



Full wwPDB EM Validation Report ⓘ

Oct 28, 2024 – 09:59 am GMT

PDB ID : 5GAH
EMDB ID : EMD-8004
Title : RNC in complex with SRP with detached NG domain
Authors : Jomaa, A.; Boehringer, D.; Leibundgut, M.; Ban, N.
Deposited on : 2015-11-26
Resolution : 3.80 Å(reported)

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

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

A user guide is available at

<https://www.wwpdb.org/validation/2017/EMValidationReportHelp>

with specific help available everywhere you see the ⓘ 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.dev113
MolProbity : 4.02b-467
Percentile statistics : 20231227.v01 (using entries in the PDB archive December 27th 2023)
MapQ : 1.9.13
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.39

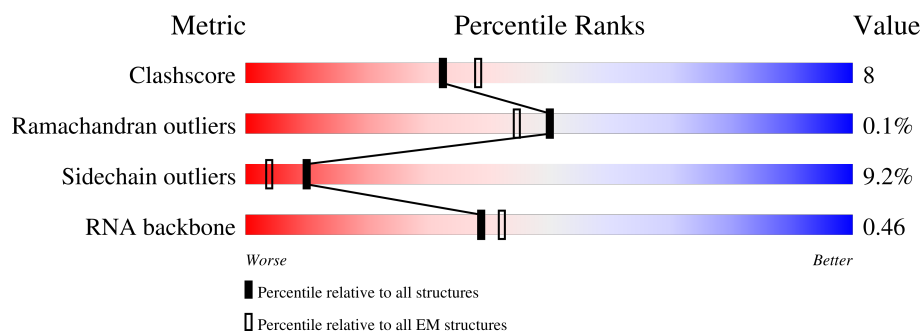
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

ELECTRON MICROSCOPY

The reported resolution of this entry is 3.80 Å.

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



| Metric | Whole archive (#Entries) | EM structures (#Entries) |
|-----------------------|-----------------------------|-----------------------------|
| Clashscore | 210492 | 15764 |
| Ramachandran outliers | 207382 | 16835 |
| Sidechain outliers | 206894 | 16415 |
| RNA backbone | 6643 | 2191 |

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 | 1 | 113 | |
| 2 | 2 | 3 | |
| 3 | A | 2903 | |
| 4 | B | 120 | |
| 5 | C | 273 | |
| 6 | D | 209 | |
| 7 | E | 201 | |

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| Mol | Chain | Length | Quality of chain |
|-----|-------|--------|------------------|
| 8 | F | 179 | |
| 9 | G | 177 | |
| 10 | H | 149 | |
| 11 | I | 165 | |
| 12 | J | 142 | |
| 13 | K | 142 | |
| 14 | L | 123 | |
| 15 | M | 144 | |
| 16 | N | 136 | |
| 17 | O | 127 | |
| 18 | P | 117 | |
| 19 | Q | 115 | |
| 20 | R | 118 | |
| 21 | S | 103 | |
| 22 | T | 110 | |
| 23 | U | 100 | |
| 24 | V | 104 | |
| 25 | W | 94 | |
| 26 | X | 85 | |
| 27 | Y | 78 | |
| 28 | Z | 63 | |
| 29 | a | 59 | |
| 30 | b | 57 | |
| 31 | c | 55 | |
| 32 | d | 46 | |

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| Mol | Chain | Length | Quality of chain |
|-----|-------|--------|--|
| 33 | e | 65 | <div><div></div><div>92%</div><div>6%</div><div></div></div> |
| 34 | f | 38 | <div><div></div><div>92%</div><div>8%</div><div></div></div> |
| 35 | i | 453 | <div><div>9%</div><div>26%</div><div></div><div>72%</div><div></div></div> |
| 36 | k | 18 | <div><div>22%</div><div>89%</div><div>11%</div><div></div></div> |

2 Entry composition

There are 38 unique types of molecules in this entry. The entry contains 94027 atoms, of which 0 are hydrogens and 0 are deuteriums.

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

- Molecule 1 is a RNA chain called SRP 4.5S RNA.

| Mol | Chain | Residues | Atoms | | | | | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|----|---------|-------|
| 1 | 1 | 43 | Total | C | N | O | P | 0 | 0 |
| | | | 926 | 413 | 174 | 296 | 43 | | |

- Molecule 2 is a RNA chain called tRNA CCAend.

| Mol | Chain | Residues | Atoms | | | | | AltConf | Trace |
|-----|-------|----------|-------|----|----|----|---|---------|-------|
| 2 | 2 | 3 | Total | C | N | O | P | 0 | 0 |
| | | | 62 | 28 | 11 | 20 | 3 | | |

- Molecule 3 is a RNA chain called 23S rRNA.

| Mol | Chain | Residues | Atoms | | | | | AltConf | Trace |
|-----|-------|----------|-------|-------|-------|-------|------|---------|-------|
| 3 | A | 2883 | Total | C | N | O | P | 0 | 0 |
| | | | 61902 | 27613 | 11397 | 20009 | 2883 | | |

- Molecule 4 is a RNA chain called 5S rRNA.

| Mol | Chain | Residues | Atoms | | | | | AltConf | Trace |
|-----|-------|----------|-------|------|-----|-----|-----|---------|-------|
| 4 | B | 120 | Total | C | N | O | P | 0 | 0 |
| | | | 2569 | 1144 | 468 | 837 | 120 | | |

- Molecule 5 is a protein called 50S ribosomal protein L2.

| Mol | Chain | Residues | Atoms | | | | | AltConf | Trace |
|-----|-------|----------|-------|------|-----|-----|---|---------|-------|
| 5 | C | 271 | Total | C | N | O | S | 0 | 0 |
| | | | 2082 | 1288 | 423 | 364 | 7 | | |

- Molecule 6 is a protein called 50S ribosomal protein L3.

| Mol | Chain | Residues | Atoms | | | | | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|-------|
| 6 | D | 209 | Total | C | N | O | S | 0 | 0 |
| | | | 1565 | 979 | 288 | 294 | 4 | | |

- Molecule 7 is a protein called 50S ribosomal protein L4.

| Mol | Chain | Residues | Atoms | | | | | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|-------|
| 7 | E | 201 | Total | C | N | O | S | 0 | 0 |
| | | | 1552 | 974 | 283 | 290 | 5 | | |

- Molecule 8 is a protein called 50S ribosomal protein L5.

| Mol | Chain | Residues | Atoms | | | | | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|-------|
| 8 | F | 177 | Total | C | N | O | S | 0 | 0 |
| | | | 1410 | 899 | 249 | 256 | 6 | | |

- Molecule 9 is a protein called 50S ribosomal protein L6.

| Mol | Chain | Residues | Atoms | | | | | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|-------|
| 9 | G | 176 | Total | C | N | O | S | 0 | 0 |
| | | | 1323 | 832 | 243 | 246 | 2 | | |

- Molecule 10 is a protein called 50S ribosomal protein L9.

| Mol | Chain | Residues | Atoms | | | | | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|-------|
| 10 | H | 149 | Total | C | N | O | S | 0 | 0 |
| | | | 1110 | 699 | 197 | 213 | 1 | | |

- Molecule 11 is a protein called 50S ribosomal protein L10.

| Mol | Chain | Residues | Atoms | | | | | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|-------|
| 11 | I | 125 | Total | C | N | O | S | 0 | 0 |
| | | | 946 | 599 | 169 | 175 | 3 | | |

There are 2 discrepancies between the modelled and reference sequences:

| Chain | Residue | Modelled | Actual | Comment | Reference |
|-------|---------|----------|--------|----------|------------|
| I | 85 | VAL | SER | conflict | UNP P0A7J3 |
| I | 86 | THR | MET | conflict | UNP P0A7J3 |

- Molecule 12 is a protein called 50S ribosomal protein L11.

| Mol | Chain | Residues | Atoms | | | | | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|-------|
| 12 | J | 134 | Total | C | N | O | S | 0 | 0 |
| | | | 979 | 619 | 169 | 185 | 6 | | |

- Molecule 13 is a protein called 50S ribosomal protein L13.

| Mol | Chain | Residues | Atoms | | | | | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|-------|
| 13 | K | 142 | Total | C | N | O | S | 0 | 0 |
| | | | 1129 | 714 | 212 | 199 | 4 | | |

- Molecule 14 is a protein called 50S ribosomal protein L14.

| Mol | Chain | Residues | Atoms | | | | | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|-------|
| 14 | L | 123 | Total | C | N | O | S | 0 | 0 |
| | | | 946 | 593 | 181 | 166 | 6 | | |

- Molecule 15 is a protein called 50S ribosomal protein L15.

| Mol | Chain | Residues | Atoms | | | | | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|-------|
| 15 | M | 144 | Total | C | N | O | S | 0 | 0 |
| | | | 1053 | 654 | 207 | 190 | 2 | | |

- Molecule 16 is a protein called 50S ribosomal protein L16.

| Mol | Chain | Residues | Atoms | | | | | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|-------|
| 16 | N | 136 | Total | C | N | O | S | 0 | 0 |
| | | | 1074 | 686 | 205 | 177 | 6 | | |

- Molecule 17 is a protein called 50S ribosomal protein L17.

| Mol | Chain | Residues | Atoms | | | | | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|-------|
| 17 | O | 125 | Total | C | N | O | S | 0 | 0 |
| | | | 993 | 613 | 202 | 173 | 5 | | |

- Molecule 18 is a protein called 50S ribosomal protein L18.

| Mol | Chain | Residues | Atoms | | | | | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|-------|
| 18 | P | 117 | Total | C | N | O | S | 0 | 0 |
| | | | 900 | 557 | 179 | 163 | 1 | | |

- Molecule 19 is a protein called 50S ribosomal protein L19.

| Mol | Chain | Residues | Atoms | | | | | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|-------|
| 19 | Q | 114 | Total | C | N | O | S | 0 | 0 |
| | | | 917 | 574 | 179 | 163 | 1 | | |

- Molecule 20 is a protein called 50S ribosomal protein L20.

| Mol | Chain | Residues | Atoms | | | | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---------|-------|
| 20 | R | 117 | Total | C | N | O | 0 | 0 |
| | | | 947 | 604 | 192 | 151 | | |

- Molecule 21 is a protein called 50S ribosomal protein L21.

| Mol | Chain | Residues | Atoms | | | | | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|-------|
| 21 | S | 103 | Total | C | N | O | S | 0 | 0 |
| | | | 816 | 516 | 153 | 145 | 2 | | |

- Molecule 22 is a protein called 50S ribosomal protein L22.

| Mol | Chain | Residues | Atoms | | | | | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|-------|
| 22 | T | 110 | Total | C | N | O | S | 0 | 0 |
| | | | 857 | 532 | 166 | 156 | 3 | | |

- Molecule 23 is a protein called 50S ribosomal protein L23.

| Mol | Chain | Residues | Atoms | | | | | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|-------|
| 23 | U | 95 | Total | C | N | O | S | 0 | 0 |
| | | | 756 | 479 | 141 | 135 | 1 | | |

- Molecule 24 is a protein called 50S ribosomal protein L24.

| Mol | Chain | Residues | Atoms | | | | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---------|-------|
| 24 | V | 102 | Total | C | N | O | 0 | 0 |
| | | | 779 | 492 | 146 | 141 | | |

- Molecule 25 is a protein called 50S ribosomal protein L25.

| Mol | Chain | Residues | Atoms | | | | | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|-------|
| 25 | W | 94 | Total | C | N | O | S | 0 | 0 |
| | | | 753 | 479 | 137 | 134 | 3 | | |

- Molecule 26 is a protein called 50S ribosomal protein L27.

| Mol | Chain | Residues | Atoms | | | | | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|-------|
| 26 | X | 76 | Total | C | N | O | S | 0 | 0 |
| | | | 580 | 359 | 117 | 103 | 1 | | |

- Molecule 27 is a protein called 50S ribosomal protein L28.

| Mol | Chain | Residues | Atoms | | | | | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|-------|
| 27 | Y | 77 | Total | C | N | O | S | 0 | 0 |
| | | | 625 | 388 | 129 | 106 | 2 | | |

- Molecule 28 is a protein called 50S ribosomal protein L29.

| Mol | Chain | Residues | Atoms | | | | | AltConf | Trace |
|-----|-------|----------|-------|-----|----|----|---|---------|-------|
| 28 | Z | 62 | Total | C | N | O | S | 0 | 0 |
| | | | 501 | 308 | 98 | 94 | 1 | | |

- Molecule 29 is a protein called 50S ribosomal protein L30.

| Mol | Chain | Residues | Atoms | | | | | AltConf | Trace |
|-----|-------|----------|-------|-----|----|----|---|---------|-------|
| 29 | a | 58 | Total | C | N | O | S | 0 | 0 |
| | | | 449 | 281 | 87 | 79 | 2 | | |

- Molecule 30 is a protein called 50S ribosomal protein L32.

| Mol | Chain | Residues | Atoms | | | | | AltConf | Trace |
|-----|-------|----------|-------|-----|----|----|---|---------|-------|
| 30 | b | 56 | Total | C | N | O | S | 0 | 0 |
| | | | 444 | 269 | 94 | 80 | 1 | | |

- Molecule 31 is a protein called 50S ribosomal protein L33.

| Mol | Chain | Residues | Atoms | | | | AltConf | Trace |
|-----|-------|----------|-------|-----|----|----|---------|-------|
| 31 | c | 51 | Total | C | N | O | 0 | 0 |
| | | | 414 | 266 | 76 | 72 | | |

- Molecule 32 is a protein called 50S ribosomal protein L34.

| Mol | Chain | Residues | Atoms | | | | | AltConf | Trace |
|-----|-------|----------|-------|-----|----|----|---|---------|-------|
| 32 | d | 46 | Total | C | N | O | S | 0 | 0 |
| | | | 377 | 228 | 90 | 57 | 2 | | |

- Molecule 33 is a protein called 50S ribosomal protein L35.

| Mol | Chain | Residues | Atoms | | | | | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|----|---|---------|-------|
| 33 | e | 64 | Total | C | N | O | S | 0 | 0 |
| | | | 504 | 323 | 105 | 74 | 2 | | |

- Molecule 34 is a protein called 50S ribosomal protein L36.

| Mol | Chain | Residues | Atoms | | | | | AltConf | Trace |
|-----|-------|----------|-------|-----|----|----|---|---------|-------|
| 34 | f | 38 | Total | C | N | O | S | 0 | 0 |
| | | | 302 | 185 | 65 | 48 | 4 | | |

- Molecule 35 is a protein called Signal recognition particle protein Ffh.

| Mol | Chain | Residues | Atoms | | | | | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|----|---------|-------|
| 35 | i | 126 | Total | C | N | O | S | 0 | 0 |
| | | | 916 | 575 | 169 | 161 | 11 | | |

- Molecule 36 is a protein called 1A9L SS.

| Mol | Chain | Residues | Atoms | | | | | AltConf | Trace |
|-----|-------|----------|-------|----|----|----|---|---------|-------|
| 36 | k | 18 | Total | C | N | O | S | 0 | 0 |
| | | | 137 | 94 | 20 | 22 | 1 | | |

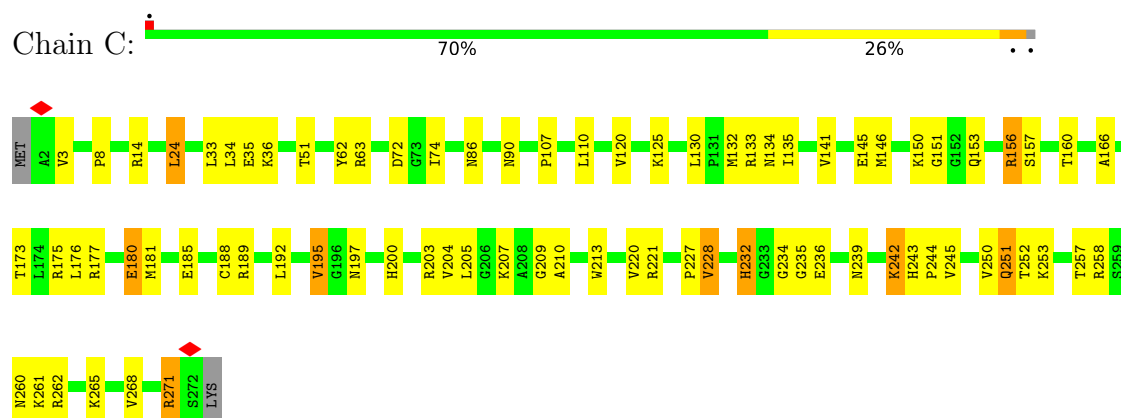
- Molecule 37 is MAGNESIUM ION (three-letter code: MG) (formula: Mg).

| Mol | Chain | Residues | Atoms | | AltConf |
|-----|-------|----------|-------|-----|---------|
| 37 | 2 | 1 | Total | Mg | 0 |
| | | | 1 | 1 | |
| 37 | A | 412 | Total | Mg | 0 |
| | | | 412 | 412 | |
| 37 | B | 11 | Total | Mg | 0 |
| | | | 11 | 11 | |
| 37 | C | 2 | Total | Mg | 0 |
| | | | 2 | 2 | |
| 37 | D | 1 | Total | Mg | 0 |
| | | | 1 | 1 | |
| 37 | E | 1 | Total | Mg | 0 |
| | | | 1 | 1 | |
| 37 | P | 1 | Total | Mg | 0 |
| | | | 1 | 1 | |
| 37 | R | 1 | Total | Mg | 0 |
| | | | 1 | 1 | |
| 37 | b | 1 | Total | Mg | 0 |
| | | | 1 | 1 | |

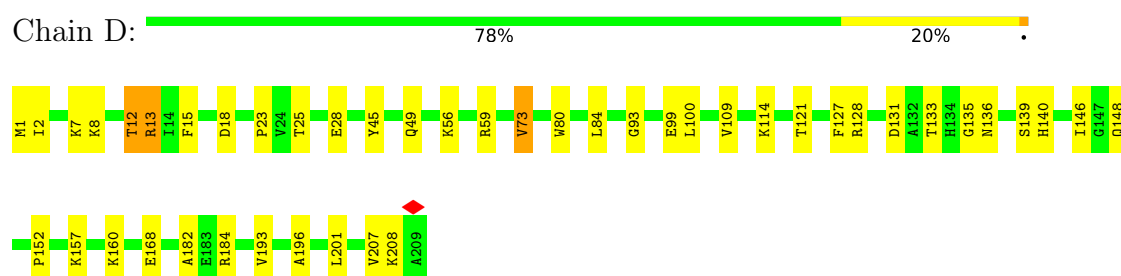
- Molecule 38 is ZINC ION (three-letter code: ZN) (formula: Zn).

| Mol | Chain | Residues | Atoms | | AltConf |
|-----|-------|----------|-------|----|---------|
| 38 | f | 1 | Total | Zn | 0 |
| | | | 1 | 1 | |

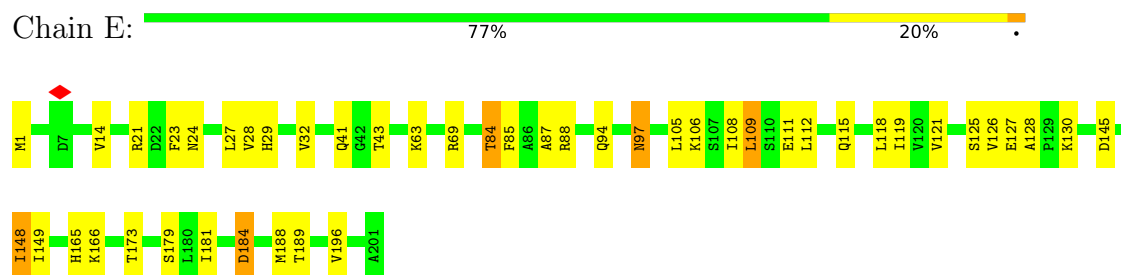
| | | | | | | | | | | | | | |
|-------|-------|-------|-------|-------|-------|-------|-------|-------|------|------|------|------|------|
| G1774 | U1775 | A1672 | U1578 | G1492 | G1410 | U1199 | G1100 | U1023 | U931 | A845 | G776 | A670 | A504 |
| G1673 | G1674 | G1673 | G1581 | C1493 | G1410 | U1199 | G1100 | G1024 | U932 | U846 | G777 | C671 | A505 |
| A1780 | U1781 | G1674 | C1582 | A1494 | C1414 | G1205 | U1101 | G1025 | A933 | U847 | G778 | C672 | C509 |
| U1782 | U1782 | A1677 | U1583 | A1495 | U1415 | A1206 | A1103 | G1026 | C946 | C848 | U779 | C673 | A592 |
| A1785 | A1785 | A1678 | U1584 | U1496 | U1416 | G1210 | U1105 | A1027 | A947 | A849 | G780 | G674 | C510 |
| A1786 | A1786 | A1678 | C1585 | C1498 | C1417 | G1211 | G1106 | A1028 | C948 | U850 | A781 | A677 | U611 |
| A1789 | A1789 | A1681 | C1499 | C1499 | U1418 | G1212 | G1110 | U1033 | G949 | G857 | A782 | C677 | G512 |
| C1790 | C1790 | A1689 | G1500 | U1506 | A1420 | G1218 | G1111 | G1038 | C953 | G858 | A783 | C678 | A513 |
| A1791 | A1791 | G1685 | G1501 | C1507 | G1421 | U1230 | G1112 | A1039 | C957 | U859 | G784 | C679 | A514 |
| A1794 | A1794 | A1700 | A1592 | C1507 | G1422 | U1231 | G1115 | A1040 | C958 | G861 | G785 | C680 | A515 |
| C1795 | C1795 | A1603 | A1598 | C1507 | G1424 | G1236 | G1116 | C1044 | A959 | G862 | A788 | C681 | C516 |
| U1796 | U1796 | A1604 | A1508 | U1508 | G1426 | A1237 | G1125 | A1045 | C961 | U863 | A789 | A685 | G517 |
| G1797 | G1797 | G1605 | U1509 | C1507 | G1427 | G1238 | A1126 | A1046 | C961 | A864 | A790 | U686 | U519 |
| U1798 | U1798 | C1708 | A1609 | G1510 | A1428 | G1243 | A1127 | G1047 | C968 | G869 | A791 | A706 | U521 |
| C1799 | C1799 | C1607 | A1610 | G1511 | G1432 | U1247 | A1129 | A1048 | C969 | U870 | A792 | G707 | C610 |
| A1801 | A1801 | A1608 | A1611 | G1512 | A1433 | G1248 | U1130 | G1056 | C970 | U871 | A793 | A707 | C611 |
| A1802 | A1802 | A1612 | A1612 | G1513 | A1434 | U1249 | U1131 | A1057 | A972 | U872 | A794 | A707 | A526 |
| G1807 | G1807 | A1614 | A1614 | G1514 | A1435 | G1250 | U1132 | U1060 | C973 | C876 | C795 | G711 | C527 |
| A1808 | A1808 | C1615 | A1615 | C1526 | A1436 | G1251 | A1133 | G1061 | A974 | A878 | C796 | G712 | A528 |
| A1809 | A1809 | A1616 | A1616 | C1527 | A1437 | G1252 | A1134 | G1062 | A975 | C879 | C797 | G713 | A529 |
| A1810 | A1810 | C1617 | A1617 | G1528 | A1438 | G1253 | C1135 | G1063 | C976 | G880 | A799 | U714 | G530 |
| G1811 | G1811 | U1725 | A1617 | G1529 | A1439 | A1254 | G1136 | U1066 | A981 | U881 | A800 | U715 | C531 |
| C1815 | C1815 | U1729 | A1618 | G1530 | U1442 | A1255 | G1139 | A1067 | A982 | C877 | A801 | C717 | A532 |
| G1817 | G1817 | G1730 | U1631 | A1531 | U1443 | G1256 | U1141 | G1068 | A983 | A878 | A802 | A718 | G533 |
| U1818 | U1818 | G1731 | G1631 | A1532 | C1446 | G1257 | U1142 | G1069 | A984 | C879 | A803 | C719 | G543 |
| A1819 | A1819 | G1732 | A1634 | U1533 | C1447 | U1258 | A1143 | A1070 | C987 | G880 | A804 | C720 | C544 |
| U1820 | U1820 | U1634 | A1634 | A1534 | G1448 | G1259 | A1144 | G1071 | C988 | U881 | A805 | C721 | U |
| A1821 | A1821 | A1735 | A1637 | C1535 | G1449 | A1260 | G1149 | G1072 | C989 | C882 | A806 | A722 | A |
| C1822 | C1822 | U1736 | C1638 | G1536 | G1450 | A1262 | C1150 | G1073 | C990 | G883 | A807 | G729 | G548 |
| U1825 | U1825 | G1738 | C1639 | U1537 | G1451 | A1266 | G1154 | G1074 | C991 | U884 | U807 | A730 | C549 |
| G1826 | G1826 | G1743 | G1642 | G1542 | A1463 | U1267 | A1155 | C1075 | C992 | C885 | A808 | G733 | C550 |
| U1827 | U1827 | G1744 | G1643 | A1544 | C1463 | A1268 | A1156 | C1076 | C993 | C886 | A809 | U734 | C551 |
| G1828 | G1828 | A1744 | A1545 | G1546 | G1464 | C1269 | G1168 | A1077 | C994 | C887 | A810 | U735 | U552 |
| A1829 | A1829 | U1751 | G1645 | G1546 | G1465 | G1271 | A1169 | U1078 | C995 | C888 | A811 | U736 | U558 |
| C1837 | C1837 | C1752 | C1646 | U1554 | U1466 | A1272 | G1170 | C1079 | C996 | C889 | A812 | U737 | G561 |
| C1838 | C1838 | G1756 | U1647 | G1560 | U1467 | A1275 | C1172 | U1082 | C997 | C890 | A813 | U738 | U562 |
| G1839 | G1839 | A1757 | G1648 | G1560 | U1468 | U1275 | U1173 | U1083 | C998 | C891 | A814 | U739 | C565 |
| G1845 | G1845 | U1758 | G1649 | U1563 | A1470 | A1287 | U | A1084 | C999 | C892 | A815 | U741 | C566 |
| A1847 | A1847 | U1759 | A1652 | C1564 | A1395 | G1288 | U | A1085 | C999 | C893 | C816 | U742 | U567 |
| A1848 | A1848 | C1760 | G1653 | G1565 | U1396 | C1289 | G1177 | A1086 | C999 | C894 | C816 | A743 | U568 |
| G1850 | G1850 | G1761 | A1654 | U1566 | U1397 | C1290 | C1178 | G1087 | C999 | C895 | A819 | U746 | A563 |
| A1853 | A1853 | C1763 | A1655 | A1569 | U1398 | U1294 | G1179 | U1088 | C999 | C896 | A820 | U747 | C564 |
| C1858 | C1858 | A1764 | G1659 | A1570 | C1399 | U1294 | U1180 | A1089 | C999 | C897 | A821 | A753 | C565 |
| U1859 | U1859 | U1769 | G1660 | A1571 | G1401 | U1300 | U1181 | A1090 | C999 | C898 | A822 | U754 | U567 |
| G1869 | G1869 | G1770 | A1664 | A1572 | U1402 | G1301 | G1182 | A1091 | C999 | C899 | A823 | U755 | U568 |
| | | | U1576 | U1576 | A1403 | A1302 | G1187 | A1092 | C999 | C900 | A824 | A756 | U569 |
| | | | U1577 | U1577 | C1404 | A1303 | U1188 | A1093 | C999 | C901 | A825 | G757 | G570 |
| | | | G1667 | G1667 | U1406 | G1303 | U1188 | A1094 | C999 | C902 | A826 | C758 | U571 |
| | | | | | | U1406 | U1198 | A1095 | C999 | C903 | A827 | C759 | A572 |
| | | | | | | | U1198 | A1096 | C999 | C904 | A828 | G763 | A573 |
| | | | | | | | U1198 | A1097 | C999 | C905 | A829 | A764 | A574 |
| | | | | | | | U1198 | A1098 | C999 | C906 | A830 | A765 | A575 |
| | | | | | | | U1198 | A1099 | C999 | C907 | A831 | C765 | U576 |
| | | | | | | | U1198 | A1100 | C999 | C908 | A832 | C772 | G577 |
| | | | | | | | U1198 | A1101 | C999 | C909 | A833 | U773 | C581 |
| | | | | | | | U1198 | A1102 | C999 | C910 | A834 | G774 | G585 |
| | | | | | | | U1198 | A1103 | C999 | C911 | A835 | G775 | |
| | | | | | | | U1198 | A1104 | C999 | C912 | A836 | | |
| | | | | | | | U1198 | A1105 | C999 | C913 | A837 | | |
| | | | | | | | U1198 | A1106 | C999 | C914 | A838 | | |
| | | | | | | | U1198 | A1107 | C999 | C915 | A839 | | |
| | | | | | | | U1198 | A1108 | C999 | C916 | A840 | | |
| | | | | | | | U1198 | A1109 | C999 | C917 | A841 | | |
| | | | | | | | U1198 | A1110 | C999 | C918 | A842 | | |
| | | | | | | | U1198 | A1111 | C999 | C919 | A843 | | |
| | | | | | | | U1198 | A1112 | C999 | C920 | A844 | | |
| | | | | | | | U1198 | A1113 | C999 | C921 | A845 | | |
| | | | | | | | U1198 | A1114 | C999 | C922 | A846 | | |
| | | | | | | | U1198 | A1115 | C999 | C923 | A847 | | |
| | | | | | | | U1198 | A1116 | C999 | C924 | A848 | | |
| | | | | | | | U1198 | A1117 | C999 | C925 | A849 | | |
| | | | | | | | U1198 | A1118 | C999 | C926 | A850 | | |
| | | | | | | | U1198 | A1119 | C999 | C927 | A851 | | |
| | | | | | | | U1198 | A1120 | C999 | C928 | A852 | | |
| | | | | | | | U1198 | A1121 | C999 | C929 | A853 | | |
| | | | | | | | U1198 | A1122 | C999 | C930 | A854 | | |
| | | | | | | | U1198 | A1123 | C999 | C931 | A855 | | |
| | | | | | | | U1198 | A1124 | C999 | C932 | A856 | | |
| | | | | | | | U1198 | A1125 | C999 | C933 | A857 | | |
| | | | | | | | U1198 | A1126 | C999 | C934 | A858 | | |
| | | | | | | | U1198 | A1127 | C999 | C935 | A859 | | |
| | | | | | | | U1198 | A1128 | C999 | C936 | A860 | | |
| | | | | | | | U1198 | A1129 | C999 | C937 | A861 | | |
| | | | | | | | U1198 | A1130 | C999 | C938 | A862 | | |
| | | | | | | | U1198 | A1131 | C999 | C939 | A863 | | |
| | | | | | | | U1198 | A1132 | C999 | C940 | A864 | | |
| | | | | | | | U1198 | A1133 | C999 | C941 | A865 | | |
| | | | | | | | U1198 | A1134 | C999 | C942 | A866 | | |
| | | | | | | | U1198 | A1135 | C999 | C943 | A867 | | |
| | | | | | | | U1198 | A1136 | C999 | C944 | A868 | | |
| | | | | | | | U1198 | A1137 | C999 | C945 | A869 | | |
| | | | | | | | U1198 | A1138 | C999 | C946 | A870 | | |
| | | | | | | | U1198 | A1139 | C999 | C947 | A871 | | |
| | | | | | | | U1198 | A1140 | C999 | C948 | A872 | | |
| | | | | | | | U1198 | A1141 | C999 | C949 | A873 | | |
| | | | | | | | U1198 | A1142 | C999 | C950 | A874 | | |
| | | | | | | | U1198 | A1143 | C999 | C951 | A875 | | |
| | | | | | | | U1198 | A1144 | C999 | C952 | A876 | | |
| | | | | | | | U1198 | A1145 | C999 | C953 | A877 | | |
| | | | | | | | U1198 | A1146 | C999 | C954 | A878 | | |
| | | | | | | | U1198 | A1147 | C999 | C955 | A879 | | |
| | | | | | | | U1198 | A1148 | C999 | C956 | A880 | | |
| | | | | | | | U1198 | A1149 | C999 | C957 | A881 | | |
| | | | | | | | U1198 | A1150 | C999 | C958 | A882 | | |
| | | | | | | | U1198 | A1151 | C999 | C959 | A883 | | |
| | | | | | | | U1198 | A1152 | C999 | C960 | A884 | | |
| | | | | | | | U1198 | A1153 | C999 | C961 | A885 | | |
| | | | | | | | U1198 | A1154 | C999 | C962 | A886 | | |
| | | | | | | | U1198 | A1155 | C999 | C963 | A887 | | |
| | | | | | | | U1198 | A1156 | C999 | C964 | A888 | | |
| | | | | | | | U1198 | A1157 | C999 | C965 | A889 | | |
| | | | | | | | U1198 | A1158 | C999 | C966 | A890 | | |
| | | | | | | | U1198 | A1159 | C999 | C967 | A891 | | |
| | | | | | | | U1198 | A1160 | C999 | C968 | A892 | | |
| | | | | | | | U1198 | A1161 | C999 | C969 | A893 | | |
| | | | | | | | U1198 | A1162 | C999 | C970 | A894 | | |
| | | | | | | | U1198 | A1163 | C999 | C971 | A895 | | |
| | | | | | | | U1198 | A1164 | C999 | C972 | A896 | | |
| | | | | | | | U1198 | A1165 | C999 | C973 | A897 | | |
| | | | | | | | U1198 | A1166 | C999 | C974 | A898 | | |
| | | | | | | | U1198 | A1167 | C999 | C975 | A899 | | |
| | | | | | | | U1198 | | | | | | |



