



Full wwPDB EM Validation Report ⓘ

Oct 1, 2025 – 02:35 PM JST

PDB ID : 9V1I / pdb_00009v1i
EMDB ID : EMD-64694
Title : Cryo- EM structure of ribosomal large subunit (LSU) from Entamoeba histolytica at 2.8 angstrom resolution
Authors : Sharma, S.; Mishra, S.; Gourinath, S.; Kaushal, P.S.
Deposited on : 2025-05-19
Resolution : 2.80 Å (reported)
Based on initial models : 4UG0, 5XXB

This is a Full wwPDB EM Validation Report for a publicly released PDB entry.

We welcome your comments at validation@mail.wwpdb.org

A user guide is available at

<https://www.wwpdb.org/validation/2017/EMValidationReportHelp>
with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

<http://www.wwpdb.org/validation/2017/FAQs#types>.

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

EMDB validation analysis : 0.0.1.dev129
MolProbity : 4-5-2 with Phenix2.0
Percentile statistics : 20231227.v01 (using entries in the PDB archive December 27th 2023)
EM percentile statistics : 202505.v01 (Using data in the EMDB archive up until May 2025)
MapQ : 1.9.13
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.46

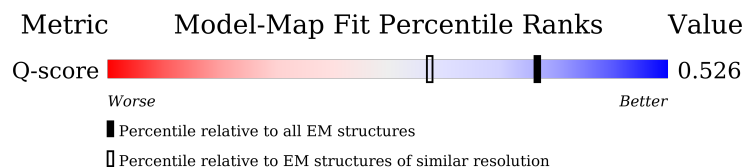
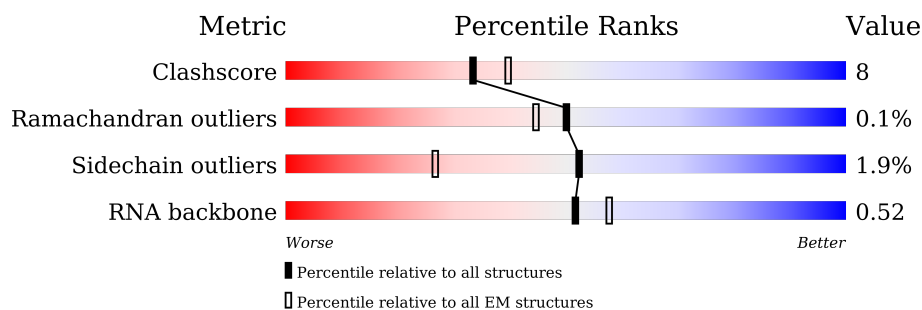
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

ELECTRON MICROSCOPY

The reported resolution of this entry is 2.80 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.















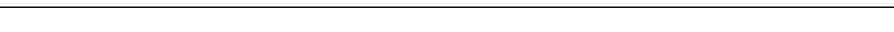

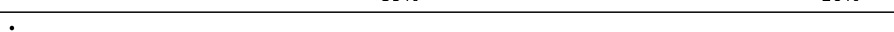

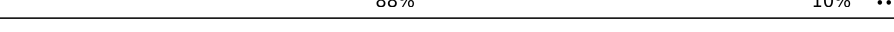



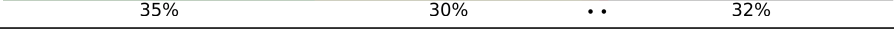




| Metric | Whole archive (#Entries) | EM structures (#Entries) | Similar EM resolution (#Entries, resolution range(Å)) |
|-----------------------|-----------------------------|-----------------------------|--|
| Clashscore | 210492 | 15764 | - |
| Ramachandran outliers | 207382 | 16835 | - |
| Sidechain outliers | 206894 | 16415 | - |
| RNA backbone | 6643 | 2191 | - |
| Q-score | - | 25397 | 11806 (2.30 - 3.30) |

The table below summarises the geometric issues observed across the polymeric chains and their fit to the map. The red, orange, yellow and green segments of the bar indicate the fraction of residues that contain outliers for ≥ 3 , 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions $\leq 5\%$. The upper red bar (where present) indicates the fraction of residues that have poor fit to the EM map (all-atom inclusion $< 40\%$). The numeric value is given above the bar.

| Mol | Chain | Length | Quality of chain |
|-----|-------|--------|------------------|
| 1 | 1A | 3503 | |
| 2 | 1B | 155 | |
| 3 | 1C | 117 | |











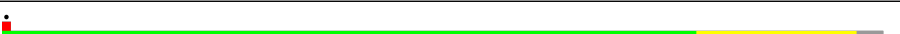


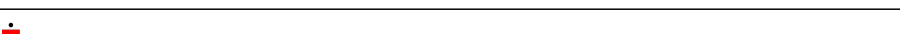
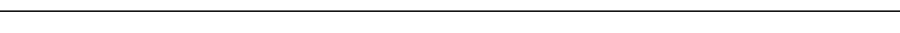
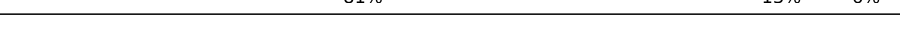
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| Mol | Chain | Length | Quality of chain |
|-----|-------|--------|--|
| 4 | ID | 257 |  |
| 5 | IE | 402 |  |
| 6 | IF | 431 |  |
| 7 | IG | 286 |  |
| 8 | IH | 204 |  |
| 9 | II | 230 |  |
| 10 | IJ | 286 |  |
| 11 | IK | 197 |  |
| 12 | IL | 210 |  |
| 13 | IM | 174 |  |
| 14 | IN | 291 |  |
| 15 | IO | 205 |  |
| 16 | IP | 135 |  |
| 17 | IQ | 205 |  |
| 18 | IR | 179 |  |
| 19 | IS | 168 |  |
| 20 | IT | 173 |  |
| 21 | IU | 198 |  |
| 22 | IV | 166 |  |
| 23 | IW | 137 |  |
| 24 | IX | 140 |  |
| 25 | IY | 121 |  |
| 26 | IZ | 163 |  |
| 27 | la | 213 |  |
| 28 | lb | 139 |  |

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| Mol | Chain | Length | Quality of chain |
|-----|-------|--------|--|
| 29 | lc | 149 |  86% 13% .. |
| 30 | ld | 64 |  88% 6% 6% |
| 31 | le | 109 |  15% 72% 22% 6% |
| 32 | lf | 150 |  13% 79% 17% .. |
| 33 | lg | 134 |  81% 16% . |
| 34 | lh | 137 |  64% 12% 23% |
| 35 | li | 122 |  87% 13% |
| 36 | lj | 108 |  86% 12% . |
| 37 | lk | 104 |  70% 15% 14% |
| 38 | ll | 77 |  71% 21% . 6% |
| 39 | lm | 93 |  78% 18% . |
| 40 | ln | 84 |  10% 63% 23% . 13% |
| 41 | lo | 51 |  86% 10% .. |
| 42 | lp | 56 |  59% 32% . 5% |
| 43 | lq | 98 |  81% 13% 6% |
| 44 | lr | 13 |  100% |

2 Entry composition

There are 44 unique types of molecules in this entry. The entry contains 121291 atoms, of which 0 are hydrogens and 0 are deuteriums.

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

- Molecule 1 is a RNA chain called 25S rRNA (3068-MER).

| Mol | Chain | Residues | Atoms | | | | | AltConf | Trace |
|-----|-------|----------|-------|-------|-------|-------|------|---------|-------|
| 1 | 1A | 3067 | Total | C | N | O | P | 0 | 0 |
| | | | 65572 | 29397 | 11934 | 21174 | 3067 | | |

- Molecule 2 is a RNA chain called 5.8S rRNA (145-MER).

| Mol | Chain | Residues | Atoms | | | | | AltConf | Trace |
|-----|-------|----------|-------|------|-----|------|-----|---------|-------|
| 2 | 1B | 145 | Total | C | N | O | P | 0 | 0 |
| | | | 3097 | 1390 | 560 | 1002 | 145 | | |

- Molecule 3 is a RNA chain called 5S rRNA (117-MER).

| Mol | Chain | Residues | Atoms | | | | | AltConf | Trace |
|-----|-------|----------|-------|------|-----|-----|-----|---------|-------|
| 3 | 1C | 117 | Total | C | N | O | P | 0 | 0 |
| | | | 2477 | 1108 | 425 | 827 | 117 | | |

- Molecule 4 is a protein called Large ribosomal subunit protein uL2.

| Mol | Chain | Residues | Atoms | | | | | AltConf | Trace |
|-----|-------|----------|-------|------|-----|-----|---|---------|-------|
| 4 | 1D | 246 | Total | C | N | O | S | 0 | 0 |
| | | | 1881 | 1165 | 382 | 326 | 8 | | |

- Molecule 5 is a protein called 60S ribosomal protein L3, putative.

| Mol | Chain | Residues | Atoms | | | | | AltConf | Trace |
|-----|-------|----------|-------|------|-----|-----|----|---------|-------|
| 5 | 1E | 387 | Total | C | N | O | S | 0 | 0 |
| | | | 3076 | 1956 | 578 | 527 | 15 | | |

- Molecule 6 is a protein called 60S ribosomal protein L4, putative.

| Mol | Chain | Residues | Atoms | | | | | AltConf | Trace |
|-----|-------|----------|-------|------|-----|-----|----|---------|-------|
| 6 | 1F | 424 | Total | C | N | O | S | 0 | 0 |
| | | | 3272 | 2085 | 622 | 551 | 14 | | |

- Molecule 7 is a protein called 60S ribosomal protein L5, putative.

| Mol | Chain | Residues | Atoms | | | | | AltConf | Trace |
|-----|-------|----------|-------|------|-----|-----|---|---------|-------|
| 7 | lG | 279 | Total | C | N | O | S | 0 | 0 |
| | | | 2222 | 1421 | 400 | 393 | 8 | | |

- Molecule 8 is a protein called 60S ribosomal protein L6, putative.

| Mol | Chain | Residues | Atoms | | | | | AltConf | Trace |
|-----|-------|----------|-------|------|-----|-----|---|---------|-------|
| 8 | lH | 203 | Total | C | N | O | S | 0 | 0 |
| | | | 1607 | 1053 | 272 | 278 | 4 | | |

- Molecule 9 is a protein called 60S ribosomal protein L7, putative.

| Mol | Chain | Residues | Atoms | | | | | AltConf | Trace |
|-----|-------|----------|-------|------|-----|-----|---|---------|-------|
| 9 | lI | 210 | Total | C | N | O | S | 0 | 0 |
| | | | 1658 | 1067 | 301 | 282 | 8 | | |

- Molecule 10 is a protein called 60S ribosomal protein L7a.

| Mol | Chain | Residues | Atoms | | | | | AltConf | Trace |
|-----|-------|----------|-------|------|-----|-----|---|---------|-------|
| 10 | lJ | 213 | Total | C | N | O | S | 0 | 0 |
| | | | 1727 | 1114 | 317 | 291 | 5 | | |

- Molecule 11 is a protein called 60S ribosomal protein L9, putative.

| Mol | Chain | Residues | Atoms | | | | | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|-------|
| 11 | lK | 193 | Total | C | N | O | S | 0 | 0 |
| | | | 1538 | 974 | 279 | 279 | 6 | | |

- Molecule 12 is a protein called Ribosomal protein L10, putative.

| Mol | Chain | Residues | Atoms | | | | | AltConf | Trace |
|-----|-------|----------|-------|------|-----|-----|----|---------|-------|
| 12 | lL | 200 | Total | C | N | O | S | 0 | 0 |
| | | | 1597 | 1017 | 302 | 264 | 14 | | |

- Molecule 13 is a protein called 60S ribosomal protein L11, putative.

| Mol | Chain | Residues | Atoms | | | | | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|-------|
| 13 | lM | 170 | Total | C | N | O | S | 0 | 0 |
| | | | 1350 | 857 | 243 | 245 | 5 | | |

- Molecule 14 is a protein called 60S ribosomal protein L13, putative.

| Mol | Chain | Residues | Atoms | | | | | AltConf | Trace |
|-----|-------|----------|-------|------|-----|-----|---|---------|-------|
| 14 | lN | 232 | Total | C | N | O | S | 0 | 0 |
| | | | 1872 | 1186 | 369 | 309 | 8 | | |

- Molecule 15 is a protein called 60S ribosomal protein L13, putative.

| Mol | Chain | Residues | Atoms | | | | | AltConf | Trace |
|-----|-------|----------|-------|------|-----|-----|---|---------|-------|
| 15 | lO | 204 | Total | C | N | O | S | 0 | 0 |
| | | | 1616 | 1030 | 302 | 275 | 9 | | |

- Molecule 16 is a protein called 60S ribosomal protein L14, putative.

| Mol | Chain | Residues | Atoms | | | | | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|-------|
| 16 | lP | 132 | Total | C | N | O | S | 0 | 0 |
| | | | 1039 | 666 | 192 | 177 | 4 | | |

- Molecule 17 is a protein called Ribosomal protein L15.

| Mol | Chain | Residues | Atoms | | | | | AltConf | Trace |
|-----|-------|----------|-------|------|-----|-----|---|---------|-------|
| 17 | lQ | 204 | Total | C | N | O | S | 0 | 0 |
| | | | 1676 | 1051 | 356 | 264 | 5 | | |

- Molecule 18 is a protein called 60S ribosomal protein L17, putative.

| Mol | Chain | Residues | Atoms | | | | | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|-------|
| 18 | lR | 158 | Total | C | N | O | S | 0 | 0 |
| | | | 1232 | 779 | 238 | 210 | 5 | | |

- Molecule 19 is a protein called 60S ribosomal protein L18, putative.

| Mol | Chain | Residues | Atoms | | | | | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|-------|
| 19 | lS | 167 | Total | C | N | O | S | 0 | 0 |
| | | | 1321 | 835 | 258 | 219 | 9 | | |

- Molecule 20 is a protein called 60S ribosomal protein L18a.

| Mol | Chain | Residues | Atoms | | | | | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|-------|
| 20 | lT | 173 | Total | C | N | O | S | 0 | 0 |
| | | | 1413 | 910 | 259 | 235 | 9 | | |

- Molecule 21 is a protein called Ribosomal protein L19.

| Mol | Chain | Residues | Atoms | | | | | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|-------|
| 21 | IU | 150 | Total | C | N | O | S | 0 | 0 |
| | | | 1235 | 787 | 246 | 197 | 5 | | |

- Molecule 22 is a protein called 60S ribosomal protein L21, putative.

| Mol | Chain | Residues | Atoms | | | | | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|-------|
| 22 | IV | 165 | Total | C | N | O | S | 0 | 0 |
| | | | 1320 | 846 | 254 | 217 | 3 | | |

- Molecule 23 is a protein called Large ribosomal subunit protein eL22.

| Mol | Chain | Residues | Atoms | | | | | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|-------|
| 23 | IW | 93 | Total | C | N | O | S | 0 | 0 |
| | | | 763 | 493 | 132 | 133 | 5 | | |

- Molecule 24 is a protein called 60S ribosomal protein L23, putative.

| Mol | Chain | Residues | Atoms | | | | | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|-------|
| 24 | IX | 133 | Total | C | N | O | S | 0 | 0 |
| | | | 1015 | 629 | 196 | 182 | 8 | | |

- Molecule 25 is a protein called Ribosomal protein L23A, putative.

| Mol | Chain | Residues | Atoms | | | | | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|-------|
| 25 | IY | 116 | Total | C | N | O | S | 0 | 0 |
| | | | 926 | 597 | 166 | 159 | 4 | | |

- Molecule 26 is a protein called 60S ribosomal protein L24, putative.

| Mol | Chain | Residues | Atoms | | | | | AltConf | Trace |
|-----|-------|----------|-------|-----|----|----|---|---------|-------|
| 26 | IZ | 57 | Total | C | N | O | S | 0 | 0 |
| | | | 481 | 318 | 88 | 73 | 2 | | |

- Molecule 27 is a protein called 60S ribosomal protein L26, putative.

| Mol | Chain | Residues | Atoms | | | | | AltConf | Trace |
|-----|-------|----------|-------|------|-----|-----|---|---------|-------|
| 27 | la | 210 | Total | C | N | O | S | 0 | 0 |
| | | | 1651 | 1055 | 304 | 285 | 7 | | |

- Molecule 28 is a protein called 60S ribosomal protein L27, putative.

| Mol | Chain | Residues | Atoms | | | | | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|-------|
| 28 | lb | 137 | Total | C | N | O | S | 0 | 0 |
| | | | 1094 | 707 | 196 | 187 | 4 | | |

- Molecule 29 is a protein called Large ribosomal subunit protein uL15A.

| Mol | Chain | Residues | Atoms | | | | | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|-------|
| 29 | lc | 148 | Total | C | N | O | S | 0 | 0 |
| | | | 1192 | 757 | 236 | 194 | 5 | | |

- Molecule 30 is a protein called 60S ribosomal protein L29.

| Mol | Chain | Residues | Atoms | | | | | AltConf | Trace |
|-----|-------|----------|-------|-----|----|----|---|---------|-------|
| 30 | ld | 60 | Total | C | N | O | S | 0 | 0 |
| | | | 478 | 297 | 97 | 82 | 2 | | |

- Molecule 31 is a protein called 60S ribosomal protein L30, putative.

| Mol | Chain | Residues | Atoms | | | | | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|-------|
| 31 | le | 103 | Total | C | N | O | S | 0 | 0 |
| | | | 768 | 486 | 131 | 149 | 2 | | |

- Molecule 32 is a protein called 60S ribosomal protein L31, putative.

| Mol | Chain | Residues | Atoms | | | | | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|-------|
| 32 | lf | 146 | Total | C | N | O | S | 0 | 0 |
| | | | 1184 | 759 | 219 | 200 | 6 | | |

- Molecule 33 is a protein called 60S ribosomal protein L32, putative.

| Mol | Chain | Residues | Atoms | | | | | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|-------|
| 33 | lg | 129 | Total | C | N | O | S | 0 | 0 |
| | | | 1058 | 672 | 209 | 172 | 5 | | |

- Molecule 34 is a protein called 60S ribosomal protein L34, putative.

| Mol | Chain | Residues | Atoms | | | | | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|-------|
| 34 | lh | 105 | Total | C | N | O | S | 0 | 0 |
| | | | 820 | 512 | 169 | 133 | 6 | | |

- Molecule 35 is a protein called uL29.

| Mol | Chain | Residues | Atoms | | | | | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|-------|
| 35 | li | 122 | Total | C | N | O | S | 0 | 0 |
| | | | 974 | 620 | 188 | 162 | 4 | | |

- Molecule 36 is a protein called 60S ribosomal protein L35a, putative.

| Mol | Chain | Residues | Atoms | | | | | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|-------|
| 36 | lj | 106 | Total | C | N | O | S | 0 | 0 |
| | | | 841 | 545 | 158 | 135 | 3 | | |

- Molecule 37 is a protein called 60S ribosomal protein L36, putative.

| Mol | Chain | Residues | Atoms | | | | | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|-------|
| 37 | lk | 89 | Total | C | N | O | S | 0 | 0 |
| | | | 712 | 447 | 144 | 116 | 5 | | |

- Molecule 38 is a protein called 60S ribosomal protein L37-A, putative.

| Mol | Chain | Residues | Atoms | | | | | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|----|---|---------|-------|
| 38 | ll | 72 | Total | C | N | O | S | 0 | 0 |
| | | | 591 | 361 | 132 | 91 | 7 | | |

- Molecule 39 is a protein called 60S ribosomal protein L37A, putative.

| Mol | Chain | Residues | Atoms | | | | | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|-------|
| 39 | lm | 90 | Total | C | N | O | S | 0 | 0 |
| | | | 688 | 428 | 135 | 119 | 6 | | |

- Molecule 40 is a protein called 60S ribosomal protein L38, putative.

| Mol | Chain | Residues | Atoms | | | | | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|-------|
| 40 | ln | 73 | Total | C | N | O | S | 0 | 0 |
| | | | 584 | 378 | 104 | 100 | 2 | | |

- Molecule 41 is a protein called Ribosomal protein L39, putative.

| Mol | Chain | Residues | Atoms | | | | | AltConf | Trace |
|-----|-------|----------|-------|-----|----|----|---|---------|-------|
| 41 | lo | 50 | Total | C | N | O | S | 0 | 0 |
| | | | 432 | 275 | 91 | 63 | 3 | | |

- Molecule 42 is a protein called 60S ribosomal protein L40, putative.

| Mol | Chain | Residues | Atoms | | | | | AltConf | Trace |
|-----|-------|----------|-------|-----|----|----|---|---------|-------|
| 42 | lp | 53 | Total | C | N | O | S | 0 | 0 |
| | | | 420 | 259 | 86 | 69 | 6 | | |

- Molecule 43 is a protein called 60S ribosomal protein L44, putative.

| Mol | Chain | Residues | Atoms | | | | | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|-------|
| 43 | lq | 92 | Total | C | N | O | S | 0 | 0 |
| | | | 756 | 480 | 148 | 122 | 6 | | |

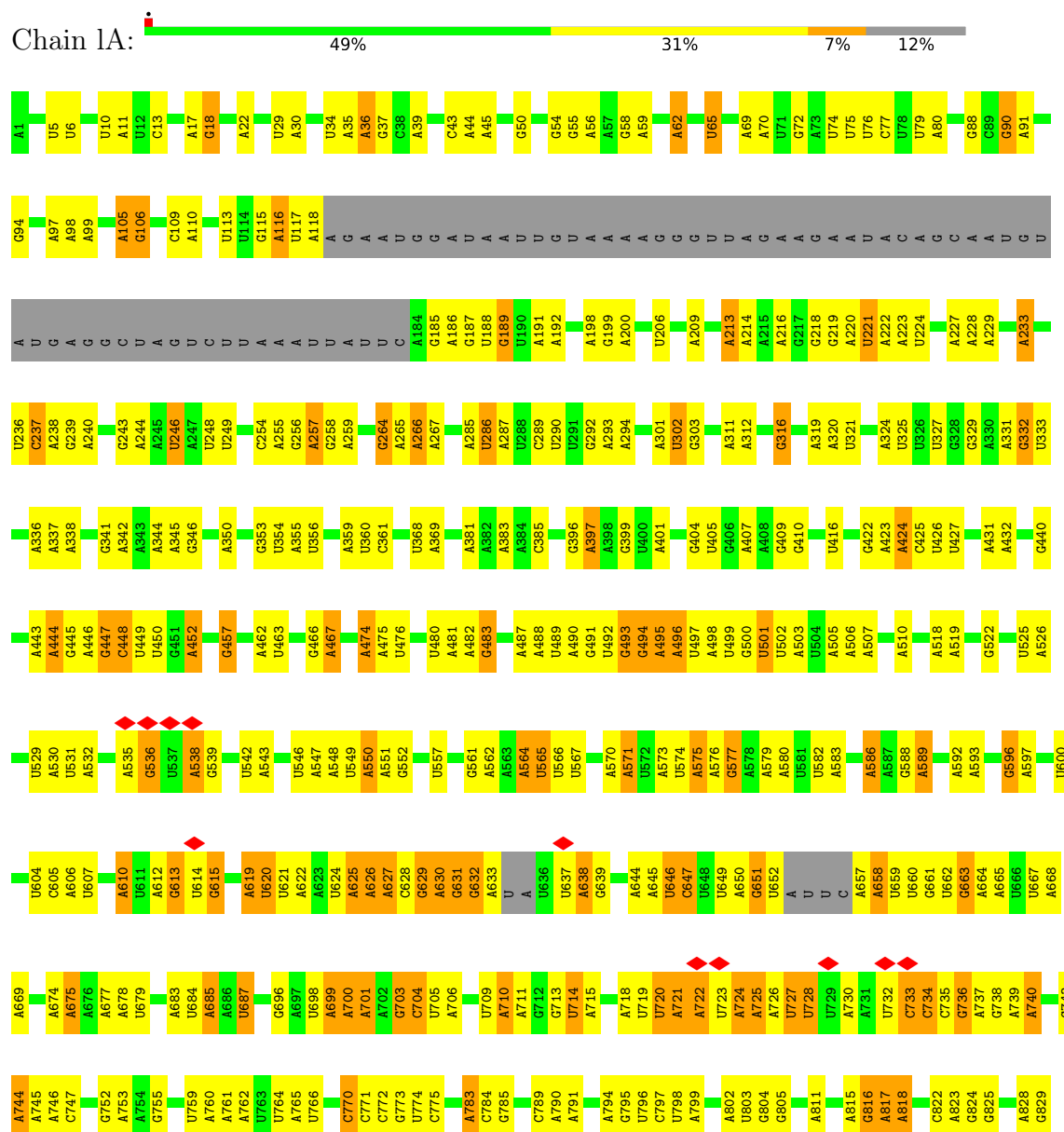
- Molecule 44 is a protein called Unknown peptide.

| Mol | Chain | Residues | Atoms | | | | AltConf | Trace |
|-----|-------|----------|-------|----|----|----|---------|-------|
| 44 | lr | 13 | Total | C | N | O | 0 | 0 |
| | | | 65 | 39 | 13 | 13 | | |

3 Residue-property plots

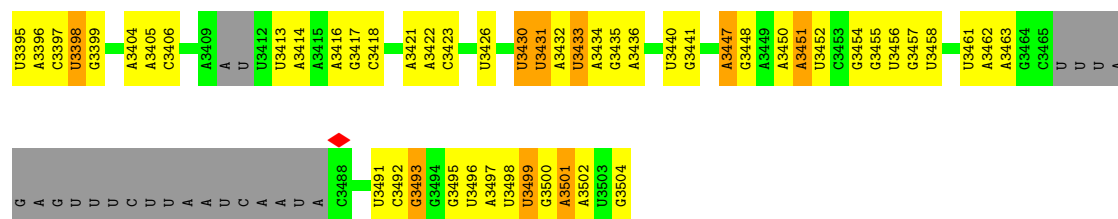
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and atom inclusion in map density. Residues are color-coded according to the number of geometric quality criteria for which they contain at least one outlier: green = 0, yellow = 1, orange = 2 and red = 3 or more. A red diamond above a residue indicates a poor fit to the EM map for this residue (all-atom inclusion < 40%). Stretches of 2 or more consecutive residues without any outlier are shown as a green connector. Residues present in the sample, but not in the model, are shown in grey.

• Molecule 1: 25S rRNA (3068-MER)



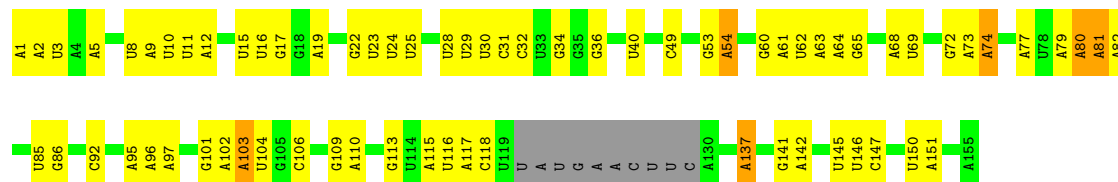
| | | | | | | | | | | | | |
|-------|-------|-------|---|-------|-------|-------|-------|-------|-------|-------|-------|------|
| G2025 | G1956 | U1870 | U | G1601 | U1508 | C1399 | A1326 | A1204 | U1130 | G1035 | G934 | A832 |
| G2034 | U1959 | U1876 | C | A1602 | A1509 | U1400 | A1327 | C1205 | G1131 | A1036 | A935 | U833 |
| U2035 | U1960 | A1877 | U | A1603 | A1610 | A1328 | A1328 | C1207 | U1132 | C1042 | A936 | A834 |
| A2036 | G1961 | A1878 | A | A1604 | G1511 | A1402 | U1334 | U1208 | A | G1043 | U938 | A835 |
| A2040 | U1962 | A1882 | A | A1605 | A1516 | G1409 | U1335 | C1210 | U | A1044 | A939 | C836 |
| A2041 | G1963 | A1883 | G | A1606 | C1517 | A1410 | G1336 | A1211 | G | U1047 | U940 | A837 |
| A2042 | G1964 | A1884 | U | A1607 | A1518 | A1411 | A1337 | U1217 | G | A1048 | A941 | A841 |
| A2043 | U1965 | A1885 | C | A1615 | A1519 | A1417 | U1338 | U1218 | G | G1053 | C942 | A846 |
| C2044 | U1966 | A1886 | A | G1621 | A1520 | G1417 | U1342 | U1219 | U | G1056 | C948 | A847 |
| C2050 | U1967 | A1887 | A | A1622 | A1521 | G1430 | A1343 | A1219 | A | C1057 | C949 | A851 |
| A2051 | U1968 | A1888 | U | A1623 | G1522 | G1431 | U1344 | A1220 | G | U1058 | U953 | A852 |
| G2052 | A1974 | U1890 | A | G1624 | A1524 | A1432 | U1345 | A1221 | U | C1063 | G954 | A853 |
| A2062 | G1975 | C1991 | U | A1631 | A1527 | U1433 | A1347 | U1222 | A | U1079 | U954 | A854 |
| A2063 | U1976 | U1892 | A | G1632 | A1533 | A1437 | C1356 | A1225 | U | A1071 | G960 | A855 |
| A2064 | U1977 | G1997 | A | G1633 | U1534 | A1440 | G | G1240 | U | U1072 | A961 | A858 |
| A2067 | U1979 | A1903 | U | G1634 | U1535 | U1441 | U | G1241 | C | A1073 | A | G864 |
| U2072 | A1982 | U1904 | C | U1635 | G1538 | C1447 | G | C1243 | C | C1078 | A | A868 |
| A2079 | A1983 | G1905 | A | U1639 | U1539 | U1456 | G | U1247 | U | U1097 | A | G869 |
| A2080 | A1984 | A1906 | G | A1641 | A1540 | A1456 | U | U1248 | A | G1086 | C | A870 |
| U2081 | A1985 | A1907 | A | A1642 | A1541 | U1459 | G | C1249 | C | U1087 | U | A871 |
| U2082 | U1986 | U1908 | U | U1648 | A1545 | G1454 | A | G1256 | A | U1088 | U | A872 |
| A2083 | A1988 | C1909 | A | U1649 | G1546 | U1465 | G | U1263 | U | C1089 | A | U873 |
| G2084 | A1989 | U1910 | U | A1652 | A1547 | U1467 | C | U1269 | A | A1090 | U | A874 |
| A2085 | G1994 | G1911 | G | U1653 | U1548 | A1468 | G | G1277 | A | A1091 | G | C875 |
| G2095 | G1995 | G1912 | A | G1661 | U1549 | U1469 | A | A1278 | U | A1092 | U | G881 |
| A2098 | U1998 | U1913 | U | U1667 | G1550 | G1474 | A | G1282 | A | G1093 | C996 | A886 |
| G2099 | C | A1921 | U | C1667 | A1551 | A1475 | G | A1284 | U | U1094 | U993 | U892 |
| G2100 | U | U1922 | A | U1752 | A1552 | G1476 | U | A1290 | A | U1095 | G997 | A896 |
| G2101 | U | U1923 | U | G1668 | A1553 | A1477 | C | G1291 | A | U1103 | U998 | A897 |
| G2102 | U | U1924 | U | G1669 | C1554 | U1478 | G | A1292 | A | U1104 | G999 | U898 |
| G2103 | U | A1925 | U | U1674 | U1555 | U1479 | U | U1293 | A | U1105 | A1015 | A899 |
| G2104 | U | U1926 | U | A1675 | G1556 | U1480 | A | A1305 | U | G1107 | A1006 | A904 |
| G2105 | U | U1927 | U | A1676 | U1557 | A1484 | A1383 | A1306 | A | U1108 | C1007 | A905 |
| G2106 | U | U1928 | U | A1677 | C1558 | U1485 | G1384 | A1307 | U | G1112 | A1015 | A908 |
| G2107 | U | U1929 | U | U1678 | U1559 | C1486 | A1385 | A1310 | U | A1115 | G1019 | A909 |
| G2108 | U | U1930 | U | A1679 | U1560 | A1486 | A1386 | C1311 | A | U1118 | G1026 | A910 |
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| G2110 | U | U1932 | U | A1681 | U1562 | U1488 | U1388 | U1313 | A | A1120 | G1028 | G918 |
| G2111 | U | U1933 | U | A1682 | G1563 | U1489 | U1389 | A1314 | U | A1121 | G1029 | G919 |
| G2112 | U | U1934 | U | A1683 | U1564 | U1490 | G1390 | A1315 | U | U1126 | C1030 | A920 |
| G2113 | U | U1935 | U | A1684 | U1565 | U1491 | U1391 | A1316 | U | A1127 | A1033 | A925 |
| G2114 | U | U1936 | U | A1685 | U1566 | U1492 | U1392 | A1324 | U | A1127 | A1034 | |
| G2115 | U | U1937 | U | A1686 | U1567 | U1493 | U1393 | A1325 | U | | | |
| G2116 | U | U1938 | U | A1687 | C1571 | U1494 | U1394 | | | | | |
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| G2118 | U | U1940 | U | A1689 | U1569 | U1496 | C1396 | | | | | |
| G2119 | U | U1941 | U | A1690 | U1570 | U1497 | A1397 | | | | | |
| G2120 | U | U1942 | U | A1691 | C1571 | U1498 | A1398 | | | | | |
| G2121 | U | U1943 | U | A1692 | U1571 | U1499 | U1399 | | | | | |
| G2122 | U | U1944 | U | A1693 | U1572 | U1500 | U1400 | | | | | |
| G2123 | U | U1945 | U | A1694 | U1573 | U1501 | U1401 | | | | | |
| G2124 | U | U1946 | U | A1695 | U1574 | U1502 | U1402 | | | | | |
| G2125 | U | U1947 | U | A1696 | U1575 | U1503 | U1403 | | | | | |
| G2126 | U | U1948 | U | A1697 | U1576 | U1504 | U1404 | | | | | |
| G2127 | U | U1949 | U | A1698 | U1577 | U1505 | U1405 | | | | | |
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| G2136 | U | U1958 | U | U | U1586 | U1514 | U1414 | | | | | |
| G2137 | U | U1959 | U | U | U1587 | U1515 | U1415 | | | | | |
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| G2141 | U | U1963 | U | U | U1591 | U1519 | U1419 | | | | | |
| G2142 | U | U1964 | U | U | U1592 | U1520 | U1420 | | | | | |
| G2143 | U | U1965 | U | U | U1593 | U1521 | U1421 | | | | | |
| G2144 | U | U1966 | U | U | U1594 | U1522 | U1422 | | | | | |
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| G2148 | U | U1970 | U | U | U1598 | U1526 | U1426 | | | | | |
| G2149 | U | U1971 | U | U | U1599 | U1527 | U1427 | | | | | |
| G2150 | U | U1972 | U | U | U1600 | U1528 | U1428 | | | | | |
| G2151 | U | U1973 | U | U | U1601 | U1529 | U1429 | | | | | |
| G2152 | U | U1974 | U | U | U1602 | U1530 | U1430 | | | | | |
| G2153 | U | U1975 | U | U | U1603 | U1531 | U1431 | | | | | |
| G2154 | U | U1976 | U | U | U1604 | U1532 | U1432 | | | | | |
| G2155 | U | U1977 | U | U | U1605 | U1533 | U1433 | | | | | |
| G2156 | U | U1978 | U | U | U1606 | U1534 | U1434 | | | | | |
| G2157 | U | U1979 | U | U | U1607 | U1535 | U1435 | | | | | |
| G2158 | U | U1980 | U | U | U1608 | U1536 | U1436 | | | | | |
| G2159 | U | U1981 | U | U | U1609 | U1537 | U1437 | | | | | |
| G2160 | U | U1982 | U | U | U1610 | U1538 | U1438 | | | | | |
| G2161 | U | U1983 | U | U | U1611 | U1539 | U1439 | | | | | |
| G2162 | U | U1984 | U | U | U1612 | U1540 | U1440 | | | | | |
| G2163 | U | U1985 | U | U | U1613 | U1541 | U1441 | | | | | |
| G2164 | U | U1986 | U | U | U1614 | U1542 | U1442 | | | | | |
| G2165 | U | U1987 | U | U | U1615 | U1543 | U1443 | | | | | |
| G2166 | U | U1988 | U | U | U1616 | U1544 | U1444 | | | | | |
| G2167 | U | U1989 | U | U | U1617 | U1545 | U1445 | | | | | |
| G2168 | U | U1990 | U | U | U1618 | U1546 | U1446 | | | | | |
| G2169 | U | U1991 | U | U | U1619 | U1547 | U1447 | | | | | |
| G2170 | U | U1992 | U | U | U1620 | U1548 | U1448 | | | | | |
| G2171 | U | U1993 | U | U | U1621 | U1549 | U1449 | | | | | |
| G2172 | U | U1994 | U | U | U1622 | U1550 | U1450 | | | | | |
| G2173 | U | U1995 | U | U | U1623 | U1551 | U1451 | | | | | |
| G2174 | U | U1996 | U | U | U1624 | U1552 | U1452 | | | | | |
| G2175 | U | U1997 | U | U | U1625 | U1553 | U1453 | | | | | |
| G2176 | U | U1998 | U | U | U1626 | U1554 | U1454 | | | | | |
| G2177 | U | U1999 | U | U | U1627 | U1555 | U1455 | | | | | |
| G2178 | U | U2000 | U | U | U1628 | U1556 | U1456 | | | | | |
| G2179 | U | U2001 | U | U | U1629 | U1557 | U1457 | | | | | |
| G2180 | U | U2002 | U | U | U1630 | U1558 | U1458 | | | | | |
| G2181 | U | U2003 | U | U | U1631 | U1559 | U1459 | | | | | |
| G2182 | U | U2004 | U | U | U1632 | U1560 | U1460 | | | | | |
| G2183 | U | U2005 | U | U | U1633 | U1561 | U1461 | | | | | |
| G2184 | U | U2006 | U | U | U1634 | U1562 | U1462 | | | | | |
| G2185 | U | U2007 | U | U | U1635 | U1563 | U1463 | | | | | |
| G2186 | U | U2008 | U | U | U1636 | U1564 | U1464 | | | | | |
| G2187 | U | U2009 | U | U | U1637 | U1565 | U1465 | | | | | |
| G2188 | U | U2010 | U | U | U1638 | U1566 | U1466 | | | | | |
| G2189 | U | U2011 | U | U | U1639 | U1567 | U1467 | | | | | |
| G2190 | U | U2012 | U | U | U1640 | U1568 | U1468 | | | | | |
| G2191 | U | U2013 | U | U | U1641 | U1569 | U1469 | | | | | |
| G2192 | U | U2014 | U | U | U1642 | U1570 | U1470 | | | | | |
| G2193 | U | U2015 | U | U | U1643 | U1571 | U1471 | | | | | |
| G2194 | U | U2016 | U | U | U1644 | | | | | | | |





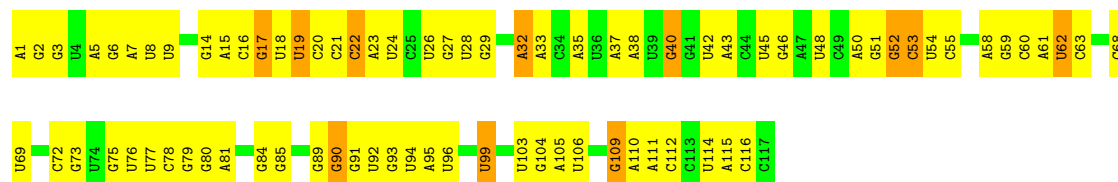
• Molecule 2: 5.8S rRNA (145-MER)

Chain IB: 48% 41% 6%



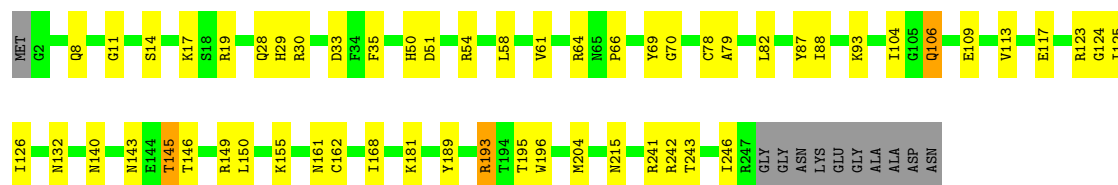
• Molecule 3: 5S rRNA (117-MER)

Chain IC: 32% 58% 9%



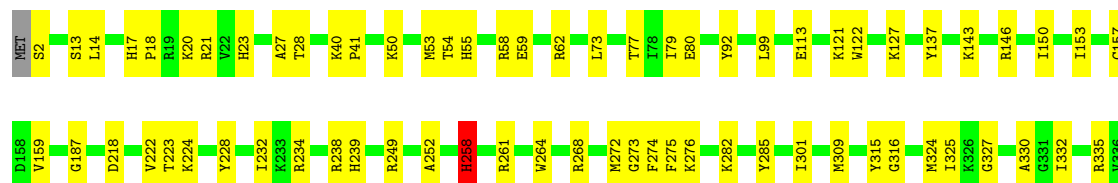
• Molecule 4: Large ribosomal subunit protein uL2

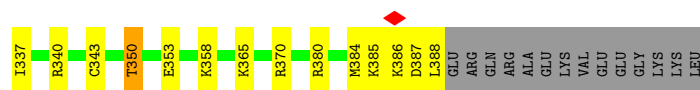
Chain ID: 74% 21% . .



• Molecule 5: 60S ribosomal protein L3, putative

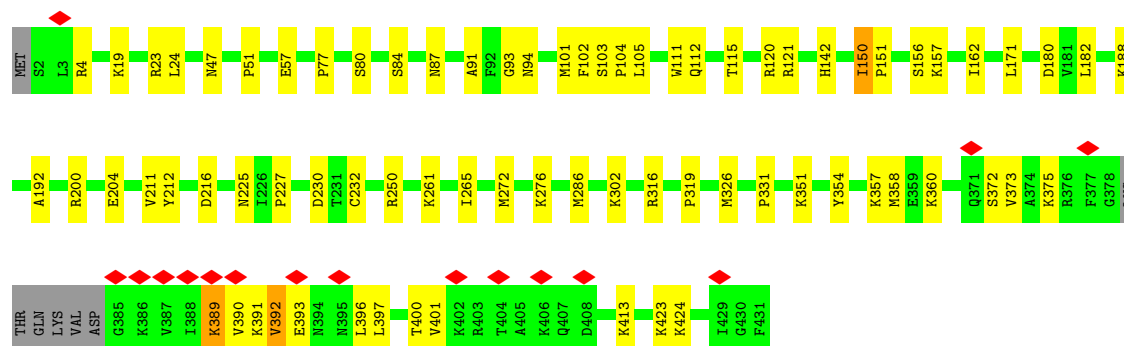
Chain IE: 76% 20% .





