:G:O6 | 34:2:575:G:N1 | 2.51 | 0.44 |
| 34:2:954:A:H2' | 34:2:955:C:O4' | 2.17 | 0.44 |
| 6:F:78:ARG:NH2 | 34:2:1410:G:OP1 | 2.51 | 0.44 |
| 7:G:175:ILE:HD13 | 34:2:78:A:O2' | 2.16 | 0.44 |
| 21:U:39:ALA:HA | 21:U:42:ILE:HG12 | 1.99 | 0.44 |
| 10:J:140:ILE:HD12 | 25:Y:65:GLY:HA3 | 1.99 | 0.44 |
| 26:Z:49:ARG:CG | 26:Z:49:ARG:HH11 | 2.12 | 0.44 |
| 34:2:1218:A:N6 | 34:2:1264:G:H4' | 2.32 | 0.44 |
| 34:2:1219:C:C4 | 34:2:1263:G:N2 | 2.86 | 0.44 |
| 34:2:1498:C:N3 | 34:2:1499:C:C5 | 2.86 | 0.44 |
| 34:2:251:U:O2' | 34:2:252:A:O4' | 2.31 | 0.44 |
| 34:2:267:C:N4 | 34:2:286:G:N1 | 2.47 | 0.44 |
| 34:2:288:U:C2 | 34:2:289:G:C8 | 3.06 | 0.44 |
| 34:2:560:G:C6 | 34:2:584:A:N1 | 2.86 | 0.44 |
| 34:2:734:A:H2' | 34:2:735:C:C6 | 2.53 | 0.44 |
| 34:2:952:G:H2' | 34:2:953:G:C8 | 2.52 | 0.44 |
| 23:W:75:ILE:HA | 34:2:1099:G:O2' | 2.17 | 0.44 |
| 34:2:1014:U:C5 | 34:2:1015:C:N3 | 2.86 | 0.44 |
| 34:2:1080:A:C6 | 34:2:1090:A:C6 | 3.06 | 0.44 |
| 34:2:1209:C:H2' | 34:2:1210:A:C8 | 2.52 | 0.44 |
| 34:2:268:G:N2 | 34:2:269:C:C2 | 2.86 | 0.44 |
| 34:2:268:G:O6 | 34:2:286:G:C4 | 2.71 | 0.44 |
| 34:2:508:G:H2' | 34:2:509:G:C1' | 2.47 | 0.44 |
| 34:2:564:C:C5 | 34:2:575:G:C8 | 3.06 | 0.44 |
| 8:H:41:LEU:HD22 | 8:H:70:TYR:CD2 | 2.52 | 0.44 |
| 6:F:125:VAL:CG1 | 26:Z:59:TYR:HB3 | 2.44 | 0.44 |
| 26:Z:61:SER:O | 26:Z:63:SER:N | 2.51 | 0.44 |
| 34:2:1218:A:C8 | 34:2:1263:G:N2 | 2.85 | 0.44 |
| 34:2:157:U:H4' | 34:2:158:U:OP1 | 2.18 | 0.44 |
| 34:2:514:A:C6 | 34:2:542:C:C6 | 3.06 | 0.44 |
| 34:2:515:G:C6 | 34:2:536:G:C2 | 3.06 | 0.44 |
| 34:2:922:A:C6 | 34:2:923:A:N6 | 2.86 | 0.44 |
| 7:G:5:ILE:HD12 | 7:G:16:ILE:HD13 | 2.00 | 0.44 |
| 34:2:1232:G:N2 | 34:2:1252:U:H1' | 2.32 | 0.44 |
| 34:2:1287:G:N7 | 34:2:1313:U:H2' | 2.33 | 0.44 |
| 34:2:1671:G:C4 | 34:2:1672:C:C5 | 3.06 | 0.44 |
| 34:2:53:G:C6 | 34:2:54:C:C4 | 3.05 | 0.44 |
| 34:2:955:C:H2' | 34:2:956:G:C8 | 2.52 | 0.44 |

Continued on next page...

Continued from previous page...

| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 34:2:8:U:H3' | 34:2:9:U:H5' | 1.97 | 0.44 |
| 19:S:103:ASN:O | 19:S:106:GLU:HG2 | 2.18 | 0.44 |
| 16:P:18:LYS:HA | 19:S:91:ASP:C | 2.37 | 0.44 |
| 34:2:1042:A:C6 | 34:2:1075:A:C2 | 3.06 | 0.43 |
| 34:2:168:A:C8 | 34:2:170:A:N7 | 2.86 | 0.43 |
| 34:2:911:U:O2 | 34:2:911:U:C2' | 2.66 | 0.43 |
| 34:2:979:G:H2' | 34:2:980:U:O4' | 2.18 | 0.43 |
| 34:2:1217:G:C5' | 34:2:1442:A:H62 | 2.31 | 0.43 |
| 34:2:1316:C:H2' | 34:2:1317:G:O4' | 2.18 | 0.43 |
| 34:2:151:U:O2 | 34:2:162:G:H8 | 2.00 | 0.43 |
| 34:2:429:G:C2 | 34:2:430:C:C2 | 3.06 | 0.43 |
| 34:2:519:A:C2 | 34:2:532:U:O2 | 2.71 | 0.43 |
| 34:2:53:G:C2 | 34:2:54:C:C2 | 3.06 | 0.43 |
| 34:2:623:G:C6 | 34:2:624:C:C4 | 3.06 | 0.43 |
| 34:2:776:G:N1 | 34:2:777:C:C4 | 2.86 | 0.43 |
| 34:2:782:G:C6 | 34:2:783:C:C4 | 3.05 | 0.43 |
| 10:J:11:THR:HB | 10:J:12:TYR:CE1 | 2.53 | 0.43 |
| 6:F:113:VAL:HG12 | 17:Q:43:ILE:HD11 | 2.00 | 0.43 |
| 16:P:19:GLY:C | 19:S:93:ASN:H | 2.21 | 0.43 |
| 26:Z:96:SER:O | 26:Z:97:LYS:HG3 | 2.18 | 0.43 |
| 34:2:1015:C:H2' | 34:2:1016:U:O4' | 2.18 | 0.43 |
| 34:2:1123:A:C6 | 34:2:1124:A:C6 | 3.06 | 0.43 |
| 1:A:162:CYS:SG | 1:A:163:ASN:N | 2.91 | 0.43 |
| 25:Y:121:THR:N | 34:2:148:C:OP1 | 2.50 | 0.43 |
| 34:2:1046:G:C2 | 34:2:1071:C:O2 | 2.72 | 0.43 |
| 34:2:1437:C:C2 | 34:2:1438:C:C5 | 3.06 | 0.43 |
| 7:G:136:LYS:O | 7:G:175:ILE:HG23 | 2.18 | 0.43 |
| 20:T:99:SER:HA | 20:T:102:ARG:NH2 | 2.33 | 0.43 |
| 34:2:1031:G:C2 | 34:2:1032:C:C2 | 3.06 | 0.43 |
| 34:2:1270:G:C2 | 34:2:1438:C:C2 | 3.06 | 0.43 |
| 34:2:1417:G:H2' | 34:2:1418:C:O4' | 2.18 | 0.43 |
| 34:2:551:G:C2 | 34:2:572:C:C2 | 3.06 | 0.43 |
| 34:2:886:A:C2 | 34:2:925:A:C2 | 3.06 | 0.43 |
| 14:N:127:ARG:NH2 | 34:2:628:U:OP1 | 2.51 | 0.43 |
| 34:2:1217:G:C5 | 34:2:1442:A:C8 | 3.06 | 0.43 |
| 34:2:1222:A:C2 | 34:2:1260:G:C2 | 3.07 | 0.43 |
| 34:2:1482:G:N2 | 34:2:1483:C:C2 | 2.86 | 0.43 |
| 34:2:1540:G:O2' | 34:2:1541:A:O4' | 2.35 | 0.43 |
| 34:2:1546:G:C2 | 34:2:1547:C:C2 | 3.07 | 0.43 |
| 34:2:213:G:C5' | 34:2:241:U:O2 | 2.66 | 0.43 |
| 34:2:266:U:H3 | 34:2:267:C:N4 | 2.17 | 0.43 |

Continued on next page...

Continued from previous page...

| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 34:2:452:U:O2 | 34:2:452:U:H2' | 2.19 | 0.43 |
| 1:A:29:VAL:HG13 | 1:A:150:ASP:HB3 | 2.00 | 0.43 |
| 10:J:109:LEU:HD11 | 10:J:134:ILE:HG21 | 1.98 | 0.43 |
| 34:2:1222:A:N1 | 34:2:1259:U:C2 | 2.86 | 0.43 |
| 34:2:207:U:N3 | 34:2:208:U:C4 | 2.87 | 0.43 |
| 34:2:560:G:O6 | 34:2:584:A:N6 | 2.51 | 0.43 |
| 1:A:53:THR:HA | 1:A:161:PRO:HD2 | 2.00 | 0.43 |
| 6:F:194:GLU:OE2 | 26:Z:59:TYR:CE2 | 2.72 | 0.43 |
| 34:2:1182:A:C2 | 34:2:1209:C:O2 | 2.72 | 0.43 |
| 34:2:1210:A:H2' | 34:2:1211:G:O4' | 2.18 | 0.43 |
| 34:2:366:A:H2' | 34:2:367:U:O4' | 2.19 | 0.43 |
| 34:2:828:A:O2' | 34:2:829:U:OP2 | 2.37 | 0.43 |
| 2:B:137:ILE:HG21 | 2:B:176:VAL:HG21 | 1.99 | 0.43 |
| 7:G:174:LYS:CD | 34:2:65:A:H5' | 2.48 | 0.43 |
| 17:Q:47:LYS:O | 17:Q:50:GLU:HB2 | 2.18 | 0.43 |
| 26:Z:61:SER:H | 26:Z:64:VAL:HB | 1.84 | 0.43 |
| 34:2:1220:A:C4 | 34:2:1262:G:C2 | 3.07 | 0.43 |
| 16:P:79:HIS:HB2 | 34:2:1240:G:C8 | 2.54 | 0.43 |
| 34:2:1292:U:O4 | 34:2:1293:G:C5 | 2.72 | 0.43 |
| 34:2:1598:A:H4' | 34:2:1599:G:OP1 | 2.18 | 0.43 |
| 34:2:1785:C:H2' | 34:2:1786:G:C8 | 2.54 | 0.43 |
| 34:2:252:A:O2' | 34:2:253:A:O4' | 2.35 | 0.43 |
| 34:2:429:G:C6 | 34:2:430:C:C4 | 3.07 | 0.43 |
| 34:2:452:U:O2 | 34:2:452:U:C2' | 2.66 | 0.43 |
| 34:2:1171:G:C2 | 34:2:1172:C:C2 | 3.06 | 0.43 |
| 34:2:1178:G:C2 | 34:2:1179:C:C2 | 3.07 | 0.43 |
| 34:2:1258:U:C6 | 34:2:1259:U:C4 | 3.06 | 0.43 |
| 34:2:1222:A:N1 | 34:2:1260:G:C6 | 2.87 | 0.43 |
| 34:2:1783:U:H2' | 34:2:1784:G:H8 | 1.83 | 0.43 |
| 7:G:173:PRO:HG3 | 34:2:66:U:C2 | 2.54 | 0.43 |
| 34:2:978:A:N3 | 34:2:1773:U:O2' | 2.42 | 0.43 |
| 10:J:126:ARG:HD3 | 10:J:144:PRO:HB3 | 2.01 | 0.43 |
| 10:J:149:ARG:O | 10:J:151:GLU:N | 2.49 | 0.43 |
| 11:K:42:VAL:HG12 | 11:K:46:LEU:HD12 | 2.01 | 0.43 |
| 34:2:1073:G:O2' | 34:2:1074:C:H5'' | 2.19 | 0.42 |
| 34:2:1240:G:C2' | 34:2:1241:A:O5' | 2.65 | 0.42 |
| 34:2:1551:G:N1 | 34:2:1554:A:OP2 | 2.52 | 0.42 |
| 34:2:851:C:H2' | 34:2:852:G:O4' | 2.19 | 0.42 |
| 1:A:25:GLY:O | 1:A:26:ALA:HB3 | 2.19 | 0.42 |
| 9:I:9:HIS:O | 9:I:10:LYS:HB2 | 2.19 | 0.42 |
| 23:W:2:THR:N | 34:2:1033:C:HO2' | 2.16 | 0.42 |

Continued on next page...