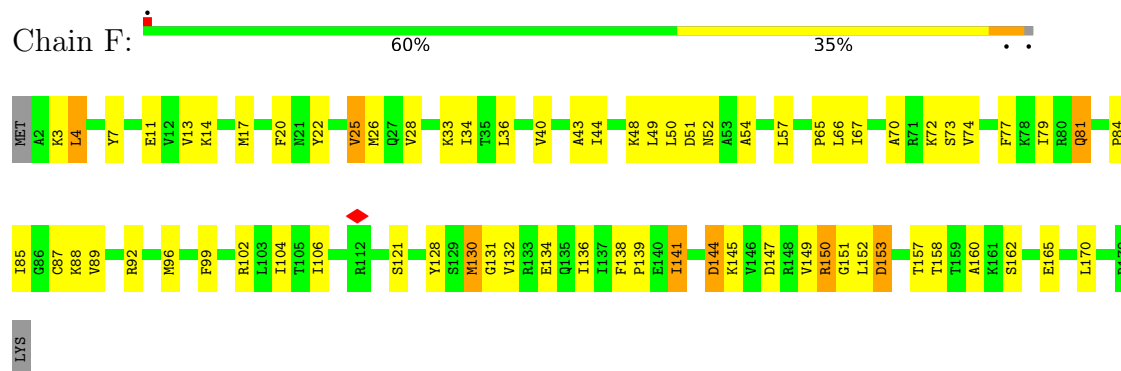
- Molecule 6: 50S ribosomal protein L3



- Molecule 7: 50S ribosomal protein L4

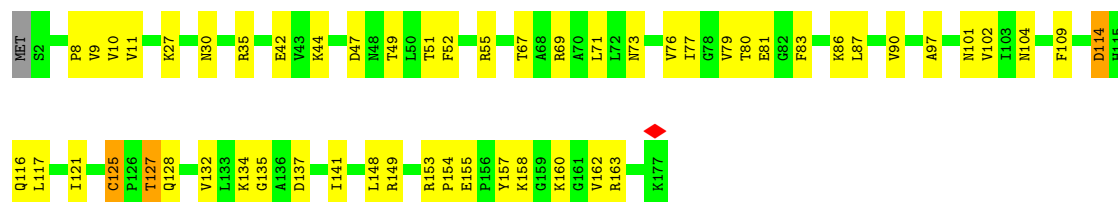


- Molecule 8: 50S ribosomal protein L5

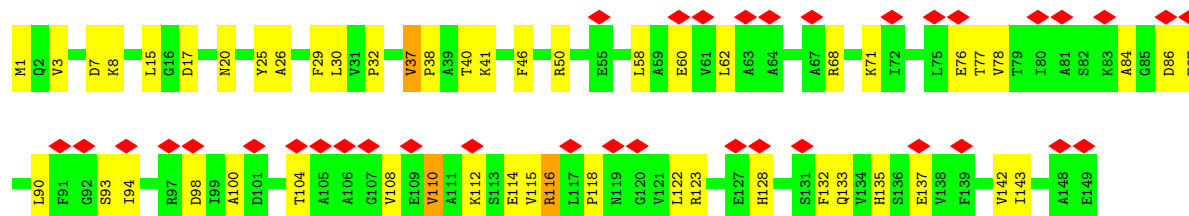


- Molecule 9: 50S ribosomal protein L6

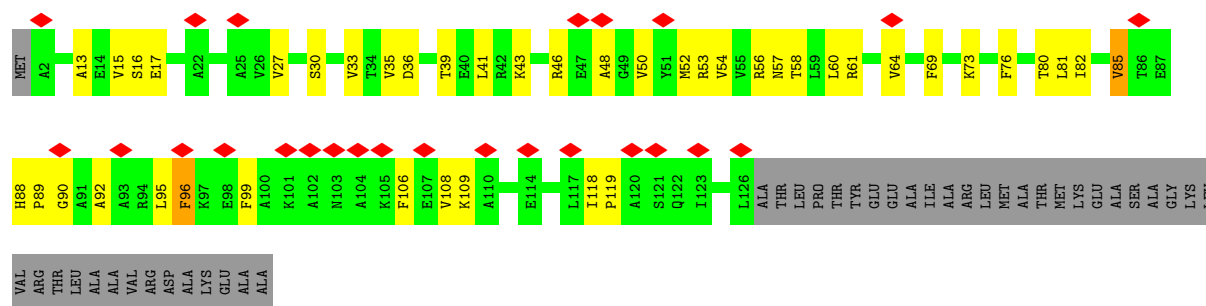




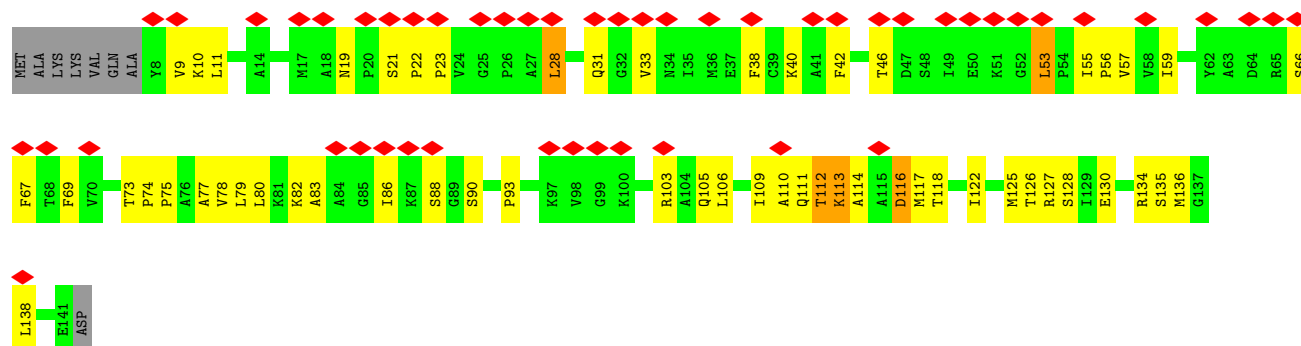
• Molecule 10: 50S ribosomal protein L9



• Molecule 11: 50S ribosomal protein L10

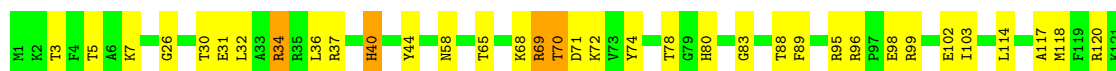


• Molecule 12: 50S ribosomal protein L11



• Molecule 13: 50S ribosomal protein L13





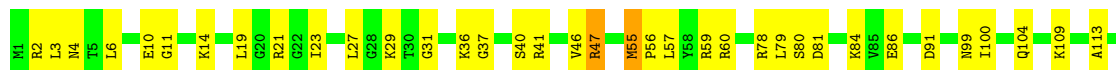
- Molecule 14: 50S ribosomal protein L14

Chain L: 68% 30% .



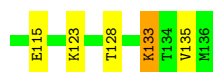
- Molecule 15: 50S ribosomal protein L15

Chain M: 74% 24% .



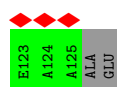
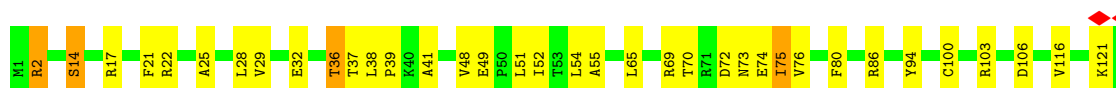
- Molecule 16: 50S ribosomal protein L16

Chain N: 72% 26% .



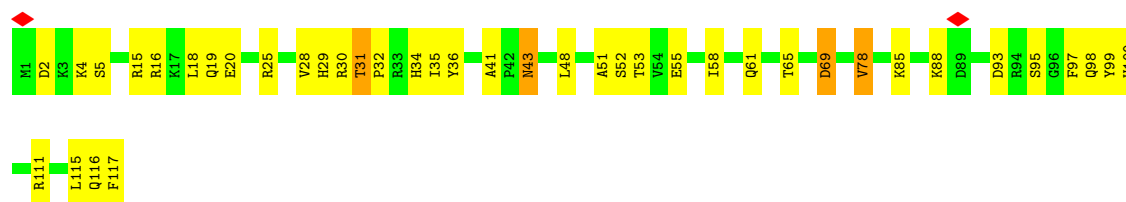
- Molecule 17: 50S ribosomal protein L17

Chain O: 70% 25% . .




- Molecule 18: 50S ribosomal protein L18

Chain P:  65% 32% .




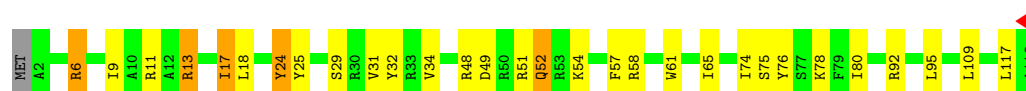
- Molecule 19: 50S ribosomal protein L19

Chain Q:  74% 24% ..



- Molecule 20: 50S ribosomal protein L20

Chain R:  74% 21% ..




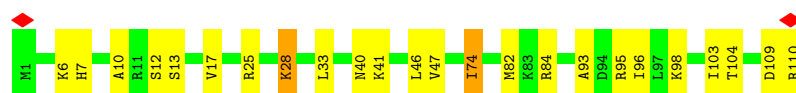
- Molecule 21: 50S ribosomal protein L21

Chain S:  70% 28% .



- Molecule 22: 50S ribosomal protein L22

Chain T:  78% 20% .



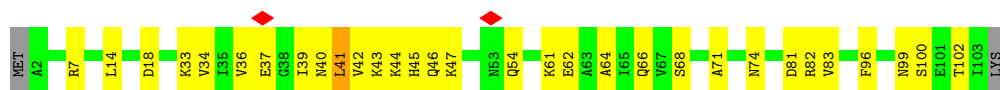
- Molecule 23: 50S ribosomal protein L23

Chain U:  71% 23% . 5%



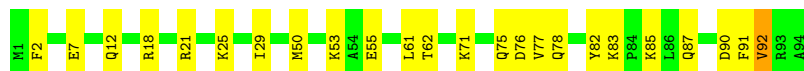
- Molecule 24: 50S ribosomal protein L24

Chain V:  68% 29% ..



- Molecule 25: 50S ribosomal protein L25

Chain W: 74% 24%



- Molecule 26: 50S ribosomal protein L27

Chain X: 59% 28% 11%



- Molecule 27: 50S ribosomal protein L28

Chain Y: 62% 36%



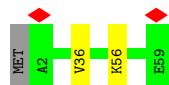
- Molecule 28: 50S ribosomal protein L29

Chain Z: 67% 27% 5%



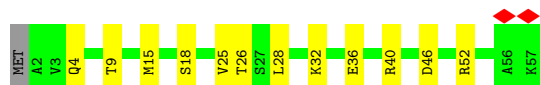
- Molecule 29: 50S ribosomal protein L30

Chain a: 95%



- Molecule 30: 50S ribosomal protein L32

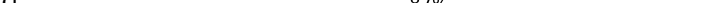
Chain b: 77% 21%

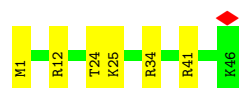


- Molecule 31: 50S ribosomal protein L33



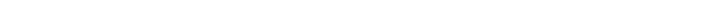
 MET ALA LYS G4 I5 R6 K10 T22 V47 I54 LYS

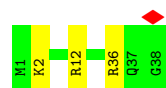
- Chain d:  87% 13%



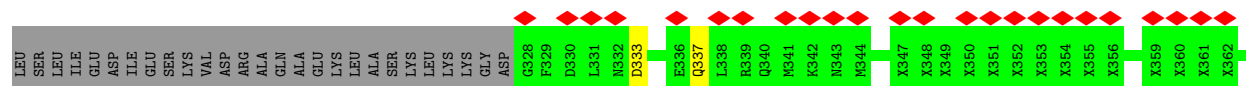
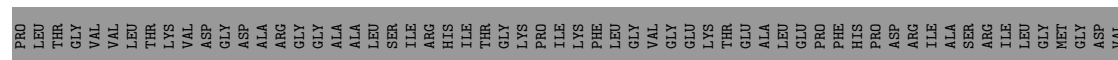
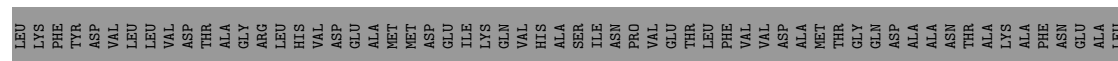
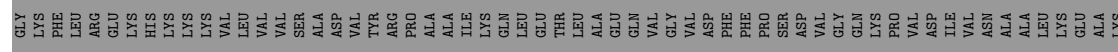
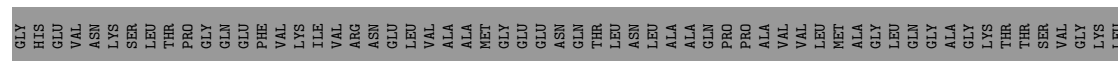
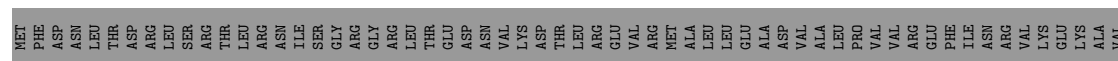
- Chain e: 92% 6%

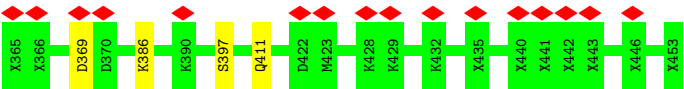


- Chain f:  92% 8%

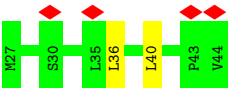
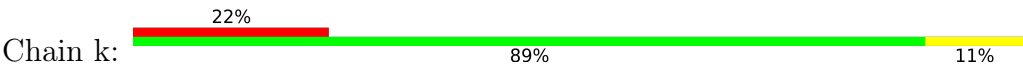


- Chain i:  9% 26% 72%





• Molecule 36: 1A9L SS



4 Experimental information

| Property | Value | Source |
|--------------------------------------|---|-----------|
| EM reconstruction method | SINGLE PARTICLE | Depositor |
| Imposed symmetry | POINT, Not provided | |
| Number of particles used | 46409 | Depositor |
| Resolution determination method | FSC 0.143 CUT-OFF | Depositor |
| CTF correction method | PHASE FLIPPING AND AMPLITUDE CORRECTION | Depositor |
| Microscope | FEI TITAN KRIOS | Depositor |
| Voltage (kV) | 300 | Depositor |
| Electron dose ($e^-/\text{\AA}^2$) | 20 | Depositor |
| Minimum defocus (nm) | Not provided | |
| Maximum defocus (nm) | Not provided | |
| Magnification | Not provided | |
| Image detector | FEI FALCON II (4k x 4k) | Depositor |
| Maximum map value | 0.390 | Depositor |
| Minimum map value | -0.215 | Depositor |
| Average map value | 0.001 | Depositor |
| Map value standard deviation | 0.023 | Depositor |
| Recommended contour level | 0.05 | Depositor |
| Map size (Å) | 398.88, 398.88, 398.88 | wwPDB |
| Map dimensions | 288, 288, 288 | wwPDB |
| Map angles (°) | 90.0, 90.0, 90.0 | wwPDB |
| Pixel spacing (Å) | 1.385, 1.385, 1.385 | Depositor |

5 Model quality

5.1 Standard geometry

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

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

| Mol | Chain | Bond lengths | | Bond angles | |
|-----|-------|--------------|-----------------|-------------|-------------------|
| | | RMSZ | $\# Z > 5$ | RMSZ | $\# Z > 5$ |
| 1 | 1 | 0.79 | 0/1037 | 1.29 | 7/1616 (0.4%) |
| 2 | 2 | 0.57 | 0/68 | 1.25 | 1/103 (1.0%) |
| 3 | A | 0.68 | 14/69329 (0.0%) | 1.17 | 187/108152 (0.2%) |
| 4 | B | 0.51 | 0/2872 | 1.04 | 1/4478 (0.0%) |
| 5 | C | 0.47 | 0/2121 | 0.65 | 0/2852 |
| 6 | D | 0.47 | 0/1586 | 0.63 | 0/2134 |
| 7 | E | 0.44 | 0/1571 | 0.61 | 1/2113 (0.0%) |
| 8 | F | 0.39 | 0/1434 | 0.56 | 0/1926 |
| 9 | G | 0.39 | 0/1343 | 0.58 | 0/1816 |
| 10 | H | 0.42 | 0/1121 | 0.57 | 0/1515 |
| 11 | I | 0.48 | 0/958 | 0.62 | 1/1292 (0.1%) |
| 12 | J | 0.58 | 0/993 | 0.69 | 1/1341 (0.1%) |
| 13 | K | 0.46 | 0/1152 | 0.57 | 0/1551 |
| 14 | L | 0.45 | 0/955 | 0.63 | 0/1279 |
| 15 | M | 0.47 | 0/1062 | 0.64 | 0/1413 |
| 16 | N | 0.48 | 0/1093 | 0.59 | 0/1460 |
| 17 | O | 0.47 | 0/1006 | 0.67 | 0/1345 |
| 18 | P | 0.41 | 0/910 | 0.56 | 0/1219 |
| 19 | Q | 0.48 | 0/929 | 0.60 | 0/1242 |
| 20 | R | 0.56 | 0/960 | 0.59 | 0/1278 |
| 21 | S | 0.46 | 0/829 | 0.62 | 0/1107 |
| 22 | T | 0.52 | 0/864 | 0.71 | 0/1156 |
| 23 | U | 0.45 | 0/763 | 0.61 | 0/1021 |
| 24 | V | 0.38 | 0/787 | 0.54 | 0/1051 |
| 25 | W | 0.40 | 0/766 | 0.57 | 0/1025 |
| 26 | X | 0.50 | 0/587 | 0.60 | 0/776 |
| 27 | Y | 0.48 | 0/635 | 0.61 | 0/848 |
| 28 | Z | 0.41 | 0/502 | 0.54 | 0/667 |
| 29 | a | 0.38 | 0/453 | 0.56 | 0/605 |
| 30 | b | 0.43 | 0/450 | 0.62 | 0/599 |
| 31 | c | 0.44 | 0/421 | 0.61 | 0/561 |
| 32 | d | 0.51 | 0/380 | 0.66 | 0/498 |

| Mol | Chain | Bond lengths | | Bond angles | |
|-----|-------|--------------|------------------|-------------|-------------------|
| | | RMSZ | # Z >5 | RMSZ | # Z >5 |
| 33 | e | 0.47 | 0/513 | 0.62 | 0/676 |
| 34 | f | 0.49 | 0/303 | 0.58 | 0/397 |
| 35 | i | 0.44 | 0/672 | 0.56 | 0/883 |
| 36 | k | 0.62 | 0/137 | 0.85 | 0/186 |
| All | All | 0.63 | 14/101562 (0.0%) | 1.05 | 199/152181 (0.1%) |

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 | C | 0 | 1 |
| 9 | G | 0 | 1 |
| 12 | J | 0 | 1 |
| All | All | 0 | 3 |

All (14) bond length outliers are listed below:

| Mol | Chain | Res | Type | Atoms | Z | Observed(Å) | Ideal(Å) |
|-----|-------|------|------|-------|-------|-------------|----------|
| 3 | A | 2542 | A | N9-C4 | -6.90 | 1.33 | 1.37 |
| 3 | A | 1254 | A | N9-C4 | -6.39 | 1.34 | 1.37 |
| 3 | A | 1321 | A | N9-C4 | 6.27 | 1.41 | 1.37 |
| 3 | A | 1490 | A | N9-C4 | 6.00 | 1.41 | 1.37 |
| 3 | A | 2114 | A | N9-C4 | 5.98 | 1.41 | 1.37 |
| 3 | A | 776 | G | N9-C4 | 5.94 | 1.42 | 1.38 |
| 3 | A | 563 | A | N9-C4 | -5.70 | 1.34 | 1.37 |
| 3 | A | 1254 | A | N3-C4 | -5.57 | 1.31 | 1.34 |
| 3 | A | 586 | A | N3-C4 | -5.30 | 1.31 | 1.34 |
| 3 | A | 1010 | A | N9-C4 | -5.29 | 1.34 | 1.37 |
| 3 | A | 1678 | A | N9-C4 | -5.17 | 1.34 | 1.37 |
| 3 | A | 960 | A | N9-C4 | -5.15 | 1.34 | 1.37 |
| 3 | A | 514 | A | N9-C4 | -5.09 | 1.34 | 1.37 |
| 3 | A | 1269 | A | N9-C4 | -5.01 | 1.34 | 1.37 |

All (199) bond angle outliers are listed below:

| Mol | Chain | Res | Type | Atoms | Z | Observed(°) | Ideal(°) |
|-----|-------|------|------|------------|--------|-------------|----------|
| 3 | A | 2423 | U | C6-N1-C2 | -12.25 | 113.65 | 121.00 |
| 3 | A | 1838 | C | C6-N1-C2 | 9.39 | 124.06 | 120.30 |
| 3 | A | 2422 | C | O4'-C1'-N1 | 9.31 | 115.65 | 108.20 |
| 3 | A | 2423 | U | C5-C6-N1 | 8.80 | 127.10 | 122.70 |

Continued on next page...

Continued from previous page...

| Mol | Chain | Res | Type | Atoms | Z | Observed(°) | Ideal(°) |
|-----|-------|------|------|------------|-------|-------------|----------|
| 3 | A | 1584 | U | C2-N1-C1' | 8.52 | 127.92 | 117.70 |
| 3 | A | 776 | G | C8-N9-C4 | -8.06 | 103.17 | 106.40 |
| 3 | A | 2431 | U | N3-C2-O2 | -7.90 | 116.67 | 122.20 |
| 3 | A | 275 | C | C6-N1-C2 | -7.75 | 117.20 | 120.30 |
| 3 | A | 1760 | C | C6-N1-C2 | 7.62 | 123.35 | 120.30 |
| 3 | A | 1584 | U | N1-C2-O2 | 7.29 | 127.91 | 122.80 |
| 3 | A | 2422 | C | N3-C2-O2 | -7.29 | 116.80 | 121.90 |
| 3 | A | 2431 | U | C5-C4-O4 | 6.99 | 130.10 | 125.90 |
| 3 | A | 1992 | G | C4-C5-N7 | 6.99 | 113.59 | 110.80 |
| 3 | A | 2177 | C | C6-N1-C2 | -6.98 | 117.51 | 120.30 |
| 3 | A | 2614 | A | C6-N1-C2 | -6.84 | 114.49 | 118.60 |
| 3 | A | 2424 | C | O4'-C1'-N1 | 6.83 | 113.66 | 108.20 |
| 3 | A | 2207 | C | C6-N1-C2 | -6.82 | 117.57 | 120.30 |
| 3 | A | 137 | U | C5-C4-O4 | -6.82 | 121.81 | 125.90 |
| 3 | A | 2636 | C | C2-N1-C1' | 6.81 | 126.29 | 118.80 |
| 3 | A | 214 | G | N3-C4-C5 | -6.78 | 125.21 | 128.60 |
| 1 | 1 | 42 | A | O4'-C1'-N9 | 6.62 | 113.49 | 108.20 |
| 3 | A | 1064 | C | C6-N1-C2 | -6.61 | 117.66 | 120.30 |
| 3 | A | 1027 | A | C8-N9-C4 | 6.60 | 108.44 | 105.80 |
| 3 | A | 102 | U | C2-N1-C1' | 6.60 | 125.62 | 117.70 |
| 3 | A | 2422 | C | C6-N1-C2 | -6.60 | 117.66 | 120.30 |
| 3 | A | 776 | G | C4-N9-C1' | 6.57 | 135.04 | 126.50 |
| 3 | A | 1849 | G | C8-N9-C4 | -6.56 | 103.78 | 106.40 |
| 3 | A | 1607 | C | C6-N1-C2 | -6.56 | 117.68 | 120.30 |
| 3 | A | 2542 | A | C2-N3-C4 | -6.54 | 107.33 | 110.60 |
| 3 | A | 2000 | C | C6-N1-C2 | 6.53 | 122.91 | 120.30 |
| 3 | A | 784 | G | P-O3'-C3' | 6.45 | 127.44 | 119.70 |
| 3 | A | 2456 | C | C6-N1-C2 | -6.45 | 117.72 | 120.30 |
| 3 | A | 1531 | C | C5-C6-N1 | 6.45 | 124.22 | 121.00 |
| 3 | A | 2104 | C | C6-N1-C2 | -6.41 | 117.74 | 120.30 |
| 3 | A | 1313 | U | N3-C2-O2 | -6.38 | 117.74 | 122.20 |
| 3 | A | 906 | U | C5-C4-O4 | 6.37 | 129.72 | 125.90 |
| 3 | A | 1849 | G | N7-C8-N9 | 6.36 | 116.28 | 113.10 |
| 3 | A | 1652 | A | C8-N9-C4 | 6.34 | 108.34 | 105.80 |
| 3 | A | 1128 | G | C8-N9-C4 | 6.33 | 108.93 | 106.40 |
| 3 | A | 12 | U | N3-C2-O2 | -6.26 | 117.82 | 122.20 |
| 3 | A | 1695 | G | N9-C4-C5 | -6.24 | 102.91 | 105.40 |
| 3 | A | 1606 | C | N3-C2-O2 | -6.20 | 117.56 | 121.90 |
| 3 | A | 758 | C | C6-N1-C2 | -6.19 | 117.82 | 120.30 |
| 3 | A | 832 | U | C5-C6-N1 | -6.19 | 119.60 | 122.70 |
| 3 | A | 805 | G | C8-N9-C4 | 6.17 | 108.87 | 106.40 |
| 3 | A | 483 | A | C8-N9-C4 | 6.17 | 108.27 | 105.80 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(°) | Ideal(°) |
|-----|-------|------|------|------------|-------|-------------|----------|
| 3 | A | 1470 | A | C8-N9-C4 | -6.14 | 103.34 | 105.80 |
| 3 | A | 1848 | A | C8-N9-C4 | -6.13 | 103.35 | 105.80 |
| 3 | A | 611 | C | C6-N1-C2 | -6.12 | 117.85 | 120.30 |
| 3 | A | 733 | G | C4-C5-N7 | 6.11 | 113.25 | 110.80 |
| 3 | A | 2499 | C | N1-C2-O2 | 6.09 | 122.56 | 118.90 |
| 3 | A | 776 | G | N3-C4-C5 | -6.08 | 125.56 | 128.60 |
| 3 | A | 804 | A | C8-N9-C4 | 6.06 | 108.23 | 105.80 |
| 3 | A | 2704 | C | C6-N1-C2 | -6.06 | 117.88 | 120.30 |
| 3 | A | 1072 | C | C6-N1-C2 | -6.05 | 117.88 | 120.30 |
| 3 | A | 1272 | A | C8-N9-C4 | 6.04 | 108.22 | 105.80 |
| 3 | A | 2542 | A | N3-C4-C5 | 6.04 | 131.03 | 126.80 |
| 3 | A | 1362 | C | C6-N1-C2 | -6.02 | 117.89 | 120.30 |
| 3 | A | 102 | U | N1-C2-O2 | 6.01 | 127.01 | 122.80 |
| 3 | A | 2691 | C | C6-N1-C2 | 6.00 | 122.70 | 120.30 |
| 3 | A | 2109 | U | C6-N1-C2 | -5.99 | 117.40 | 121.00 |
| 3 | A | 2171 | A | O4'-C1'-N9 | 5.97 | 112.98 | 108.20 |
| 1 | 1 | 42 | A | C4-N9-C1' | 5.97 | 137.05 | 126.30 |
| 3 | A | 130 | C | N3-C4-C5 | 5.97 | 124.29 | 121.90 |
| 3 | A | 2077 | A | C6-N1-C2 | -5.97 | 115.02 | 118.60 |
| 3 | A | 1584 | U | C5-C6-N1 | 5.93 | 125.67 | 122.70 |
| 3 | A | 2433 | A | N1-C2-N3 | 5.93 | 132.27 | 129.30 |
| 3 | A | 774 | G | C8-N9-C4 | 5.93 | 108.77 | 106.40 |
| 3 | A | 1261 | C | C6-N1-C2 | 5.90 | 122.66 | 120.30 |
| 3 | A | 1531 | C | C6-N1-C2 | -5.89 | 117.94 | 120.30 |
| 3 | A | 832 | U | C2-N3-C4 | -5.88 | 123.47 | 127.00 |
| 3 | A | 2052 | A | N1-C6-N6 | 5.88 | 122.13 | 118.60 |
| 3 | A | 1992 | G | N9-C4-C5 | -5.85 | 103.06 | 105.40 |
| 3 | A | 2440 | C | C6-N1-C2 | 5.85 | 122.64 | 120.30 |
| 3 | A | 1584 | U | N3-C2-O2 | -5.84 | 118.11 | 122.20 |
| 3 | A | 2153 | C | C5-C6-N1 | 5.84 | 123.92 | 121.00 |
| 12 | J | 53 | LEU | CA-CB-CG | 5.83 | 128.71 | 115.30 |
| 3 | A | 790 | U | N1-C2-O2 | 5.82 | 126.88 | 122.80 |
| 3 | A | 776 | G | O4'-C1'-N9 | 5.81 | 112.85 | 108.20 |
| 3 | A | 2423 | U | N3-C4-C5 | -5.79 | 111.12 | 114.60 |
| 3 | A | 205 | G | O4'-C1'-N9 | 5.79 | 112.83 | 108.20 |
| 3 | A | 141 | G | N7-C8-N9 | 5.77 | 115.98 | 113.10 |
| 3 | A | 816 | C | C6-N1-C2 | -5.74 | 118.00 | 120.30 |
| 3 | A | 2580 | U | C6-N1-C2 | -5.73 | 117.56 | 121.00 |
| 3 | A | 2582 | G | N3-C4-C5 | -5.72 | 125.74 | 128.60 |
| 3 | A | 2588 | G | N3-C4-C5 | 5.72 | 131.46 | 128.60 |
| 3 | A | 1643 | G | C8-N9-C4 | -5.70 | 104.12 | 106.40 |
| 3 | A | 2820 | A | C8-N9-C4 | 5.70 | 108.08 | 105.80 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(°) | Ideal(°) |
|-----|-------|------|------|-----------|-------|-------------|----------|
| 7 | E | 109 | LEU | CA-CB-CG | -5.70 | 102.20 | 115.30 |
| 3 | A | 987 | C | N3-C4-C5 | 5.68 | 124.17 | 121.90 |
| 3 | A | 2845 | U | C2-N3-C4 | -5.68 | 123.59 | 127.00 |
| 3 | A | 783 | A | C8-N9-C4 | -5.67 | 103.53 | 105.80 |
| 3 | A | 1526 | C | C6-N1-C2 | -5.67 | 118.03 | 120.30 |
| 3 | A | 741 | U | C5-C6-N1 | -5.66 | 119.87 | 122.70 |
| 3 | A | 1871 | A | C8-N9-C4 | -5.64 | 103.54 | 105.80 |
| 11 | I | 95 | LEU | CA-CB-CG | 5.64 | 128.27 | 115.30 |
| 3 | A | 793 | A | C5-C6-N6 | -5.64 | 119.19 | 123.70 |
| 3 | A | 1659 | G | N3-C4-C5 | 5.64 | 131.42 | 128.60 |
| 3 | A | 2243 | U | C5-C6-N1 | -5.64 | 119.88 | 122.70 |
| 3 | A | 1045 | C | C6-N1-C2 | 5.62 | 122.55 | 120.30 |
| 3 | A | 793 | A | C2-N3-C4 | 5.60 | 113.40 | 110.60 |
| 3 | A | 1993 | U | C5-C6-N1 | -5.59 | 119.90 | 122.70 |
| 3 | A | 76 | C | C5-C6-N1 | 5.58 | 123.79 | 121.00 |
| 3 | A | 410 | G | N3-C4-C5 | -5.57 | 125.81 | 128.60 |
| 3 | A | 2636 | C | C6-N1-C1' | -5.57 | 114.11 | 120.80 |
| 3 | A | 2145 | C | C6-N1-C2 | -5.56 | 118.08 | 120.30 |
| 3 | A | 776 | G | N7-C8-N9 | 5.54 | 115.87 | 113.10 |
| 3 | A | 2498 | C | C6-N1-C2 | -5.54 | 118.08 | 120.30 |
| 3 | A | 972 | A | N1-C6-N6 | -5.53 | 115.28 | 118.60 |
| 3 | A | 1303 | G | C8-N9-C4 | 5.53 | 108.61 | 106.40 |
| 3 | A | 1314 | C | C6-N1-C2 | -5.50 | 118.10 | 120.30 |
| 3 | A | 1351 | C | C6-N1-C2 | 5.48 | 122.49 | 120.30 |
| 3 | A | 1584 | U | C6-N1-C1' | -5.45 | 113.57 | 121.20 |
| 3 | A | 2022 | U | C6-N1-C2 | 5.45 | 124.27 | 121.00 |
| 3 | A | 1078 | U | C5-C6-N1 | 5.45 | 125.42 | 122.70 |
| 3 | A | 2153 | C | C6-N1-C2 | -5.45 | 118.12 | 120.30 |
| 3 | A | 825 | A | C6-N1-C2 | -5.43 | 115.34 | 118.60 |
| 3 | A | 613 | A | P-O3'-C3' | 5.42 | 126.20 | 119.70 |
| 3 | A | 12 | U | N1-C2-O2 | 5.41 | 126.59 | 122.80 |
| 3 | A | 1604 | C | C5-C6-N1 | -5.41 | 118.29 | 121.00 |
| 3 | A | 793 | A | C5-C6-N1 | 5.40 | 120.40 | 117.70 |
| 3 | A | 206 | U | C2-N1-C1' | 5.40 | 124.18 | 117.70 |
| 3 | A | 280 | U | P-O3'-C3' | 5.40 | 126.18 | 119.70 |
| 3 | A | 2614 | A | C5-C6-N1 | 5.40 | 120.40 | 117.70 |
| 3 | A | 1125 | G | C8-N9-C4 | -5.40 | 104.24 | 106.40 |
| 3 | A | 2595 | G | C4-N9-C1' | -5.39 | 119.49 | 126.50 |
| 3 | A | 2380 | C | C6-N1-C2 | -5.39 | 118.14 | 120.30 |
| 3 | A | 2423 | U | N1-C2-N3 | 5.38 | 118.13 | 114.90 |
| 3 | A | 130 | C | C6-N1-C2 | 5.38 | 122.45 | 120.30 |
| 3 | A | 1642 | G | N3-C4-C5 | 5.37 | 131.29 | 128.60 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(°) | Ideal(°) |
|-----|-------|------|------|------------|-------|-------------|----------|
| 3 | A | 755 | U | C5-C6-N1 | -5.37 | 120.02 | 122.70 |
| 3 | A | 642 | U | O4'-C1'-N1 | 5.35 | 112.48 | 108.20 |
| 3 | A | 1172 | C | C6-N1-C2 | -5.35 | 118.16 | 120.30 |
| 3 | A | 946 | C | N3-C2-O2 | -5.34 | 118.17 | 121.90 |
| 3 | A | 790 | U | C2-N1-C1' | 5.33 | 124.10 | 117.70 |
| 3 | A | 1072 | C | C5-C6-N1 | 5.33 | 123.66 | 121.00 |
| 3 | A | 1970 | A | N1-C2-N3 | 5.32 | 131.96 | 129.30 |
| 1 | 1 | 33 | C | C5-C6-N1 | 5.31 | 123.65 | 121.00 |
| 3 | A | 2645 | G | C4-N9-C1' | 5.30 | 133.39 | 126.50 |
| 3 | A | 2645 | G | N3-C4-C5 | -5.30 | 125.95 | 128.60 |
| 1 | 1 | 42 | A | N7-C8-N9 | 5.30 | 116.45 | 113.80 |
| 3 | A | 128 | C | C6-N1-C2 | 5.29 | 122.42 | 120.30 |
| 3 | A | 1848 | A | N7-C8-N9 | 5.29 | 116.44 | 113.80 |
| 3 | A | 2000 | C | C5-C6-N1 | -5.29 | 118.35 | 121.00 |
| 3 | A | 906 | U | O4'-C1'-N1 | 5.29 | 112.43 | 108.20 |
| 3 | A | 135 | U | C5-C6-N1 | 5.29 | 125.34 | 122.70 |
| 3 | A | 264 | C | N3-C2-O2 | -5.29 | 118.20 | 121.90 |
| 3 | A | 1494 | A | P-O3'-C3' | 5.28 | 126.04 | 119.70 |
| 3 | A | 809 | G | N3-C4-C5 | -5.28 | 125.96 | 128.60 |
| 3 | A | 569 | U | C5-C6-N1 | -5.27 | 120.06 | 122.70 |
| 3 | A | 1606 | C | N1-C2-O2 | 5.26 | 122.06 | 118.90 |
| 3 | A | 1664 | A | C8-N9-C4 | -5.25 | 103.70 | 105.80 |
| 4 | B | 42 | C | C6-N1-C2 | -5.25 | 118.20 | 120.30 |
| 1 | 1 | 42 | A | C6-C5-N7 | -5.25 | 128.62 | 132.30 |
| 3 | A | 375 | G | N3-C4-N9 | 5.24 | 129.15 | 126.00 |
| 3 | A | 1848 | A | O4'-C1'-N9 | 5.24 | 112.39 | 108.20 |
| 3 | A | 2022 | U | C5-C6-N1 | -5.24 | 120.08 | 122.70 |
| 1 | 1 | 42 | A | C8-N9-C1' | -5.23 | 118.28 | 127.70 |
| 3 | A | 972 | A | N9-C4-C5 | 5.23 | 107.89 | 105.80 |
| 3 | A | 672 | C | N3-C2-O2 | -5.22 | 118.25 | 121.90 |
| 3 | A | 2090 | A | C8-N9-C4 | 5.22 | 107.89 | 105.80 |
| 2 | 2 | 74 | C | C5-C6-N1 | 5.20 | 123.60 | 121.00 |
| 3 | A | 828 | U | C5-C6-N1 | -5.20 | 120.10 | 122.70 |
| 3 | A | 2542 | A | C8-N9-C4 | 5.18 | 107.87 | 105.80 |
| 3 | A | 906 | U | C2-N1-C1' | -5.18 | 111.49 | 117.70 |
| 1 | 1 | 70 | G | N3-C4-N9 | 5.17 | 129.10 | 126.00 |
| 3 | A | 2074 | U | C2-N1-C1' | 5.17 | 123.90 | 117.70 |
| 3 | A | 375 | G | N3-C4-C5 | -5.17 | 126.02 | 128.60 |
| 3 | A | 2114 | A | C8-N9-C4 | -5.16 | 103.74 | 105.80 |
| 3 | A | 1769 | U | C5-C6-N1 | -5.15 | 120.12 | 122.70 |
| 3 | A | 981 | A | C8-N9-C4 | 5.12 | 107.85 | 105.80 |
| 3 | A | 30 | G | C8-N9-C4 | 5.10 | 108.44 | 106.40 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(°) | Ideal(°) |
|-----|-------|------|------|-------------|-------|-------------|----------|
| 3 | A | 2115 | G | N3-C4-C5 | -5.10 | 126.05 | 128.60 |
| 3 | A | 2074 | U | N3-C2-O2 | -5.09 | 118.63 | 122.20 |
| 3 | A | 211 | C | C6-N1-C2 | 5.09 | 122.33 | 120.30 |
| 3 | A | 2847 | U | C5-C6-N1 | -5.08 | 120.16 | 122.70 |
| 3 | A | 2267 | A | C8-N9-C4 | -5.08 | 103.77 | 105.80 |
| 3 | A | 646 | U | C6-N1-C2 | -5.07 | 117.96 | 121.00 |
| 3 | A | 271 | G | C8-N9-C4 | 5.07 | 108.43 | 106.40 |
| 3 | A | 2516 | A | C8-N9-C4 | 5.07 | 107.83 | 105.80 |
| 3 | A | 1617 | C | C5-C6-N1 | -5.06 | 118.47 | 121.00 |
| 3 | A | 1958 | C | C6-N1-C2 | -5.06 | 118.28 | 120.30 |
| 3 | A | 1652 | A | N7-C8-N9 | -5.05 | 111.28 | 113.80 |
| 3 | A | 906 | U | C6-N1-C1' | 5.04 | 128.26 | 121.20 |
| 3 | A | 66 | C | N3-C2-O2 | -5.04 | 118.38 | 121.90 |
| 3 | A | 1102 | C | C6-N1-C2 | -5.04 | 118.29 | 120.30 |
| 3 | A | 2580 | U | N3-C2-O2 | -5.03 | 118.68 | 122.20 |
| 3 | A | 2421 | G | C4-C5-N7 | 5.03 | 112.81 | 110.80 |
| 3 | A | 878 | A | C8-N9-C4 | -5.03 | 103.79 | 105.80 |
| 3 | A | 2424 | C | C5'-C4'-O4' | 5.02 | 115.13 | 109.10 |
| 3 | A | 2614 | A | C8-N9-C4 | -5.02 | 103.79 | 105.80 |
| 3 | A | 783 | A | N1-C6-N6 | -5.02 | 115.59 | 118.60 |
| 3 | A | 102 | U | C6-N1-C1' | -5.01 | 114.18 | 121.20 |
| 3 | A | 2013 | A | C6-N1-C2 | -5.01 | 115.59 | 118.60 |
| 3 | A | 1570 | A | C8-N9-C4 | 5.01 | 107.80 | 105.80 |
| 3 | A | 804 | A | C2-N3-C4 | -5.01 | 108.10 | 110.60 |
| 3 | A | 1617 | C | C2-N3-C4 | -5.00 | 117.40 | 119.90 |
| 3 | A | 1314 | C | C2-N1-C1' | 5.00 | 124.31 | 118.80 |
| 3 | A | 516 | C | C6-N1-C2 | 5.00 | 122.30 | 120.30 |

