# Full wwPDB EM Validation Report ⓘ

Dec 10, 2022 – 11:32 pm GMT

| | | |
|---|---|---|
| PDB ID | : | 4UY8 |
| EMDB ID | : | EMD-2773 |
| Title | : | Molecular basis for the ribosome functioning as a L-tryptophan sensor - Cryo-EM structure of a TnaC stalled E.coli ribosome |
| Authors | : | Bischoff, L.; Berninghausen, O.; Beckmann, R. |
| Deposited on | : | 2014-08-29 |
| 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:

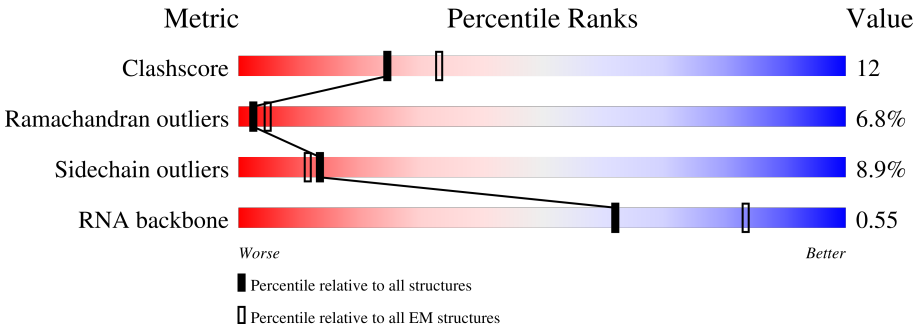
| | | |
|---|---|---|
| EMDB validation analysis | : | 0.0.1.dev43 |
| Mogul | : | 1.8.4, CSD as541be (2020) |
| MolProbity | : | 4.02b-467 |
| Percentile statistics | : | 20191225.v01 (using entries in the PDB archive December 25th 2019) |
| MapQ | : | 1.9.9 |
| Ideal geometry (proteins) | : | Engh & Huber (2001) |
| Ideal geometry (DNA, RNA) | : | Parkinson et al. (1996) |
| Validation Pipeline (wwPDB-VP) | : | 2.31.3 |

# 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 | 158937 | 4297 |
| Ramachandran outliers | 154571 | 4023 |
| Sidechain outliers | 154315 | 3826 |
| RNA backbone | 4643 | 859 |

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

| Mol | Chain | Length | Quality of chain |
|---|---|---|---|
| 1 | 0 | 56 | 75% 71% 25% |
| 2 | 1 | 50 | 94% 64% 28% 8% |
| 3 | 2 | 46 | 59% 76% 22% |
| 4 | 3 | 64 | 88% 77% 19% 5% |
| 5 | 4 | 38 | 68% 55% 39% |
| 6 | 5 | 148 | 100% 29% 41% 20% 9% |
| 7 | 6 | 30 | 100% 60% 30% 10% |