Continued from previous page...

| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|-------------------|--------------------------|-------------------|
| 34:2:1079:U:H3 | 34:2:1090:A:H61 | 1.67 | 0.42 |
| 34:2:1482:G:C6 | 34:2:1483:C:N4 | 2.88 | 0.42 |
| 34:2:1590:A:C2 | 34:2:1602:U:N3 | 2.87 | 0.42 |
| 34:2:144:A:C6 | 34:2:170:A:C6 | 3.07 | 0.42 |
| 34:2:1784:G:C6 | 34:2:1785:C:N3 | 2.87 | 0.42 |
| 34:2:535:C:C2' | 34:2:536:G:O4' | 2.65 | 0.42 |
| 34:2:556:G:N1 | 34:2:558:C:C4 | 2.87 | 0.42 |
| 34:2:571:C:C4 | 34:2:572:C:C5 | 3.07 | 0.42 |
| 1:A:15:GLN:HG3 | 18:R:117:LEU:HD23 | 2.00 | 0.42 |
| 6:F:125:VAL:HG11 | 26:Z:59:TYR:CB | 2.43 | 0.42 |
| 10:J:7:THR:HG21 | 34:2:758:U:H5'' | 2.00 | 0.42 |
| 14:N:4:MET:SD | 14:N:124:ARG:NH1 | 2.92 | 0.42 |
| 34:2:1083:A:C2 | 34:2:1089:C:N3 | 2.87 | 0.42 |
| 34:2:1218:A:H62 | 34:2:1263:G:C2' | 2.26 | 0.42 |
| 34:2:1460:G:C2 | 34:2:1461:C:C2 | 3.07 | 0.42 |
| 34:2:1491:A:O2' | 34:2:1492:C:OP2 | 2.28 | 0.42 |
| 34:2:515:G:C5 | 34:2:536:G:N2 | 2.85 | 0.42 |
| 34:2:513:G:N1 | 34:2:542:C:C4 | 2.57 | 0.42 |
| 34:2:566:A:C2 | 34:2:582:C:H1' | 2.55 | 0.42 |
| 34:2:549:A:C2 | 34:2:588:C:C6 | 3.07 | 0.42 |
| 16:P:18:LYS:N | 19:S:93:ASN:O | 2.41 | 0.42 |
| 12:L:99:ARG:CB | 24:X:12:ALA:HB2 | 2.49 | 0.42 |
| 25:Y:29:HIS:N | 25:Y:30:PRO:CD | 2.82 | 0.42 |
| 34:2:1460:G:C6 | 34:2:1461:C:C4 | 3.07 | 0.42 |
| 34:2:1672:C:H2' | 34:2:1673:C:C6 | 2.54 | 0.42 |
| 9:I:96:LEU:HD11 | 9:I:180:CYS:SG | 2.59 | 0.42 |
| 34:2:1073:G:O2' | 34:2:1074:C:O5' | 2.37 | 0.42 |
| 34:2:1074:C:O2' | 34:2:1074:C:O2 | 2.37 | 0.42 |
| 34:2:1083:A:C2 | 34:2:1089:C:C2 | 3.07 | 0.42 |
| 34:2:1126:G:C2 | 34:2:1127:C:C2 | 3.08 | 0.42 |
| 34:2:1230:U:O3' | 34:2:1258:U:H5' | 2.19 | 0.42 |
| 34:2:1307:G:C6 | 34:2:1308:C:N4 | 2.87 | 0.42 |
| 34:2:1444:A:C8 | 34:2:1446:G:C5 | 3.08 | 0.42 |
| 34:2:1154:G:N2 | 34:2:1622:C:C2 | 2.87 | 0.42 |
| 34:2:127:G:O2' | 34:2:178:A:N7 | 2.46 | 0.42 |
| 34:2:506:U:O4' | 34:2:506:U:O2 | 2.37 | 0.42 |
| 34:2:630:G:C5 | 34:2:631:U:C4 | 3.07 | 0.42 |
| 34:2:1171:G:C6 | 34:2:1172:C:C4 | 3.07 | 0.42 |
| 34:2:1315:G:C2 | 34:2:1316:C:C2 | 3.07 | 0.42 |
| 34:2:647:G:N3 | 34:2:647:G:H2' | 2.34 | 0.42 |
| 16:P:19:GLY:H | 19:S:92:VAL:C | 2.22 | 0.42 |

Continued on next page...

Continued from previous page...

| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 16:P:20:VAL:N | 19:S:94:ASP:H | 2.18 | 0.42 |
| 18:R:45:ARG:NH2 | 34:2:1413:U:OP1 | 2.52 | 0.42 |
| 16:P:17:TYR:CA | 19:S:92:VAL:O | 2.68 | 0.42 |
| 34:2:1588:G:N2 | 34:2:1589:C:C2 | 2.87 | 0.42 |
| 34:2:407:C:HO2' | 34:2:1730:A:HO2' | 1.66 | 0.42 |
| 34:2:1629:A:N6 | 34:2:1761:A:O2' | 2.53 | 0.42 |
| 34:2:16:G:C2 | 34:2:17:C:N3 | 2.87 | 0.42 |
| 34:2:564:C:C4 | 34:2:576:G:C5 | 3.07 | 0.42 |
| 6:F:138:ALA:HA | 6:F:203:ALA:HB1 | 2.01 | 0.42 |
| 7:G:160:ARG:HB3 | 7:G:171:LYS:HB2 | 2.01 | 0.42 |
| 17:Q:49:TYR:O | 17:Q:52:LEU:HG | 2.20 | 0.42 |
| 34:2:1217:G:H2' | 34:2:1442:A:N6 | 2.34 | 0.42 |
| 34:2:1378:U:H2' | 34:2:1379:U:O4' | 2.19 | 0.42 |
| 34:2:549:A:C6 | 34:2:556:G:O6 | 2.73 | 0.42 |
| 34:2:566:A:C2' | 34:2:567:G:O4' | 2.60 | 0.42 |
| 34:2:885:U:N3 | 34:2:886:A:C5 | 2.87 | 0.42 |
| 13:M:21:LEU:HD21 | 13:M:80:ILE:HD13 | 2.01 | 0.42 |
| 19:S:38:VAL:HG22 | 19:S:101:LEU:HB3 | 2.02 | 0.42 |
| 34:2:1431:G:H2' | 34:2:1432:U:O4' | 2.19 | 0.42 |
| 34:2:1531:C:H4' | 34:2:1537:G:C6 | 2.55 | 0.42 |
| 34:2:1602:U:C4 | 34:2:1603:G:N7 | 2.88 | 0.42 |
| 34:2:922:A:H2' | 34:2:923:A:O4' | 2.19 | 0.42 |
| 34:2:941:G:C2 | 34:2:942:C:C2 | 3.08 | 0.42 |
| 34:2:1070:U:O3' | 34:2:1071:C:O4' | 2.38 | 0.42 |
| 34:2:63:G:O2' | 34:2:64:U:O5' | 2.38 | 0.42 |
| 34:2:1083:A:C6 | 34:2:1089:C:N4 | 2.88 | 0.41 |
| 34:2:1255:A:C1' | 34:2:1257:U:C5 | 3.02 | 0.41 |
| 34:2:1220:A:C2 | 34:2:1262:G:C5 | 3.08 | 0.41 |
| 34:2:15:U:H2' | 34:2:16:G:O4' | 2.21 | 0.41 |
| 34:2:363:G:C2 | 34:2:380:C:N3 | 2.88 | 0.41 |
| 34:2:60:U:H4' | 34:2:454:C:N4 | 2.35 | 0.41 |
| 34:2:629:A:C8 | 34:2:630:G:C8 | 3.08 | 0.41 |
| 34:2:922:A:N1 | 34:2:923:A:N6 | 2.67 | 0.41 |
| 10:J:127:VAL:HG21 | 34:2:477:A:H5' | 2.02 | 0.41 |
| 18:R:110:VAL:HG13 | 18:R:117:LEU:HD22 | 2.02 | 0.41 |
| 24:X:63:GLN:CG | 24:X:64:PRO:HD2 | 2.49 | 0.41 |
| 34:2:1040:G:C5 | 34:2:1076:C:N4 | 2.86 | 0.41 |
| 34:2:1183:A:O2' | 34:2:1184:U:H4' | 2.21 | 0.41 |
| 34:2:1260:G:C5 | 34:2:1261:U:C4 | 3.08 | 0.41 |
| 34:2:391:G:C2 | 34:2:392:C:C2 | 3.08 | 0.41 |
| 34:2:50:C:N3 | 34:2:429:G:C6 | 2.88 | 0.41 |

Continued on next page...

Continued from previous page...

| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|-------------------|--------------------------|-------------------|
| 34:2:584:A:N6 | 34:2:585:G:O6 | 2.53 | 0.41 |
| 9:I:5:ARG:NH1 | 9:I:29:LEU:O | 2.44 | 0.41 |
| 10:J:171:ARG:N | 10:J:171:ARG:HD2 | 2.35 | 0.41 |
| 23:W:76:SER:CB | 23:W:77:PRO:CD | 2.98 | 0.41 |
| 34:2:1073:G:O2' | 34:2:1074:C:C5' | 2.68 | 0.41 |
| 34:2:1222:A:C2 | 34:2:1260:G:N3 | 2.88 | 0.41 |
| 34:2:1441:U:H4' | 34:2:1444:A:N3 | 2.35 | 0.41 |
| 34:2:268:G:C5 | 34:2:269:C:C5 | 3.09 | 0.41 |
| 34:2:300:A:H2' | 34:2:301:U:O4' | 2.20 | 0.41 |
| 34:2:31:C:N4 | 34:2:32:U:C4 | 2.88 | 0.41 |
| 34:2:407:C:H2' | 34:2:408:C:C6 | 2.54 | 0.41 |
| 1:A:185:ARG:HG3 | 22:V:45:ALA:HB3 | 2.01 | 0.41 |
| 34:2:1206:C:C2 | 34:2:1207:A:C6 | 3.09 | 0.41 |
| 34:2:1315:G:C6 | 34:2:1316:C:C4 | 3.08 | 0.41 |
| 34:2:1560:G:N2 | 34:2:1561:C:C2 | 2.89 | 0.41 |
| 34:2:511:A:C3' | 34:2:512:U:C5' | 2.96 | 0.41 |
| 34:2:642:G:C6 | 34:2:692:C:N3 | 2.88 | 0.41 |
| 34:2:878:G:C6 | 34:2:879:C:C4 | 3.08 | 0.41 |
| 34:2:978:A:C2 | 34:2:1773:U:H4' | 2.55 | 0.41 |
| 1:A:124:THR:HG22 | 1:A:174:TRP:HE1 | 1.85 | 0.41 |
| 3:C:144:ILE:CD1 | 3:C:196:ALA:HB1 | 2.51 | 0.41 |
| 13:M:45:LEU:HD13 | 13:M:71:LEU:HB3 | 2.02 | 0.41 |
| 26:Z:66:VAL:HA | 26:Z:67:ASP:HA | 1.56 | 0.41 |
| 34:2:1471:U:O2 | 34:2:1471:U:H2' | 2.19 | 0.41 |
| 34:2:146:A:C5 | 34:2:147:U:C5 | 3.08 | 0.41 |
| 34:2:146:A:C6 | 34:2:147:U:C5 | 3.08 | 0.41 |
| 5:E:47:PHE:CE2 | 5:E:52:LEU:HD11 | 2.56 | 0.41 |
| 10:J:133:HIS:HB2 | 10:J:134:ILE:HD12 | 2.02 | 0.41 |
| 24:X:53:VAL:HG13 | 24:X:72:VAL:HG13 | 2.02 | 0.41 |
| 34:2:1290:G:C2 | 34:2:1324:A:C2 | 3.08 | 0.41 |
| 34:2:1463:C:C5 | 34:2:1464:G:C8 | 3.09 | 0.41 |
| 34:2:59:C:O2' | 34:2:60:U:C6 | 2.72 | 0.41 |
| 34:2:690:A:H2' | 34:2:691:U:O4' | 2.20 | 0.41 |
| 34:2:8:U:C3' | 34:2:9:U:C5' | 2.90 | 0.41 |
| 34:2:8:U:HO2' | 34:2:9:U:H5' | 1.85 | 0.41 |
| 16:P:98:ASN:O | 34:2:1182:A:N6 | 2.54 | 0.41 |
| 34:2:1250:U:C2 | 34:2:1251:C:C5 | 3.08 | 0.41 |
| 34:2:1307:G:C6 | 34:2:1308:C:C4 | 3.09 | 0.41 |
| 34:2:1546:G:N2 | 34:2:1547:C:C2 | 2.89 | 0.41 |
| 34:2:209:A:H2' | 34:2:210:U:H5' | 2.00 | 0.41 |
| 34:2:211:U:C2 | 34:2:253:A:C2 | 3.09 | 0.41 |

Continued on next page...

Continued from previous page...

| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 34:2:46:A:N1 | 34:2:431:G:O2' | 2.45 | 0.41 |
| 34:2:566:A:C8 | 34:2:575:G:N2 | 2.86 | 0.41 |
| 34:2:776:G:C2 | 34:2:777:C:C2 | 3.08 | 0.41 |
| 23:W:8:ALA:HA | 23:W:74:VAL:HG21 | 2.01 | 0.41 |
| 34:2:1255:A:O4' | 34:2:1257:U:H5 | 2.04 | 0.41 |
| 21:U:70:THR:HG22 | 34:2:1279:C:O2' | 2.20 | 0.41 |
| 19:S:41:ARG:NH1 | 34:2:1563:C:OP1 | 2.46 | 0.41 |
| 34:2:556:G:N2 | 34:2:558:C:N3 | 2.68 | 0.41 |
| 34:2:564:C:C2' | 34:2:576:G:N2 | 2.78 | 0.41 |
| 34:2:885:U:O4 | 34:2:886:A:N6 | 2.54 | 0.41 |
| 1:A:102:PHE:CE2 | 1:A:132:ALA:HA | 2.55 | 0.41 |
| 4:D:20:GLU:HG2 | 11:K:61:TRP:CZ3 | 2.55 | 0.41 |
| 15:O:124:ASP:OD1 | 34:2:926:C:O2' | 2.33 | 0.41 |
| 34:2:391:G:C6 | 34:2:392:C:C4 | 3.08 | 0.41 |
| 34:2:564:C:C5 | 34:2:576:G:C5 | 3.09 | 0.41 |
| 7:G:36:VAL:HB | 7:G:50:PHE:HB2 | 2.03 | 0.41 |
| 7:G:56:ASN:ND2 | 7:G:61:PHE:O | 2.54 | 0.41 |
| 11:K:3:ILE:HG21 | 11:K:8:ARG:HB2 | 2.02 | 0.41 |
| 15:O:50:ALA:O | 15:O:52:ARG:N | 2.53 | 0.41 |
| 25:Y:35:VAL:HG21 | 25:Y:40:LEU:HD11 | 2.02 | 0.41 |
| 34:2:1002:A:O2' | 34:2:1004:A:N7 | 2.44 | 0.41 |
| 34:2:935:G:P | 34:2:1074:C:N3 | 2.91 | 0.41 |
| 34:2:1041:G:H1 | 34:2:1075:A:H2 | 1.69 | 0.41 |
| 34:2:1245:C:C4 | 34:2:1246:U:O2 | 2.74 | 0.41 |
| 34:2:1464:G:C6 | 34:2:1465:C:C4 | 3.08 | 0.41 |
| 34:2:151:U:C2 | 34:2:162:G:C8 | 3.08 | 0.41 |
| 34:2:1592:G:OP2 | 34:2:1594:C:N4 | 2.54 | 0.41 |
| 34:2:185:C:O2 | 34:2:185:C:H2' | 2.21 | 0.41 |
| 34:2:216:A:N1 | 34:2:844:G:H1' | 2.36 | 0.41 |
| 10:J:173:ALA:HB3 | 34:2:511:A:OP1 | 2.20 | 0.41 |
| 13:M:70:GLY:O | 13:M:73:THR:OG1 | 2.39 | 0.41 |
| 34:2:1038:A:H61 | 34:2:1077:C:N4 | 2.19 | 0.41 |
| 34:2:1187:G:C6 | 34:2:1197:G:C6 | 3.09 | 0.41 |
| 34:2:268:G:O6 | 34:2:286:G:N3 | 2.54 | 0.41 |
| 34:2:403:G:C6 | 34:2:404:C:C4 | 3.09 | 0.41 |
| 34:2:425:G:C2 | 34:2:426:C:C2 | 3.09 | 0.41 |
| 34:2:425:G:C6 | 34:2:426:C:C4 | 3.09 | 0.41 |
| 34:2:821:U:C4 | 34:2:822:G:C2 | 3.09 | 0.41 |
| 13:M:55:LEU:HB3 | 13:M:68:VAL:HG11 | 2.03 | 0.41 |
| 23:W:4:THR:O | 23:W:5:SER:C | 2.58 | 0.41 |
| 34:2:1076:C:HO2' | 34:2:1077:C:C5' | 2.34 | 0.40 |