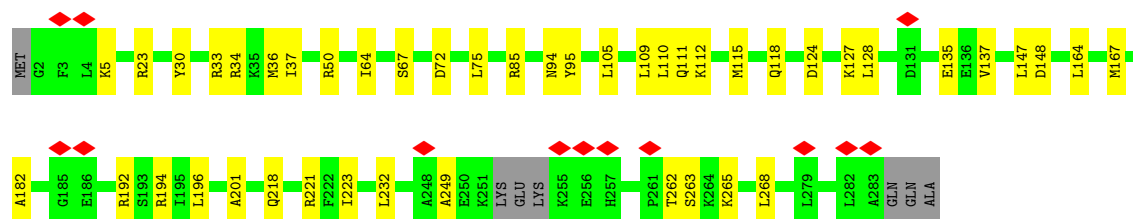
- Molecule 6: 60S ribosomal protein L4, putative

Chain IF: 81% 17% ..



- Molecule 7: 60S ribosomal protein L5, putative

Chain IG: 5% 82% 16% .



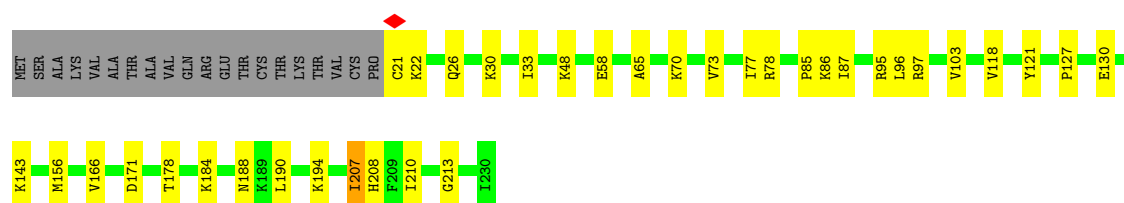
- Molecule 8: 60S ribosomal protein L6, putative


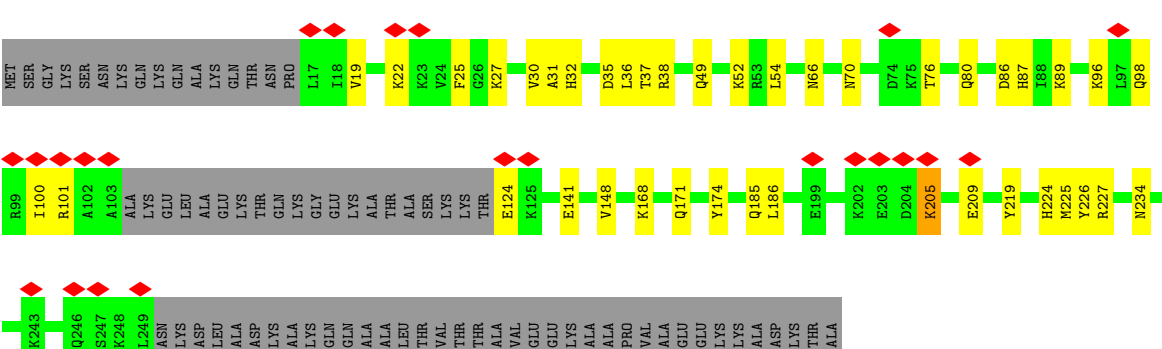
Chain IH: 78% 21%

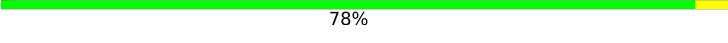





- Molecule 9: 60S ribosomal protein L7, putative


Chain II: 76% 15% 9%



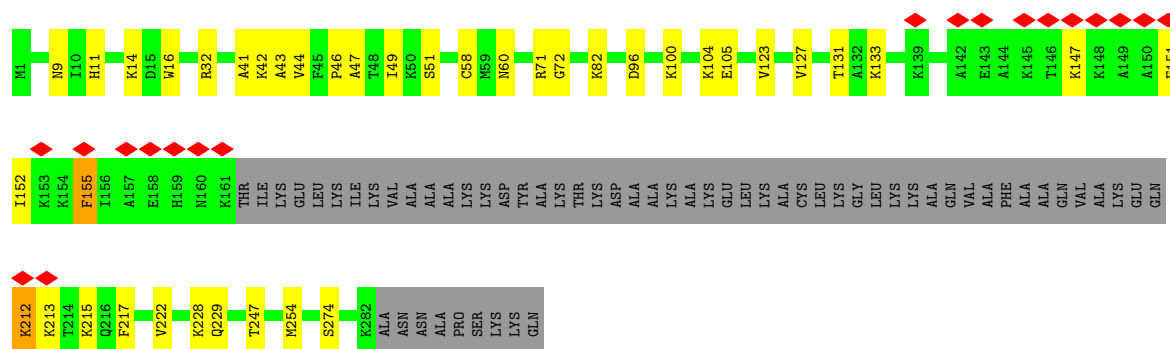
- Chain 1J: 
- 
- | Position | Amino Acid | Frequency (bits) |
|----------|------------|------------------|
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| 2 | Ser | 0.00 |
| 3 | Gly | 0.00 |
| 4 | Lys | 0.00 |
| 5 | Ser | 0.00 |
| 6 | Asn | 0.00 |
| 7 | Gln | 0.00 |
| 8 | Lys | 0.00 |
| 9 | Gln | 0.00 |
| 10 | Ala | 0.00 |
| 11 | Lys | 0.00 |
| 12 | Gln | 0.00 |
| 13 | Thr | 0.00 |
| 14 | Asn | 0.00 |
| 15 | Pro | 0.00 |
| 16 | Lys | 0.00 |
| 17 | Lys | 0.00 |
| 18 | Lys | 0.00 |
| 19 | Lys | 0.00 |
| 20 | Lys | 0.00 |
| 21 | Lys | 0.00 |
| 22 | Lys | 0.00 |
| 23 | Lys | 0.00 |
| 24 | Lys | 0.00 |
| 25 | Lys | 0.00 |
| 26 | Lys | 0.00 |
| 27 | Lys | 0.00 |
| 28 | Lys | 0.00 |
| 29 | Lys | 0.00 |
| 30 | Lys | 0.00 |
| 31 | Lys | 0.00 |
| 32 | Lys | 0.00 |
| 33 | Lys | 0.00 |
| 34 | Lys | 0.00 |
| 35 | Lys | 0.00 |
| 36 | Lys | 0.00 |
| 37 | Lys | 0.00 |
| 38 | Lys | 0.00 |
| 39 | Lys | 0.00 |
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| 65 | Lys | 0.00 |
| 66 | Lys | 0.00 |
| 67 | Lys | 0.00 |
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| 88 | Lys | 0.00 |
| 89 | Lys | 0.00 |
| 90 | Lys | 0.00 |
| 91 | Lys | 0.00 |
| 92 | Lys | 0.00 |
| 93 | Lys | 0.00 |
| 94 | Lys | 0.00 |
| 95 | Lys | 0.00 |
| 96 | Lys | 0.00 |
| 97 | Lys | 0.00 |
| 98 | Lys | 0.00 |
| 99 | Lys | 0.00 |
| 100 | Lys | 0.00 |
| 101 | Lys | 0.00 |
| 102 | Lys | 0.00 |
| 103 | Lys | 0.00 |
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| 107 | Lys | 0.00 |
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| 110 | Lys | 0.00 |
| 111 | Lys | 0.00 |
| 112 | Lys | 0.00 |
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| 115 | Lys | 0.00 |
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| 135 | Lys | 0.00 |
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| 139 | Lys | 0.00 |
| 140 | Lys | 0.00 |
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| 143 | Lys | |

- Chain 1K: 

- Chain 1L: 
- 
- 

- Chain IM: 

- Chain IN: 



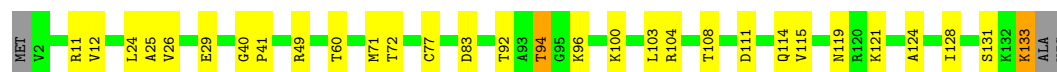
- Molecule 15: 60S ribosomal protein L13, putative

Chain IO: 84% 16%



- Molecule 16: 60S ribosomal protein L14, putative

Chain IP: 76% 21% ..



- Molecule 17: Ribosomal protein L15

Chain IQ: 89% 10%



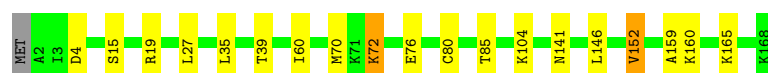
- Molecule 18: 60S ribosomal protein L17, putative

Chain IR: 79% 8% 12%



- Molecule 19: 60S ribosomal protein L18, putative

Chain IS: 88% 10% ..



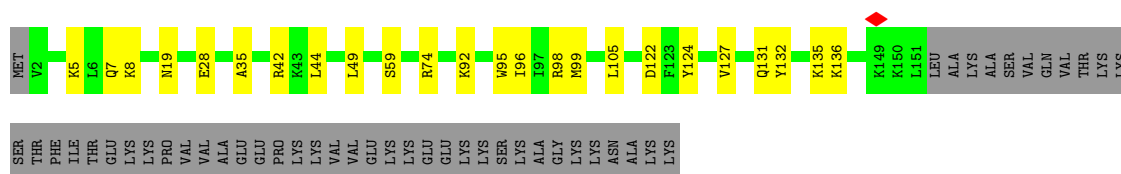
- Molecule 20: 60S ribosomal protein L18a

Chain IT:  86% 13% .



- Molecule 21: Ribosomal protein L19

Chain IU:  64% 12% 24%



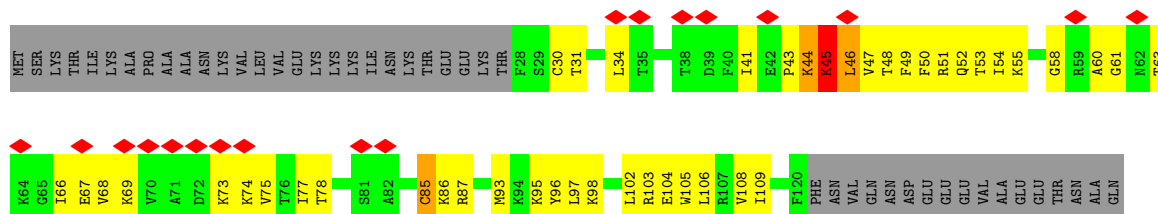
- Molecule 22: 60S ribosomal protein L21, putative

Chain IV:  86% 13% ..



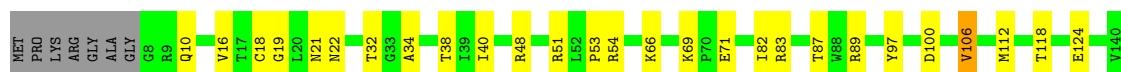
- Molecule 23: Large ribosomal subunit protein eL22

Chain IW:  13% 35% 30% .. 32%




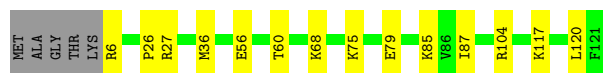
- Molecule 24: 60S ribosomal protein L23, putative

Chain IX:  76% 19% . 5%

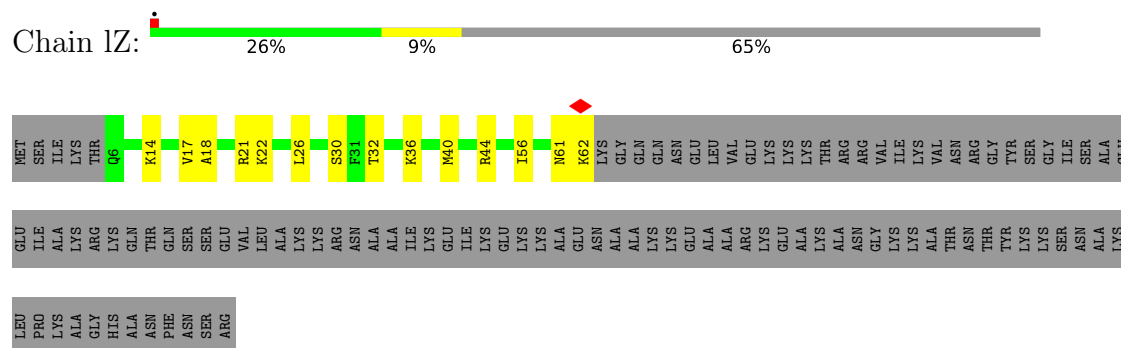


- Molecule 25: Ribosomal protein L23A, putative

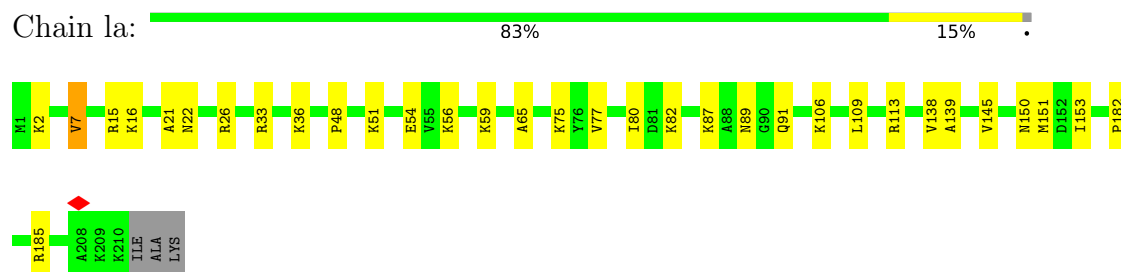
Chain IY:  84% 12% .



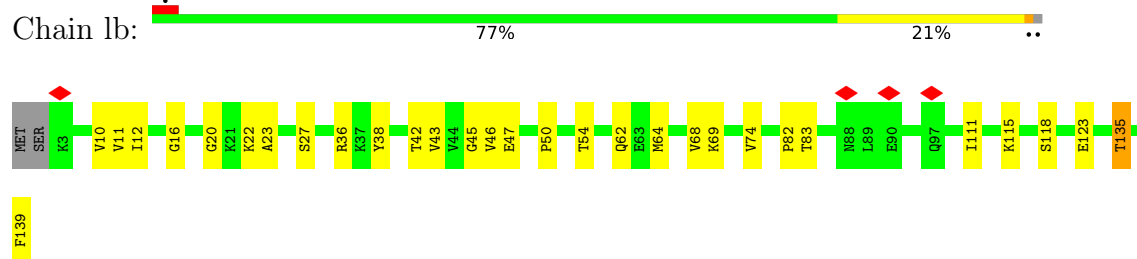
- Molecule 26: 60S ribosomal protein L24, putative



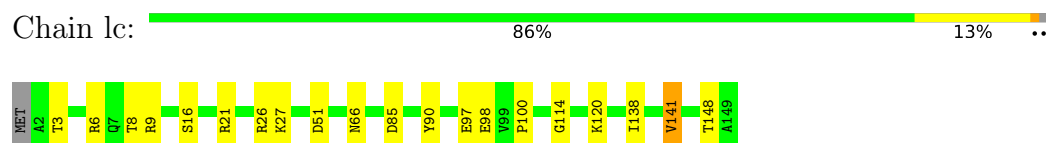
- Molecule 27: 60S ribosomal protein L26, putative



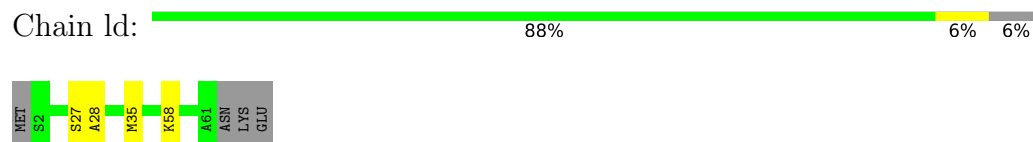
- Molecule 28: 60S ribosomal protein L27, putative



- Molecule 29: Large ribosomal subunit protein uL15A

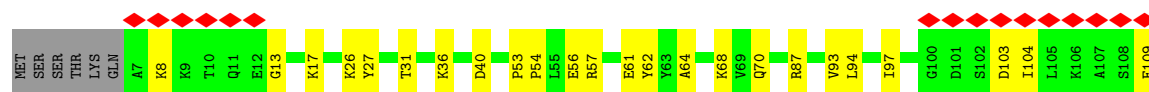


- Molecule 30: 60S ribosomal protein L29

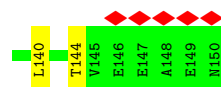
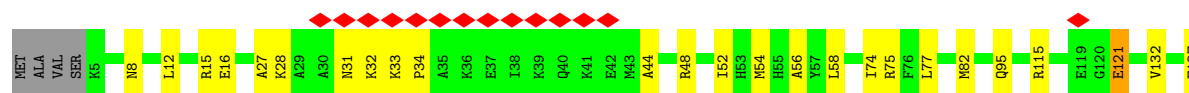
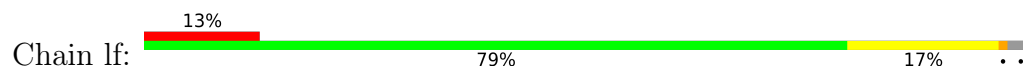


- Molecule 31: 60S ribosomal protein L30, putative

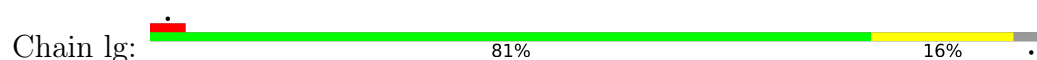




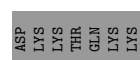
- Molecule 32: 60S ribosomal protein L31, putative



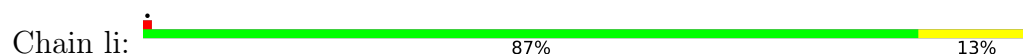
- Molecule 33: 60S ribosomal protein L32, putative



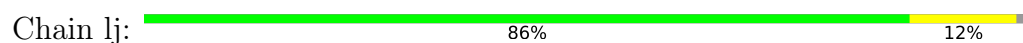
- Molecule 34: 60S ribosomal protein L34, putative



- Molecule 35: uL29

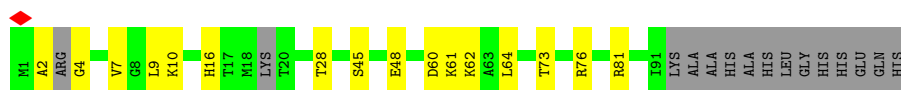


- Molecule 36: 60S ribosomal protein L35a, putative

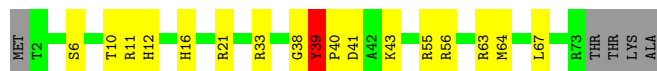


- Molecule 37: 60S ribosomal protein L36, putative

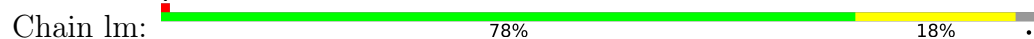




- Molecule 38: 60S ribosomal protein L37-A, putative



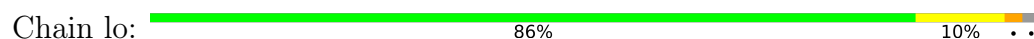
- Molecule 39: 60S ribosomal protein L37A, putative



- Molecule 40: 60S ribosomal protein L38, putative



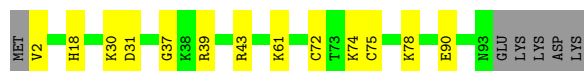
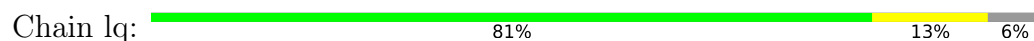
- Molecule 41: Ribosomal protein L39, putative



- Molecule 42: 60S ribosomal protein L40, putative



- Molecule 43: 60S ribosomal protein L44, putative



- Molecule 44: Unknown peptide

Chain lr:

100%

There are no outlier residues recorded for this chain.

4 Experimental information

| Property | Value | Source |
|--------------------------------------|---|-----------|
| EM reconstruction method | SINGLE PARTICLE | Depositor |
| Imposed symmetry | POINT, Not provided | |
| Number of particles used | 378061 | Depositor |
| Resolution determination method | FSC 0.143 CUT-OFF | Depositor |
| CTF correction method | PHASE FLIPPING AND AMPLITUDE CORRECTION | Depositor |
| Microscope | TFS KRIOS | Depositor |
| Voltage (kV) | 300 | Depositor |
| Electron dose ($e^-/\text{\AA}^2$) | 1.34 | Depositor |
| Minimum defocus (nm) | 1800 | Depositor |
| Maximum defocus (nm) | 3000 | Depositor |
| Magnification | 75000 | Depositor |
| Image detector | FEI FALCON III (4k x 4k) | Depositor |
| Maximum map value | 18.211 | Depositor |
| Minimum map value | -6.837 | Depositor |
| Average map value | -0.000 | Depositor |
| Map value standard deviation | 1.000 | Depositor |
| Recommended contour level | 2 | Depositor |
| Map size (Å) | 321.00003, 321.00003, 321.00003 | wwPDB |
| Map dimensions | 300, 300, 300 | wwPDB |
| Map angles (°) | 90.0, 90.0, 90.0 | wwPDB |
| Pixel spacing (Å) | 1.07, 1.07, 1.07 | Depositor |

5 Model quality ⓘ

5.1 Standard geometry ⓘ

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

| Mol | Chain | Bond lengths | | Bond angles | |
|-----|-------|--------------|---------|-------------|---------------|
| | | RMSZ | # Z >5 | RMSZ | # Z >5 |
| 1 | 1A | 0.19 | 0/73480 | 0.30 | 0/114456 |
| 2 | 1B | 0.19 | 0/3470 | 0.30 | 0/5401 |
| 3 | 1C | 0.20 | 0/2765 | 0.37 | 2/4303 (0.0%) |
| 4 | 1D | 0.18 | 0/1920 | 0.29 | 0/2582 |
| 5 | 1E | 0.18 | 0/3140 | 0.33 | 0/4216 |
| 6 | 1F | 0.19 | 0/3330 | 0.30 | 1/4468 (0.0%) |
| 7 | 1G | 0.14 | 0/2261 | 0.29 | 0/3028 |
| 8 | 1H | 0.14 | 0/1639 | 0.31 | 0/2203 |
| 9 | 1I | 0.16 | 0/1680 | 0.29 | 0/2252 |
| 10 | 1J | 0.12 | 0/1757 | 0.28 | 0/2360 |
| 11 | 1K | 0.13 | 0/1562 | 0.23 | 0/2103 |
| 12 | 1L | 0.16 | 0/1633 | 0.31 | 0/2184 |
| 13 | 1M | 0.11 | 0/1369 | 0.26 | 0/1834 |
| 14 | 1N | 0.16 | 0/1900 | 0.29 | 0/2534 |
| 15 | 1O | 0.17 | 0/1646 | 0.28 | 0/2209 |
| 16 | 1P | 0.23 | 0/1051 | 0.34 | 1/1411 (0.1%) |
| 17 | 1Q | 0.18 | 0/1707 | 0.24 | 0/2276 |
| 18 | 1R | 0.18 | 0/1251 | 0.26 | 0/1675 |
| 19 | 1S | 0.16 | 0/1342 | 0.25 | 0/1796 |
| 20 | 1T | 0.16 | 0/1445 | 0.26 | 0/1946 |
| 21 | 1U | 0.14 | 0/1253 | 0.24 | 0/1666 |
| 22 | 1V | 0.17 | 0/1351 | 0.27 | 0/1819 |
| 23 | 1W | 0.27 | 0/774 | 0.67 | 1/1031 (0.1%) |
| 24 | 1X | 0.17 | 0/1030 | 0.29 | 0/1384 |
| 25 | 1Y | 0.14 | 0/941 | 0.22 | 0/1262 |
| 26 | 1Z | 0.12 | 0/492 | 0.24 | 0/656 |
| 27 | 1a | 0.14 | 0/1673 | 0.23 | 0/2236 |
| 28 | 1b | 0.13 | 0/1112 | 0.26 | 0/1489 |
| 29 | 1c | 0.19 | 0/1223 | 0.27 | 0/1636 |
| 30 | 1d | 0.18 | 0/485 | 0.31 | 0/639 |
| 31 | 1e | 0.13 | 0/776 | 0.29 | 0/1044 |
| 32 | 1f | 0.15 | 0/1205 | 0.28 | 0/1609 |
| 33 | 1g | 0.18 | 0/1075 | 0.26 | 0/1434 |
| 34 | 1h | 0.16 | 0/833 | 0.23 | 0/1115 |

| Mol | Chain | Bond lengths | | Bond angles | |
|-----|-------|--------------|----------|-------------|-----------------|
| | | RMSZ | # Z >5 | RMSZ | # Z >5 |
| 35 | li | 0.14 | 0/984 | 0.23 | 0/1310 |
| 36 | lj | 0.19 | 0/862 | 0.29 | 0/1163 |
| 37 | lk | 0.11 | 0/721 | 0.22 | 0/955 |
| 38 | ll | 0.20 | 0/602 | 0.33 | 0/797 |
| 39 | lm | 0.16 | 0/696 | 0.33 | 0/928 |
| 40 | ln | 0.15 | 0/592 | 0.29 | 0/789 |
| 41 | lo | 0.19 | 0/444 | 0.23 | 0/587 |
| 42 | lp | 0.17 | 0/425 | 0.54 | 2/563 (0.4%) |
| 43 | lq | 0.16 | 0/770 | 0.24 | 0/1019 |
| All | All | 0.18 | 0/130667 | 0.30 | 7/192368 (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 |
|-----|-------|---------------------|---------------------|
| 5 | lE | 0 | 1 |
| 20 | lT | 0 | 1 |
| 23 | lW | 0 | 1 |
| 38 | ll | 0 | 1 |
| All | All | 0 | 4 |

There are no bond length outliers.

All (7) bond angle outliers are listed below:

| Mol | Chain | Res | Type | Atoms | Z | Observed(°) | Ideal(°) |
|-----|-------|-----|------|-----------|-------|-------------|----------|
| 3 | lC | 62 | U | OP2-P-O3' | -8.80 | 81.60 | 108.00 |
| 3 | lC | 62 | U | OP1-P-O3' | -8.53 | 82.40 | 108.00 |
| 42 | lp | 24 | CYS | CA-CB-SG | 6.31 | 128.92 | 114.40 |
| 42 | lp | 35 | CYS | CA-CB-SG | 5.99 | 128.18 | 114.40 |
| 6 | lF | 389 | LYS | CA-CB-CG | 5.92 | 125.94 | 114.10 |
| 16 | lP | 133 | LYS | CA-CB-CG | 5.82 | 125.74 | 114.10 |
| 23 | lW | 45 | LYS | CA-CB-CG | 5.32 | 124.73 | 114.10 |

There are no chirality outliers.

All (4) planarity outliers are listed below:

| Mol | Chain | Res | Type | Group |
|-----|-------|-----|------|---------|
| 5 | lE | 258 | HIS | Peptide |
| 20 | lT | 172 | LEU | Peptide |

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| Mol | Chain | Res | Type | Group |
|-----|-------|-----|------|---------|
| 23 | IW | 44 | LYS | Peptide |
| 38 | II | 39 | TYR | 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 | IA | 65572 | 0 | 32902 | 942 | 0 |
| 2 | IB | 3097 | 0 | 1552 | 41 | 0 |
| 3 | IC | 2477 | 0 | 1252 | 95 | 0 |
| 4 | ID | 1881 | 0 | 1928 | 40 | 0 |
| 5 | IE | 3076 | 0 | 3209 | 62 | 0 |
| 6 | IF | 3272 | 0 | 3500 | 63 | 0 |
| 7 | IG | 2222 | 0 | 2304 | 35 | 0 |
| 8 | IH | 1607 | 0 | 1726 | 31 | 0 |
| 9 | II | 1658 | 0 | 1802 | 29 | 0 |
| 10 | IJ | 1727 | 0 | 1849 | 25 | 0 |
| 11 | IK | 1538 | 0 | 1598 | 28 | 0 |
| 12 | IL | 1597 | 0 | 1654 | 23 | 0 |
| 13 | IM | 1350 | 0 | 1390 | 28 | 0 |
| 14 | IN | 1872 | 0 | 2034 | 37 | 0 |
| 15 | IO | 1616 | 0 | 1700 | 21 | 0 |
| 16 | IP | 1039 | 0 | 1133 | 23 | 0 |
| 17 | IQ | 1676 | 0 | 1777 | 16 | 0 |
| 18 | IR | 1232 | 0 | 1307 | 12 | 0 |
| 19 | IS | 1321 | 0 | 1427 | 14 | 0 |
| 20 | IT | 1413 | 0 | 1479 | 17 | 0 |
| 21 | IU | 1235 | 0 | 1369 | 21 | 0 |
| 22 | IV | 1320 | 0 | 1406 | 18 | 0 |
| 23 | IW | 763 | 0 | 818 | 38 | 0 |
| 24 | IX | 1015 | 0 | 1054 | 24 | 0 |
| 25 | IY | 926 | 0 | 997 | 11 | 0 |
| 26 | IZ | 481 | 0 | 518 | 10 | 0 |
| 27 | la | 1651 | 0 | 1822 | 23 | 0 |
| 28 | lb | 1094 | 0 | 1174 | 22 | 0 |
| 29 | lc | 1192 | 0 | 1205 | 18 | 0 |
| 30 | ld | 478 | 0 | 507 | 3 | 0 |
| 31 | le | 768 | 0 | 810 | 15 | 0 |

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| Mol | Chain | Non-H | H(model) | H(added) | Clashes | Symm-Clashes |
|-----|-------|--------|----------|----------|---------|--------------|
| 32 | lf | 1184 | 0 | 1270 | 18 | 0 |
| 33 | lg | 1058 | 0 | 1140 | 15 | 0 |
| 34 | lh | 820 | 0 | 864 | 13 | 0 |
| 35 | li | 974 | 0 | 1093 | 14 | 0 |
| 36 | lj | 841 | 0 | 878 | 9 | 0 |
| 37 | lk | 712 | 0 | 755 | 11 | 0 |
| 38 | ll | 591 | 0 | 617 | 13 | 0 |
| 39 | lm | 688 | 0 | 728 | 14 | 0 |
| 40 | ln | 584 | 0 | 643 | 13 | 0 |
| 41 | lo | 432 | 0 | 444 | 6 | 0 |
| 42 | lp | 420 | 0 | 450 | 15 | 0 |
| 43 | lq | 756 | 0 | 821 | 10 | 0 |
| 44 | lr | 65 | 0 | 16 | 0 | 0 |
| All | All | 121291 | 0 | 88922 | 1660 | 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 8.