There are no chirality outliers.

All (3) planarity outliers are listed below:

| Mol | Chain | Res | Type | Group |
|-----|-------|-----|------|---------|
| 5 | C | 232 | HIS | Peptide |
| 9 | G | 47 | ASP | Peptide |
| 12 | J | 19 | ASN | Peptide |

5.2 Too-close contacts [i](#)

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 | 1 | 926 | 0 | 467 | 10 | 0 |
| 2 | 2 | 62 | 0 | 34 | 1 | 0 |
| 3 | A | 61902 | 0 | 31133 | 683 | 0 |
| 4 | B | 2569 | 0 | 1301 | 19 | 0 |
| 5 | C | 2082 | 0 | 2154 | 51 | 0 |
| 6 | D | 1565 | 0 | 1616 | 32 | 0 |
| 7 | E | 1552 | 0 | 1619 | 27 | 0 |
| 8 | F | 1410 | 0 | 1444 | 42 | 0 |
| 9 | G | 1323 | 0 | 1371 | 35 | 0 |
| 10 | H | 1110 | 0 | 1148 | 23 | 0 |
| 11 | I | 946 | 0 | 978 | 31 | 0 |
| 12 | J | 979 | 0 | 1028 | 39 | 0 |
| 13 | K | 1129 | 0 | 1162 | 24 | 0 |
| 14 | L | 946 | 0 | 1023 | 21 | 0 |
| 15 | M | 1053 | 0 | 1129 | 26 | 0 |
| 16 | N | 1074 | 0 | 1157 | 23 | 0 |
| 17 | O | 993 | 0 | 1034 | 25 | 0 |
| 18 | P | 900 | 0 | 935 | 23 | 0 |
| 19 | Q | 917 | 0 | 962 | 19 | 0 |
| 20 | R | 947 | 0 | 1019 | 24 | 0 |
| 21 | S | 816 | 0 | 839 | 20 | 0 |
| 22 | T | 857 | 0 | 922 | 14 | 0 |
| 23 | U | 756 | 0 | 817 | 14 | 0 |
| 24 | V | 779 | 0 | 831 | 18 | 0 |
| 25 | W | 753 | 0 | 780 | 14 | 0 |
| 26 | X | 580 | 0 | 594 | 16 | 0 |
| 27 | Y | 625 | 0 | 652 | 17 | 0 |
| 28 | Z | 501 | 0 | 531 | 13 | 0 |
| 29 | a | 449 | 0 | 488 | 0 | 0 |
| 30 | b | 444 | 0 | 458 | 0 | 0 |
| 31 | c | 414 | 0 | 442 | 0 | 0 |
| 32 | d | 377 | 0 | 418 | 0 | 0 |
| 33 | e | 504 | 0 | 572 | 0 | 0 |
| 34 | f | 302 | 0 | 340 | 0 | 0 |
| 35 | i | 916 | 0 | 944 | 0 | 0 |
| 36 | k | 137 | 0 | 168 | 0 | 0 |
| 37 | 2 | 1 | 0 | 0 | 0 | 0 |
| 37 | A | 412 | 0 | 0 | 0 | 0 |
| 37 | B | 11 | 0 | 0 | 0 | 0 |
| 37 | C | 2 | 0 | 0 | 0 | 0 |
| 37 | D | 1 | 0 | 0 | 0 | 0 |
| 37 | E | 1 | 0 | 0 | 0 | 0 |