Continued on next page...

Continued from previous page...

| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 34:2:1570:G:N3 | 34:2:1570:G:H5'' | 2.36 | 0.40 |
| 34:2:179:A:H2' | 34:2:180:A:O4' | 2.20 | 0.40 |
| 34:2:26:A:HO2' | 34:2:27:U:C5' | 2.34 | 0.40 |
| 34:2:99:C:C2 | 34:2:360:C:C5 | 3.09 | 0.40 |
| 34:2:883:A:O2' | 34:2:884:G:H5'' | 2.21 | 0.40 |
| 34:2:947:G:C2 | 34:2:948:C:C2 | 3.09 | 0.40 |
| 8:H:20:VAL:HG21 | 8:H:46:ILE:HD13 | 2.02 | 0.40 |
| 25:Y:20:ARG:CZ | 25:Y:74:LEU:HD13 | 2.51 | 0.40 |
| 34:2:16:G:C2 | 34:2:17:C:C2 | 3.09 | 0.40 |
| 34:2:16:G:C6 | 34:2:17:C:N4 | 2.89 | 0.40 |
| 3:C:156:PRO:HG3 | 22:V:9:VAL:HG11 | 2.04 | 0.40 |
| 6:F:122:ILE:HD12 | 26:Z:59:TYR:CE2 | 2.55 | 0.40 |
| 16:P:18:LYS:C | 19:S:93:ASN:C | 2.80 | 0.40 |
| 34:2:1140:G:H2' | 34:2:1141:A:C8 | 2.57 | 0.40 |
| 34:2:1354:C:H2' | 34:2:1355:U:O4' | 2.21 | 0.40 |
| 34:2:1437:C:H2' | 34:2:1438:C:H6 | 1.86 | 0.40 |
| 34:2:149:U:C4 | 34:2:150:G:N7 | 2.90 | 0.40 |
| 34:2:1588:G:C6 | 34:2:1589:C:C4 | 3.10 | 0.40 |
| 9:I:138:LYS:NZ | 34:2:186:G:O2' | 2.45 | 0.40 |
| 34:2:392:C:H2' | 34:2:393:C:C6 | 2.56 | 0.40 |
| 34:2:531:U:H2' | 34:2:532:U:O4' | 2.21 | 0.40 |
| 34:2:566:A:N1 | 34:2:582:C:H1' | 2.36 | 0.40 |
| 34:2:65:A:H2 | 34:2:84:A:N7 | 2.19 | 0.40 |
| 34:2:776:G:C6 | 34:2:777:C:C4 | 3.09 | 0.40 |
| 34:2:946:U:H2' | 34:2:947:G:O4' | 2.21 | 0.40 |
| 34:2:958:U:C2' | 34:2:958:U:O2 | 2.69 | 0.40 |
| 5:E:126:VAL:HG13 | 5:E:139:VAL:CG2 | 2.52 | 0.40 |
| 6:F:98:SER:HB2 | 6:F:178:THR:HG21 | 2.03 | 0.40 |
| 6:F:66:ILE:HG22 | 6:F:66:ILE:O | 2.21 | 0.40 |
| 34:2:1020:C:H2' | 34:2:1021:C:O4' | 2.22 | 0.40 |
| 34:2:1256:U:C5 | 34:2:1257:U:H1' | 2.57 | 0.40 |
| 34:2:1231:U:P | 34:2:1258:U:H5' | 2.62 | 0.40 |
| 34:2:208:U:C2 | 34:2:209:A:C8 | 3.09 | 0.40 |
| 34:2:941:G:C6 | 34:2:942:C:C4 | 3.09 | 0.40 |
| 26:Z:67:ASP:CA | 26:Z:69:PHE:H | 2.35 | 0.40 |
| 34:2:1040:G:C6 | 34:2:1041:G:C6 | 3.09 | 0.40 |
| 34:2:1072:G:N3 | 34:2:1073:G:N7 | 2.64 | 0.40 |
| 34:2:1765:G:H4' | 34:2:1766:G:O5' | 2.21 | 0.40 |
| 34:2:214:A:C4 | 34:2:241:U:C4 | 3.09 | 0.40 |
| 34:2:604:A:C4 | 34:2:605:A:C2 | 3.09 | 0.40 |
| 34:2:65:A:O2' | 34:2:83:G:N1 | 2.55 | 0.40 |

Continued on next page...

Continued from previous page...

| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|----------------|----------------|--------------------------|-------------------|
| 6:F:138:ALA:HA | 6:F:203:ALA:CB | 2.51 | 0.40 |

There are no symmetry-related clashes.

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 | Percentiles | |
|-----|-------|---------------|-----------|----------|----------|-------------|----|
| 1 | A | 204/206 (99%) | 168 (82%) | 25 (12%) | 11 (5%) | 2 | 28 |
| 2 | B | 212/214 (99%) | 174 (82%) | 32 (15%) | 6 (3%) | 6 | 42 |
| 3 | C | 215/217 (99%) | 187 (87%) | 21 (10%) | 7 (3%) | 4 | 39 |
| 4 | D | 221/223 (99%) | 198 (90%) | 17 (8%) | 6 (3%) | 6 | 43 |
| 5 | E | 258/260 (99%) | 214 (83%) | 36 (14%) | 8 (3%) | 5 | 40 |
| 6 | F | 204/206 (99%) | 174 (85%) | 21 (10%) | 9 (4%) | 3 | 32 |
| 7 | G | 224/226 (99%) | 186 (83%) | 29 (13%) | 9 (4%) | 3 | 34 |
| 8 | H | 182/184 (99%) | 155 (85%) | 16 (9%) | 11 (6%) | 2 | 26 |
| 9 | I | 184/200 (92%) | 154 (84%) | 22 (12%) | 8 (4%) | 3 | 32 |
| 10 | J | 180/182 (99%) | 151 (84%) | 17 (9%) | 12 (7%) | 1 | 23 |
| 11 | K | 94/96 (98%) | 80 (85%) | 7 (7%) | 7 (7%) | 1 | 20 |
| 12 | L | 153/155 (99%) | 129 (84%) | 17 (11%) | 7 (5%) | 3 | 31 |
| 13 | M | 120/122 (98%) | 94 (78%) | 21 (18%) | 5 (4%) | 3 | 33 |
| 14 | N | 148/150 (99%) | 130 (88%) | 14 (10%) | 4 (3%) | 6 | 43 |
| 15 | O | 125/127 (98%) | 108 (86%) | 11 (9%) | 6 (5%) | 2 | 30 |
| 16 | P | 121/123 (98%) | 96 (79%) | 16 (13%) | 9 (7%) | 1 | 20 |
| 17 | Q | 139/141 (99%) | 122 (88%) | 12 (9%) | 5 (4%) | 4 | 37 |
| 18 | R | 127/129 (98%) | 106 (84%) | 14 (11%) | 7 (6%) | 2 | 28 |
| 19 | S | 143/145 (99%) | 119 (83%) | 17 (12%) | 7 (5%) | 2 | 30 |

Continued on next page...

Continued from previous page...

| Mol | Chain | Analysed | Favoured | Allowed | Outliers | Percentiles | |
|-----|-------|-----------------|------------|-----------|----------|-------------|-----|
| 20 | T | 141/143 (99%) | 126 (89%) | 10 (7%) | 5 (4%) | 4 | 38 |
| 21 | U | 104/106 (98%) | 93 (89%) | 7 (7%) | 4 (4%) | 4 | 36 |
| 22 | V | 85/87 (98%) | 69 (81%) | 10 (12%) | 6 (7%) | 1 | 21 |
| 23 | W | 127/129 (98%) | 107 (84%) | 14 (11%) | 6 (5%) | 3 | 31 |
| 24 | X | 143/145 (99%) | 121 (85%) | 15 (10%) | 7 (5%) | 2 | 30 |
| 25 | Y | 132/134 (98%) | 113 (86%) | 9 (7%) | 10 (8%) | 1 | 19 |
| 26 | Z | 68/70 (97%) | 58 (85%) | 5 (7%) | 5 (7%) | 1 | 20 |
| 27 | a | 98/100 (98%) | 74 (76%) | 13 (13%) | 11 (11%) | 0 | 9 |
| 28 | b | 80/82 (98%) | 64 (80%) | 12 (15%) | 4 (5%) | 2 | 30 |
| 29 | c | 61/63 (97%) | 55 (90%) | 6 (10%) | 0 | 100 | 100 |
| 30 | d | 51/53 (96%) | 41 (80%) | 10 (20%) | 0 | 100 | 100 |
| 31 | e | 53/55 (96%) | 47 (89%) | 3 (6%) | 3 (6%) | 2 | 27 |
| 32 | f | 67/69 (97%) | 50 (75%) | 11 (16%) | 6 (9%) | 1 | 15 |
| 33 | g | 312/324 (96%) | 261 (84%) | 44 (14%) | 7 (2%) | 8 | 46 |
| All | All | 4776/4866 (98%) | 4024 (84%) | 534 (11%) | 218 (5%) | 5 | 31 |

All (218) Ramachandran outliers are listed below:

| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1 | A | 130 | ALA |
| 2 | B | 100 | PHE |
| 3 | C | 149 | TRP |
| 4 | D | 164 | VAL |
| 6 | F | 59 | SER |
| 6 | F | 206 | GLY |
| 7 | G | 154 | ARG |
| 8 | H | 32 | PRO |
| 8 | H | 64 | VAL |
| 8 | H | 74 | GLN |
| 9 | I | 10 | LYS |
| 10 | J | 121 | SER |
| 11 | K | 88 | PRO |
| 12 | L | 105 | LYS |
| 14 | N | 24 | ALA |
| 14 | N | 133 | SER |
| 15 | O | 91 | SER |
| 16 | P | 20 | VAL |

Continued on next page...

Continued from previous page...

| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 16 | P | 29 | PRO |
| 17 | Q | 40 | GLN |
| 17 | Q | 138 | PHE |
| 18 | R | 26 | MET |
| 18 | R | 121 | VAL |
| 19 | S | 92 | VAL |
| 20 | T | 11 | ALA |
| 21 | U | 107 | THR |
| 21 | U | 118 | ILE |
| 22 | V | 30 | SER |
| 23 | W | 83 | ILE |
| 24 | X | 42 | PRO |
| 24 | X | 64 | PRO |
| 24 | X | 131 | SER |
| 25 | Y | 30 | PRO |
| 25 | Y | 60 | PHE |
| 26 | Z | 73 | GLY |
| 26 | Z | 104 | ALA |
| 27 | a | 18 | VAL |
| 27 | a | 75 | ILE |
| 27 | a | 81 | ALA |
| 27 | a | 86 | VAL |
| 28 | b | 21 | LEU |
| 32 | f | 143 | HIS |
| 1 | A | 26 | ALA |
| 1 | A | 72 | ASP |
| 1 | A | 94 | GLY |
| 3 | C | 141 | VAL |
| 3 | C | 153 | LEU |
| 4 | D | 217 | VAL |
| 5 | E | 38 | LEU |
| 5 | E | 195 | ILE |
| 5 | E | 201 | HIS |
| 7 | G | 122 | GLU |
| 8 | H | 10 | SER |
| 8 | H | 13 | PRO |
| 8 | H | 53 | GLY |
| 8 | H | 132 | PRO |
| 9 | I | 11 | ARG |
| 9 | I | 153 | ILE |
| 10 | J | 65 | LYS |
| 10 | J | 118 | LEU |

Continued on next page...