All (1660) 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) |
|-----------------|------------------|--------------------------|-------------------|
| 3:IC:79:G:N1 | 3:IC:95:A:C2 | 2.13 | 1.17 |
| 3:IC:79:G:N1 | 3:IC:95:A:H2 | 1.41 | 1.15 |
| 3:IC:81:A:H2 | 3:IC:93:G:N1 | 1.44 | 1.13 |
| 1:1A:3454:G:N1 | 1:1A:3502:A:H2 | 1.50 | 1.09 |
| 1:1A:3454:G:N1 | 1:1A:3502:A:C2 | 2.20 | 1.05 |
| 3:IC:27:G:H1 | 3:IC:50:A:N6 | 1.55 | 1.03 |
| 5:IE:17:HIS:HD2 | 5:IE:18:PRO:HA | 1.23 | 1.03 |
| 1:1A:638:A:N6 | 1:1A:651:G:H1 | 1.64 | 0.95 |
| 1:1A:869:G:H21 | 1:1A:872:A:N6 | 1.64 | 0.94 |
| 3:IC:81:A:C2 | 3:IC:93:G:N1 | 2.24 | 0.94 |
| 1:1A:638:A:H61 | 1:1A:651:G:H1 | 0.98 | 0.94 |
| 2:1B:49:C:HO2' | 2:1B:63:A:HO2' | 1.06 | 0.92 |
| 1:1A:869:G:N2 | 1:1A:872:A:N6 | 2.17 | 0.91 |
| 3:IC:18:U:H3 | 3:IC:58:A:H61 | 1.20 | 0.90 |
| 3:IC:27:G:H1 | 3:IC:50:A:H61 | 0.91 | 0.89 |
| 23:1W:52:GLN:HA | 23:1W:61:GLY:HA2 | 1.54 | 0.89 |
| 23:1W:45:LYS:O | 23:1W:49:PHE:N | 2.07 | 0.87 |
| 1:1A:631:G:H1 | 1:1A:659:U:H3 | 1.16 | 0.86 |
| 1:1A:3457:G:H1 | 1:1A:3496:U:H3 | 1.18 | 0.86 |
| 3:IC:52:G:N2 | 3:IC:54:U:O4 | 2.08 | 0.86 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|-------------------|--------------------------|-------------------|
| 1:1A:774:U:OP1 | 29:lc:21:ARG:NH2 | 2.09 | 0.85 |
| 1:1A:737:A:H3' | 1:1A:738:G:H21 | 1.40 | 0.85 |
| 3:1C:26:U:H3 | 3:1C:51:G:H22 | 1.26 | 0.83 |
| 3:1C:81:A:N1 | 3:1C:93:G:O6 | 2.11 | 0.83 |
| 1:1A:2269:U:H5' | 1:1A:2270:G:H5' | 1.59 | 0.83 |
| 1:1A:17:A:H2 | 2:1B:137:A:H61 | 1.25 | 0.83 |
| 3:1C:75:G:H1 | 3:1C:99:U:H5 | 1.22 | 0.83 |
| 1:1A:3146:U:H4' | 1:1A:3147:U:H5'' | 1.61 | 0.81 |
| 3:1C:27:G:N2 | 3:1C:50:A:N1 | 2.28 | 0.81 |
| 1:1A:1118:A:H2 | 1:1A:1165:A:H62 | 1.27 | 0.81 |
| 13:1M:110:ILE:HD12 | 13:1M:111:ASP:H | 1.44 | 0.81 |
| 1:1A:3455:G:H22 | 1:1A:3501:A:H2 | 1.30 | 0.80 |
| 6:1F:389:LYS:HD2 | 6:1F:389:LYS:O | 1.81 | 0.79 |
| 1:1A:493:G:H21 | 1:1A:580:A:H61 | 1.31 | 0.79 |
| 1:1A:1841:G:H22 | 1:1A:1975:G:H1 | 1.27 | 0.79 |
| 1:1A:869:G:N2 | 1:1A:872:A:H62 | 1.78 | 0.79 |
| 1:1A:1818:C:OP2 | 34:lh:74:ARG:NH2 | 2.16 | 0.78 |
| 1:1A:869:G:N2 | 1:1A:872:A:C6 | 2.51 | 0.78 |
| 3:1C:69:U:H3 | 3:1C:104:G:H1 | 1.28 | 0.78 |
| 3:1C:79:G:O6 | 3:1C:95:A:N1 | 2.16 | 0.78 |
| 5:1E:17:HIS:CD2 | 5:1E:18:PRO:HA | 2.15 | 0.77 |
| 23:1W:45:LYS:HB2 | 23:1W:45:LYS:HZ2 | 1.48 | 0.77 |
| 1:1A:1605:A:H2 | 1:1A:3430:U:H3 | 1.33 | 0.76 |
| 1:1A:409:G:OP2 | 38:ll:56:ARG:NH2 | 2.19 | 0.76 |
| 1:1A:3211:A:H2 | 1:1A:3239:G:H21 | 1.32 | 0.75 |
| 1:1A:3454:G:O6 | 1:1A:3502:A:N1 | 2.18 | 0.75 |
| 3:1C:68:C:H42 | 3:1C:105:A:H61 | 1.31 | 0.75 |
| 1:1A:3498:U:H4' | 1:1A:3499:U:H5' | 1.69 | 0.75 |
| 1:1A:2721:G:H1 | 1:1A:2941:C:H5 | 1.34 | 0.75 |
| 6:1F:375:LYS:HB2 | 6:1F:390:VAL:HG11 | 1.69 | 0.75 |
| 9:1I:30:LYS:H | 9:1I:30:LYS:HD2 | 1.51 | 0.74 |
| 17:1Q:14:LYS:O | 17:1Q:23:ARG:NH2 | 2.19 | 0.73 |
| 1:1A:869:G:N2 | 1:1A:872:A:C5 | 2.56 | 0.73 |
| 25:1Y:60:THR:HG22 | 25:1Y:104:ARG:HG3 | 1.71 | 0.73 |
| 35:li:-7:LEU:HD22 | 35:li:42:ASP:HB3 | 1.70 | 0.73 |
| 1:1A:816:G:N2 | 1:1A:829:G:OP2 | 2.21 | 0.73 |
| 6:1F:101:MET:HE3 | 6:1F:104:PRO:HA | 1.71 | 0.73 |
| 25:1Y:56:GLU:OE2 | 25:1Y:56:GLU:N | 2.18 | 0.72 |
| 42:lp:21:CYS:HB3 | 42:lp:24:CYS:HB2 | 1.71 | 0.72 |
| 1:1A:1086:G:H1 | 1:1A:1240:C:H5 | 1.38 | 0.72 |
| 8:1H:56:ARG:NH1 | 36:lj:108:ILE:O | 2.22 | 0.72 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|--------------------|--------------------------|-------------------|
| 1:1A:1661:G:O2' | 1:1A:1751:A:N6 | 2.22 | 0.72 |
| 1:1A:631:G:N2 | 1:1A:659:U:O2 | 2.22 | 0.72 |
| 39:1m:8:VAL:HG13 | 39:1m:11:VAL:HG23 | 1.72 | 0.71 |
| 12:1L:179:GLU:OE2 | 12:1L:179:GLU:N | 2.21 | 0.71 |
| 13:1M:108:GLU:HG2 | 13:1M:122:ILE:HD11 | 1.72 | 0.71 |
| 33:1g:41:ASN:HB3 | 33:1g:44:ARG:HG2 | 1.72 | 0.71 |
| 20:1T:5:TYR:HB2 | 20:1T:60:ILE:HD11 | 1.73 | 0.71 |
| 7:1G:50:ARG:NH2 | 7:1G:72:ASP:OD2 | 2.23 | 0.71 |
| 1:1A:1883:A:H62 | 1:1A:1931:U:H3 | 1.36 | 0.71 |
| 3:1C:6:G:H1 | 3:1C:111:A:H2 | 1.39 | 0.71 |
| 3:1C:59:G:H5' | 7:1G:265:LYS:HG2 | 1.71 | 0.71 |
| 28:1b:68:VAL:O | 28:1b:118:SER:OG | 2.08 | 0.71 |
| 1:1A:1502:A:N6 | 19:1S:15:SER:OG | 2.24 | 0.70 |
| 1:1A:1247:G:H1 | 3:1C:92:U:H5 | 1.37 | 0.70 |
| 1:1A:3456:U:H3 | 1:1A:3497:A:H2 | 1.38 | 0.70 |
| 23:1W:45:LYS:HB2 | 23:1W:45:LYS:NZ | 2.01 | 0.70 |
| 3:1C:3:G:H1 | 3:1C:114:U:H3 | 1.37 | 0.70 |
| 9:1I:130:GLU:N | 9:1I:130:GLU:OE2 | 2.25 | 0.70 |
| 1:1A:50:G:HO2' | 1:1A:1688:A:HO2' | 1.39 | 0.69 |
| 3:1C:84:G:H22 | 3:1C:91:G:N2 | 1.91 | 0.69 |
| 1:1A:3302:U:H2' | 1:1A:3303:A:H8 | 1.56 | 0.69 |
| 1:1A:804:G:H22 | 1:1A:911:U:H3 | 1.39 | 0.69 |
| 4:1D:117:GLU:HG2 | 4:1D:124:GLY:H | 1.58 | 0.69 |
| 32:1f:27:ALA:O | 32:1f:31:ASN:ND2 | 2.25 | 0.69 |
| 16:1P:25:ALA:HA | 16:1P:40:GLY:HA3 | 1.73 | 0.69 |
| 14:1N:82:LYS:NZ | 14:1N:215:LYS:O | 2.26 | 0.69 |
| 22:1V:88:ARG:NH2 | 30:1d:28:ALA:O | 2.25 | 0.69 |
| 1:1A:920:A:OP1 | 29:1c:27:LYS:NZ | 2.25 | 0.69 |
| 40:1n:31:ARG:HG3 | 40:1n:42:LYS:HB2 | 1.75 | 0.69 |
| 37:1k:45:SER:HB2 | 37:1k:48:GLU:HG3 | 1.75 | 0.69 |
| 1:1A:1187:A:H62 | 1:1A:1217:U:H3 | 1.41 | 0.68 |
| 3:1C:22:C:H2' | 3:1C:23:A:H8 | 1.58 | 0.68 |
| 12:1L:170:LYS:HA | 12:1L:177:THR:HA | 1.74 | 0.68 |
| 1:1A:2416:U:O2' | 1:1A:3246:A:N1 | 2.22 | 0.68 |
| 1:1A:3204:C:O2 | 24:1X:89:ARG:NH1 | 2.26 | 0.68 |
| 1:1A:1864:C:OP1 | 23:1W:98:LYS:NZ | 2.27 | 0.68 |
| 1:1A:3246:A:O2' | 24:1X:54:ARG:NH2 | 2.27 | 0.68 |
| 1:1A:3458:U:H3 | 1:1A:3495:G:H1 | 1.41 | 0.68 |
| 3:1C:79:G:C6 | 3:1C:95:A:N1 | 2.61 | 0.68 |
| 6:1F:230:ASP:OD2 | 6:1F:250:ARG:NH2 | 2.24 | 0.68 |
| 1:1A:638:A:N1 | 1:1A:651:G:N2 | 2.36 | 0.68 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|--------------------|--------------------------|-------------------|
| 3:IC:26:U:O2 | 3:IC:52:G:N2 | 2.27 | 0.67 |
| 11:IK:112:VAL:HB | 11:IK:121:GLN:HB2 | 1.75 | 0.67 |
| 34:lh:81:CYS:SG | 34:lh:84:CYS:N | 2.64 | 0.67 |
| 3:IC:17:G:H1 | 3:IC:59:G:H1 | 1.42 | 0.67 |
| 1:IA:2906:U:H2' | 1:IA:2907:C:H6 | 1.60 | 0.67 |
| 1:IA:3336:G:O2' | 15:IO:115:LYS:O | 2.12 | 0.67 |
| 1:IA:3454:G:H1 | 1:IA:3502:A:H2 | 0.74 | 0.67 |
| 4:ID:106:GLN:O | 39:lm:90:LYS:NZ | 2.28 | 0.67 |
| 1:IA:1127:A:H4' | 12:IL:39:ARG:HD2 | 1.77 | 0.67 |
| 1:IA:2688:G:O2' | 1:IA:3008:U:OP1 | 2.11 | 0.67 |
| 1:IA:2261:G:O2' | 1:IA:2390:U:OP2 | 2.13 | 0.66 |
| 6:IF:77:PRO:HB2 | 6:IF:91:ALA:HB3 | 1.77 | 0.66 |
| 1:IA:331:A:OP2 | 43:lq:39:ARG:NH1 | 2.28 | 0.66 |
| 1:IA:610:A:N6 | 1:IA:687:U:O4 | 2.28 | 0.66 |
| 33:lg:91:ARG:HG3 | 33:lg:91:ARG:HH11 | 1.60 | 0.66 |
| 1:IA:43:C:H5'' | 14:IN:14:LYS:HG3 | 1.78 | 0.66 |
| 1:IA:1763:C:H2' | 1:IA:1764:A:H8 | 1.60 | 0.66 |
| 1:IA:1841:G:N2 | 1:IA:1975:G:H22 | 1.94 | 0.66 |
| 1:IA:993:U:OP2 | 1:IA:2109:C:O2' | 2.12 | 0.66 |
| 3:IC:79:G:C2 | 3:IC:95:A:H2 | 2.10 | 0.66 |
| 1:IA:2906:U:H2' | 1:IA:2907:C:C6 | 2.31 | 0.66 |
| 2:IB:60:G:O6 | 38:ll:63:ARG:NH2 | 2.28 | 0.66 |
| 1:IA:2466:G:N2 | 5:IE:228:TYR:OH | 2.24 | 0.66 |
| 1:IA:116:A:N6 | 10:IJ:124:GLU:O | 2.30 | 0.65 |
| 1:IA:1744:A:H2' | 1:IA:1745:A:C8 | 2.32 | 0.65 |
| 9:II:95:ARG:NH2 | 9:II:190:LEU:O | 2.29 | 0.65 |
| 1:IA:189:G:OP1 | 17:IQ:4:TYR:OH | 2.12 | 0.65 |
| 1:IA:1749:U:OP2 | 21:IU:42:ARG:NH2 | 2.30 | 0.65 |
| 4:ID:126:ILE:HG21 | 4:ID:150:LEU:HD22 | 1.77 | 0.65 |
| 5:IE:370:ARG:HH22 | 5:IE:380:ARG:HH21 | 1.45 | 0.65 |
| 9:II:87:ILE:HG23 | 9:II:118:VAL:HG12 | 1.79 | 0.65 |
| 1:IA:2213:U:OP2 | 1:IA:2218:A:N6 | 2.23 | 0.65 |
| 10:IJ:76:THR:O | 10:IJ:80:GLN:NE2 | 2.28 | 0.65 |
| 10:IJ:89:LYS:HE2 | 10:IJ:186:LEU:HD23 | 1.78 | 0.65 |
| 1:IA:1763:C:H2' | 1:IA:1764:A:C8 | 2.32 | 0.65 |
| 1:IA:2178:A:HO2' | 1:IA:2179:U:H6 | 1.42 | 0.65 |
| 8:IH:56:ARG:NH2 | 8:IH:107:GLN:O | 2.30 | 0.65 |
| 1:IA:1356:C:N4 | 1:IA:1386:G:OP2 | 2.30 | 0.65 |
| 3:IC:94:U:H2' | 3:IC:95:A:C8 | 2.32 | 0.65 |
| 8:IH:98:ASN:ND2 | 8:IH:187:MET:O | 2.29 | 0.65 |
| 12:IL:171:TRP:CD1 | 12:IL:172:GLY:H | 2.14 | 0.65 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|--------------------|--------------------------|-------------------|
| 1:1A:218:G:H1 | 1:1A:290:U:H3 | 1.45 | 0.64 |
| 1:1A:597:A:N3 | 8:1H:51:ASN:ND2 | 2.44 | 0.64 |
| 1:1A:732:U:O2' | 1:1A:733:C:O5' | 2.13 | 0.64 |
| 3:1C:17:G:H22 | 3:1C:59:G:H22 | 1.44 | 0.64 |
| 1:1A:570:A:H2' | 1:1A:571:A:C8 | 2.33 | 0.64 |
| 1:1A:3107:G:N2 | 1:1A:3110:A:OP2 | 2.26 | 0.64 |
| 1:1A:3454:G:C6 | 1:1A:3502:A:N1 | 2.65 | 0.64 |
| 20:1T:39:MET:HE2 | 20:1T:43:LYS:HE2 | 1.78 | 0.64 |
| 14:1N:104:LYS:HB2 | 37:1k:16:HIS:HB2 | 1.79 | 0.64 |
| 32:1f:48:ARG:HG2 | 32:1f:48:ARG:HH11 | 1.63 | 0.64 |
| 1:1A:1648:U:OP2 | 1:1A:2081:A:O2' | 2.14 | 0.64 |
| 3:1C:14:G:H2' | 3:1C:15:A:H8 | 1.61 | 0.64 |
| 10:1J:66:ASN:OD1 | 10:1J:70:ASN:ND2 | 2.30 | 0.64 |
| 13:1M:32:ARG:NH1 | 13:1M:119:GLN:O | 2.31 | 0.64 |
| 38:1l:39:TYR:O | 38:1l:41:ASP:N | 2.30 | 0.64 |
| 1:1A:118:A:N6 | 1:1A:189:G:O2' | 2.28 | 0.64 |
| 9:1I:65:ALA:HB1 | 22:1V:142:ARG:HH12 | 1.62 | 0.64 |
| 1:1A:341:G:OP2 | 17:1Q:15:GLN:NE2 | 2.31 | 0.64 |
| 1:1A:1293:U:O4 | 1:1A:1454:G:O2' | 2.14 | 0.64 |
| 24:1X:71:GLU:OE1 | 24:1X:71:GLU:N | 2.20 | 0.64 |
| 1:1A:2114:U:N3 | 1:1A:2198:G:OP2 | 2.31 | 0.64 |
| 20:1T:19:GLU:OE1 | 22:1V:153:LYS:NZ | 2.31 | 0.64 |
| 1:1A:457:G:N2 | 18:1R:5:CYS:SG | 2.71 | 0.64 |
| 34:1h:25:THR:HG22 | 34:1h:26:ALA:H | 1.63 | 0.64 |
| 1:1A:621:U:OP1 | 6:1F:372:SER:OG | 2.12 | 0.63 |
| 1:1A:896:A:O2' | 1:1A:2790:U:OP1 | 2.13 | 0.63 |
| 1:1A:1892:C:H2' | 1:1A:1893:A:H8 | 1.63 | 0.63 |
| 1:1A:220:A:H2' | 1:1A:221:U:H6 | 1.61 | 0.63 |
| 1:1A:919:G:H22 | 6:1F:103:SER:HB2 | 1.64 | 0.63 |
| 14:1N:47:ALA:HB2 | 35:1i:109:PHE:HA | 1.80 | 0.63 |
| 28:1b:10:VAL:O | 28:1b:83:THR:OG1 | 2.16 | 0.63 |
| 36:1j:5:ARG:NH1 | 36:1j:7:HIS:O | 2.30 | 0.63 |
| 1:1A:440:G:N1 | 1:1A:443:A:OP2 | 2.28 | 0.63 |
| 18:1R:18:ARG:NH1 | 18:1R:20:ASP:OD1 | 2.32 | 0.63 |
| 37:1k:2:ALA:O | 37:1k:4:GLY:N | 2.32 | 0.63 |
| 1:1A:2381:G:OP2 | 1:1A:2381:G:N2 | 2.26 | 0.63 |
| 1:1A:2958:G:O2' | 1:1A:2959:G:OP1 | 2.16 | 0.63 |
| 1:1A:58:G:H22 | 1:1A:75:U:H4' | 1.63 | 0.63 |
| 1:1A:626:A:OP1 | 1:1A:664:A:N6 | 2.32 | 0.63 |
| 1:1A:3306:U:HO2' | 1:1A:3322:A:HO2' | 1.45 | 0.63 |
| 1:1A:536:G:O6 | 14:1N:212:LYS:N | 2.32 | 0.62 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|-------------------|--------------------------|-------------------|
| 7:IG:85:ARG:NH1 | 7:IG:249:ALA:O | 2.30 | 0.62 |
| 12:IL:76:MET:HE1 | 12:IL:148:MET:HG2 | 1.81 | 0.62 |
| 1:IA:897:A:H8 | 1:IA:898:U:HO2' | 1.46 | 0.62 |
| 10:IJ:98:GLN:HA | 10:IJ:101:ARG:HD2 | 1.81 | 0.62 |
| 1:IA:626:A:HO2' | 1:IA:627:A:H8 | 1.46 | 0.62 |
| 6:IF:84:SER:OG | 6:IF:87:ASN:OD1 | 2.16 | 0.62 |
| 22:IV:80:VAL:HG12 | 22:IV:81:ASN:H | 1.65 | 0.62 |
| 28:lb:54:THR:O | 28:lb:62:GLN:NE2 | 2.32 | 0.62 |
| 28:lb:27:SER:HG | 28:lb:42:THR:HG1 | 1.45 | 0.62 |
| 33:lg:36:PRO:HG2 | 33:lg:44:ARG:HB3 | 1.81 | 0.62 |
| 1:IA:2991:G:OP1 | 42:lp:25:TYR:OH | 2.18 | 0.62 |
| 2:IB:101:G:OP2 | 2:IB:103:A:O2' | 2.16 | 0.62 |
| 1:IA:3462:A:H2' | 1:IA:3463:A:C8 | 2.34 | 0.62 |
| 3:IC:84:G:H1 | 3:IC:91:G:H22 | 1.45 | 0.62 |
| 1:IA:589:A:OP1 | 8:IH:35:ARG:NH2 | 2.33 | 0.62 |
| 1:IA:628:C:H2' | 1:IA:629:G:C8 | 2.34 | 0.62 |
| 1:IA:871:A:H2' | 1:IA:872:A:C8 | 2.34 | 0.62 |
| 7:IG:50:ARG:NH1 | 7:IG:148:ASP:OD2 | 2.33 | 0.62 |
| 35:li:71:GLU:OE2 | 35:li:71:GLU:N | 2.32 | 0.62 |
| 5:IE:50:LYS:HB2 | 5:IE:337:ILE:HD11 | 1.82 | 0.62 |
| 7:IG:64:ILE:HG13 | 7:IG:105:LEU:HD21 | 1.81 | 0.62 |
| 13:IM:41:THR:O | 13:IM:75:LYS:NZ | 2.32 | 0.62 |
| 24:IX:22:ASN:ND2 | 24:IX:40:ILE:O | 2.33 | 0.62 |
| 17:IQ:31:ARG:NH1 | 17:IQ:124:ASP:OD2 | 2.32 | 0.62 |
| 1:IA:881:G:OP1 | 19:IS:72:LYS:NZ | 2.30 | 0.61 |
| 1:IA:3367:U:H2' | 1:IA:3368:G:C8 | 2.35 | 0.61 |
| 5:IE:80:GLU:OE1 | 5:IE:315:TYR:OH | 2.14 | 0.61 |
| 1:IA:625:A:O2' | 1:IA:664:A:N6 | 2.34 | 0.61 |
| 1:IA:897:A:O2' | 1:IA:899:A:N1 | 2.29 | 0.61 |
| 4:ID:109:GLU:CD | 4:ID:109:GLU:H | 2.08 | 0.61 |
| 13:IM:110:ILE:HD12 | 13:IM:111:ASP:N | 2.15 | 0.61 |
| 1:IA:815:A:H4' | 1:IA:817:A:OP1 | 2.01 | 0.61 |
| 5:IE:222:VAL:O | 5:IE:335:ARG:NH1 | 2.34 | 0.61 |
| 6:IF:319:PRO:HB2 | 6:IF:326:MET:HE2 | 1.82 | 0.61 |
| 33:lg:130:GLN:HA | 33:lg:134:GLN:HB3 | 1.82 | 0.61 |
| 1:IA:570:A:H2' | 1:IA:571:A:H8 | 1.66 | 0.61 |
| 1:IA:1555:U:H2' | 1:IA:1556:G:H8 | 1.66 | 0.61 |
| 24:IX:83:ARG:NH2 | 24:IX:118:THR:O | 2.34 | 0.61 |
| 27:la:138:VAL:HG12 | 27:la:151:MET:HE1 | 1.81 | 0.61 |
| 1:IA:490:A:N1 | 1:IA:583:A:N6 | 2.49 | 0.61 |
| 1:IA:698:U:O2' | 1:IA:699:A:N3 | 2.32 | 0.61 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 1:1A:3170:A:H2' | 1:1A:3171:A:H8 | 1.66 | 0.61 |
| 3:1C:22:C:H2' | 3:1C:23:A:C8 | 2.36 | 0.61 |
| 9:1I:21:CYS:SG | 9:1I:22:LYS:N | 2.73 | 0.61 |
| 1:1A:1209:U:OP1 | 1:1A:1211:A:O2' | 2.19 | 0.61 |
| 1:1A:2767:A:H2' | 1:1A:2768:G:C8 | 2.36 | 0.61 |
| 3:1C:80:G:H1 | 3:1C:94:U:H3 | 1.47 | 0.60 |
| 1:1A:1605:A:O2' | 1:1A:1607:A:OP2 | 2.17 | 0.60 |
| 1:1A:2908:U:H2' | 1:1A:2909:A:C8 | 2.36 | 0.60 |
| 1:1A:3372:U:O2' | 1:1A:3374:C:OP2 | 2.19 | 0.60 |
| 3:1C:75:G:N1 | 3:1C:99:U:H5 | 1.98 | 0.60 |
| 5:1E:17:HIS:HD2 | 5:1E:18:PRO:CA | 2.08 | 0.60 |
| 13:1M:18:VAL:HG13 | 13:1M:70:THR:HG22 | 1.83 | 0.60 |
| 23:1W:104:GLU:OE2 | 23:1W:104:GLU:N | 2.26 | 0.60 |
| 1:1A:191:A:H2' | 1:1A:192:A:C8 | 2.37 | 0.60 |
| 1:1A:209:A:O3' | 14:1N:215:LYS:NZ | 2.34 | 0.60 |
| 1:1A:1476:G:O2' | 1:1A:1477:A:H5' | 2.01 | 0.60 |
| 1:1A:2429:G:H5'' | 18:1R:86:LYS:HB2 | 1.82 | 0.60 |
| 1:1A:893:U:H3 | 1:1A:897:A:H2 | 1.47 | 0.60 |
| 1:1A:495:A:N6 | 1:1A:577:G:O2' | 2.31 | 0.60 |
| 1:1A:1269:U:OP2 | 33:1g:44:ARG:NH2 | 2.33 | 0.60 |
| 1:1A:1737:A:OP2 | 34:1h:11:HIS:ND1 | 2.32 | 0.60 |
| 1:1A:2461:G:O2' | 1:1A:2462:G:OP2 | 2.17 | 0.60 |
| 1:1A:3044:G:O2' | 1:1A:3178:A:N1 | 2.34 | 0.60 |
| 1:1A:1523:U:OP1 | 33:1g:105:LYS:NZ | 2.32 | 0.60 |
| 1:1A:2101:G:O2' | 1:1A:2410:U:O4 | 2.15 | 0.60 |
| 1:1A:2944:A:O2' | 1:1A:2945:A:H2' | 2.02 | 0.60 |
| 1:1A:3352:G:H4' | 1:1A:3353:U:H5'' | 1.84 | 0.60 |
| 28:1b:42:THR:HG22 | 28:1b:74:VAL:HG22 | 1.83 | 0.60 |
| 1:1A:2414:C:OP1 | 5:1E:238:ARG:NH1 | 2.31 | 0.60 |
| 14:1N:9:ASN:HB2 | 19:1S:165:LYS:HB2 | 1.84 | 0.60 |
| 1:1A:725:A:OP2 | 6:1F:413:LYS:NZ | 2.34 | 0.60 |
| 1:1A:822:C:H2' | 1:1A:823:A:C8 | 2.37 | 0.60 |
| 1:1A:873:U:H2' | 1:1A:874:A:C8 | 2.37 | 0.59 |
| 1:1A:1327:A:H2' | 1:1A:1328:A:C8 | 2.37 | 0.59 |
| 16:1P:49:ARG:NH2 | 16:1P:71:MET:O | 2.28 | 0.59 |
| 1:1A:1912:A:H61 | 39:1m:42:CYS:HA | 1.67 | 0.59 |
| 1:1A:2062:A:O2' | 1:1A:3220:U:OP1 | 2.16 | 0.59 |
| 10:1J:35:ASP:OD1 | 25:1Y:6:ARG:N | 2.35 | 0.59 |
| 11:1K:43:LYS:HE3 | 15:1O:132:PRO:HG2 | 1.84 | 0.59 |
| 1:1A:1208:U:C4 | 1:1A:1211:A:H5'' | 2.38 | 0.59 |
| 3:1C:17:G:H22 | 3:1C:59:G:N2 | 2.00 | 0.59 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 2:1B:11:U:H2' | 2:1B:12:A:H8 | 1.67 | 0.59 |
| 15:1O:127:ILE:HD12 | 20:1T:170:THR:HG23 | 1.84 | 0.59 |
| 28:1b:20:GLY:HA3 | 28:1b:139:PHE:CZ | 2.37 | 0.59 |
| 1:1A:492:U:O2' | 1:1A:493:G:O5' | 2.20 | 0.59 |
| 1:1A:705:U:H2' | 1:1A:706:A:H8 | 1.68 | 0.59 |
| 1:1A:796:U:H2' | 1:1A:797:C:C6 | 2.38 | 0.59 |
| 3:1C:29:G:O6 | 3:1C:46:G:O6 | 2.20 | 0.59 |
| 4:1D:64:ARG:NH1 | 4:1D:70:GLY:O | 2.35 | 0.59 |
| 1:1A:759:U:H2' | 1:1A:760:A:H8 | 1.66 | 0.59 |
| 1:1A:1277:G:OP2 | 1:1A:1277:G:N2 | 2.31 | 0.59 |
| 1:1A:1384:A:O2' | 1:1A:1385:G:O4' | 2.20 | 0.59 |
| 1:1A:213:A:H5' | 14:1N:133:LYS:H | 1.68 | 0.59 |
| 1:1A:246:U:N3 | 1:1A:266:A:OP2 | 2.34 | 0.59 |
| 1:1A:2632:A:O2' | 28:1b:139:PHE:O | 2.19 | 0.59 |
| 8:1H:11:LYS:NZ | 8:1H:27:ILE:O | 2.34 | 0.59 |
| 5:1E:28:THR:O | 5:1E:276:LYS:NZ | 2.35 | 0.59 |
| 27:1a:48:PRO:O | 27:1a:113:ARG:NH2 | 2.36 | 0.59 |
| 1:1A:639:G:H1 | 1:1A:650:A:H2 | 1.50 | 0.59 |
| 1:1A:1290:A:OP1 | 36:1j:85:ARG:NH2 | 2.35 | 0.59 |
| 1:1A:220:A:H2' | 1:1A:221:U:C6 | 2.38 | 0.59 |
| 1:1A:663:G:OP2 | 16:1P:72:THR:OG1 | 2.12 | 0.59 |
| 1:1A:1846:A:H2' | 1:1A:1847:A:H8 | 1.68 | 0.59 |
| 2:1B:1:A:H2' | 2:1B:2:A:C8 | 2.38 | 0.59 |
| 1:1A:1823:C:H2' | 1:1A:1824:A:C4 | 2.37 | 0.58 |
| 1:1A:3302:U:H2' | 1:1A:3303:A:C8 | 2.37 | 0.58 |
| 3:1C:28:U:H3' | 3:1C:29:G:H21 | 1.67 | 0.58 |
| 3:1C:81:A:N1 | 3:1C:93:G:C6 | 2.71 | 0.58 |
| 3:1C:85:G:H22 | 3:1C:90:G:H1 | 1.49 | 0.58 |
| 1:1A:424:A:O2' | 1:1A:425:C:OP2 | 2.22 | 0.58 |
| 1:1A:1225:A:H5'' | 9:1I:95:ARG:HD2 | 1.84 | 0.58 |
| 1:1A:1992:A:H2' | 1:1A:1993:G:H8 | 1.67 | 0.58 |
| 24:1X:51:ARG:HH21 | 24:1X:54:ARG:HH12 | 1.51 | 0.58 |
| 1:1A:547:A:H2' | 1:1A:548:A:H8 | 1.68 | 0.58 |
| 1:1A:550:A:H2' | 1:1A:551:A:C8 | 2.38 | 0.58 |
| 1:1A:789:C:H2' | 1:1A:790:A:H8 | 1.67 | 0.58 |
| 1:1A:2739:U:H2' | 1:1A:2740:G:H8 | 1.66 | 0.58 |
| 1:1A:816:G:H22 | 1:1A:829:G:P | 2.25 | 0.58 |
| 1:1A:3368:G:H2' | 1:1A:3369:U:C6 | 2.37 | 0.58 |
| 1:1A:3454:G:C2 | 1:1A:3502:A:H2 | 2.18 | 0.58 |
| 3:1C:79:G:H1 | 3:1C:95:A:H2 | 0.67 | 0.58 |
| 6:1F:389:LYS:HD3 | 6:1F:391:LYS:HE2 | 1.85 | 0.58 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 29:lc:6:ARG:HB3 | 29:lc:8:THR:HG22 | 1.86 | 0.58 |
| 1:lA:1877:A:H2' | 1:lA:1878:A:C8 | 2.38 | 0.58 |
| 1:lA:3008:U:O2' | 1:lA:3009:C:OP1 | 2.22 | 0.58 |
| 20:IT:69:LYS:NZ | 20:IT:93:VAL:O | 2.36 | 0.58 |
| 10:lJ:52:LYS:NZ | 17:lQ:29:GLU:OE2 | 2.29 | 0.58 |
| 1:lA:3336:G:H5' | 1:lA:3373:A:H61 | 1.69 | 0.58 |
| 1:lA:852:A:O2' | 1:lA:854:A:OP2 | 2.22 | 0.57 |
| 1:lA:1846:A:H2' | 1:lA:1847:A:C8 | 2.39 | 0.57 |
| 1:lA:2637:A:H61 | 1:lA:2649:G:H2' | 1.69 | 0.57 |
| 1:lA:3397:C:OP2 | 1:lA:3398:U:O2' | 2.22 | 0.57 |
| 1:lA:227:A:H2' | 1:lA:228:A:C8 | 2.38 | 0.57 |
| 4:lD:193:ARG:HG3 | 4:lD:195:THR:HG23 | 1.86 | 0.57 |
| 22:IV:75:MET:SD | 22:IV:88:ARG:NH1 | 2.77 | 0.57 |
| 27:la:21:ALA:O | 27:la:26:ARG:NH1 | 2.36 | 0.57 |
| 1:lA:476:U:OP1 | 36:lJ:66:ARG:NH1 | 2.37 | 0.57 |
| 3:lC:2:G:O2' | 3:lC:24:U:O2 | 2.21 | 0.57 |
| 6:lF:101:MET:HE1 | 6:lF:105:LEU:HG | 1.85 | 0.57 |
| 1:lA:13:C:OP2 | 25:IY:27:ARG:NH2 | 2.35 | 0.57 |
| 1:lA:2346:A:H2' | 1:lA:2347:A:C8 | 2.38 | 0.57 |
| 1:lA:586:A:N6 | 8:lH:43:THR:O | 2.38 | 0.57 |
| 1:lA:1729:G:O2' | 1:lA:1730:G:O4' | 2.15 | 0.57 |
| 1:lA:191:A:H2' | 1:lA:192:A:H8 | 1.68 | 0.57 |
| 1:lA:1220:A:H2' | 1:lA:1220:A:N3 | 2.19 | 0.57 |
| 1:lA:3368:G:H2' | 1:lA:3369:U:H6 | 1.69 | 0.57 |
| 8:lH:23:THR:H | 8:lH:26:MET:HE2 | 1.70 | 0.57 |
| 13:lM:49:GLU:HA | 13:lM:64:GLN:HA | 1.87 | 0.57 |
| 1:lA:286:U:H4' | 14:lN:43:ALA:HA | 1.87 | 0.57 |
| 1:lA:873:U:H2' | 1:lA:874:A:H8 | 1.69 | 0.57 |
| 1:lA:1019:G:H1' | 1:lA:1737:A:N6 | 2.19 | 0.57 |
| 1:lA:1186:G:H21 | 1:lA:1220:A:N6 | 2.02 | 0.57 |
| 1:lA:2634:A:OP2 | 4:lD:64:ARG:NH2 | 2.36 | 0.57 |
| 1:lA:2767:A:H2' | 1:lA:2768:G:H8 | 1.69 | 0.57 |
| 1:lA:2848:A:N1 | 1:lA:2911:U:H5 | 2.02 | 0.57 |
| 1:lA:3129:U:H2' | 1:lA:3130:A:H8 | 1.68 | 0.57 |
| 10:lJ:174:TYR:HH | 10:lJ:226:TYR:HH | 1.53 | 0.57 |
| 31:le:26:LYS:HG3 | 31:le:97:ILE:HB | 1.87 | 0.57 |
| 1:lA:505:A:H2' | 1:lA:506:A:C8 | 2.39 | 0.57 |
| 1:lA:721:A:H2' | 1:lA:722:A:C8 | 2.39 | 0.57 |
| 1:lA:2236:A:H2' | 1:lA:2237:A:C8 | 2.39 | 0.57 |
| 10:lJ:37:THR:HG22 | 10:lJ:38:ARG:H | 1.70 | 0.57 |
| 23:IW:102:LEU:HD12 | 23:IW:106:LEU:HD13 | 1.87 | 0.57 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|-------------------|--------------------------|-------------------|
| 40:ln:14:GLU:HG2 | 40:ln:17:GLN:OE1 | 2.05 | 0.57 |
| 1:lA:99:A:H5'' | 14:lN:58:CYS:HB3 | 1.87 | 0.57 |
| 1:lA:493:G:H1' | 1:lA:579:A:H61 | 1.68 | 0.57 |
| 24:lX:18:CYS:HB2 | 24:lX:54:ARG:HB3 | 1.86 | 0.57 |
| 1:lA:785:G:O2' | 1:lA:1569:A:OP1 | 2.23 | 0.57 |
| 1:lA:2236:A:H2' | 1:lA:2237:A:H8 | 1.70 | 0.57 |
| 1:lA:975:G:OP1 | 21:lU:92:LYS:NZ | 2.38 | 0.56 |
| 1:lA:1553:A:OP1 | 2:lB:22:G:O2' | 2.22 | 0.56 |
| 1:lA:1639:U:H2' | 1:lA:1640:A:H8 | 1.69 | 0.56 |
| 2:lB:11:U:H2' | 2:lB:12:A:C8 | 2.39 | 0.56 |
| 29:lc:85:ASP:N | 29:lc:85:ASP:OD2 | 2.38 | 0.56 |
| 1:lA:1115:A:O2' | 3:lC:76:U:O2 | 2.22 | 0.56 |
| 1:lA:2746:A:H5' | 1:lA:2747:G:C8 | 2.40 | 0.56 |
| 1:lA:2751:C:P | 13:lM:51:ARG:HE | 2.28 | 0.56 |
| 9:ll:30:LYS:HD2 | 9:ll:30:LYS:N | 2.20 | 0.56 |
| 1:lA:737:A:O5' | 1:lA:738:G:N2 | 2.37 | 0.56 |
| 3:lC:85:G:N2 | 3:lC:90:G:H22 | 2.03 | 0.56 |
| 1:lA:2979:C:H5 | 1:lA:2995:C:H42 | 1.52 | 0.56 |
| 1:lA:3452:U:H3 | 1:lA:3504:G:H22 | 1.53 | 0.56 |
| 10:lJ:168:LYS:O | 10:lJ:171:GLN:NE2 | 2.38 | 0.56 |
| 1:lA:605:C:H2' | 1:lA:606:A:H8 | 1.70 | 0.56 |
| 1:lA:721:A:H2' | 1:lA:722:A:H8 | 1.70 | 0.56 |
| 1:lA:1814:G:N2 | 1:lA:1817:A:OP2 | 2.36 | 0.56 |
| 8:lH:64:ILE:HD12 | 8:lH:115:GLN:HB3 | 1.85 | 0.56 |
| 1:lA:675:A:H5'' | 6:lF:354:TYR:CE2 | 2.41 | 0.56 |
| 1:lA:1346:G:H21 | 1:lA:1410:A:H62 | 1.54 | 0.56 |
| 1:lA:3139:G:H1' | 2:lB:1:A:C2 | 2.40 | 0.56 |
| 21:lU:95:TRP:CH2 | 21:lU:99:MET:HE3 | 2.40 | 0.56 |
| 3:lC:17:G:H1 | 3:lC:59:G:H22 | 1.53 | 0.56 |
| 12:lL:140:CYS:SG | 12:lL:148:MET:HG3 | 2.46 | 0.56 |
| 1:lA:502:U:H2' | 1:lA:503:A:C8 | 2.41 | 0.56 |
| 1:lA:624:U:H2' | 1:lA:625:A:O4' | 2.06 | 0.56 |
| 1:lA:1764:A:H2' | 1:lA:1765:A:C8 | 2.41 | 0.56 |
| 1:lA:1847:A:H2' | 1:lA:1848:A:C8 | 2.41 | 0.56 |
| 15:lO:12:CYS:HB3 | 15:lO:42:LEU:HG | 1.88 | 0.56 |
| 23:lW:53:THR:HA | 23:lW:60:ALA:HB1 | 1.87 | 0.56 |
| 1:lA:227:A:H2' | 1:lA:228:A:H8 | 1.71 | 0.56 |
| 1:lA:2468:C:O2' | 5:lE:268:ARG:NH1 | 2.39 | 0.56 |
| 5:lE:27:ALA:HB1 | 5:lE:276:LYS:HD2 | 1.88 | 0.56 |
| 1:lA:760:A:H2' | 1:lA:761:A:H8 | 1.71 | 0.55 |
| 1:lA:797:C:H2' | 1:lA:798:U:H6 | 1.71 | 0.55 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|-------------------|--------------------------|-------------------|
| 13:IM:64:GLN:N | 13:IM:64:GLN:OE1 | 2.38 | 0.55 |
| 1:IA:2632:A:OP2 | 4:ID:87:TYR:OH | 2.20 | 0.55 |
| 27:la:80:ILE:HG22 | 27:la:82:LYS:H | 1.71 | 0.55 |
| 1:IA:941:A:H2' | 1:IA:942:C:C6 | 2.41 | 0.55 |
| 1:IA:2745:C:H42 | 13:IM:22:SER:HB3 | 1.72 | 0.55 |
| 5:IE:223:THR:OG1 | 5:IE:273:GLY:O | 2.23 | 0.55 |
| 31:le:17:LYS:NZ | 31:le:103:ASP:OD1 | 2.40 | 0.55 |
| 1:IA:265:A:H1' | 1:IA:266:A:H2 | 1.71 | 0.55 |
| 1:IA:918:G:O2' | 14:IN:16:TRP:NE1 | 2.32 | 0.55 |
| 3:IC:109:G:H2' | 3:IC:110:A:C8 | 2.41 | 0.55 |
| 1:IA:1095:A:H2 | 1:IA:1099:A:H2 | 1.54 | 0.55 |
| 1:IA:2732:A:H2' | 1:IA:2733:A:H8 | 1.71 | 0.55 |
| 22:IV:129:LEU:HD23 | 22:IV:129:LEU:H | 1.71 | 0.55 |
| 1:IA:665:A:OP1 | 20:IT:64:ASN:ND2 | 2.39 | 0.55 |
| 1:IA:1476:G:N3 | 1:IA:1476:G:H2' | 2.21 | 0.55 |
| 1:IA:1640:A:H2' | 1:IA:1641:A:C8 | 2.41 | 0.55 |
| 1:IA:2485:G:H3' | 1:IA:2486:U:H4' | 1.88 | 0.55 |
| 1:IA:3038:C:O2' | 42:lp:25:TYR:O | 2.24 | 0.55 |
| 1:IA:3450:A:H2' | 1:IA:3451:A:C8 | 2.42 | 0.55 |
| 1:IA:447:G:N2 | 2:IB:17:G:OP2 | 2.40 | 0.55 |
| 1:IA:1327:A:H2' | 1:IA:1328:A:H8 | 1.71 | 0.55 |
| 1:IA:2499:U:H2' | 1:IA:2500:A:H8 | 1.72 | 0.55 |
| 1:IA:2730:U:H2' | 1:IA:2731:G:H8 | 1.71 | 0.55 |
| 5:IE:384:MET:O | 5:IE:388:LEU:N | 2.36 | 0.55 |
| 1:IA:1558:C:H4' | 27:la:182:PRO:HG2 | 1.89 | 0.55 |
| 1:IA:2721:G:H5'' | 1:IA:2722:U:O4' | 2.07 | 0.55 |
| 1:IA:674:A:OP1 | 6:IF:357:LYS:NZ | 2.40 | 0.55 |
| 1:IA:1841:G:H22 | 1:IA:1975:G:H22 | 1.55 | 0.55 |
| 11:IK:182:LEU:HB3 | 42:lp:11:ALA:HB1 | 1.89 | 0.55 |
| 22:IV:8:ASN:O | 22:IV:11:THR:OG1 | 2.25 | 0.55 |
| 24:IX:106:VAL:HG12 | 24:IX:112:MET:HG2 | 1.89 | 0.55 |
| 1:IA:462:A:H2' | 1:IA:463:U:C6 | 2.42 | 0.55 |
| 1:IA:1027:G:H4' | 1:IA:1028:G:O5' | 2.07 | 0.55 |
| 3:IC:17:G:N2 | 3:IC:59:G:H22 | 2.05 | 0.55 |
| 1:IA:1562:A:H2' | 29:lc:3:THR:HG21 | 1.89 | 0.54 |
| 1:IA:3413:U:O2' | 36:lj:58:LYS:NZ | 2.36 | 0.54 |
| 1:IA:3457:G:N2 | 1:IA:3496:U:O2 | 2.30 | 0.54 |
| 1:IA:450:U:H4' | 1:IA:1550:G:H4' | 1.89 | 0.54 |
| 1:IA:774:U:H2' | 1:IA:775:C:C6 | 2.42 | 0.54 |
| 1:IA:1639:U:H2' | 1:IA:1640:A:C8 | 2.41 | 0.54 |
| 1:IA:3139:G:H1' | 2:IB:1:A:H2 | 1.71 | 0.54 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|--------------------|--------------------------|-------------------|
| 1:1A:76:U:H2' | 1:1A:77:C:H6 | 1.73 | 0.54 |
| 1:1A:401:A:N1 | 6:1F:84:SER:HB3 | 2.22 | 0.54 |
| 1:1A:502:U:H2' | 1:1A:503:A:H8 | 1.73 | 0.54 |
| 1:1A:1177:A:H2' | 1:1A:1178:A:C8 | 2.43 | 0.54 |
| 1:1A:1912:A:N6 | 39:1m:42:CYS:HA | 2.23 | 0.54 |
| 3:1C:78:C:H2' | 3:1C:79:G:H8 | 1.72 | 0.54 |
| 1:1A:720:U:O2' | 1:1A:721:A:OP1 | 2.25 | 0.54 |
| 1:1A:886:A:H4' | 30:1d:27:SER:HB2 | 1.89 | 0.54 |
| 1:1A:2908:U:H2' | 1:1A:2909:A:H8 | 1.73 | 0.54 |
| 2:1B:25:U:OP2 | 27:1a:15:ARG:NH1 | 2.41 | 0.54 |
| 1:1A:1090:A:H2' | 1:1A:1091:A:C8 | 2.41 | 0.54 |
| 1:1A:1886:A:H2' | 1:1A:1887:A:C8 | 2.43 | 0.54 |
| 2:1B:25:U:H4' | 27:1a:16:LYS:HB2 | 1.90 | 0.54 |
| 6:1F:4:ARG:HD2 | 6:1F:24:LEU:O | 2.06 | 0.54 |
| 42:1p:11:ALA:O | 42:1p:15:ASN:ND2 | 2.35 | 0.54 |
| 1:1A:10:U:H2' | 1:1A:11:A:H8 | 1.73 | 0.54 |
| 1:1A:106:G:OP2 | 14:1N:71:ARG:NH2 | 2.40 | 0.54 |
| 1:1A:632:G:H2' | 1:1A:633:A:C8 | 2.43 | 0.54 |
| 1:1A:1401:C:H2' | 1:1A:1402:A:H8 | 1.72 | 0.54 |
| 1:1A:2981:A:N6 | 1:1A:2993:G:O2' | 2.39 | 0.54 |
| 1:1A:3393:A:H2' | 1:1A:3394:A:C8 | 2.42 | 0.54 |
| 3:1C:84:G:H22 | 3:1C:91:G:H22 | 1.56 | 0.54 |
| 5:1E:21:ARG:HB2 | 5:1E:274:PHE:HB3 | 1.90 | 0.54 |
| 5:1E:59:GLU:HG2 | 5:1E:358:LYS:HD2 | 1.89 | 0.54 |
| 1:1A:667:U:H2' | 1:1A:668:A:N3 | 2.23 | 0.54 |
| 1:1A:1071:A:H4' | 1:1A:1087:G:N2 | 2.22 | 0.54 |
| 1:1A:1538:G:N2 | 1:1A:1541:A:OP2 | 2.34 | 0.54 |
| 1:1A:1848:A:H2' | 1:1A:1849:A:C8 | 2.41 | 0.54 |
| 1:1A:2985:C:OP1 | 1:1A:2987:C:N4 | 2.40 | 0.54 |
| 3:1C:84:G:N2 | 3:1C:91:G:H22 | 2.05 | 0.54 |
| 14:1N:46:PRO:HB2 | 35:1i:109:PHE:HB3 | 1.90 | 0.54 |
| 16:1P:11:ARG:NH1 | 16:1P:60:THR:O | 2.36 | 0.54 |
| 21:1U:95:TRP:CZ2 | 21:1U:99:MET:HE3 | 2.43 | 0.54 |
| 31:1e:62:TYR:HE2 | 34:1h:97:GLU:HG2 | 1.72 | 0.54 |
| 33:1g:95:ALA:HB3 | 33:1g:120:VAL:HG22 | 1.89 | 0.54 |
| 1:1A:501:U:H2' | 1:1A:502:U:H6 | 1.72 | 0.54 |
| 1:1A:2272:C:O2' | 1:1A:2346:A:N3 | 2.38 | 0.54 |
| 1:1A:2732:A:H2' | 1:1A:2733:A:C8 | 2.42 | 0.54 |
| 1:1A:244:A:N3 | 1:1A:264:G:O2' | 2.39 | 0.54 |
| 1:1A:699:A:H2' | 1:1A:700:A:C8 | 2.42 | 0.54 |
| 1:1A:1006:A:H2' | 1:1A:1007:C:C6 | 2.43 | 0.54 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|--------------------|--------------------------|-------------------|
| 1:1A:3023:U:H1' | 5:1E:252:ALA:HB3 | 1.90 | 0.54 |
| 19:1S:152:VAL:HA | 19:1S:159:ALA:H | 1.73 | 0.54 |
| 1:1A:789:C:H2' | 1:1A:790:A:C8 | 2.43 | 0.53 |
| 1:1A:1459:U:H5'' | 9:1I:194:LYS:HB3 | 1.91 | 0.53 |
| 15:1O:63:VAL:HG12 | 15:1O:66:ASN:H | 1.72 | 0.53 |
| 1:1A:660:U:H2' | 1:1A:661:G:H8 | 1.74 | 0.53 |
| 1:1A:804:G:H2' | 1:1A:805:G:C8 | 2.44 | 0.53 |
| 1:1A:1103:U:H2' | 1:1A:1104:A:H8 | 1.73 | 0.53 |
| 1:1A:1305:A:H1' | 1:1A:1306:A:C8 | 2.44 | 0.53 |
| 1:1A:2489:A:H2' | 1:1A:2490:G:H8 | 1.72 | 0.53 |
| 3:1C:78:C:H2' | 3:1C:79:G:C8 | 2.44 | 0.53 |
| 5:1E:232:ILE:HG13 | 5:1E:249:ARG:HB3 | 1.90 | 0.53 |
| 13:1M:92:LYS:HA | 13:1M:172:LEU:HB3 | 1.90 | 0.53 |
| 32:1f:48:ARG:HG2 | 32:1f:48:ARG:NH1 | 2.23 | 0.53 |
| 35:1i:-9:ALA:HA | 35:1i:38:VAL:HG13 | 1.90 | 0.53 |
| 1:1A:500:G:O6 | 1:1A:573:A:N6 | 2.41 | 0.53 |
| 1:1A:675:A:H2' | 6:1F:354:TYR:CD2 | 2.43 | 0.53 |
| 1:1A:765:A:N3 | 36:1j:92:PRO:HG2 | 2.24 | 0.53 |
| 1:1A:2099:G:O2' | 24:1X:19:GLY:O | 2.26 | 0.53 |
| 5:1E:92:TYR:HB3 | 5:1E:99:LEU:HD22 | 1.90 | 0.53 |
| 25:1Y:26:PRO:HD2 | 35:1i:69:PRO:HG3 | 1.89 | 0.53 |
| 1:1A:759:U:H2' | 1:1A:760:A:C8 | 2.43 | 0.53 |
| 1:1A:1545:A:H4' | 33:1g:122:ASN:HD21 | 1.73 | 0.53 |
| 1:1A:3024:C:H2' | 1:1A:3025:U:C6 | 2.43 | 0.53 |
| 23:1W:85:CYS:SG | 23:1W:86:LYS:N | 2.81 | 0.53 |
| 1:1A:700:A:H5'' | 1:1A:745:A:H62 | 1.73 | 0.53 |
| 1:1A:1206:A:H2' | 1:1A:1207:C:C6 | 2.43 | 0.53 |
| 1:1A:979:G:C5 | 4:1D:181:LYS:HB3 | 2.44 | 0.53 |
| 1:1A:2427:U:H2' | 1:1A:2428:A:H8 | 1.74 | 0.53 |
| 1:1A:3250:G:O2' | 5:1E:282:LYS:NZ | 2.42 | 0.53 |
| 1:1A:646:U:O2' | 1:1A:647:C:O5' | 2.26 | 0.53 |
| 1:1A:728:U:OP2 | 9:1I:48:LYS:NZ | 2.33 | 0.53 |
| 1:1A:3237:G:O3' | 26:1Z:44:ARG:NH2 | 2.41 | 0.53 |
| 29:1c:3:THR:HA | 29:1c:6:ARG:HD3 | 1.89 | 0.53 |
| 6:1F:372:SER:HB2 | 6:1F:392:VAL:HG11 | 1.89 | 0.53 |
| 7:1G:36:MET:HE1 | 7:1G:148:ASP:CG | 2.34 | 0.53 |
| 11:1K:94:LYS:HB3 | 11:1K:194:GLU:HB2 | 1.89 | 0.53 |
| 11:1K:101:ARG:HG3 | 11:1K:188:SER:HB3 | 1.90 | 0.53 |
| 15:1O:173:GLN:O | 15:1O:177:LYS:HD3 | 2.08 | 0.53 |
| 21:1U:44:LEU:HD22 | 21:1U:49:LEU:HD12 | 1.91 | 0.53 |
| 1:1A:3088:G:O2' | 1:1A:3091:C:OP2 | 2.19 | 0.53 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 11:IK:67:MET:HE1 | 11:IK:74:ASP:HB3 | 1.90 | 0.53 |
| 14:IN:105:GLU:N | 14:IN:105:GLU:OE1 | 2.41 | 0.53 |
| 15:IO:190:GLU:O | 15:IO:193:LYS:NZ | 2.42 | 0.53 |
| 1:IA:65:U:O2' | 1:IA:97:A:O2' | 2.22 | 0.53 |
| 1:IA:3103:C:H2' | 1:IA:3104:G:H8 | 1.74 | 0.53 |
| 3:IC:32:A:H2' | 3:IC:33:A:C8 | 2.43 | 0.53 |
| 38:II:21:ARG:NH2 | 38:II:38:GLY:O | 2.42 | 0.53 |
| 3:IC:2:G:H2' | 3:IC:3:G:H8 | 1.73 | 0.52 |
| 3:IC:103:U:H2' | 3:IC:104:G:C8 | 2.44 | 0.52 |
| 36:IJ:40:THR:HG21 | 36:IJ:75:PRO:HB3 | 1.91 | 0.52 |
| 1:IA:3198:A:H4' | 5:IE:13:SER:HB2 | 1.90 | 0.52 |
| 28:IB:46:VAL:HG13 | 28:IB:68:VAL:HG13 | 1.91 | 0.52 |
| 1:IA:236:U:O4' | 27:IA:33:ARG:NH1 | 2.43 | 0.52 |
| 1:IA:761:A:H2' | 1:IA:762:A:C8 | 2.44 | 0.52 |
| 1:IA:816:G:H5' | 1:IA:817:A:OP1 | 2.09 | 0.52 |
| 1:IA:2041:U:H4' | 1:IA:2042:A:H5'' | 1.91 | 0.52 |
| 1:IA:2308:A:H2' | 1:IA:2309:A:C8 | 2.44 | 0.52 |
| 3:IC:14:G:H2' | 3:IC:15:A:C8 | 2.42 | 0.52 |
| 8:IH:64:ILE:O | 8:IH:113:THR:OG1 | 2.21 | 0.52 |
| 1:IA:1593:A:OP1 | 32:IF:75:ARG:NH2 | 2.43 | 0.52 |
| 1:IA:2123:A:H2' | 1:IA:2124:A:C8 | 2.44 | 0.52 |
| 7:IG:128:LEU:HB3 | 7:IG:192:ARG:HG3 | 1.91 | 0.52 |
| 8:IH:122:VAL:HG12 | 8:IH:169:VAL:HG13 | 1.92 | 0.52 |
| 35:II:85:THR:HG22 | 35:II:87:ALA:H | 1.73 | 0.52 |
| 38:II:64:MET:HE2 | 38:II:67:LEU:HB3 | 1.91 | 0.52 |
| 1:IA:622:A:H5'' | 6:IF:391:LYS:HG3 | 1.90 | 0.52 |
| 1:IA:772:C:N4 | 1:IA:773:G:O6 | 2.43 | 0.52 |
| 2:IB:116:U:H2' | 2:IB:117:A:C8 | 2.44 | 0.52 |
| 6:IF:80:SER:O | 6:IF:87:ASN:ND2 | 2.38 | 0.52 |
| 9:II:166:VAL:HG13 | 9:II:171:ASP:HB2 | 1.91 | 0.52 |
| 1:IA:301:A:H2' | 1:IA:302:U:C6 | 2.45 | 0.52 |
| 1:IA:337:A:H2' | 1:IA:338:A:H8 | 1.74 | 0.52 |
| 1:IA:1509:A:H2' | 1:IA:1510:A:C8 | 2.43 | 0.52 |
| 1:IA:1848:A:H2' | 1:IA:1849:A:H8 | 1.74 | 0.52 |
| 11:IK:71:ASN:OD1 | 11:IK:71:ASN:N | 2.40 | 0.52 |
| 19:IS:35:LEU:O | 19:IS:39:THR:OG1 | 2.26 | 0.52 |
| 32:IF:52:ILE:HD13 | 32:IF:77:LEU:HD12 | 1.90 | 0.52 |
| 1:IA:361:C:OP1 | 14:IN:100:LYS:NZ | 2.41 | 0.52 |
| 1:IA:452:A:C2 | 2:IB:19:A:H1' | 2.45 | 0.52 |
| 1:IA:2128:A:OP1 | 39:IM:23:ARG:NH2 | 2.42 | 0.52 |