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| Mol | Chain | Non-H | H(model) | H(added) | Clashes | Symm-Clashes |
|-----|-------|-------|----------|----------|---------|--------------|
| 37 | P | 1 | 0 | 0 | 0 | 0 |
| 37 | R | 1 | 0 | 0 | 0 | 0 |
| 37 | b | 1 | 0 | 0 | 0 | 0 |
| 38 | f | 1 | 0 | 0 | 0 | 0 |
| All | All | 94027 | 0 | 62510 | 1167 | 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 (1167) 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:A:1818:U:OP2 | 5:C:156:ARG:NH1 | 2.00 | 0.95 |
| 3:A:1168:G:H1 | 3:A:1181:U:H3 | 1.20 | 0.90 |
| 3:A:276:U:O2 | 3:A:278:A:N6 | 2.08 | 0.87 |
| 3:A:1827:U:OP2 | 5:C:221:ARG:NH1 | 2.08 | 0.86 |
| 10:H:3:VAL:HG12 | 10:H:38:PRO:HA | 1.57 | 0.86 |
| 3:A:2135:A:N6 | 3:A:2156:G:O2' | 2.10 | 0.84 |
| 3:A:287:G:O6 | 3:A:352:A:N6 | 2.10 | 0.84 |
| 3:A:2107:G:H1 | 3:A:2182:U:H3 | 1.22 | 0.83 |
| 5:C:107:PRO:HD2 | 5:C:110:LEU:HD22 | 1.59 | 0.82 |
| 3:A:807:U:OP2 | 15:M:41:ARG:NH1 | 2.14 | 0.81 |
| 15:M:109:LYS:HG2 | 15:M:126:ARG:HB2 | 1.64 | 0.80 |
| 3:A:994:C:O2 | 21:S:10:LYS:NZ | 2.16 | 0.79 |
| 3:A:2128:G:N3 | 3:A:2173:A:O2' | 2.14 | 0.79 |
| 18:P:15:ARG:NH2 | 18:P:95:SER:OG | 2.18 | 0.77 |
| 11:I:41:LEU:HD21 | 11:I:96:PHE:HE1 | 1.50 | 0.77 |
| 5:C:245:VAL:HG12 | 5:C:251:GLN:HA | 1.67 | 0.76 |
| 3:A:614:A:O2' | 3:A:616:A:N7 | 2.18 | 0.76 |
| 3:A:2135:A:HO2' | 3:A:2159:G:HO2' | 1.32 | 0.76 |
| 3:A:2599:G:N7 | 5:C:236:GLU:HB2 | 2.02 | 0.74 |
| 3:A:545:U:O2 | 3:A:548:G:N1 | 2.19 | 0.74 |
| 3:A:2848:G:O2' | 3:A:2867:G:N2 | 2.19 | 0.73 |
| 5:C:181:MET:HB2 | 5:C:268:VAL:HB | 1.69 | 0.73 |
| 3:A:720:U:H2' | 3:A:721:A:C8 | 2.24 | 0.72 |
| 13:K:131:ASN:OD1 | 13:K:131:ASN:N | 2.22 | 0.72 |
| 3:A:2119:A:N6 | 3:A:2167:U:O2 | 2.22 | 0.72 |
| 3:A:331:C:H41 | 3:A:1210:G:H22 | 1.37 | 0.72 |
| 7:E:1:MET:HG3 | 7:E:14:VAL:HG23 | 1.71 | 0.71 |
| 13:K:70:THR:OG1 | 13:K:71:ASP:OD1 | 2.08 | 0.71 |
| 3:A:331:C:H41 | 3:A:1210:G:N2 | 1.89 | 0.71 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|-------------------|--------------------------|-------------------|
| 3:A:2423:U:H2' | 3:A:2424:C:O4' | 1.89 | 0.71 |
| 14:L:70:ARG:HD3 | 14:L:76:VAL:HG22 | 1.72 | 0.70 |
| 3:A:1801:A:OP2 | 5:C:150:LYS:NZ | 2.18 | 0.70 |
| 3:A:2310:C:H2' | 8:F:77:PHE:HE2 | 1.54 | 0.70 |
| 3:A:2163:A:OP1 | 3:A:2170:A:O2' | 2.08 | 0.70 |
| 11:I:50:VAL:HG22 | 11:I:85:VAL:HG13 | 1.74 | 0.70 |
| 3:A:1069:A:H4' | 3:A:1070:A:H5'' | 1.71 | 0.70 |
| 3:A:971:G:H2' | 3:A:972:A:O4' | 1.92 | 0.70 |
| 3:A:258:G:H1' | 15:M:104:GLN:HE22 | 1.56 | 0.69 |
| 3:A:513:A:O2' | 20:R:11:ARG:NH1 | 2.26 | 0.69 |
| 9:G:35:ARG:HD3 | 9:G:71:LEU:HD13 | 1.74 | 0.69 |
| 11:I:43:LYS:HG2 | 11:I:46:ARG:HH22 | 1.56 | 0.68 |
| 14:L:79:PHE:HD1 | 19:Q:70:VAL:HG22 | 1.58 | 0.68 |
| 3:A:1536:C:H4' | 3:A:1537:G:H5'' | 1.75 | 0.68 |
| 3:A:2830:C:H5'' | 6:D:56:LYS:HE3 | 1.75 | 0.68 |
| 3:A:362:A:H3' | 3:A:363:G:H8 | 1.59 | 0.68 |
| 3:A:2135:A:O2' | 3:A:2159:G:O2' | 2.06 | 0.68 |
| 12:J:79:LEU:HB3 | 12:J:109:ILE:HG12 | 1.76 | 0.68 |
| 14:L:21:CYS:HA | 14:L:41:ILE:HG22 | 1.76 | 0.68 |
| 3:A:878:A:H3' | 3:A:879:G:H8 | 1.60 | 0.67 |
| 3:A:358:U:H2' | 3:A:359:G:H8 | 1.60 | 0.67 |
| 18:P:31:THR:HG22 | 18:P:34:HIS:H | 1.59 | 0.67 |
| 3:A:1340:U:OP1 | 23:U:19:LYS:NZ | 2.26 | 0.67 |
| 3:A:286:U:H2' | 3:A:287:G:H8 | 1.60 | 0.67 |
| 3:A:2103:C:O2 | 3:A:2186:G:N1 | 2.27 | 0.67 |
| 3:A:2122:U:OP1 | 3:A:2168:G:N2 | 2.26 | 0.67 |
| 3:A:196:A:OP2 | 15:M:47:ARG:NH1 | 2.28 | 0.66 |
| 3:A:1105:U:H2' | 3:A:1106:G:C8 | 2.29 | 0.66 |
| 3:A:286:U:H2' | 3:A:287:G:C8 | 2.31 | 0.66 |
| 27:Y:32:ASN:O | 27:Y:52:SER:HA | 1.95 | 0.66 |
| 3:A:2209:G:H1 | 3:A:2215:C:H42 | 1.44 | 0.66 |
| 3:A:2590:A:H2' | 3:A:2591:C:H6 | 1.61 | 0.66 |
| 13:K:31:GLU:HG3 | 13:K:142:ILE:HG13 | 1.77 | 0.66 |
| 3:A:2305:U:C2 | 8:F:151:GLY:HA3 | 2.31 | 0.66 |
| 3:A:2713:U:H3' | 3:A:2714:G:H5'' | 1.77 | 0.66 |
| 10:H:84:ALA:HA | 10:H:90:LEU:HA | 1.78 | 0.66 |
| 4:B:43:C:O2 | 8:F:92:ARG:NH2 | 2.28 | 0.66 |
| 3:A:2216:G:H2' | 3:A:2217:G:H8 | 1.60 | 0.66 |
| 3:A:572:A:OP2 | 21:S:80:ARG:NH2 | 2.27 | 0.66 |
| 3:A:2303:G:O2' | 8:F:121:SER:O | 2.13 | 0.65 |
| 28:Z:10:SER:N | 28:Z:13:GLU:OE1 | 2.26 | 0.65 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|-------------------|--------------------------|-------------------|
| 3:A:1344:U:O2' | 3:A:1345:C:OP1 | 2.14 | 0.65 |
| 3:A:1597:A:H5'' | 3:A:1598:A:H5' | 1.78 | 0.65 |
| 9:G:9:VAL:HG22 | 9:G:69:ARG:HE | 1.61 | 0.65 |
| 3:A:860:U:H1' | 3:A:2268:A:H5' | 1.78 | 0.65 |
| 7:E:87:ALA:O | 7:E:88:ARG:NH2 | 2.30 | 0.65 |
| 1:1:49:G:H1 | 1:1:60:A:H61 | 1.43 | 0.65 |
| 8:F:158:THR:HG22 | 8:F:160:ALA:H | 1.62 | 0.65 |
| 3:A:370:G:O2' | 3:A:424:G:OP1 | 2.11 | 0.65 |
| 3:A:1794:A:H2' | 3:A:1795:C:H6 | 1.61 | 0.65 |
| 16:N:50:ARG:O | 16:N:54:THR:OG1 | 2.13 | 0.64 |
| 3:A:1869:G:N2 | 3:A:1871:A:O2' | 2.30 | 0.64 |
| 3:A:1007:C:OP1 | 13:K:37:ARG:NH2 | 2.29 | 0.64 |
| 3:A:1342:A:O2' | 3:A:1344:U:OP2 | 2.16 | 0.64 |
| 3:A:2674:G:H4' | 14:L:30:ARG:HG3 | 1.78 | 0.64 |
| 3:A:1510:G:H2' | 3:A:1511:G:C8 | 2.32 | 0.64 |
| 3:A:2788:C:O2' | 3:A:2809:A:N3 | 2.28 | 0.64 |
| 26:X:65:GLY:HA2 | 26:X:85:GLU:HG2 | 1.78 | 0.64 |
| 3:A:2424:C:H5'' | 3:A:2425:A:H5' | 1.79 | 0.64 |
| 3:A:968:C:H2' | 3:A:969:G:H8 | 1.62 | 0.64 |
| 3:A:1105:U:H2' | 3:A:1106:G:H8 | 1.63 | 0.64 |
| 3:A:322:A:H5' | 3:A:340:A:H1' | 1.78 | 0.63 |
| 3:A:2102:G:N2 | 3:A:2187:U:O2 | 2.31 | 0.63 |
| 20:R:74:ILE:HD11 | 20:R:78:LYS:HB3 | 1.80 | 0.63 |
| 3:A:1094:U:N3 | 3:A:1097:U:OP2 | 2.30 | 0.63 |
| 3:A:1614:A:N1 | 22:T:93:ALA:HB2 | 2.13 | 0.63 |
| 8:F:74:VAL:HG22 | 8:F:79:ILE:HD11 | 1.79 | 0.63 |
| 8:F:144:ASP:N | 8:F:144:ASP:OD1 | 2.30 | 0.63 |
| 16:N:14:LYS:O | 16:N:71:LYS:NZ | 2.32 | 0.63 |
| 3:A:1980:G:O2' | 3:A:1982:U:OP2 | 2.16 | 0.63 |
| 21:S:41:ILE:HB | 21:S:48:LYS:HD2 | 1.79 | 0.63 |
| 22:T:82:MET:HB3 | 22:T:84:ARG:HH22 | 1.63 | 0.63 |
| 3:A:284:U:H3 | 3:A:356:G:H1 | 1.44 | 0.63 |
| 3:A:2151:U:H2' | 3:A:2152:G:C8 | 2.34 | 0.63 |
| 19:Q:91:ALA:HB2 | 19:Q:113:ARG:HA | 1.80 | 0.63 |
| 3:A:1187:G:OP1 | 21:S:85:LYS:NZ | 2.31 | 0.62 |
| 3:A:2116:G:N7 | 3:A:2165:C:N4 | 2.44 | 0.62 |
| 25:W:21:ARG:NH2 | 25:W:87:GLN:O | 2.28 | 0.62 |
| 3:A:1433:A:N1 | 3:A:1434:A:N6 | 2.47 | 0.62 |
| 13:K:117:ALA:HA | 13:K:120:ARG:HH21 | 1.64 | 0.62 |
| 3:A:514:A:N3 | 3:A:581:C:O2' | 2.32 | 0.62 |
| 17:O:49:GLU:HA | 17:O:52:ILE:HD12 | 1.79 | 0.62 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|-------------------|--------------------------|-------------------|
| 20:R:58:ARG:HA | 20:R:61:TRP:CE3 | 2.34 | 0.62 |
| 3:A:784:G:C6 | 5:C:228:VAL:HG11 | 2.35 | 0.62 |
| 19:Q:4:ILE:HD12 | 19:Q:4:ILE:H | 1.65 | 0.62 |
| 3:A:825:A:H2' | 3:A:826:U:O4' | 1.98 | 0.62 |
| 3:A:2809:A:H2' | 3:A:2810:A:C8 | 2.34 | 0.62 |
| 3:A:2590:A:H2' | 3:A:2591:C:C6 | 2.35 | 0.62 |
| 10:H:68:ARG:HA | 10:H:71:LYS:HD2 | 1.81 | 0.62 |
| 3:A:2822:G:O6 | 17:O:2:ARG:NH1 | 2.32 | 0.61 |
| 12:J:53:LEU:HD11 | 12:J:82:LYS:HD2 | 1.83 | 0.61 |
| 11:I:57:ASN:ND2 | 11:I:76:PHE:O | 2.33 | 0.61 |
| 3:A:1079:C:O2' | 12:J:134:ARG:NH1 | 2.33 | 0.61 |
| 15:M:57:LEU:HD13 | 15:M:60:ARG:HH11 | 1.65 | 0.61 |
| 3:A:2636:C:HO2' | 6:D:45:TYR:HH | 1.47 | 0.61 |
| 3:A:2310:C:H2' | 8:F:77:PHE:CE2 | 2.35 | 0.61 |
| 3:A:2639:A:H2' | 3:A:2640:G:O4' | 2.01 | 0.61 |
| 17:O:54:LEU:HD21 | 17:O:65:LEU:HD23 | 1.82 | 0.61 |
| 3:A:1001:A:H2' | 3:A:1002:G:O4' | 2.01 | 0.61 |
| 5:C:235:GLY:HA3 | 5:C:239:ASN:HB2 | 1.83 | 0.61 |
| 11:I:41:LEU:HD21 | 11:I:96:PHE:CE1 | 2.34 | 0.61 |
| 3:A:585:G:N7 | 20:R:6:ARG:NH1 | 2.48 | 0.60 |
| 3:A:503:A:H4' | 3:A:504:A:H5' | 1.83 | 0.60 |
| 6:D:12:THR:OG1 | 6:D:13:ARG:N | 2.34 | 0.60 |
| 3:A:2060:A:H3' | 7:E:63:LYS:HZ1 | 1.65 | 0.60 |
| 22:T:6:LYS:HG2 | 22:T:104:THR:HG23 | 1.82 | 0.60 |
| 3:A:570:G:H2' | 3:A:2030:A:N7 | 2.16 | 0.60 |
| 9:G:137:ASP:O | 9:G:141:ILE:HG22 | 2.01 | 0.60 |
| 26:X:56:ASP:OD1 | 26:X:56:ASP:N | 2.28 | 0.60 |
| 3:A:1076:C:H2' | 3:A:1077:A:C8 | 2.37 | 0.60 |
| 3:A:1363:C:O2' | 3:A:1809:A:N3 | 2.33 | 0.60 |
| 3:A:1794:A:H2' | 3:A:1795:C:C6 | 2.37 | 0.60 |
| 6:D:2:ILE:HG13 | 6:D:100:LEU:HD21 | 1.83 | 0.60 |
| 11:I:27:VAL:HG22 | 11:I:82:ILE:HG22 | 1.83 | 0.60 |
| 7:E:97:ASN:N | 7:E:97:ASN:OD1 | 2.34 | 0.60 |
| 15:M:81:ASP:HA | 15:M:84:LYS:HD2 | 1.82 | 0.60 |
| 3:A:776:G:O2' | 3:A:777:G:OP1 | 2.19 | 0.60 |
| 3:A:2831:G:OP1 | 6:D:56:LYS:NZ | 2.35 | 0.60 |
| 3:A:355:U:H2' | 3:A:356:G:C8 | 2.37 | 0.59 |
| 8:F:44:ILE:HG21 | 8:F:79:ILE:HG22 | 1.83 | 0.59 |
| 3:A:1796:U:H2' | 3:A:1797:G:H8 | 1.67 | 0.59 |
| 3:A:2584:U:H3' | 3:A:2585:U:H5'' | 1.84 | 0.59 |
| 3:A:2819:G:H2' | 3:A:2821:A:N7 | 2.17 | 0.59 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|-------------------|--------------------------|-------------------|
| 13:K:36:LEU:HD11 | 13:K:122:LEU:HB2 | 1.83 | 0.59 |
| 9:G:27:LYS:NZ | 9:G:27:LYS:HB3 | 2.17 | 0.59 |
| 18:P:99:TYR:OH | 18:P:111:ARG:NH1 | 2.36 | 0.59 |
| 3:A:878:A:H3' | 3:A:879:G:C8 | 2.38 | 0.59 |
| 3:A:2205:A:H61 | 3:A:2219:U:H3 | 1.50 | 0.59 |
| 11:I:64:VAL:HG22 | 11:I:69:PHE:HB2 | 1.84 | 0.59 |
| 24:V:81:ASP:OD1 | 24:V:82:ARG:N | 2.35 | 0.59 |
| 4:B:7:G:OP1 | 18:P:4:LYS:NZ | 2.27 | 0.59 |
| 3:A:1170:C:O2 | 3:A:1179:G:N2 | 2.33 | 0.58 |
| 3:A:2021:C:OP1 | 20:R:25:TYR:OH | 2.21 | 0.58 |
| 3:A:2127:G:O2' | 3:A:2128:G:O5' | 2.19 | 0.58 |
| 3:A:1808:A:H3' | 3:A:1809:A:C8 | 2.38 | 0.58 |
| 3:A:396:G:OP2 | 27:Y:10:LYS:NZ | 2.36 | 0.58 |
| 3:A:833:A:H2' | 3:A:834:G:C8 | 2.38 | 0.58 |
| 3:A:1130:U:O2' | 3:A:1131:G:H8 | 1.87 | 0.58 |
| 3:A:2127:G:O2' | 3:A:2128:G:O4' | 2.20 | 0.58 |
| 17:O:73:ASN:HA | 17:O:76:VAL:HG22 | 1.86 | 0.58 |
| 21:S:37:GLU:HB3 | 21:S:53:PHE:CE1 | 2.39 | 0.58 |
| 25:W:76:ASP:OD1 | 25:W:77:VAL:N | 2.37 | 0.58 |
| 12:J:106:LEU:HB3 | 12:J:126:THR:HG23 | 1.85 | 0.58 |
| 18:P:41:ALA:HB2 | 18:P:48:LEU:HD21 | 1.86 | 0.58 |
| 6:D:148:GLN:HB2 | 6:D:152:PRO:HD2 | 1.85 | 0.58 |
| 3:A:1715:G:O2' | 3:A:1743:G:O6 | 2.17 | 0.57 |
| 3:A:2412:A:H2' | 3:A:2413:G:O4' | 2.04 | 0.57 |
| 7:E:21:ARG:HD3 | 7:E:106:LYS:HB3 | 1.85 | 0.57 |
| 3:A:2291:U:H2' | 3:A:2292:U:C6 | 2.38 | 0.57 |
| 3:A:2602:A:H4' | 3:A:2603:G:O5' | 2.04 | 0.57 |
| 5:C:227:PRO:HG3 | 5:C:234:GLY:H | 1.69 | 0.57 |
| 12:J:59:ILE:HD13 | 12:J:69:PHE:HB3 | 1.86 | 0.57 |
| 3:A:849:A:H2' | 3:A:850:U:C6 | 2.39 | 0.57 |
| 6:D:157:LYS:HD2 | 13:K:80:HIS:CE1 | 2.40 | 0.57 |
| 17:O:94:TYR:O | 17:O:116:VAL:HG23 | 2.05 | 0.57 |
| 3:A:1645:G:H5'' | 3:A:1646:C:H5' | 1.86 | 0.57 |
| 3:A:2447:G:N2 | 3:A:2450:A:OP2 | 2.37 | 0.57 |
| 10:H:37:VAL:HG22 | 10:H:38:PRO:HD2 | 1.85 | 0.57 |
| 3:A:340:A:H2' | 3:A:341:C:O4' | 2.05 | 0.57 |
| 3:A:839:U:H2' | 3:A:840:C:C6 | 2.40 | 0.57 |
| 6:D:13:ARG:HD2 | 6:D:15:PHE:CZ | 2.38 | 0.57 |
| 7:E:112:LEU:HB3 | 7:E:118:LEU:HB2 | 1.87 | 0.57 |
| 3:A:876:C:H2' | 3:A:877:A:O4' | 2.05 | 0.57 |
| 6:D:1:MET:HG2 | 6:D:2:ILE:H | 1.70 | 0.57 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|-------------------|--------------------------|-------------------|
| 3:A:2216:G:H2' | 3:A:2217:G:C8 | 2.40 | 0.56 |
| 8:F:33:LYS:HG2 | 8:F:157:THR:HB | 1.87 | 0.56 |
| 24:V:18:ASP:OD2 | 24:V:40:ASN:N | 2.38 | 0.56 |
| 3:A:299:A:N1 | 3:A:322:A:O2' | 2.27 | 0.56 |
| 3:A:1905:C:H2' | 3:A:1930:G:C8 | 2.40 | 0.56 |
| 3:A:26:G:C6 | 3:A:27:G:N1 | 2.73 | 0.56 |
| 3:A:721:A:H2' | 3:A:722:A:C8 | 2.41 | 0.56 |
| 3:A:1063:G:H5' | 12:J:77:ALA:HB1 | 1.87 | 0.56 |
| 3:A:1796:U:H2' | 3:A:1797:G:C8 | 2.40 | 0.56 |
| 11:I:60:LEU:O | 11:I:64:VAL:HB | 2.06 | 0.56 |
| 3:A:480:A:OP2 | 24:V:44:LYS:NZ | 2.23 | 0.56 |
| 3:A:1800:C:H5' | 5:C:146:MET:HE1 | 1.87 | 0.56 |
| 5:C:166:ALA:HB3 | 5:C:173:THR:HB | 1.86 | 0.56 |
| 3:A:2162:G:H5'' | 3:A:2171:A:H2' | 1.86 | 0.56 |
| 3:A:388:G:N7 | 3:A:390:U:H2' | 2.21 | 0.56 |
| 3:A:1790:C:H3' | 3:A:1828:G:N2 | 2.21 | 0.56 |
| 9:G:30:ASN:HB3 | 9:G:79:VAL:HA | 1.88 | 0.56 |
| 3:A:1076:C:H2' | 3:A:1077:A:H8 | 1.69 | 0.56 |
| 3:A:2491:U:H5'' | 3:A:2570:G:H5'' | 1.88 | 0.56 |
| 4:B:42:C:C5 | 8:F:66:LEU:HD22 | 2.41 | 0.56 |
| 3:A:2133:G:H2' | 3:A:2157:G:H1 | 1.70 | 0.56 |
| 3:A:2430:A:N3 | 3:A:2430:A:H2' | 2.21 | 0.56 |
| 3:A:2584:U:H3' | 3:A:2585:U:C5' | 2.36 | 0.56 |
| 12:J:73:THR:HB | 12:J:112:THR:HG22 | 1.87 | 0.56 |
| 3:A:812:C:H4' | 20:R:13:ARG:NH1 | 2.21 | 0.56 |
| 3:A:1251:C:OP2 | 20:R:6:ARG:NH2 | 2.35 | 0.56 |
| 3:A:2298:A:H2' | 3:A:2299:U:O4' | 2.05 | 0.56 |
| 12:J:53:LEU:HD22 | 12:J:78:VAL:HG13 | 1.87 | 0.56 |
| 13:K:72:LYS:HE3 | 13:K:74:TYR:CE1 | 2.39 | 0.56 |
| 3:A:1442:U:H2' | 3:A:1443:U:C6 | 2.41 | 0.55 |
| 17:O:2:ARG:NH1 | 17:O:2:ARG:HB3 | 2.21 | 0.55 |
| 25:W:62:THR:HG22 | 25:W:71:LYS:HG2 | 1.88 | 0.55 |
| 12:J:127:ARG:HA | 12:J:130:GLU:HB2 | 1.89 | 0.55 |
| 18:P:16:ARG:HA | 18:P:16:ARG:HH21 | 1.71 | 0.55 |
| 3:A:19:A:H2' | 3:A:20:C:C6 | 2.41 | 0.55 |
| 3:A:849:A:H2' | 3:A:850:U:H6 | 1.70 | 0.55 |
| 3:A:2171:A:H3' | 3:A:2173:A:C8 | 2.41 | 0.55 |
| 3:A:2783:U:H2' | 3:A:2784:U:C6 | 2.42 | 0.55 |
| 10:H:7:ASP:OD1 | 10:H:8:LYS:N | 2.40 | 0.55 |
| 24:V:33:LYS:HB3 | 24:V:64:ALA:HB1 | 1.87 | 0.55 |
| 3:A:184:C:H2' | 3:A:185:G:C8 | 2.41 | 0.55 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 3:A:591:U:H2' | 3:A:592:A:H8 | 1.72 | 0.55 |
| 3:A:882:G:H1 | 3:A:894:U:H3 | 1.54 | 0.55 |
| 5:C:160:THR:HG22 | 5:C:177:ARG:HG2 | 1.89 | 0.55 |
| 3:A:639:U:H2' | 3:A:640:C:C6 | 2.42 | 0.55 |
| 3:A:2591:C:H2' | 3:A:2592:G:C8 | 2.41 | 0.55 |
| 17:O:48:VAL:O | 17:O:51:LEU:HB2 | 2.05 | 0.55 |
| 3:A:2070:A:H2' | 3:A:2071:A:C8 | 2.42 | 0.55 |
| 6:D:8:LYS:HB2 | 6:D:201:LEU:HD11 | 1.88 | 0.55 |
| 8:F:132:VAL:HG22 | 8:F:152:LEU:HB3 | 1.88 | 0.55 |
| 18:P:69:ASP:N | 18:P:69:ASP:OD1 | 2.40 | 0.55 |
| 3:A:2262:U:H2' | 3:A:2263:C:H6 | 1.72 | 0.54 |
| 8:F:134:GLU:HB3 | 8:F:136:ILE:HG12 | 1.89 | 0.54 |
| 3:A:833:A:H2' | 3:A:834:G:H8 | 1.72 | 0.54 |
| 6:D:184:ARG:NH1 | 19:Q:7:GLN:OE1 | 2.40 | 0.54 |
| 7:E:88:ARG:HA | 7:E:88:ARG:HH21 | 1.72 | 0.54 |
| 13:K:34:ARG:HH22 | 13:K:40:HIS:HB3 | 1.71 | 0.54 |
| 3:A:586:A:H5' | 7:E:84:THR:HG21 | 1.90 | 0.54 |
| 3:A:609:A:H2' | 3:A:610:C:O4' | 2.08 | 0.54 |
| 3:A:1837:C:H2' | 3:A:1899:A:H61 | 1.73 | 0.54 |
| 3:A:2619:C:H5'' | 6:D:157:LYS:HG3 | 1.89 | 0.54 |
| 3:A:996:A:OP2 | 21:S:10:LYS:HD3 | 2.07 | 0.54 |
| 3:A:2424:C:H5'' | 3:A:2425:A:C5' | 2.37 | 0.54 |
| 12:J:79:LEU:HA | 12:J:82:LYS:HG2 | 1.88 | 0.54 |
| 3:A:1923:U:H2' | 3:A:1924:C:C6 | 2.43 | 0.54 |
| 3:A:2267:A:H5'' | 3:A:2268:A:H5'' | 1.89 | 0.54 |
| 12:J:56:PRO:HD3 | 12:J:75:PRO:HD3 | 1.90 | 0.54 |
| 3:A:172:A:H2' | 3:A:173:A:C8 | 2.43 | 0.54 |
| 21:S:48:LYS:HE3 | 21:S:103:ALA:HB1 | 1.90 | 0.54 |
| 23:U:68:LYS:HG3 | 23:U:77:ARG:NH2 | 2.23 | 0.54 |
| 23:U:56:GLU:HA | 23:U:88:LYS:HE3 | 1.89 | 0.54 |
| 3:A:2579:C:O2' | 6:D:136:ASN:ND2 | 2.41 | 0.54 |
| 3:A:2845:U:H5'' | 19:Q:52:ASN:O | 2.08 | 0.54 |
| 9:G:104:ASN:ND2 | 9:G:114:ASP:OD1 | 2.41 | 0.54 |
| 3:A:2834:G:O6 | 3:A:2879:A:H2' | 2.08 | 0.54 |
| 21:S:20:VAL:HG13 | 21:S:96:VAL:HG23 | 1.89 | 0.53 |
| 3:A:2443:C:H2' | 3:A:2444:G:C8 | 2.43 | 0.53 |
| 3:A:2808:G:O2' | 3:A:2890:G:O6 | 2.21 | 0.53 |
| 5:C:145:GLU:HB2 | 5:C:188:CYS:HB3 | 1.89 | 0.53 |
| 3:A:284:U:O2 | 3:A:356:G:N2 | 2.37 | 0.53 |
| 3:A:608:A:H2' | 3:A:609:A:C8 | 2.44 | 0.53 |
| 14:L:38:ILE:HD11 | 14:L:112:PHE:HZ | 1.73 | 0.53 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|------------------|--------------------------|-------------------|
| 3:A:2547:A:H4' | 14:L:29:HIS:CD2 | 2.44 | 0.53 |
| 14:L:40:LYS:HE3 | 14:L:57:VAL:HG12 | 1.91 | 0.53 |
| 3:A:9:G:O2' | 3:A:2800:A:N6 | 2.42 | 0.53 |
| 3:A:720:U:H2' | 3:A:721:A:H8 | 1.72 | 0.53 |
| 3:A:1056:G:H5'' | 3:A:1057:A:H5' | 1.90 | 0.53 |
| 11:I:88:HIS:ND1 | 11:I:89:PRO:O | 2.42 | 0.53 |
| 17:O:36:THR:OG1 | 17:O:37:THR:N | 2.42 | 0.53 |
| 3:A:788:A:OP1 | 3:A:791:C:N4 | 2.41 | 0.53 |
| 3:A:1069:A:C2 | 3:A:1096:A:H5'' | 2.44 | 0.53 |
| 11:I:54:VAL:HG22 | 11:I:81:LEU:HD13 | 1.90 | 0.53 |
| 3:A:2171:A:H3' | 3:A:2173:A:H8 | 1.74 | 0.53 |
| 3:A:1056:G:O2' | 3:A:1103:A:N6 | 2.40 | 0.52 |
| 3:A:1873:G:H2' | 3:A:1874:C:H6 | 1.74 | 0.52 |
| 10:H:116:ARG:HH21 | 10:H:133:GLN:HB3 | 1.74 | 0.52 |
| 17:O:36:THR:HG23 | 17:O:41:ALA:HB2 | 1.90 | 0.52 |
| 3:A:2086:U:H2' | 3:A:2087:G:C8 | 2.44 | 0.52 |
| 3:A:2210:U:H4' | 3:A:2211:A:H5' | 1.91 | 0.52 |
| 3:A:2280:G:O2' | 3:A:2388:A:N1 | 2.37 | 0.52 |
| 5:C:62:TYR:HA | 5:C:86:ASN:HD21 | 1.73 | 0.52 |
| 3:A:68:G:H2' | 3:A:69:C:O4' | 2.10 | 0.52 |
| 3:A:653:U:H1' | 3:A:654:A:H5'' | 1.91 | 0.52 |
| 3:A:679:C:H2' | 3:A:680:C:C6 | 2.44 | 0.52 |
| 3:A:1425:G:H2' | 3:A:1426:G:O4' | 2.09 | 0.52 |
| 3:A:1428:C:C5 | 3:A:1569:A:H5'' | 2.45 | 0.52 |
| 3:A:1993:U:H4' | 6:D:133:THR:OG1 | 2.10 | 0.52 |
| 25:W:55:GLU:H | 25:W:55:GLU:CD | 2.12 | 0.52 |
| 1:1:60:A:H2' | 1:1:61:G:O4' | 2.09 | 0.52 |
| 3:A:671:C:H2' | 3:A:672:C:H6 | 1.74 | 0.52 |
| 3:A:1410:G:H1 | 3:A:1592:C:H42 | 1.57 | 0.52 |
| 8:F:99:PHE:HD1 | 8:F:102:ARG:HH22 | 1.57 | 0.52 |
| 13:K:3:THR:HB | 20:R:57:PHE:HE1 | 1.75 | 0.52 |
| 3:A:1421:G:C2 | 3:A:1422:G:C8 | 2.98 | 0.52 |
| 1:1:47:A:OP2 | 1:1:61:G:N1 | 2.42 | 0.52 |
| 1:1:48:G:H3' | 1:1:49:G:H8 | 1.75 | 0.52 |
| 3:A:845:A:H61 | 3:A:932:U:H3 | 1.58 | 0.52 |
| 3:A:1791:A:N6 | 3:A:1828:G:O2' | 2.42 | 0.52 |
| 3:A:2127:G:H2' | 3:A:2128:G:C8 | 2.45 | 0.52 |
| 6:D:114:LYS:HD3 | 6:D:196:ALA:HB2 | 1.92 | 0.52 |
| 3:A:898:C:H2' | 3:A:899:A:O4' | 2.10 | 0.52 |
| 21:S:52:PRO:HG2 | 21:S:53:PHE:CD2 | 2.45 | 0.52 |
| 3:A:1289:C:H2' | 3:A:1290:C:C6 | 2.45 | 0.52 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 3:A:1798:U:H5'' | 5:C:258:ARG:HB2 | 1.92 | 0.52 |
| 3:A:2637:U:C2' | 3:A:2638:G:H5' | 2.39 | 0.52 |
| 4:B:93:C:OP2 | 25:W:18:ARG:NH1 | 2.42 | 0.52 |
| 7:E:28:VAL:O | 7:E:32:VAL:HG13 | 2.09 | 0.52 |
| 23:U:93:LEU:HD13 | 23:U:95:PHE:CZ | 2.44 | 0.52 |
| 3:A:90:U:H3' | 3:A:91:A:H8 | 1.74 | 0.52 |
| 3:A:1451:C:H1' | 3:A:1452:G:C2 | 2.45 | 0.52 |
| 3:A:1681:G:H21 | 3:A:1762:A:H3' | 1.75 | 0.52 |
| 3:A:120:U:H4' | 3:A:121:G:H5'' | 1.89 | 0.52 |
| 3:A:2133:G:H21 | 3:A:2158:A:H62 | 1.58 | 0.52 |
| 24:V:74:ASN:HD21 | 24:V:99:ASN:HD21 | 1.58 | 0.52 |
| 3:A:1437:C:H2' | 3:A:1438:U:C6 | 2.45 | 0.51 |
| 12:J:73:THR:OG1 | 12:J:113:LYS:NZ | 2.40 | 0.51 |
| 3:A:256:A:H2' | 3:A:257:C:H6 | 1.74 | 0.51 |
| 3:A:2439:A:H4' | 3:A:2440:C:H5'' | 1.91 | 0.51 |
| 3:A:2850:A:N7 | 3:A:2868:A:O2' | 2.39 | 0.51 |
| 28:Z:2:LYS:HG3 | 28:Z:5:GLU:OE1 | 2.10 | 0.51 |
| 3:A:1790:C:H2' | 3:A:1791:A:C5 | 2.45 | 0.51 |
| 8:F:128:TYR:HE2 | 8:F:130:MET:HG2 | 1.76 | 0.51 |
| 3:A:968:C:H2' | 3:A:969:G:C8 | 2.42 | 0.51 |
| 3:A:1000:A:OP2 | 3:A:1154:G:N1 | 2.32 | 0.51 |
| 3:A:1115:G:O2' | 3:A:1116:G:H5'' | 2.10 | 0.51 |
| 3:A:1414:C:H2' | 3:A:1415:U:O4' | 2.11 | 0.51 |
| 7:E:24:ASN:ND2 | 7:E:27:LEU:HB2 | 2.25 | 0.51 |
| 3:A:948:C:H2' | 3:A:949:G:C8 | 2.45 | 0.51 |
| 3:A:2647:U:H2' | 3:A:2648:G:H8 | 1.76 | 0.51 |
| 3:A:2720:U:OP1 | 19:Q:53:ARG:NH2 | 2.41 | 0.51 |
| 17:O:55:ALA:HA | 17:O:80:PHE:CE2 | 2.45 | 0.51 |
| 3:A:141:G:H2' | 3:A:142:A:O4' | 2.11 | 0.51 |
| 3:A:499:U:H2' | 3:A:500:G:O4' | 2.10 | 0.51 |
| 7:E:145:ASP:HA | 7:E:166:LYS:HB3 | 1.92 | 0.51 |
| 20:R:24:TYR:N | 20:R:24:TYR:CD1 | 2.78 | 0.51 |
| 3:A:364:C:H2' | 3:A:365:U:C6 | 2.45 | 0.51 |
| 3:A:576:U:H2' | 3:A:577:G:C8 | 2.46 | 0.51 |
| 7:E:41:GLN:HG2 | 7:E:43:THR:HG23 | 1.92 | 0.51 |
| 15:M:36:LYS:O | 15:M:40:SER:HB3 | 2.11 | 0.51 |
| 3:A:621:A:OP2 | 15:M:99:ASN:ND2 | 2.40 | 0.51 |
| 19:Q:16:ASP:OD1 | 19:Q:16:ASP:N | 2.33 | 0.51 |
| 21:S:28:ALA:HB3 | 21:S:31:GLU:HG3 | 1.93 | 0.51 |
| 3:A:645:C:O2' | 3:A:646:U:OP1 | 2.24 | 0.51 |
| 3:A:2271:G:H5'' | 26:X:18:ALA:HB1 | 1.93 | 0.51 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 3:A:2502:G:H5'' | 3:A:2503:A:H5'' | 1.93 | 0.51 |
| 3:A:1405:U:H2' | 3:A:1406:U:C6 | 2.46 | 0.51 |
| 3:A:2333:A:P | 26:X:77:ARG:HH22 | 2.34 | 0.51 |
| 12:J:113:LYS:HE3 | 12:J:116:ASP:HB3 | 1.92 | 0.50 |
| 16:N:1:MET:HA | 16:N:47:GLU:HG3 | 1.94 | 0.50 |
| 3:A:1394:U:H4' | 3:A:1603:A:H4' | 1.92 | 0.50 |
| 13:K:32:LEU:O | 13:K:36:LEU:HB2 | 2.12 | 0.50 |
| 3:A:357:C:H2' | 3:A:358:U:C6 | 2.47 | 0.50 |
| 3:A:1132:U:H2' | 3:A:1133:A:C8 | 2.46 | 0.50 |
| 3:A:1927:A:H2' | 3:A:1928:A:C8 | 2.46 | 0.50 |
| 8:F:40:VAL:HG11 | 8:F:43:ALA:HB2 | 1.92 | 0.50 |
| 16:N:30:SER:H | 16:N:106:ASP:HB3 | 1.75 | 0.50 |
| 22:T:40:ASN:O | 22:T:41:LYS:HG2 | 2.10 | 0.50 |
| 3:A:256:A:H2' | 3:A:257:C:C6 | 2.46 | 0.50 |
| 3:A:1342:A:OP1 | 23:U:40:LYS:NZ | 2.33 | 0.50 |
| 3:A:2024:G:H2' | 3:A:2025:C:H6 | 1.76 | 0.50 |
| 3:A:2282:G:C6 | 3:A:2425:A:C2 | 3.00 | 0.50 |
| 14:L:64:ARG:NH1 | 14:L:102:PRO:O | 2.44 | 0.50 |
| 15:M:23:ILE:HG12 | 21:S:82:HIS:CD2 | 2.47 | 0.50 |
| 3:A:128:C:H2' | 3:A:129:C:C6 | 2.46 | 0.50 |
| 23:U:7:LEU:HD13 | 23:U:46:ALA:HA | 1.92 | 0.50 |
| 20:R:65:ILE:HD11 | 20:R:95:LEU:HB2 | 1.93 | 0.50 |
| 24:V:46:GLN:OE1 | 24:V:54:GLN:NE2 | 2.44 | 0.50 |
| 3:A:90:U:C2 | 3:A:91:A:N7 | 2.80 | 0.50 |
| 3:A:2183:A:H2' | 3:A:2184:A:C8 | 2.46 | 0.50 |
| 10:H:94:ILE:HB | 10:H:122:LEU:HB2 | 1.94 | 0.50 |
| 28:Z:39:GLN:HB3 | 28:Z:41:HIS:CE1 | 2.47 | 0.50 |
| 3:A:738:G:H1' | 3:A:759:G:N2 | 2.27 | 0.50 |
| 3:A:2308:G:H3' | 3:A:2310:C:OP2 | 2.11 | 0.50 |
| 4:B:2:G:H2' | 4:B:3:C:C6 | 2.47 | 0.50 |
| 5:C:132:MET:HG2 | 5:C:135:ILE:HD12 | 1.94 | 0.50 |
| 9:G:127:THR:HG22 | 9:G:128:GLN:H | 1.77 | 0.50 |
| 20:R:76:TYR:CZ | 20:R:80:ILE:HG13 | 2.46 | 0.50 |
| 8:F:17:MET:SD | 8:F:22:TYR:HB2 | 2.52 | 0.50 |
| 9:G:83:PHE:O | 9:G:134:LYS:HA | 2.12 | 0.50 |
| 12:J:83:ALA:O | 12:J:105:GLN:NE2 | 2.45 | 0.50 |
| 3:A:878:A:N6 | 3:A:899:A:O2' | 2.45 | 0.49 |