Continued from previous page...

| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 11 | K | 81 | ASN |
| 11 | K | 83 | PRO |
| 12 | L | 5 | LEU |
| 12 | L | 7 | VAL |
| 12 | L | 55 | ASP |
| 13 | M | 48 | GLY |
| 13 | M | 82 | VAL |
| 13 | M | 85 | ALA |
| 16 | P | 12 | PHE |
| 16 | P | 101 | VAL |
| 17 | Q | 27 | GLY |
| 18 | R | 127 | VAL |
| 19 | S | 26 | ILE |
| 19 | S | 51 | ASP |
| 20 | T | 43 | ASN |
| 22 | V | 22 | ARG |
| 23 | W | 5 | SER |
| 23 | W | 57 | ARG |
| 23 | W | 120 | HIS |
| 24 | X | 130 | VAL |
| 25 | Y | 64 | TYR |
| 27 | a | 10 | ARG |
| 27 | a | 83 | ILE |
| 27 | a | 85 | ARG |
| 32 | f | 89 | LYS |
| 32 | f | 97 | LYS |
| 32 | f | 111 | GLU |
| 33 | g | 293 | ASP |
| 1 | A | 35 | PRO |
| 2 | B | 209 | ASN |
| 3 | C | 41 | VAL |
| 3 | C | 111 | ASP |
| 4 | D | 44 | THR |
| 4 | D | 93 | ASP |
| 5 | E | 80 | THR |
| 5 | E | 95 | THR |
| 5 | E | 120 | SER |
| 5 | E | 205 | PHE |
| 6 | F | 53 | VAL |
| 6 | F | 101 | MET |
| 7 | G | 89 | ASN |
| 8 | H | 29 | ASN |

Continued on next page...

Continued from previous page...

| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 9 | I | 22 | ARG |
| 9 | I | 40 | THR |
| 9 | I | 52 | ASN |
| 10 | J | 97 | LEU |
| 10 | J | 171 | ARG |
| 12 | L | 133 | LYS |
| 13 | M | 78 | PRO |
| 15 | O | 18 | ARG |
| 15 | O | 124 | ASP |
| 17 | Q | 116 | LEU |
| 20 | T | 50 | SER |
| 22 | V | 4 | ASP |
| 22 | V | 44 | ARG |
| 23 | W | 107 | SER |
| 25 | Y | 61 | ARG |
| 25 | Y | 63 | GLN |
| 27 | a | 8 | ASN |
| 31 | e | 11 | ALA |
| 31 | e | 61 | SER |
| 32 | f | 88 | PRO |
| 33 | g | 4 | SER |
| 33 | g | 244 | LYS |
| 1 | A | 9 | LEU |
| 1 | A | 39 | LYS |
| 1 | A | 103 | THR |
| 1 | A | 167 | LYS |
| 1 | A | 193 | GLN |
| 2 | B | 148 | ASN |
| 2 | B | 210 | VAL |
| 5 | E | 77 | ARG |
| 6 | F | 83 | ARG |
| 7 | G | 165 | GLY |
| 7 | G | 173 | PRO |
| 7 | G | 177 | ARG |
| 8 | H | 110 | GLN |
| 9 | I | 116 | HIS |
| 10 | J | 35 | GLY |
| 10 | J | 120 | LYS |
| 10 | J | 147 | MET |
| 15 | O | 51 | ASP |
| 16 | P | 28 | MET |
| 16 | P | 80 | LEU |

Continued on next page...

Continued from previous page...

| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 16 | P | 121 | ILE |
| 17 | Q | 115 | THR |
| 18 | R | 100 | LEU |
| 20 | T | 39 | THR |
| 21 | U | 21 | LYS |
| 25 | Y | 34 | ASN |
| 26 | Z | 56 | THR |
| 26 | Z | 57 | TYR |
| 27 | a | 16 | GLY |
| 28 | b | 3 | LEU |
| 32 | f | 106 | TYR |
| 33 | g | 168 | ASP |
| 1 | A | 68 | PRO |
| 2 | B | 190 | PRO |
| 3 | C | 44 | THR |
| 3 | C | 65 | SER |
| 6 | F | 40 | GLN |
| 6 | F | 52 | ASP |
| 6 | F | 102 | ASN |
| 7 | G | 8 | PRO |
| 7 | G | 70 | PRO |
| 7 | G | 224 | ALA |
| 10 | J | 18 | PRO |
| 10 | J | 67 | PRO |
| 10 | J | 122 | VAL |
| 10 | J | 134 | ILE |
| 11 | K | 54 | PHE |
| 11 | K | 87 | PHE |
| 11 | K | 94 | GLY |
| 12 | L | 30 | LYS |
| 14 | N | 70 | LYS |
| 15 | O | 114 | ARG |
| 18 | R | 72 | LYS |
| 19 | S | 14 | ILE |
| 19 | S | 144 | ARG |
| 21 | U | 71 | PRO |
| 24 | X | 4 | GLY |
| 25 | Y | 51 | GLU |
| 25 | Y | 133 | ASN |
| 28 | b | 62 | VAL |
| 31 | e | 47 | VAL |
| 2 | B | 221 | PRO |

Continued on next page...

Continued from previous page...

| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 4 | D | 4 | ILE |
| 11 | K | 2 | LEU |
| 12 | L | 113 | PRO |
| 14 | N | 3 | ARG |
| 15 | O | 25 | ASP |
| 16 | P | 69 | GLU |
| 19 | S | 12 | GLN |
| 20 | T | 45 | LEU |
| 22 | V | 46 | ILE |
| 22 | V | 82 | VAL |
| 24 | X | 144 | ARG |
| 25 | Y | 31 | ASN |
| 26 | Z | 62 | VAL |
| 27 | a | 84 | VAL |
| 33 | g | 139 | GLY |
| 27 | a | 36 | ILE |
| 33 | g | 278 | ILE |
| 6 | F | 77 | GLY |
| 8 | H | 8 | ILE |
| 13 | M | 97 | ILE |
| 18 | R | 38 | ILE |
| 18 | R | 124 | VAL |
| 23 | W | 76 | SER |
| 4 | D | 163 | PRO |
| 8 | H | 98 | ILE |
| 9 | I | 39 | GLY |
| 24 | X | 63 | GLN |
| 28 | b | 39 | GLY |
| 33 | g | 31 | PRO |
| 16 | P | 53 | PRO |
| 19 | S | 76 | PRO |
| 25 | Y | 29 | HIS |

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 | |
|-----|-------|----------------|-----------|----------|-------------|----|
| 1 | A | 174/174 (100%) | 160 (92%) | 14 (8%) | 14 | 50 |
| 2 | B | 196/196 (100%) | 182 (93%) | 14 (7%) | 17 | 55 |
| 3 | C | 176/176 (100%) | 154 (88%) | 22 (12%) | 5 | 29 |
| 4 | D | 185/185 (100%) | 165 (89%) | 20 (11%) | 7 | 37 |
| 5 | E | 223/223 (100%) | 204 (92%) | 19 (8%) | 12 | 48 |
| 6 | F | 174/174 (100%) | 158 (91%) | 16 (9%) | 11 | 43 |
| 7 | G | 192/192 (100%) | 175 (91%) | 17 (9%) | 11 | 45 |
| 8 | H | 164/164 (100%) | 149 (91%) | 15 (9%) | 11 | 44 |
| 9 | I | 148/158 (94%) | 126 (85%) | 22 (15%) | 3 | 23 |
| 10 | J | 153/153 (100%) | 135 (88%) | 18 (12%) | 6 | 32 |
| 11 | K | 88/88 (100%) | 82 (93%) | 6 (7%) | 18 | 56 |
| 12 | L | 136/136 (100%) | 126 (93%) | 10 (7%) | 16 | 53 |
| 13 | M | 97/97 (100%) | 91 (94%) | 6 (6%) | 21 | 59 |
| 14 | N | 127/127 (100%) | 116 (91%) | 11 (9%) | 12 | 46 |
| 15 | O | 96/96 (100%) | 90 (94%) | 6 (6%) | 21 | 58 |
| 16 | P | 105/106 (99%) | 96 (91%) | 9 (9%) | 12 | 47 |
| 17 | Q | 117/117 (100%) | 109 (93%) | 8 (7%) | 18 | 56 |
| 18 | R | 117/117 (100%) | 104 (89%) | 13 (11%) | 7 | 35 |
| 19 | S | 128/128 (100%) | 111 (87%) | 17 (13%) | 4 | 28 |
| 20 | T | 117/117 (100%) | 106 (91%) | 11 (9%) | 10 | 42 |
| 21 | U | 96/96 (100%) | 92 (96%) | 4 (4%) | 34 | 68 |
| 22 | V | 73/73 (100%) | 69 (94%) | 4 (6%) | 25 | 63 |
| 23 | W | 110/110 (100%) | 97 (88%) | 13 (12%) | 6 | 32 |
| 24 | X | 120/120 (100%) | 105 (88%) | 15 (12%) | 5 | 29 |
| 25 | Y | 108/108 (100%) | 94 (87%) | 14 (13%) | 5 | 28 |
| 26 | Z | 60/60 (100%) | 55 (92%) | 5 (8%) | 13 | 49 |
| 27 | a | 85/85 (100%) | 73 (86%) | 12 (14%) | 4 | 26 |
| 28 | b | 72/72 (100%) | 68 (94%) | 4 (6%) | 25 | 62 |
| 29 | c | 55/55 (100%) | 52 (94%) | 3 (6%) | 25 | 63 |
| 30 | d | 46/46 (100%) | 42 (91%) | 4 (9%) | 12 | 46 |
| 31 | e | 49/49 (100%) | 45 (92%) | 4 (8%) | 13 | 49 |
| 32 | f | 58/60 (97%) | 48 (83%) | 10 (17%) | 2 | 17 |

Continued on next page...

Continued from previous page...

| Mol | Chain | Analysed | Rotameric | Outliers | Percentiles | |
|-----|-------|------------------|------------|----------|-------------|----|
| 33 | g | 265/270 (98%) | 251 (95%) | 14 (5%) | 26 | 64 |
| All | All | 4110/4128 (100%) | 3730 (91%) | 380 (9%) | 15 | 43 |

All (380) residues with a non-rotameric sidechain are listed below:

| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1 | A | 9 | LEU |
| 1 | A | 21 | ARG |
| 1 | A | 32 | HIS |
| 1 | A | 56 | LYS |
| 1 | A | 59 | LEU |
| 1 | A | 79 | ARG |
| 1 | A | 108 | THR |
| 1 | A | 109 | ASN |
| 1 | A | 135 | GLU |
| 1 | A | 146 | LEU |
| 1 | A | 151 | SER |
| 1 | A | 177 | LEU |
| 1 | A | 198 | MET |
| 1 | A | 205 | ARG |
| 2 | B | 47 | LEU |
| 2 | B | 48 | VAL |
| 2 | B | 70 | LEU |
| 2 | B | 84 | VAL |
| 2 | B | 96 | LEU |
| 2 | B | 100 | PHE |
| 2 | B | 120 | LEU |
| 2 | B | 127 | VAL |
| 2 | B | 167 | VAL |
| 2 | B | 179 | SER |
| 2 | B | 181 | LEU |
| 2 | B | 191 | GLU |
| 2 | B | 194 | ASN |
| 2 | B | 228 | LEU |
| 3 | C | 43 | VAL |
| 3 | C | 49 | LEU |
| 3 | C | 51 | LYS |
| 3 | C | 58 | ILE |
| 3 | C | 59 | GLU |
| 3 | C | 71 | PHE |
| 3 | C | 86 | MET |
| 3 | C | 92 | GLN |

Continued on next page...

Continued from previous page...

| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 3 | C | 93 | LYS |
| 3 | C | 94 | GLN |
| 3 | C | 99 | GLN |
| 3 | C | 100 | ARG |
| 3 | C | 111 | ASP |
| 3 | C | 122 | THR |
| 3 | C | 142 | ILE |
| 3 | C | 145 | ARG |
| 3 | C | 149 | TRP |
| 3 | C | 166 | LYS |
| 3 | C | 167 | CYS |
| 3 | C | 190 | LYS |
| 3 | C | 223 | ILE |
| 3 | C | 235 | TRP |
| 4 | D | 5 | ILE |
| 4 | D | 7 | LYS |
| 4 | D | 11 | LEU |
| 4 | D | 17 | PHE |
| 4 | D | 51 | ARG |
| 4 | D | 65 | ARG |
| 4 | D | 101 | GLN |
| 4 | D | 113 | LEU |
| 4 | D | 122 | VAL |
| 4 | D | 134 | CYS |
| 4 | D | 135 | GLU |
| 4 | D | 141 | LYS |
| 4 | D | 143 | ARG |
| 4 | D | 146 | ARG |
| 4 | D | 157 | LEU |
| 4 | D | 162 | GLN |
| 4 | D | 173 | ARG |
| 4 | D | 178 | ARG |
| 4 | D | 179 | GLN |
| 4 | D | 222 | VAL |
| 5 | E | 6 | LYS |
| 5 | E | 9 | LEU |
| 5 | E | 11 | ARG |
| 5 | E | 18 | TRP |
| 5 | E | 37 | LYS |
| 5 | E | 38 | LEU |
| 5 | E | 42 | LEU |
| 5 | E | 51 | ARG |

Continued on next page...