| 1:IA:2589:C:OP2 | 1:IA:2656:G:N2 | 2.42 | 0.52 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 1:1A:3148:C:H2' | 1:1A:3149:A:H8 | 1.74 | 0.52 |
| 1:1A:3315:U:O2' | 1:1A:3418:C:OP2 | 2.27 | 0.52 |
| 4:1D:143:ASN:N | 4:1D:143:ASN:OD1 | 2.43 | 0.52 |
| 27:1a:87:LYS:O | 27:1a:89:ASN:N | 2.43 | 0.52 |
| 35:1i:-6:LYS:O | 35:1i:-3:ALA:N | 2.39 | 0.52 |
| 1:1A:237:C:H2' | 1:1A:238:A:H8 | 1.74 | 0.52 |
| 1:1A:709:U:O2' | 1:1A:710:A:OP1 | 2.27 | 0.52 |
| 1:1A:941:A:H2' | 1:1A:942:C:H6 | 1.75 | 0.52 |
| 1:1A:1409:G:H5'' | 11:1K:55:LYS:HE3 | 1.91 | 0.52 |
| 1:1A:3431:U:H3 | 1:1A:3441:G:H1 | 1.58 | 0.52 |
| 12:1L:66:GLU:OE1 | 12:1L:69:ARG:NH2 | 2.42 | 0.52 |
| 1:1A:797:C:H2' | 1:1A:798:U:C6 | 2.45 | 0.52 |
| 1:1A:1342:U:H2' | 1:1A:1343:A:H4' | 1.91 | 0.52 |
| 1:1A:1640:A:H2' | 1:1A:1641:A:H8 | 1.75 | 0.52 |
| 10:1J:30:VAL:HG12 | 10:1J:31:ALA:H | 1.74 | 0.52 |
| 12:1L:55:LEU:HD21 | 12:1L:164:LYS:HE2 | 1.92 | 0.52 |
| 1:1A:701:A:C5 | 1:1A:703:G:H1' | 2.45 | 0.52 |
| 1:1A:832:A:O2' | 1:1A:833:U:OP1 | 2.26 | 0.52 |
| 1:1A:835:A:H2' | 1:1A:836:C:O4' | 2.10 | 0.52 |
| 1:1A:2357:A:H8 | 1:1A:3117:U:H1' | 1.75 | 0.52 |
| 2:1B:74:A:OP2 | 27:1a:51:LYS:HB2 | 2.10 | 0.52 |
| 11:1K:101:ARG:NH1 | 11:1K:149:GLU:OE1 | 2.43 | 0.52 |
| 39:1m:57:CYS:SG | 39:1m:60:CYS:HB3 | 2.50 | 0.52 |
| 1:1A:678:A:H2' | 1:1A:679:U:C6 | 2.45 | 0.51 |
| 1:1A:1130:U:H2' | 1:1A:1131:G:H8 | 1.75 | 0.51 |
| 1:1A:2730:U:H2' | 1:1A:2731:G:C8 | 2.45 | 0.51 |
| 1:1A:1887:A:H2' | 1:1A:1888:A:C8 | 2.45 | 0.51 |
| 1:1A:1992:A:H2' | 1:1A:1993:G:C8 | 2.44 | 0.51 |
| 2:1B:141:G:H5'' | 17:1Q:60:VAL:HG11 | 1.92 | 0.51 |
| 1:1A:1856:G:H2' | 1:1A:1857:A:H8 | 1.75 | 0.51 |
| 1:1A:1956:G:OP2 | 40:1n:79:LYS:NZ | 2.35 | 0.51 |
| 31:1e:27:TYR:OH | 31:1e:87:ARG:NH1 | 2.43 | 0.51 |
| 1:1A:5:U:H2' | 1:1A:6:U:C6 | 2.46 | 0.51 |
| 1:1A:869:G:C5 | 1:1A:870:A:H1' | 2.45 | 0.51 |
| 1:1A:1752:U:H2' | 1:1A:1753:A:O4' | 2.11 | 0.51 |
| 1:1A:1809:A:C8 | 28:1b:64:MET:HG2 | 2.45 | 0.51 |
| 1:1A:255:A:N3 | 6:1F:225:ASN:ND2 | 2.55 | 0.51 |
| 1:1A:2483:C:H2' | 1:1A:2484:U:H6 | 1.75 | 0.51 |
| 1:1A:2837:U:H2' | 1:1A:2838:A:H8 | 1.75 | 0.51 |
| 1:1A:3350:U:OP2 | 1:1A:3351:U:O2' | 2.23 | 0.51 |
| 4:1D:19:ARG:NH1 | 4:1D:189:TYR:O | 2.42 | 0.51 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 1:1A:18:G:H5' | 38:1L:43:LYS:HG2 | 1.93 | 0.51 |
| 1:1A:59:A:N3 | 1:1A:74:U:O2' | 2.37 | 0.51 |
| 1:1A:546:U:N3 | 1:1A:547:A:N7 | 2.59 | 0.51 |
| 1:1A:2414:C:O2 | 24:1X:21:ASN:ND2 | 2.40 | 0.51 |
| 11:1K:13:ILE:HD11 | 11:1K:63:VAL:HG23 | 1.93 | 0.51 |
| 23:1W:49:PHE:CD2 | 23:1W:96:TYR:HD1 | 2.28 | 0.51 |
| 39:1m:51:ALA:HB3 | 39:1m:54:ILE:HD12 | 1.93 | 0.51 |
| 1:1A:575:A:H2' | 1:1A:576:A:O4' | 2.10 | 0.51 |
| 1:1A:1112:G:O2' | 1:1A:1172:G:O6 | 2.21 | 0.51 |
| 1:1A:2683:U:H5 | 1:1A:2948:G:N7 | 2.08 | 0.51 |
| 1:1A:3203:A:H4' | 5:1E:365:LYS:HD2 | 1.92 | 0.51 |
| 14:1N:49:ILE:HG22 | 14:1N:51:SER:H | 1.76 | 0.51 |
| 22:1V:52:LEU:HD12 | 22:1V:53:PRO:HD2 | 1.93 | 0.51 |
| 23:1W:55:LYS:HE2 | 23:1W:58:GLY:HA2 | 1.92 | 0.51 |
| 23:1W:63:THR:HB | 23:1W:66:ILE:HD13 | 1.93 | 0.51 |
| 1:1A:501:U:H2' | 1:1A:502:U:C6 | 2.46 | 0.51 |
| 1:1A:3285:A:C6 | 1:1A:3287:U:H1' | 2.45 | 0.51 |
| 1:1A:3462:A:H2' | 1:1A:3463:A:H8 | 1.75 | 0.51 |
| 6:1F:115:THR:HB | 6:1F:120:ARG:HD2 | 1.93 | 0.51 |
| 24:1X:87:THR:HA | 24:1X:97:TYR:HB3 | 1.92 | 0.51 |
| 1:1A:482:A:N1 | 1:1A:752:G:O2' | 2.42 | 0.51 |
| 1:1A:1325:C:H42 | 1:1A:3000:C:H5'' | 1.76 | 0.51 |
| 1:1A:1635:U:OP1 | 41:1o:42:ARG:NH2 | 2.44 | 0.51 |
| 1:1A:1888:A:N1 | 1:1A:1922:U:H5 | 2.08 | 0.51 |
| 1:1A:2079:A:H2' | 1:1A:2080:A:O4' | 2.10 | 0.51 |
| 3:1C:3:G:H22 | 3:1C:114:U:H3 | 1.58 | 0.51 |
| 1:1A:592:A:H2' | 1:1A:593:A:H8 | 1.75 | 0.51 |
| 1:1A:2841:A:O2' | 1:1A:2842:U:OP2 | 2.22 | 0.51 |
| 1:1A:3396:A:H5'' | 16:1P:121:LYS:HD3 | 1.93 | 0.51 |
| 43:1q:72:CYS:SG | 43:1q:75:CYS:N | 2.84 | 0.51 |
| 1:1A:312:A:OP2 | 37:1k:28:THR:OG1 | 2.22 | 0.50 |
| 1:1A:467:A:N1 | 1:1A:2438:C:O2' | 2.32 | 0.50 |
| 1:1A:1337:A:H2' | 1:1A:1338:U:H6 | 1.76 | 0.50 |
| 1:1A:1430:G:O6 | 1:1A:2442:C:O2' | 2.25 | 0.50 |
| 1:1A:2482:C:H2' | 1:1A:2483:C:C6 | 2.46 | 0.50 |
| 3:1C:8:U:H3 | 3:1C:109:G:H1 | 1.58 | 0.50 |
| 11:1K:100:MET:HE1 | 11:1K:167:ILE:HB | 1.92 | 0.50 |
| 22:1V:26:ASN:HB2 | 22:1V:29:THR:HG23 | 1.93 | 0.50 |
| 27:1a:54:GLU:HG3 | 27:1a:106:LYS:HB3 | 1.93 | 0.50 |
| 1:1A:1107:G:H2' | 1:1A:1108:A:C8 | 2.46 | 0.50 |
| 1:1A:1633:G:H1' | 1:1A:2044:C:H5'' | 1.92 | 0.50 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|--------------------|--------------------------|-------------------|
| 1:1A:2052:G:O2' | 38:1L:6:SER:OG | 2.29 | 0.50 |
| 1:1A:2739:U:H2' | 1:1A:2740:G:C8 | 2.46 | 0.50 |
| 1:1A:3222:U:OP1 | 21:1U:59:SER:N | 2.34 | 0.50 |
| 3:1C:85:G:N2 | 3:1C:90:G:H1 | 2.10 | 0.50 |
| 5:1E:234:ARG:HG3 | 5:1E:272:MET:HB3 | 1.93 | 0.50 |
| 8:1H:93:GLY:O | 8:1H:98:ASN:HB2 | 2.11 | 0.50 |
| 17:1Q:80:VAL:HB | 17:1Q:82:ARG:HD2 | 1.92 | 0.50 |
| 5:1E:224:LYS:HB2 | 5:1E:332:ILE:HG23 | 1.93 | 0.50 |
| 23:1W:67:GLU:HB3 | 23:1W:69:LYS:HE2 | 1.94 | 0.50 |
| 1:1A:213:A:H2' | 14:1N:127:VAL:HG21 | 1.94 | 0.50 |
| 1:1A:663:G:H5' | 16:1P:72:THR:HG23 | 1.93 | 0.50 |
| 1:1A:1157:A:H4' | 7:1G:5:LYS:H | 1.77 | 0.50 |
| 1:1A:1479:A:H4' | 1:1A:1480:U:O5' | 2.11 | 0.50 |
| 1:1A:1524:A:H5'' | 33:1g:102:SER:HB3 | 1.92 | 0.50 |
| 1:1A:1974:A:H2' | 1:1A:1975:G:C8 | 2.46 | 0.50 |
| 5:1E:386:LYS:HD3 | 5:1E:386:LYS:C | 2.36 | 0.50 |
| 29:1c:51:ASP:OD1 | 29:1c:51:ASP:N | 2.44 | 0.50 |
| 1:1A:855:A:OP1 | 30:1d:58:LYS:NZ | 2.43 | 0.50 |
| 1:1A:1752:U:H4' | 1:1A:2036:A:H4' | 1.92 | 0.50 |
| 3:1C:6:G:OP1 | 7:1G:33:ARG:NH1 | 2.44 | 0.50 |
| 1:1A:493:G:H21 | 1:1A:580:A:N6 | 2.05 | 0.50 |
| 1:1A:1310:A:N3 | 20:1T:108:SER:OG | 2.43 | 0.50 |
| 1:1A:1847:A:H2' | 1:1A:1848:A:H8 | 1.76 | 0.50 |
| 1:1A:1892:C:H2' | 1:1A:1893:A:C8 | 2.46 | 0.50 |
| 1:1A:3154:A:H2' | 1:1A:3155:U:C6 | 2.46 | 0.50 |
| 4:1D:161:ASN:OD1 | 4:1D:161:ASN:N | 2.43 | 0.50 |
| 6:1F:121:ARG:HG2 | 6:1F:276:LYS:HD3 | 1.92 | 0.50 |
| 1:1A:10:U:H2' | 1:1A:11:A:C8 | 2.47 | 0.50 |
| 1:1A:823:A:H2' | 1:1A:824:G:H2' | 1.94 | 0.50 |
| 1:1A:1200:A:H1' | 7:1G:115:MET:HE1 | 1.94 | 0.50 |
| 1:1A:2433:A:H2' | 1:1A:2434:A:C8 | 2.47 | 0.50 |
| 3:1C:81:A:C2 | 3:1C:93:G:C6 | 2.97 | 0.50 |
| 26:1Z:36:LYS:O | 26:1Z:40:MET:HG2 | 2.12 | 0.50 |
| 1:1A:802:A:H2' | 1:1A:803:U:C6 | 2.47 | 0.50 |
| 1:1A:1468:A:H2' | 1:1A:1469:A:C8 | 2.47 | 0.50 |
| 1:1A:1555:U:H2' | 1:1A:1556:G:C8 | 2.47 | 0.50 |
| 1:1A:1982:U:H2' | 4:1D:50:HIS:CD2 | 2.46 | 0.50 |
| 3:1C:9:U:OP2 | 22:1V:26:ASN:ND2 | 2.41 | 0.50 |
| 1:1A:868:A:H2' | 1:1A:869:G:C8 | 2.47 | 0.50 |
| 1:1A:2504:U:H2' | 1:1A:2505:A:H8 | 1.77 | 0.50 |
| 1:1A:3025:U:H2' | 1:1A:3026:U:C6 | 2.47 | 0.50 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 11:IK:102:VAL:HG21 | 11:IK:111:LEU:HD11 | 1.93 | 0.50 |
| 40:ln:18:ILE:O | 40:ln:22:LEU:HD12 | 2.10 | 0.50 |
| 1:IA:213:A:N6 | 14:IN:131:THR:OG1 | 2.41 | 0.49 |
| 1:IA:547:A:H2' | 1:IA:548:A:C8 | 2.47 | 0.49 |
| 1:IA:2634:A:OP1 | 4:ID:69:TYR:OH | 2.25 | 0.49 |
| 1:IA:3393:A:H2' | 1:IA:3394:A:H8 | 1.75 | 0.49 |
| 4:ID:168:ILE:HD11 | 39:lm:79:VAL:HG21 | 1.93 | 0.49 |
| 1:IA:926:A:N1 | 1:IA:2487:U:O2' | 2.38 | 0.49 |
| 12:IL:138:GLY:C | 12:IL:148:MET:HE1 | 2.37 | 0.49 |
| 28:lb:23:ALA:HA | 28:lb:45:GLY:HA2 | 1.93 | 0.49 |
| 1:IA:316:G:OP1 | 17:IQ:47:ARG:NE | 2.45 | 0.49 |
| 1:IA:466:G:O2' | 1:IA:2441:U:OP2 | 2.20 | 0.49 |
| 1:IA:1130:U:H2' | 1:IA:1131:G:C8 | 2.48 | 0.49 |
| 1:IA:1225:A:OP2 | 9:II:184:LYS:NZ | 2.45 | 0.49 |
| 14:IN:152:ILE:HA | 14:IN:155:PHE:HB2 | 1.94 | 0.49 |
| 21:IU:99:MET:HE1 | 21:IU:127:VAL:O | 2.11 | 0.49 |
| 1:IA:662:U:H2' | 1:IA:663:G:O4' | 2.11 | 0.49 |
| 1:IA:1198:U:H3 | 1:IA:1204:A:H62 | 1.59 | 0.49 |
| 1:IA:1904:U:OP2 | 21:IU:124:TYR:OH | 2.24 | 0.49 |
| 1:IA:2505:A:H2' | 1:IA:2506:U:C6 | 2.47 | 0.49 |
| 1:IA:2839:A:H5'' | 43:lq:78:LYS:HD2 | 1.93 | 0.49 |
| 1:IA:3038:C:H5'' | 42:lp:27:ARG:HH21 | 1.77 | 0.49 |
| 2:IB:80:A:O2' | 2:IB:81:A:OP1 | 2.29 | 0.49 |
| 26:IZ:61:ASN:OD1 | 26:IZ:61:ASN:N | 2.46 | 0.49 |
| 28:lb:23:ALA:HB1 | 28:lb:43:VAL:HB | 1.92 | 0.49 |
| 28:lb:27:SER:OG | 28:lb:42:THR:OG1 | 2.18 | 0.49 |
| 1:IA:443:A:H4' | 1:IA:444:A:OP1 | 2.12 | 0.49 |
| 1:IA:1631:A:O2' | 38:II:12:HIS:O | 2.29 | 0.49 |
| 1:IA:2149:U:OP1 | 21:IU:136:LYS:HE3 | 2.11 | 0.49 |
| 1:IA:2289:A:H2' | 1:IA:2290:A:C8 | 2.48 | 0.49 |
| 1:IA:2416:U:OP2 | 5:IE:239:HIS:ND1 | 2.27 | 0.49 |
| 1:IA:3084:A:H8 | 1:IA:3084:A:OP2 | 1.94 | 0.49 |
| 2:IB:2:A:H2' | 2:IB:3:U:H6 | 1.76 | 0.49 |
| 3:IC:7:A:H5'' | 22:IV:27:THR:OG1 | 2.12 | 0.49 |
| 12:IL:30:ARG:HG3 | 12:IL:63:GLU:HG3 | 1.95 | 0.49 |
| 28:lb:123:GLU:HA | 28:lb:123:GLU:OE2 | 2.12 | 0.49 |
| 1:IA:1026:G:OP1 | 17:IQ:76:ARG:NH2 | 2.45 | 0.49 |
| 1:IA:1312:A:H62 | 1:IA:1441:U:H3 | 1.60 | 0.49 |
| 1:IA:1855:G:H2' | 1:IA:1856:G:O4' | 2.12 | 0.49 |
| 1:IA:2084:G:H2' | 1:IA:2085:A:H8 | 1.77 | 0.49 |
| 1:IA:2226:G:O2' | 1:IA:2265:U:OP1 | 2.27 | 0.49 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|--------------------|--------------------------|-------------------|
| 1:1A:3103:C:H2' | 1:1A:3104:G:C8 | 2.48 | 0.49 |
| 3:1C:7:A:OP1 | 22:1V:27:THR:HG21 | 2.11 | 0.49 |
| 16:1P:41:PRO:HB3 | 16:1P:77:CYS:SG | 2.53 | 0.49 |
| 23:1W:73:LYS:HG3 | 23:1W:74:LYS:HD3 | 1.94 | 0.49 |
| 37:1k:73:THR:HB | 37:1k:76:ARG:HB2 | 1.94 | 0.49 |
| 1:1A:1090:A:H2' | 1:1A:1091:A:H8 | 1.77 | 0.49 |
| 1:1A:2499:U:H2' | 1:1A:2500:A:C8 | 2.48 | 0.49 |
| 2:1B:141:G:H2' | 2:1B:142:A:C8 | 2.47 | 0.49 |
| 3:1C:35:A:H2 | 3:1C:40:G:H22 | 1.61 | 0.49 |
| 1:1A:506:A:H2' | 1:1A:507:A:C8 | 2.48 | 0.49 |
| 1:1A:2299:A:H2' | 1:1A:2300:A:C8 | 2.48 | 0.49 |
| 1:1A:3168:A:H2' | 1:1A:3169:C:C6 | 2.48 | 0.49 |
| 3:1C:6:G:H2' | 3:1C:7:A:C8 | 2.47 | 0.49 |
| 1:1A:58:G:N2 | 1:1A:75:U:H4' | 2.28 | 0.49 |
| 1:1A:493:G:H2' | 1:1A:494:G:C4 | 2.48 | 0.49 |
| 1:1A:668:A:H2' | 1:1A:669:A:H8 | 1.77 | 0.49 |
| 1:1A:3170:A:H2' | 1:1A:3171:A:C8 | 2.48 | 0.49 |
| 1:1A:3499:U:H5'' | 32:1f:56:ALA:HB1 | 1.93 | 0.49 |
| 2:1B:116:U:H2' | 2:1B:117:A:H8 | 1.77 | 0.49 |
| 3:1C:84:G:H1 | 3:1C:91:G:N2 | 2.10 | 0.49 |
| 23:1W:105:TRP:HB2 | 23:1W:106:LEU:HD12 | 1.94 | 0.49 |
| 1:1A:239:G:H2' | 1:1A:240:A:C8 | 2.48 | 0.49 |
| 1:1A:764:U:H2' | 1:1A:765:A:H8 | 1.78 | 0.49 |
| 1:1A:1533:U:O2' | 1:1A:1534:U:OP1 | 2.30 | 0.49 |
| 1:1A:1669:G:O2' | 1:1A:1736:A:N3 | 2.42 | 0.49 |
| 1:1A:1897:A:C2 | 1:1A:1913:G:N2 | 2.74 | 0.49 |
| 1:1A:3083:A:N7 | 5:1E:2:SER:N | 2.61 | 0.49 |
| 1:1A:3344:U:C5 | 20:1T:172:LEU:HG | 2.48 | 0.49 |
| 6:1F:375:LYS:HB2 | 6:1F:390:VAL:CG1 | 2.42 | 0.49 |
| 14:1N:42:LYS:O | 14:1N:44:VAL:N | 2.45 | 0.49 |
| 1:1A:90:G:H2' | 1:1A:91:A:C8 | 2.48 | 0.48 |
| 1:1A:404:G:N2 | 1:1A:407:A:OP2 | 2.34 | 0.48 |
| 3:1C:80:G:H22 | 3:1C:94:U:H3 | 1.59 | 0.48 |
| 7:1G:75:LEU:O | 7:1G:112:LYS:NZ | 2.45 | 0.48 |
| 27:1a:2:LYS:HD3 | 27:1a:7:VAL:HG22 | 1.94 | 0.48 |
| 1:1A:897:A:H8 | 1:1A:898:U:O2' | 1.96 | 0.48 |
| 1:1A:3260:A:H2' | 1:1A:3261:A:C8 | 2.47 | 0.48 |
| 5:1E:77:THR:OG1 | 5:1E:327:GLY:O | 2.30 | 0.48 |
| 1:1A:43:C:OP1 | 14:1N:14:LYS:HD2 | 2.12 | 0.48 |
| 1:1A:525:U:H2' | 1:1A:526:A:C8 | 2.48 | 0.48 |
| 1:1A:675:A:H8 | 6:1F:354:TYR:HD2 | 1.59 | 0.48 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 1:1A:790:A:H2' | 1:1A:791:A:C8 | 2.48 | 0.48 |
| 1:1A:2780:A:H2' | 1:1A:2781:U:C6 | 2.49 | 0.48 |
| 1:1A:3440:U:O2' | 5:1E:23:HIS:O | 2.29 | 0.48 |
| 2:1B:145:U:H2' | 2:1B:146:U:C6 | 2.47 | 0.48 |
| 14:1N:247:THR:OG1 | 29:1c:98:GLU:HB3 | 2.14 | 0.48 |
| 28:1b:16:GLY:O | 34:1h:74:ARG:HG3 | 2.13 | 0.48 |
| 1:1A:97:A:H2' | 1:1A:98:A:O4' | 2.13 | 0.48 |
| 1:1A:992:U:H3' | 1:1A:993:U:H4' | 1.94 | 0.48 |
| 1:1A:2064:G:N1 | 1:1A:2067:A:OP2 | 2.46 | 0.48 |
| 4:1D:149:ARG:HG3 | 4:1D:155:LYS:HD3 | 1.96 | 0.48 |
| 16:1P:29:GLU:HG2 | 20:1T:68:VAL:HG21 | 1.95 | 0.48 |
| 37:1k:60:ASP:O | 37:1k:81:ARG:NH1 | 2.46 | 0.48 |
| 1:1A:113:U:OP2 | 17:1Q:2:GLY:N | 2.47 | 0.48 |
| 1:1A:243:G:O2' | 1:1A:264:G:N2 | 2.47 | 0.48 |
| 1:1A:764:U:H2' | 1:1A:765:A:C8 | 2.49 | 0.48 |
| 1:1A:1073:A:H62 | 1:1A:1086:G:H21 | 1.59 | 0.48 |
| 1:1A:1675:A:H2' | 1:1A:1676:A:C8 | 2.49 | 0.48 |
| 1:1A:2230:U:H2' | 1:1A:2231:C:C6 | 2.49 | 0.48 |
| 26:1Z:22:LYS:HE3 | 26:1Z:30:SER:HB2 | 1.95 | 0.48 |
| 1:1A:1201:A:H2' | 1:1A:1202:A:O4' | 2.13 | 0.48 |
| 1:1A:2129:G:C8 | 39:1m:16:THR:HG22 | 2.49 | 0.48 |
| 1:1A:2178:A:O2' | 1:1A:2179:U:H6 | 1.95 | 0.48 |
| 1:1A:2492:U:H2' | 1:1A:2493:U:C6 | 2.49 | 0.48 |
| 1:1A:2836:C:O2' | 43:1q:31:ASP:OD1 | 2.31 | 0.48 |
| 1:1A:3426:U:O4 | 5:1E:121:LYS:NZ | 2.44 | 0.48 |
| 1:1A:1431:G:OP2 | 15:1O:60:ARG:NH1 | 2.47 | 0.48 |
| 1:1A:1502:A:H3' | 1:1A:1502:A:N3 | 2.29 | 0.48 |
| 1:1A:2503:U:H2' | 1:1A:2504:U:C6 | 2.49 | 0.48 |
| 1:1A:2959:G:N7 | 1:1A:3013:C:H5' | 2.29 | 0.48 |
| 1:1A:3168:A:H2' | 1:1A:3169:C:H6 | 1.79 | 0.48 |
| 5:1E:285:TYR:HB2 | 5:1E:324:MET:HG2 | 1.95 | 0.48 |
| 28:1b:50:PRO:HG3 | 28:1b:68:VAL:HG22 | 1.96 | 0.48 |
| 1:1A:564:A:H4' | 1:1A:565:U:O5' | 2.12 | 0.48 |
| 12:1L:142:GLU:OE2 | 12:1L:142:GLU:HA | 2.13 | 0.48 |
| 14:1N:46:PRO:HA | 14:1N:229:GLN:HG3 | 1.95 | 0.48 |
| 18:1R:18:ARG:NH2 | 18:1R:147:GLU:HG2 | 2.29 | 0.48 |
| 1:1A:718:A:H2' | 1:1A:719:U:C6 | 2.49 | 0.48 |
| 1:1A:2034:G:O2' | 41:1o:3:GLY:O | 2.31 | 0.48 |
| 3:1C:54:U:H4' | 13:1M:152:HIS:HB2 | 1.96 | 0.48 |
| 6:1F:286:MET:HE1 | 19:1S:27:LEU:HD13 | 1.95 | 0.48 |
| 9:1I:207:ILE:HG13 | 9:1I:213:GLY:HA3 | 1.96 | 0.48 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 12:IL:98:ARG:HB3 | 12:IL:120:GLY:HA3 | 1.95 | 0.48 |
| 20:IT:147:MET:HE2 | 20:IT:173:CYS:SG | 2.54 | 0.48 |
| 23:IW:95:LYS:HB3 | 23:IW:95:LYS:HE2 | 1.68 | 0.48 |
| 1:IA:94:G:N7 | 14:IN:11:HIS:NE2 | 2.57 | 0.48 |
| 1:IA:494:G:H4' | 1:IA:495:A:OP1 | 2.13 | 0.48 |
| 1:IA:1219:A:H4' | 1:IA:1220:A:H5' | 1.96 | 0.48 |
| 1:IA:1745:A:H5' | 1:IA:1877:A:H1' | 1.96 | 0.48 |
| 1:IA:3148:C:H2' | 1:IA:3149:A:C8 | 2.49 | 0.48 |
| 3:IC:55:C:O2' | 13:IM:146:ASP:OD2 | 2.32 | 0.48 |
| 3:IC:60:C:H2' | 3:IC:61:A:C8 | 2.49 | 0.48 |
| 8:IH:23:THR:OG1 | 8:IH:25:ASP:OD1 | 2.21 | 0.48 |
| 20:IT:3:GLU:OE2 | 20:IT:95:ARG:NH1 | 2.47 | 0.48 |
| 41:IO:46:ARG:HD3 | 41:IO:46:ARG:HA | 1.60 | 0.48 |
| 1:IA:668:A:H2' | 1:IA:669:A:C8 | 2.48 | 0.47 |
| 1:IA:1035:G:H5' | 1:IA:1036:A:OP1 | 2.14 | 0.47 |
| 1:IA:1508:U:H2' | 1:IA:1509:A:C8 | 2.49 | 0.47 |
| 1:IA:3493:G:H4' | 5:IE:385:LYS:HD3 | 1.95 | 0.47 |
| 11:IK:147:LYS:HE3 | 11:IK:147:LYS:HB3 | 1.76 | 0.47 |
| 24:IX:48:ARG:HD2 | 24:IX:51:ARG:NH1 | 2.29 | 0.47 |
| 40:IN:56:ASP:HB3 | 40:IN:59:LYS:HG3 | 1.95 | 0.47 |
| 1:IA:216:A:N6 | 1:IA:292:G:H1 | 2.12 | 0.47 |
| 1:IA:255:A:H4' | 1:IA:257:A:N7 | 2.29 | 0.47 |
| 1:IA:724:A:O2' | 1:IA:725:A:H5'' | 2.14 | 0.47 |
| 1:IA:1738:G:C2 | 1:IA:1739:G:C8 | 3.02 | 0.47 |
| 1:IA:1869:U:H2' | 1:IA:1870:U:C6 | 2.50 | 0.47 |
| 1:IA:2844:U:H2' | 1:IA:2845:U:C6 | 2.49 | 0.47 |
| 3:IC:89:G:H4' | 12:IL:11:LEU:HD22 | 1.96 | 0.47 |
| 7:IG:167:MET:HE2 | 7:IG:167:MET:HB3 | 1.67 | 0.47 |
| 15:IO:158:GLU:O | 15:IO:162:LYS:HG2 | 2.14 | 0.47 |
| 38:IL:33:ARG:NH2 | 38:IL:41:ASP:OD2 | 2.44 | 0.47 |
| 1:IA:592:A:H2' | 1:IA:593:A:C8 | 2.48 | 0.47 |
| 1:IA:2123:A:H2' | 1:IA:2124:A:H8 | 1.78 | 0.47 |
| 6:IF:150:ILE:HG22 | 6:IF:151:PRO:HD3 | 1.96 | 0.47 |
| 7:IG:37:ILE:HD12 | 7:IG:67:SER:HB2 | 1.95 | 0.47 |
| 7:IG:223:ILE:HD12 | 7:IG:223:ILE:H | 1.78 | 0.47 |
| 1:IA:732:U:O2' | 1:IA:733:C:H6 | 1.97 | 0.47 |
| 1:IA:1856:G:H2' | 1:IA:1857:A:C8 | 2.50 | 0.47 |
| 1:IA:2432:A:H61 | 1:IA:3126:C:H5 | 1.62 | 0.47 |
| 1:IA:2838:A:H2' | 1:IA:2839:A:C8 | 2.48 | 0.47 |
| 1:IA:3362:U:H2' | 1:IA:3363:C:C6 | 2.49 | 0.47 |
| 6:IF:212:TYR:HB2 | 6:IF:216:ASP:HB2 | 1.96 | 0.47 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 6:1F:357:LYS:HA | 6:1F:360:LYS:HE3 | 1.95 | 0.47 |
| 10:1J:89:LYS:NZ | 10:1J:185:GLN:O | 2.44 | 0.47 |
| 35:li:-5:ILE:HG12 | 35:li:45:ARG:HD3 | 1.96 | 0.47 |
| 1:1A:223:A:H2' | 1:1A:224:U:C6 | 2.49 | 0.47 |
| 1:1A:858:A:O2' | 1:1A:1185:A:N7 | 2.48 | 0.47 |
| 1:1A:871:A:O2' | 1:1A:872:A:O5' | 2.29 | 0.47 |
| 1:1A:3447:A:H2' | 1:1A:3448:G:O4' | 2.14 | 0.47 |
| 1:1A:3462:A:O4' | 1:1A:3493:G:N2 | 2.44 | 0.47 |
| 24:1X:22:ASN:HB2 | 24:1X:53:PRO:HD2 | 1.97 | 0.47 |
| 27:1a:75:LYS:HB2 | 27:1a:77:VAL:HG22 | 1.95 | 0.47 |
| 31:le:36:LYS:HE3 | 31:le:36:LYS:HB3 | 1.52 | 0.47 |
| 1:1A:353:G:H2' | 1:1A:354:U:C6 | 2.49 | 0.47 |
| 1:1A:426:U:H2' | 1:1A:427:U:C6 | 2.49 | 0.47 |
| 1:1A:525:U:H2' | 1:1A:526:A:H8 | 1.79 | 0.47 |
| 1:1A:1222:U:O2' | 22:1V:136:ARG:O | 2.31 | 0.47 |
| 3:1C:2:G:H2' | 3:1C:3:G:C8 | 2.49 | 0.47 |
| 8:1H:158:LYS:HD3 | 8:1H:158:LYS:N | 2.29 | 0.47 |
| 8:1H:165:LYS:HE3 | 8:1H:165:LYS:HB3 | 1.63 | 0.47 |
| 13:1M:48:SER:N | 13:1M:66:ALA:O | 2.48 | 0.47 |
| 20:1T:147:MET:HG3 | 20:1T:150:CYS:SG | 2.55 | 0.47 |
| 31:le:57:ARG:O | 31:le:61:GLU:HG3 | 2.14 | 0.47 |
| 42:lp:8:GLU:O | 42:lp:12:ARG:HG3 | 2.14 | 0.47 |
| 1:1A:43:C:OP2 | 1:1A:44:A:O2' | 2.20 | 0.47 |
| 1:1A:557:U:OP2 | 6:1F:23:ARG:NH1 | 2.47 | 0.47 |
| 1:1A:605:C:H2' | 1:1A:606:A:C8 | 2.49 | 0.47 |
| 1:1A:619:A:O2' | 1:1A:620:U:O5' | 2.28 | 0.47 |
| 1:1A:817:A:H2' | 1:1A:818:A:C8 | 2.49 | 0.47 |
| 1:1A:1086:G:H2' | 1:1A:1087:G:H8 | 1.79 | 0.47 |
| 1:1A:1189:U:H2' | 1:1A:1190:U:C6 | 2.50 | 0.47 |
| 1:1A:1739:G:OP1 | 34:lh:37:LYS:NZ | 2.47 | 0.47 |
| 1:1A:1749:U:P | 21:1U:42:ARG:HH22 | 2.37 | 0.47 |
| 1:1A:1841:G:H22 | 1:1A:1975:G:N2 | 2.12 | 0.47 |
| 1:1A:2766:A:H2' | 1:1A:2767:A:C8 | 2.50 | 0.47 |
| 1:1A:2856:G:C8 | 1:1A:2903:A:N6 | 2.76 | 0.47 |
| 1:1A:2978:C:H2' | 1:1A:2979:C:O2 | 2.15 | 0.47 |
| 2:1B:10:U:H2' | 2:1B:11:U:C6 | 2.50 | 0.47 |
| 23:1W:63:THR:HB | 23:1W:66:ILE:HB | 1.96 | 0.47 |
| 33:lg:33:TRP:O | 33:lg:34:ARG:NH1 | 2.48 | 0.47 |
| 1:1A:405:U:OP1 | 38:ll:11:ARG:NH2 | 2.48 | 0.47 |
| 1:1A:491:G:C6 | 1:1A:582:U:C2 | 3.02 | 0.47 |
| 1:1A:685:A:O4' | 1:1A:1450:A:N6 | 2.48 | 0.47 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 1:1A:700:A:H5'' | 1:1A:745:A:N6 | 2.28 | 0.47 |
| 1:1A:892:U:H2' | 1:1A:893:U:C6 | 2.49 | 0.47 |
| 1:1A:1605:A:H2 | 1:1A:3430:U:N3 | 2.08 | 0.47 |
| 5:1E:40:LYS:HA | 5:1E:40:LYS:HD3 | 1.70 | 0.47 |
| 6:1F:47:ASN:HA | 6:1F:112:GLN:HG3 | 1.97 | 0.47 |
| 28:1b:36:ARG:HG3 | 28:1b:38:TYR:CZ | 2.50 | 0.47 |
| 1:1A:727:U:H2' | 9:1I:48:LYS:HE2 | 1.96 | 0.47 |
| 1:1A:1985:A:H2' | 1:1A:1986:A:C8 | 2.49 | 0.47 |
| 7:1G:262:THR:OG1 | 7:1G:263:SER:N | 2.47 | 0.47 |
| 11:1K:157:VAL:O | 11:1K:161:SER:OG | 2.21 | 0.47 |
| 13:1M:111:ASP:HB3 | 13:1M:112:LEU:H | 1.52 | 0.47 |
| 23:1W:48:THR:O | 23:1W:49:PHE:C | 2.58 | 0.47 |
| 1:1A:221:U:H2' | 1:1A:222:A:H8 | 1.80 | 0.47 |
| 1:1A:631:G:N1 | 1:1A:659:U:N3 | 2.36 | 0.47 |
| 1:1A:701:A:C4 | 1:1A:703:G:H1' | 2.50 | 0.47 |
| 1:1A:2637:A:H2' | 1:1A:2638:A:H8 | 1.79 | 0.47 |
| 2:1B:28:U:H2' | 2:1B:29:U:C6 | 2.50 | 0.47 |
| 5:1E:79:ILE:HD12 | 5:1E:325:ILE:HG13 | 1.97 | 0.47 |
| 7:1G:182:ALA:HB1 | 7:1G:194:ARG:HD2 | 1.97 | 0.47 |
| 14:1N:215:LYS:NZ | 14:1N:217:PHE:O | 2.46 | 0.47 |
| 1:1A:2112:C:C2 | 1:1A:2113:A:C8 | 3.03 | 0.46 |
| 1:1A:2142:G:H2' | 1:1A:2143:C:C6 | 2.50 | 0.46 |
| 1:1A:2209:U:O4 | 1:1A:2223:A:H2 | 1.98 | 0.46 |
| 1:1A:2433:A:H2' | 1:1A:2434:A:H8 | 1.80 | 0.46 |
| 1:1A:3370:A:H2' | 1:1A:3371:U:C6 | 2.50 | 0.46 |
| 1:1A:3404:A:H2' | 8:1H:95:PHE:CZ | 2.49 | 0.46 |
| 2:1B:115:A:H2' | 2:1B:116:U:C6 | 2.49 | 0.46 |
| 6:1F:112:GLN:HB3 | 17:1Q:203:TYR:CE2 | 2.51 | 0.46 |
| 10:1J:205:LYS:O | 10:1J:209:GLU:HG2 | 2.16 | 0.46 |
| 12:1L:50:VAL:HG22 | 12:1L:148:MET:HE3 | 1.97 | 0.46 |
| 14:1N:47:ALA:C | 14:1N:49:ILE:H | 2.23 | 0.46 |
| 16:1P:100:LYS:O | 16:1P:104:ARG:HG2 | 2.16 | 0.46 |
| 27:1a:2:LYS:HB3 | 27:1a:2:LYS:HE3 | 1.63 | 0.46 |
| 1:1A:187:G:H5'' | 1:1A:188:U:H3' | 1.96 | 0.46 |
| 1:1A:228:A:H2' | 1:1A:229:A:C8 | 2.49 | 0.46 |
| 1:1A:677:A:OP1 | 6:1F:351:LYS:NZ | 2.36 | 0.46 |
| 1:1A:1103:U:H2' | 1:1A:1104:A:C8 | 2.50 | 0.46 |
| 1:1A:1621:G:O2' | 1:1A:2072:U:O4 | 2.21 | 0.46 |
| 1:1A:1883:A:N6 | 1:1A:1931:U:H3 | 2.11 | 0.46 |
| 1:1A:3395:U:H2' | 1:1A:3396:A:C8 | 2.51 | 0.46 |
| 11:1K:35:LEU:HD13 | 11:1K:88:MET:HG2 | 1.97 | 0.46 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 18:IR:126:ARG:NH1 | 18:IR:140:SER:OG | 2.47 | 0.46 |
| 24:IX:32:THR:O | 24:IX:34:ALA:N | 2.48 | 0.46 |
| 1:IA:631:G:H2' | 1:IA:631:G:N3 | 2.30 | 0.46 |
| 1:IA:1189:U:H2' | 1:IA:1190:U:H6 | 1.79 | 0.46 |
| 1:IA:1270:G:O2' | 33:lg:46:LYS:O | 2.31 | 0.46 |
| 1:IA:2262:U:H2' | 1:IA:2263:G:O4' | 2.14 | 0.46 |
| 1:IA:2486:U:H5 | 1:IA:2944:A:N1 | 2.13 | 0.46 |
| 31:le:62:TYR:CE2 | 34:lh:97:GLU:HG2 | 2.50 | 0.46 |
| 1:IA:410:G:O6 | 38:ll:56:ARG:HD3 | 2.15 | 0.46 |
| 1:IA:573:A:H2' | 1:IA:574:U:C6 | 2.50 | 0.46 |
| 1:IA:735:C:H2' | 1:IA:736:G:O4' | 2.15 | 0.46 |
| 1:IA:953:U:H2' | 1:IA:954:G:O4' | 2.15 | 0.46 |
| 1:IA:1961:G:H2' | 1:IA:1962:U:O4' | 2.16 | 0.46 |
| 8:IH:72:TYR:CD2 | 8:IH:103:MET:HE1 | 2.50 | 0.46 |
| 1:IA:355:A:H2' | 1:IA:356:U:C6 | 2.50 | 0.46 |
| 1:IA:2904:U:H2' | 1:IA:2905:U:H6 | 1.80 | 0.46 |
| 1:IA:3254:U:H4' | 1:IA:3255:G:H5' | 1.97 | 0.46 |
| 1:IA:3286:A:C2 | 1:IA:3287:U:H5' | 2.51 | 0.46 |
| 2:IB:15:U:H5' | 18:IR:2:VAL:HG13 | 1.98 | 0.46 |
| 3:IC:38:A:C2 | 13:IM:70:THR:HG23 | 2.50 | 0.46 |
| 12:IL:51:HIS:ND1 | 12:IL:137:SER:OG | 2.39 | 0.46 |
| 15:IO:202:PHE:CZ | 16:IP:111:ASP:HB3 | 2.51 | 0.46 |
| 16:IP:108:THR:OG1 | 16:IP:111:ASP:OD1 | 2.32 | 0.46 |
| 32:lf:28:LYS:O | 32:lf:32:LYS:HB2 | 2.16 | 0.46 |
| 1:IA:795:G:H4' | 1:IA:796:U:H6 | 1.81 | 0.46 |
| 1:IA:798:U:C2 | 1:IA:799:A:C8 | 3.03 | 0.46 |
| 1:IA:1876:U:H2' | 1:IA:1936:A:N6 | 2.31 | 0.46 |
| 1:IA:1889:U:H2' | 1:IA:1890:U:C6 | 2.50 | 0.46 |
| 1:IA:3136:U:H2' | 1:IA:3137:C:C6 | 2.50 | 0.46 |
| 1:IA:3349:G:OP1 | 16:IP:94:THR:OG1 | 2.29 | 0.46 |
| 3:IC:21:C:H4' | 3:IC:22:C:C5 | 2.51 | 0.46 |
| 23:IW:85:CYS:SG | 23:IW:87:ARG:N | 2.86 | 0.46 |
| 32:lf:8:ASN:O | 32:lf:12:LEU:HG | 2.15 | 0.46 |
| 32:lf:82:MET:HE3 | 32:lf:115:ARG:HB2 | 1.97 | 0.46 |
| 1:IA:258:G:C8 | 6:IF:227:PRO:HG3 | 2.51 | 0.46 |
| 1:IA:474:A:H2' | 1:IA:475:A:H8 | 1.81 | 0.46 |
| 1:IA:760:A:H2' | 1:IA:761:A:C8 | 2.49 | 0.46 |
| 1:IA:836:C:H2' | 1:IA:837:A:C8 | 2.51 | 0.46 |
| 1:IA:1509:A:H2' | 1:IA:1510:A:H8 | 1.80 | 0.46 |
| 1:IA:2445:G:H2' | 1:IA:2446:G:C8 | 2.50 | 0.46 |
| 1:IA:2504:U:H2' | 1:IA:2505:A:C8 | 2.50 | 0.46 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 1:1A:2753:U:H2' | 1:1A:2754:C:C6 | 2.51 | 0.46 |
| 1:1A:3262:U:OP1 | 42:lp:39:LYS:HE2 | 2.16 | 0.46 |
| 12:1L:190:ILE:HG23 | 12:1L:197:PHE:HB2 | 1.98 | 0.46 |
| 13:1M:21:ILE:HG13 | 13:1M:125:MET:HG3 | 1.97 | 0.46 |
| 23:1W:45:LYS:NZ | 23:1W:96:TYR:OH | 2.24 | 0.46 |
| 1:1A:105:A:N1 | 1:1A:368:U:O2' | 2.43 | 0.46 |
| 1:1A:337:A:H2' | 1:1A:338:A:C8 | 2.51 | 0.46 |
| 1:1A:565:U:H2' | 1:1A:566:U:C6 | 2.50 | 0.46 |
| 1:1A:668:A:C8 | 1:1A:669:A:C8 | 3.04 | 0.46 |
| 1:1A:1764:A:H2' | 1:1A:1765:A:H8 | 1.77 | 0.46 |
| 1:1A:2427:U:H2' | 1:1A:2428:A:C8 | 2.50 | 0.46 |
| 1:1A:3311:U:H2' | 1:1A:3312:U:C6 | 2.51 | 0.46 |
| 3:1C:16:C:H2' | 3:1C:17:G:O4' | 2.15 | 0.46 |
| 4:1D:79:ALA:HB3 | 4:1D:82:LEU:HD13 | 1.98 | 0.46 |
| 6:1F:360:LYS:NZ | 6:1F:400:THR:OG1 | 2.48 | 0.46 |
| 1:1A:474:A:H2' | 1:1A:475:A:C8 | 2.51 | 0.46 |
| 1:1A:564:A:H1' | 1:1A:565:U:OP2 | 2.15 | 0.46 |
| 1:1A:1086:G:H2' | 1:1A:1087:G:C8 | 2.51 | 0.46 |
| 1:1A:1968:U:H2' | 1:1A:1969:U:C6 | 2.51 | 0.46 |
| 1:1A:2818:A:N3 | 7:1G:36:MET:HG2 | 2.31 | 0.46 |
| 1:1A:2903:A:H2' | 1:1A:2904:U:O4' | 2.16 | 0.46 |
| 2:1B:141:G:H2' | 2:1B:142:A:H8 | 1.80 | 0.46 |
| 23:1W:43:PRO:O | 23:1W:47:VAL:HG23 | 2.15 | 0.46 |
| 23:1W:48:THR:O | 23:1W:51:ARG:N | 2.49 | 0.46 |
| 32:1f:48:ARG:NH1 | 32:1f:144:THR:OG1 | 2.48 | 0.46 |
| 33:1g:91:ARG:HG3 | 33:1g:91:ARG:NH1 | 2.27 | 0.46 |
| 36:1j:48:VAL:HG22 | 36:1j:101:VAL:HG22 | 1.98 | 0.46 |
| 1:1A:1520:A:H4' | 1:1A:1521:A:O5' | 2.15 | 0.46 |
| 1:1A:3207:G:H2' | 1:1A:3208:A:C8 | 2.51 | 0.46 |
| 3:1C:1:A:H61 | 3:1C:116:C:H42 | 1.64 | 0.46 |
| 3:1C:76:U:H2' | 3:1C:77:U:O4' | 2.16 | 0.46 |
| 20:1T:78:VAL:HG22 | 20:1T:83:ILE:HG12 | 1.98 | 0.46 |
| 24:1X:10:GLN:HA | 24:1X:10:GLN:OE1 | 2.15 | 0.46 |
| 42:lp:29:PRO:HG2 | 42:lp:32:ALA:HB2 | 1.97 | 0.46 |
| 1:1A:480:U:H2' | 1:1A:481:A:O4' | 2.16 | 0.45 |
| 1:1A:2273:C:H4' | 1:1A:2274:A:O5' | 2.15 | 0.45 |
| 1:1A:3312:U:H2' | 1:1A:3313:U:H6 | 1.80 | 0.45 |
| 1:1A:3501:A:H2' | 1:1A:3502:A:H8 | 1.81 | 0.45 |
| 2:1B:15:U:C2 | 2:1B:16:U:C5 | 3.05 | 0.45 |
| 6:1F:272:MET:HE1 | 19:1S:104:LYS:HE3 | 1.99 | 0.45 |
| 16:1P:124:ALA:O | 16:1P:128:ILE:HG12 | 2.17 | 0.45 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|--------------------|--------------------------|-------------------|
| 32:lf:33:LYS:N | 32:lf:34:PRO:HD3 | 2.31 | 0.45 |
| 1:lA:489:U:H2' | 1:lA:490:A:C8 | 2.51 | 0.45 |
| 1:lA:745:A:H4' | 8:lH:50:TRP:HB2 | 1.99 | 0.45 |
| 1:lA:1741:A:N3 | 1:lA:1763:C:O2' | 2.47 | 0.45 |
| 5:lE:223:THR:HG22 | 5:lE:330:ALA:HB1 | 1.99 | 0.45 |
| 8:lH:113:THR:HG22 | 8:lH:204:PHE:HB3 | 1.98 | 0.45 |
| 1:lA:828:A:OP1 | 17:lQ:202:ARG:NH2 | 2.48 | 0.45 |
| 1:lA:1688:A:H2' | 1:lA:1689:A:C8 | 2.52 | 0.45 |
| 5:lE:137:TYR:O | 5:lE:146:ARG:NH1 | 2.49 | 0.45 |
| 1:lA:1389:U:H2' | 1:lA:1390:G:C8 | 2.52 | 0.45 |
| 1:lA:1391:U:H2' | 1:lA:1392:G:O4' | 2.17 | 0.45 |
| 1:lA:2495:A:H2' | 1:lA:2496:C:C6 | 2.51 | 0.45 |
| 1:lA:2835:C:O3' | 43:lq:37:GLY:HA3 | 2.16 | 0.45 |
| 1:lA:2847:A:H2' | 1:lA:2848:A:C8 | 2.52 | 0.45 |
| 4:lD:140:ASN:HB3 | 4:lD:145:THR:HG22 | 1.98 | 0.45 |
| 5:lE:58:ARG:NH1 | 5:lE:353:GLU:OE2 | 2.50 | 0.45 |
| 10:lJ:219:TYR:CD1 | 10:lJ:225:MET:HE1 | 2.52 | 0.45 |
| 15:lO:77:PRO:O | 15:lO:81:VAL:HG23 | 2.17 | 0.45 |
| 39:lm:92:SER:O | 39:lm:92:SER:OG | 2.34 | 0.45 |
| 1:lA:961:A:H5' | 21:lU:131:GLN:NE2 | 2.31 | 0.45 |
| 1:lA:996:C:O2' | 1:lA:999:G:O2' | 2.30 | 0.45 |
| 1:lA:1337:A:H2' | 1:lA:1338:U:C6 | 2.51 | 0.45 |
| 1:lA:1729:G:H2' | 1:lA:1730:G:C8 | 2.52 | 0.45 |
| 1:lA:1934:G:O3' | 40:ln:51:THR:HG21 | 2.16 | 0.45 |
| 1:lA:2297:G:N7 | 37:lk:61:LYS:NZ | 2.63 | 0.45 |
| 1:lA:3396:A:H2' | 1:lA:3397:C:C6 | 2.52 | 0.45 |
| 2:lB:1:A:H2' | 2:lB:2:A:H8 | 1.80 | 0.45 |
| 6:lF:162:ILE:HD11 | 6:lF:171:LEU:HD13 | 1.97 | 0.45 |
| 9:lI:70:LYS:NZ | 9:lI:178:THR:O | 2.44 | 0.45 |
| 9:lI:73:VAL:HG12 | 9:lI:127:PRO:HD3 | 1.97 | 0.45 |
| 35:li:-9:ALA:HB3 | 35:li:45:ARG:HH22 | 1.82 | 0.45 |
| 1:lA:1033:A:C2 | 4:lD:204:MET:HG2 | 2.52 | 0.45 |
| 1:lA:1078:C:O2' | 1:lA:2486:U:O4 | 2.34 | 0.45 |
| 1:lA:1183:G:H5' | 1:lA:1187:A:OP1 | 2.17 | 0.45 |
| 1:lA:3188:C:H42 | 11:lK:129:LYS:HG2 | 1.82 | 0.45 |
| 4:lD:35:PHE:CD1 | 4:lD:66:PRO:HB2 | 2.51 | 0.45 |
| 4:lD:189:TYR:CD2 | 4:lD:196:TRP:HB2 | 2.51 | 0.45 |
| 13:lM:12:ILE:HD12 | 13:lM:154:LEU:HD21 | 1.98 | 0.45 |
| 19:lS:160:LYS:HD3 | 19:lS:160:LYS:HA | 1.59 | 0.45 |
| 1:lA:327:U:O2' | 1:lA:329:G:N7 | 2.40 | 0.45 |
| 1:lA:960:G:H2' | 1:lA:961:A:C8 | 2.51 | 0.45 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 1:1A:2851:A:H2' | 1:1A:2852:G:C8 | 2.52 | 0.45 |
| 1:1A:2979:C:H5 | 1:1A:2995:C:N4 | 2.13 | 0.45 |
| 6:1F:102:PHE:O | 6:1F:103:SER:C | 2.59 | 0.45 |
| 7:1G:95:TYR:CG | 7:1G:194:ARG:HG2 | 2.52 | 0.45 |
| 18:1R:61:ARG:O | 18:1R:64:ASN:ND2 | 2.50 | 0.45 |
| 28:1b:47:GLU:HB3 | 28:1b:69:LYS:HG2 | 1.99 | 0.45 |
| 29:1c:148:THR:HA | 37:1k:2:ALA:HB3 | 1.99 | 0.45 |
| 32:1f:54:MET:HG3 | 32:1f:58:LEU:HG | 1.98 | 0.45 |
| 1:1A:34:U:H2' | 1:1A:35:A:O4' | 2.17 | 0.45 |
| 1:1A:770:C:O2 | 1:1A:2453:G:O2' | 2.26 | 0.45 |
| 1:1A:1105:U:H2' | 1:1A:1106:U:C6 | 2.52 | 0.45 |
| 1:1A:1476:G:O2' | 1:1A:1477:A:N3 | 2.45 | 0.45 |
| 1:1A:1921:A:H2' | 1:1A:1922:U:O2 | 2.17 | 0.45 |
| 1:1A:2482:C:H2' | 1:1A:2483:C:H6 | 1.81 | 0.45 |
| 1:1A:3262:U:H2' | 1:1A:3263:G:C8 | 2.52 | 0.45 |
| 3:1C:48:U:OP1 | 7:1G:221:ARG:HB2 | 2.17 | 0.45 |
| 5:1E:73:LEU:HD22 | 26:1Z:18:ALA:HB1 | 1.99 | 0.45 |
| 5:1E:387:ASP:C | 5:1E:387:ASP:OD2 | 2.59 | 0.45 |
| 6:1F:358:MET:HE3 | 6:1F:358:MET:HB3 | 1.81 | 0.45 |
| 6:1F:393:GLU:HB3 | 6:1F:396:LEU:HG | 1.99 | 0.45 |
| 12:1L:175:LYS:HD2 | 12:1L:175:LYS:HA | 1.66 | 0.45 |
| 23:1W:77:ILE:HD12 | 23:1W:78:THR:N | 2.31 | 0.45 |
| 1:1A:1844:U:H2' | 1:1A:1845:G:H8 | 1.82 | 0.45 |
| 1:1A:1876:U:H2' | 1:1A:1936:A:H61 | 1.82 | 0.45 |
| 1:1A:1989:U:H2' | 1:1A:1990:A:C8 | 2.52 | 0.45 |
| 3:1C:104:G:H2' | 3:1C:105:A:C8 | 2.51 | 0.45 |
| 4:1D:51:ASP:HB2 | 4:1D:58:LEU:HD22 | 1.99 | 0.45 |
| 5:1E:153:ILE:O | 5:1E:157:CYS:HB2 | 2.16 | 0.45 |
| 5:1E:218:ASP:OD2 | 5:1E:340:ARG:NH2 | 2.48 | 0.45 |
| 5:1E:273:GLY:O | 5:1E:275:PHE:N | 2.49 | 0.45 |
| 23:1W:44:LYS:O | 23:1W:45:LYS:HG3 | 2.17 | 0.45 |
| 39:1m:16:THR:O | 39:1m:16:THR:OG1 | 2.35 | 0.45 |
| 42:1p:17:ASP:HB3 | 42:1p:30:LEU:HD11 | 1.98 | 0.45 |
| 1:1A:223:A:H2' | 1:1A:224:U:H6 | 1.81 | 0.45 |
| 1:1A:498:A:N1 | 1:1A:575:A:N6 | 2.64 | 0.45 |
| 1:1A:551:A:H2' | 1:1A:552:G:O4' | 2.16 | 0.45 |
| 1:1A:732:U:O2' | 1:1A:733:C:O4' | 2.35 | 0.45 |
| 1:1A:1606:A:H5'' | 18:1R:53:ILE:HB | 1.98 | 0.45 |
| 1:1A:2720:U:O2' | 1:1A:2721:G:H5' | 2.17 | 0.45 |
| 1:1A:3150:A:H2' | 1:1A:3151:A:H8 | 1.82 | 0.45 |
| 5:1E:122:TRP:CZ2 | 5:1E:127:LYS:HG2 | 2.51 | 0.45 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|--------------------|--------------------------|-------------------|
| 26:lZ:40:MET:O | 26:lZ:44:ARG:HG3 | 2.17 | 0.45 |
| 1:lA:610:A:N6 | 1:lA:687:U:C4 | 2.85 | 0.44 |
| 1:lA:1882:A:H1' | 1:lA:1883:A:H2 | 1.82 | 0.44 |
| 1:lA:2632:A:C8 | 34:lh:91:ARG:HD2 | 2.52 | 0.44 |
| 1:lA:3344:U:OP1 | 11:lK:24:LYS:NZ | 2.45 | 0.44 |
| 3:lC:26:U:H2' | 3:lC:27:G:C8 | 2.52 | 0.44 |
| 7:lG:201:ALA:HB2 | 7:lG:232:LEU:HD12 | 2.00 | 0.44 |
| 14:lN:147:LYS:H | 14:lN:147:LYS:HD2 | 1.81 | 0.44 |
| 28:lb:22:LYS:NZ | 28:lb:135:THR:HG23 | 2.32 | 0.44 |
| 33:lg:50:THR:O | 33:lg:50:THR:OG1 | 2.28 | 0.44 |
| 42:lp:45:ASP:O | 42:lp:46:LEU:HD23 | 2.17 | 0.44 |
| 1:lA:548:A:H2' | 1:lA:549:U:C6 | 2.53 | 0.44 |
| 1:lA:596:G:C2 | 1:lA:597:A:C8 | 3.05 | 0.44 |
| 1:lA:713:G:H3' | 1:lA:714:U:C5' | 2.47 | 0.44 |
| 1:lA:720:U:H2' | 1:lA:721:A:C8 | 2.53 | 0.44 |
| 1:lA:2320:A:O4' | 4:lD:243:THR:HG21 | 2.18 | 0.44 |
| 1:lA:3033:C:H2' | 1:lA:3034:A:C8 | 2.52 | 0.44 |
| 1:lA:3090:G:C2 | 5:lE:252:ALA:HB1 | 2.52 | 0.44 |
| 4:lD:104:ILE:HD11 | 4:lD:113:VAL:HG21 | 2.00 | 0.44 |
| 6:lF:372:SER:HB3 | 6:lF:396:LEU:HD13 | 1.98 | 0.44 |
| 9:lI:143:LYS:HE3 | 9:lI:143:LYS:HB2 | 1.72 | 0.44 |
| 20:lT:93:VAL:HG23 | 20:lT:94:THR:HG23 | 1.99 | 0.44 |