| 3:A:1021:A:H3' | 3:A:1021:A:N3 | 2.27 | 0.49 |
| 3:A:1327:A:N6 | 3:A:1647:U:O2 | 2.45 | 0.49 |
| 3:A:1638:C:H1' | 3:A:2698:U:O2' | 2.12 | 0.49 |
| 17:O:14:SER:HA | 17:O:17:ARG:NH1 | 2.27 | 0.49 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|------------------|--------------------------|-------------------|
| 25:W:75:GLN:HB2 | 25:W:92:VAL:HG12 | 1.94 | 0.49 |
| 3:A:613:A:O2' | 3:A:614:A:O5' | 2.30 | 0.49 |
| 3:A:1187:G:HO2' | 3:A:1188:U:H6 | 1.60 | 0.49 |
| 3:A:2171:A:H5' | 3:A:2173:A:N7 | 2.26 | 0.49 |
| 9:G:8:PRO:HB3 | 9:G:51:THR:HG22 | 1.94 | 0.49 |
| 19:Q:23:GLY:O | 19:Q:90:GLY:HA3 | 2.11 | 0.49 |
| 3:A:1506:U:H2' | 3:A:1507:C:C6 | 2.48 | 0.49 |
| 3:A:2747:G:O2' | 9:G:67:THR:HG23 | 2.12 | 0.49 |
| 3:A:2809:A:H2' | 3:A:2810:A:H8 | 1.75 | 0.49 |
| 8:F:50:LEU:O | 8:F:54:ALA:N | 2.38 | 0.49 |
| 18:P:30:ARG:HG3 | 18:P:35:ILE:HD12 | 1.94 | 0.49 |
| 26:X:34:GLY:N | 26:X:61:ALA:O | 2.37 | 0.49 |
| 3:A:1088:A:N6 | 12:J:135:SER:HB3 | 2.26 | 0.49 |
| 3:A:2576:G:O2' | 3:A:2579:C:OP2 | 2.23 | 0.49 |
| 3:A:2626:C:H2' | 3:A:2627:G:O4' | 2.12 | 0.49 |
| 7:E:184:ASP:OD1 | 7:E:184:ASP:N | 2.43 | 0.49 |
| 9:G:101:ASN:ND2 | 9:G:116:GLN:OE1 | 2.46 | 0.49 |
| 15:M:4:ASN:OD1 | 15:M:4:ASN:N | 2.39 | 0.49 |
| 3:A:27:G:N2 | 3:A:512:G:H1' | 2.28 | 0.49 |
| 3:A:671:C:H2' | 3:A:672:C:C6 | 2.47 | 0.49 |
| 3:A:1939:U:OP1 | 3:A:2604:U:O2' | 2.28 | 0.49 |
| 3:A:2073:C:H2' | 3:A:2074:U:H6 | 1.77 | 0.49 |
| 3:A:563:A:C4 | 3:A:2018:G:C2 | 3.01 | 0.49 |
| 3:A:1243:C:H1' | 15:M:4:ASN:O | 2.13 | 0.49 |
| 11:I:33:VAL:HG21 | 11:I:106:PHE:CE2 | 2.47 | 0.49 |
| 15:M:19:LEU:HD23 | 15:M:27:LEU:HD13 | 1.95 | 0.49 |
| 3:A:1606:C:H5' | 3:A:1607:C:OP1 | 2.13 | 0.49 |
| 21:S:65:ALA:HB3 | 21:S:95:ASP:HB2 | 1.94 | 0.49 |
| 3:A:1005:C:H2' | 3:A:1006:C:C6 | 2.47 | 0.49 |
| 3:A:1903:G:C2 | 3:A:1904:G:C8 | 3.00 | 0.49 |
| 3:A:2564:A:OP1 | 3:A:2648:G:O2' | 2.19 | 0.49 |
| 7:E:23:PHE:CD1 | 7:E:111:GLU:HG3 | 2.48 | 0.49 |
| 10:H:110:VAL:HG12 | 10:H:114:GLU:HB2 | 1.94 | 0.49 |
| 14:L:10:VAL:HG12 | 14:L:12:ASP:H | 1.78 | 0.49 |
| 3:A:184:C:H2' | 3:A:185:G:H8 | 1.77 | 0.48 |
| 3:A:1093:G:C2' | 3:A:1098:A:H61 | 2.26 | 0.48 |
| 3:A:1819:A:H5'' | 5:C:160:THR:HG21 | 1.94 | 0.48 |
| 3:A:2151:U:H2' | 3:A:2152:G:H8 | 1.77 | 0.48 |
| 3:A:2483:C:N3 | 16:N:123:LYS:NZ | 2.60 | 0.48 |
| 3:A:784:G:H5' | 3:A:785:G:OP1 | 2.13 | 0.48 |
| 12:J:113:LYS:O | 12:J:117:MET:N | 2.46 | 0.48 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|------------------|--------------------------|-------------------|
| 3:A:1654:A:H2' | 3:A:1655:A:H8 | 1.78 | 0.48 |
| 3:A:1790:C:H3' | 3:A:1828:G:H22 | 1.77 | 0.48 |
| 3:A:2290:G:H2' | 3:A:2291:U:O4' | 2.12 | 0.48 |
| 4:B:116:G:H2' | 4:B:117:G:C8 | 2.49 | 0.48 |
| 27:Y:6:GLN:NE2 | 27:Y:76:GLU:OE2 | 2.39 | 0.48 |
| 27:Y:17:ASN:HB2 | 27:Y:25:THR:OG1 | 2.13 | 0.48 |
| 3:A:719:C:H2' | 3:A:720:U:H6 | 1.78 | 0.48 |
| 3:A:140:C:H4' | 3:A:141:G:OP1 | 2.13 | 0.48 |
| 3:A:813:U:H2' | 3:A:814:C:C6 | 2.49 | 0.48 |
| 3:A:2116:G:C5 | 3:A:2165:C:N4 | 2.82 | 0.48 |
| 9:G:86:LYS:HG2 | 9:G:132:VAL:HG22 | 1.96 | 0.48 |
| 27:Y:17:ASN:OD1 | 27:Y:27:ARG:HD2 | 2.13 | 0.48 |
| 3:A:136:G:H2' | 3:A:137:U:O4' | 2.13 | 0.48 |
| 3:A:467:G:H2' | 3:A:468:G:O4' | 2.13 | 0.48 |
| 3:A:1179:G:H2' | 3:A:1180:U:C6 | 2.48 | 0.48 |
| 3:A:1773:A:N7 | 3:A:1829:A:H1' | 2.28 | 0.48 |
| 3:A:2158:A:H4' | 3:A:2159:G:O5' | 2.14 | 0.48 |
| 5:C:145:GLU:HG2 | 5:C:151:GLY:C | 2.34 | 0.48 |
| 9:G:80:THR:OG1 | 9:G:81:GLU:N | 2.46 | 0.48 |
| 18:P:51:ALA:HB3 | 18:P:78:VAL:HG13 | 1.95 | 0.48 |
| 23:U:68:LYS:HG3 | 23:U:77:ARG:HH21 | 1.79 | 0.48 |
| 26:X:40:GLN:NE2 | 26:X:43:THR:HA | 2.29 | 0.48 |
| 1:1:49:G:H1 | 1:1:60:A:N6 | 2.10 | 0.48 |
| 3:A:2209:G:H1 | 3:A:2215:C:N4 | 2.11 | 0.48 |
| 17:O:38:LEU:HB3 | 17:O:39:PRO:HD3 | 1.95 | 0.48 |
| 3:A:175:G:N2 | 3:A:176:A:N3 | 2.62 | 0.48 |
| 3:A:428:A:H2' | 3:A:429:A:C8 | 2.49 | 0.48 |
| 3:A:914:G:H5' | 3:A:915:C:OP2 | 2.13 | 0.48 |
| 3:A:2428:G:H21 | 15:M:60:ARG:NH2 | 2.12 | 0.48 |
| 13:K:72:LYS:HE3 | 13:K:74:TYR:CZ | 2.49 | 0.48 |
| 28:Z:14:LEU:HB3 | 28:Z:57:LEU:HD21 | 1.96 | 0.48 |
| 3:A:160:A:N3 | 3:A:2208:C:O2' | 2.43 | 0.48 |
| 3:A:782:A:N7 | 5:C:220:VAL:HG21 | 2.29 | 0.48 |
| 3:A:1132:U:H3' | 3:A:1133:A:H5'' | 1.95 | 0.48 |
| 3:A:2433:A:H2 | 27:Y:21:ALA:HB1 | 1.79 | 0.48 |
| 5:C:175:ARG:HG3 | 5:C:181:MET:HE1 | 1.96 | 0.48 |
| 6:D:25:THR:HG21 | 6:D:193:VAL:HG22 | 1.95 | 0.48 |
| 8:F:7:TYR:CD1 | 8:F:11:GLU:HG3 | 2.48 | 0.48 |
| 10:H:115:VAL:HG22 | 10:H:132:PHE:CE2 | 2.48 | 0.48 |
| 16:N:11:LYS:HD3 | 16:N:86:LYS:HD3 | 1.96 | 0.48 |
| 23:U:58:VAL:HG22 | 23:U:85:VAL:HG22 | 1.96 | 0.48 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|------------------|--------------------------|-------------------|
| 3:A:1268:A:H2' | 3:A:1269:A:O4' | 2.13 | 0.48 |
| 3:A:1386:C:H2' | 3:A:1387:A:C8 | 2.49 | 0.48 |
| 3:A:1527:G:N1 | 3:A:1544:A:OP2 | 2.32 | 0.48 |
| 3:A:1846:G:H5'' | 3:A:1847:A:OP2 | 2.14 | 0.48 |
| 3:A:2305:U:H5'' | 8:F:131:GLY:HA3 | 1.96 | 0.48 |
| 3:A:2570:G:H2' | 3:A:2571:U:O4' | 2.14 | 0.48 |
| 3:A:2834:G:H2' | 3:A:2879:A:N6 | 2.29 | 0.48 |
| 5:C:260:ASN:OD1 | 5:C:262:ARG:N | 2.37 | 0.48 |
| 13:K:58:ASN:ND2 | 13:K:128:ASN:OD1 | 2.42 | 0.48 |
| 16:N:41:LEU:HG | 16:N:96:ILE:HG13 | 1.95 | 0.48 |
| 3:A:156:A:H2' | 3:A:157:C:O4' | 2.13 | 0.47 |
| 3:A:483:A:O4' | 24:V:45:HIS:HB3 | 2.14 | 0.47 |
| 3:A:2226:C:H2' | 3:A:2227:A:O4' | 2.13 | 0.47 |
| 9:G:155:GLU:OE1 | 9:G:157:TYR:N | 2.45 | 0.47 |
| 10:H:142:VAL:HG12 | 10:H:143:ILE:H | 1.79 | 0.47 |
| 3:A:208:C:H2' | 3:A:209:C:H6 | 1.78 | 0.47 |
| 3:A:477:A:H2' | 3:A:478:A:C8 | 2.49 | 0.47 |
| 3:A:910:A:H2' | 3:A:911:A:C8 | 2.48 | 0.47 |
| 3:A:2060:A:H3' | 7:E:63:LYS:NZ | 2.29 | 0.47 |
| 3:A:2444:G:OP2 | 7:E:63:LYS:HD2 | 2.14 | 0.47 |
| 13:K:32:LEU:O | 13:K:36:LEU:HG | 3.31 | 0.47 |
| 13:K:78:THR:HG23 | 13:K:83:GLY:O | 2.13 | 0.47 |
| 6:D:56:LYS:HB2 | 6:D:59:ARG:HB2 | 1.95 | 0.47 |
| 9:G:35:ARG:CD | 9:G:71:LEU:HD13 | 2.44 | 0.47 |
| 10:H:93:SER:HB3 | 10:H:123:ARG:HG2 | 1.95 | 0.47 |
| 12:J:10:LYS:O | 12:J:11:LEU:HD12 | 2.15 | 0.47 |
| 12:J:42:PHE:O | 12:J:46:THR:OG1 | 2.32 | 0.47 |
| 22:T:96:ILE:HD13 | 22:T:96:ILE:HA | 1.74 | 0.47 |
| 3:A:112:U:H5' | 28:Z:58:ASN:HD21 | 1.80 | 0.47 |
| 3:A:795:C:H2' | 3:A:796:C:C6 | 2.49 | 0.47 |
| 3:A:957:C:C5 | 3:A:959:A:C5 | 3.01 | 0.47 |
| 3:A:995:C:OP2 | 20:R:54:LYS:NZ | 2.44 | 0.47 |
| 3:A:1027:A:C6 | 3:A:1126:A:C4 | 3.02 | 0.47 |
| 3:A:1438:U:H2' | 3:A:1439:A:H8 | 1.79 | 0.47 |
| 13:K:114:LEU:O | 13:K:118:MET:HG3 | 2.14 | 0.47 |
| 3:A:1446:C:H2' | 3:A:1447:C:C6 | 2.49 | 0.47 |
| 3:A:1873:G:H2' | 3:A:1874:C:C6 | 2.49 | 0.47 |
| 11:I:85:VAL:HG22 | 11:I:92:ALA:HB2 | 1.96 | 0.47 |
| 12:J:40:LYS:N | 12:J:40:LYS:HD2 | 2.30 | 0.47 |
| 15:M:55:MET:SD | 15:M:56:PRO:HD2 | 2.55 | 0.47 |
| 24:V:14:LEU:HD11 | 24:V:71:ALA:HB2 | 1.95 | 0.47 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|-------------------|--------------------------|-------------------|
| 3:A:127:A:H5'' | 3:A:128:C:O4' | 2.14 | 0.47 |
| 3:A:1007:C:H5'' | 13:K:37:ARG:NH2 | 2.28 | 0.47 |
| 3:A:2592:G:C6 | 3:A:2593:U:N3 | 2.83 | 0.47 |
| 18:P:30:ARG:HB3 | 18:P:97:PHE:CE1 | 2.50 | 0.47 |
| 18:P:31:THR:HG23 | 18:P:32:PRO:HD2 | 1.96 | 0.47 |
| 18:P:43:ASN:ND2 | 18:P:43:ASN:H | 2.13 | 0.47 |
| 25:W:2:PHE:HB3 | 25:W:50:MET:CE | 2.45 | 0.47 |
| 1:1:45:U:H3 | 1:1:64:G:H1 | 1.63 | 0.47 |
| 3:A:911:A:H2' | 16:N:9:PHE:HZ | 1.78 | 0.47 |
| 3:A:911:A:H2' | 16:N:9:PHE:CZ | 2.50 | 0.47 |
| 3:A:1085:A:H61 | 11:I:35:VAL:HG22 | 1.78 | 0.47 |
| 3:A:1672:A:C6 | 3:A:1673:G:C6 | 3.03 | 0.47 |
| 3:A:2431:U:H5 | 3:A:2433:A:H5'' | 1.79 | 0.47 |
| 3:A:2557:G:H2' | 3:A:2558:C:C6 | 2.49 | 0.47 |
| 6:D:121:THR:HB | 6:D:127:PHE:CD2 | 2.50 | 0.47 |
| 7:E:125:SER:OG | 7:E:126:VAL:N | 2.46 | 0.47 |
| 7:E:149:ILE:HB | 7:E:188:MET:HG2 | 1.96 | 0.47 |
| 9:G:102:VAL:HG22 | 9:G:116:GLN:HE22 | 1.78 | 0.47 |
| 10:H:29:PHE:O | 10:H:32:PRO:HD2 | 2.15 | 0.47 |
| 27:Y:62:LYS:HE3 | 27:Y:66:THR:HG21 | 1.96 | 0.47 |
| 3:A:323:C:C4 | 3:A:333:G:C8 | 3.03 | 0.47 |
| 8:F:25:VAL:O | 8:F:28:VAL:HG12 | 2.14 | 0.47 |
| 22:T:7:HIS:CE1 | 22:T:10:ALA:HB2 | 2.49 | 0.47 |
| 3:A:713:G:H2' | 3:A:714:U:C6 | 2.50 | 0.47 |
| 3:A:825:A:C2 | 3:A:833:A:C2 | 3.03 | 0.47 |
| 3:A:975:A:H1' | 3:A:990:A:C2 | 2.50 | 0.47 |
| 3:A:998:C:H2' | 3:A:999:U:O4' | 2.14 | 0.47 |
| 3:A:1799:G:C5 | 5:C:176:LEU:HD13 | 2.50 | 0.47 |
| 3:A:2419:U:O2' | 3:A:2420:C:H5' | 2.15 | 0.47 |
| 12:J:28:LEU:HD11 | 12:J:33:VAL:HG11 | 1.97 | 0.47 |
| 12:J:75:PRO:HD2 | 12:J:78:VAL:HB | 1.96 | 0.47 |
| 17:O:25:ALA:O | 17:O:29:VAL:HG23 | 2.15 | 0.47 |
| 19:Q:100:LEU:HA | 19:Q:100:LEU:HD23 | 1.67 | 0.47 |
| 27:Y:40:VAL:HG12 | 27:Y:43:GLU:H | 1.80 | 0.47 |
| 1:1:37:U:O4 | 1:1:68:A:N6 | 2.49 | 0.47 |
| 3:A:861:A:C6 | 3:A:917:A:C8 | 3.03 | 0.47 |
| 3:A:1060:U:C2 | 3:A:1062:G:H5' | 2.50 | 0.47 |
| 3:A:1689:A:C6 | 3:A:1700:A:C2 | 3.03 | 0.47 |
| 3:A:2339:C:H2' | 3:A:2340:A:H8 | 1.80 | 0.47 |
| 8:F:73:SER:OG | 8:F:81:GLN:N | 2.33 | 0.47 |
| 24:V:41:LEU:HD22 | 24:V:62:GLU:HG2 | 1.96 | 0.47 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 3:A:857:G:H2' | 3:A:858:G:O4' | 2.16 | 0.46 |
| 3:A:2039:U:H2' | 3:A:2040:G:C8 | 2.51 | 0.46 |
| 5:C:252:THR:OG1 | 5:C:253:LYS:N | 2.48 | 0.46 |
| 9:G:42:GLU:CG | 9:G:55:ARG:HH21 | 2.29 | 0.46 |
| 11:I:39:THR:HG22 | 11:I:43:LYS:HE3 | 1.98 | 0.46 |
| 19:Q:88:ARG:NH2 | 19:Q:112:GLU:HB2 | 2.31 | 0.46 |
| 3:A:144:A:H1' | 23:U:3:ARG:HH22 | 1.80 | 0.46 |
| 3:A:1038:G:H2' | 3:A:1039:A:C8 | 2.50 | 0.46 |
| 3:A:1097:U:H2' | 3:A:1098:A:O4' | 2.15 | 0.46 |
| 3:A:1808:A:H3' | 3:A:1809:A:H8 | 1.79 | 0.46 |
| 3:A:1946:U:H2' | 3:A:1947:C:C6 | 2.51 | 0.46 |
| 10:H:40:THR:HG22 | 10:H:41:LYS:H | 1.79 | 0.46 |
| 21:S:38:VAL:O | 21:S:54:VAL:HG23 | 2.15 | 0.46 |
| 3:A:75:G:H4' | 28:Z:48:ARG:CZ | 2.45 | 0.46 |
| 3:A:796:C:H2' | 3:A:797:G:C8 | 2.51 | 0.46 |
| 3:A:861:A:H2' | 3:A:862:G:O4' | 2.15 | 0.46 |
| 3:A:871:U:H2' | 3:A:872:U:C6 | 2.50 | 0.46 |
| 3:A:2230:G:H2' | 3:A:2231:U:C6 | 2.51 | 0.46 |
| 9:G:121:ILE:HD13 | 9:G:135:GLY:HA3 | 1.98 | 0.46 |
| 11:I:27:VAL:HG13 | 11:I:80:THR:HG23 | 1.97 | 0.46 |
| 18:P:53:THR:HB | 18:P:65:THR:HB | 1.98 | 0.46 |
| 20:R:49:ASP:HA | 20:R:52:GLN:HB2 | 1.96 | 0.46 |
| 1:I:59:A:H2' | 1:I:60:A:C8 | 2.50 | 0.46 |
| 3:A:247:G:H4' | 3:A:386:G:C5 | 2.50 | 0.46 |
| 3:A:1028:A:N6 | 3:A:1125:G:H2' | 2.30 | 0.46 |
| 3:A:1420:A:N7 | 3:A:2211:A:N6 | 2.62 | 0.46 |
| 3:A:2047:C:O2' | 3:A:2823:A:N1 | 2.42 | 0.46 |
| 4:B:116:G:H2' | 4:B:117:G:H8 | 1.80 | 0.46 |
| 13:K:98:GLU:OE1 | 13:K:98:GLU:N | 2.41 | 0.46 |
| 20:R:18:LEU:HD11 | 20:R:32:TYR:HA | 1.97 | 0.46 |
| 3:A:483:A:H5'' | 24:V:47:LYS:HG2 | 1.97 | 0.46 |
| 3:A:1062:G:N2 | 12:J:93:PRO:HG2 | 2.30 | 0.46 |
| 3:A:1510:G:H2' | 3:A:1511:G:H8 | 1.78 | 0.46 |
| 3:A:2788:C:H2' | 3:A:2789:C:C6 | 2.50 | 0.46 |
| 5:C:176:LEU:HD23 | 5:C:176:LEU:HA | 1.80 | 0.46 |
| 5:C:232:HIS:NE2 | 5:C:244:PRO:HA | 2.30 | 0.46 |
| 15:M:21:ARG:HD3 | 15:M:21:ARG:HA | 1.66 | 0.46 |
| 3:A:2821:A:H2' | 3:A:2822:G:C8 | 2.51 | 0.46 |
| 14:L:73:ASP:OD1 | 14:L:73:ASP:N | 2.39 | 0.46 |
| 3:A:358:U:H2' | 3:A:359:G:C8 | 2.44 | 0.46 |
| 3:A:2126:A:H61 | 3:A:2163:A:H5' | 1.80 | 0.46 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 5:C:125:LYS:HE2 | 5:C:125:LYS:HB2 | 1.77 | 0.46 |
| 13:K:95:ARG:HG2 | 13:K:96:ARG:N | 2.30 | 0.46 |
| 16:N:66:ARG:HB2 | 16:N:101:VAL:O | 2.16 | 0.46 |
| 3:A:878:A:H5' | 3:A:879:G:OP2 | 2.16 | 0.46 |
| 3:A:1342:A:C6 | 3:A:1397:U:C5 | 3.04 | 0.46 |
| 3:A:1709:U:H2' | 3:A:1710:G:H8 | 1.80 | 0.46 |
| 3:A:2786:U:H2' | 3:A:2787:C:H6 | 1.79 | 0.46 |
| 5:C:33:LEU:HD23 | 5:C:33:LEU:HA | 1.58 | 0.46 |
| 14:L:25:LEU:HA | 14:L:25:LEU:HD23 | 1.67 | 0.46 |
| 22:T:25:ARG:NH2 | 22:T:74:ILE:O | 2.49 | 0.46 |
| 3:A:532:A:N3 | 3:A:532:A:H2' | 2.31 | 0.46 |
| 3:A:880:G:N2 | 3:A:898:C:C2 | 2.84 | 0.46 |
| 3:A:1387:A:H5' | 3:A:1469:A:H1' | 1.97 | 0.46 |
| 3:A:2069:G:N2 | 3:A:2443:C:C2 | 2.83 | 0.46 |
| 4:B:95:U:H2' | 4:B:96:G:H8 | 1.81 | 0.46 |
| 9:G:155:GLU:OE2 | 9:G:158:LYS:N | 2.48 | 0.46 |
| 11:I:30:SER:HB3 | 11:I:81:LEU:HB2 | 1.98 | 0.46 |
| 19:Q:106:LYS:O | 19:Q:109:ARG:NH2 | 2.45 | 0.46 |
| 3:A:1785:A:O2' | 3:A:1786:A:H2' | 2.16 | 0.46 |
| 3:A:1869:G:N2 | 3:A:1873:G:C5 | 2.83 | 0.46 |
| 3:A:2229:U:H2' | 3:A:2230:G:C8 | 2.51 | 0.46 |
| 6:D:99:GLU:OE2 | 6:D:182:ALA:HB2 | 2.15 | 0.46 |
| 17:O:28:LEU:O | 17:O:32:GLU:N | 2.45 | 0.46 |
| 3:A:1563:U:H2' | 3:A:1564:C:C6 | 2.51 | 0.45 |
| 12:J:80:LEU:HB3 | 12:J:138:LEU:CD1 | 2.46 | 0.45 |
| 24:V:81:ASP:OD2 | 24:V:96:PHE:HB3 | 2.16 | 0.45 |
| 3:A:208:C:H2' | 3:A:209:C:C6 | 2.52 | 0.45 |
| 3:A:1570:A:H5' | 5:C:36:LYS:HB2 | 1.98 | 0.45 |
| 6:D:184:ARG:HH11 | 19:Q:7:GLN:CD | 2.20 | 0.45 |
| 22:T:13:SER:O | 22:T:17:VAL:HG23 | 2.17 | 0.45 |
| 3:A:772:C:H2' | 3:A:773:U:C6 | 2.52 | 0.45 |
| 3:A:1706:C:O2' | 3:A:1757:A:H5' | 2.17 | 0.45 |
| 3:A:1848:A:H3' | 3:A:1849:G:H8 | 1.80 | 0.45 |
| 5:C:160:THR:O | 5:C:195:VAL:HG23 | 2.17 | 0.45 |
| 14:L:17:ARG:HA | 14:L:17:ARG:HD3 | 1.77 | 0.45 |
| 14:L:79:PHE:CD1 | 19:Q:70:VAL:HG22 | 2.46 | 0.45 |
| 15:M:27:LEU:O | 15:M:31:GLY:HA2 | 2.16 | 0.45 |
| 3:A:1086:A:H4' | 3:A:1103:A:C2 | 2.52 | 0.45 |
| 3:A:1149:G:H2' | 3:A:1150:C:C6 | 2.50 | 0.45 |
| 8:F:20:PHE:CZ | 8:F:165:GLU:HA | 2.51 | 0.45 |
| 24:V:37:GLU:O | 24:V:39:ILE:HG12 | 2.17 | 0.45 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|-------------------|--------------------------|-------------------|
| 3:A:1466:U:H5'' | 3:A:1467:U:H5' | 1.98 | 0.45 |
| 3:A:1653:G:H3' | 17:O:2:ARG:HG3 | 1.98 | 0.45 |
| 3:A:2052:A:OP1 | 6:D:146:ILE:HG12 | 2.17 | 0.45 |
| 6:D:207:VAL:HG13 | 6:D:208:LYS:HG3 | 1.98 | 0.45 |
| 10:H:62:LEU:HD23 | 10:H:135:HIS:CD2 | 2.52 | 0.45 |
| 11:I:53:ARG:O | 11:I:81:LEU:HD12 | 2.16 | 0.45 |
| 14:L:66:LYS:HB3 | 14:L:66:LYS:HE2 | 1.64 | 0.45 |
| 18:P:88:LYS:HG2 | 18:P:116:GLN:HB2 | 1.98 | 0.45 |
| 25:W:25:LYS:HB3 | 25:W:25:LYS:HE2 | 1.71 | 0.45 |
| 3:A:111:A:H2' | 3:A:112:U:O4' | 2.16 | 0.45 |
| 3:A:172:A:H2' | 3:A:173:A:H8 | 1.81 | 0.45 |
| 3:A:257:C:H2' | 3:A:258:G:O4' | 2.15 | 0.45 |
| 3:A:831:G:H5'' | 15:M:37:GLY:HA2 | 1.97 | 0.45 |
| 3:A:908:C:O2' | 16:N:70:ASP:OD2 | 2.30 | 0.45 |
| 3:A:1545:A:H2' | 3:A:1546:G:O4' | 2.17 | 0.45 |
| 3:A:1848:A:N3 | 3:A:1849:G:C8 | 2.85 | 0.45 |
| 3:A:2667:C:H1' | 9:G:109:PHE:CD1 | 2.52 | 0.45 |
| 6:D:49:GLN:HA | 6:D:80:TRP:O | 2.16 | 0.45 |
| 23:U:34:VAL:HG21 | 23:U:43:ILE:HD11 | 1.99 | 0.45 |
| 25:W:83:LYS:HB3 | 25:W:85:LYS:HG3 | 1.98 | 0.45 |
| 26:X:23:VAL:HG22 | 26:X:38:VAL:HB | 1.99 | 0.45 |
| 3:A:499:U:H5'' | 24:V:43:LYS:HE3 | 1.99 | 0.45 |
| 3:A:1313:U:H2' | 3:A:1610:A:C2 | 2.51 | 0.45 |
| 3:A:1416:G:N2 | 3:A:1582:C:O2 | 2.33 | 0.45 |
| 3:A:1631:G:N2 | 3:A:1634:A:OP2 | 2.32 | 0.45 |
| 3:A:2165:C:H2' | 3:A:2166:U:O4' | 2.16 | 0.45 |
| 3:A:2433:A:H5' | 3:A:2434:A:P | 2.57 | 0.45 |
| 14:L:99:ILE:HG12 | 14:L:118:LEU:HB2 | 1.98 | 0.45 |
| 3:A:239:C:H2' | 3:A:240:C:O4' | 2.16 | 0.45 |
| 3:A:629:G:H5'' | 3:A:650:C:O2' | 2.16 | 0.45 |
| 3:A:657:U:H2' | 3:A:658:U:C6 | 2.52 | 0.45 |
| 3:A:706:A:C2 | 3:A:707:G:H1' | 2.52 | 0.45 |
| 3:A:1022:G:O2' | 3:A:1024:G:O6 | 2.27 | 0.45 |
| 3:A:1287:A:H3' | 3:A:1288:G:N2 | 2.32 | 0.45 |
| 3:A:1972:G:H2' | 3:A:1973:G:H8 | 1.81 | 0.45 |
| 3:A:2134:A:H1' | 3:A:2159:G:H21 | 1.82 | 0.45 |
| 3:A:2396:G:N3 | 3:A:2421:G:N2 | 2.64 | 0.45 |
| 3:A:2667:C:H1' | 9:G:109:PHE:HD1 | 1.82 | 0.45 |
| 10:H:100:ALA:O | 10:H:104:THR:HG23 | 2.17 | 0.45 |
| 18:P:18:LEU:HA | 18:P:18:LEU:HD23 | 1.71 | 0.45 |
| 3:A:593:U:H2' | 3:A:594:U:C6 | 2.52 | 0.45 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|-------------------|--------------------------|-------------------|
| 3:A:718:A:H2' | 3:A:719:C:O4' | 2.16 | 0.45 |
| 3:A:764:A:H5' | 5:C:209:GLY:HA2 | 1.98 | 0.45 |
| 3:A:948:C:H1' | 3:A:984:A:C8 | 2.52 | 0.45 |
| 3:A:2327:A:H2' | 3:A:2328:A:C8 | 2.52 | 0.45 |
| 3:A:2524:G:H2' | 3:A:2525:G:O4' | 2.16 | 0.45 |
| 12:J:117:MET:HB2 | 12:J:125:MET:HG2 | 1.99 | 0.45 |
| 17:O:2:ARG:HB3 | 17:O:2:ARG:CZ | 2.47 | 0.45 |
| 17:O:17:ARG:HG2 | 17:O:21:PHE:HE2 | 1.82 | 0.45 |
| 3:A:1177:G:H2' | 3:A:1178:C:C6 | 2.51 | 0.45 |
| 3:A:1918:A:O2' | 3:A:1920:C:N4 | 2.50 | 0.45 |
| 5:C:243:HIS:HA | 5:C:244:PRO:HD3 | 1.79 | 0.45 |
| 8:F:136:ILE:HG22 | 8:F:141:ILE:HG21 | 1.98 | 0.45 |
| 9:G:148:LEU:HD23 | 9:G:148:LEU:HA | 1.71 | 0.45 |
| 11:I:41:LEU:HB2 | 11:I:99:PHE:CE1 | 2.52 | 0.45 |
| 13:K:69:ARG:O | 13:K:89:PHE:HB3 | 2.17 | 0.45 |
| 16:N:65:ILE:HG12 | 16:N:103:TYR:CD2 | 2.51 | 0.45 |
| 21:S:4:VAL:HA | 21:S:12:HIS:O | 2.16 | 0.45 |
| 3:A:154:U:H2' | 3:A:155:A:C8 | 2.53 | 0.44 |
| 3:A:2273:A:H2' | 3:A:2274:A:C8 | 2.52 | 0.44 |
| 3:A:2313:C:H5'' | 8:F:88:LYS:HD3 | 1.98 | 0.44 |
| 3:A:2683:C:H4' | 6:D:13:ARG:HH12 | 1.81 | 0.44 |
| 6:D:7:LYS:HB3 | 6:D:7:LYS:HE2 | 1.78 | 0.44 |
| 12:J:86:ILE:CD1 | 12:J:138:LEU:HD21 | 2.46 | 0.44 |
| 12:J:130:GLU:HB3 | 12:J:134:ARG:NH2 | 2.32 | 0.44 |
| 19:Q:89:ARG:HB3 | 19:Q:113:ARG:NH1 | 2.32 | 0.44 |
| 3:A:594:U:H2' | 3:A:595:C:C6 | 2.51 | 0.44 |
| 3:A:620:G:H4' | 3:A:621:A:O5' | 2.17 | 0.44 |
| 3:A:1450:G:C6 | 3:A:1451:C:N4 | 2.86 | 0.44 |
| 3:A:1667:G:N2 | 3:A:1992:G:OP2 | 2.44 | 0.44 |
| 3:A:2230:G:H1' | 27:Y:32:ASN:HB2 | 1.99 | 0.44 |
| 3:A:2396:G:C2 | 3:A:2421:G:C2 | 3.05 | 0.44 |
| 7:E:121:VAL:O | 7:E:189:THR:HA | 2.18 | 0.44 |
| 11:I:52:MET:HE3 | 11:I:81:LEU:HD11 | 1.99 | 0.44 |
| 13:K:65:THR:O | 13:K:68:LYS:HB2 | 2.16 | 0.44 |
| 16:N:90:GLU:HB3 | 16:N:91:TYR:CD1 | 2.53 | 0.44 |
| 26:X:55:ARG:HE | 26:X:55:ARG:HB2 | 1.45 | 0.44 |
| 3:A:198:C:O2' | 3:A:199:A:H5' | 2.17 | 0.44 |
| 3:A:2489:U:C4 | 3:A:2490:G:C6 | 3.06 | 0.44 |
| 3:A:2569:G:C2 | 3:A:2570:G:C8 | 3.05 | 0.44 |
| 3:A:2776:A:C8 | 3:A:2782:G:C5 | 3.05 | 0.44 |
| 9:G:117:LEU:HD13 | 9:G:121:ILE:HG22 | 1.99 | 0.44 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 15:M:10:GLU:OE2 | 15:M:11:GLY:N | 2.50 | 0.44 |
| 21:S:27:ILE:HG22 | 21:S:28:ALA:O | 2.18 | 0.44 |
| 3:A:77:G:H2' | 3:A:78:U:O4' | 2.16 | 0.44 |
| 3:A:1198:U:H2' | 3:A:1199:U:C6 | 2.52 | 0.44 |
| 3:A:2387:U:H1' | 26:X:41:ARG:NH1 | 2.32 | 0.44 |
| 3:A:2704:C:H2' | 3:A:2705:A:O4' | 2.17 | 0.44 |
| 19:Q:62:ARG:NH2 | 19:Q:101:ARG:HG2 | 2.32 | 0.44 |
| 25:W:21:ARG:HE | 25:W:87:GLN:HA | 1.83 | 0.44 |
| 26:X:36:ILE:HG23 | 26:X:58:THR:HG23 | 2.00 | 0.44 |
| 28:Z:56:LEU:HD22 | 28:Z:56:LEU:HA | 1.82 | 0.44 |
| 3:A:141:G:C8 | 3:A:141:G:H3' | 2.51 | 0.44 |
| 3:A:1420:A:N7 | 3:A:2211:A:C6 | 2.85 | 0.44 |
| 3:A:1508:A:O2' | 3:A:1509:A:O4' | 2.19 | 0.44 |
| 3:A:2318:G:C6 | 3:A:2319:G:N1 | 2.86 | 0.44 |
| 12:J:122:ILE:O | 12:J:126:THR:OG1 | 2.22 | 0.44 |
| 14:L:3:GLN:HE21 | 14:L:3:GLN:HB3 | 1.66 | 0.44 |
| 3:A:57:C:H2' | 3:A:58:G:O4' | 2.18 | 0.44 |
| 3:A:149:A:C2 | 3:A:150:U:C2 | 3.06 | 0.44 |
| 3:A:356:G:H2' | 3:A:357:C:O4' | 2.18 | 0.44 |
| 3:A:870:U:OP1 | 16:N:6:ARG:NH1 | 2.51 | 0.44 |
| 3:A:1591:A:H2' | 3:A:1592:C:C6 | 2.53 | 0.44 |
| 3:A:2377:A:H2' | 3:A:2378:A:C8 | 2.53 | 0.44 |
| 8:F:67:ILE:HD12 | 8:F:84:PRO:HB3 | 2.00 | 0.44 |
| 8:F:147:ASP:OD1 | 8:F:150:ARG:NH2 | 2.51 | 0.44 |
| 3:A:181:A:H1' | 3:A:435:C:O4' | 2.17 | 0.44 |
| 3:A:630:G:N2 | 3:A:633:A:OP2 | 2.43 | 0.44 |
| 3:A:997:G:H5'' | 20:R:92:ARG:NH1 | 2.33 | 0.44 |
| 3:A:1082:U:O2' | 11:I:39:THR:HG23 | 2.18 | 0.44 |
| 3:A:1301:A:H2' | 3:A:1301:A:N3 | 2.33 | 0.44 |
| 3:A:2683:C:H4' | 6:D:13:ARG:NH1 | 2.33 | 0.44 |
| 3:A:746:U:HO2' | 3:A:2611:C:HO2' | 1.66 | 0.44 |
| 3:A:1056:G:H1' | 3:A:1103:A:N6 | 2.33 | 0.44 |
| 3:A:1082:U:H4' | 11:I:46:ARG:NH1 | 2.32 | 0.44 |
| 3:A:1093:G:H1' | 3:A:1099:G:N1 | 2.32 | 0.44 |
| 3:A:2024:G:H2' | 3:A:2025:C:C6 | 2.53 | 0.44 |
| 3:A:2678:C:H2' | 3:A:2679:A:O4' | 2.18 | 0.44 |
| 10:H:26:ALA:HA | 10:H:30:LEU:HB2 | 1.99 | 0.44 |
| 18:P:52:SER:O | 18:P:58:ILE:HD12 | 2.18 | 0.44 |
| 19:Q:53:ARG:HB2 | 19:Q:56:HIS:HB2 | 1.99 | 0.44 |
| 27:Y:59:ILE:HG12 | 27:Y:67:VAL:HG21 | 1.99 | 0.44 |
| 3:A:33:C:N4 | 3:A:446:G:O2' | 2.45 | 0.44 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|-------------------|--------------------------|-------------------|
| 3:A:277:G:H4' | 3:A:278:A:N7 | 2.33 | 0.44 |
| 3:A:1205:A:H2' | 7:E:165:HIS:HE1 | 1.83 | 0.44 |
| 3:A:1230:A:H2' | 3:A:1231:U:O4' | 2.18 | 0.44 |
| 3:A:1614:A:C2 | 22:T:93:ALA:HB2 | 2.52 | 0.44 |
| 3:A:2443:C:H2' | 3:A:2444:G:H8 | 1.82 | 0.44 |
| 5:C:141:VAL:HG12 | 5:C:192:LEU:HA | 1.98 | 0.44 |
| 8:F:128:TYR:CE2 | 8:F:130:MET:HG2 | 2.53 | 0.44 |
| 9:G:42:GLU:HG3 | 9:G:55:ARG:HH21 | 1.83 | 0.44 |
| 18:P:85:LYS:HE2 | 18:P:85:LYS:HB3 | 1.79 | 0.44 |
| 19:Q:25:THR:HB | 19:Q:88:ARG:HG2 | 1.99 | 0.44 |
| 3:A:1266:G:N2 | 3:A:2012:G:H2' | 2.33 | 0.43 |
| 3:A:1266:G:O2' | 3:A:2012:G:O6 | 2.34 | 0.43 |
| 3:A:1287:A:H5' | 17:O:103:ARG:HD2 | 1.98 | 0.43 |
| 3:A:1710:G:H2' | 3:A:1711:A:C8 | 2.53 | 0.43 |
| 3:A:1853:A:N6 | 3:A:1888:G:O2' | 2.51 | 0.43 |
| 3:A:2292:U:H2' | 3:A:2293:G:C8 | 2.52 | 0.43 |
| 4:B:114:C:H2' | 4:B:115:A:H8 | 1.83 | 0.43 |
| 12:J:110:ALA:O | 12:J:114:ALA:HB2 | 2.18 | 0.43 |
| 23:U:31:VAL:O | 23:U:32:LEU:HD23 | 2.18 | 0.43 |
| 3:A:475:C:N4 | 3:A:476:G:C6 | 2.86 | 0.43 |
| 3:A:677:A:O2' | 3:A:2071:A:H5' | 2.17 | 0.43 |
| 3:A:1962:C:H4' | 3:A:1963:U:C5 | 2.52 | 0.43 |
| 3:A:2654:A:OP1 | 3:A:2654:A:H8 | 2.01 | 0.43 |
| 12:J:90:SER:HB2 | 12:J:136:MET:O | 2.18 | 0.43 |
| 3:A:380:G:H2' | 3:A:381:G:O4' | 2.18 | 0.43 |
| 3:A:969:G:H2' | 3:A:970:U:C6 | 2.53 | 0.43 |
| 3:A:1048:A:N1 | 3:A:1112:G:O2' | 2.36 | 0.43 |
| 3:A:1351:C:H4' | 3:A:1572:A:O4' | 2.18 | 0.43 |