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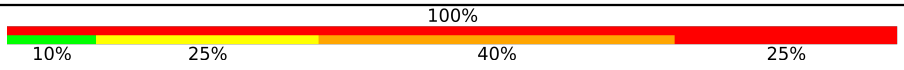
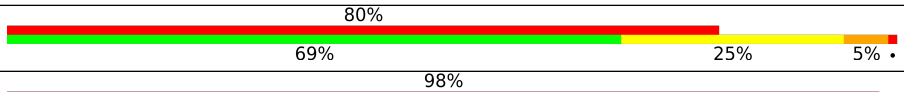
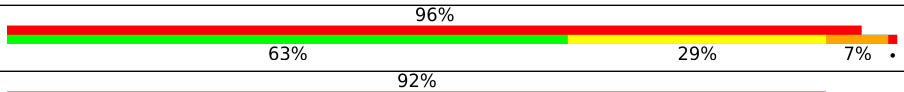
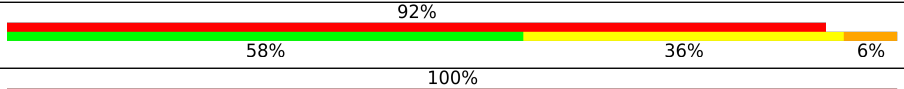
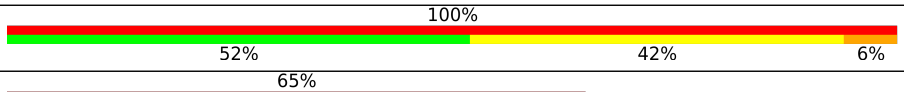
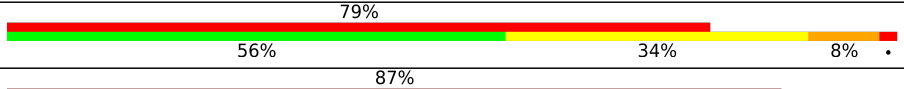
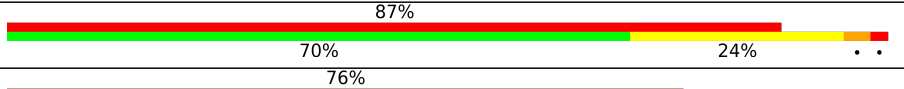
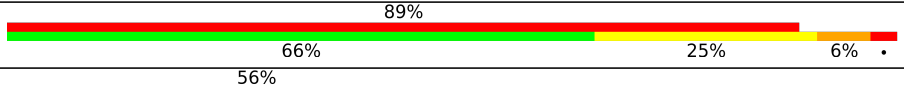
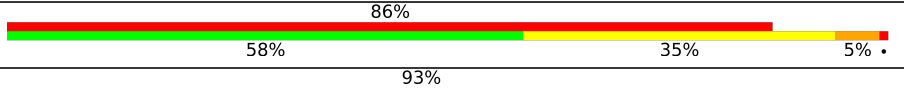
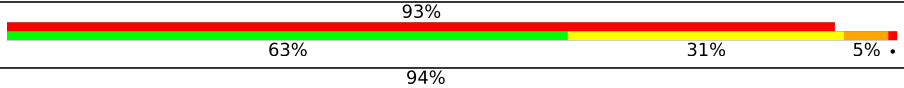
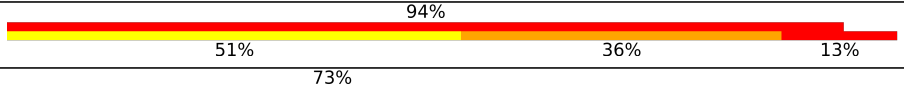
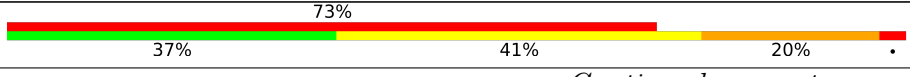
| Mol | Chain | Length | Quality of chain |
|---|---|---|---|
| 8 | 7 | 20 |   |
| 9 | 8 | 94 |   |
| 10 | A | 2854 |   |
| 11 | B | 118 |   |
| 12 | C | 271 |   |
| 13 | D | 209 |   |
| 14 | E | 201 |   |
| 15 | F | 177 |   |
| 16 | G | 176 |   |
| 17 | H | 50 |   |
| 18 | I | 141 |   |
| 19 | J | 142 |   |
| 20 | K | 122 |   |
| 21 | L | 143 |   |
| 22 | M | 136 |   |
| 23 | N | 120 |   |
| 24 | O | 116 |   |
| 25 | P | 114 |   |
| 26 | Q | 117 |   |
| 27 | R | 103 |   |
| 28 | S | 110 |   |
| 29 | T | 93 |   |
| 30 | U | 102 |   |
| 31 | V | 77 |   |
| 32 | W | 79 |   |

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| Mol | Chain | Length | Quality of chain |
|---|---|---|---|
| 33 | X | 77 | 78% 70% 23% 5% |
| 34 | Y | 63 | 87% 60% 38% |
| 35 | Z | 58 | 78% 53% 36% 9% |

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

| Mol | Type | Chain | Res | Chirality | Geometry | Clashes | Electron density |
|---|---|---|---|---|---|---|---|
| 38 | TRP | 7 | 1001 | - | - | X | - |
| 38 | TRP | 7 | 1002 | - | - | X | - |

# 2 Entry composition (i)

There are 39 unique types of molecules in this entry. The entry contains 92995 atoms, of which 8 are hydrogens and 0 are deuteriums.

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

- Molecule 1 is a protein called 50S RIBOSOMAL PROTEIN L32.

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

- Molecule 2 is a protein called 50S RIBOSOMAL PROTEIN L33.

| Mol | Chain | Residues | Atoms | | | | AltConf | Trace |
|---|---|---|---|---|---|---|---|---|
| | | | Total | C | N | O | | |
| 2 | 1 | 50 | 409 | 263 | 75 | 71 | 0 | 0 |

- Molecule 3 is a protein called 50S RIBOSOMAL PROTEIN L34.

| Mol | Chain | Residues | Atoms | | | | | AltConf | Trace |
|---|---|---|---|---|---|---|---|---|---|
| | | | Total | C | N | O | S | | |
| 3 | 2 | 46 | 377 | 228 | 90 | 57 | 2 | 0 | 0 |

- Molecule 4 is a protein called 50S RIBOSOMAL PROTEIN L35.