| 1:lA:467:A:C2 | 1:lA:2439:A:H4' | 2.52 | 0.44 |
| 1:lA:542:U:H2' | 1:lA:543:A:C8 | 2.52 | 0.44 |
| 1:lA:700:A:O2' | 1:lA:701:A:OP1 | 2.31 | 0.44 |
| 1:lA:1263:U:O3' | 9:lI:85:PRO:HD3 | 2.17 | 0.44 |
| 1:lA:1392:G:H21 | 1:lA:1397:A:H62 | 1.65 | 0.44 |
| 1:lA:1534:U:H2' | 1:lA:1535:A:C8 | 2.52 | 0.44 |
| 1:lA:2633:C:H2' | 1:lA:2634:A:O4' | 2.18 | 0.44 |
| 1:lA:2903:A:O5' | 1:lA:2903:A:H8 | 1.98 | 0.44 |
| 24:lX:38:THR:HG21 | 24:lX:66:LYS:HD2 | 2.00 | 0.44 |
| 1:lA:1057:C:OP2 | 29:lc:26:ARG:NH1 | 2.51 | 0.44 |
| 1:lA:1093:G:OP1 | 19:lS:19:ARG:NH1 | 2.44 | 0.44 |
| 1:lA:1744:A:H2' | 1:lA:1745:A:H8 | 1.80 | 0.44 |
| 1:lA:2851:A:H2' | 1:lA:2852:G:H8 | 1.81 | 0.44 |
| 3:lC:84:G:N3 | 3:lC:84:G:H2' | 2.33 | 0.44 |
| 3:lC:85:G:H1 | 3:lC:90:G:H1 | 1.65 | 0.44 |
| 4:lD:93:LYS:HB3 | 4:lD:93:LYS:HE3 | 1.84 | 0.44 |
| 5:lE:53:MET:HE2 | 5:lE:53:MET:HB3 | 1.77 | 0.44 |
| 6:lF:4:ARG:HA | 6:lF:4:ARG:HD3 | 1.73 | 0.44 |
| 6:lF:157:LYS:HE2 | 27:la:145:VAL:HG12 | 2.00 | 0.44 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 28:lb:83:THR:HG22 | 34:lh:93:PHE:CZ | 2.53 | 0.44 |
| 1:1A:336:A:H5'' | 17:lQ:97:SER:HB3 | 1.98 | 0.44 |
| 1:1A:490:A:C6 | 1:1A:583:A:N6 | 2.85 | 0.44 |
| 1:1A:2303:U:H2' | 1:1A:2304:A:H8 | 1.82 | 0.44 |
| 9:II:26:GLN:OE1 | 9:II:30:LYS:NZ | 2.45 | 0.44 |
| 11:IK:35:LEU:HD23 | 11:IK:35:LEU:HA | 1.90 | 0.44 |
| 19:IS:70:MET:HE3 | 19:IS:70:MET:HB3 | 1.80 | 0.44 |
| 23:IW:68:VAL:HG22 | 23:IW:77:ILE:HG22 | 2.00 | 0.44 |
| 1:1A:630:A:C4 | 1:1A:631:G:C8 | 3.06 | 0.44 |
| 1:1A:632:G:H2' | 1:1A:633:A:N9 | 2.32 | 0.44 |
| 1:1A:2230:U:H2' | 1:1A:2231:C:H6 | 1.82 | 0.44 |
| 1:1A:2910:G:H2' | 1:1A:2911:U:O4' | 2.17 | 0.44 |
| 1:1A:3141:A:N6 | 1:1A:3151:A:OP1 | 2.46 | 0.44 |
| 1:1A:3337:A:C5 | 15:IO:115:LYS:HG2 | 2.53 | 0.44 |
| 1:1A:3432:A:O2' | 1:1A:3433:U:OP1 | 2.34 | 0.44 |
| 2:IB:23:U:O2' | 2:IB:24:U:H5' | 2.17 | 0.44 |
| 12:IL:43:CYS:O | 12:IL:171:TRP:NE1 | 2.48 | 0.44 |
| 14:IN:228:LYS:HA | 14:IN:228:LYS:HD3 | 1.90 | 0.44 |
| 19:IS:60:ILE:HD12 | 19:IS:85:THR:HG21 | 2.00 | 0.44 |
| 35:li:79:LYS:O | 35:li:83:GLN:HG2 | 2.17 | 0.44 |
| 40:ln:47:LYS:HD3 | 40:ln:48:TYR:CE2 | 2.53 | 0.44 |
| 1:1A:237:C:H2' | 1:1A:238:A:C8 | 2.52 | 0.44 |
| 1:1A:431:A:H2' | 1:1A:432:A:C8 | 2.52 | 0.44 |
| 1:1A:1667:U:O2 | 1:1A:1743:U:H5' | 2.18 | 0.44 |
| 1:1A:1841:G:N2 | 1:1A:1975:G:H1 | 2.05 | 0.44 |
| 1:1A:3314:U:O2' | 1:1A:3417:G:OP2 | 2.33 | 0.44 |
| 2:IB:29:U:H2' | 2:IB:30:U:C6 | 2.53 | 0.44 |
| 9:II:96:LEU:HD21 | 9:II:103:VAL:HG22 | 1.99 | 0.44 |
| 10:IJ:141:GLU:OE2 | 17:IQ:6:TYR:OH | 2.27 | 0.44 |
| 11:IK:133:HIS:CD2 | 11:IK:133:HIS:O | 2.71 | 0.44 |
| 21:IU:122:ASP:N | 21:IU:122:ASP:OD1 | 2.50 | 0.44 |
| 27:la:139:ALA:HA | 27:la:151:MET:SD | 2.58 | 0.44 |
| 31:le:70:GLN:HE22 | 31:le:109:GLU:H | 1.66 | 0.44 |
| 1:1A:625:A:O2' | 1:1A:626:A:OP1 | 2.35 | 0.44 |
| 1:1A:1095:A:C2 | 1:1A:1099:A:H2 | 2.34 | 0.44 |
| 1:1A:1904:U:O2' | 1:1A:1906:A:N7 | 2.41 | 0.44 |
| 1:1A:1922:U:H2' | 1:1A:1923:U:C6 | 2.52 | 0.44 |
| 1:1A:2207:A:C8 | 1:1A:2264:A:C8 | 3.06 | 0.44 |
| 1:1A:2303:U:H2' | 1:1A:2304:A:C8 | 2.52 | 0.44 |
| 2:IB:8:U:H2' | 2:IB:9:A:H8 | 1.82 | 0.44 |
| 3:IC:45:U:H2' | 3:IC:46:G:H8 | 1.83 | 0.44 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 5:IE:41:PRO:HA | 5:IE:187:GLY:HA3 | 1.99 | 0.44 |
| 8:IH:155:TYR:O | 8:IH:159:LYS:HG2 | 2.17 | 0.44 |
| 28:lb:11:VAL:HG12 | 28:lb:82:PRO:HA | 2.00 | 0.44 |
| 1:IA:219:G:H2' | 1:IA:220:A:H8 | 1.83 | 0.44 |
| 1:IA:246:U:OP1 | 27:la:59:LYS:NZ | 2.47 | 0.44 |
| 1:IA:743:G:H2' | 1:IA:744:A:C4 | 2.53 | 0.44 |
| 1:IA:765:A:H2' | 1:IA:766:U:C6 | 2.53 | 0.44 |
| 1:IA:2122:U:O2' | 1:IA:2134:A:N7 | 2.44 | 0.44 |
| 1:IA:2483:C:H2' | 1:IA:2484:U:C6 | 2.52 | 0.44 |
| 2:IB:79:A:O2' | 2:IB:80:A:OP1 | 2.29 | 0.44 |
| 14:IN:72:GLY:HA3 | 14:IN:96:ASP:HB2 | 1.99 | 0.44 |
| 16:IP:92:THR:O | 16:IP:96:LYS:HG3 | 2.18 | 0.44 |
| 1:IA:13:C:P | 25:IY:27:ARG:HH22 | 2.41 | 0.43 |
| 1:IA:62:A:N6 | 1:IA:72:G:H1' | 2.33 | 0.43 |
| 1:IA:908:A:H2' | 1:IA:909:A:C8 | 2.53 | 0.43 |
| 1:IA:1485:A:H2' | 1:IA:1486:C:O4' | 2.18 | 0.43 |
| 1:IA:1592:U:H2' | 1:IA:1593:A:H8 | 1.82 | 0.43 |
| 1:IA:3163:G:O2' | 5:IE:14:LEU:O | 2.31 | 0.43 |
| 1:IA:3169:C:H2' | 1:IA:3170:A:H8 | 1.83 | 0.43 |
| 3:IC:45:U:H2' | 3:IC:46:G:C8 | 2.53 | 0.43 |
| 7:IG:118:GLN:HB2 | 7:IG:137:VAL:HG11 | 1.99 | 0.43 |
| 21:IU:5:LYS:HB3 | 21:IU:5:LYS:HE3 | 1.71 | 0.43 |
| 23:IW:45:LYS:HZ2 | 23:IW:46:LEU:H | 1.66 | 0.43 |
| 29:lc:97:GLU:OE1 | 29:lc:97:GLU:N | 2.40 | 0.43 |
| 31:le:64:ALA:O | 31:le:68:LYS:N | 2.51 | 0.43 |
| 1:IA:426:U:H2' | 1:IA:427:U:H6 | 1.82 | 0.43 |
| 1:IA:909:A:H2' | 1:IA:910:A:H8 | 1.82 | 0.43 |
| 1:IA:2744:A:C2 | 13:IM:124:GLY:HA3 | 2.53 | 0.43 |
| 1:IA:3149:A:H2' | 1:IA:3150:A:C8 | 2.53 | 0.43 |
| 1:IA:3501:A:H2' | 1:IA:3502:A:C8 | 2.52 | 0.43 |
| 7:IG:127:LYS:HB2 | 7:IG:127:LYS:HE3 | 1.75 | 0.43 |
| 12:IL:52:ILE:HD12 | 12:IL:136:ILE:HB | 2.00 | 0.43 |
| 23:IW:49:PHE:CE2 | 23:IW:96:TYR:HD1 | 2.35 | 0.43 |
| 34:lh:80:LYS:HB3 | 34:lh:85:VAL:HG23 | 2.00 | 0.43 |
| 1:IA:797:C:C2 | 1:IA:798:U:C5 | 3.06 | 0.43 |
| 3:IC:5:A:H61 | 3:IC:112:C:H42 | 1.65 | 0.43 |
| 6:IF:354:TYR:HD1 | 6:IF:354:TYR:O | 2.01 | 0.43 |
| 14:IN:60:ASN:OD1 | 29:lc:66:ASN:HB3 | 2.19 | 0.43 |
| 1:IA:399:G:O6 | 38:ll:55:ARG:NH2 | 2.44 | 0.43 |
| 1:IA:496:A:H2' | 1:IA:497:U:O4' | 2.18 | 0.43 |
| 1:IA:606:A:H2' | 1:IA:607:U:C6 | 2.54 | 0.43 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 1:1A:996:C:HO2' | 1:1A:999:G:HO2' | 1.64 | 0.43 |
| 1:1A:1207:C:H2' | 1:1A:1208:U:O4' | 2.18 | 0.43 |
| 1:1A:2639:A:H2' | 1:1A:2640:A:C8 | 2.53 | 0.43 |
| 1:1A:3262:U:H2' | 1:1A:3263:G:H8 | 1.83 | 0.43 |
| 1:1A:3455:G:N2 | 1:1A:3501:A:H2 | 2.07 | 0.43 |
| 11:1K:97:GLN:HE21 | 11:1K:99:LYS:HD2 | 1.83 | 0.43 |
| 13:1M:91:LEU:HD23 | 13:1M:91:LEU:HA | 1.84 | 0.43 |
| 16:1P:103:LEU:HD12 | 16:1P:103:LEU:HA | 1.82 | 0.43 |
| 21:1U:105:LEU:HD13 | 21:1U:135:LYS:HE2 | 2.01 | 0.43 |
| 26:1Z:14:LYS:HE2 | 26:1Z:14:LYS:HB2 | 1.78 | 0.43 |
| 27:1a:87:LYS:N | 27:1a:91:GLN:O | 2.39 | 0.43 |
| 32:1f:54:MET:HE1 | 32:1f:74:ILE:HG13 | 2.00 | 0.43 |
| 34:1h:69:LYS:HE3 | 34:1h:69:LYS:HB3 | 1.83 | 0.43 |
| 1:1A:582:U:H2' | 1:1A:583:A:C8 | 2.54 | 0.43 |
| 1:1A:619:A:H2' | 1:1A:619:A:N3 | 2.33 | 0.43 |
| 1:1A:632:G:C2 | 1:1A:657:A:C2 | 3.06 | 0.43 |
| 1:1A:703:G:C8 | 1:1A:704:C:C6 | 3.07 | 0.43 |
| 1:1A:790:A:H2' | 1:1A:791:A:H8 | 1.82 | 0.43 |
| 1:1A:1495:A:H2' | 1:1A:1496:A:H8 | 1.83 | 0.43 |
| 1:1A:1592:U:H2' | 1:1A:1593:A:C8 | 2.54 | 0.43 |
| 1:1A:2254:A:H5'' | 4:1D:132:ASN:OD1 | 2.18 | 0.43 |
| 1:1A:3142:G:N3 | 1:1A:3143:A:N6 | 2.65 | 0.43 |
| 3:1C:35:A:O5' | 3:1C:35:A:H8 | 2.02 | 0.43 |
| 6:1F:91:ALA:O | 6:1F:93:GLY:N | 2.52 | 0.43 |
| 7:1G:147:LEU:HD22 | 7:1G:164:LEU:HD13 | 2.00 | 0.43 |
| 10:1J:37:THR:HG22 | 10:1J:38:ARG:N | 2.32 | 0.43 |
| 12:1L:191:ILE:HD11 | 12:1L:200:ALA:HB2 | 1.99 | 0.43 |
| 19:1S:141:ASN:HA | 19:1S:146:LEU:HD12 | 1.99 | 0.43 |
| 32:1f:121:GLU:N | 32:1f:121:GLU:OE1 | 2.51 | 0.43 |
| 1:1A:333:U:O2' | 17:1Q:180:ARG:O | 2.34 | 0.43 |
| 1:1A:491:G:C5 | 1:1A:492:U:C4 | 3.06 | 0.43 |
| 1:1A:529:U:H2' | 1:1A:530:A:H8 | 1.84 | 0.43 |
| 1:1A:1030:C:OP1 | 4:1D:14:SER:OG | 2.36 | 0.43 |
| 1:1A:2815:G:N2 | 1:1A:2818:A:OP2 | 2.39 | 0.43 |
| 1:1A:2958:G:N2 | 1:1A:2961:U:O2 | 2.48 | 0.43 |
| 1:1A:3291:G:C5 | 1:1A:3292:U:C5 | 3.07 | 0.43 |
| 1:1A:3311:U:H2' | 1:1A:3312:U:H6 | 1.84 | 0.43 |
| 16:1P:108:THR:N | 16:1P:111:ASP:OD1 | 2.44 | 0.43 |
| 25:1Y:85:LYS:HD2 | 25:1Y:85:LYS:HA | 1.71 | 0.43 |
| 1:1A:2835:C:H2' | 1:1A:2836:C:H6 | 1.83 | 0.43 |
| 1:1A:2848:A:H2' | 1:1A:2849:U:C6 | 2.54 | 0.43 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|--------------------|--------------------------|-------------------|
| 1:1A:2979:C:H2' | 1:1A:2980:A:O4' | 2.19 | 0.43 |
| 1:1A:3303:A:H2' | 1:1A:3304:C:C6 | 2.53 | 0.43 |
| 1:1A:3346:U:C2 | 1:1A:3347:A:C8 | 3.06 | 0.43 |
| 3:1C:85:G:H22 | 3:1C:90:G:N2 | 2.17 | 0.43 |
| 3:1C:114:U:H2' | 3:1C:115:A:N3 | 2.34 | 0.43 |
| 6:1F:424:LYS:NZ | 9:1I:58:GLU:OE1 | 2.52 | 0.43 |
| 41:1o:29:MET:HE2 | 41:1o:29:MET:HB2 | 1.87 | 0.43 |
| 1:1A:360:U:H2' | 1:1A:361:C:H6 | 1.84 | 0.43 |
| 1:1A:1058:U:O2' | 1:1A:2478:A:N1 | 2.48 | 0.43 |
| 1:1A:1187:A:N6 | 1:1A:1217:U:H3 | 2.13 | 0.43 |
| 1:1A:2721:G:N1 | 1:1A:2941:C:H5 | 2.09 | 0.43 |
| 1:1A:2744:A:H1' | 13:1M:107:GLU:OE2 | 2.18 | 0.43 |
| 1:1A:3312:U:H2' | 1:1A:3313:U:C6 | 2.54 | 0.43 |
| 1:1A:3328:G:H2' | 1:1A:3329:U:O4' | 2.19 | 0.43 |
| 1:1A:3332:A:H2' | 1:1A:3333:A:C8 | 2.53 | 0.43 |
| 1:1A:3370:A:H2' | 1:1A:3371:U:H6 | 1.84 | 0.43 |
| 1:1A:3452:U:H3 | 1:1A:3504:G:H1 | 1.66 | 0.43 |
| 4:1D:17:LYS:HE3 | 4:1D:17:LYS:HB2 | 1.73 | 0.43 |
| 7:1G:110:LEU:HD22 | 7:1G:115:MET:HG3 | 2.01 | 0.43 |
| 16:1P:133:LYS:HD2 | 16:1P:133:LYS:O | 2.18 | 0.43 |
| 23:1W:50:PHE:O | 23:1W:54:ILE:HD12 | 2.19 | 0.43 |
| 37:1k:10:LYS:HB3 | 37:1k:10:LYS:HE2 | 1.87 | 0.43 |
| 1:1A:324:A:H2' | 1:1A:325:U:C6 | 2.53 | 0.43 |
| 1:1A:498:A:H2' | 1:1A:499:U:C6 | 2.53 | 0.43 |
| 1:1A:739:A:H2' | 1:1A:740:A:C8 | 2.53 | 0.43 |
| 1:1A:836:C:H2' | 1:1A:837:A:H8 | 1.84 | 0.43 |
| 1:1A:2432:A:H2 | 18:1R:131:ARG:HH22 | 1.66 | 0.43 |
| 1:1A:2937:G:O2' | 1:1A:2938:U:OP2 | 2.33 | 0.43 |
| 1:1A:3130:A:O2' | 5:1E:261:ARG:HB3 | 2.19 | 0.43 |
| 1:1A:3195:G:H2' | 1:1A:3196:U:C6 | 2.53 | 0.43 |
| 1:1A:3292:U:N3 | 1:1A:3293:C:C5 | 2.87 | 0.43 |
| 1:1A:3392:G:H2' | 1:1A:3393:A:H8 | 1.83 | 0.43 |
| 3:1C:46:G:N3 | 7:1G:218:GLN:NE2 | 2.66 | 0.43 |
| 4:1D:61:VAL:HG11 | 4:1D:88:ILE:HD11 | 2.01 | 0.43 |
| 4:1D:246:ILE:HD12 | 4:1D:246:ILE:H | 1.84 | 0.43 |
| 6:1F:51:PRO:HA | 6:1F:111:TRP:CE2 | 2.54 | 0.43 |
| 6:1F:286:MET:HE1 | 19:1S:27:LEU:HB3 | 2.00 | 0.43 |
| 7:1G:111:GLN:HE21 | 7:1G:111:GLN:HB2 | 1.62 | 0.43 |
| 11:1K:54:LYS:HB3 | 11:1K:57:GLY:H | 1.84 | 0.43 |
| 36:1j:43:TYR:HA | 36:1j:46:LYS:HG3 | 2.01 | 0.43 |
| 1:1A:332:G:C6 | 43:1q:43:ARG:HD3 | 2.53 | 0.43 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|--------------------|--------------------------|-------------------|
| 1:lA:359:A:H2' | 1:lA:360:U:C6 | 2.54 | 0.43 |
| 1:lA:632:G:H2' | 1:lA:633:A:C4 | 2.53 | 0.43 |
| 1:lA:851:A:H5'' | 29:lc:114:GLY:O | 2.19 | 0.43 |
| 1:lA:948:C:O2' | 1:lA:949:G:N7 | 2.51 | 0.43 |
| 1:lA:1194:A:O2' | 1:lA:1195:G:H5' | 2.19 | 0.43 |
| 1:lA:2239:U:O2' | 4:lD:11:GLY:HA3 | 2.19 | 0.43 |
| 1:lA:2240:C:OP1 | 4:lD:8:GLN:NE2 | 2.41 | 0.43 |
| 4:lD:104:ILE:N | 4:lD:162:CYS:O | 2.44 | 0.43 |
| 5:lE:143:LYS:HE2 | 5:lE:143:LYS:HB2 | 1.73 | 0.43 |
| 13:lM:133:ARG:HG2 | 13:lM:134:PRO:HD2 | 2.00 | 0.43 |
| 32:lf:44:ALA:O | 32:lf:115:ARG:NH1 | 2.52 | 0.43 |
| 42:lp:35:CYS:O | 42:lp:42:HIS:HA | 2.19 | 0.43 |
| 1:lA:531:U:H2' | 1:lA:532:A:C8 | 2.54 | 0.42 |
| 1:lA:531:U:H2' | 1:lA:532:A:H8 | 1.83 | 0.42 |
| 1:lA:705:U:C2 | 1:lA:706:A:C8 | 3.07 | 0.42 |
| 1:lA:940:U:H2' | 1:lA:941:A:C8 | 2.54 | 0.42 |
| 1:lA:1569:A:H5'' | 1:lA:1570:U:O5' | 2.19 | 0.42 |
| 1:lA:2731:G:H2' | 1:lA:2732:A:H8 | 1.84 | 0.42 |
| 1:lA:2773:U:OP2 | 7:lG:23:ARG:NE | 2.48 | 0.42 |
| 1:lA:3226:C:H2' | 1:lA:3227:A:O4' | 2.19 | 0.42 |
| 2:lB:54:A:H5' | 41:lo:21:ARG:HD3 | 2.00 | 0.42 |
| 6:lF:423:LYS:HE2 | 6:lF:423:LYS:HB3 | 1.80 | 0.42 |
| 11:lK:136:MET:HE1 | 11:lK:167:ILE:HD11 | 1.99 | 0.42 |
| 14:lN:151:GLU:O | 14:lN:155:PHE:N | 2.50 | 0.42 |
| 31:le:8:LYS:HA | 31:le:8:LYS:HD2 | 1.73 | 0.42 |
| 42:lp:24:CYS:HA | 42:lp:40:CYS:HB3 | 2.00 | 0.42 |
| 1:lA:1909:C:H2' | 1:lA:1910:A:C8 | 2.53 | 0.42 |
| 1:lA:3421:A:H2' | 1:lA:3422:A:C8 | 2.55 | 0.42 |
| 1:lA:3432:A:N6 | 1:lA:3434:A:N3 | 2.67 | 0.42 |
| 3:lC:62:U:O2' | 12:lL:203:LYS:HA | 2.20 | 0.42 |
| 8:lH:150:PHE:O | 8:lH:154:GLN:HG2 | 2.19 | 0.42 |
| 13:lM:63:ASP:N | 13:lM:63:ASP:OD1 | 2.49 | 0.42 |
| 20:IT:3:GLU:HG2 | 20:IT:60:ILE:HD12 | 2.01 | 0.42 |
| 40:ln:30:VAL:HG11 | 40:ln:67:ILE:HD13 | 2.01 | 0.42 |
| 1:lA:979:G:H1' | 1:lA:1015:A:OP1 | 2.19 | 0.42 |
| 1:lA:1131:G:H2' | 1:lA:1132:U:C6 | 2.54 | 0.42 |
| 1:lA:1271:C:H4' | 1:lA:1456:U:C4 | 2.53 | 0.42 |
| 1:lA:1440:A:OP2 | 15:lO:134:ARG:HD3 | 2.19 | 0.42 |
| 1:lA:1527:A:O2' | 1:lA:1551:A:N1 | 2.40 | 0.42 |
| 1:lA:3104:G:H2' | 1:lA:3105:U:C6 | 2.54 | 0.42 |
| 3:lC:53:C:O2' | 13:lM:152:HIS:ND1 | 2.47 | 0.42 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|--------------------|--------------------------|-------------------|
| 6:1F:19:LYS:HD3 | 6:1F:19:LYS:HA | 1.73 | 0.42 |
| 23:1W:49:PHE:CD2 | 23:1W:96:TYR:CD1 | 3.08 | 0.42 |
| 24:1X:16:VAL:HG21 | 24:1X:124:GLU:HG2 | 2.01 | 0.42 |
| 27:1a:56:LYS:HD2 | 27:1a:65:ALA:HB2 | 2.01 | 0.42 |
| 32:1f:137:PHE:HA | 32:1f:140:LEU:HD12 | 2.01 | 0.42 |
| 1:1A:487:A:H2' | 1:1A:488:A:C8 | 2.54 | 0.42 |
| 1:1A:613:G:O2' | 1:1A:615:G:OP2 | 2.33 | 0.42 |
| 1:1A:683:A:H2' | 1:1A:684:U:O4' | 2.18 | 0.42 |
| 1:1A:733:C:H3' | 1:1A:734:C:H5'' | 2.01 | 0.42 |
| 1:1A:1689:A:C5 | 1:1A:1690:A:H1' | 2.55 | 0.42 |
| 1:1A:2731:G:H2' | 1:1A:2732:A:C8 | 2.54 | 0.42 |
| 3:1C:42:U:C2 | 3:1C:43:A:C8 | 3.07 | 0.42 |
| 11:1K:129:LYS:HA | 11:1K:129:LYS:HD2 | 1.80 | 0.42 |
| 21:1U:28:GLU:N | 21:1U:28:GLU:OE2 | 2.52 | 0.42 |
| 31:1e:13:GLY:O | 31:1e:17:LYS:HG3 | 2.20 | 0.42 |
| 1:1A:846:A:H2' | 1:1A:847:A:C8 | 2.54 | 0.42 |
| 1:1A:974:U:O4 | 39:1m:4:ARG:NH1 | 2.52 | 0.42 |
| 1:1A:1176:A:OP1 | 9:1I:86:LYS:NZ | 2.48 | 0.42 |
| 1:1A:1314:A:H2 | 15:1O:135:LYS:H | 1.67 | 0.42 |
| 1:1A:2348:G:OP2 | 1:1A:2348:G:N2 | 2.34 | 0.42 |
| 1:1A:2634:A:O2' | 10:1J:30:VAL:HG13 | 2.19 | 0.42 |
| 1:1A:2835:C:H2' | 1:1A:2836:C:C6 | 2.55 | 0.42 |
| 1:1A:3265:C:H2' | 1:1A:3266:U:C6 | 2.54 | 0.42 |
| 3:1C:103:U:H2' | 3:1C:104:G:H8 | 1.82 | 0.42 |
| 7:1G:115:MET:H | 7:1G:115:MET:HG2 | 1.71 | 0.42 |
| 8:1H:171:GLU:OE2 | 8:1H:172:SER:N | 2.52 | 0.42 |
| 8:1H:198:HIS:HB3 | 8:1H:200:HIS:CE1 | 2.54 | 0.42 |
| 10:1J:27:LYS:HG2 | 10:1J:32:HIS:HB2 | 2.00 | 0.42 |
| 10:1J:224:HIS:HA | 10:1J:227:ARG:HG2 | 2.02 | 0.42 |
| 13:1M:151:ASP:N | 13:1M:151:ASP:OD1 | 2.51 | 0.42 |
| 23:1W:30:CYS:H | 23:1W:77:ILE:HD11 | 1.84 | 0.42 |
| 24:1X:69:LYS:HA | 24:1X:69:LYS:HD2 | 1.82 | 0.42 |
| 24:1X:100:ASP:OD1 | 26:1Z:26:LEU:HD21 | 2.19 | 0.42 |
| 1:1A:505:A:H2' | 1:1A:506:A:H8 | 1.84 | 0.42 |
| 1:1A:795:G:H4' | 1:1A:796:U:C6 | 2.54 | 0.42 |
| 1:1A:798:U:H2' | 1:1A:799:A:H8 | 1.84 | 0.42 |
| 1:1A:1187:A:H2' | 1:1A:1188:A:O4' | 2.19 | 0.42 |
| 1:1A:1539:U:C4 | 33:1g:56:ILE:HD12 | 2.53 | 0.42 |
| 1:1A:2098:A:H61 | 1:1A:2415:C:H42 | 1.67 | 0.42 |
| 3:1C:17:G:H1 | 3:1C:59:G:N2 | 2.16 | 0.42 |
| 7:1G:30:TYR:O | 7:1G:34:ARG:HG3 | 2.19 | 0.42 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|-------------------|--------------------------|-------------------|
| 8:IH:93:GLY:O | 8:IH:94:PRO:C | 2.62 | 0.42 |
| 14:IN:49:ILE:C | 14:IN:51:SER:H | 2.26 | 0.42 |
| 20:IT:41:LEU:HB3 | 20:IT:47:VAL:HB | 2.01 | 0.42 |
| 31:le:53:PRO:HB2 | 31:le:56:GLU:OE1 | 2.20 | 0.42 |
| 1:lA:37:G:N2 | 1:lA:2946:A:H62 | 2.18 | 0.42 |
| 1:lA:631:G:O6 | 1:lA:659:U:O4 | 2.37 | 0.42 |
| 1:lA:703:G:H3' | 1:lA:704:C:H6 | 1.85 | 0.42 |
| 1:lA:713:G:H3' | 1:lA:714:U:H5' | 2.02 | 0.42 |
| 1:lA:1346:G:HO2' | 1:lA:1347:A:P | 2.42 | 0.42 |
| 1:lA:1508:U:H2' | 1:lA:1509:A:H8 | 1.85 | 0.42 |
| 1:lA:2224:U:H2' | 1:lA:2225:A:C8 | 2.54 | 0.42 |
| 1:lA:2488:G:H2' | 1:lA:2489:A:C8 | 2.54 | 0.42 |
| 1:lA:2701:U:H2' | 1:lA:2702:G:H8 | 1.83 | 0.42 |
| 1:lA:2747:G:N3 | 1:lA:2747:G:H2' | 2.35 | 0.42 |
| 1:lA:3369:U:H2' | 1:lA:3370:A:C8 | 2.55 | 0.42 |
| 2:IB:117:A:H2' | 2:IB:118:C:C6 | 2.55 | 0.42 |
| 8:IH:31:LYS:HA | 8:IH:31:LYS:HD2 | 1.88 | 0.42 |
| 29:lc:8:THR:HG23 | 29:lc:9:ARG:HD2 | 2.02 | 0.42 |
| 40:ln:23:LYS:HA | 40:ln:23:LYS:HD3 | 1.72 | 0.42 |
| 43:lq:2:VAL:O | 43:lq:90:GLU:N | 2.50 | 0.42 |
| 43:lq:30:LYS:HB3 | 43:lq:30:LYS:HE3 | 1.75 | 0.42 |
| 1:lA:663:G:OP1 | 16:IP:71:MET:HA | 2.20 | 0.42 |
| 1:lA:775:C:OP1 | 29:lc:21:ARG:HB3 | 2.20 | 0.42 |
| 1:lA:937:C:O2' | 1:lA:2214:A:N1 | 2.44 | 0.42 |
| 1:lA:2084:G:H2' | 1:lA:2085:A:C8 | 2.55 | 0.42 |
| 1:lA:2144:U:OP2 | 21:IU:74:ARG:NE | 2.39 | 0.42 |
| 1:lA:2388:A:H2' | 1:lA:2391:G:H21 | 1.85 | 0.42 |
| 1:lA:2459:U:H5' | 15:IO:72:PHE:CE2 | 2.54 | 0.42 |
| 5:IE:238:ARG:HE | 5:IE:238:ARG:HB2 | 1.55 | 0.42 |
| 11:IK:4:LEU:HD12 | 11:IK:4:LEU:HA | 1.80 | 0.42 |
| 13:IM:117:ASP:OD1 | 13:IM:117:ASP:N | 2.49 | 0.42 |
| 21:IU:74:ARG:HD3 | 21:IU:74:ARG:HA | 1.87 | 0.42 |
| 22:IV:120:ILE:HD12 | 22:IV:121:GLN:N | 2.34 | 0.42 |
| 23:IW:44:LYS:O | 23:IW:45:LYS:HE3 | 2.20 | 0.42 |
| 25:IY:87:ILE:HD11 | 25:IY:104:ARG:HD3 | 2.01 | 0.42 |
| 40:ln:18:ILE:HG23 | 40:ln:19:LEU:HD22 | 2.02 | 0.42 |
| 1:lA:445:G:H5'' | 1:lA:448:C:H1' | 2.01 | 0.42 |
| 1:lA:2443:A:H2' | 1:lA:2444:A:C8 | 2.54 | 0.42 |
| 1:lA:2489:A:H2' | 1:lA:2490:G:C8 | 2.54 | 0.42 |
| 1:lA:2939:G:N7 | 43:lq:61:LYS:NZ | 2.67 | 0.42 |
| 1:lA:3101:A:H2' | 1:lA:3102:C:H6 | 1.84 | 0.42 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 2:1B:2:A:H2' | 2:1B:3:U:C6 | 2.54 | 0.42 |
| 2:1B:68:A:H2' | 2:1B:69:U:C6 | 2.54 | 0.42 |
| 8:1H:144:LYS:HB3 | 8:1H:144:LYS:HE3 | 1.68 | 0.42 |
| 15:1O:17:LEU:HD13 | 15:1O:139:LEU:HD11 | 2.01 | 0.42 |
| 22:1V:120:ILE:HD12 | 22:1V:120:ILE:C | 2.45 | 0.42 |
| 31:1e:53:PRO:HA | 31:1e:54:PRO:HD3 | 1.93 | 0.42 |
| 32:1f:16:GLU:OE2 | 32:1f:16:GLU:C | 2.63 | 0.42 |
| 37:1k:62:LYS:HA | 37:1k:62:LYS:HD2 | 1.63 | 0.42 |
| 1:1A:639:G:H22 | 1:1A:650:A:H2 | 1.67 | 0.42 |
| 1:1A:723:U:O2' | 1:1A:724:A:N3 | 2.44 | 0.42 |
| 1:1A:2142:G:H2' | 1:1A:2143:C:H6 | 1.85 | 0.42 |
| 1:1A:2508:A:H5'' | 1:1A:2509:U:OP2 | 2.20 | 0.42 |
| 1:1A:2661:U:H2' | 1:1A:2662:G:O4' | 2.20 | 0.42 |
| 1:1A:3432:A:HO2' | 1:1A:3433:U:P | 2.42 | 0.42 |
| 3:1C:6:G:N1 | 3:1C:111:A:H2 | 2.12 | 0.42 |
| 3:1C:106:U:H5'' | 7:1G:268:LEU:HD21 | 2.02 | 0.42 |
| 5:1E:54:THR:OG1 | 5:1E:55:HIS:N | 2.53 | 0.42 |
| 6:1F:150:ILE:HD12 | 6:1F:150:ILE:HA | 1.71 | 0.42 |
| 6:1F:188:LYS:HG3 | 6:1F:204:GLU:HG2 | 2.02 | 0.42 |
| 10:1J:30:VAL:HG12 | 10:1J:31:ALA:N | 2.35 | 0.42 |
| 10:1J:86:ASP:OD1 | 10:1J:87:HIS:N | 2.53 | 0.42 |
| 15:1O:101:LYS:HB3 | 15:1O:101:LYS:HE2 | 1.76 | 0.42 |
| 16:1P:12:VAL:HG22 | 16:1P:26:VAL:HG22 | 2.01 | 0.42 |
| 21:1U:8:LYS:NZ | 21:1U:19:ASN:O | 2.52 | 0.42 |
| 24:1X:18:CYS:CB | 24:1X:54:ARG:HB3 | 2.50 | 0.42 |
| 1:1A:221:U:C2 | 1:1A:222:A:C8 | 3.08 | 0.41 |
| 1:1A:493:G:H1' | 1:1A:579:A:N6 | 2.34 | 0.41 |
| 1:1A:1342:U:N3 | 1:1A:1343:A:H1' | 2.35 | 0.41 |
| 1:1A:1606:A:C8 | 18:1R:53:ILE:HG22 | 2.55 | 0.41 |
| 1:1A:2682:U:H2' | 1:1A:2683:U:O4' | 2.20 | 0.41 |
| 3:1C:19:U:H2' | 3:1C:20:C:C6 | 2.55 | 0.41 |
| 4:1D:54:ARG:HD3 | 4:1D:58:LEU:HD13 | 2.02 | 0.41 |
| 5:1E:92:TYR:HB2 | 5:1E:159:VAL:HB | 2.02 | 0.41 |
| 6:1F:142:HIS:ND1 | 6:1F:180:ASP:OD2 | 2.44 | 0.41 |
| 6:1F:211:VAL:HA | 6:1F:232:CYS:O | 2.20 | 0.41 |
| 7:1G:124:ASP:OD1 | 7:1G:124:ASP:N | 2.47 | 0.41 |
| 9:1I:97:ARG:NH1 | 19:1S:4:ASP:O | 2.53 | 0.41 |
| 11:1K:19:ILE:HG12 | 11:1K:28:VAL:HG22 | 2.02 | 0.41 |
| 25:1Y:117:LYS:HB3 | 25:1Y:117:LYS:HE3 | 1.91 | 0.41 |
| 1:1A:248:U:H2' | 1:1A:249:U:C6 | 2.56 | 0.41 |
| 1:1A:491:G:C6 | 1:1A:492:U:C4 | 3.07 | 0.41 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 1:1A:566:U:H2' | 1:1A:567:U:C6 | 2.55 | 0.41 |
| 1:1A:658:A:H1' | 1:1A:659:U:C6 | 2.55 | 0.41 |
| 1:1A:675:A:H8 | 6:1F:354:TYR:CD2 | 2.37 | 0.41 |
| 1:1A:1219:A:H4' | 1:1A:1220:A:OP2 | 2.20 | 0.41 |
| 1:1A:1547:A:H2' | 1:1A:1548:U:C6 | 2.55 | 0.41 |
| 1:1A:1757:C:H2' | 1:1A:1758:U:C6 | 2.55 | 0.41 |
| 1:1A:2924:A:OP1 | 14:1N:274:SER:HB3 | 2.20 | 0.41 |
| 1:1A:3129:U:H2' | 1:1A:3130:A:C8 | 2.53 | 0.41 |
| 4:1D:30:ARG:NH2 | 4:1D:33:ASP:OD1 | 2.52 | 0.41 |
| 5:1E:301:ILE:H | 5:1E:301:ILE:HG13 | 1.71 | 0.41 |
| 6:1F:261:LYS:HG2 | 6:1F:265:ILE:HG13 | 2.01 | 0.41 |
| 16:1P:24:LEU:HD23 | 16:1P:24:LEU:HA | 1.82 | 0.41 |
| 18:1R:52:ILE:O | 18:1R:54:LYS:NZ | 2.52 | 0.41 |
| 23:1W:54:ILE:HD12 | 23:1W:54:ILE:H | 1.86 | 0.41 |
| 24:1X:87:THR:HG21 | 26:1Z:21:ARG:HD3 | 2.01 | 0.41 |
| 26:1Z:56:ILE:H | 26:1Z:56:ILE:HG12 | 1.66 | 0.41 |
| 1:1A:219:G:H2' | 1:1A:220:A:C8 | 2.55 | 0.41 |
| 1:1A:518:A:H2' | 1:1A:519:A:O4' | 2.20 | 0.41 |
| 1:1A:1581:G:N7 | 18:1R:27:LYS:HB2 | 2.35 | 0.41 |
| 1:1A:1822:U:H2' | 1:1A:1823:C:C4' | 2.50 | 0.41 |
| 1:1A:1889:U:H2' | 1:1A:1890:U:H6 | 1.84 | 0.41 |
| 1:1A:1978:U:H2' | 1:1A:1979:U:C6 | 2.55 | 0.41 |
| 1:1A:2185:C:H2' | 1:1A:2186:U:C6 | 2.55 | 0.41 |
| 1:1A:2417:A:H2' | 1:1A:2418:U:O4' | 2.20 | 0.41 |
| 1:1A:3491:U:P | 5:1E:385:LYS:HD2 | 2.59 | 0.41 |
| 4:1D:29:HIS:O | 4:1D:123:ARG:NE | 2.34 | 0.41 |
| 7:1G:94:ASN:N | 7:1G:94:ASN:OD1 | 2.54 | 0.41 |
| 12:1L:13:ARG:HE | 12:1L:13:ARG:HB3 | 1.60 | 0.41 |
| 16:1P:83:ASP:OD2 | 16:1P:83:ASP:N | 2.53 | 0.41 |
| 17:1Q:103:GLU:OE2 | 17:1Q:118:SER:OG | 2.30 | 0.41 |
| 20:1T:58:GLN:HE21 | 20:1T:58:GLN:HB2 | 1.67 | 0.41 |
| 23:1W:93:MET:O | 23:1W:97:LEU:HD12 | 2.20 | 0.41 |
| 31:1e:31:THR:HG23 | 31:1e:93:VAL:HG21 | 2.02 | 0.41 |
| 42:1p:24:CYS:SG | 42:1p:37:LYS:HB2 | 2.61 | 0.41 |
| 1:1A:36:A:O2' | 1:1A:1056:G:O6 | 2.35 | 0.41 |
| 1:1A:783:A:H2' | 1:1A:784:C:C6 | 2.55 | 0.41 |
| 1:1A:1121:A:N1 | 1:1A:1168:C:O2' | 2.48 | 0.41 |
| 1:1A:1484:A:H2' | 1:1A:1485:A:C8 | 2.56 | 0.41 |
| 1:1A:2383:G:O2' | 1:1A:2386:U:OP2 | 2.39 | 0.41 |
| 2:1B:31:C:H2' | 2:1B:32:C:H6 | 1.84 | 0.41 |
| 6:1F:4:ARG:NH1 | 6:1F:4:ARG:HG2 | 2.34 | 0.41 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 8:1H:79:PHE:HA | 8:1H:91:VAL:HG12 | 2.02 | 0.41 |
| 11:1K:113:ILE:HG12 | 11:1K:120:ILE:HG13 | 2.02 | 0.41 |
| 15:1O:17:LEU:HA | 15:1O:42:LEU:HD22 | 2.02 | 0.41 |
| 23:1W:67:GLU:HB2 | 23:1W:78:THR:HG23 | 2.01 | 0.41 |
| 24:1X:112:MET:HE3 | 24:1X:112:MET:HB3 | 1.83 | 0.41 |
| 25:1Y:36:MET:HE1 | 25:1Y:68:LYS:HB2 | 2.03 | 0.41 |
| 40:1n:21:LEU:HD12 | 40:1n:21:LEU:HA | 1.92 | 0.41 |
| 40:1n:27:ILE:HG13 | 40:1n:43:VAL:HG13 | 2.01 | 0.41 |
| 1:1A:491:G:C5 | 1:1A:492:U:C5 | 3.09 | 0.41 |
| 1:1A:960:G:H2' | 1:1A:961:A:H8 | 1.86 | 0.41 |
| 1:1A:1047:U:H2' | 1:1A:1048:A:C8 | 2.56 | 0.41 |
| 1:1A:1641:A:H2' | 1:1A:1642:A:O4' | 2.20 | 0.41 |
| 1:1A:2656:G:H5' | 10:1J:54:LEU:HD11 | 2.03 | 0.41 |
| 1:1A:3502:A:H4' | 5:1E:316:GLY:HA2 | 2.03 | 0.41 |
| 3:1C:69:U:H3 | 3:1C:104:G:H22 | 1.68 | 0.41 |
| 6:1F:4:ARG:HG2 | 6:1F:4:ARG:HH11 | 1.85 | 0.41 |
| 6:1F:316:ARG:HE | 6:1F:316:ARG:HB3 | 1.64 | 0.41 |
| 9:1I:87:ILE:HG21 | 9:1I:121:TYR:CD2 | 2.56 | 0.41 |
| 12:1L:183:GLN:C | 12:1L:183:GLN:OE1 | 2.63 | 0.41 |
| 21:1U:92:LYS:O | 21:1U:96:ILE:HG13 | 2.21 | 0.41 |
| 1:1A:529:U:H2' | 1:1A:530:A:C8 | 2.55 | 0.41 |
| 1:1A:1615:A:O2' | 32:1f:95:GLN:OE1 | 2.38 | 0.41 |
| 1:1A:1842:U:H2' | 1:1A:1843:G:C8 | 2.56 | 0.41 |
| 1:1A:2595:G:H2' | 1:1A:2596:U:C6 | 2.55 | 0.41 |
| 1:1A:2953:C:OP2 | 1:1A:3098:U:O2' | 2.37 | 0.41 |
| 1:1A:3084:A:OP2 | 5:1E:258:HIS:HB2 | 2.20 | 0.41 |
| 6:1F:331:PRO:HB2 | 9:1I:33:ILE:HD11 | 2.03 | 0.41 |
| 11:1K:61:ASN:OD1 | 11:1K:61:ASN:N | 2.53 | 0.41 |
| 11:1K:119:SER:HG | 11:1K:133:HIS:CD2 | 2.38 | 0.41 |
| 15:1O:62:ARG:HD2 | 15:1O:67:PRO:HB3 | 2.03 | 0.41 |
| 22:1V:107:GLU:C | 22:1V:107:GLU:OE2 | 2.63 | 0.41 |
| 25:1Y:75:LYS:O | 25:1Y:79:GLU:HG3 | 2.20 | 0.41 |
| 34:1h:71:THR:OG1 | 34:1h:72:VAL:N | 2.53 | 0.41 |
| 35:1i:-6:LYS:HD3 | 35:1i:-6:LYS:HA | 1.74 | 0.41 |
| 1:1A:678:A:H2' | 1:1A:679:U:H6 | 1.85 | 0.41 |
| 1:1A:761:A:H2' | 1:1A:762:A:H8 | 1.82 | 0.41 |
| 1:1A:1242:G:H2' | 1:1A:1243:C:C6 | 2.55 | 0.41 |
| 1:1A:2131:A:OP2 | 1:1A:2132:A:O2' | 2.32 | 0.41 |
| 1:1A:2485:G:O2' | 1:1A:2487:U:H5'' | 2.21 | 0.41 |
| 1:1A:3434:A:H2' | 1:1A:3435:G:O4' | 2.21 | 0.41 |
| 5:1E:113:GLU:H | 5:1E:113:GLU:HG3 | 1.70 | 0.41 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|--------------------|--------------------------|-------------------|
| 6:IF:302:LYS:HB2 | 6:IF:302:LYS:HE2 | 1.94 | 0.41 |
| 8:IH:22:PRO:HG2 | 8:IH:27:ILE:HD11 | 2.01 | 0.41 |
| 9:II:156:MET:HE3 | 9:II:156:MET:HB2 | 1.98 | 0.41 |
| 10:IJ:205:LYS:HE3 | 10:IJ:205:LYS:HB2 | 1.82 | 0.41 |
| 23:IW:103:ARG:NH1 | 23:IW:103:ARG:O | 2.53 | 0.41 |
| 1:IA:79:U:H2' | 1:IA:80:A:O4' | 2.20 | 0.41 |
| 1:IA:940:U:H2' | 1:IA:941:A:H8 | 1.86 | 0.41 |
| 1:IA:1089:C:H2' | 1:IA:1090:A:C8 | 2.56 | 0.41 |
| 1:IA:1249:C:O2' | 1:IA:2705:A:OP1 | 2.39 | 0.41 |
| 1:IA:2232:U:OP2 | 4:ID:241:ARG:NH2 | 2.48 | 0.41 |
| 1:IA:2425:U:O2' | 1:IA:3436:A:N3 | 2.53 | 0.41 |
| 1:IA:2683:U:H5 | 1:IA:2948:G:C8 | 2.38 | 0.41 |
| 1:IA:3112:A:N7 | 4:ID:215:ASN:ND2 | 2.69 | 0.41 |
| 1:IA:3373:A:H1' | 1:IA:3385:G:C4 | 2.56 | 0.41 |
| 2:IB:28:U:H2' | 2:IB:29:U:H6 | 1.86 | 0.41 |
| 27:la:150:ASN:O | 27:la:153:ILE:HG12 | 2.20 | 0.41 |
| 1:IA:233:A:N3 | 1:IA:254:C:O2' | 2.51 | 0.41 |
| 1:IA:336:A:H2' | 1:IA:337:A:C8 | 2.56 | 0.41 |
| 1:IA:526:A:H5'' | 1:IA:538:A:N1 | 2.35 | 0.41 |
| 1:IA:619:A:C6 | 16:IP:77:CYS:HB3 | 2.55 | 0.41 |
| 1:IA:926:A:H62 | 1:IA:1053:G:H1 | 1.68 | 0.41 |
| 1:IA:1107:G:H2' | 1:IA:1108:A:H8 | 1.85 | 0.41 |
| 1:IA:1126:U:H2' | 1:IA:1127:A:O4' | 2.21 | 0.41 |
| 1:IA:1168:C:H2' | 1:IA:1169:U:C6 | 2.56 | 0.41 |
| 1:IA:1188:A:H2' | 1:IA:1189:U:C6 | 2.56 | 0.41 |
| 1:IA:1282:G:OP1 | 9:II:78:ARG:NH1 | 2.54 | 0.41 |
| 1:IA:1392:G:C2 | 1:IA:1393:U:C4 | 3.08 | 0.41 |
| 1:IA:1511:G:OP1 | 6:IF:200:ARG:NH1 | 2.52 | 0.41 |
| 1:IA:1554:C:C5 | 6:IF:192:ALA:HB2 | 2.56 | 0.41 |
| 1:IA:1845:G:N2 | 1:IA:1924:U:O2' | 2.53 | 0.41 |
| 1:IA:1863:U:O2 | 23:IW:95:LYS:HD2 | 2.21 | 0.41 |
| 1:IA:2415:C:OP1 | 24:IX:54:ARG:NH2 | 2.54 | 0.41 |
| 1:IA:3086:G:H2' | 1:IA:3087:U:O4' | 2.21 | 0.41 |
| 1:IA:3196:U:H2' | 1:IA:3197:C:C6 | 2.56 | 0.41 |
| 2:IB:117:A:H2' | 2:IB:118:C:H6 | 1.86 | 0.41 |
| 14:IN:254:MET:H | 14:IN:254:MET:HG3 | 1.74 | 0.41 |
| 15:IO:93:ASN:O | 15:IO:97:LYS:HG2 | 2.21 | 0.41 |
| 21:IU:98:ARG:NH1 | 21:IU:132:TYR:O | 2.52 | 0.41 |
| 27:la:22:ASN:OD1 | 27:la:22:ASN:N | 2.53 | 0.41 |
| 28:lb:20:GLY:HA3 | 28:lb:139:PHE:HZ | 1.83 | 0.41 |
| 40:ln:71:ILE:HD12 | 40:ln:71:ILE:HA | 1.85 | 0.41 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|--------------------|--------------------------|-------------------|
| 43:lq:74:LYS:HE2 | 43:lq:74:LYS:HB2 | 1.86 | 0.41 |
| 1:lA:542:U:H2' | 1:lA:543:A:H8 | 1.86 | 0.41 |
| 1:lA:739:A:H2' | 1:lA:740:A:H8 | 1.85 | 0.41 |
| 1:lA:897:A:H4' | 1:lA:898:U:OP1 | 2.19 | 0.41 |
| 1:lA:934:G:OP1 | 38:ll:16:HIS:NE2 | 2.42 | 0.41 |
| 1:lA:937:C:H2' | 1:lA:938:U:O4' | 2.21 | 0.41 |
| 1:lA:1465:G:H2' | 1:lA:1466:U:C6 | 2.56 | 0.41 |
| 1:lA:1822:U:H2' | 1:lA:1823:C:H4' | 2.03 | 0.41 |
| 1:lA:1823:C:H2' | 1:lA:1824:A:N3 | 2.35 | 0.41 |
| 1:lA:2759:A:H2' | 1:lA:2759:A:N3 | 2.36 | 0.41 |
| 5:lE:62:ARG:HD3 | 5:lE:350:THR:HA | 2.03 | 0.41 |
| 7:lG:196:LEU:HD23 | 7:lG:196:LEU:HA | 1.92 | 0.41 |
| 14:lN:41:ALA:O | 14:lN:229:GLN:NE2 | 2.54 | 0.41 |
| 23:lW:46:LEU:HD13 | 23:lW:50:PHE:HE2 | 1.86 | 0.41 |
| 29:lc:138:ILE:O | 29:lc:141:VAL:HG12 | 2.21 | 0.41 |
| 1:lA:109:C:C2 | 1:lA:110:A:C8 | 3.09 | 0.40 |
| 1:lA:604:U:H2' | 1:lA:605:C:H6 | 1.85 | 0.40 |
| 1:lA:1887:A:H2' | 1:lA:1888:A:H8 | 1.85 | 0.40 |
| 1:lA:2150:G:C2 | 1:lA:2176:G:C2 | 3.08 | 0.40 |
| 1:lA:2295:A:H2' | 1:lA:2296:U:C6 | 2.55 | 0.40 |
| 1:lA:2346:A:H2' | 1:lA:2347:A:H8 | 1.85 | 0.40 |
| 1:lA:3243:C:H2' | 1:lA:3244:U:O4' | 2.22 | 0.40 |
| 1:lA:3360:U:H3 | 8:lH:185:GLU:HG2 | 1.86 | 0.40 |
| 5:lE:146:ARG:O | 5:lE:150:ILE:HG12 | 2.21 | 0.40 |
| 8:lH:114:SER:OG | 8:lH:204:PHE:O | 2.37 | 0.40 |
| 9:ll:58:GLU:C | 9:ll:58:GLU:OE2 | 2.64 | 0.40 |
| 16:lP:115:VAL:O | 16:lP:119:ASN:HB2 | 2.20 | 0.40 |
| 35:li:-9:ALA:HB1 | 35:li:45:ARG:HH12 | 1.86 | 0.40 |
| 35:li:-7:LEU:HD23 | 35:li:-2:ILE:HD11 | 2.01 | 0.40 |
| 37:lk:64:LEU:HB2 | 37:lk:81:ARG:NH1 | 2.36 | 0.40 |
| 39:lm:48:ARG:NH2 | 39:lm:58:LYS:HD3 | 2.37 | 0.40 |
| 1:lA:1310:A:H2' | 1:lA:1311:C:C6 | 2.56 | 0.40 |
| 1:lA:1324:A:H5' | 1:lA:1325:C:O5' | 2.20 | 0.40 |
| 1:lA:1437:A:O3' | 15:lO:18:GLY:HA3 | 2.21 | 0.40 |
| 1:lA:1468:A:H2' | 1:lA:1469:A:H8 | 1.86 | 0.40 |
| 1:lA:2981:A:H2' | 1:lA:2982:G:O4' | 2.21 | 0.40 |
| 1:lA:3287:U:H2' | 1:lA:3288:U:C6 | 2.56 | 0.40 |
| 7:lG:135:GLU:OE1 | 7:lG:135:GLU:N | 2.54 | 0.40 |
| 10:lJ:96:LYS:O | 10:lJ:100:ILE:HG13 | 2.21 | 0.40 |
| 14:lN:49:ILE:HG22 | 14:lN:51:SER:N | 2.35 | 0.40 |
| 14:lN:123:VAL:O | 14:lN:222:VAL:HA | 2.21 | 0.40 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 23:1W:102:LEU:HD12 | 23:1W:106:LEU:CD1 | 2.52 | 0.40 |
| 29:1c:90:TYR:CG | 29:1c:100:PRO:HD3 | 2.56 | 0.40 |
| 39:1m:49:ARG:HB2 | 39:1m:55:TRP:CZ3 | 2.56 | 0.40 |
| 1:1A:320:A:H2' | 1:1A:321:U:C6 | 2.56 | 0.40 |
| 1:1A:397:A:N6 | 41:1o:35:ILE:HG23 | 2.36 | 0.40 |
| 1:1A:993:U:O4 | 1:1A:3122:U:H5 | 2.05 | 0.40 |
| 1:1A:1157:A:H5' | 7:1G:5:LYS:HD3 | 2.03 | 0.40 |
| 1:1A:2486:U:C5 | 1:1A:2944:A:N1 | 2.89 | 0.40 |
| 1:1A:2989:U:H2' | 42:1p:22:ARG:HD3 | 2.04 | 0.40 |
| 1:1A:3452:U:H3 | 1:1A:3504:G:N2 | 2.19 | 0.40 |
| 1:1A:3456:U:H5'' | 5:1E:309:MET:HE3 | 2.03 | 0.40 |
| 5:1E:365:LYS:HA | 5:1E:365:LYS:HD3 | 1.97 | 0.40 |
| 9:1I:208:HIS:CE1 | 9:1I:210:ILE:HD12 | 2.56 | 0.40 |
| 13:1M:51:ARG:O | 13:1M:61:ARG:NH1 | 2.55 | 0.40 |
| 13:1M:105:GLY:HA2 | 13:1M:126:ASP:HA | 2.03 | 0.40 |
| 31:1e:68:LYS:HE2 | 31:1e:68:LYS:HB2 | 1.70 | 0.40 |
| 1:1A:236:U:O4 | 27:1a:36:LYS:HG2 | 2.22 | 0.40 |
| 1:1A:483:G:H5'' | 1:1A:753:A:N6 | 2.36 | 0.40 |
| 1:1A:1107:G:H21 | 22:1V:101:CYS:HA | 1.86 | 0.40 |
| 1:1A:1186:G:H2' | 1:1A:1187:A:H5'' | 2.03 | 0.40 |
| 1:1A:1217:U:H2' | 1:1A:1218:U:O4' | 2.21 | 0.40 |
| 1:1A:1467:U:H2' | 1:1A:1468:A:C8 | 2.56 | 0.40 |
| 1:1A:1564:U:O4 | 29:1c:3:THR:HG23 | 2.22 | 0.40 |
| 1:1A:2420:U:H2' | 1:1A:2421:G:C8 | 2.57 | 0.40 |
| 4:1D:28:GLN:HB2 | 4:1D:123:ARG:HB3 | 2.04 | 0.40 |
| 8:1H:21:TYR:CZ | 33:1g:115:ILE:HG23 | 2.57 | 0.40 |
| 10:1J:234:ASN:HD22 | 10:1J:238:HIS:CE1 | 2.40 | 0.40 |
| 21:1U:7:GLN:NE2 | 21:1U:35:ALA:O | 2.41 | 0.40 |
| 22:1V:17:ARG:HB2 | 22:1V:22:HIS:CE1 | 2.55 | 0.40 |
| 28:1b:115:LYS:HA | 28:1b:115:LYS:HD3 | 1.70 | 0.40 |
| 1:1A:487:A:H2' | 1:1A:488:A:H8 | 1.86 | 0.40 |
| 1:1A:718:A:H2' | 1:1A:719:U:H6 | 1.86 | 0.40 |
| 1:1A:1158:U:H2' | 1:1A:1159:C:C6 | 2.57 | 0.40 |
| 1:1A:1334:U:H2' | 1:1A:1335:U:C6 | 2.57 | 0.40 |
| 1:1A:1475:A:H8 | 27:1a:185:ARG:HH12 | 1.69 | 0.40 |
| 1:1A:2243:A:H2' | 1:1A:2244:A:C8 | 2.57 | 0.40 |
| 1:1A:3300:A:H2' | 1:1A:3301:A:C8 | 2.55 | 0.40 |
| 2:1B:96:A:H2' | 2:1B:97:A:O4' | 2.22 | 0.40 |
| 4:1D:125:ILE:HD13 | 4:1D:125:ILE:HA | 1.94 | 0.40 |
| 5:1E:17:HIS:HE1 | 5:1E:264:TRP:HB2 | 1.87 | 0.40 |
| 24:1X:82:ILE:HG13 | 24:1X:83:ARG:HG2 | 2.04 | 0.40 |