Continued from previous page...

| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 5 | E | 68 | ARG |
| 5 | E | 77 | ARG |
| 5 | E | 79 | ASP |
| 5 | E | 123 | LEU |
| 5 | E | 133 | LYS |
| 5 | E | 143 | ASP |
| 5 | E | 187 | ARG |
| 5 | E | 208 | VAL |
| 5 | E | 225 | VAL |
| 5 | E | 245 | LYS |
| 5 | E | 247 | THR |
| 6 | F | 81 | ASN |
| 6 | F | 94 | ARG |
| 6 | F | 101 | MET |
| 6 | F | 114 | ARG |
| 6 | F | 121 | GLU |
| 6 | F | 158 | ARG |
| 6 | F | 165 | SER |
| 6 | F | 173 | SER |
| 6 | F | 186 | PHE |
| 6 | F | 187 | ARG |
| 6 | F | 188 | ASN |
| 6 | F | 192 | ILE |
| 6 | F | 196 | LEU |
| 6 | F | 210 | SER |
| 6 | F | 211 | TYR |
| 6 | F | 220 | GLU |
| 7 | G | 52 | ILE |
| 7 | G | 75 | LEU |
| 7 | G | 92 | ARG |
| 7 | G | 96 | SER |
| 7 | G | 97 | VAL |
| 7 | G | 136 | LYS |
| 7 | G | 141 | ILE |
| 7 | G | 152 | ASP |
| 7 | G | 153 | VAL |
| 7 | G | 155 | ASP |
| 7 | G | 159 | ARG |
| 7 | G | 164 | LYS |
| 7 | G | 178 | LEU |
| 7 | G | 180 | THR |
| 7 | G | 182 | GLN |

Continued on next page...

Continued from previous page...

| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 7 | G | 183 | ARG |
| 7 | G | 215 | ARG |
| 8 | H | 11 | GLN |
| 8 | H | 16 | LEU |
| 8 | H | 24 | PHE |
| 8 | H | 27 | LEU |
| 8 | H | 33 | GLU |
| 8 | H | 47 | ARG |
| 8 | H | 80 | GLU |
| 8 | H | 81 | LEU |
| 8 | H | 93 | LEU |
| 8 | H | 114 | ARG |
| 8 | H | 122 | HIS |
| 8 | H | 126 | LEU |
| 8 | H | 129 | LEU |
| 8 | H | 139 | ARG |
| 8 | H | 174 | ASN |
| 9 | I | 8 | ARG |
| 9 | I | 10 | LYS |
| 9 | I | 24 | LYS |
| 9 | I | 25 | ARG |
| 9 | I | 29 | LEU |
| 9 | I | 35 | ASN |
| 9 | I | 62 | THR |
| 9 | I | 66 | SER |
| 9 | I | 72 | VAL |
| 9 | I | 75 | LYS |
| 9 | I | 77 | ARG |
| 9 | I | 86 | SER |
| 9 | I | 96 | LEU |
| 9 | I | 107 | THR |
| 9 | I | 138 | LYS |
| 9 | I | 140 | THR |
| 9 | I | 144 | TRP |
| 9 | I | 159 | SER |
| 9 | I | 160 | GLN |
| 9 | I | 161 | PHE |
| 9 | I | 170 | ILE |
| 9 | I | 190 | LEU |
| 10 | J | 8 | TYR |
| 10 | J | 11 | THR |
| 10 | J | 28 | LEU |

Continued on next page...

Continued from previous page...

| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 10 | J | 30 | LEU |
| 10 | J | 37 | LYS |
| 10 | J | 49 | LEU |
| 10 | J | 61 | THR |
| 10 | J | 64 | GLU |
| 10 | J | 69 | ARG |
| 10 | J | 89 | ASP |
| 10 | J | 97 | LEU |
| 10 | J | 126 | ARG |
| 10 | J | 132 | ARG |
| 10 | J | 145 | SER |
| 10 | J | 149 | ARG |
| 10 | J | 153 | GLU |
| 10 | J | 175 | LYS |
| 10 | J | 176 | ARG |
| 11 | K | 15 | LEU |
| 11 | K | 40 | LEU |
| 11 | K | 59 | PHE |
| 11 | K | 76 | LEU |
| 11 | K | 80 | LEU |
| 11 | K | 86 | ILE |
| 12 | L | 8 | GLN |
| 12 | L | 10 | GLU |
| 12 | L | 80 | MET |
| 12 | L | 83 | THR |
| 12 | L | 84 | ILE |
| 12 | L | 87 | ARG |
| 12 | L | 94 | VAL |
| 12 | L | 101 | GLU |
| 12 | L | 105 | LYS |
| 12 | L | 136 | ARG |
| 13 | M | 55 | LEU |
| 13 | M | 67 | LEU |
| 13 | M | 69 | GLN |
| 13 | M | 91 | TRP |
| 13 | M | 104 | ARG |
| 13 | M | 105 | LYS |
| 14 | N | 3 | ARG |
| 14 | N | 12 | SER |
| 14 | N | 25 | TRP |
| 14 | N | 36 | GLN |
| 14 | N | 64 | LYS |

Continued on next page...

Continued from previous page...

| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 14 | N | 88 | LEU |
| 14 | N | 89 | TYR |
| 14 | N | 115 | LEU |
| 14 | N | 121 | ARG |
| 14 | N | 139 | TRP |
| 14 | N | 142 | GLU |
| 15 | O | 53 | ASP |
| 15 | O | 67 | VAL |
| 15 | O | 71 | CYS |
| 15 | O | 114 | ARG |
| 15 | O | 124 | ASP |
| 15 | O | 127 | ARG |
| 16 | P | 17 | TYR |
| 16 | P | 40 | ARG |
| 16 | P | 52 | LYS |
| 16 | P | 57 | MET |
| 16 | P | 77 | ARG |
| 16 | P | 79 | HIS |
| 16 | P | 84 | ILE |
| 16 | P | 111 | MET |
| 16 | P | 127 | ARG |
| 17 | Q | 8 | GLN |
| 17 | Q | 19 | VAL |
| 17 | Q | 46 | PHE |
| 17 | Q | 53 | LEU |
| 17 | Q | 55 | VAL |
| 17 | Q | 121 | SER |
| 17 | Q | 128 | LYS |
| 17 | Q | 142 | TYR |
| 18 | R | 6 | THR |
| 18 | R | 16 | LEU |
| 18 | R | 17 | ILE |
| 18 | R | 27 | ASP |
| 18 | R | 36 | ASP |
| 18 | R | 45 | ARG |
| 18 | R | 47 | ARG |
| 18 | R | 66 | VAL |
| 18 | R | 67 | ARG |
| 18 | R | 88 | VAL |
| 18 | R | 127 | VAL |
| 18 | R | 128 | ARG |
| 18 | R | 130 | ARG |

Continued on next page...

Continued from previous page...

| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 19 | S | 16 | ARG |
| 19 | S | 25 | ASN |
| 19 | S | 36 | ARG |
| 19 | S | 38 | VAL |
| 19 | S | 41 | ARG |
| 19 | S | 49 | LYS |
| 19 | S | 73 | MET |
| 19 | S | 74 | GLN |
| 19 | S | 85 | PHE |
| 19 | S | 93 | ASN |
| 19 | S | 96 | LYS |
| 19 | S | 100 | SER |
| 19 | S | 105 | LEU |
| 19 | S | 126 | ARG |
| 19 | S | 128 | PHE |
| 19 | S | 131 | LEU |
| 19 | S | 144 | ARG |
| 20 | T | 45 | LEU |
| 20 | T | 53 | TRP |
| 20 | T | 57 | ARG |
| 20 | T | 63 | ARG |
| 20 | T | 68 | ARG |
| 20 | T | 85 | ASN |
| 20 | T | 86 | ARG |
| 20 | T | 100 | ILE |
| 20 | T | 102 | ARG |
| 20 | T | 124 | ILE |
| 20 | T | 139 | THR |
| 21 | U | 52 | LYS |
| 21 | U | 84 | MET |
| 21 | U | 94 | GLU |
| 21 | U | 103 | ILE |
| 22 | V | 12 | TYR |
| 22 | V | 33 | GLN |
| 22 | V | 38 | GLN |
| 22 | V | 50 | TYR |
| 23 | W | 6 | VAL |
| 23 | W | 7 | LEU |
| 23 | W | 11 | LEU |
| 23 | W | 15 | ASN |
| 23 | W | 19 | LYS |
| 23 | W | 23 | ARG |

Continued on next page...

Continued from previous page...

| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 23 | W | 24 | GLN |
| 23 | W | 25 | VAL |
| 23 | W | 28 | ARG |
| 23 | W | 61 | ILE |
| 23 | W | 66 | ASN |
| 23 | W | 70 | ASN |
| 23 | W | 107 | SER |
| 24 | X | 9 | LEU |
| 24 | X | 17 | VAL |
| 24 | X | 19 | ARG |
| 24 | X | 63 | GLN |
| 24 | X | 64 | PRO |
| 24 | X | 70 | LYS |
| 24 | X | 73 | ARG |
| 24 | X | 93 | LEU |
| 24 | X | 98 | GLU |
| 24 | X | 99 | ASN |
| 24 | X | 102 | VAL |
| 24 | X | 107 | PHE |
| 24 | X | 109 | ARG |
| 24 | X | 114 | LYS |
| 24 | X | 130 | VAL |
| 25 | Y | 3 | ASP |
| 25 | Y | 6 | THR |
| 25 | Y | 15 | ASN |
| 25 | Y | 29 | HIS |
| 25 | Y | 31 | ASN |
| 25 | Y | 35 | VAL |
| 25 | Y | 46 | GLU |
| 25 | Y | 57 | VAL |
| 25 | Y | 74 | LEU |
| 25 | Y | 98 | GLU |
| 25 | Y | 110 | GLN |
| 25 | Y | 113 | ASN |
| 25 | Y | 116 | LYS |
| 25 | Y | 125 | ILE |
| 26 | Z | 49 | ARG |
| 26 | Z | 59 | TYR |
| 26 | Z | 63 | SER |
| 26 | Z | 68 | ARG |
| 26 | Z | 97 | LYS |
| 27 | a | 1 | MET |

Continued on next page...

Continued from previous page...

| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 27 | a | 5 | ARG |
| 27 | a | 7 | SER |
| 27 | a | 8 | ASN |
| 27 | a | 18 | VAL |
| 27 | a | 30 | VAL |
| 27 | a | 32 | LYS |
| 27 | a | 33 | ASP |
| 27 | a | 34 | LYS |
| 27 | a | 39 | MET |
| 27 | a | 64 | LEU |
| 27 | a | 75 | ILE |
| 28 | b | 7 | LEU |
| 28 | b | 9 | HIS |
| 28 | b | 26 | GLN |
| 28 | b | 67 | THR |
| 29 | c | 16 | LEU |
| 29 | c | 32 | PHE |
| 29 | c | 56 | LEU |
| 30 | d | 21 | CYS |
| 30 | d | 40 | ARG |
| 30 | d | 45 | GLU |
| 30 | d | 49 | ASP |
| 31 | e | 17 | GLN |
| 31 | e | 22 | GLU |
| 31 | e | 33 | ARG |
| 31 | e | 53 | LYS |
| 32 | f | 82 | LYS |
| 32 | f | 89 | LYS |
| 32 | f | 99 | LYS |
| 32 | f | 103 | LEU |
| 32 | f | 106 | TYR |
| 32 | f | 113 | LYS |
| 32 | f | 117 | LEU |
| 32 | f | 120 | GLU |
| 32 | f | 136 | ARG |
| 32 | f | 139 | CYS |
| 33 | g | 27 | SER |
| 33 | g | 43 | LEU |
| 33 | g | 55 | PHE |
| 33 | g | 60 | ARG |
| 33 | g | 67 | HIS |
| 33 | g | 99 | ASN |

Continued on next page...

Continued from previous page...

| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 33 | g | 175 | VAL |
| 33 | g | 188 | LEU |
| 33 | g | 244 | LYS |
| 33 | g | 273 | GLU |
| 33 | g | 275 | GLU |
| 33 | g | 292 | GLN |
| 33 | g | 299 | LEU |
| 33 | g | 321 | GLN |

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (23) such sidechains are listed below:

| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1 | A | 92 | HIS |
| 1 | A | 109 | ASN |
| 2 | B | 160 | HIS |
| 5 | E | 224 | ASN |
| 6 | F | 141 | ASN |
| 6 | F | 202 | ASN |
| 7 | G | 4 | ASN |
| 7 | G | 190 | GLN |
| 14 | N | 78 | ASN |
| 15 | O | 29 | HIS |
| 16 | P | 79 | HIS |
| 16 | P | 98 | ASN |
| 17 | Q | 83 | GLN |
| 19 | S | 89 | GLN |
| 20 | T | 25 | GLN |
| 23 | W | 92 | ASN |
| 24 | X | 18 | HIS |
| 24 | X | 22 | ASN |
| 24 | X | 63 | GLN |
| 24 | X | 79 | ASN |
| 25 | Y | 29 | HIS |
| 25 | Y | 34 | ASN |
| 28 | b | 49 | HIS |

5.3.3 RNA [i](#)

| Mol | Chain | Analysed | Backbone Outliers | Pucker Outliers |
|-----|-------|-----------------|-------------------|-----------------|
| 34 | 2 | 1778/1780 (99%) | 767 (43%) | 111 (6%) |

Continued on next page...

Continued from previous page...

| Mol | Chain | Analysed | Backbone Outliers | Pucker Outliers |
|-----|-------|-----------------|-------------------|-----------------|
| 35 | i | 184/192 (95%) | 107 (58%) | 0 |
| All | All | 1962/1972 (99%) | 874 (44%) | 111 (5%) |

All (874) RNA backbone outliers are listed below:

| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 34 | 2 | 2 | A |
| 34 | 2 | 3 | U |
| 34 | 2 | 4 | C |
| 34 | 2 | 5 | U |
| 34 | 2 | 9 | U |
| 34 | 2 | 10 | G |
| 34 | 2 | 14 | C |
| 34 | 2 | 17 | C |
| 34 | 2 | 25 | C |
| 34 | 2 | 26 | A |
| 34 | 2 | 32 | U |
| 34 | 2 | 34 | G |
| 34 | 2 | 39 | A |
| 34 | 2 | 40 | A |
| 34 | 2 | 42 | G |
| 34 | 2 | 45 | U |
| 34 | 2 | 47 | A |
| 34 | 2 | 51 | A |
| 34 | 2 | 57 | G |
| 34 | 2 | 59 | C |
| 34 | 2 | 60 | U |
| 34 | 2 | 61 | A |
| 34 | 2 | 63 | G |
| 34 | 2 | 64 | U |
| 34 | 2 | 65 | A |
| 34 | 2 | 66 | U |
| 34 | 2 | 67 | A |
| 34 | 2 | 68 | A |
| 34 | 2 | 69 | G |
| 34 | 2 | 71 | A |
| 34 | 2 | 72 | A |
| 34 | 2 | 73 | U |
| 34 | 2 | 74 | U |
| 34 | 2 | 75 | U |
| 34 | 2 | 76 | A |
| 34 | 2 | 77 | U |

Continued on next page...