| 3:A:2172:U:H4' | 3:A:2173:A:H5' | 2.00 | 0.43 |
| 8:F:145:LYS:HA | 8:F:145:LYS:HD3 | 1.89 | 0.43 |
| 15:M:80:SER:O | 15:M:84:LYS:HE3 | 2.19 | 0.43 |
| 21:S:91:GLN:NE2 | 21:S:92:TRP:H | 2.16 | 0.43 |
| 3:A:776:G:HO2' | 3:A:777:G:P | 2.39 | 0.43 |
| 3:A:973:A:OP2 | 21:S:81:LYS:HE3 | 2.18 | 0.43 |
| 3:A:1735:A:H2' | 3:A:1736:U:O4' | 2.18 | 0.43 |
| 3:A:2647:U:H2' | 3:A:2648:G:C8 | 2.54 | 0.43 |
| 22:T:47:VAL:HG22 | 22:T:103:ILE:HD13 | 2.00 | 0.43 |
| 3:A:93:G:H2' | 3:A:94:A:H8 | 1.84 | 0.43 |
| 3:A:1044:C:O2' | 3:A:1111:A:N1 | 2.45 | 0.43 |
| 3:A:1354:A:H2' | 3:A:1355:G:O4' | 2.19 | 0.43 |
| 3:A:1515:A:H3' | 3:A:1516:G:H8 | 1.84 | 0.43 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 3:A:1627:G:C2 | 3:A:1628:G:C8 | 3.07 | 0.43 |
| 3:A:2292:U:H2' | 3:A:2293:G:H8 | 1.84 | 0.43 |
| 4:B:49:C:H2' | 4:B:50:A:C8 | 2.54 | 0.43 |
| 10:H:46:PHE:HD1 | 10:H:50:ARG:NH2 | 2.16 | 0.43 |
| 17:O:86:ARG:HD3 | 17:O:121:LYS:HG3 | 1.98 | 0.43 |
| 20:R:24:TYR:O | 20:R:29:SER:HB3 | 2.19 | 0.43 |
| 3:A:11:C:H2' | 3:A:12:U:H5' | 2.00 | 0.43 |
| 3:A:112:U:H5' | 28:Z:58:ASN:ND2 | 2.34 | 0.43 |
| 3:A:463:G:N1 | 3:A:467:G:C6 | 2.86 | 0.43 |
| 3:A:834:G:C2 | 3:A:835:C:C2 | 3.06 | 0.43 |
| 3:A:976:G:HO2' | 3:A:1155:A:HO2' | 1.60 | 0.43 |
| 3:A:1434:A:C2 | 3:A:1435:G:C5 | 3.07 | 0.43 |
| 3:A:2786:U:H2' | 3:A:2787:C:C6 | 2.53 | 0.43 |
| 5:C:153:GLN:O | 5:C:156:ARG:HG3 | 2.18 | 0.43 |
| 6:D:131:ASP:O | 6:D:140:HIS:HD2 | 2.01 | 0.43 |
| 7:E:108:ILE:O | 7:E:112:LEU:HG | 2.18 | 0.43 |
| 8:F:138:PHE:HA | 8:F:139:PRO:HD3 | 1.90 | 0.43 |
| 1:1:55:A:H2' | 1:1:56:A:C8 | 2.53 | 0.43 |
| 3:A:14:A:C6 | 3:A:526:A:C2 | 3.07 | 0.43 |
| 3:A:76:C:H6 | 3:A:76:C:O5' | 2.02 | 0.43 |
| 3:A:2138:G:C6 | 3:A:2154:A:C2 | 3.06 | 0.43 |
| 3:A:2847:U:H2' | 3:A:2848:G:O4' | 2.18 | 0.43 |
| 5:C:90:ASN:ND2 | 5:C:197:ASN:HB2 | 2.34 | 0.43 |
| 10:H:62:LEU:HD22 | 10:H:137:GLU:OE1 | 2.19 | 0.43 |
| 15:M:6:LEU:HD23 | 15:M:6:LEU:HA | 1.82 | 0.43 |
| 20:R:74:ILE:HG12 | 20:R:75:SER:N | 2.34 | 0.43 |
| 22:T:46:LEU:HA | 22:T:46:LEU:HD23 | 1.82 | 0.43 |
| 3:A:239:C:HO2' | 3:A:622:G:HO2' | 1.62 | 0.43 |
| 3:A:566:U:H5'' | 15:M:29:LYS:HE3 | 1.99 | 0.43 |
| 3:A:591:U:H2' | 3:A:592:A:C8 | 2.54 | 0.43 |
| 3:A:783:A:C5 | 3:A:785:G:H1' | 2.53 | 0.43 |
| 3:A:1542:U:H2' | 3:A:1543:G:O4' | 2.18 | 0.43 |
| 3:A:1597:A:C5' | 3:A:1598:A:H5' | 2.47 | 0.43 |
| 3:A:1858:A:H2' | 3:A:1859:U:O4' | 2.17 | 0.43 |
| 3:A:2114:A:C2 | 3:A:2166:U:H2' | 2.53 | 0.43 |
| 3:A:2130:U:O2' | 3:A:2133:G:O2' | 2.32 | 0.43 |
| 3:A:2512:C:H5'' | 3:A:2513:A:OP2 | 2.17 | 0.43 |
| 3:A:2588:G:O6 | 3:A:2607:G:C6 | 2.72 | 0.43 |
| 7:E:128:ALA:O | 7:E:130:LYS:N | 2.51 | 0.43 |
| 11:I:118:ILE:HA | 11:I:119:PRO:HD2 | 1.84 | 0.43 |
| 16:N:26:VAL:HB | 16:N:133:LYS:HB2 | 2.00 | 0.43 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 20:R:9:ILE:H | 20:R:9:ILE:HD12 | 1.84 | 0.43 |
| 21:S:4:VAL:HG12 | 21:S:39:LEU:HB2 | 2.00 | 0.43 |
| 3:A:493:G:H2' | 3:A:494:G:O4' | 2.19 | 0.43 |
| 3:A:1473:G:H2' | 3:A:1474:U:O4' | 2.19 | 0.43 |
| 3:A:1517:G:C2 | 3:A:1732:C:N3 | 2.86 | 0.43 |
| 5:C:8:PRO:HB3 | 5:C:14:ARG:HG3 | 1.99 | 0.43 |
| 6:D:109:VAL:HG12 | 6:D:201:LEU:HD22 | 2.01 | 0.43 |
| 6:D:148:GLN:OE1 | 6:D:148:GLN:N | 2.51 | 0.43 |
| 10:H:104:THR:HA | 10:H:108:VAL:O | 2.19 | 0.43 |
| 13:K:26:GLY:O | 13:K:30:THR:HG23 | 2.18 | 0.43 |
| 16:N:33:LEU:HD11 | 16:N:128:THR:HB | 2.00 | 0.43 |
| 20:R:17:ILE:HD13 | 20:R:17:ILE:HA | 1.63 | 0.43 |
| 25:W:29:ILE:O | 25:W:91:PHE:HB2 | 2.19 | 0.43 |
| 26:X:47:ALA:HB1 | 26:X:51:VAL:O | 2.19 | 0.43 |
| 3:A:1141:U:H4' | 3:A:1142:A:O4' | 2.19 | 0.43 |
| 3:A:1341:G:O2' | 23:U:59:ASN:ND2 | 2.47 | 0.43 |
| 3:A:1501:G:H2' | 3:A:1502:A:H8 | 1.84 | 0.43 |
| 3:A:2038:G:H2' | 3:A:2039:U:O4' | 2.17 | 0.43 |
| 3:A:2843:G:H2' | 3:A:2844:G:C8 | 2.54 | 0.43 |
| 8:F:170:LEU:HD23 | 8:F:170:LEU:HA | 1.75 | 0.43 |
| 9:G:44:LYS:HE3 | 9:G:44:LYS:HB2 | 1.80 | 0.43 |
| 12:J:33:VAL:HG13 | 12:J:67:PHE:CD2 | 2.54 | 0.43 |
| 17:O:72:ASP:OD1 | 17:O:73:ASN:N | 2.51 | 0.43 |
| 23:U:34:VAL:HG11 | 23:U:43:ILE:HD13 | 2.01 | 0.43 |
| 3:A:5:A:H2' | 3:A:6:A:C8 | 2.54 | 0.42 |
| 3:A:141:G:C8 | 3:A:142:A:O4' | 2.72 | 0.42 |
| 3:A:195:A:H5'' | 15:M:47:ARG:HH22 | 1.84 | 0.42 |
| 3:A:1494:A:H2' | 3:A:1495:A:H8 | 1.83 | 0.42 |
| 3:A:1759:A:H2' | 3:A:1760:C:C6 | 2.54 | 0.42 |
| 3:A:2144:G:N2 | 3:A:2148:G:O6 | 2.52 | 0.42 |
| 3:A:2771:C:H2' | 3:A:2772:C:C6 | 2.54 | 0.42 |
| 5:C:245:VAL:HA | 5:C:252:THR:HG22 | 2.01 | 0.42 |
| 3:A:461:C:H2' | 3:A:462:C:H6 | 1.84 | 0.42 |
| 3:A:464:U:C2 | 3:A:788:A:C6 | 3.07 | 0.42 |
| 3:A:1088:A:H61 | 12:J:135:SER:HB3 | 1.82 | 0.42 |
| 3:A:1614:A:H8 | 3:A:1614:A:O5' | 2.02 | 0.42 |
| 3:A:2533:U:OP1 | 3:A:2665:A:O2' | 2.34 | 0.42 |
| 3:A:2646:C:OP2 | 3:A:2732:G:O2' | 2.35 | 0.42 |
| 5:C:200:HIS:CD2 | 5:C:200:HIS:C | 2.92 | 0.42 |
| 5:C:210:ALA:HA | 5:C:213:TRP:CE3 | 2.53 | 0.42 |
| 3:A:674:G:H2' | 3:A:804:A:H61 | 1.83 | 0.42 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 3:A:1064:C:H5'' | 12:J:88:SER:HB2 | 2.01 | 0.42 |
| 3:A:1524:G:H2' | 3:A:1525:A:O4' | 2.20 | 0.42 |
| 3:A:1590:A:H2' | 3:A:1591:A:C8 | 2.54 | 0.42 |
| 3:A:1736:U:H2' | 3:A:1737:G:O4' | 2.18 | 0.42 |
| 3:A:1922:G:H2' | 3:A:1923:U:O4' | 2.18 | 0.42 |
| 3:A:2184:A:H2' | 3:A:2185:U:C6 | 2.53 | 0.42 |
| 3:A:2700:A:H2' | 3:A:2701:U:C6 | 2.54 | 0.42 |
| 3:A:2790:U:H5' | 3:A:2893:A:N7 | 2.34 | 0.42 |
| 4:B:66:A:H61 | 4:B:107:G:H2' | 1.84 | 0.42 |
| 4:B:106:G:H2' | 4:B:107:G:O4' | 2.19 | 0.42 |
| 5:C:133:ARG:HD2 | 10:H:123:ARG:NH1 | 2.35 | 0.42 |
| 7:E:29:HIS:O | 7:E:32:VAL:HG22 | 2.19 | 0.42 |
| 8:F:79:ILE:HG21 | 8:F:85:ILE:HD11 | 2.01 | 0.42 |
| 9:G:149:ARG:HG3 | 9:G:162:VAL:O | 2.20 | 0.42 |
| 14:L:65:THR:HB | 14:L:68:GLY:H | 1.84 | 0.42 |
| 1:1:48:G:H3' | 1:1:49:G:C8 | 2.54 | 0.42 |
| 3:A:543:G:H5' | 3:A:544:C:OP2 | 2.18 | 0.42 |
| 3:A:571:U:H3' | 21:S:80:ARG:NH2 | 2.34 | 0.42 |
| 3:A:1387:A:H2' | 3:A:1388:G:O4' | 2.18 | 0.42 |
| 3:A:1637:A:H2' | 3:A:1638:C:C6 | 2.54 | 0.42 |
| 5:C:24:LEU:HA | 5:C:24:LEU:HD12 | 1.66 | 0.42 |
| 12:J:38:PHE:CD1 | 12:J:59:ILE:HD11 | 2.54 | 0.42 |
| 12:J:113:LYS:HA | 12:J:116:ASP:HB2 | 2.01 | 0.42 |
| 16:N:36:VAL:HG13 | 25:W:82:TYR:CD2 | 2.55 | 0.42 |
| 20:R:24:TYR:N | 20:R:24:TYR:HD1 | 2.17 | 0.42 |
| 24:V:61:LYS:HG2 | 24:V:62:GLU:H | 1.85 | 0.42 |
| 3:A:123:G:N2 | 3:A:129:C:C2 | 2.87 | 0.42 |
| 3:A:653:U:C1' | 3:A:654:A:H5'' | 2.49 | 0.42 |
| 3:A:729:G:H2' | 3:A:1775:U:H1' | 2.01 | 0.42 |
| 3:A:729:G:C5 | 5:C:207:LYS:HB2 | 2.55 | 0.42 |
| 3:A:1039:A:H2' | 3:A:1040:A:O4' | 2.20 | 0.42 |
| 3:A:1751:U:H2' | 3:A:1752:C:C6 | 2.54 | 0.42 |
| 3:A:1759:A:C2 | 3:A:2697:G:H1' | 2.54 | 0.42 |
| 3:A:2518:A:H2' | 3:A:2518:A:N3 | 2.34 | 0.42 |
| 8:F:48:LYS:HB2 | 8:F:48:LYS:HE2 | 1.85 | 0.42 |
| 12:J:103:ARG:H | 12:J:103:ARG:HD2 | 1.83 | 0.42 |
| 3:A:307:G:N1 | 3:A:310:A:OP2 | 2.52 | 0.42 |
| 3:A:794:A:H2' | 3:A:795:C:C6 | 2.55 | 0.42 |
| 3:A:812:C:C2 | 3:A:1250:G:N1 | 2.87 | 0.42 |
| 3:A:877:A:C6 | 3:A:899:A:C6 | 3.08 | 0.42 |
| 3:A:1798:U:OP2 | 5:C:271:ARG:NH2 | 2.52 | 0.42 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|------------------|--------------------------|-------------------|
| 3:A:1902:C:H4' | 5:C:242:LYS:O | 2.19 | 0.42 |
| 3:A:2304:G:H22 | 3:A:2312:U:H3 | 1.67 | 0.42 |
| 3:A:2322:A:C4 | 3:A:2323:G:C8 | 3.07 | 0.42 |
| 10:H:94:ILE:HG23 | 10:H:98:ASP:HB2 | 2.01 | 0.42 |
| 11:I:15:VAL:HG11 | 11:I:60:LEU:CD2 | 2.50 | 0.42 |
| 12:J:22:PRO:HB2 | 12:J:23:PRO:HD3 | 2.02 | 0.42 |
| 12:J:74:PRO:HA | 12:J:75:PRO:HD3 | 1.89 | 0.42 |
| 19:Q:106:LYS:O | 19:Q:109:ARG:HD3 | 2.20 | 0.42 |
| 20:R:117:LEU:HD23 | 20:R:117:LEU:HA | 1.77 | 0.42 |
| 25:W:2:PHE:HE1 | 25:W:53:LYS:HD2 | 1.84 | 0.42 |
| 3:A:819:A:N3 | 3:A:819:A:H2' | 2.34 | 0.42 |
| 3:A:1110:G:HO2' | 3:A:1111:A:P | 2.43 | 0.42 |
| 3:A:1327:A:H2' | 3:A:1328:A:O4' | 2.19 | 0.42 |
| 3:A:1400:U:H2' | 3:A:1401:G:O4' | 2.19 | 0.42 |
| 4:B:57:A:C4 | 8:F:26:MET:HB3 | 2.54 | 0.42 |
| 10:H:1:MET:O | 10:H:20:ASN:HA | 2.20 | 0.42 |
| 11:I:85:VAL:HG21 | 11:I:90:GLY:O | 2.20 | 0.42 |
| 17:O:75:ILE:HD12 | 17:O:75:ILE:HA | 1.82 | 0.42 |
| 3:A:647:G:H2' | 3:A:648:G:C8 | 2.55 | 0.42 |
| 3:A:1047:G:OP1 | 11:I:56:ARG:NH1 | 2.52 | 0.42 |
| 3:A:1463:C:H2' | 3:A:1464:G:H8 | 1.85 | 0.42 |
| 3:A:2796:U:HO2' | 3:A:2797:U:H6 | 1.63 | 0.42 |
| 17:O:103:ARG:HB3 | 17:O:106:ASP:OD1 | 2.20 | 0.42 |
| 3:A:669:G:N2 | 3:A:670:A:C2 | 2.88 | 0.42 |
| 3:A:910:A:C6 | 3:A:911:A:C6 | 3.08 | 0.42 |
| 3:A:1065:U:H2' | 3:A:1066:U:O4' | 2.19 | 0.42 |
| 3:A:1068:G:N2 | 3:A:1095:A:O3' | 2.44 | 0.42 |
| 3:A:1324:G:C4 | 3:A:1328:A:N6 | 2.88 | 0.42 |
| 3:A:1509:A:O2' | 3:A:1510:G:H8 | 2.03 | 0.42 |
| 3:A:2119:A:H62 | 3:A:2167:U:H1' | 1.85 | 0.42 |
| 3:A:2433:A:H5' | 3:A:2434:A:OP2 | 2.19 | 0.42 |
| 3:A:2776:A:C2 | 3:A:2778:A:C4 | 3.07 | 0.42 |
| 8:F:34:ILE:HB | 8:F:96:MET:HG3 | 2.02 | 0.42 |
| 11:I:43:LYS:HE2 | 12:J:118:THR:HA | 2.01 | 0.42 |
| 14:L:11:ALA:O | 14:L:100:PHE:N | 2.46 | 0.42 |
| 16:N:42:THR:N | 16:N:45:GLN:OE1 | 2.47 | 0.42 |
| 20:R:31:VAL:HG12 | 20:R:34:VAL:H | 1.85 | 0.42 |
| 3:A:565:C:H4' | 3:A:1253:A:C6 | 2.55 | 0.42 |
| 3:A:1499:C:H2' | 3:A:1500:G:H8 | 1.85 | 0.42 |
| 3:A:1880:U:H2' | 3:A:1881:C:C6 | 2.55 | 0.42 |
| 8:F:4:LEU:HD23 | 8:F:4:LEU:HA | 1.73 | 0.42 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 9:G:97:ALA:HB3 | 9:G:104:ASN:HB2 | 2.01 | 0.42 |
| 22:T:28:LYS:HB2 | 22:T:28:LYS:HE2 | 1.41 | 0.42 |
| 3:A:648:G:C2 | 3:A:649:G:C5 | 3.08 | 0.41 |
| 3:A:1417:C:H2' | 3:A:1418:G:C8 | 2.55 | 0.41 |
| 3:A:1463:C:H2' | 3:A:1464:G:C8 | 2.55 | 0.41 |
| 5:C:205:LEU:HD23 | 5:C:205:LEU:HA | 1.68 | 0.41 |
| 7:E:109:LEU:HA | 7:E:109:LEU:HD23 | 1.79 | 0.41 |
| 8:F:57:LEU:HD12 | 8:F:87:CYS:SG | 2.60 | 0.41 |
| 8:F:79:ILE:HD12 | 8:F:79:ILE:O | 2.20 | 0.41 |
| 3:A:449:A:C4 | 3:A:450:G:C8 | 3.08 | 0.41 |
| 3:A:1056:G:H5' | 11:I:35:VAL:HG21 | 2.02 | 0.41 |
| 3:A:1449:G:N2 | 3:A:1463:C:C2 | 2.88 | 0.41 |
| 3:A:1770:G:C6 | 3:A:1983:G:C6 | 3.07 | 0.41 |
| 3:A:1825:U:O2 | 5:C:253:LYS:NZ | 2.31 | 0.41 |
| 3:A:1877:A:H2' | 3:A:1878:G:O4' | 2.20 | 0.41 |
| 3:A:2706:A:C2 | 3:A:2707:U:C2 | 3.08 | 0.41 |
| 9:G:73:ASN:O | 9:G:77:ILE:HG13 | 2.20 | 0.41 |
| 3:A:53:A:H2' | 3:A:54:G:O4' | 2.20 | 0.41 |
| 3:A:118:A:N3 | 3:A:178:G:H1' | 2.36 | 0.41 |
| 3:A:393:C:H2' | 3:A:394:C:H6 | 1.85 | 0.41 |
| 3:A:981:A:N1 | 3:A:2027:G:O2' | 2.42 | 0.41 |
| 3:A:1005:C:H2' | 3:A:1006:C:H6 | 1.84 | 0.41 |
| 3:A:1484:U:H2' | 3:A:1485:U:C6 | 2.55 | 0.41 |
| 3:A:1780:A:H3' | 3:A:1781:U:H2' | 2.01 | 0.41 |
| 3:A:1946:U:H2' | 3:A:1947:C:H6 | 1.84 | 0.41 |
| 3:A:2209:G:C2 | 3:A:2216:G:C2 | 3.08 | 0.41 |
| 3:A:2339:C:O3' | 4:B:41:G:N2 | 2.52 | 0.41 |
| 3:A:2838:G:H2' | 3:A:2839:G:O4' | 2.20 | 0.41 |
| 5:C:176:LEU:HB2 | 5:C:180:GLU:O | 2.20 | 0.41 |
| 7:E:181:ILE:H | 7:E:181:ILE:HG13 | 1.70 | 0.41 |
| 8:F:70:ALA:HB3 | 8:F:81:GLN:HA | 2.02 | 0.41 |
| 9:G:76:VAL:O | 9:G:80:THR:HG23 | 2.20 | 0.41 |
| 14:L:93:GLN:HA | 14:L:94:PRO:HD3 | 1.88 | 0.41 |
| 3:A:335:C:H5'' | 24:V:82:ARG:HD2 | 2.02 | 0.41 |
| 3:A:848:C:H42 | 3:A:930:G:H1 | 1.68 | 0.41 |
| 3:A:1432:G:H2' | 3:A:1433:A:C8 | 2.55 | 0.41 |
| 3:A:1482:G:H2' | 3:A:1483:G:H8 | 1.84 | 0.41 |
| 3:A:2860:A:H5'' | 3:A:2861:U:OP2 | 2.21 | 0.41 |
| 3:A:2895:G:H2' | 3:A:2896:C:C6 | 2.56 | 0.41 |
| 6:D:73:VAL:HG11 | 6:D:93:GLY:HA2 | 2.02 | 0.41 |
| 9:G:83:PHE:HB2 | 9:G:135:GLY:O | 2.20 | 0.41 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 16:N:133:LYS:HB3 | 16:N:133:LYS:HE3 | 1.42 | 0.41 |
| 3:A:297:G:H2' | 3:A:298:G:O4' | 2.20 | 0.41 |
| 3:A:1078:U:O2 | 3:A:1088:A:H3' | 2.21 | 0.41 |
| 3:A:1972:G:H2' | 3:A:1973:G:C8 | 2.55 | 0.41 |
| 3:A:2267:A:H5'' | 3:A:2268:A:C5' | 2.49 | 0.41 |
| 4:B:48:U:H4' | 18:P:100:HIS:HD2 | 1.84 | 0.41 |
| 4:B:71:C:C2 | 4:B:106:G:C2 | 3.08 | 0.41 |
| 8:F:13:VAL:O | 8:F:17:MET:HB2 | 2.21 | 0.41 |
| 14:L:71:ARG:HA | 14:L:71:ARG:HD3 | 1.81 | 0.41 |
| 3:A:75:G:H4' | 28:Z:48:ARG:NH2 | 2.35 | 0.41 |
| 3:A:528:A:C8 | 3:A:2042:A:C2 | 3.09 | 0.41 |
| 3:A:558:U:OP1 | 13:K:114:LEU:N | 2.47 | 0.41 |
| 3:A:807:U:H2' | 3:A:808:G:H8 | 1.84 | 0.41 |
| 3:A:2102:G:C2 | 3:A:2187:U:O2 | 2.73 | 0.41 |
| 3:A:2352:A:N1 | 26:X:34:GLY:HA3 | 2.35 | 0.41 |
| 3:A:2365:G:H4' | 26:X:60:PHE:CE2 | 2.55 | 0.41 |
| 3:A:2812:G:H2' | 3:A:2813:A:O4' | 2.20 | 0.41 |
| 27:Y:3:ARG:NE | 27:Y:30:LEU:HD13 | 2.35 | 0.41 |
| 28:Z:21:LEU:HD23 | 28:Z:21:LEU:HA | 1.82 | 0.41 |
| 2:2:74:C:O5' | 2:2:74:C:H6 | 2.04 | 0.41 |
| 3:A:31:C:O3' | 3:A:1238:G:H5' | 2.21 | 0.41 |
| 3:A:678:C:H2' | 3:A:679:C:H6 | 1.84 | 0.41 |
| 3:A:1073:A:H2' | 3:A:1074:G:O4' | 2.21 | 0.41 |
| 3:A:1709:U:H2' | 3:A:1710:G:C8 | 2.55 | 0.41 |
| 3:A:1821:A:H2' | 3:A:1822:C:C6 | 2.55 | 0.41 |
| 3:A:2286:G:C8 | 3:A:2287:A:N6 | 2.88 | 0.41 |
| 3:A:2550:G:C6 | 3:A:2551:C:C4 | 3.09 | 0.41 |
| 3:A:2682:A:C2 | 6:D:23:PRO:HB3 | 2.56 | 0.41 |
| 4:B:95:U:H2' | 4:B:96:G:C8 | 2.56 | 0.41 |
| 15:M:78:ARG:HG2 | 15:M:113:ALA:HB3 | 2.03 | 0.41 |
| 22:T:33:LEU:HD23 | 22:T:33:LEU:HA | 1.66 | 0.41 |
| 3:A:561:G:H4' | 20:R:48:ARG:HH22 | 1.86 | 0.41 |
| 3:A:799:G:C6 | 3:A:800:A:C6 | 3.08 | 0.41 |
| 3:A:1057:A:N7 | 3:A:1086:A:H2' | 2.35 | 0.41 |
| 3:A:1275:A:OP2 | 3:A:1646:C:N4 | 2.52 | 0.41 |
| 3:A:1366:A:H2' | 3:A:1367:A:O4' | 2.21 | 0.41 |
| 3:A:1789:A:H2' | 3:A:1790:C:O4' | 2.21 | 0.41 |
| 3:A:2343:U:H2' | 3:A:2344:U:C6 | 2.55 | 0.41 |
| 3:A:2785:C:H2' | 3:A:2786:U:H6 | 1.85 | 0.41 |
| 8:F:36:LEU:HA | 8:F:153:ASP:O | 2.21 | 0.41 |
| 9:G:71:LEU:HA | 9:G:71:LEU:HD23 | 1.83 | 0.41 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 9:G:154:PRO:HA | 9:G:160:LYS:O | 2.21 | 0.41 |
| 27:Y:54:LYS:O | 27:Y:58:VAL:HG23 | 2.19 | 0.41 |
| 3:A:64:A:C6 | 3:A:65:U:C4 | 3.09 | 0.41 |
| 3:A:328:U:H4' | 24:V:66:GLN:HE21 | 1.86 | 0.41 |
| 3:A:396:G:H1' | 27:Y:29:PHE:HB3 | 2.02 | 0.41 |
| 3:A:465:G:C6 | 3:A:466:A:N6 | 2.89 | 0.41 |
| 3:A:520:G:H2' | 3:A:521:U:C6 | 2.56 | 0.41 |
| 3:A:601:C:O2' | 3:A:605:G:H5'' | 2.21 | 0.41 |
| 3:A:681:G:C2 | 3:A:797:G:C2 | 3.09 | 0.41 |
| 3:A:743:A:OP1 | 6:D:135:GLY:HA2 | 2.21 | 0.41 |
| 3:A:779:U:H2' | 3:A:780:G:C8 | 2.56 | 0.41 |
| 3:A:997:G:OP1 | 20:R:92:ARG:HD2 | 2.21 | 0.41 |
| 3:A:1341:G:C2 | 3:A:1398:C:H4' | 2.56 | 0.41 |
| 3:A:1374:G:H8 | 3:A:1374:G:OP2 | 2.04 | 0.41 |
| 3:A:1423:G:N2 | 3:A:1576:U:O2 | 2.54 | 0.41 |
| 3:A:1869:G:C2 | 3:A:1873:G:C6 | 3.09 | 0.41 |
| 3:A:2061:G:H2' | 3:A:2501:C:O2' | 2.21 | 0.41 |
| 4:B:7:G:H5'' | 18:P:29:HIS:CE1 | 2.56 | 0.41 |
| 11:I:48:ALA:HB3 | 11:I:50:VAL:HG23 | 2.03 | 0.41 |
| 14:L:103:VAL:HB | 14:L:107:LEU:HD12 | 2.02 | 0.41 |
| 15:M:81:ASP:HB3 | 15:M:100:ILE:HD13 | 2.02 | 0.41 |
| 16:N:6:ARG:CZ | 16:N:6:ARG:HB2 | 2.50 | 0.41 |
| 18:P:115:LEU:HD23 | 18:P:117:PHE:CE2 | 2.56 | 0.41 |
| 25:W:2:PHE:HB3 | 25:W:50:MET:HE3 | 2.03 | 0.41 |
| 26:X:41:ARG:HD3 | 26:X:41:ARG:HA | 1.53 | 0.41 |
| 27:Y:72:ARG:HG3 | 27:Y:78:TYR:HE2 | 1.86 | 0.41 |
| 27:Y:74:ARG:HE | 27:Y:74:ARG:HB3 | 1.45 | 0.41 |
| 28:Z:37:LEU:HD12 | 28:Z:37:LEU:HA | 1.82 | 0.41 |
| 3:A:141:G:C8 | 3:A:141:G:C3' | 3.04 | 0.41 |
| 3:A:199:A:N6 | 3:A:2434:A:C5 | 2.89 | 0.41 |
| 3:A:948:C:H2' | 3:A:949:G:H8 | 1.85 | 0.41 |
| 3:A:2578:G:OP2 | 3:A:2578:G:H4' | 2.20 | 0.41 |
| 10:H:128:HIS:O | 10:H:143:ILE:HA | 2.20 | 0.41 |
| 11:I:61:ARG:HG2 | 11:I:73:LYS:HG2 | 2.02 | 0.41 |
| 16:N:38:ARG:HB2 | 16:N:98:PRO:HD3 | 2.03 | 0.41 |
| 21:S:85:LYS:HE2 | 21:S:85:LYS:HB3 | 1.80 | 0.41 |
| 28:Z:38:GLN:HG3 | 28:Z:39:GLN:H | 1.85 | 0.41 |
| 3:A:778:G:H5'' | 3:A:779:U:OP2 | 2.21 | 0.40 |
| 3:A:811:U:C2 | 3:A:1251:C:C5 | 3.09 | 0.40 |
| 3:A:1045:C:OP1 | 3:A:1046:A:O2' | 2.37 | 0.40 |
| 3:A:1818:U:C5 | 5:C:156:ARG:NH2 | 2.90 | 0.40 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|------------------|--------------------------|-------------------|
| 3:A:2229:U:H2' | 3:A:2230:G:H8 | 1.85 | 0.40 |
| 3:A:2663:G:H2' | 3:A:2664:G:O4' | 2.21 | 0.40 |
| 3:A:2804:U:H2' | 3:A:2805:C:C6 | 2.56 | 0.40 |
| 16:N:65:ILE:HG12 | 16:N:103:TYR:HD2 | 1.86 | 0.40 |
| 17:O:72:ASP:O | 17:O:76:VAL:HG13 | 2.21 | 0.40 |
| 19:Q:40:LEU:HD23 | 19:Q:40:LEU:HA | 1.75 | 0.40 |
| 27:Y:3:ARG:O | 27:Y:12:PRO:HD3 | 2.21 | 0.40 |
| 3:A:42:A:C6 | 3:A:43:G:C5 | 3.10 | 0.40 |
| 3:A:118:A:C8 | 3:A:119:A:C8 | 3.09 | 0.40 |
| 3:A:277:G:H4' | 3:A:278:A:C5 | 2.57 | 0.40 |
| 3:A:501:A:H2' | 3:A:502:A:C8 | 2.56 | 0.40 |
| 3:A:1024:G:C6 | 3:A:1025:G:C6 | 3.09 | 0.40 |
| 3:A:1071:G:O2' | 3:A:1089:A:OP2 | 2.36 | 0.40 |
| 3:A:2143:C:H2' | 3:A:2144:G:O4' | 2.21 | 0.40 |
| 3:A:2388:A:H5' | 3:A:2389:G:OP2 | 2.21 | 0.40 |
| 3:A:2431:U:O2 | 3:A:2431:U:O4' | 2.39 | 0.40 |
| 3:A:2603:G:C6 | 3:A:2604:U:C4 | 3.09 | 0.40 |
| 3:A:2847:U:C5 | 3:A:2848:G:C5 | 3.09 | 0.40 |
| 5:C:34:LEU:HD21 | 5:C:63:ARG:HG3 | 2.03 | 0.40 |
| 9:G:9:VAL:HG23 | 9:G:52:PHE:HE1 | 1.86 | 0.40 |
| 12:J:42:PHE:CE1 | 12:J:57:VAL:HB | 2.56 | 0.40 |
| 22:T:109:ASP:OD1 | 22:T:110:ARG:N | 2.54 | 0.40 |
| 26:X:70:GLU:HG3 | 26:X:72:LYS:HE2 | 2.04 | 0.40 |
| 3:A:719:C:H2' | 3:A:720:U:C6 | 2.57 | 0.40 |
| 3:A:863:A:H2' | 3:A:864:G:C8 | 2.57 | 0.40 |
| 3:A:863:A:H2' | 3:A:864:G:H8 | 1.86 | 0.40 |
| 3:A:1127:A:N7 | 3:A:2488:G:O2' | 2.55 | 0.40 |
| 3:A:1807:G:N2 | 3:A:1811:G:C5 | 2.89 | 0.40 |
| 3:A:1838:C:H4' | 3:A:1839:G:H8 | 1.85 | 0.40 |
| 3:A:2421:G:H4' | 3:A:2421:G:OP1 | 2.21 | 0.40 |
| 3:A:2600:A:H2' | 3:A:2601:C:C6 | 2.56 | 0.40 |
| 3:A:2627:G:H1' | 3:A:2777:G:N2 | 2.36 | 0.40 |
| 11:I:99:PHE:HD2 | 11:I:106:PHE:HZ | 1.69 | 0.40 |
| 17:O:22:ARG:HG3 | 17:O:70:THR:HA | 2.03 | 0.40 |
| 18:P:115:LEU:HD23 | 18:P:117:PHE:HE2 | 1.86 | 0.40 |
| 24:V:96:PHE:O | 24:V:100:SER:HA | 2.21 | 0.40 |
| 26:X:45:PHE:CD1 | 26:X:80:ILE:HD11 | 2.56 | 0.40 |
| 3:A:1:G:H2' | 3:A:2:G:C8 | 2.57 | 0.40 |
| 3:A:445:C:H2' | 3:A:446:G:O4' | 2.22 | 0.40 |
| 3:A:822:G:H2' | 3:A:823:C:C6 | 2.57 | 0.40 |
| 3:A:871:U:H4' | 16:N:68:PHE:CD2 | 2.56 | 0.40 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 3:A:987:C:O2' | 3:A:1000:A:N3 | 2.44 | 0.40 |
| 3:A:1672:A:N6 | 3:A:1673:G:C6 | 2.89 | 0.40 |
| 3:A:2423:U:H2' | 3:A:2424:C:C1' | 2.51 | 0.40 |
| 4:B:49:C:H2' | 4:B:50:A:H8 | 1.87 | 0.40 |
| 5:C:157:SER:O | 5:C:160:THR:OG1 | 2.38 | 0.40 |
| 7:E:148:ILE:H | 7:E:148:ILE:HG12 | 1.64 | 0.40 |
| 8:F:65:PRO:HA | 8:F:89:VAL:HG22 | 2.01 | 0.40 |
| 9:G:90:VAL:HG21 | 9:G:163:ARG:NH1 | 2.37 | 0.40 |
| 9:G:125:CYS:HB2 | 9:G:127:THR:O | 2.22 | 0.40 |
| 11:I:13:ALA:O | 11:I:17:GLU:HB2 | 2.22 | 0.40 |
| 13:K:99:ARG:HD2 | 13:K:102:GLU:OE1 | 2.22 | 0.40 |
| 15:M:79:LEU:HB2 | 15:M:113:ALA:O | 2.21 | 0.40 |
| 18:P:28:VAL:HG12 | 18:P:93:ASP:O | 2.21 | 0.40 |
| 28:Z:46:VAL:O | 28:Z:50:VAL:HG23 | 2.21 | 0.40 |
| 3:A:339:U:H6 | 3:A:339:U:O5' | 2.05 | 0.40 |
| 3:A:353:C:H2' | 3:A:354:A:O4' | 2.22 | 0.40 |
| 3:A:717:C:C5 | 3:A:718:A:C8 | 3.10 | 0.40 |
| 3:A:729:G:C6 | 5:C:207:LYS:HB2 | 2.56 | 0.40 |
| 3:A:991:C:H2' | 3:A:992:C:H6 | 1.85 | 0.40 |
| 3:A:1139:G:H8 | 3:A:1139:G:OP2 | 2.05 | 0.40 |
| 3:A:1258:U:C2 | 3:A:1259:G:C8 | 3.09 | 0.40 |
| 3:A:1707:G:C5 | 3:A:1756:G:C6 | 3.10 | 0.40 |
| 3:A:2394:C:H42 | 3:A:2422:C:N4 | 2.19 | 0.40 |
| 3:A:2586:U:OP2 | 3:A:2608:G:N1 | 2.48 | 0.40 |
| 7:E:69:ARG:H | 7:E:69:ARG:HG2 | 1.76 | 0.40 |
| 15:M:3:LEU:HD23 | 15:M:3:LEU:HA | 1.77 | 0.40 |
| 17:O:65:LEU:HD12 | 17:O:65:LEU:HA | 1.85 | 0.40 |
| 18:P:25:ARG:O | 18:P:25:ARG:HG3 | 2.22 | 0.40 |
| 23:U:49:LYS:HG3 | 23:U:50:LEU:HD23 | 2.03 | 0.40 |
| 24:V:36:VAL:HB | 24:V:39:ILE:HB | 2.03 | 0.40 |
| 27:Y:36:HIS:O | 27:Y:48:THR:HA | 2.21 | 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 | |
|-----|-------|---------------|-----------|---------|----------|-------------|-----|
| 5 | C | 269/273 (98%) | 261 (97%) | 8 (3%) | 0 | 100 | 100 |
| 6 | D | 207/209 (99%) | 201 (97%) | 6 (3%) | 0 | 100 | 100 |
| 7 | E | 199/201 (99%) | 190 (96%) | 9 (4%) | 0 | 100 | 100 |
| 8 | F | 175/179 (98%) | 166 (95%) | 9 (5%) | 0 | 100 | 100 |
| 9 | G | 174/177 (98%) | 171 (98%) | 3 (2%) | 0 | 100 | 100 |
| 10 | H | 147/149 (99%) | 138 (94%) | 8 (5%) | 1 (1%) | 19 | 52 |
| 11 | I | 123/165 (74%) | 113 (92%) | 9 (7%) | 1 (1%) | 16 | 49 |
| 12 | J | 132/142 (93%) | 126 (96%) | 6 (4%) | 0 | 100 | 100 |
| 13 | K | 140/142 (99%) | 135 (96%) | 5 (4%) | 0 | 100 | 100 |
| 14 | L | 121/123 (98%) | 117 (97%) | 4 (3%) | 0 | 100 | 100 |
| 15 | M | 142/144 (99%) | 140 (99%) | 2 (1%) | 0 | 100 | 100 |
| 16 | N | 134/136 (98%) | 131 (98%) | 3 (2%) | 0 | 100 | 100 |
| 17 | O | 123/127 (97%) | 118 (96%) | 5 (4%) | 0 | 100 | 100 |
| 18 | P | 115/117 (98%) | 112 (97%) | 3 (3%) | 0 | 100 | 100 |
| 19 | Q | 112/115 (97%) | 110 (98%) | 2 (2%) | 0 | 100 | 100 |
| 20 | R | 115/118 (98%) | 114 (99%) | 1 (1%) | 0 | 100 | 100 |
| 21 | S | 101/103 (98%) | 99 (98%) | 2 (2%) | 0 | 100 | 100 |
| 22 | T | 108/110 (98%) | 105 (97%) | 3 (3%) | 0 | 100 | 100 |
| 23 | U | 93/100 (93%) | 90 (97%) | 3 (3%) | 0 | 100 | 100 |
| 24 | V | 100/104 (96%) | 99 (99%) | 1 (1%) | 0 | 100 | 100 |
| 25 | W | 92/94 (98%) | 89 (97%) | 3 (3%) | 0 | 100 | 100 |
| 26 | X | 74/85 (87%) | 73 (99%) | 1 (1%) | 0 | 100 | 100 |
| 27 | Y | 75/78 (96%) | 72 (96%) | 3 (4%) | 0 | 100 | 100 |
| 28 | Z | 60/63 (95%) | 58 (97%) | 2 (3%) | 0 | 100 | 100 |
| 29 | a | 56/59 (95%) | 55 (98%) | 1 (2%) | 0 | 100 | 100 |
| 30 | b | 54/57 (95%) | 50 (93%) | 4 (7%) | 0 | 100 | 100 |
| 31 | c | 49/55 (89%) | 48 (98%) | 1 (2%) | 0 | 100 | 100 |
| 32 | d | 44/46 (96%) | 43 (98%) | 1 (2%) | 0 | 100 | 100 |
| 33 | e | 62/65 (95%) | 59 (95%) | 3 (5%) | 0 | 100 | 100 |
| 34 | f | 36/38 (95%) | 36 (100%) | 0 | 0 | 100 | 100 |