There are no symmetry-related clashes.

5.3 Torsion angles

5.3.1 Protein backbone

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

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

| Mol | Chain | Analysed | Favoured | Allowed | Outliers | Percentiles | |
|-----|-------|---------------|-----------|---------|----------|-------------|-----|
| 4 | ID | 244/257 (95%) | 229 (94%) | 15 (6%) | 0 | 100 | 100 |
| 5 | IE | 385/402 (96%) | 373 (97%) | 12 (3%) | 0 | 100 | 100 |
| 6 | IF | 420/431 (97%) | 404 (96%) | 16 (4%) | 0 | 100 | 100 |
| 7 | IG | 275/286 (96%) | 259 (94%) | 16 (6%) | 0 | 100 | 100 |
| 8 | IH | 201/204 (98%) | 183 (91%) | 18 (9%) | 0 | 100 | 100 |
| 9 | II | 208/230 (90%) | 200 (96%) | 8 (4%) | 0 | 100 | 100 |
| 10 | IJ | 209/286 (73%) | 200 (96%) | 9 (4%) | 0 | 100 | 100 |
| 11 | IK | 191/197 (97%) | 185 (97%) | 6 (3%) | 0 | 100 | 100 |
| 12 | IL | 196/210 (93%) | 187 (95%) | 9 (5%) | 0 | 100 | 100 |
| 13 | IM | 166/174 (95%) | 158 (95%) | 7 (4%) | 1 (1%) | 22 | 51 |
| 14 | IN | 228/291 (78%) | 212 (93%) | 16 (7%) | 0 | 100 | 100 |
| 15 | IO | 202/205 (98%) | 197 (98%) | 5 (2%) | 0 | 100 | 100 |
| 16 | IP | 130/135 (96%) | 128 (98%) | 2 (2%) | 0 | 100 | 100 |
| 17 | IQ | 202/205 (98%) | 197 (98%) | 5 (2%) | 0 | 100 | 100 |
| 18 | IR | 156/179 (87%) | 153 (98%) | 3 (2%) | 0 | 100 | 100 |
| 19 | IS | 165/168 (98%) | 153 (93%) | 12 (7%) | 0 | 100 | 100 |
| 20 | IT | 171/173 (99%) | 165 (96%) | 6 (4%) | 0 | 100 | 100 |
| 21 | IU | 148/198 (75%) | 145 (98%) | 3 (2%) | 0 | 100 | 100 |
| 22 | IV | 163/166 (98%) | 158 (97%) | 5 (3%) | 0 | 100 | 100 |
| 23 | IW | 91/137 (66%) | 82 (90%) | 8 (9%) | 1 (1%) | 12 | 37 |
| 24 | IX | 131/140 (94%) | 128 (98%) | 3 (2%) | 0 | 100 | 100 |
| 25 | IY | 114/121 (94%) | 112 (98%) | 2 (2%) | 0 | 100 | 100 |