Continued from previous page...

| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 34 | 2 | 78 | A |
| 34 | 2 | 80 | A |
| 34 | 2 | 81 | G |
| 34 | 2 | 82 | U |
| 34 | 2 | 86 | A |
| 34 | 2 | 93 | A |
| 34 | 2 | 101 | U |
| 34 | 2 | 104 | A |
| 34 | 2 | 111 | U |
| 34 | 2 | 113 | U |
| 34 | 2 | 114 | C |
| 34 | 2 | 115 | G |
| 34 | 2 | 123 | G |
| 34 | 2 | 124 | A |
| 34 | 2 | 125 | U |
| 34 | 2 | 127 | G |
| 34 | 2 | 129 | U |
| 34 | 2 | 130 | C |
| 34 | 2 | 131 | C |
| 34 | 2 | 132 | U |
| 34 | 2 | 133 | U |
| 34 | 2 | 134 | U |
| 34 | 2 | 136 | C |
| 34 | 2 | 137 | U |
| 34 | 2 | 138 | A |
| 34 | 2 | 139 | C |
| 34 | 2 | 140 | A |
| 34 | 2 | 141 | U |
| 34 | 2 | 146 | A |
| 34 | 2 | 148 | C |
| 34 | 2 | 149 | U |
| 34 | 2 | 150 | G |
| 34 | 2 | 152 | G |
| 34 | 2 | 153 | G |
| 34 | 2 | 154 | U |
| 34 | 2 | 155 | A |
| 34 | 2 | 157 | U |
| 34 | 2 | 158 | U |
| 34 | 2 | 159 | C |
| 34 | 2 | 160 | U |
| 34 | 2 | 161 | A |
| 34 | 2 | 167 | A |

Continued on next page...

Continued from previous page...

| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 34 | 2 | 169 | U |
| 34 | 2 | 170 | A |
| 34 | 2 | 173 | U |
| 34 | 2 | 175 | C |
| 34 | 2 | 176 | U |
| 34 | 2 | 177 | U |
| 34 | 2 | 178 | A |
| 34 | 2 | 180 | A |
| 34 | 2 | 183 | C |
| 34 | 2 | 184 | U |
| 34 | 2 | 186 | G |
| 34 | 2 | 187 | A |
| 34 | 2 | 190 | C |
| 34 | 2 | 191 | U |
| 34 | 2 | 192 | U |
| 34 | 2 | 194 | G |
| 34 | 2 | 195 | G |
| 34 | 2 | 198 | G |
| 34 | 2 | 199 | A |
| 34 | 2 | 203 | G |
| 34 | 2 | 205 | A |
| 34 | 2 | 210 | U |
| 34 | 2 | 217 | A |
| 34 | 2 | 218 | A |
| 34 | 2 | 220 | A |
| 34 | 2 | 224 | A |
| 34 | 2 | 225 | A |
| 34 | 2 | 226 | U |
| 34 | 2 | 228 | U |
| 34 | 2 | 230 | U |
| 34 | 2 | 231 | U |
| 34 | 2 | 232 | C |
| 34 | 2 | 233 | G |
| 34 | 2 | 234 | G |
| 34 | 2 | 235 | A |
| 34 | 2 | 239 | C |
| 34 | 2 | 240 | U |
| 34 | 2 | 241 | U |
| 34 | 2 | 249 | C |
| 34 | 2 | 253 | A |
| 34 | 2 | 256 | A |
| 34 | 2 | 259 | U |

Continued on next page...

Continued from previous page...

| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 34 | 2 | 264 | A |
| 34 | 2 | 265 | A |
| 34 | 2 | 266 | U |
| 34 | 2 | 267 | C |
| 34 | 2 | 268 | G |
| 34 | 2 | 269 | C |
| 34 | 2 | 270 | A |
| 34 | 2 | 274 | C |
| 34 | 2 | 275 | C |
| 34 | 2 | 276 | U |
| 34 | 2 | 277 | U |
| 34 | 2 | 278 | G |
| 34 | 2 | 279 | U |
| 34 | 2 | 280 | G |
| 34 | 2 | 284 | G |
| 34 | 2 | 286 | G |
| 34 | 2 | 288 | U |
| 34 | 2 | 294 | A |
| 34 | 2 | 298 | A |
| 34 | 2 | 301 | U |
| 34 | 2 | 305 | U |
| 34 | 2 | 308 | C |
| 34 | 2 | 309 | C |
| 34 | 2 | 311 | A |
| 34 | 2 | 312 | U |
| 34 | 2 | 313 | C |
| 34 | 2 | 314 | A |
| 34 | 2 | 315 | A |
| 34 | 2 | 319 | U |
| 34 | 2 | 320 | C |
| 34 | 2 | 321 | G |
| 34 | 2 | 322 | A |
| 34 | 2 | 328 | G |
| 34 | 2 | 332 | A |
| 34 | 2 | 336 | G |
| 34 | 2 | 337 | C |
| 34 | 2 | 342 | C |
| 34 | 2 | 351 | A |
| 34 | 2 | 359 | A |
| 34 | 2 | 360 | C |
| 34 | 2 | 374 | U |
| 34 | 2 | 377 | A |

Continued on next page...

Continued from previous page...

| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 34 | 2 | 382 | G |
| 34 | 2 | 389 | G |
| 34 | 2 | 392 | C |
| 34 | 2 | 397 | G |
| 34 | 2 | 399 | A |
| 34 | 2 | 400 | A |
| 34 | 2 | 401 | C |
| 34 | 2 | 403 | G |
| 34 | 2 | 406 | A |
| 34 | 2 | 410 | C |
| 34 | 2 | 411 | A |
| 34 | 2 | 412 | U |
| 34 | 2 | 414 | C |
| 34 | 2 | 415 | A |
| 34 | 2 | 416 | A |
| 34 | 2 | 417 | G |
| 34 | 2 | 419 | A |
| 34 | 2 | 421 | G |
| 34 | 2 | 422 | G |
| 34 | 2 | 423 | C |
| 34 | 2 | 424 | A |
| 34 | 2 | 425 | G |
| 34 | 2 | 433 | G |
| 34 | 2 | 436 | A |
| 34 | 2 | 438 | U |
| 34 | 2 | 442 | C |
| 34 | 2 | 443 | C |
| 34 | 2 | 444 | A |
| 34 | 2 | 447 | C |
| 34 | 2 | 452 | U |
| 34 | 2 | 458 | G |
| 34 | 2 | 459 | A |
| 34 | 2 | 460 | G |
| 34 | 2 | 463 | A |
| 34 | 2 | 467 | A |
| 34 | 2 | 474 | A |
| 34 | 2 | 476 | A |
| 34 | 2 | 479 | G |
| 34 | 2 | 480 | A |
| 34 | 2 | 483 | C |
| 34 | 2 | 490 | C |
| 34 | 2 | 491 | A |

Continued on next page...

Continued from previous page...

| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 34 | 2 | 492 | U |
| 34 | 2 | 493 | U |
| 34 | 2 | 494 | C |
| 34 | 2 | 497 | G |
| 34 | 2 | 499 | C |
| 34 | 2 | 500 | U |
| 34 | 2 | 503 | U |
| 34 | 2 | 504 | A |
| 34 | 2 | 505 | A |
| 34 | 2 | 506 | U |
| 34 | 2 | 507 | U |
| 34 | 2 | 509 | G |
| 34 | 2 | 510 | A |
| 34 | 2 | 512 | U |
| 34 | 2 | 513 | G |
| 34 | 2 | 514 | A |
| 34 | 2 | 516 | U |
| 34 | 2 | 518 | C |
| 34 | 2 | 521 | U |
| 34 | 2 | 524 | A |
| 34 | 2 | 526 | A |
| 34 | 2 | 527 | U |
| 34 | 2 | 532 | U |
| 34 | 2 | 533 | A |
| 34 | 2 | 534 | A |
| 34 | 2 | 535 | C |
| 34 | 2 | 536 | G |
| 34 | 2 | 537 | A |
| 34 | 2 | 538 | G |
| 34 | 2 | 539 | G |
| 34 | 2 | 540 | A |
| 34 | 2 | 541 | A |
| 34 | 2 | 542 | C |
| 34 | 2 | 543 | A |
| 34 | 2 | 544 | A |
| 34 | 2 | 545 | C |
| 34 | 2 | 547 | G |
| 34 | 2 | 548 | G |
| 34 | 2 | 550 | G |
| 34 | 2 | 551 | G |
| 34 | 2 | 553 | C |
| 34 | 2 | 554 | A |

Continued on next page...

Continued from previous page...

| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 34 | 2 | 556 | G |
| 34 | 2 | 557 | U |
| 34 | 2 | 558 | C |
| 34 | 2 | 561 | G |
| 34 | 2 | 564 | C |
| 34 | 2 | 565 | C |
| 34 | 2 | 570 | G |
| 34 | 2 | 573 | G |
| 34 | 2 | 574 | C |
| 34 | 2 | 575 | G |
| 34 | 2 | 576 | G |
| 34 | 2 | 577 | U |
| 34 | 2 | 578 | A |
| 34 | 2 | 579 | A |
| 34 | 2 | 581 | U |
| 34 | 2 | 593 | A |
| 34 | 2 | 594 | G |
| 34 | 2 | 596 | G |
| 34 | 2 | 600 | A |
| 34 | 2 | 605 | A |
| 34 | 2 | 606 | G |
| 34 | 2 | 607 | U |
| 34 | 2 | 610 | U |
| 34 | 2 | 613 | C |
| 34 | 2 | 618 | A |
| 34 | 2 | 619 | A |
| 34 | 2 | 622 | A |
| 34 | 2 | 623 | G |
| 34 | 2 | 629 | A |
| 34 | 2 | 632 | U |
| 34 | 2 | 634 | A |
| 34 | 2 | 637 | U |
| 34 | 2 | 638 | U |
| 34 | 2 | 639 | U |
| 34 | 2 | 640 | G |
| 34 | 2 | 642 | G |
| 34 | 2 | 647 | G |
| 34 | 2 | 648 | U |
| 34 | 2 | 649 | U |
| 34 | 2 | 652 | C |
| 34 | 2 | 653 | C |
| 34 | 2 | 654 | G |

Continued on next page...

Continued from previous page...

| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 34 | 2 | 655 | G |
| 34 | 2 | 677 | G |
| 34 | 2 | 678 | U |
| 34 | 2 | 679 | U |
| 34 | 2 | 683 | C |
| 34 | 2 | 684 | A |
| 34 | 2 | 691 | U |
| 34 | 2 | 694 | U |
| 34 | 2 | 695 | U |
| 34 | 2 | 696 | C |
| 34 | 2 | 697 | C |
| 34 | 2 | 698 | U |
| 34 | 2 | 701 | U |
| 34 | 2 | 704 | C |
| 34 | 2 | 705 | U |
| 34 | 2 | 708 | C |
| 34 | 2 | 709 | C |
| 34 | 2 | 710 | U |
| 34 | 2 | 712 | U |
| 34 | 2 | 713 | A |
| 34 | 2 | 714 | C |
| 34 | 2 | 716 | C |
| 34 | 2 | 717 | C |
| 34 | 2 | 718 | U |
| 34 | 2 | 719 | U |
| 34 | 2 | 722 | G |
| 34 | 2 | 724 | G |
| 34 | 2 | 725 | U |
| 34 | 2 | 727 | C |
| 34 | 2 | 731 | C |
| 34 | 2 | 732 | G |
| 34 | 2 | 733 | A |
| 34 | 2 | 734 | A |
| 34 | 2 | 735 | C |
| 34 | 2 | 736 | C |
| 34 | 2 | 737 | A |
| 34 | 2 | 738 | G |
| 34 | 2 | 740 | A |
| 34 | 2 | 741 | C |
| 34 | 2 | 742 | U |
| 34 | 2 | 743 | U |
| 34 | 2 | 754 | A |

Continued on next page...

Continued from previous page...

| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 34 | 2 | 756 | A |
| 34 | 2 | 765 | G |
| 34 | 2 | 766 | U |
| 34 | 2 | 767 | U |
| 34 | 2 | 769 | A |
| 34 | 2 | 771 | A |
| 34 | 2 | 774 | A |
| 34 | 2 | 778 | G |
| 34 | 2 | 779 | A |
| 34 | 2 | 780 | A |
| 34 | 2 | 781 | A |
| 34 | 2 | 782 | G |
| 34 | 2 | 785 | C |
| 34 | 2 | 786 | G |
| 34 | 2 | 787 | A |
| 34 | 2 | 788 | A |
| 34 | 2 | 789 | U |
| 34 | 2 | 792 | A |
| 34 | 2 | 793 | U |
| 34 | 2 | 794 | U |
| 34 | 2 | 795 | A |
| 34 | 2 | 802 | A |
| 34 | 2 | 806 | A |
| 34 | 2 | 809 | G |
| 34 | 2 | 811 | A |
| 34 | 2 | 812 | U |
| 34 | 2 | 813 | A |
| 34 | 2 | 815 | G |
| 34 | 2 | 817 | C |
| 34 | 2 | 819 | U |
| 34 | 2 | 820 | U |
| 34 | 2 | 821 | U |
| 34 | 2 | 822 | G |
| 34 | 2 | 823 | G |
| 34 | 2 | 825 | U |
| 34 | 2 | 826 | C |
| 34 | 2 | 828 | A |
| 34 | 2 | 829 | U |
| 34 | 2 | 830 | U |
| 34 | 2 | 831 | U |
| 34 | 2 | 832 | U |
| 34 | 2 | 834 | U |

Continued on next page...