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| Mol | Chain | Analysed | Favoured | Allowed | Outliers | Percentiles | |
|-----|-------|-----------------|------------|----------|----------|-------------|-----|
| 35 | i | 84/453 (18%) | 84 (100%) | 0 | 0 | 100 | 100 |
| 36 | k | 16/18 (89%) | 12 (75%) | 4 (25%) | 0 | 100 | 100 |
| All | All | 3532/4045 (87%) | 3415 (97%) | 115 (3%) | 2 (0%) | 50 | 79 |

All (2) Ramachandran outliers are listed below:

| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 10 | H | 118 | PRO |
| 11 | I | 108 | VAL |

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 | |
|-----|-------|----------------|-----------|----------|-------------|----|
| 5 | C | 216/218 (99%) | 192 (89%) | 24 (11%) | 5 | 21 |
| 6 | D | 164/164 (100%) | 154 (94%) | 10 (6%) | 15 | 41 |
| 7 | E | 165/165 (100%) | 152 (92%) | 13 (8%) | 10 | 34 |
| 8 | F | 148/150 (99%) | 130 (88%) | 18 (12%) | 4 | 19 |
| 9 | G | 137/138 (99%) | 129 (94%) | 8 (6%) | 17 | 42 |
| 10 | H | 114/114 (100%) | 100 (88%) | 14 (12%) | 4 | 19 |
| 11 | I | 95/123 (77%) | 89 (94%) | 6 (6%) | 15 | 40 |
| 12 | J | 104/110 (94%) | 93 (89%) | 11 (11%) | 5 | 23 |
| 13 | K | 116/116 (100%) | 105 (90%) | 11 (10%) | 7 | 26 |
| 14 | L | 104/104 (100%) | 94 (90%) | 10 (10%) | 7 | 26 |
| 15 | M | 103/103 (100%) | 94 (91%) | 9 (9%) | 8 | 30 |
| 16 | N | 109/109 (100%) | 100 (92%) | 9 (8%) | 9 | 32 |
| 17 | O | 102/103 (99%) | 95 (93%) | 7 (7%) | 13 | 37 |
| 18 | P | 87/87 (100%) | 75 (86%) | 12 (14%) | 3 | 17 |
| 19 | Q | 99/100 (99%) | 90 (91%) | 9 (9%) | 7 | 28 |
| 20 | R | 89/90 (99%) | 82 (92%) | 7 (8%) | 10 | 34 |

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| Mol | Chain | Analysed | Rotameric | Outliers | Percentiles | |
|-----|-------|-----------------|------------|----------|-------------|----|
| 21 | S | 84/84 (100%) | 76 (90%) | 8 (10%) | 7 | 26 |
| 22 | T | 93/93 (100%) | 88 (95%) | 5 (5%) | 18 | 43 |
| 23 | U | 82/84 (98%) | 77 (94%) | 5 (6%) | 15 | 41 |
| 24 | V | 83/85 (98%) | 76 (92%) | 7 (8%) | 9 | 32 |
| 25 | W | 78/78 (100%) | 72 (92%) | 6 (8%) | 10 | 34 |
| 26 | X | 57/63 (90%) | 51 (90%) | 6 (10%) | 5 | 23 |
| 27 | Y | 67/68 (98%) | 63 (94%) | 4 (6%) | 16 | 41 |
| 28 | Z | 54/55 (98%) | 47 (87%) | 7 (13%) | 3 | 18 |
| 29 | a | 48/49 (98%) | 46 (96%) | 2 (4%) | 25 | 49 |
| 30 | b | 47/48 (98%) | 35 (74%) | 12 (26%) | 0 | 3 |
| 31 | c | 45/49 (92%) | 40 (89%) | 5 (11%) | 5 | 21 |
| 32 | d | 38/38 (100%) | 32 (84%) | 6 (16%) | 2 | 13 |
| 33 | e | 51/52 (98%) | 47 (92%) | 4 (8%) | 10 | 34 |
| 34 | f | 34/34 (100%) | 31 (91%) | 3 (9%) | 8 | 30 |
| 35 | i | 71/341 (21%) | 65 (92%) | 6 (8%) | 8 | 31 |
| 36 | k | 17/17 (100%) | 15 (88%) | 2 (12%) | 4 | 20 |
| All | All | 2901/3232 (90%) | 2635 (91%) | 266 (9%) | 10 | 28 |

All (266) residues with a non-rotameric sidechain are listed below:

| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 5 | C | 3 | VAL |
| 5 | C | 24 | LEU |
| 5 | C | 35 | GLU |
| 5 | C | 51 | THR |
| 5 | C | 72 | ASP |
| 5 | C | 74 | ILE |
| 5 | C | 120 | VAL |
| 5 | C | 130 | LEU |
| 5 | C | 134 | ASN |
| 5 | C | 156 | ARG |
| 5 | C | 180 | GLU |
| 5 | C | 185 | GLU |
| 5 | C | 189 | ARG |
| 5 | C | 195 | VAL |
| 5 | C | 203 | ARG |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 5 | C | 204 | VAL |
| 5 | C | 228 | VAL |
| 5 | C | 242 | LYS |
| 5 | C | 250 | VAL |
| 5 | C | 251 | GLN |
| 5 | C | 257 | THR |
| 5 | C | 261 | LYS |
| 5 | C | 265 | LYS |
| 5 | C | 271 | ARG |
| 6 | D | 12 | THR |
| 6 | D | 13 | ARG |
| 6 | D | 18 | ASP |
| 6 | D | 28 | GLU |
| 6 | D | 73 | VAL |
| 6 | D | 84 | LEU |
| 6 | D | 128 | ARG |
| 6 | D | 139 | SER |
| 6 | D | 160 | LYS |
| 6 | D | 168 | GLU |
| 7 | E | 84 | THR |
| 7 | E | 85 | PHE |
| 7 | E | 94 | GLN |
| 7 | E | 97 | ASN |
| 7 | E | 105 | LEU |
| 7 | E | 115 | GLN |
| 7 | E | 119 | ILE |
| 7 | E | 127 | GLU |
| 7 | E | 148 | ILE |
| 7 | E | 173 | THR |
| 7 | E | 179 | SER |
| 7 | E | 184 | ASP |
| 7 | E | 196 | VAL |
| 8 | F | 3 | LYS |
| 8 | F | 4 | LEU |
| 8 | F | 14 | LYS |
| 8 | F | 25 | VAL |
| 8 | F | 49 | LEU |
| 8 | F | 51 | ASP |
| 8 | F | 52 | ASN |
| 8 | F | 72 | LYS |
| 8 | F | 81 | GLN |
| 8 | F | 104 | ILE |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 8 | F | 106 | ILE |
| 8 | F | 130 | MET |
| 8 | F | 141 | ILE |
| 8 | F | 144 | ASP |
| 8 | F | 149 | VAL |
| 8 | F | 150 | ARG |
| 8 | F | 153 | ASP |
| 8 | F | 162 | SER |
| 9 | G | 10 | VAL |
| 9 | G | 11 | VAL |
| 9 | G | 49 | THR |
| 9 | G | 87 | LEU |
| 9 | G | 114 | ASP |
| 9 | G | 125 | CYS |
| 9 | G | 127 | THR |
| 9 | G | 153 | ARG |
| 10 | H | 15 | LEU |
| 10 | H | 17 | ASP |
| 10 | H | 25 | TYR |
| 10 | H | 37 | VAL |
| 10 | H | 58 | LEU |
| 10 | H | 60 | GLU |
| 10 | H | 76 | GLU |
| 10 | H | 77 | THR |
| 10 | H | 78 | VAL |
| 10 | H | 86 | ASP |
| 10 | H | 87 | GLU |
| 10 | H | 110 | VAL |
| 10 | H | 112 | LYS |
| 10 | H | 116 | ARG |
| 11 | I | 16 | SER |
| 11 | I | 36 | ASP |
| 11 | I | 58 | THR |
| 11 | I | 85 | VAL |
| 11 | I | 96 | PHE |
| 11 | I | 109 | LYS |
| 12 | J | 9 | VAL |
| 12 | J | 21 | SER |
| 12 | J | 28 | LEU |
| 12 | J | 31 | GLN |
| 12 | J | 55 | ILE |
| 12 | J | 66 | SER |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 12 | J | 111 | GLN |
| 12 | J | 112 | THR |
| 12 | J | 113 | LYS |
| 12 | J | 116 | ASP |
| 12 | J | 128 | SER |
| 13 | K | 5 | THR |
| 13 | K | 7 | LYS |
| 13 | K | 34 | ARG |
| 13 | K | 40 | HIS |
| 13 | K | 44 | TYR |
| 13 | K | 69 | ARG |
| 13 | K | 70 | THR |
| 13 | K | 88 | THR |
| 13 | K | 103 | ILE |
| 13 | K | 122 | LEU |
| 13 | K | 131 | ASN |
| 14 | L | 1 | MET |
| 14 | L | 21 | CYS |
| 14 | L | 42 | THR |
| 14 | L | 49 | ARG |
| 14 | L | 56 | ASP |
| 14 | L | 58 | LEU |
| 14 | L | 65 | THR |
| 14 | L | 84 | CYS |
| 14 | L | 106 | GLU |
| 14 | L | 116 | ILE |
| 15 | M | 2 | ARG |
| 15 | M | 14 | LYS |
| 15 | M | 46 | VAL |
| 15 | M | 47 | ARG |
| 15 | M | 55 | MET |
| 15 | M | 59 | ARG |
| 15 | M | 86 | GLU |
| 15 | M | 91 | ASP |
| 15 | M | 126 | ARG |
| 16 | N | 6 | ARG |
| 16 | N | 7 | THR |
| 16 | N | 12 | MET |
| 16 | N | 25 | ASP |
| 16 | N | 54 | THR |
| 16 | N | 58 | LYS |
| 16 | N | 115 | GLU |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 16 | N | 133 | LYS |
| 16 | N | 135 | VAL |
| 17 | O | 2 | ARG |
| 17 | O | 14 | SER |
| 17 | O | 36 | THR |
| 17 | O | 69 | ARG |
| 17 | O | 74 | GLU |
| 17 | O | 75 | ILE |
| 17 | O | 100 | CYS |
| 18 | P | 2 | ASP |
| 18 | P | 5 | SER |
| 18 | P | 19 | GLN |
| 18 | P | 20 | GLU |
| 18 | P | 31 | THR |
| 18 | P | 36 | TYR |
| 18 | P | 43 | ASN |
| 18 | P | 55 | GLU |
| 18 | P | 61 | GLN |
| 18 | P | 69 | ASP |
| 18 | P | 78 | VAL |
| 18 | P | 98 | GLN |
| 19 | Q | 3 | ASN |
| 19 | Q | 7 | GLN |
| 19 | Q | 21 | ARG |
| 19 | Q | 26 | VAL |
| 19 | Q | 51 | ARG |
| 19 | Q | 65 | SER |
| 19 | Q | 68 | GLU |
| 19 | Q | 92 | VAL |
| 19 | Q | 115 | ASN |
| 20 | R | 6 | ARG |
| 20 | R | 13 | ARG |
| 20 | R | 17 | ILE |
| 20 | R | 24 | TYR |
| 20 | R | 51 | ARG |
| 20 | R | 52 | GLN |
| 20 | R | 109 | LEU |
| 21 | S | 20 | VAL |
| 21 | S | 25 | LEU |
| 21 | S | 38 | VAL |
| 21 | S | 45 | GLU |
| 21 | S | 71 | LYS |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 21 | S | 72 | VAL |
| 21 | S | 83 | TYR |
| 21 | S | 101 | ILE |
| 22 | T | 12 | SER |
| 22 | T | 28 | LYS |
| 22 | T | 74 | ILE |
| 22 | T | 95 | ARG |
| 22 | T | 98 | LYS |
| 23 | U | 7 | LEU |
| 23 | U | 16 | VAL |
| 23 | U | 17 | SER |
| 23 | U | 48 | GLN |
| 23 | U | 72 | GLN |
| 24 | V | 7 | ARG |
| 24 | V | 34 | VAL |
| 24 | V | 41 | LEU |
| 24 | V | 42 | VAL |
| 24 | V | 68 | SER |
| 24 | V | 83 | VAL |
| 24 | V | 102 | THR |
| 25 | W | 7 | GLU |
| 25 | W | 12 | GLN |
| 25 | W | 61 | LEU |
| 25 | W | 78 | GLN |
| 25 | W | 90 | ASP |
| 25 | W | 92 | VAL |
| 26 | X | 11 | ARG |
| 26 | X | 12 | ASN |
| 26 | X | 21 | LEU |
| 26 | X | 35 | SER |
| 26 | X | 41 | ARG |
| 26 | X | 56 | ASP |
| 27 | Y | 2 | SER |
| 27 | Y | 4 | VAL |
| 27 | Y | 42 | SER |
| 27 | Y | 74 | ARG |
| 28 | Z | 2 | LYS |
| 28 | Z | 16 | THR |
| 28 | Z | 28 | LEU |
| 28 | Z | 44 | LYS |
| 28 | Z | 45 | GLN |
| 28 | Z | 48 | ARG |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 28 | Z | 56 | LEU |
| 29 | a | 36 | VAL |
| 29 | a | 56 | LYS |
| 30 | b | 4 | GLN |
| 30 | b | 9 | THR |
| 30 | b | 15 | MET |
| 30 | b | 18 | SER |
| 30 | b | 25 | VAL |
| 30 | b | 26 | THR |
| 30 | b | 28 | LEU |
| 30 | b | 32 | LYS |
| 30 | b | 36 | GLU |
| 30 | b | 40 | ARG |
| 30 | b | 46 | ASP |
| 30 | b | 52 | ARG |
| 31 | c | 5 | ILE |
| 31 | c | 6 | ARG |
| 31 | c | 10 | LYS |
| 31 | c | 22 | THR |
| 31 | c | 47 | VAL |
| 32 | d | 1 | MET |
| 32 | d | 12 | ARG |
| 32 | d | 24 | THR |
| 32 | d | 25 | LYS |
| 32 | d | 34 | ARG |
| 32 | d | 41 | ARG |
| 33 | e | 8 | ARG |
| 33 | e | 31 | HIS |
| 33 | e | 32 | ILE |
| 33 | e | 51 | SER |
| 34 | f | 2 | LYS |
| 34 | f | 12 | ARG |
| 34 | f | 36 | ARG |
| 35 | i | 333 | ASP |
| 35 | i | 337 | GLN |
| 35 | i | 369 | ASP |
| 35 | i | 386 | LYS |
| 35 | i | 397 | SER |
| 35 | i | 411 | GLN |
| 36 | k | 36 | LEU |
| 36 | k | 40 | LEU |

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (36)

such sidechains are listed below:

| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 5 | C | 86 | ASN |
| 5 | C | 90 | ASN |
| 5 | C | 200 | HIS |
| 5 | C | 251 | GLN |
| 6 | D | 136 | ASN |
| 6 | D | 140 | HIS |
| 7 | E | 165 | HIS |
| 8 | F | 81 | GLN |
| 8 | F | 127 | ASN |
| 10 | H | 11 | ASN |
| 10 | H | 33 | GLN |
| 10 | H | 43 | ASN |
| 12 | J | 31 | GLN |
| 13 | K | 80 | HIS |
| 13 | K | 86 | GLN |
| 14 | L | 3 | GLN |
| 14 | L | 89 | ASN |
| 15 | M | 104 | GLN |
| 16 | N | 3 | GLN |
| 17 | O | 18 | GLN |
| 18 | P | 100 | HIS |
| 19 | Q | 52 | ASN |
| 19 | Q | 66 | ASN |
| 20 | R | 81 | ASN |
| 21 | S | 82 | HIS |
| 22 | T | 7 | HIS |
| 23 | U | 48 | GLN |
| 23 | U | 59 | ASN |
| 26 | X | 46 | HIS |
| 28 | Z | 39 | GLN |
| 28 | Z | 58 | ASN |
| 32 | d | 26 | ASN |
| 32 | d | 29 | GLN |
| 35 | i | 332 | ASN |
| 35 | i | 381 | ASN |
| 35 | i | 411 | GLN |

5.3.3 RNA ⓘ

| Mol | Chain | Analysed | Backbone Outliers | Pucker Outliers |
|-----|-------|--------------|-------------------|-----------------|
| 1 | 1 | 42/113 (37%) | 13 (30%) | 0 |

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| Mol | Chain | Analysed | Backbone Outliers | Pucker Outliers |
|-----|-------|-----------------|-------------------|-----------------|
| 2 | 2 | 2/3 (66%) | 1 (50%) | 0 |
| 3 | A | 2878/2903 (99%) | 518 (17%) | 19 (0%) |
| 4 | B | 119/120 (99%) | 13 (10%) | 0 |
| All | All | 3041/3139 (96%) | 545 (17%) | 19 (0%) |

All (545) RNA backbone outliers are listed below:

| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1 | 1 | 33 | C |
| 1 | 1 | 36 | U |
| 1 | 1 | 37 | U |
| 1 | 1 | 38 | U |
| 1 | 1 | 39 | A |
| 1 | 1 | 41 | C |
| 1 | 1 | 42 | A |
| 1 | 1 | 43 | G |
| 1 | 1 | 46 | C |
| 1 | 1 | 57 | G |
| 1 | 1 | 58 | G |
| 1 | 1 | 67 | A |
| 1 | 1 | 70 | G |
| 2 | 2 | 76 | A |
| 3 | A | 10 | A |
| 3 | A | 12 | U |
| 3 | A | 33 | C |
| 3 | A | 34 | U |
| 3 | A | 35 | G |
| 3 | A | 45 | G |
| 3 | A | 46 | G |
| 3 | A | 49 | A |
| 3 | A | 50 | U |
| 3 | A | 51 | G |
| 3 | A | 62 | U |
| 3 | A | 63 | A |
| 3 | A | 65 | U |
| 3 | A | 71 | A |
| 3 | A | 72 | U |
| 3 | A | 74 | A |
| 3 | A | 75 | G |
| 3 | A | 84 | A |
| 3 | A | 93 | G |
| 3 | A | 96 | C |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 3 | A | 101 | A |
| 3 | A | 102 | U |
| 3 | A | 103 | A |
| 3 | A | 110 | G |
| 3 | A | 118 | A |
| 3 | A | 119 | A |
| 3 | A | 120 | U |
| 3 | A | 136 | G |
| 3 | A | 137 | U |
| 3 | A | 138 | U |
| 3 | A | 139 | U |
| 3 | A | 142 | A |
| 3 | A | 156 | A |
| 3 | A | 162 | U |
| 3 | A | 181 | A |
| 3 | A | 188 | G |
| 3 | A | 196 | A |
| 3 | A | 199 | A |
| 3 | A | 215 | G |
| 3 | A | 216 | A |
| 3 | A | 220 | G |
| 3 | A | 221 | A |
| 3 | A | 222 | A |
| 3 | A | 226 | A |
| 3 | A | 248 | G |
| 3 | A | 266 | G |
| 3 | A | 272 | A |
| 3 | A | 275 | C |
| 3 | A | 276 | U |
| 3 | A | 285 | G |
| 3 | A | 291 | G |
| 3 | A | 302 | C |
| 3 | A | 311 | A |
| 3 | A | 329 | G |
| 3 | A | 330 | A |
| 3 | A | 335 | C |
| 3 | A | 349 | U |
| 3 | A | 353 | C |
| 3 | A | 356 | G |
| 3 | A | 361 | G |
| 3 | A | 362 | A |
| 3 | A | 372 | G |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 3 | A | 386 | G |
| 3 | A | 396 | G |
| 3 | A | 399 | U |
| 3 | A | 411 | G |
| 3 | A | 419 | U |
| 3 | A | 424 | G |
| 3 | A | 454 | A |
| 3 | A | 455 | C |
| 3 | A | 475 | C |
| 3 | A | 477 | A |
| 3 | A | 479 | A |
| 3 | A | 480 | A |
| 3 | A | 481 | G |
| 3 | A | 491 | G |
| 3 | A | 504 | A |
| 3 | A | 505 | A |
| 3 | A | 509 | C |
| 3 | A | 510 | C |
| 3 | A | 513 | A |
| 3 | A | 518 | G |
| 3 | A | 529 | A |
| 3 | A | 531 | C |
| 3 | A | 532 | A |
| 3 | A | 533 | G |
| 3 | A | 543 | G |
| 3 | A | 544 | C |
| 3 | A | 550 | C |
| 3 | A | 552 | U |
| 3 | A | 558 | U |
| 3 | A | 563 | A |
| 3 | A | 567 | U |
| 3 | A | 568 | U |
| 3 | A | 573 | U |
| 3 | A | 575 | A |
| 3 | A | 586 | A |
| 3 | A | 603 | A |
| 3 | A | 613 | A |
| 3 | A | 614 | A |
| 3 | A | 615 | U |
| 3 | A | 627 | A |
| 3 | A | 632 | A |
| 3 | A | 634 | C |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 3 | A | 637 | A |
| 3 | A | 645 | C |
| 3 | A | 646 | U |
| 3 | A | 647 | G |
| 3 | A | 653 | U |
| 3 | A | 654 | A |
| 3 | A | 655 | A |
| 3 | A | 668 | A |
| 3 | A | 685 | A |
| 3 | A | 686 | U |
| 3 | A | 711 | G |
| 3 | A | 712 | G |
| 3 | A | 713 | G |
| 3 | A | 718 | A |
| 3 | A | 730 | A |
| 3 | A | 747 | U |
| 3 | A | 753 | A |
| 3 | A | 757 | G |
| 3 | A | 763 | G |
| 3 | A | 764 | A |
| 3 | A | 765 | C |
| 3 | A | 775 | G |
| 3 | A | 777 | G |
| 3 | A | 782 | A |
| 3 | A | 784 | G |
| 3 | A | 785 | G |
| 3 | A | 788 | A |
| 3 | A | 789 | A |
| 3 | A | 790 | U |
| 3 | A | 791 | C |
| 3 | A | 793 | A |
| 3 | A | 794 | A |
| 3 | A | 801 | G |
| 3 | A | 805 | G |
| 3 | A | 812 | C |
| 3 | A | 827 | U |
| 3 | A | 828 | U |
| 3 | A | 831 | G |
| 3 | A | 846 | U |
| 3 | A | 859 | G |
| 3 | A | 865 | C |
| 3 | A | 869 | G |

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| Mol | Chain | Res | Type |
|-----|-------|------|------|
| 3 | A | 878 | A |
| 3 | A | 896 | A |
| 3 | A | 897 | C |
| 3 | A | 899 | A |
| 3 | A | 907 | G |
| 3 | A | 910 | A |
| 3 | A | 914 | G |
| 3 | A | 915 | C |
| 3 | A | 932 | U |
| 3 | A | 933 | A |
| 3 | A | 946 | C |
| 3 | A | 953 | G |
| 3 | A | 957 | C |
| 3 | A | 961 | C |
| 3 | A | 974 | G |
| 3 | A | 983 | A |
| 3 | A | 990 | A |
| 3 | A | 996 | A |
| 3 | A | 999 | U |
| 3 | A | 1005 | C |
| 3 | A | 1009 | A |
| 3 | A | 1012 | U |
| 3 | A | 1013 | C |
| 3 | A | 1022 | G |
| 3 | A | 1023 | U |
| 3 | A | 1027 | A |
| 3 | A | 1033 | U |
| 3 | A | 1040 | A |
| 3 | A | 1046 | A |
| 3 | A | 1056 | G |
| 3 | A | 1057 | A |
| 3 | A | 1070 | A |
| 3 | A | 1071 | G |
| 3 | A | 1073 | A |
| 3 | A | 1083 | U |
| 3 | A | 1087 | G |
| 3 | A | 1088 | A |
| 3 | A | 1090 | A |
| 3 | A | 1101 | U |
| 3 | A | 1111 | A |
| 3 | A | 1112 | G |
| 3 | A | 1116 | G |

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| Mol | Chain | Res | Type |
|-----|-------|------|------|
| 3 | A | 1129 | A |
| 3 | A | 1130 | U |
| 3 | A | 1132 | U |
| 3 | A | 1133 | A |
| 3 | A | 1135 | C |
| 3 | A | 1136 | G |
| 3 | A | 1139 | G |
| 3 | A | 1142 | A |
| 3 | A | 1143 | A |
| 3 | A | 1155 | A |
| 3 | A | 1173 | U |
| 3 | A | 1179 | G |
| 3 | A | 1182 | G |
| 3 | A | 1206 | G |
| 3 | A | 1212 | G |
| 3 | A | 1218 | G |
| 3 | A | 1236 | G |
| 3 | A | 1238 | G |
| 3 | A | 1247 | A |
| 3 | A | 1249 | U |
| 3 | A | 1252 | G |
| 3 | A | 1253 | A |
| 3 | A | 1256 | G |
| 3 | A | 1262 | A |
| 3 | A | 1271 | G |
| 3 | A | 1272 | A |
| 3 | A | 1294 | U |
| 3 | A | 1300 | G |
| 3 | A | 1301 | A |
| 3 | A | 1302 | A |
| 3 | A | 1308 | A |
| 3 | A | 1329 | U |
| 3 | A | 1332 | G |
| 3 | A | 1337 | G |
| 3 | A | 1338 | G |
| 3 | A | 1345 | C |
| 3 | A | 1346 | G |
| 3 | A | 1365 | A |
| 3 | A | 1379 | U |
| 3 | A | 1383 | A |
| 3 | A | 1395 | A |
| 3 | A | 1403 | A |

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| Mol | Chain | Res | Type |
|-----|-------|------|------|
| 3 | A | 1416 | G |
| 3 | A | 1417 | C |
| 3 | A | 1424 | G |
| 3 | A | 1428 | C |
| 3 | A | 1434 | A |
| 3 | A | 1437 | C |
| 3 | A | 1449 | G |
| 3 | A | 1451 | C |
| 3 | A | 1452 | G |
| 3 | A | 1453 | A |
| 3 | A | 1482 | G |
| 3 | A | 1489 | C |
| 3 | A | 1491 | G |
| 3 | A | 1493 | C |
| 3 | A | 1494 | A |
| 3 | A | 1495 | A |
| 3 | A | 1497 | U |
| 3 | A | 1498 | C |
| 3 | A | 1509 | A |
| 3 | A | 1510 | G |
| 3 | A | 1515 | A |
| 3 | A | 1524 | G |
| 3 | A | 1529 | G |
| 3 | A | 1533 | C |
| 3 | A | 1535 | A |
| 3 | A | 1536 | C |
| 3 | A | 1537 | G |
| 3 | A | 1554 | U |
| 3 | A | 1560 | G |
| 3 | A | 1566 | A |
| 3 | A | 1569 | A |
| 3 | A | 1576 | U |
| 3 | A | 1578 | U |
| 3 | A | 1581 | G |
| 3 | A | 1583 | A |
| 3 | A | 1585 | C |
| 3 | A | 1606 | C |
| 3 | A | 1607 | C |
| 3 | A | 1608 | A |
| 3 | A | 1616 | A |
| 3 | A | 1634 | A |
| 3 | A | 1639 | C |

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| Mol | Chain | Res | Type |
|-----|-------|------|------|
| 3 | A | 1647 | U |
| 3 | A | 1648 | U |
| 3 | A | 1649 | G |
| 3 | A | 1660 | G |
| 3 | A | 1674 | G |
| 3 | A | 1677 | A |
| 3 | A | 1715 | G |
| 3 | A | 1722 | A |
| 3 | A | 1725 | U |
| 3 | A | 1729 | U |
| 3 | A | 1730 | C |
| 3 | A | 1738 | G |
| 3 | A | 1744 | A |
| 3 | A | 1757 | A |
| 3 | A | 1764 | C |
| 3 | A | 1773 | A |
| 3 | A | 1782 | U |
| 3 | A | 1786 | A |
| 3 | A | 1791 | A |
| 3 | A | 1800 | C |
| 3 | A | 1801 | A |
| 3 | A | 1802 | A |
| 3 | A | 1808 | A |
| 3 | A | 1809 | A |
| 3 | A | 1811 | G |
| 3 | A | 1816 | C |
| 3 | A | 1829 | A |
| 3 | A | 1847 | A |
| 3 | A | 1849 | G |
| 3 | A | 1850 | G |
| 3 | A | 1870 | C |
| 3 | A | 1871 | A |
| 3 | A | 1872 | A |
| 3 | A | 1876 | A |
| 3 | A | 1896 | G |
| 3 | A | 1906 | G |
| 3 | A | 1920 | C |
| 3 | A | 1927 | A |
| 3 | A | 1929 | G |
| 3 | A | 1930 | G |
| 3 | A | 1931 | U |
| 3 | A | 1934 | C |

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| Mol | Chain | Res | Type |
|-----|-------|------|------|
| 3 | A | 1936 | A |
| 3 | A | 1937 | A |
| 3 | A | 1939 | U |
| 3 | A | 1955 | U |
| 3 | A | 1956 | U |
| 3 | A | 1960 | A |
| 3 | A | 1962 | C |
| 3 | A | 1966 | A |
| 3 | A | 1967 | C |
| 3 | A | 1970 | A |
| 3 | A | 1971 | U |
| 3 | A | 1972 | G |
| 3 | A | 1974 | C |
| 3 | A | 1982 | U |
| 3 | A | 1991 | U |
| 3 | A | 1992 | G |
| 3 | A | 1993 | U |
| 3 | A | 1997 | C |
| 3 | A | 2021 | C |
| 3 | A | 2023 | C |
| 3 | A | 2030 | A |
| 3 | A | 2031 | A |
| 3 | A | 2033 | A |
| 3 | A | 2043 | C |
| 3 | A | 2050 | C |
| 3 | A | 2054 | A |
| 3 | A | 2055 | C |
| 3 | A | 2056 | G |
| 3 | A | 2060 | A |
| 3 | A | 2061 | G |
| 3 | A | 2062 | A |
| 3 | A | 2069 | G |
| 3 | A | 2072 | C |
| 3 | A | 2093 | G |
| 3 | A | 2097 | A |
| 3 | A | 2101 | A |
| 3 | A | 2103 | C |
| 3 | A | 2104 | C |
| 3 | A | 2105 | U |
| 3 | A | 2106 | U |
| 3 | A | 2111 | U |
| 3 | A | 2112 | G |

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| Mol | Chain | Res | Type |
|-----|-------|------|------|
| 3 | A | 2113 | U |
| 3 | A | 2116 | G |
| 3 | A | 2117 | A |
| 3 | A | 2118 | U |
| 3 | A | 2119 | A |
| 3 | A | 2120 | G |
| 3 | A | 2123 | G |
| 3 | A | 2126 | A |
| 3 | A | 2128 | G |
| 3 | A | 2131 | U |
| 3 | A | 2132 | U |
| 3 | A | 2133 | G |
| 3 | A | 2134 | A |
| 3 | A | 2145 | C |
| 3 | A | 2146 | C |
| 3 | A | 2147 | A |
| 3 | A | 2148 | G |
| 3 | A | 2159 | G |
| 3 | A | 2160 | C |
| 3 | A | 2161 | C |
| 3 | A | 2163 | A |
| 3 | A | 2164 | C |
| 3 | A | 2165 | C |
| 3 | A | 2167 | U |
| 3 | A | 2168 | G |
| 3 | A | 2169 | A |
| 3 | A | 2170 | A |
| 3 | A | 2171 | A |
| 3 | A | 2172 | U |
| 3 | A | 2173 | A |
| 3 | A | 2174 | C |
| 3 | A | 2177 | C |
| 3 | A | 2178 | C |
| 3 | A | 2185 | U |
| 3 | A | 2187 | U |
| 3 | A | 2190 | G |
| 3 | A | 2198 | A |
| 3 | A | 2203 | U |
| 3 | A | 2204 | G |
| 3 | A | 2211 | A |
| 3 | A | 2212 | A |
| 3 | A | 2225 | A |

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| Mol | Chain | Res | Type |
|-----|-------|------|------|
| 3 | A | 2238 | G |
| 3 | A | 2239 | G |
| 3 | A | 2250 | G |
| 3 | A | 2268 | A |
| 3 | A | 2278 | A |
| 3 | A | 2280 | G |
| 3 | A | 2283 | C |
| 3 | A | 2287 | A |
| 3 | A | 2288 | A |
| 3 | A | 2297 | A |
| 3 | A | 2305 | U |
| 3 | A | 2308 | G |
| 3 | A | 2322 | A |
| 3 | A | 2325 | G |
| 3 | A | 2331 | G |
| 3 | A | 2336 | A |
| 3 | A | 2345 | G |
| 3 | A | 2347 | C |
| 3 | A | 2350 | C |
| 3 | A | 2354 | C |
| 3 | A | 2357 | G |
| 3 | A | 2366 | A |
| 3 | A | 2383 | G |
| 3 | A | 2385 | C |
| 3 | A | 2402 | U |
| 3 | A | 2403 | C |
| 3 | A | 2406 | A |
| 3 | A | 2420 | C |
| 3 | A | 2421 | G |
| 3 | A | 2422 | C |
| 3 | A | 2423 | U |
| 3 | A | 2424 | C |
| 3 | A | 2425 | A |
| 3 | A | 2427 | C |
| 3 | A | 2429 | G |
| 3 | A | 2430 | A |
| 3 | A | 2431 | U |
| 3 | A | 2432 | A |
| 3 | A | 2434 | A |
| 3 | A | 2435 | A |
| 3 | A | 2440 | C |
| 3 | A | 2441 | U |

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| Mol | Chain | Res | Type |
|-----|-------|------|------|
| 3 | A | 2445 | G |
| 3 | A | 2448 | A |
| 3 | A | 2464 | G |
| 3 | A | 2475 | C |
| 3 | A | 2476 | A |
| 3 | A | 2478 | A |
| 3 | A | 2491 | U |
| 3 | A | 2492 | U |
| 3 | A | 2497 | A |
| 3 | A | 2502 | G |
| 3 | A | 2504 | U |
| 3 | A | 2505 | G |
| 3 | A | 2506 | U |
| 3 | A | 2507 | C |
| 3 | A | 2513 | A |
| 3 | A | 2514 | U |
| 3 | A | 2518 | A |
| 3 | A | 2520 | C |
| 3 | A | 2529 | G |
| 3 | A | 2566 | A |
| 3 | A | 2567 | G |
| 3 | A | 2578 | G |
| 3 | A | 2582 | G |
| 3 | A | 2585 | U |
| 3 | A | 2586 | U |
| 3 | A | 2602 | A |
| 3 | A | 2603 | G |
| 3 | A | 2609 | U |
| 3 | A | 2613 | U |
| 3 | A | 2615 | U |
| 3 | A | 2621 | G |
| 3 | A | 2623 | G |
| 3 | A | 2624 | G |
| 3 | A | 2629 | U |
| 3 | A | 2630 | G |
| 3 | A | 2636 | C |
| 3 | A | 2638 | G |
| 3 | A | 2669 | G |
| 3 | A | 2682 | A |
| 3 | A | 2689 | U |
| 3 | A | 2690 | U |
| 3 | A | 2714 | G |

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| Mol | Chain | Res | Type |
|-----|-------|------|------|
| 3 | A | 2716 | C |
| 3 | A | 2726 | A |
| 3 | A | 2733 | A |
| 3 | A | 2739 | U |
| 3 | A | 2744 | G |
| 3 | A | 2748 | A |
| 3 | A | 2757 | A |
| 3 | A | 2765 | A |
| 3 | A | 2778 | A |
| 3 | A | 2779 | U |
| 3 | A | 2780 | G |
| 3 | A | 2791 | G |
| 3 | A | 2792 | A |
| 3 | A | 2798 | U |
| 3 | A | 2799 | A |
| 3 | A | 2801 | G |
| 3 | A | 2820 | A |
| 3 | A | 2821 | A |
| 3 | A | 2825 | G |
| 3 | A | 2833 | U |
| 3 | A | 2835 | A |
| 3 | A | 2836 | U |
| 3 | A | 2849 | U |
| 3 | A | 2860 | A |
| 3 | A | 2861 | U |
| 3 | A | 2867 | G |
| 3 | A | 2870 | C |
| 3 | A | 2873 | A |
| 3 | A | 2879 | A |
| 3 | A | 2880 | C |
| 3 | A | 2883 | A |
| 3 | A | 2884 | U |
| 3 | A | 2885 | G |
| 3 | A | 2886 | A |
| 3 | A | 2888 | C |
| 3 | A | 2891 | U |
| 4 | B | 24 | G |
| 4 | B | 25 | U |
| 4 | B | 35 | C |
| 4 | B | 41 | G |
| 4 | B | 45 | A |
| 4 | B | 56 | G |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 4 | B | 66 | A |
| 4 | B | 67 | G |
| 4 | B | 71 | C |
| 4 | B | 88 | C |
| 4 | B | 89 | U |
| 4 | B | 90 | C |
| 4 | B | 109 | A |

All (19) RNA pucker outliers are listed below:

| Mol | Chain | Res | Type |
|-----|-------|------|------|
| 3 | A | 100 | U |
| 3 | A | 613 | A |
| 3 | A | 645 | C |
| 3 | A | 653 | U |
| 3 | A | 784 | G |
| 3 | A | 827 | U |
| 3 | A | 830 | G |
| 3 | A | 1110 | G |
| 3 | A | 1344 | U |
| 3 | A | 1494 | A |
| 3 | A | 1721 | G |
| 3 | A | 1939 | U |
| 3 | A | 2127 | G |
| 3 | A | 2158 | A |
| 3 | A | 2422 | C |
| 3 | A | 2424 | C |
| 3 | A | 2430 | A |
| 3 | A | 2602 | A |
| 3 | A | 2756 | U |

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

Of 432 ligands modelled in this entry, 432 are monoatomic - leaving 0 for Mogul analysis.