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| Mol | Chain | Analysed | Favoured | Allowed | Outliers | Percentiles | |
|-----|-------|-----------------|------------|----------|----------|-------------|-----|
| 26 | lZ | 55/163 (34%) | 54 (98%) | 1 (2%) | 0 | 100 | 100 |
| 27 | la | 208/213 (98%) | 200 (96%) | 8 (4%) | 0 | 100 | 100 |
| 28 | lb | 135/139 (97%) | 133 (98%) | 2 (2%) | 0 | 100 | 100 |
| 29 | lc | 146/149 (98%) | 140 (96%) | 6 (4%) | 0 | 100 | 100 |
| 30 | ld | 58/64 (91%) | 55 (95%) | 3 (5%) | 0 | 100 | 100 |
| 31 | le | 101/109 (93%) | 92 (91%) | 9 (9%) | 0 | 100 | 100 |
| 32 | lf | 144/150 (96%) | 135 (94%) | 9 (6%) | 0 | 100 | 100 |
| 33 | lg | 127/134 (95%) | 123 (97%) | 4 (3%) | 0 | 100 | 100 |
| 34 | lh | 103/137 (75%) | 99 (96%) | 4 (4%) | 0 | 100 | 100 |
| 35 | li | 120/122 (98%) | 117 (98%) | 3 (2%) | 0 | 100 | 100 |
| 36 | lj | 104/108 (96%) | 100 (96%) | 4 (4%) | 0 | 100 | 100 |
| 37 | lk | 83/104 (80%) | 82 (99%) | 1 (1%) | 0 | 100 | 100 |
| 38 | ll | 70/77 (91%) | 63 (90%) | 5 (7%) | 2 (3%) | 3 | 13 |
| 39 | lm | 88/93 (95%) | 82 (93%) | 6 (7%) | 0 | 100 | 100 |
| 40 | ln | 71/84 (84%) | 69 (97%) | 2 (3%) | 0 | 100 | 100 |
| 41 | lo | 48/51 (94%) | 48 (100%) | 0 | 0 | 100 | 100 |
| 42 | lp | 51/56 (91%) | 50 (98%) | 1 (2%) | 0 | 100 | 100 |
| 43 | lq | 90/98 (92%) | 88 (98%) | 2 (2%) | 0 | 100 | 100 |
| All | All | 6198/6846 (90%) | 5938 (96%) | 256 (4%) | 4 (0%) | 50 | 77 |

All (4) Ramachandran outliers are listed below:

| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 23 | lW | 45 | LYS |
| 38 | ll | 39 | TYR |
| 38 | ll | 40 | PRO |
| 13 | lM | 28 | ASP |

5.3.2 Protein sidechains ⓘ

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

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

| Mol | Chain | Analysed | Rotameric | Outliers | Percentiles | |
|-----|-------|----------------|------------|----------|-------------|-----|
| 4 | ID | 195/201 (97%) | 189 (97%) | 6 (3%) | 35 | 69 |
| 5 | IE | 330/343 (96%) | 326 (99%) | 4 (1%) | 67 | 89 |
| 6 | IF | 338/345 (98%) | 329 (97%) | 9 (3%) | 40 | 74 |
| 7 | IG | 225/231 (97%) | 224 (100%) | 1 (0%) | 89 | 96 |
| 8 | IH | 172/173 (99%) | 170 (99%) | 2 (1%) | 67 | 89 |
| 9 | II | 178/195 (91%) | 175 (98%) | 3 (2%) | 56 | 84 |
| 10 | IJ | 186/242 (77%) | 179 (96%) | 7 (4%) | 28 | 62 |
| 11 | IK | 171/174 (98%) | 170 (99%) | 1 (1%) | 84 | 95 |
| 12 | IL | 169/176 (96%) | 167 (99%) | 2 (1%) | 67 | 89 |
| 13 | IM | 144/147 (98%) | 142 (99%) | 2 (1%) | 62 | 87 |
| 14 | IN | 200/243 (82%) | 196 (98%) | 4 (2%) | 50 | 81 |
| 15 | IO | 167/168 (99%) | 163 (98%) | 4 (2%) | 44 | 77 |
| 16 | IP | 116/118 (98%) | 113 (97%) | 3 (3%) | 41 | 75 |
| 17 | IQ | 171/172 (99%) | 170 (99%) | 1 (1%) | 84 | 95 |
| 18 | IR | 129/147 (88%) | 125 (97%) | 4 (3%) | 35 | 69 |
| 19 | IS | 142/143 (99%) | 138 (97%) | 4 (3%) | 38 | 72 |
| 20 | IT | 156/156 (100%) | 154 (99%) | 2 (1%) | 65 | 88 |
| 21 | IU | 132/174 (76%) | 132 (100%) | 0 | 100 | 100 |
| 22 | IV | 144/145 (99%) | 141 (98%) | 3 (2%) | 48 | 80 |
| 23 | IW | 86/125 (69%) | 77 (90%) | 9 (10%) | 5 | 18 |
| 24 | IX | 109/113 (96%) | 108 (99%) | 1 (1%) | 75 | 92 |
| 25 | IY | 99/102 (97%) | 98 (99%) | 1 (1%) | 73 | 91 |
| 26 | IZ | 52/137 (38%) | 49 (94%) | 3 (6%) | 17 | 45 |
| 27 | la | 177/179 (99%) | 175 (99%) | 2 (1%) | 70 | 90 |
| 28 | lb | 121/123 (98%) | 118 (98%) | 3 (2%) | 42 | 75 |
| 29 | lc | 120/121 (99%) | 117 (98%) | 3 (2%) | 42 | 75 |
| 30 | ld | 50/54 (93%) | 49 (98%) | 1 (2%) | 50 | 81 |
| 31 | le | 86/92 (94%) | 83 (96%) | 3 (4%) | 31 | 65 |
| 32 | lf | 125/128 (98%) | 122 (98%) | 3 (2%) | 44 | 77 |
| 33 | lg | 112/116 (97%) | 108 (96%) | 4 (4%) | 30 | 64 |
| 34 | lh | 86/116 (74%) | 84 (98%) | 2 (2%) | 45 | 78 |
| 35 | li | 103/103 (100%) | 103 (100%) | 0 | 100 | 100 |

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| Mol | Chain | Analysed | Rotameric | Outliers | Percentiles | |
|-----|-------|-----------------|------------|----------|-------------|-----|
| 36 | lj | 89/91 (98%) | 89 (100%) | 0 | 100 | 100 |
| 37 | lk | 71/82 (87%) | 69 (97%) | 2 (3%) | 38 | 72 |
| 38 | ll | 60/64 (94%) | 59 (98%) | 1 (2%) | 56 | 84 |
| 39 | lm | 72/74 (97%) | 72 (100%) | 0 | 100 | 100 |
| 40 | ln | 63/73 (86%) | 62 (98%) | 1 (2%) | 58 | 85 |
| 41 | lo | 44/45 (98%) | 43 (98%) | 1 (2%) | 45 | 78 |
| 42 | lp | 45/48 (94%) | 45 (100%) | 0 | 100 | 100 |
| 43 | lq | 85/91 (93%) | 84 (99%) | 1 (1%) | 67 | 89 |
| All | All | 5320/5770 (92%) | 5217 (98%) | 103 (2%) | 52 | 82 |

All (103) residues with a non-rotameric sidechain are listed below:

| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 4 | lD | 78 | CYS |
| 4 | lD | 106 | GLN |
| 4 | lD | 145 | THR |
| 4 | lD | 146 | THR |
| 4 | lD | 193 | ARG |
| 4 | lD | 242 | ARG |
| 5 | lE | 20 | LYS |
| 5 | lE | 258 | HIS |
| 5 | lE | 343 | CYS |
| 5 | lE | 350 | THR |
| 6 | lF | 57 | GLU |
| 6 | lF | 94 | ASN |
| 6 | lF | 150 | ILE |
| 6 | lF | 156 | SER |
| 6 | lF | 182 | LEU |
| 6 | lF | 373 | VAL |
| 6 | lF | 392 | VAL |
| 6 | lF | 397 | LEU |
| 6 | lF | 401 | VAL |
| 7 | lG | 109 | LEU |
| 8 | lH | 122 | VAL |
| 8 | lH | 153 | LYS |
| 9 | lI | 77 | ILE |
| 9 | lI | 188 | ASN |
| 9 | lI | 207 | ILE |
| 10 | lJ | 19 | VAL |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 10 | IJ | 22 | LYS |
| 10 | IJ | 25 | PHE |
| 10 | IJ | 36 | LEU |
| 10 | IJ | 49 | GLN |
| 10 | IJ | 148 | VAL |
| 10 | IJ | 205 | LYS |
| 11 | IK | 94 | LYS |
| 12 | IL | 103 | LEU |
| 12 | IL | 111 | LEU |
| 13 | IM | 14 | ILE |
| 13 | IM | 110 | ILE |
| 14 | IN | 32 | ARG |
| 14 | IN | 155 | PHE |
| 14 | IN | 212 | LYS |
| 14 | IN | 213 | LYS |
| 15 | IO | 39 | CYS |
| 15 | IO | 41 | ASP |
| 15 | IO | 56 | GLU |
| 15 | IO | 160 | GLU |
| 16 | IP | 94 | THR |
| 16 | IP | 114 | GLN |
| 16 | IP | 131 | SER |
| 17 | IQ | 39 | VAL |
| 18 | IR | 18 | ARG |
| 18 | IR | 139 | PHE |
| 18 | IR | 147 | GLU |
| 18 | IR | 148 | LEU |
| 19 | IS | 72 | LYS |
| 19 | IS | 76 | GLU |
| 19 | IS | 80 | CYS |
| 19 | IS | 152 | VAL |
| 20 | IT | 58 | GLN |
| 20 | IT | 106 | LEU |
| 22 | IV | 27 | THR |
| 22 | IV | 123 | LYS |
| 22 | IV | 152 | ILE |
| 23 | IW | 31 | THR |
| 23 | IW | 34 | LEU |
| 23 | IW | 41 | ILE |
| 23 | IW | 45 | LYS |
| 23 | IW | 46 | LEU |
| 23 | IW | 75 | VAL |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 23 | IW | 85 | CYS |
| 23 | IW | 108 | VAL |
| 23 | IW | 109 | ILE |
| 24 | IX | 106 | VAL |
| 25 | IY | 120 | LEU |
| 26 | IZ | 17 | VAL |
| 26 | IZ | 32 | THR |
| 26 | IZ | 62 | LYS |
| 27 | la | 7 | VAL |
| 27 | la | 109 | LEU |
| 28 | lb | 12 | ILE |
| 28 | lb | 111 | ILE |
| 28 | lb | 135 | THR |
| 29 | lc | 16 | SER |
| 29 | lc | 120 | LYS |
| 29 | lc | 141 | VAL |
| 30 | ld | 35 | MET |
| 31 | le | 40 | ASP |
| 31 | le | 94 | LEU |
| 31 | le | 104 | ILE |
| 32 | lf | 15 | ARG |
| 32 | lf | 121 | GLU |
| 32 | lf | 132 | VAL |
| 33 | lg | 35 | VAL |
| 33 | lg | 53 | LEU |
| 33 | lg | 96 | GLU |
| 33 | lg | 132 | VAL |
| 34 | lh | 36 | GLN |
| 34 | lh | 56 | HIS |
| 37 | lk | 7 | VAL |
| 37 | lk | 9 | LEU |
| 38 | ll | 10 | THR |
| 40 | ln | 31 | ARG |
| 41 | lo | 29 | MET |
| 43 | lq | 18 | HIS |

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (47) such sidechains are listed below:

| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 4 | ID | 8 | GLN |
| 4 | ID | 22 | HIS |
| 4 | ID | 106 | GLN |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 4 | lD | 233 | GLN |
| 5 | lE | 17 | HIS |
| 6 | lF | 269 | GLN |
| 7 | lG | 111 | GLN |
| 7 | lG | 234 | ASN |
| 9 | lI | 81 | ASN |
| 9 | lI | 188 | ASN |
| 10 | lJ | 49 | GLN |
| 10 | lJ | 144 | GLN |
| 10 | lJ | 171 | GLN |
| 10 | lJ | 234 | ASN |
| 11 | lK | 180 | GLN |
| 12 | lL | 144 | HIS |
| 13 | lM | 43 | GLN |
| 14 | lN | 216 | GLN |
| 16 | lP | 33 | HIS |
| 16 | lP | 114 | GLN |
| 17 | lQ | 139 | ASN |
| 18 | lR | 10 | ASN |
| 18 | lR | 16 | GLN |
| 18 | lR | 97 | ASN |
| 18 | lR | 108 | ASN |
| 19 | lS | 57 | ASN |
| 20 | lT | 16 | ASN |
| 20 | lT | 89 | GLN |
| 20 | lT | 101 | GLN |
| 22 | lV | 5 | ASN |
| 22 | lV | 26 | ASN |
| 24 | lX | 12 | ASN |
| 24 | lX | 22 | ASN |
| 25 | lY | 12 | HIS |
| 25 | lY | 18 | ASN |
| 25 | lY | 58 | HIS |
| 28 | lb | 88 | ASN |
| 29 | lc | 28 | GLN |
| 30 | ld | 17 | HIS |
| 30 | ld | 19 | ASN |
| 30 | ld | 46 | GLN |
| 31 | le | 11 | GLN |
| 32 | lf | 31 | ASN |
| 33 | lg | 122 | ASN |
| 34 | lh | 34 | HIS |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 35 | li | 83 | GLN |
| 41 | lo | 18 | HIS |

5.3.3 RNA ⓘ

| Mol | Chain | Analysed | Backbone Outliers | Pucker Outliers |
|-----|-------|-----------------|-------------------|-----------------|
| 1 | lA | 3047/3503 (86%) | 553 (18%) | 0 |
| 2 | lB | 143/155 (92%) | 32 (22%) | 0 |
| 3 | lC | 116/117 (99%) | 15 (12%) | 0 |
| All | All | 3306/3775 (87%) | 600 (18%) | 0 |

All (600) RNA backbone outliers are listed below:

| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1 | lA | 18 | G |
| 1 | lA | 22 | A |
| 1 | lA | 29 | U |
| 1 | lA | 30 | A |
| 1 | lA | 36 | A |
| 1 | lA | 39 | A |
| 1 | lA | 45 | A |
| 1 | lA | 54 | G |
| 1 | lA | 55 | G |
| 1 | lA | 56 | A |
| 1 | lA | 62 | A |
| 1 | lA | 65 | U |
| 1 | lA | 69 | A |
| 1 | lA | 70 | A |
| 1 | lA | 88 | G |
| 1 | lA | 90 | G |
| 1 | lA | 105 | A |
| 1 | lA | 106 | G |
| 1 | lA | 115 | G |
| 1 | lA | 116 | A |
| 1 | lA | 117 | U |
| 1 | lA | 185 | G |
| 1 | lA | 186 | A |
| 1 | lA | 189 | G |
| 1 | lA | 198 | A |
| 1 | lA | 199 | G |
| 1 | lA | 200 | A |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1 | lA | 206 | U |
| 1 | lA | 213 | A |
| 1 | lA | 214 | A |
| 1 | lA | 221 | U |
| 1 | lA | 233 | A |
| 1 | lA | 237 | C |
| 1 | lA | 246 | U |
| 1 | lA | 256 | G |
| 1 | lA | 257 | A |
| 1 | lA | 259 | A |
| 1 | lA | 264 | G |
| 1 | lA | 266 | A |
| 1 | lA | 267 | A |
| 1 | lA | 285 | A |
| 1 | lA | 286 | U |
| 1 | lA | 287 | A |
| 1 | lA | 289 | C |
| 1 | lA | 293 | A |
| 1 | lA | 294 | A |
| 1 | lA | 302 | U |
| 1 | lA | 303 | G |
| 1 | lA | 311 | A |
| 1 | lA | 316 | G |
| 1 | lA | 319 | A |
| 1 | lA | 332 | G |
| 1 | lA | 342 | A |
| 1 | lA | 344 | A |
| 1 | lA | 345 | A |
| 1 | lA | 346 | G |
| 1 | lA | 350 | A |
| 1 | lA | 369 | A |
| 1 | lA | 381 | A |
| 1 | lA | 383 | A |
| 1 | lA | 385 | C |
| 1 | lA | 396 | G |
| 1 | lA | 397 | A |
| 1 | lA | 416 | U |
| 1 | lA | 422 | G |
| 1 | lA | 423 | A |
| 1 | lA | 424 | A |
| 1 | lA | 444 | A |
| 1 | lA | 446 | A |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1 | lA | 447 | G |
| 1 | lA | 448 | C |
| 1 | lA | 449 | U |
| 1 | lA | 452 | A |
| 1 | lA | 457 | G |
| 1 | lA | 467 | A |
| 1 | lA | 474 | A |
| 1 | lA | 483 | G |
| 1 | lA | 493 | G |
| 1 | lA | 494 | G |
| 1 | lA | 495 | A |
| 1 | lA | 496 | A |
| 1 | lA | 501 | U |
| 1 | lA | 510 | A |
| 1 | lA | 522 | G |
| 1 | lA | 535 | A |
| 1 | lA | 536 | G |
| 1 | lA | 538 | A |
| 1 | lA | 539 | G |
| 1 | lA | 550 | A |
| 1 | lA | 561 | G |
| 1 | lA | 562 | A |
| 1 | lA | 564 | A |
| 1 | lA | 565 | U |
| 1 | lA | 571 | A |
| 1 | lA | 575 | A |
| 1 | lA | 577 | G |
| 1 | lA | 586 | A |
| 1 | lA | 588 | G |
| 1 | lA | 589 | A |
| 1 | lA | 596 | G |
| 1 | lA | 600 | U |
| 1 | lA | 610 | A |
| 1 | lA | 612 | A |
| 1 | lA | 613 | G |
| 1 | lA | 614 | U |
| 1 | lA | 615 | G |
| 1 | lA | 619 | A |
| 1 | lA | 620 | U |
| 1 | lA | 625 | A |
| 1 | lA | 626 | A |
| 1 | lA | 627 | A |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1 | lA | 629 | G |
| 1 | lA | 630 | A |
| 1 | lA | 631 | G |
| 1 | lA | 632 | G |
| 1 | lA | 637 | U |
| 1 | lA | 638 | A |
| 1 | lA | 644 | A |
| 1 | lA | 645 | A |
| 1 | lA | 646 | U |
| 1 | lA | 647 | C |
| 1 | lA | 649 | U |
| 1 | lA | 651 | G |
| 1 | lA | 652 | U |
| 1 | lA | 658 | A |
| 1 | lA | 663 | G |
| 1 | lA | 675 | A |
| 1 | lA | 685 | A |
| 1 | lA | 687 | U |
| 1 | lA | 696 | G |
| 1 | lA | 699 | A |
| 1 | lA | 700 | A |
| 1 | lA | 701 | A |
| 1 | lA | 703 | G |
| 1 | lA | 704 | C |
| 1 | lA | 710 | A |
| 1 | lA | 711 | A |
| 1 | lA | 714 | U |
| 1 | lA | 715 | A |
| 1 | lA | 720 | U |
| 1 | lA | 721 | A |
| 1 | lA | 722 | A |
| 1 | lA | 724 | A |
| 1 | lA | 725 | A |
| 1 | lA | 726 | A |
| 1 | lA | 727 | U |
| 1 | lA | 728 | U |
| 1 | lA | 730 | A |
| 1 | lA | 733 | C |
| 1 | lA | 734 | C |
| 1 | lA | 736 | G |
| 1 | lA | 740 | A |
| 1 | lA | 744 | A |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1 | lA | 746 | A |
| 1 | lA | 747 | C |
| 1 | lA | 755 | G |
| 1 | lA | 770 | C |
| 1 | lA | 771 | C |
| 1 | lA | 783 | A |
| 1 | lA | 794 | A |
| 1 | lA | 811 | A |
| 1 | lA | 816 | G |
| 1 | lA | 817 | A |
| 1 | lA | 818 | A |
| 1 | lA | 825 | G |
| 1 | lA | 832 | A |
| 1 | lA | 833 | U |
| 1 | lA | 834 | A |
| 1 | lA | 835 | A |
| 1 | lA | 841 | A |
| 1 | lA | 851 | A |
| 1 | lA | 852 | A |
| 1 | lA | 853 | A |
| 1 | lA | 854 | A |
| 1 | lA | 855 | A |
| 1 | lA | 864 | G |
| 1 | lA | 872 | A |
| 1 | lA | 873 | U |
| 1 | lA | 874 | A |
| 1 | lA | 875 | C |
| 1 | lA | 881 | G |
| 1 | lA | 889 | A |
| 1 | lA | 898 | U |
| 1 | lA | 904 | A |
| 1 | lA | 905 | A |
| 1 | lA | 918 | G |
| 1 | lA | 920 | A |
| 1 | lA | 925 | A |
| 1 | lA | 934 | G |
| 1 | lA | 936 | A |
| 1 | lA | 954 | G |
| 1 | lA | 976 | G |
| 1 | lA | 980 | A |
| 1 | lA | 993 | U |
| 1 | lA | 998 | U |

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| Mol | Chain | Res | Type |
|-----|-------|------|------|
| 1 | lA | 999 | G |
| 1 | lA | 1026 | G |
| 1 | lA | 1027 | G |
| 1 | lA | 1028 | G |
| 1 | lA | 1033 | A |
| 1 | lA | 1035 | G |
| 1 | lA | 1036 | A |
| 1 | lA | 1042 | C |
| 1 | lA | 1043 | G |
| 1 | lA | 1044 | A |
| 1 | lA | 1056 | G |
| 1 | lA | 1063 | C |
| 1 | lA | 1078 | C |
| 1 | lA | 1079 | U |
| 1 | lA | 1096 | U |
| 1 | lA | 1097 | U |
| 1 | lA | 1098 | A |
| 1 | lA | 1099 | A |
| 1 | lA | 1100 | U |
| 1 | lA | 1112 | G |
| 1 | lA | 1119 | U |
| 1 | lA | 1120 | A |
| 1 | lA | 1166 | A |
| 1 | lA | 1168 | C |
| 1 | lA | 1183 | G |
| 1 | lA | 1184 | A |
| 1 | lA | 1187 | A |
| 1 | lA | 1210 | C |
| 1 | lA | 1211 | A |
| 1 | lA | 1219 | A |
| 1 | lA | 1220 | A |
| 1 | lA | 1221 | A |
| 1 | lA | 1222 | U |
| 1 | lA | 1242 | G |
| 1 | lA | 1248 | U |
| 1 | lA | 1256 | G |
| 1 | lA | 1269 | U |
| 1 | lA | 1278 | A |
| 1 | lA | 1284 | A |
| 1 | lA | 1291 | G |
| 1 | lA | 1292 | A |
| 1 | lA | 1306 | A |

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| Mol | Chain | Res | Type |
|-----|-------|------|------|
| 1 | lA | 1312 | A |
| 1 | lA | 1314 | A |
| 1 | lA | 1315 | A |
| 1 | lA | 1316 | C |
| 1 | lA | 1325 | C |
| 1 | lA | 1343 | A |
| 1 | lA | 1344 | U |
| 1 | lA | 1345 | U |
| 1 | lA | 1386 | G |
| 1 | lA | 1387 | A |
| 1 | lA | 1388 | A |
| 1 | lA | 1389 | U |
| 1 | lA | 1410 | A |
| 1 | lA | 1411 | A |
| 1 | lA | 1417 | G |
| 1 | lA | 1431 | G |
| 1 | lA | 1433 | U |
| 1 | lA | 1437 | A |
| 1 | lA | 1440 | A |
| 1 | lA | 1441 | U |
| 1 | lA | 1447 | C |
| 1 | lA | 1450 | A |
| 1 | lA | 1455 | A |
| 1 | lA | 1474 | A |
| 1 | lA | 1475 | A |
| 1 | lA | 1476 | G |
| 1 | lA | 1477 | A |
| 1 | lA | 1478 | C |
| 1 | lA | 1480 | U |
| 1 | lA | 1495 | A |
| 1 | lA | 1499 | G |
| 1 | lA | 1500 | A |
| 1 | lA | 1502 | A |
| 1 | lA | 1503 | U |
| 1 | lA | 1505 | G |
| 1 | lA | 1516 | A |
| 1 | lA | 1517 | C |
| 1 | lA | 1518 | A |
| 1 | lA | 1519 | A |
| 1 | lA | 1521 | A |
| 1 | lA | 1527 | A |
| 1 | lA | 1534 | U |

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| Mol | Chain | Res | Type |
|-----|-------|------|------|
| 1 | lA | 1551 | A |
| 1 | lA | 1553 | A |
| 1 | lA | 1568 | G |
| 1 | lA | 1570 | U |
| 1 | lA | 1571 | C |
| 1 | lA | 1580 | A |
| 1 | lA | 1584 | G |
| 1 | lA | 1589 | U |
| 1 | lA | 1601 | G |
| 1 | lA | 1602 | A |
| 1 | lA | 1603 | A |
| 1 | lA | 1604 | A |
| 1 | lA | 1605 | A |
| 1 | lA | 1606 | A |
| 1 | lA | 1607 | A |
| 1 | lA | 1622 | A |
| 1 | lA | 1624 | G |
| 1 | lA | 1648 | U |
| 1 | lA | 1649 | U |
| 1 | lA | 1652 | U |
| 1 | lA | 1674 | U |
| 1 | lA | 1677 | A |
| 1 | lA | 1690 | A |
| 1 | lA | 1698 | G |
| 1 | lA | 1729 | G |
| 1 | lA | 1735 | A |
| 1 | lA | 1737 | A |
| 1 | lA | 1738 | G |
| 1 | lA | 1751 | A |
| 1 | lA | 1752 | U |
| 1 | lA | 1754 | G |
| 1 | lA | 1810 | A |
| 1 | lA | 1818 | C |
| 1 | lA | 1821 | A |
| 1 | lA | 1822 | U |
| 1 | lA | 1823 | C |
| 1 | lA | 1837 | U |
| 1 | lA | 1864 | C |
| 1 | lA | 1865 | U |
| 1 | lA | 1883 | A |
| 1 | lA | 1897 | A |
| 1 | lA | 1903 | A |

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| Mol | Chain | Res | Type |
|-----|-------|------|------|
| 1 | lA | 1907 | A |
| 1 | lA | 1913 | G |
| 1 | lA | 1914 | A |
| 1 | lA | 1925 | A |
| 1 | lA | 1926 | U |
| 1 | lA | 1928 | G |
| 1 | lA | 1936 | A |
| 1 | lA | 1937 | A |
| 1 | lA | 1938 | G |
| 1 | lA | 1959 | U |
| 1 | lA | 1961 | G |
| 1 | lA | 1963 | G |
| 1 | lA | 1965 | U |
| 1 | lA | 1975 | G |
| 1 | lA | 1983 | A |
| 1 | lA | 1984 | A |
| 1 | lA | 1995 | G |
| 1 | lA | 2040 | A |
| 1 | lA | 2043 | A |
| 1 | lA | 2044 | C |
| 1 | lA | 2050 | C |
| 1 | lA | 2051 | A |
| 1 | lA | 2067 | A |
| 1 | lA | 2079 | A |
| 1 | lA | 2080 | A |
| 1 | lA | 2081 | A |
| 1 | lA | 2083 | A |
| 1 | lA | 2095 | G |
| 1 | lA | 2108 | G |
| 1 | lA | 2109 | C |
| 1 | lA | 2178 | A |
| 1 | lA | 2179 | U |
| 1 | lA | 2190 | A |
| 1 | lA | 2193 | G |
| 1 | lA | 2197 | G |
| 1 | lA | 2198 | G |
| 1 | lA | 2207 | A |
| 1 | lA | 2216 | U |
| 1 | lA | 2218 | A |
| 1 | lA | 2234 | A |
| 1 | lA | 2245 | A |
| 1 | lA | 2246 | G |

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| Mol | Chain | Res | Type |
|-----|-------|------|------|
| 1 | lA | 2263 | G |
| 1 | lA | 2264 | A |
| 1 | lA | 2274 | A |
| 1 | lA | 2281 | U |
| 1 | lA | 2282 | G |
| 1 | lA | 2284 | A |
| 1 | lA | 2285 | U |
| 1 | lA | 2286 | G |
| 1 | lA | 2299 | A |
| 1 | lA | 2320 | A |
| 1 | lA | 2325 | G |
| 1 | lA | 2349 | G |
| 1 | lA | 2356 | A |
| 1 | lA | 2360 | C |
| 1 | lA | 2374 | U |
| 1 | lA | 2383 | G |
| 1 | lA | 2384 | C |
| 1 | lA | 2386 | U |
| 1 | lA | 2389 | A |
| 1 | lA | 2390 | U |
| 1 | lA | 2391 | G |
| 1 | lA | 2395 | C |
| 1 | lA | 2396 | A |
| 1 | lA | 2410 | U |
| 1 | lA | 2411 | G |
| 1 | lA | 2412 | U |
| 1 | lA | 2439 | A |
| 1 | lA | 2441 | U |
| 1 | lA | 2449 | A |
| 1 | lA | 2450 | C |
| 1 | lA | 2451 | G |
| 1 | lA | 2461 | G |
| 1 | lA | 2462 | G |
| 1 | lA | 2469 | G |
| 1 | lA | 2473 | A |
| 1 | lA | 2478 | A |
| 1 | lA | 2479 | G |
| 1 | lA | 2480 | A |
| 1 | lA | 2487 | U |
| 1 | lA | 2494 | G |
| 1 | lA | 2509 | U |
| 1 | lA | 2589 | C |

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| Mol | Chain | Res | Type |
|-----|-------|------|------|
| 1 | lA | 2590 | A |
| 1 | lA | 2594 | C |
| 1 | lA | 2595 | G |
| 1 | lA | 2598 | A |
| 1 | lA | 2629 | A |
| 1 | lA | 2637 | A |
| 1 | lA | 2651 | A |
| 1 | lA | 2655 | G |
| 1 | lA | 2656 | G |
| 1 | lA | 2663 | A |
| 1 | lA | 2666 | G |
| 1 | lA | 2676 | G |
| 1 | lA | 2677 | G |
| 1 | lA | 2684 | G |
| 1 | lA | 2689 | G |
| 1 | lA | 2696 | A |
| 1 | lA | 2707 | A |
| 1 | lA | 2715 | G |
| 1 | lA | 2721 | G |
| 1 | lA | 2722 | U |
| 1 | lA | 2726 | A |
| 1 | lA | 2727 | A |
| 1 | lA | 2744 | A |
| 1 | lA | 2747 | G |
| 1 | lA | 2759 | A |
| 1 | lA | 2761 | A |
| 1 | lA | 2764 | A |
| 1 | lA | 2766 | A |
| 1 | lA | 2773 | U |
| 1 | lA | 2774 | A |
| 1 | lA | 2775 | A |
| 1 | lA | 2797 | A |
| 1 | lA | 2798 | G |
| 1 | lA | 2799 | U |
| 1 | lA | 2819 | U |
| 1 | lA | 2822 | U |
| 1 | lA | 2823 | G |
| 1 | lA | 2825 | C |
| 1 | lA | 2842 | U |
| 1 | lA | 2843 | U |
| 1 | lA | 2857 | A |
| 1 | lA | 2904 | U |

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| Mol | Chain | Res | Type |
|-----|-------|------|------|
| 1 | lA | 2905 | U |
| 1 | lA | 2910 | G |
| 1 | lA | 2920 | U |
| 1 | lA | 2925 | A |
| 1 | lA | 2926 | U |
| 1 | lA | 2931 | C |
| 1 | lA | 2939 | G |
| 1 | lA | 2943 | G |
| 1 | lA | 2944 | A |
| 1 | lA | 2945 | A |
| 1 | lA | 2946 | A |
| 1 | lA | 2951 | A |
| 1 | lA | 2953 | C |
| 1 | lA | 2957 | G |
| 1 | lA | 2959 | G |
| 1 | lA | 2960 | A |
| 1 | lA | 2977 | G |
| 1 | lA | 2985 | C |
| 1 | lA | 2987 | C |
| 1 | lA | 2988 | A |
| 1 | lA | 3004 | U |
| 1 | lA | 3009 | C |
| 1 | lA | 3015 | A |
| 1 | lA | 3030 | A |
| 1 | lA | 3041 | G |
| 1 | lA | 3047 | U |
| 1 | lA | 3066 | U |
| 1 | lA | 3070 | C |
| 1 | lA | 3073 | U |
| 1 | lA | 3076 | A |
| 1 | lA | 3078 | U |
| 1 | lA | 3079 | A |
| 1 | lA | 3085 | C |
| 1 | lA | 3090 | G |
| 1 | lA | 3094 | G |
| 1 | lA | 3114 | A |
| 1 | lA | 3126 | C |
| 1 | lA | 3133 | G |
| 1 | lA | 3141 | A |
| 1 | lA | 3142 | G |
| 1 | lA | 3143 | A |
| 1 | lA | 3144 | U |

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| Mol | Chain | Res | Type |
|-----|-------|------|------|
| 1 | lA | 3146 | U |
| 1 | lA | 3147 | U |
| 1 | lA | 3148 | C |
| 1 | lA | 3151 | A |
| 1 | lA | 3159 | G |
| 1 | lA | 3166 | G |
| 1 | lA | 3200 | G |
| 1 | lA | 3210 | U |
| 1 | lA | 3211 | A |
| 1 | lA | 3212 | U |
| 1 | lA | 3213 | U |
| 1 | lA | 3223 | G |
| 1 | lA | 3228 | A |
| 1 | lA | 3232 | G |
| 1 | lA | 3233 | U |
| 1 | lA | 3240 | A |
| 1 | lA | 3246 | A |
| 1 | lA | 3247 | C |
| 1 | lA | 3254 | U |
| 1 | lA | 3256 | A |
| 1 | lA | 3259 | U |
| 1 | lA | 3270 | A |
| 1 | lA | 3277 | C |
| 1 | lA | 3278 | A |
| 1 | lA | 3284 | G |
| 1 | lA | 3285 | A |
| 1 | lA | 3286 | A |
| 1 | lA | 3287 | U |
| 1 | lA | 3299 | G |
| 1 | lA | 3306 | U |
| 1 | lA | 3327 | A |
| 1 | lA | 3332 | A |
| 1 | lA | 3334 | U |
| 1 | lA | 3335 | U |
| 1 | lA | 3336 | G |
| 1 | lA | 3337 | A |
| 1 | lA | 3338 | A |
| 1 | lA | 3345 | A |
| 1 | lA | 3351 | U |
| 1 | lA | 3353 | U |
| 1 | lA | 3359 | U |
| 1 | lA | 3361 | A |

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| Mol | Chain | Res | Type |
|-----|-------|------|------|
| 1 | lA | 3366 | G |
| 1 | lA | 3383 | A |
| 1 | lA | 3384 | A |
| 1 | lA | 3385 | G |
| 1 | lA | 3398 | U |
| 1 | lA | 3399 | G |
| 1 | lA | 3405 | A |
| 1 | lA | 3406 | C |
| 1 | lA | 3414 | A |
| 1 | lA | 3416 | A |
| 1 | lA | 3423 | C |
| 1 | lA | 3430 | U |
| 1 | lA | 3431 | U |
| 1 | lA | 3433 | U |
| 1 | lA | 3447 | A |
| 1 | lA | 3451 | A |
| 1 | lA | 3461 | U |
| 1 | lA | 3492 | C |
| 1 | lA | 3493 | G |
| 1 | lA | 3499 | U |
| 1 | lA | 3500 | G |
| 1 | lA | 3501 | A |
| 2 | lB | 5 | A |
| 2 | lB | 34 | G |
| 2 | lB | 36 | G |
| 2 | lB | 40 | U |
| 2 | lB | 53 | G |
| 2 | lB | 54 | A |
| 2 | lB | 61 | A |
| 2 | lB | 62 | U |
| 2 | lB | 64 | A |
| 2 | lB | 65 | G |
| 2 | lB | 72 | G |
| 2 | lB | 73 | A |
| 2 | lB | 74 | A |
| 2 | lB | 77 | A |
| 2 | lB | 80 | A |
| 2 | lB | 81 | A |
| 2 | lB | 82 | A |
| 2 | lB | 85 | U |
| 2 | lB | 86 | G |
| 2 | lB | 92 | C |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 2 | lB | 95 | A |
| 2 | lB | 102 | A |
| 2 | lB | 103 | A |
| 2 | lB | 104 | U |
| 2 | lB | 106 | C |
| 2 | lB | 109 | G |
| 2 | lB | 110 | A |
| 2 | lB | 113 | G |
| 2 | lB | 137 | A |
| 2 | lB | 147 | C |
| 2 | lB | 150 | U |
| 2 | lB | 151 | A |
| 3 | lC | 17 | G |
| 3 | lC | 19 | U |
| 3 | lC | 22 | C |
| 3 | lC | 32 | A |
| 3 | lC | 37 | A |
| 3 | lC | 40 | G |
| 3 | lC | 52 | G |
| 3 | lC | 53 | C |
| 3 | lC | 63 | C |
| 3 | lC | 72 | C |
| 3 | lC | 73 | G |
| 3 | lC | 90 | G |
| 3 | lC | 96 | U |
| 3 | lC | 99 | U |
| 3 | lC | 109 | G |

There are no RNA pucker outliers to report.

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

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

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

There are no ligands in this entry.

5.7 Other polymers

There are no such residues in this entry.

5.8 Polymer linkage issues

There are no chain breaks in this entry.

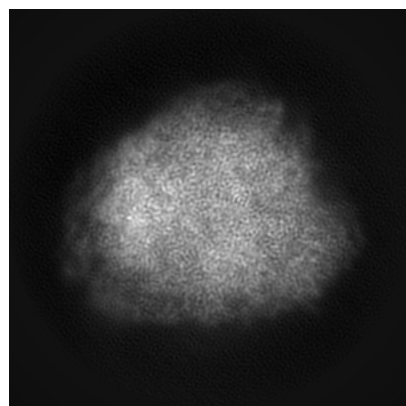
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-64694. These allow visual inspection of the internal detail of the map and identification of artifacts.