Continued from previous page...

| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 34 | 2 | 837 | G |
| 34 | 2 | 840 | U |
| 34 | 2 | 842 | U |
| 34 | 2 | 844 | G |
| 34 | 2 | 845 | G |
| 34 | 2 | 848 | C |
| 34 | 2 | 849 | A |
| 34 | 2 | 852 | G |
| 34 | 2 | 855 | A |
| 34 | 2 | 859 | U |
| 34 | 2 | 860 | U |
| 34 | 2 | 861 | A |
| 34 | 2 | 862 | A |
| 34 | 2 | 863 | U |
| 34 | 2 | 872 | U |
| 34 | 2 | 875 | G |
| 34 | 2 | 876 | G |
| 34 | 2 | 884 | G |
| 34 | 2 | 885 | U |
| 34 | 2 | 887 | U |
| 34 | 2 | 894 | G |
| 34 | 2 | 895 | U |
| 34 | 2 | 897 | A |
| 34 | 2 | 903 | G |
| 34 | 2 | 904 | A |
| 34 | 2 | 905 | A |
| 34 | 2 | 906 | A |
| 34 | 2 | 908 | U |
| 34 | 2 | 909 | C |
| 34 | 2 | 910 | U |
| 34 | 2 | 912 | G |
| 34 | 2 | 913 | G |
| 34 | 2 | 914 | A |
| 34 | 2 | 915 | U |
| 34 | 2 | 919 | U |
| 34 | 2 | 920 | U |
| 34 | 2 | 927 | U |
| 34 | 2 | 928 | A |
| 34 | 2 | 929 | A |
| 34 | 2 | 931 | U |
| 34 | 2 | 932 | A |
| 34 | 2 | 934 | U |

Continued on next page...

Continued from previous page...

| Mol | Chain | Res | Type |
|-----|-------|------|------|
| 34 | 2 | 935 | G |
| 34 | 2 | 936 | C |
| 34 | 2 | 939 | A |
| 34 | 2 | 941 | G |
| 34 | 2 | 943 | A |
| 34 | 2 | 944 | U |
| 34 | 2 | 950 | A |
| 34 | 2 | 958 | U |
| 34 | 2 | 959 | U |
| 34 | 2 | 964 | U |
| 34 | 2 | 965 | A |
| 34 | 2 | 969 | A |
| 34 | 2 | 972 | A |
| 34 | 2 | 980 | U |
| 34 | 2 | 981 | U |
| 34 | 2 | 983 | G |
| 34 | 2 | 985 | G |
| 34 | 2 | 987 | A |
| 34 | 2 | 990 | G |
| 34 | 2 | 991 | A |
| 34 | 2 | 992 | A |
| 34 | 2 | 993 | G |
| 34 | 2 | 994 | A |
| 34 | 2 | 999 | C |
| 34 | 2 | 1003 | U |
| 34 | 2 | 1004 | A |
| 34 | 2 | 1005 | C |
| 34 | 2 | 1009 | C |
| 34 | 2 | 1010 | G |
| 34 | 2 | 1011 | U |
| 34 | 2 | 1012 | A |
| 34 | 2 | 1013 | G |
| 34 | 2 | 1015 | C |
| 34 | 2 | 1020 | C |
| 34 | 2 | 1024 | A |
| 34 | 2 | 1026 | A |
| 34 | 2 | 1027 | C |
| 34 | 2 | 1028 | U |
| 34 | 2 | 1030 | U |
| 34 | 2 | 1031 | G |
| 34 | 2 | 1037 | U |
| 34 | 2 | 1038 | A |

Continued on next page...

Continued from previous page...

| Mol | Chain | Res | Type |
|-----|-------|------|------|
| 34 | 2 | 1039 | G |
| 34 | 2 | 1041 | G |
| 34 | 2 | 1042 | A |
| 34 | 2 | 1044 | C |
| 34 | 2 | 1045 | G |
| 34 | 2 | 1046 | G |
| 34 | 2 | 1050 | G |
| 34 | 2 | 1051 | U |
| 34 | 2 | 1052 | G |
| 34 | 2 | 1056 | U |
| 34 | 2 | 1057 | U |
| 34 | 2 | 1058 | C |
| 34 | 2 | 1059 | U |
| 34 | 2 | 1060 | U |
| 34 | 2 | 1063 | G |
| 34 | 2 | 1070 | U |
| 34 | 2 | 1071 | C |
| 34 | 2 | 1073 | G |
| 34 | 2 | 1074 | C |
| 34 | 2 | 1075 | A |
| 34 | 2 | 1076 | C |
| 34 | 2 | 1080 | A |
| 34 | 2 | 1081 | C |
| 34 | 2 | 1082 | G |
| 34 | 2 | 1083 | A |
| 34 | 2 | 1084 | G |
| 34 | 2 | 1087 | A |
| 34 | 2 | 1090 | A |
| 34 | 2 | 1091 | A |
| 34 | 2 | 1092 | A |
| 34 | 2 | 1094 | U |
| 34 | 2 | 1096 | U |
| 34 | 2 | 1097 | U |
| 34 | 2 | 1098 | U |
| 34 | 2 | 1099 | G |
| 34 | 2 | 1100 | G |
| 34 | 2 | 1107 | G |
| 34 | 2 | 1108 | G |
| 34 | 2 | 1110 | G |
| 34 | 2 | 1113 | G |
| 34 | 2 | 1118 | G |
| 34 | 2 | 1121 | G |

Continued on next page...

Continued from previous page...

| Mol | Chain | Res | Type |
|-----|-------|------|------|
| 34 | 2 | 1123 | A |
| 34 | 2 | 1130 | A |
| 34 | 2 | 1137 | A |
| 34 | 2 | 1142 | A |
| 34 | 2 | 1145 | G |
| 34 | 2 | 1149 | G |
| 34 | 2 | 1150 | A |
| 34 | 2 | 1157 | C |
| 34 | 2 | 1158 | C |
| 34 | 2 | 1159 | A |
| 34 | 2 | 1162 | A |
| 34 | 2 | 1163 | G |
| 34 | 2 | 1166 | G |
| 34 | 2 | 1174 | U |
| 34 | 2 | 1175 | G |
| 34 | 2 | 1183 | A |
| 34 | 2 | 1184 | U |
| 34 | 2 | 1185 | U |
| 34 | 2 | 1189 | C |
| 34 | 2 | 1190 | U |
| 34 | 2 | 1192 | A |
| 34 | 2 | 1193 | A |
| 34 | 2 | 1195 | A |
| 34 | 2 | 1196 | C |
| 34 | 2 | 1198 | G |
| 34 | 2 | 1199 | G |
| 34 | 2 | 1200 | G |
| 34 | 2 | 1201 | A |
| 34 | 2 | 1202 | A |
| 34 | 2 | 1203 | A |
| 34 | 2 | 1204 | C |
| 34 | 2 | 1211 | G |
| 34 | 2 | 1212 | G |
| 34 | 2 | 1213 | U |
| 34 | 2 | 1215 | C |
| 34 | 2 | 1216 | A |
| 34 | 2 | 1217 | G |
| 34 | 2 | 1218 | A |
| 34 | 2 | 1219 | C |
| 34 | 2 | 1222 | A |
| 34 | 2 | 1224 | U |
| 34 | 2 | 1226 | A |

Continued on next page...

Continued from previous page...

| Mol | Chain | Res | Type |
|-----|-------|------|------|
| 34 | 2 | 1227 | G |
| 34 | 2 | 1228 | G |
| 34 | 2 | 1229 | A |
| 34 | 2 | 1230 | U |
| 34 | 2 | 1231 | U |
| 34 | 2 | 1234 | C |
| 34 | 2 | 1236 | G |
| 34 | 2 | 1238 | U |
| 34 | 2 | 1240 | G |
| 34 | 2 | 1241 | A |
| 34 | 2 | 1242 | G |
| 34 | 2 | 1243 | A |
| 34 | 2 | 1244 | G |
| 34 | 2 | 1245 | C |
| 34 | 2 | 1247 | C |
| 34 | 2 | 1250 | U |
| 34 | 2 | 1253 | U |
| 34 | 2 | 1254 | G |
| 34 | 2 | 1257 | U |
| 34 | 2 | 1258 | U |
| 34 | 2 | 1259 | U |
| 34 | 2 | 1265 | U |
| 34 | 2 | 1266 | G |
| 34 | 2 | 1268 | U |
| 34 | 2 | 1269 | G |
| 34 | 2 | 1274 | A |
| 34 | 2 | 1282 | U |
| 34 | 2 | 1284 | U |
| 34 | 2 | 1296 | G |
| 34 | 2 | 1306 | U |
| 34 | 2 | 1310 | U |
| 34 | 2 | 1313 | U |
| 34 | 2 | 1314 | U |
| 34 | 2 | 1317 | G |
| 34 | 2 | 1319 | U |
| 34 | 2 | 1320 | A |
| 34 | 2 | 1321 | A |
| 34 | 2 | 1322 | C |
| 34 | 2 | 1324 | A |
| 34 | 2 | 1336 | A |
| 34 | 2 | 1339 | U |
| 34 | 2 | 1340 | A |

Continued on next page...

Continued from previous page...

| Mol | Chain | Res | Type |
|-----|-------|------|------|
| 34 | 2 | 1343 | A |
| 34 | 2 | 1344 | A |
| 34 | 2 | 1345 | A |
| 34 | 2 | 1347 | A |
| 34 | 2 | 1349 | G |
| 34 | 2 | 1353 | G |
| 34 | 2 | 1356 | G |
| 34 | 2 | 1358 | C |
| 34 | 2 | 1359 | A |
| 34 | 2 | 1360 | C |
| 34 | 2 | 1361 | U |
| 34 | 2 | 1362 | U |
| 34 | 2 | 1363 | G |
| 34 | 2 | 1364 | C |
| 34 | 2 | 1366 | G |
| 34 | 2 | 1369 | U |
| 34 | 2 | 1370 | G |
| 34 | 2 | 1371 | A |
| 34 | 2 | 1374 | C |
| 34 | 2 | 1380 | A |
| 34 | 2 | 1388 | U |
| 34 | 2 | 1393 | G |
| 34 | 2 | 1396 | U |
| 34 | 2 | 1397 | C |
| 34 | 2 | 1398 | A |
| 34 | 2 | 1400 | G |
| 34 | 2 | 1404 | A |
| 34 | 2 | 1410 | G |
| 34 | 2 | 1411 | U |
| 34 | 2 | 1412 | U |
| 34 | 2 | 1413 | U |
| 34 | 2 | 1416 | G |
| 34 | 2 | 1417 | G |
| 34 | 2 | 1425 | A |
| 34 | 2 | 1426 | G |
| 34 | 2 | 1428 | U |
| 34 | 2 | 1430 | U |
| 34 | 2 | 1432 | U |
| 34 | 2 | 1433 | G |
| 34 | 2 | 1434 | A |
| 34 | 2 | 1435 | U |
| 34 | 2 | 1442 | A |

Continued on next page...

Continued from previous page...

| Mol | Chain | Res | Type |
|-----|-------|------|------|
| 34 | 2 | 1443 | G |
| 34 | 2 | 1444 | A |
| 34 | 2 | 1445 | C |
| 34 | 2 | 1446 | G |
| 34 | 2 | 1449 | C |
| 34 | 2 | 1452 | G |
| 34 | 2 | 1454 | C |
| 34 | 2 | 1455 | C |
| 34 | 2 | 1456 | G |
| 34 | 2 | 1457 | C |
| 34 | 2 | 1458 | A |
| 34 | 2 | 1461 | C |
| 34 | 2 | 1464 | G |
| 34 | 2 | 1467 | A |
| 34 | 2 | 1468 | C |
| 34 | 2 | 1469 | A |
| 34 | 2 | 1471 | U |
| 34 | 2 | 1475 | G |
| 34 | 2 | 1476 | G |
| 34 | 2 | 1481 | A |
| 34 | 2 | 1484 | G |
| 34 | 2 | 1485 | A |
| 34 | 2 | 1487 | U |
| 34 | 2 | 1488 | A |
| 34 | 2 | 1489 | C |
| 34 | 2 | 1490 | A |
| 34 | 2 | 1491 | A |
| 34 | 2 | 1492 | C |
| 34 | 2 | 1494 | U |
| 34 | 2 | 1495 | U |
| 34 | 2 | 1498 | C |
| 34 | 2 | 1502 | G |
| 34 | 2 | 1506 | U |
| 34 | 2 | 1507 | C |
| 34 | 2 | 1508 | U |
| 34 | 2 | 1509 | G |
| 34 | 2 | 1512 | U |
| 34 | 2 | 1513 | A |
| 34 | 2 | 1514 | A |
| 34 | 2 | 1519 | G |
| 34 | 2 | 1521 | G |
| 34 | 2 | 1522 | A |

Continued on next page...