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

No monomer is involved in short contacts.

5.7 Other polymers

There are no such residues in this entry.

5.8 Polymer linkage issues

There are no chain breaks in this entry.

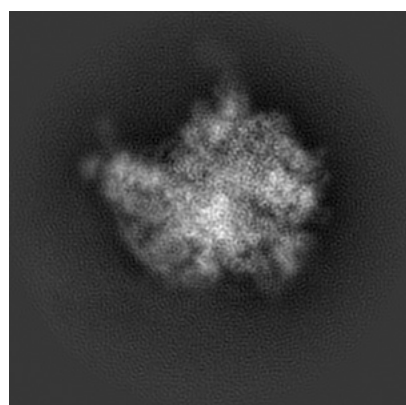
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-8004. These allow visual inspection of the internal detail of the map and identification of artifacts.

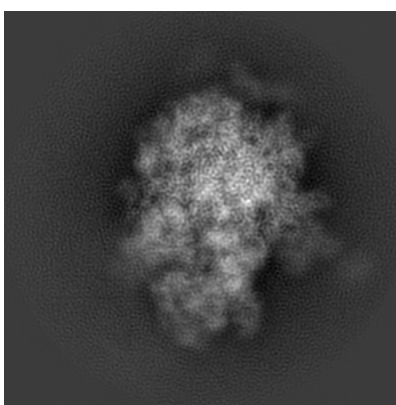
No raw map or half-maps were deposited for this entry and therefore no images, graphs, etc. pertaining to the raw map can be shown.

6.1 Orthogonal projections [i](#)

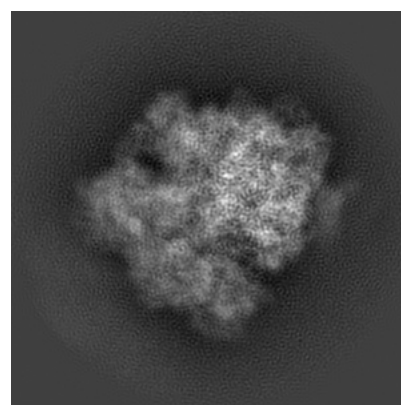
6.1.1 Primary map



X



Y

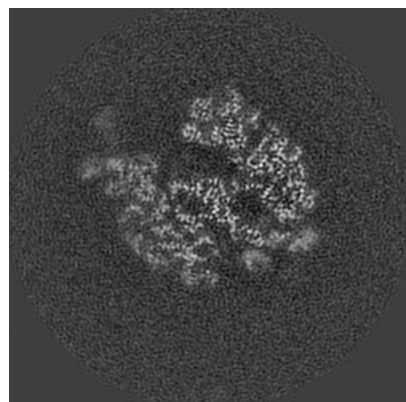


Z

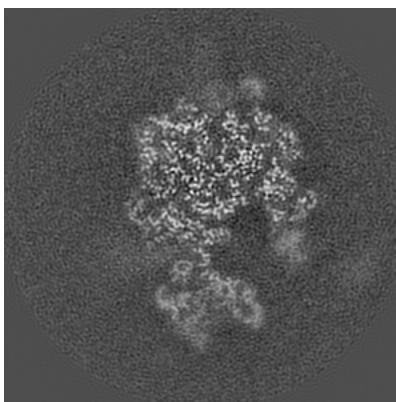
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

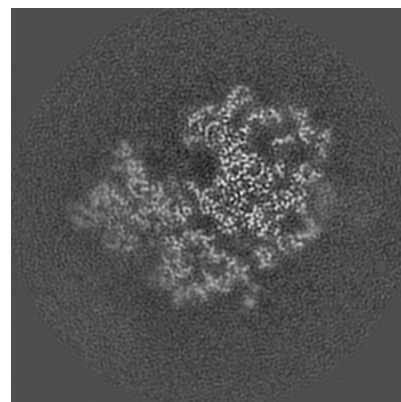
6.2.1 Primary map



X Index: 144



Y Index: 144

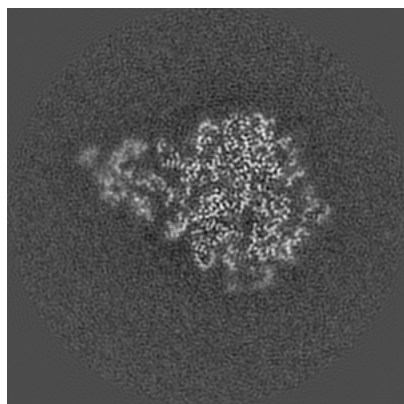


Z Index: 144

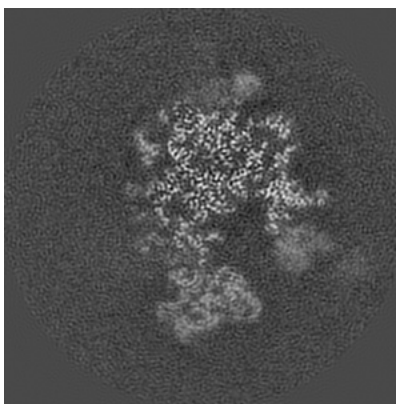
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

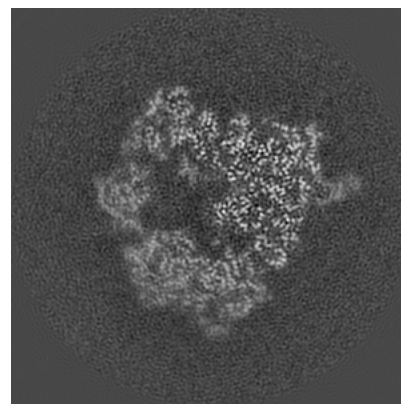
6.3.1 Primary map



X Index: 165



Y Index: 150

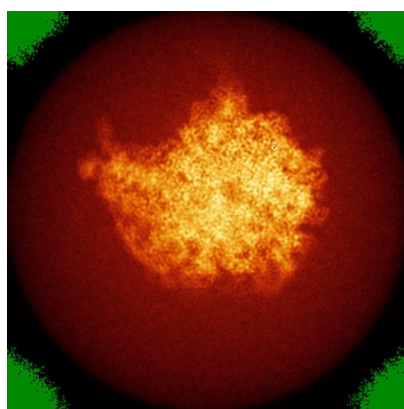


Z Index: 166

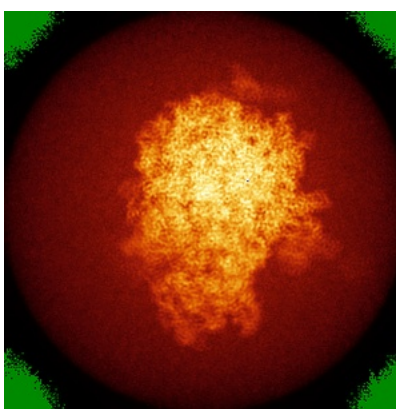
The images above show the largest variance slices of the map in three orthogonal directions.

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

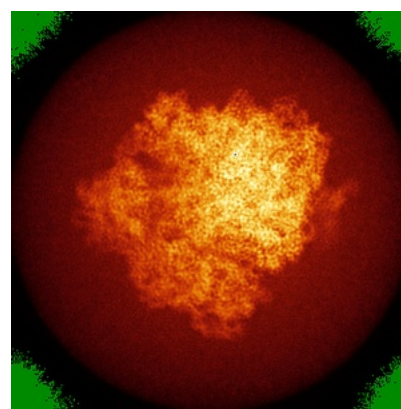
6.4.1 Primary map



X



Y



Z

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



X



Y



Z

The images above show the 3D surface view of the map at the recommended contour level 0.05. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

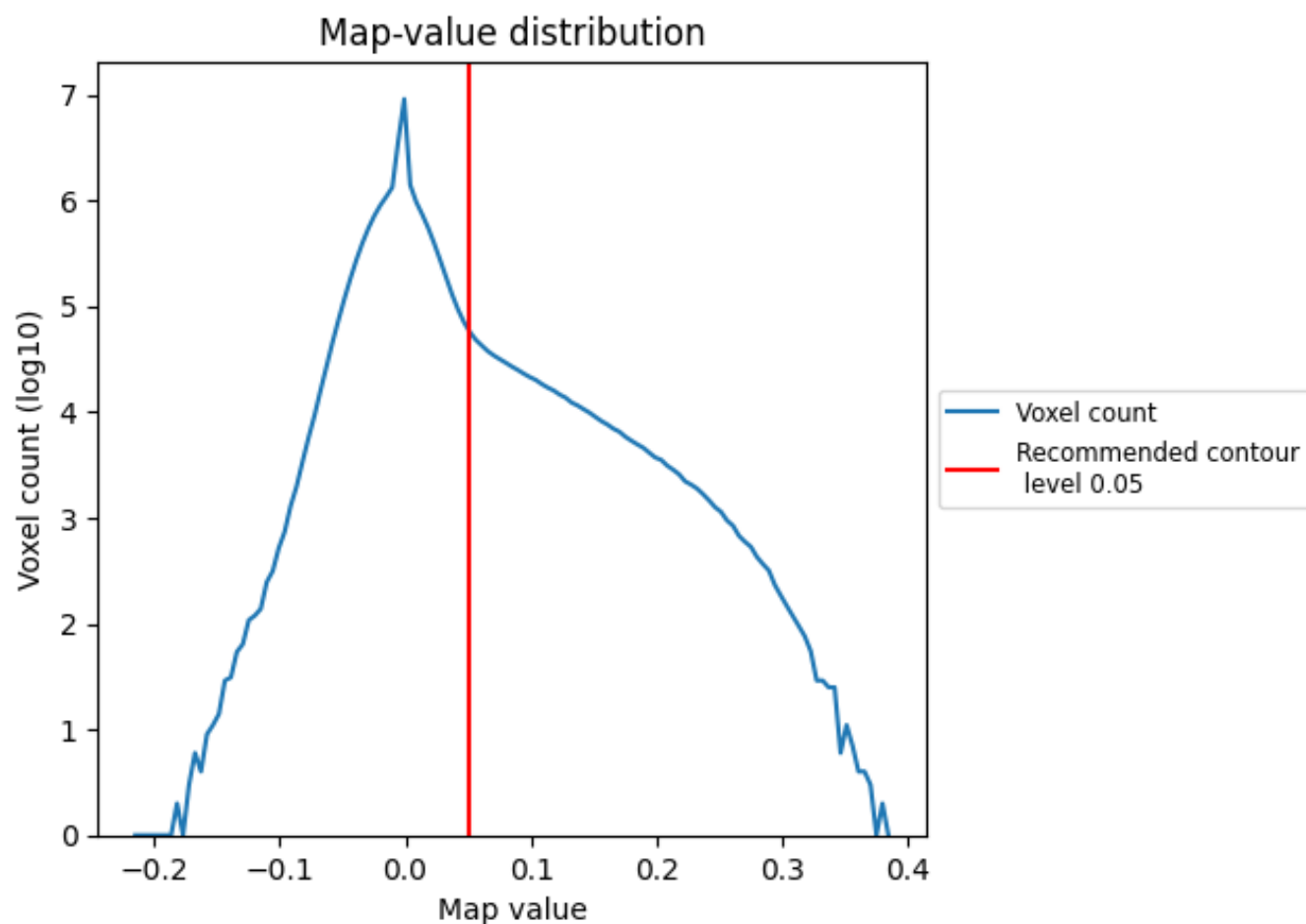
6.6 Mask visualisation [i](#)

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

7 Map analysis [i](#)

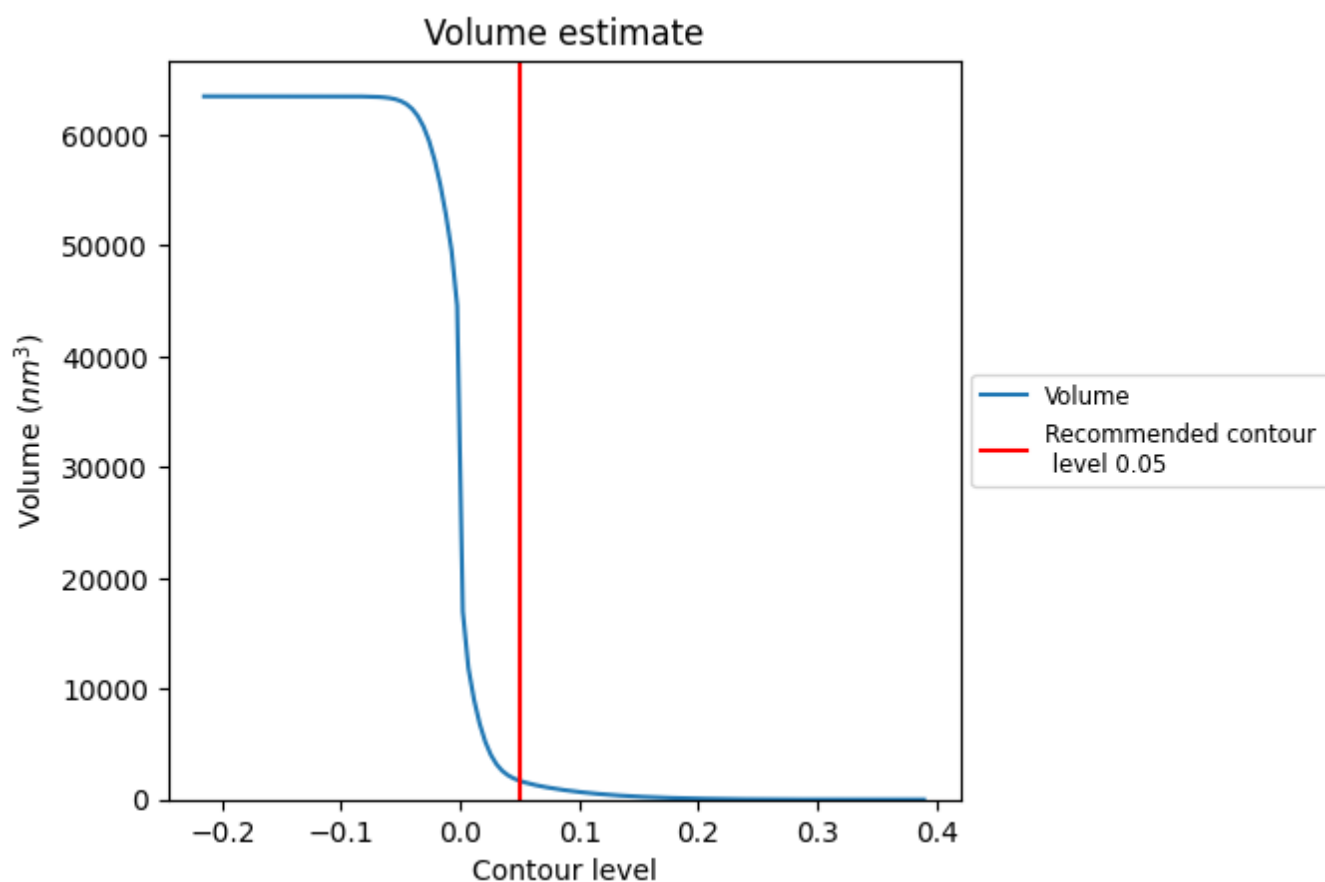
This section contains the results of statistical analysis of the map.

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.

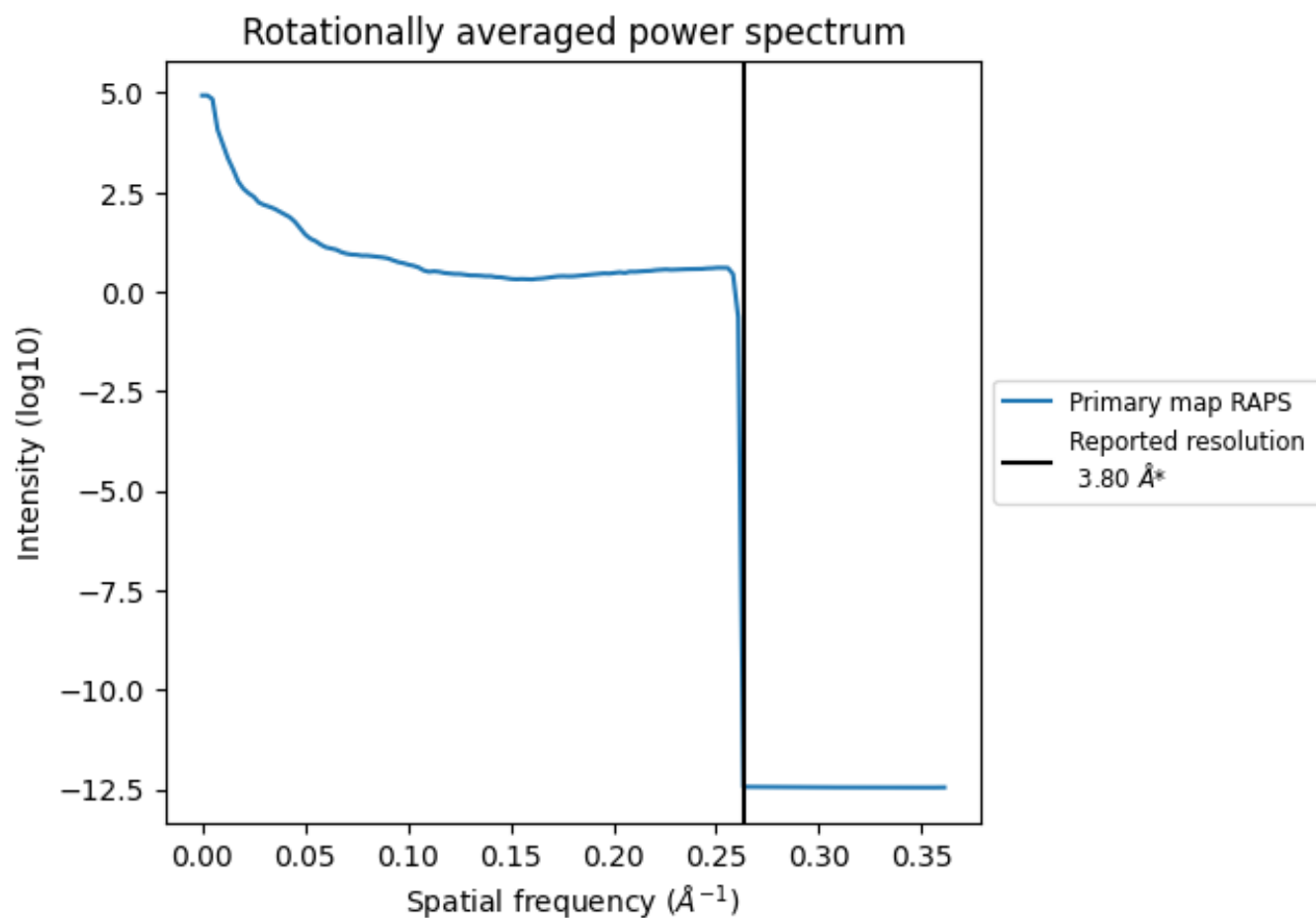
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 1693 nm³; this corresponds to an approximate mass of 1530 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 0.263 Å⁻¹

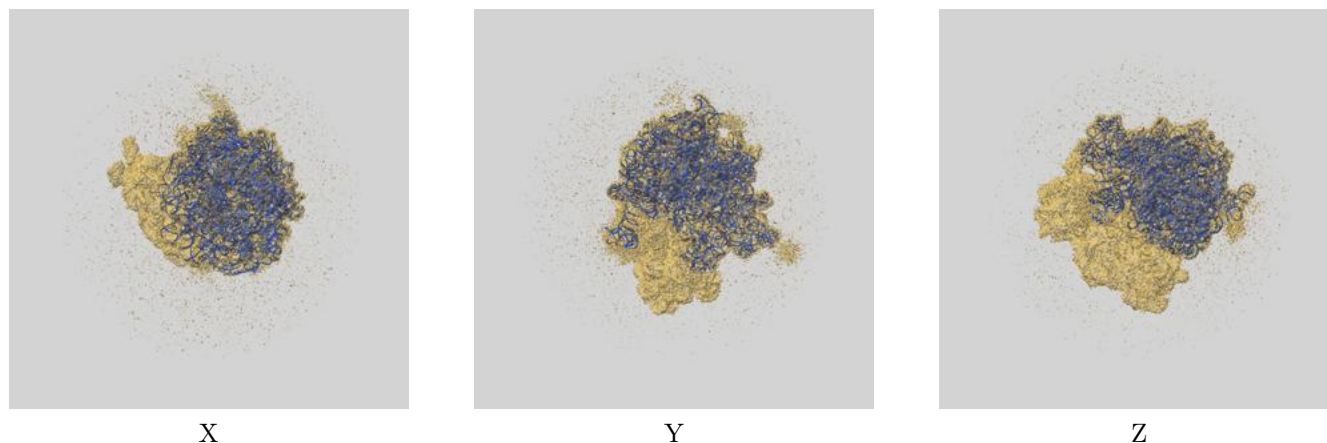
8 Fourier-Shell correlation ⓘ

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

9 Map-model fit [i](#)

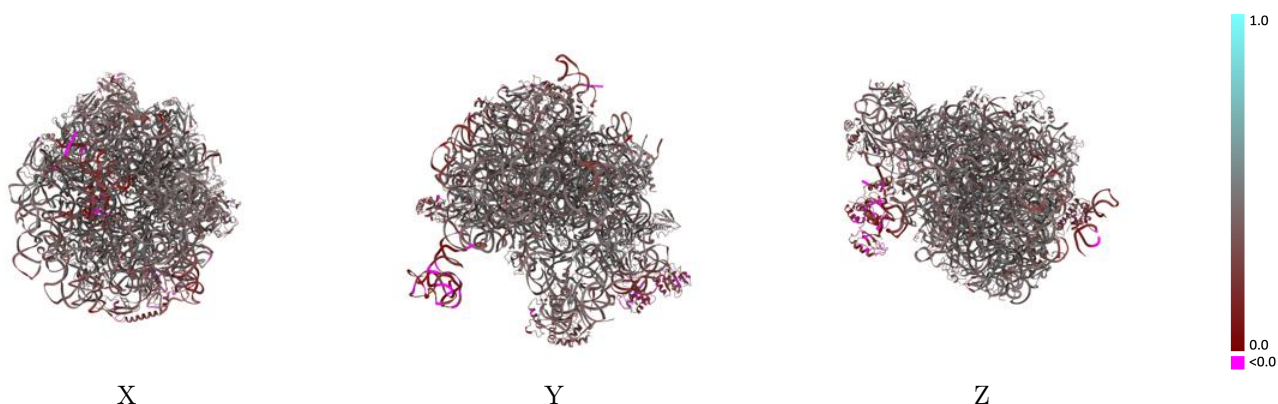
This section contains information regarding the fit between EMDB map EMD-8004 and PDB model 5GAH. Per-residue inclusion information can be found in [section 3](#) on [page 11](#).

9.1 Map-model overlay [i](#)



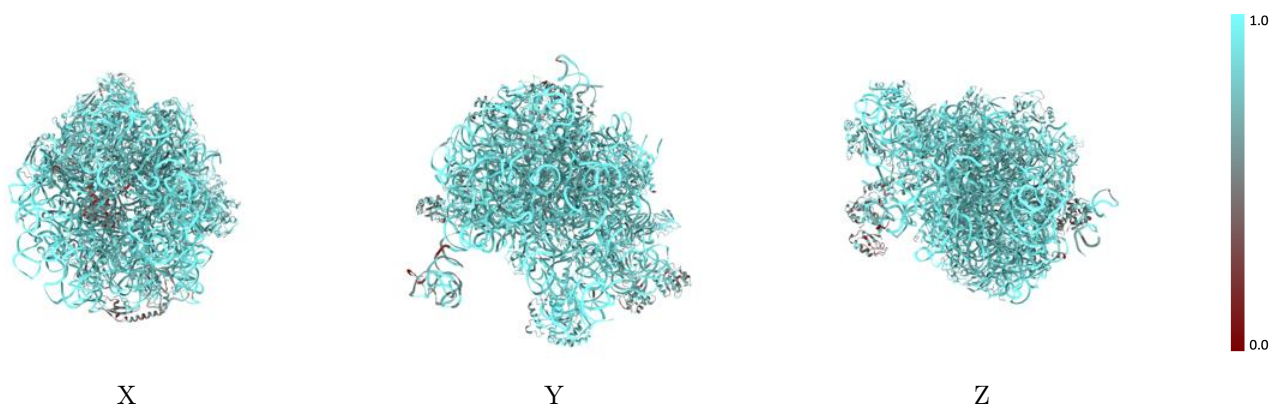
The images above show the 3D surface view of the map at the recommended contour level 0.05 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



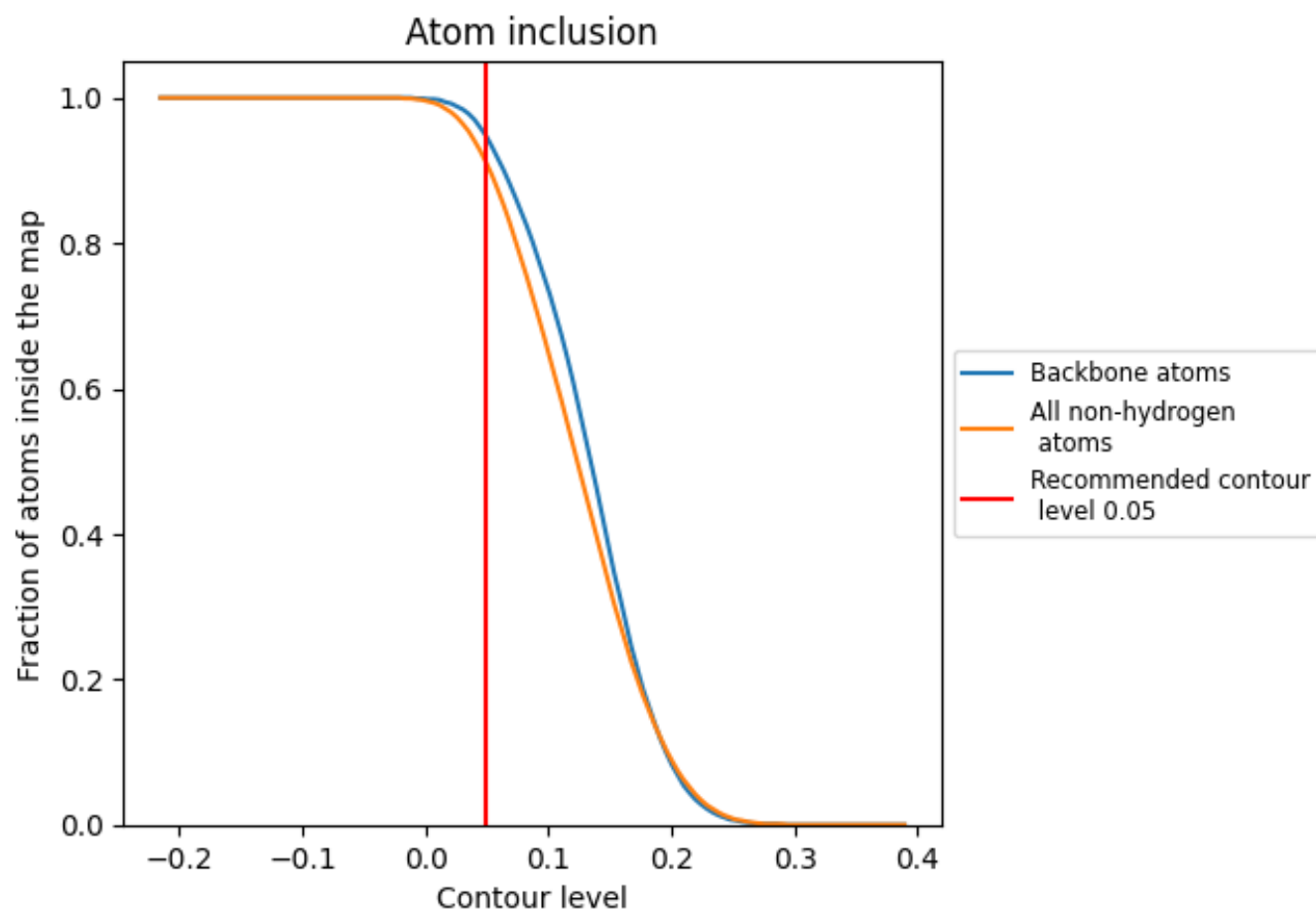
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions 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 (0.05).







































































9.4 Atom inclusion [i](#)



At the recommended contour level, 95% of all backbone atoms, 91% 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 (0.05) and Q-score for the entire model and for each chain.

| Chain | Atom inclusion | Q-score |
|-------|--|--|
| All |  0.9090 |  0.3880 |
| 1 |  0.7850 |  0.1610 |
| 2 |  0.9360 |  0.4300 |
| A |  0.9530 |  0.3920 |
| B |  0.9820 |  0.3990 |
| C |  0.8470 |  0.4420 |
| D |  0.8660 |  0.4400 |
| E |  0.8250 |  0.4010 |
| F |  0.8190 |  0.3330 |
| G |  0.8570 |  0.3810 |
| H |  0.5880 |  0.2850 |
| I |  0.6240 |  0.1910 |
| J |  0.5320 |  0.1210 |
| K |  0.8750 |  0.4340 |
| L |  0.7960 |  0.4210 |
| M |  0.8590 |  0.4120 |
| N |  0.8560 |  0.4350 |
| O |  0.8470 |  0.4110 |
| P |  0.8840 |  0.4000 |
| Q |  0.8260 |  0.4050 |
| R |  0.8740 |  0.4190 |
| S |  0.8770 |  0.4320 |
| T |  0.8130 |  0.4270 |
| U |  0.8080 |  0.3860 |
| V |  0.8360 |  0.4030 |
| W |  0.8740 |  0.4250 |
| X |  0.8650 |  0.4480 |
| Y |  0.8470 |  0.4240 |
| Z |  0.8020 |  0.3690 |
| a |  0.8700 |  0.4200 |
| b |  0.8390 |  0.4110 |
| c |  0.8180 |  0.3950 |
| d |  0.8650 |  0.4380 |
| e |  0.8720 |  0.4570 |
| f |  0.8800 |  0.4360 |



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| Chain | Atom inclusion | Q-score |
|-------|--|--|
| i |  0.5820 |  0.2390 |
| k |  0.5330 |  0.1660 |