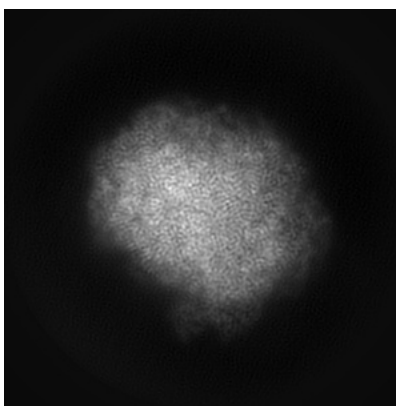
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

6.1 Orthogonal projections [i](#)

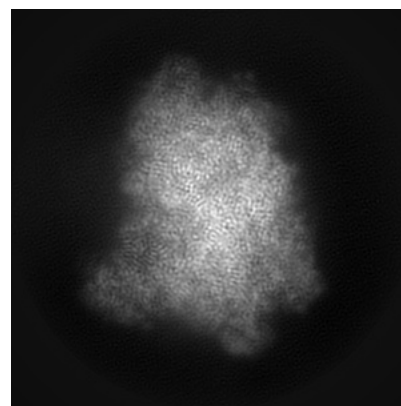
6.1.1 Primary map



X

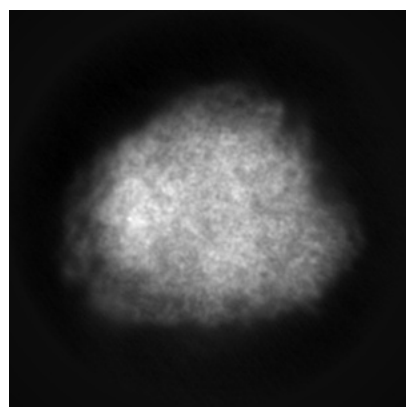


Y

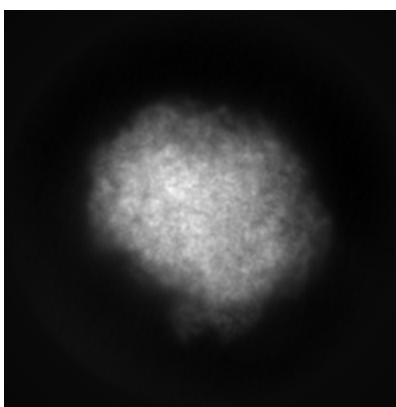


Z

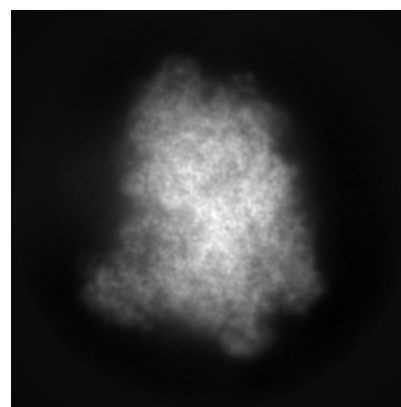
6.1.2 Raw map



X



Y

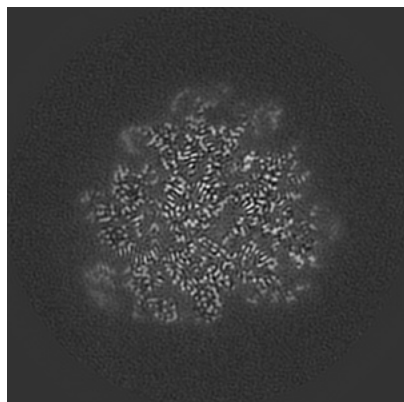


Z

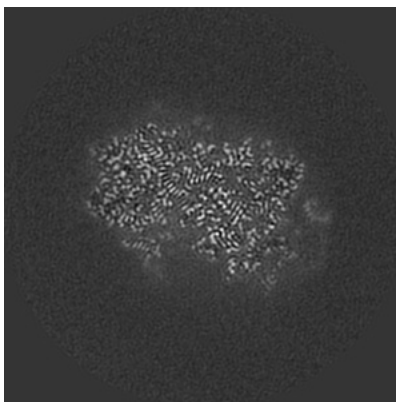
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

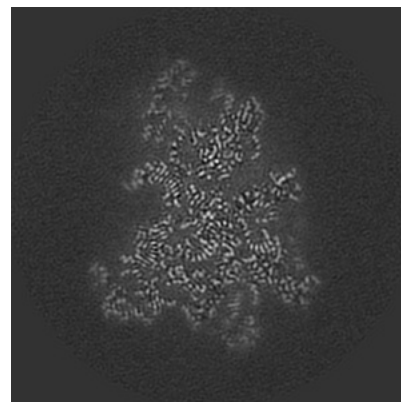
6.2.1 Primary map



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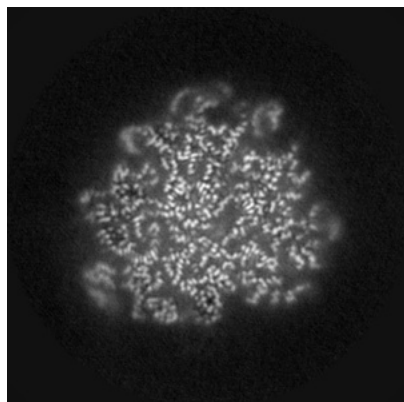


Y Index: 150

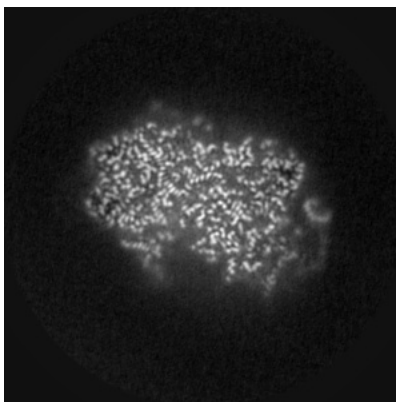


Z Index: 150

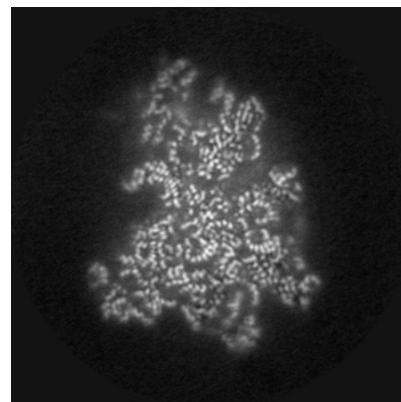
6.2.2 Raw map



X Index: 150



Y Index: 150

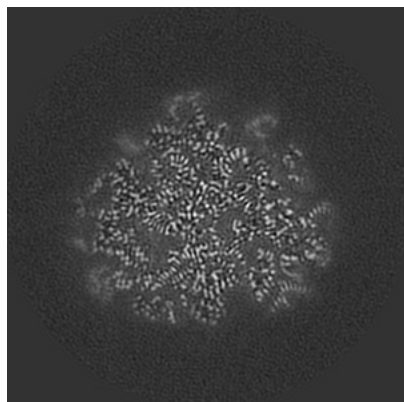


Z Index: 150

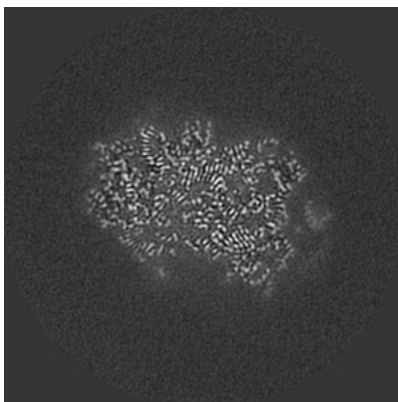
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

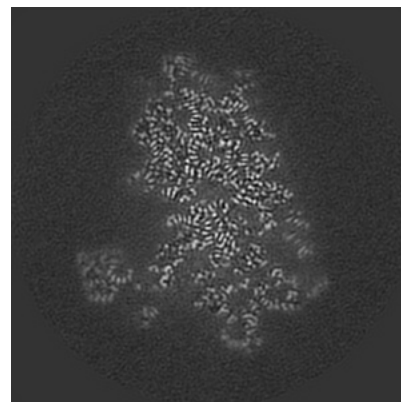
6.3.1 Primary map



X Index: 156

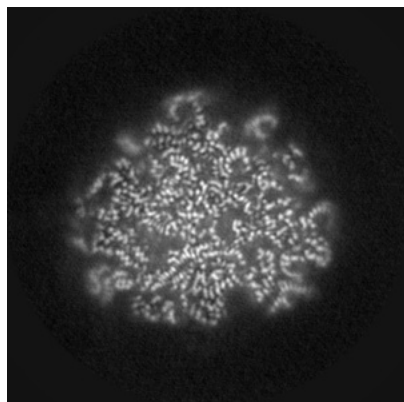


Y Index: 153

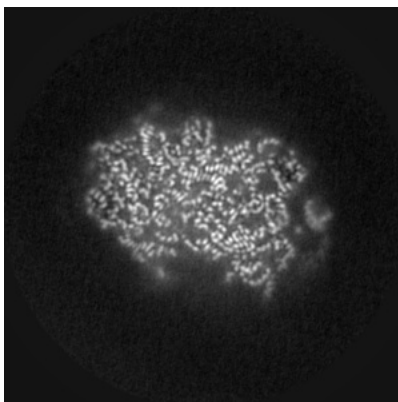


Z Index: 134

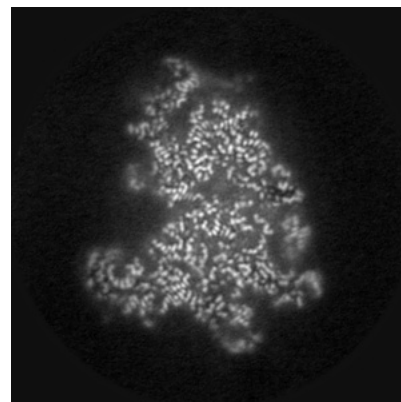
6.3.2 Raw map



X Index: 156



Y Index: 153

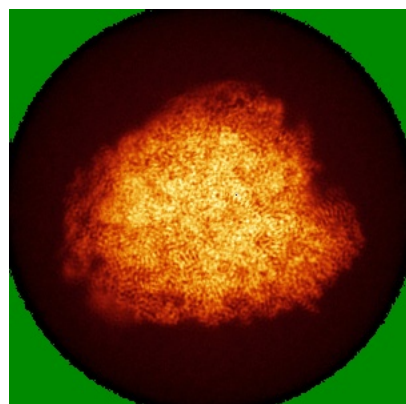


Z Index: 141

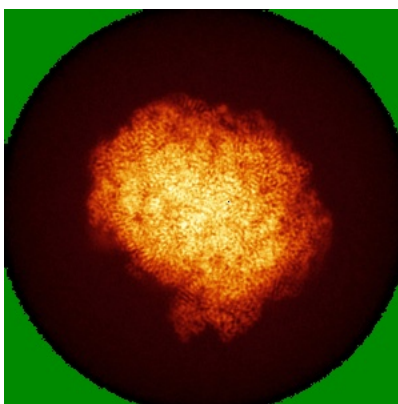
The images above show the largest variance slices of the map in three orthogonal directions.

6.4 Orthogonal standard-deviation projections (False-color) [i](#)

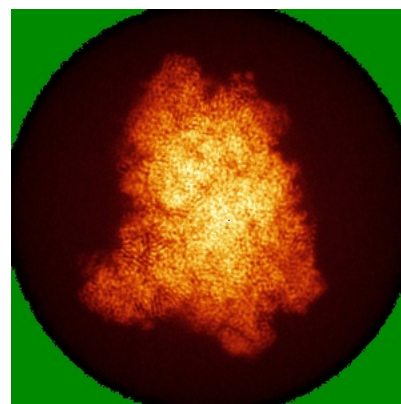
6.4.1 Primary map



X

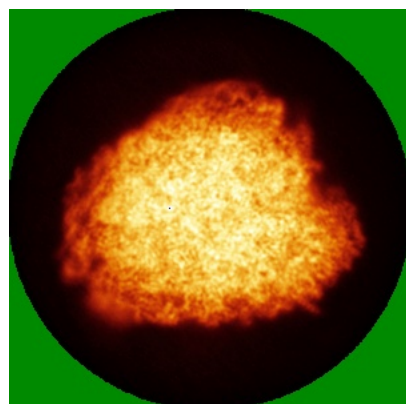


Y

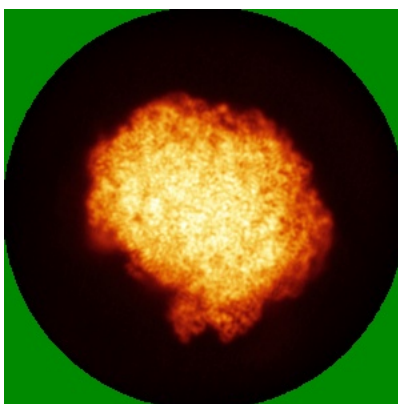


Z

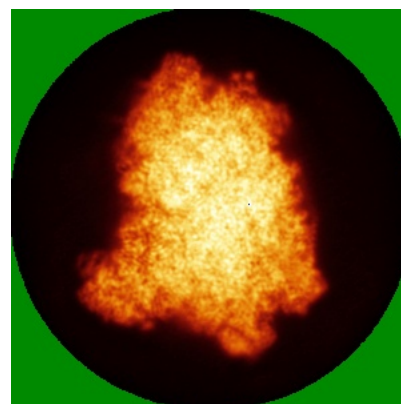
6.4.2 Raw map



X



Y

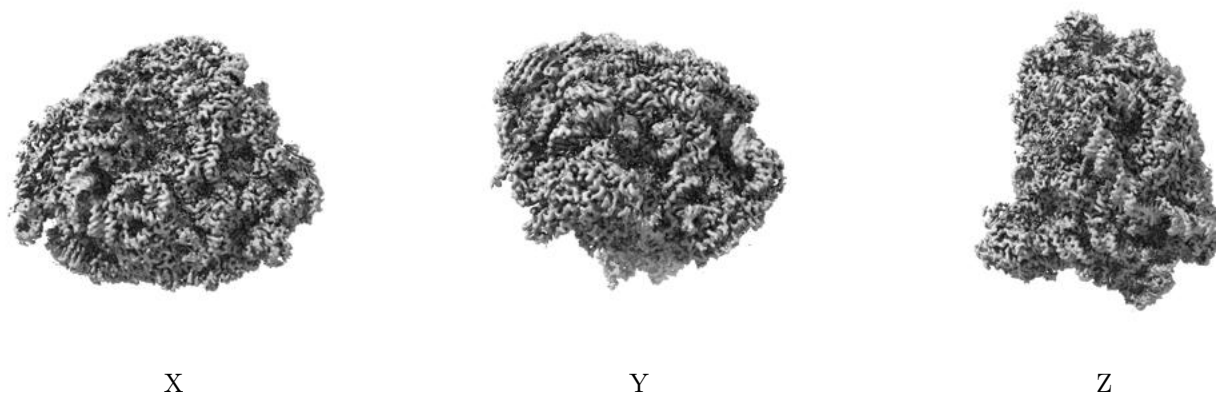


Z

The images above show the map standard deviation projections with false color in three orthogonal directions. Minimum values are shown in green, max in blue, and dark to light orange shades represent small to large values respectively.

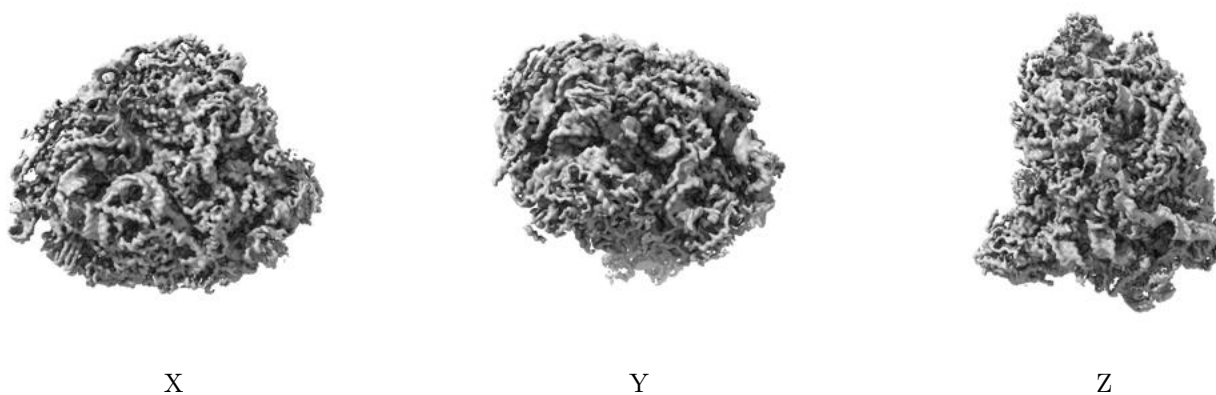
6.5 Orthogonal surface views [i](#)

6.5.1 Primary map



The images above show the 3D surface view of the map at the recommended contour level 2.0. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

6.5.2 Raw map



These images show the 3D surface of the raw map. The raw map's contour level was selected so that its surface encloses the same volume as the primary map does at its recommended contour level.

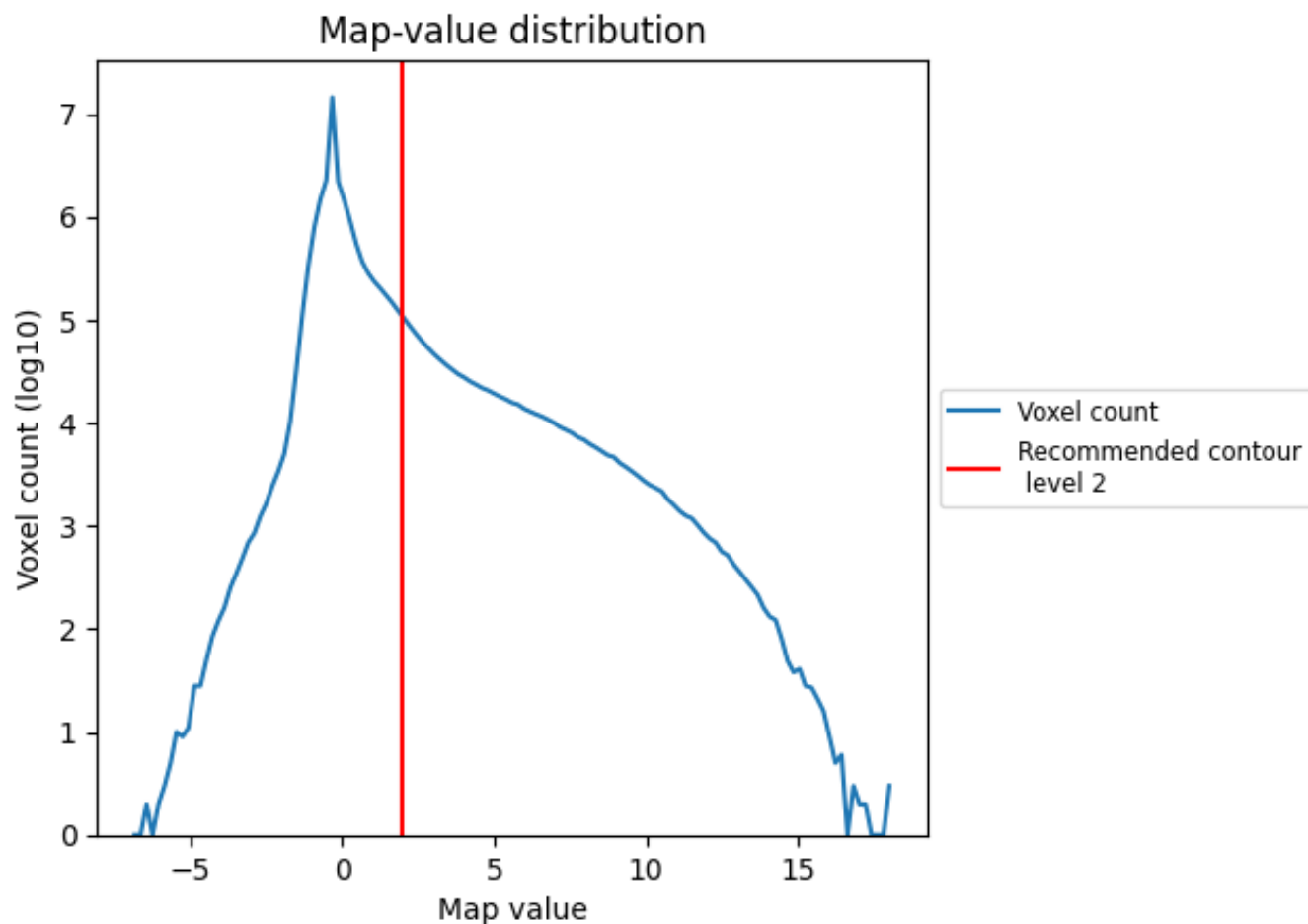
6.6 Mask visualisation [i](#)

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

7 Map analysis [i](#)

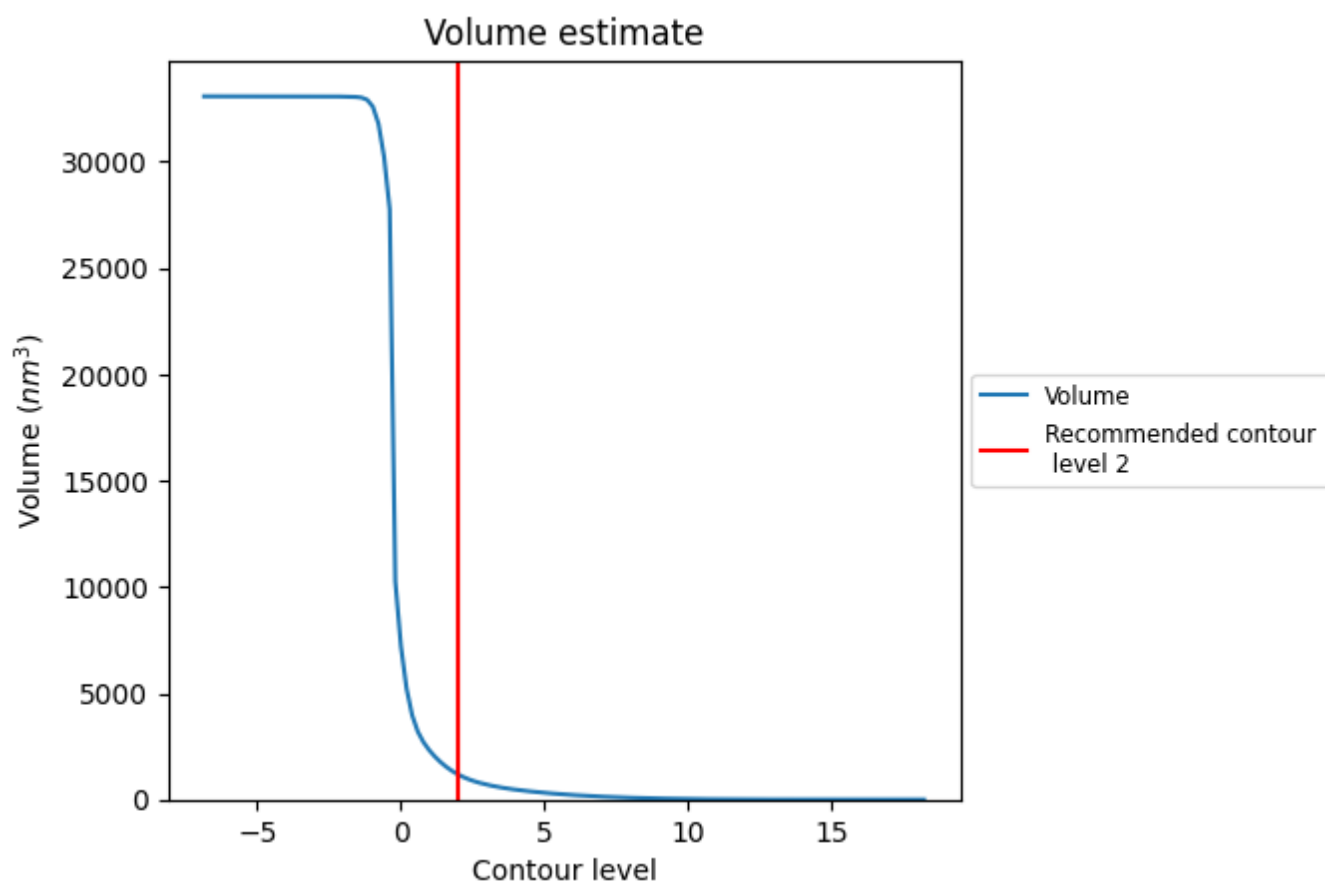
This section contains the results of statistical analysis of the map.

7.1 Map-value distribution [i](#)



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

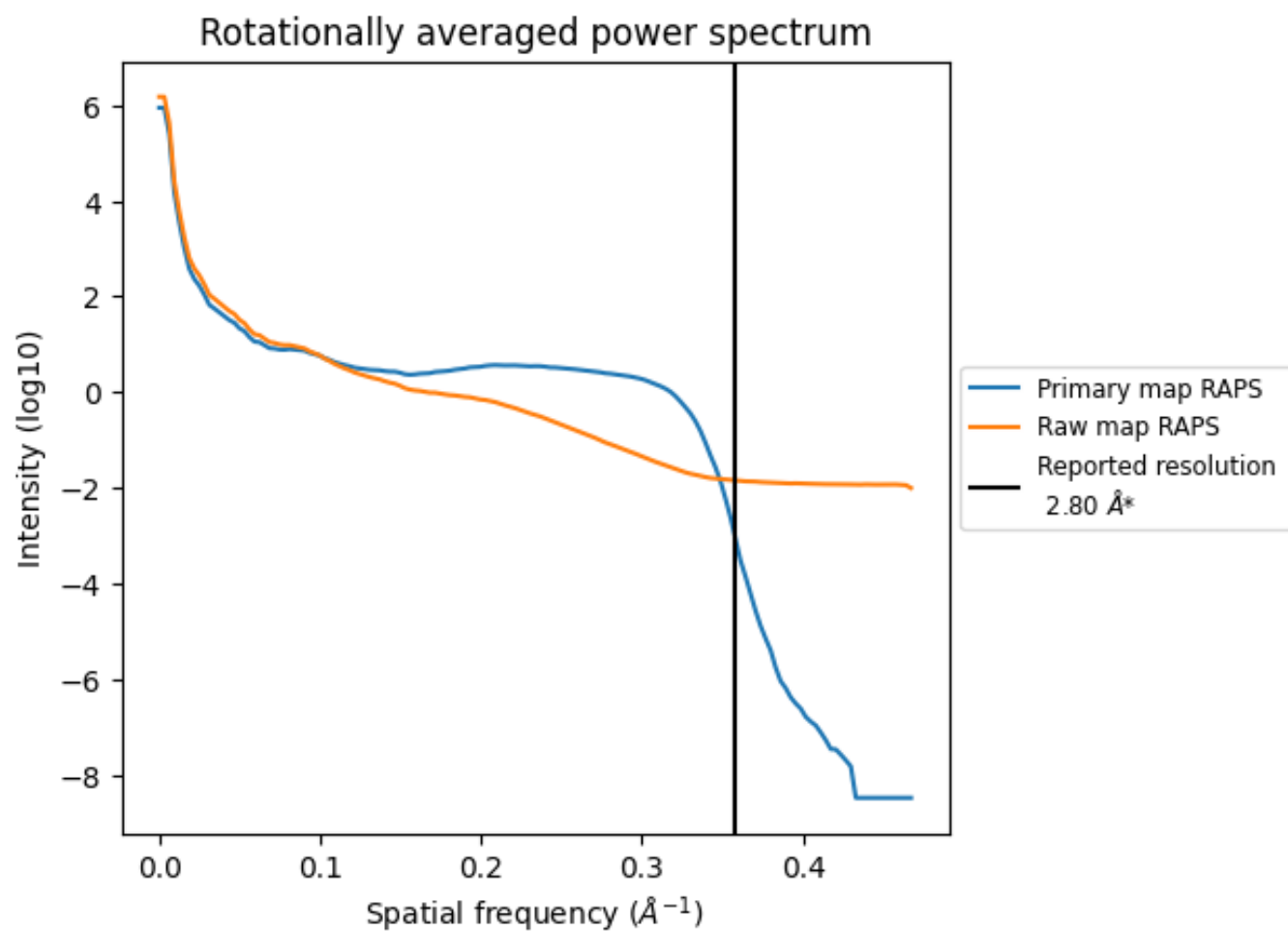
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 1183 nm^3 ; this corresponds to an approximate mass of 1069 kDa.

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

7.3 Rotationally averaged power spectrum ⓘ

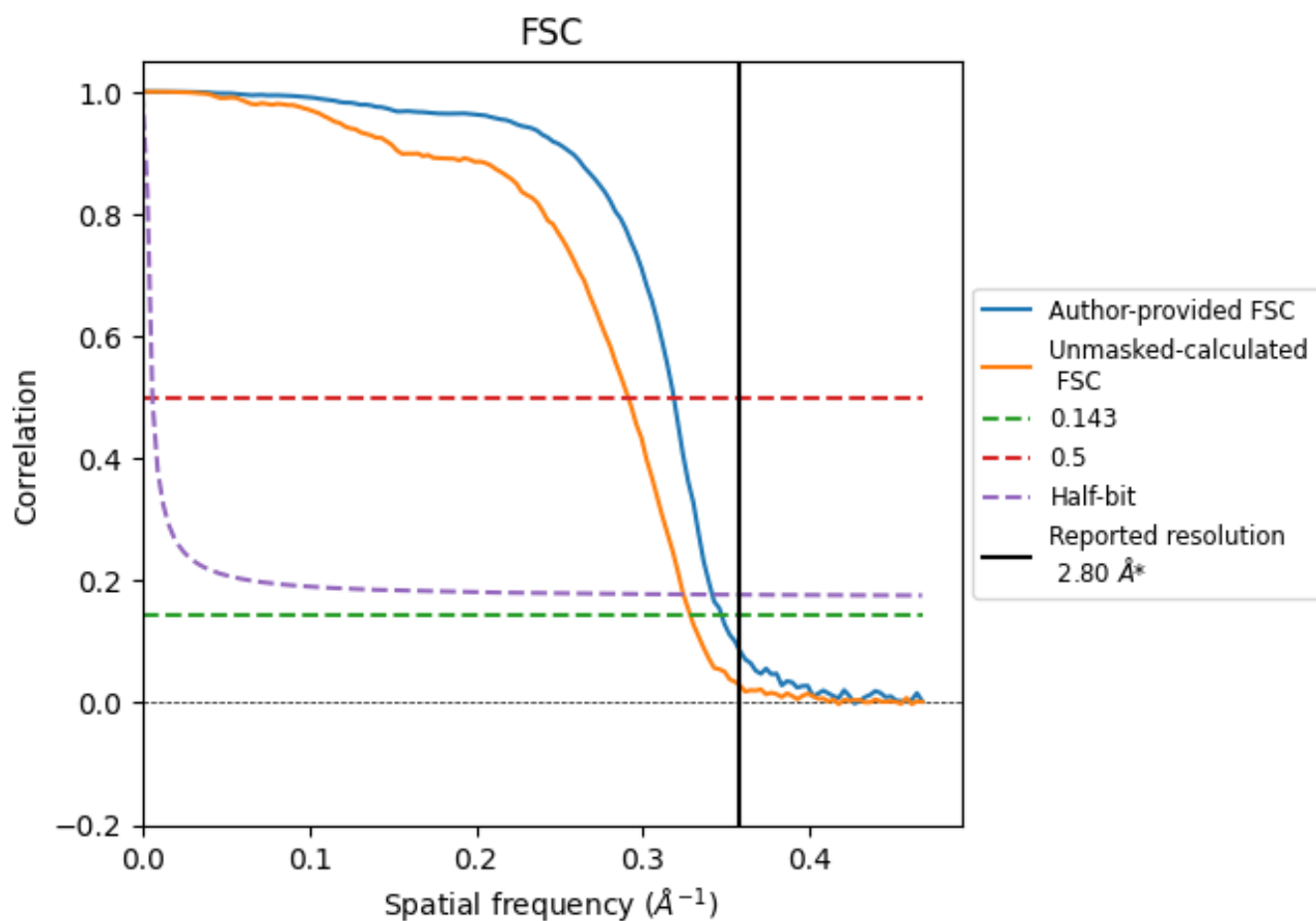


*Reported resolution corresponds to spatial frequency of 0.357 \AA^{-1}

8 Fourier-Shell correlation [i](#)

Fourier-Shell Correlation (FSC) is the most commonly used method to estimate the resolution of single-particle and subtomogram-averaged maps. The shape of the curve depends on the imposed symmetry, mask and whether or not the two 3D reconstructions used were processed from a common reference. The reported resolution is shown as a black line. A curve is displayed for the half-bit criterion in addition to lines showing the 0.143 gold standard cut-off and 0.5 cut-off.

8.1 FSC [i](#)



*Reported resolution corresponds to spatial frequency of 0.357 Å⁻¹

8.2 Resolution estimates [i](#)

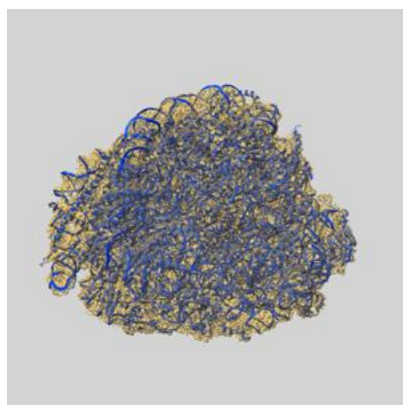
| Resolution estimate (Å) | Estimation criterion (FSC cut-off) | | |
|---------------------------|------------------------------------|------|----------|
| | 0.143 | 0.5 | Half-bit |
| Reported by author | 2.80 | - | - |
| Author-provided FSC curve | 2.88 | 3.14 | 2.93 |
| Unmasked-calculated* | 3.05 | 3.44 | 3.08 |

*Resolution estimate based on FSC curve calculated by comparison of deposited half-maps.

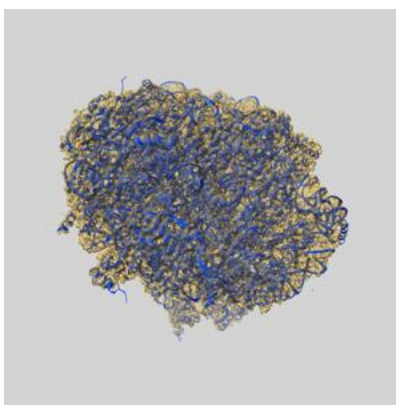
9 Map-model fit [i](#)

This section contains information regarding the fit between EMDB map EMD-64694 and PDB model 9V1I. Per-residue inclusion information can be found in section 3 on page 12.

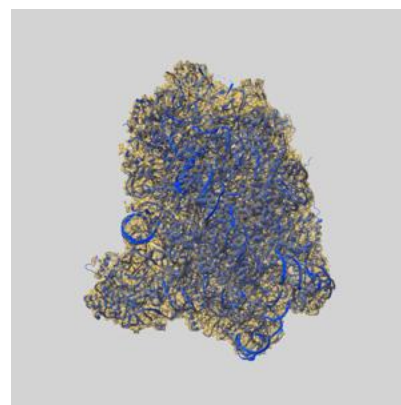
9.1 Map-model overlay [i](#)



X



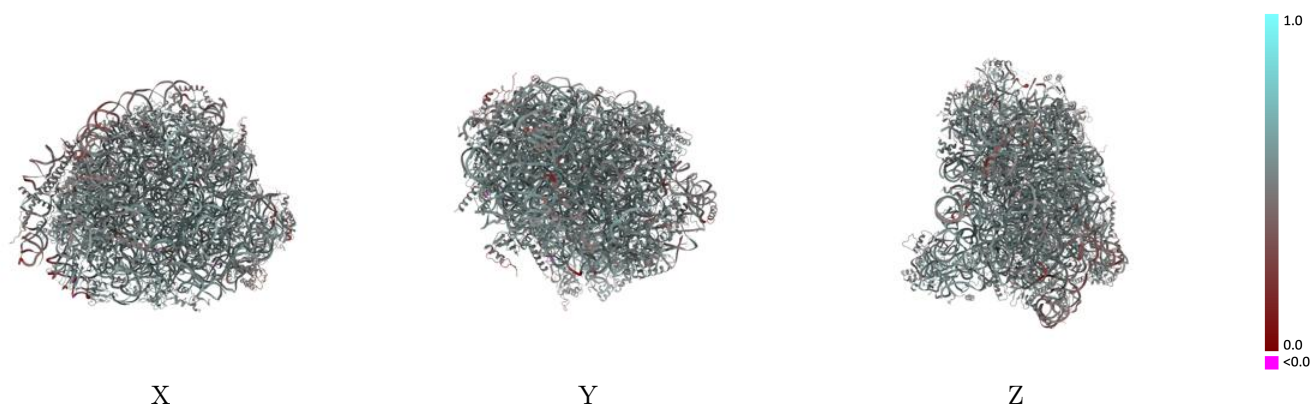
Y



Z

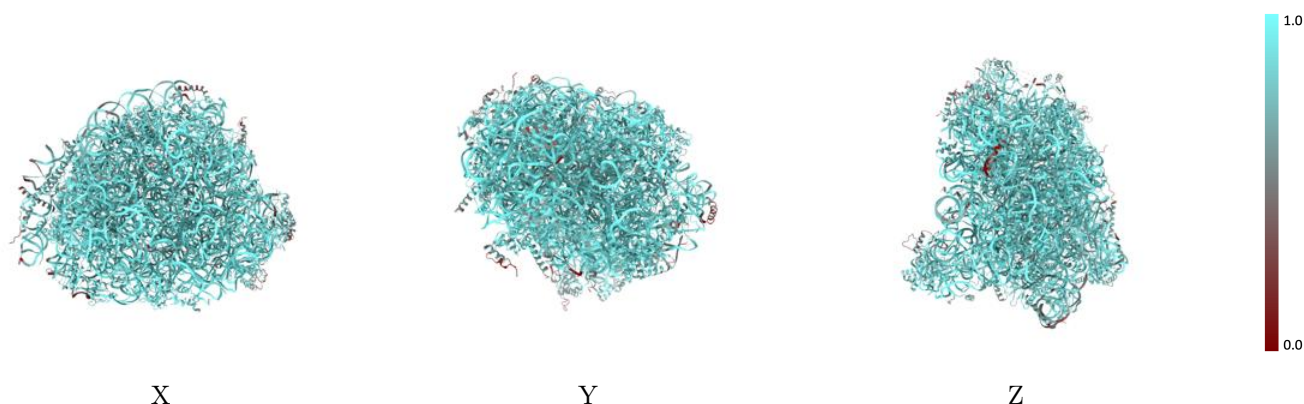
The images above show the 3D surface view of the map at the recommended contour level 2.0 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

9.2 Q-score mapped to coordinate model [i](#)



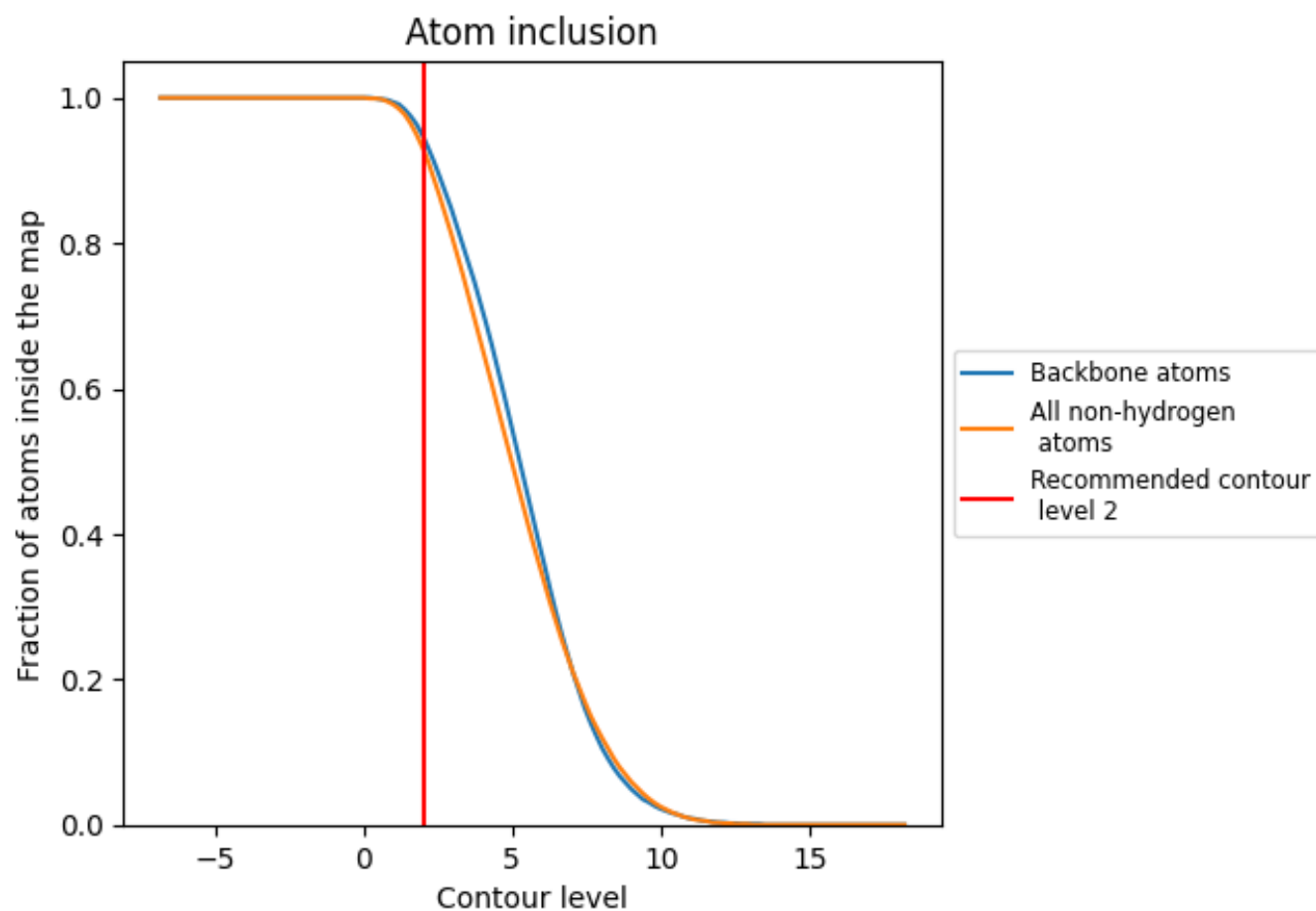
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions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

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



The images above show the model with each residue coloured according to its atom inclusion. This shows to what extent they are inside the map at the recommended contour level (2).







































































9.4 Atom inclusion [i](#)



At the recommended contour level, 95% of all backbone atoms, 93% of all non-hydrogen atoms, are inside the map.

9.5 Map-model fit summary ⓘ





















The table lists the average atom inclusion at the recommended contour level (2) and Q-score for the entire model and for each chain.

| Chain | Atom inclusion | Q-score |
|-------|--|--|
| All |  0.9300 |  0.5260 |
| 1A |  0.9560 |  0.5250 |
| 1B |  0.9860 |  0.5280 |
| 1C |  0.9780 |  0.5440 |
| 1D |  0.9510 |  0.5560 |
| 1E |  0.9400 |  0.5500 |
| 1F |  0.8800 |  0.5260 |
| 1G |  0.8320 |  0.5270 |
| 1H |  0.8100 |  0.4890 |
| 1I |  0.9320 |  0.5320 |
| 1J |  0.7750 |  0.4870 |
| 1K |  0.8960 |  0.5420 |
| 1L |  0.9260 |  0.5460 |
| 1M |  0.6820 |  0.4760 |
| 1N |  0.8290 |  0.5040 |
| 1O |  0.9300 |  0.5480 |
| 1P |  0.9200 |  0.5450 |
| 1Q |  0.9770 |  0.5550 |
| 1R |  0.9400 |  0.5380 |
| 1S |  0.9610 |  0.5370 |
| 1T |  0.9600 |  0.5540 |
| 1U |  0.9070 |  0.5310 |
| 1V |  0.9320 |  0.5550 |
| 1W |  0.6540 |  0.3900 |
| 1X |  0.9460 |  0.5520 |
| 1Y |  0.9080 |  0.5220 |
| 1Z |  0.8870 |  0.5390 |
| 1a |  0.8830 |  0.5060 |
| 1b |  0.7920 |  0.5080 |
| 1c |  0.9590 |  0.5530 |
| 1d |  0.9470 |  0.5490 |
| 1e |  0.7280 |  0.4770 |
| 1f |  0.7940 |  0.4830 |
| 1g |  0.9210 |  0.5230 |
| 1h |  0.9280 |  0.5330 |



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| Chain | Atom inclusion | Q-score |
|-------|--|--|
| li |  0.8940 |  0.5120 |
| lj |  0.9770 |  0.5530 |
| lk |  0.9190 |  0.5270 |
| ll |  0.9840 |  0.5480 |
| lm |  0.8920 |  0.5380 |
| ln |  0.7550 |  0.4650 |
| lo |  0.9830 |  0.5380 |
| lp |  0.9060 |  0.5340 |
| lq |  0.9610 |  0.5560 |
| lr |  0.9540 |  0.5150 |