Continued from previous page...

| Mol | Chain | Res | Type |
|-----|-------|------|------|
| 34 | 2 | 1523 | A |
| 34 | 2 | 1527 | C |
| 34 | 2 | 1531 | C |
| 34 | 2 | 1532 | G |
| 34 | 2 | 1533 | U |
| 34 | 2 | 1534 | G |
| 34 | 2 | 1535 | C |
| 34 | 2 | 1537 | G |
| 34 | 2 | 1538 | G |
| 34 | 2 | 1540 | G |
| 34 | 2 | 1543 | A |
| 34 | 2 | 1552 | U |
| 34 | 2 | 1555 | U |
| 34 | 2 | 1557 | A |
| 34 | 2 | 1565 | U |
| 34 | 2 | 1566 | C |
| 34 | 2 | 1569 | C |
| 34 | 2 | 1570 | G |
| 34 | 2 | 1571 | A |
| 34 | 2 | 1580 | U |
| 34 | 2 | 1583 | U |
| 34 | 2 | 1588 | G |
| 34 | 2 | 1589 | C |
| 34 | 2 | 1594 | C |
| 34 | 2 | 1595 | A |
| 34 | 2 | 1597 | C |
| 34 | 2 | 1598 | A |
| 34 | 2 | 1599 | G |
| 34 | 2 | 1602 | U |
| 34 | 2 | 1603 | G |
| 34 | 2 | 1605 | G |
| 34 | 2 | 1612 | A |
| 34 | 2 | 1614 | G |
| 34 | 2 | 1616 | C |
| 34 | 2 | 1623 | C |
| 34 | 2 | 1626 | U |
| 34 | 2 | 1629 | A |
| 34 | 2 | 1633 | A |
| 34 | 2 | 1635 | C |
| 34 | 2 | 1640 | G |
| 34 | 2 | 1643 | G |
| 34 | 2 | 1655 | U |

Continued on next page...

Continued from previous page...

| Mol | Chain | Res | Type |
|-----|-------|------|------|
| 34 | 2 | 1656 | G |
| 34 | 2 | 1667 | U |
| 34 | 2 | 1676 | A |
| 34 | 2 | 1679 | A |
| 34 | 2 | 1682 | U |
| 34 | 2 | 1685 | U |
| 34 | 2 | 1686 | U |
| 34 | 2 | 1687 | A |
| 34 | 2 | 1688 | G |
| 34 | 2 | 1692 | A |
| 34 | 2 | 1693 | G |
| 34 | 2 | 1694 | G |
| 34 | 2 | 1696 | G |
| 34 | 2 | 1697 | G |
| 34 | 2 | 1698 | C |
| 34 | 2 | 1699 | A |
| 34 | 2 | 1700 | A |
| 34 | 2 | 1701 | C |
| 34 | 2 | 1702 | U |
| 34 | 2 | 1703 | C |
| 34 | 2 | 1706 | U |
| 34 | 2 | 1707 | C |
| 34 | 2 | 1708 | U |
| 34 | 2 | 1709 | C |
| 34 | 2 | 1710 | A |
| 34 | 2 | 1711 | G |
| 34 | 2 | 1712 | A |
| 34 | 2 | 1725 | G |
| 34 | 2 | 1730 | A |
| 34 | 2 | 1740 | U |
| 34 | 2 | 1743 | G |
| 34 | 2 | 1748 | A |
| 34 | 2 | 1753 | A |
| 34 | 2 | 1754 | A |
| 34 | 2 | 1755 | G |
| 34 | 2 | 1756 | U |
| 34 | 2 | 1758 | G |
| 34 | 2 | 1759 | U |
| 34 | 2 | 1763 | A |
| 34 | 2 | 1764 | A |
| 34 | 2 | 1766 | G |
| 34 | 2 | 1767 | U |

Continued on next page...

Continued from previous page...

| Mol | Chain | Res | Type |
|-----|-------|------|------|
| 34 | 2 | 1770 | C |
| 34 | 2 | 1774 | A |
| 34 | 2 | 1776 | G |
| 34 | 2 | 1777 | U |
| 34 | 2 | 1778 | G |
| 34 | 2 | 1779 | A |
| 34 | 2 | 1780 | A |
| 34 | 2 | 1781 | C |
| 34 | 2 | 1784 | G |
| 34 | 2 | 1789 | A |
| 34 | 2 | 1790 | G |
| 34 | 2 | 1791 | G |
| 34 | 2 | 1792 | A |
| 34 | 2 | 1793 | U |
| 34 | 2 | 1794 | C |
| 34 | 2 | 1796 | U |
| 34 | 2 | 1798 | A |
| 35 | i | 6033 | A |
| 35 | i | 6034 | A |
| 35 | i | 6037 | U |
| 35 | i | 6039 | A |
| 35 | i | 6044 | G |
| 35 | i | 6046 | U |
| 35 | i | 6049 | U |
| 35 | i | 6052 | A |
| 35 | i | 6053 | U |
| 35 | i | 6056 | A |
| 35 | i | 6058 | U |
| 35 | i | 6061 | U |
| 35 | i | 6062 | G |
| 35 | i | 6063 | A |
| 35 | i | 6067 | G |
| 35 | i | 6068 | U |
| 35 | i | 6075 | A |
| 35 | i | 6076 | U |
| 35 | i | 6077 | U |
| 35 | i | 6079 | C |
| 35 | i | 6080 | A |
| 35 | i | 6081 | A |
| 35 | i | 6084 | A |
| 35 | i | 6086 | U |
| 35 | i | 6087 | G |

Continued on next page...

Continued from previous page...

| Mol | Chain | Res | Type |
|-----|-------|------|------|
| 35 | i | 6088 | C |
| 35 | i | 6090 | A |
| 35 | i | 6094 | U |
| 35 | i | 6098 | A |
| 35 | i | 6099 | U |
| 35 | i | 6101 | U |
| 35 | i | 6102 | A |
| 35 | i | 6104 | G |
| 35 | i | 6105 | U |
| 35 | i | 6106 | U |
| 35 | i | 6107 | A |
| 35 | i | 6108 | G |
| 35 | i | 6109 | C |
| 35 | i | 6110 | U |
| 35 | i | 6112 | U |
| 35 | i | 6114 | U |
| 35 | i | 6118 | U |
| 35 | i | 6119 | U |
| 35 | i | 6121 | A |
| 35 | i | 6122 | C |
| 35 | i | 6123 | G |
| 35 | i | 6124 | U |
| 35 | i | 6128 | A |
| 35 | i | 6129 | G |
| 35 | i | 6130 | G |
| 35 | i | 6132 | U |
| 35 | i | 6133 | G |
| 35 | i | 6135 | C |
| 35 | i | 6136 | U |
| 35 | i | 6137 | A |
| 35 | i | 6138 | G |
| 35 | i | 6139 | U |
| 35 | i | 6140 | G |
| 35 | i | 6142 | C |
| 35 | i | 6143 | A |
| 35 | i | 6144 | G |
| 35 | i | 6145 | C |
| 35 | i | 6146 | C |
| 35 | i | 6147 | C |
| 35 | i | 6148 | C |
| 35 | i | 6149 | A |
| 35 | i | 6153 | U |

Continued on next page...

Continued from previous page...

| Mol | Chain | Res | Type |
|-----|-------|------|------|
| 35 | i | 6154 | A |
| 35 | i | 6155 | U |
| 35 | i | 6157 | C |
| 35 | i | 6158 | A |
| 35 | i | 6159 | G |
| 35 | i | 6160 | G |
| 35 | i | 6162 | A |
| 35 | i | 6163 | G |
| 35 | i | 6165 | C |
| 35 | i | 6166 | C |
| 35 | i | 6168 | C |
| 35 | i | 6169 | U |
| 35 | i | 6170 | C |
| 35 | i | 6171 | U |
| 35 | i | 6172 | G |
| 35 | i | 6173 | C |
| 35 | i | 6174 | G |
| 35 | i | 6176 | C |
| 35 | i | 6178 | U |
| 35 | i | 6179 | U |
| 35 | i | 6180 | U |
| 35 | i | 6181 | C |
| 35 | i | 6183 | G |
| 35 | i | 6184 | A |
| 35 | i | 6186 | U |
| 35 | i | 6187 | A |
| 35 | i | 6192 | G |
| 35 | i | 6197 | A |
| 35 | i | 6198 | A |
| 35 | i | 6199 | A |
| 35 | i | 6200 | A |
| 35 | i | 6202 | C |
| 35 | i | 6210 | U |
| 35 | i | 6211 | U |
| 35 | i | 6212 | U |
| 35 | i | 6213 | A |
| 35 | i | 6218 | C |
| 35 | i | 6219 | U |
| 35 | i | 6220 | A |
| 35 | i | 6221 | C |

All (111) RNA pucker outliers are listed below:

| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 34 | 2 | 3 | U |
| 34 | 2 | 44 | U |
| 34 | 2 | 59 | C |
| 34 | 2 | 63 | G |
| 34 | 2 | 65 | A |
| 34 | 2 | 66 | U |
| 34 | 2 | 70 | C |
| 34 | 2 | 71 | A |
| 34 | 2 | 72 | A |
| 34 | 2 | 73 | U |
| 34 | 2 | 129 | U |
| 34 | 2 | 130 | C |
| 34 | 2 | 137 | U |
| 34 | 2 | 139 | C |
| 34 | 2 | 148 | C |
| 34 | 2 | 149 | U |
| 34 | 2 | 157 | U |
| 34 | 2 | 169 | U |
| 34 | 2 | 177 | U |
| 34 | 2 | 186 | G |
| 34 | 2 | 216 | A |
| 34 | 2 | 217 | A |
| 34 | 2 | 239 | C |
| 34 | 2 | 248 | U |
| 34 | 2 | 258 | U |
| 34 | 2 | 262 | C |
| 34 | 2 | 263 | G |
| 34 | 2 | 264 | A |
| 34 | 2 | 265 | A |
| 34 | 2 | 269 | C |
| 34 | 2 | 271 | U |
| 34 | 2 | 277 | U |
| 34 | 2 | 279 | U |
| 34 | 2 | 321 | G |
| 34 | 2 | 399 | A |
| 34 | 2 | 454 | C |
| 34 | 2 | 497 | G |
| 34 | 2 | 509 | G |
| 34 | 2 | 513 | G |
| 34 | 2 | 532 | U |
| 34 | 2 | 537 | A |
| 34 | 2 | 542 | C |
| 34 | 2 | 556 | G |

Continued on next page...

Continued from previous page...

| Mol | Chain | Res | Type |
|-----|-------|------|------|
| 34 | 2 | 557 | U |
| 34 | 2 | 563 | G |
| 34 | 2 | 564 | C |
| 34 | 2 | 576 | G |
| 34 | 2 | 577 | U |
| 34 | 2 | 578 | A |
| 34 | 2 | 579 | A |
| 34 | 2 | 605 | A |
| 34 | 2 | 621 | A |
| 34 | 2 | 638 | U |
| 34 | 2 | 695 | U |
| 34 | 2 | 700 | C |
| 34 | 2 | 704 | C |
| 34 | 2 | 708 | C |
| 34 | 2 | 710 | U |
| 34 | 2 | 721 | U |
| 34 | 2 | 740 | A |
| 34 | 2 | 766 | U |
| 34 | 2 | 779 | A |
| 34 | 2 | 792 | A |
| 34 | 2 | 794 | U |
| 34 | 2 | 809 | G |
| 34 | 2 | 811 | A |
| 34 | 2 | 826 | C |
| 34 | 2 | 828 | A |
| 34 | 2 | 854 | A |
| 34 | 2 | 862 | A |
| 34 | 2 | 884 | G |
| 34 | 2 | 909 | C |
| 34 | 2 | 911 | U |
| 34 | 2 | 912 | G |
| 34 | 2 | 913 | G |
| 34 | 2 | 927 | U |
| 34 | 2 | 963 | U |
| 34 | 2 | 1003 | U |
| 34 | 2 | 1010 | G |
| 34 | 2 | 1027 | C |
| 34 | 2 | 1044 | C |
| 34 | 2 | 1060 | U |
| 34 | 2 | 1073 | G |
| 34 | 2 | 1080 | A |
| 34 | 2 | 1083 | A |

Continued on next page...

Continued from previous page...

| Mol | Chain | Res | Type |
|-----|-------|------|------|
| 34 | 2 | 1107 | G |
| 34 | 2 | 1184 | U |
| 34 | 2 | 1189 | C |
| 34 | 2 | 1195 | A |
| 34 | 2 | 1217 | G |
| 34 | 2 | 1230 | U |
| 34 | 2 | 1243 | A |
| 34 | 2 | 1264 | G |
| 34 | 2 | 1343 | A |
| 34 | 2 | 1429 | C |
| 34 | 2 | 1455 | C |
| 34 | 2 | 1470 | C |
| 34 | 2 | 1491 | A |
| 34 | 2 | 1501 | A |
| 34 | 2 | 1532 | G |
| 34 | 2 | 1534 | G |
| 34 | 2 | 1556 | U |
| 34 | 2 | 1598 | A |
| 34 | 2 | 1613 | C |
| 34 | 2 | 1628 | U |
| 34 | 2 | 1634 | C |
| 34 | 2 | 1655 | U |
| 34 | 2 | 1678 | G |
| 34 | 2 | 1763 | A |
| 34 | 2 | 1765 | G |
| 34 | 2 | 1791 | G |

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

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

5.5 Carbohydrates ⓘ

There are no carbohydrates in this entry.

5.6 Ligand geometry ⓘ

Of 83 ligands modelled in this entry, 83 are monoatomic - leaving 0 for Mogul analysis.

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

No monomer is involved in short contacts.

5.7 Other polymers [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 |
|-----|-------|------------------|
| 34 | 2 | 1 |

All chain breaks are listed below:

| Model | Chain | Residue-1 | Atom-1 | Residue-2 | Atom-2 | Distance (Å) |
|-------|-------|-----------|--------|-----------|--------|--------------|
| 1 | 2 | 657:C | O3' | 676:G | P | 17.80 |