| Mol | Chain | Residues | Atoms | | | | | AltConf | Trace |
|---|---|---|---|---|---|---|---|---|---|
| | | | Total | C | N | O | S | | |
| 4 | 3 | 64 | 504 | 323 | 105 | 74 | 2 | 0 | 0 |

- Molecule 5 is a protein called 50S RIBOSOMAL PROTEIN L36.

| Mol | Chain | Residues | Atoms | | | | | AltConf | Trace |
|---|---|---|---|---|---|---|---|---|---|
| | | | Total | C | N | O | S | | |
| 5 | 4 | 38 | 302 | 185 | 65 | 48 | 4 | 0 | 0 |

- Molecule 6 is a protein called 50S RIBOSOMAL PROTEIN L10.

| Mol | Chain | Residues | Atoms | | | | | AltConf | Trace |
|---|---|---|---|---|---|---|---|---|---|
| | | | Total | C | N | O | S | | |
| 6 | 5 | 148 | 1117 | 705 | 196 | 209 | 7 | 0 | 0 |

- Molecule 7 is a protein called RIBOSOMAL L7 PROTEIN.

| Mol | Chain | Residues | Atoms | | | | | AltConf | Trace |
|---|---|---|---|---|---|---|---|---|---|
| 7 | 6 | 30 | Total | C | N | O | S | 0 | 0 |
| | | | 227 | 144 | 33 | 47 | 3 | | |

- Molecule 8 is a protein called TRYPTOPHANASE.

| Mol | Chain | Residues | Atoms | | | | | AltConf | Trace |
|---|---|---|---|---|---|---|---|---|---|
| 8 | 7 | 20 | Total | C | N | O | S | 0 | 0 |
| | | | 170 | 109 | 32 | 28 | 1 | | |

- Molecule 9 is a protein called 50S RIBOSOMAL PROTEIN L25.

| Mol | Chain | Residues | Atoms | | | | | AltConf | Trace |
|---|---|---|---|---|---|---|---|---|---|
| 9 | 8 | 94 | Total | C | N | O | S | 0 | 0 |
| | | | 753 | 479 | 137 | 134 | 3 | | |

- Molecule 10 is a RNA chain called RRNA-23S RIBOSOMAL RNA.

| Mol | Chain | Residues | Atoms | | | | | AltConf | Trace |
|---|---|---|---|---|---|---|---|---|---|
| 10 | A | 2854 | Total | C | N | O | P | 0 | 0 |
| | | | 61274 | 27334 | 11279 | 19807 | 2854 | | |

- Molecule 11 is a RNA chain called RRNA-5S RIBOSOMAL RNA.

| Mol | Chain | Residues | Atoms | | | | | AltConf | Trace |
|---|---|---|---|---|---|---|---|---|---|
| 11 | B | 118 | Total | C | N | O | P | 0 | 0 |
| | | | 2529 | 1126 | 464 | 821 | 118 | | |

- Molecule 12 is a protein called 50S RIBOSOMAL PROTEIN L2.

| Mol | Chain | Residues | Atoms | | | | | AltConf | Trace |
|---|---|---|---|---|---|---|---|---|---|
| 12 | C | 271 | Total | C | N | O | S | 0 | 0 |
| | | | 2082 | 1288 | 423 | 364 | 7 | | |

- Molecule 13 is a protein called 50S RIBOSOMAL PROTEIN L3.

| Mol | Chain | Residues | Atoms | | | | | AltConf | Trace |
|---|---|---|---|---|---|---|---|---|---|
| 13 | D | 209 | Total | C | N | O | S | 0 | 0 |
| | | | 1565 | 979 | 288 | 294 | 4 | | |

- Molecule 14 is a protein called 50S RIBOSOMAL PROTEIN L4.

| Mol | Chain | Residues | Atoms | | | | | AltConf | Trace |
|---|---|---|---|---|---|---|---|---|---|
| 14 | E | 201 | Total | C | N | O | S | 0 | 0 |
| | | | 1552 | 974 | 283 | 290 | 5 | | |

- Molecule 15 is a protein called 50S RIBOSOMAL PROTEIN L5.

| Mol | Chain | Residues | Atoms | | | | | AltConf | Trace |
|---|---|---|---|---|---|---|---|---|---|
| 15 | F | 177 | Total | C | N | O | S | 0 | 0 |
| | | | 1410 | 899 | 249 | 256 | 6 | | |

- Molecule 16 is a protein called 50S RIBOSOMAL PROTEIN L6.

| Mol | Chain | Residues | Atoms | | | | | AltConf | Trace |
|---|---|---|---|---|---|---|---|---|---|
| 16 | G | 176 | Total | C | N | O | S | 0 | 0 |
| | | | 1323 | 832 | 243 | 246 | 2 | | |

- Molecule 17 is a protein called RIBOSOMAL PROTEIN L9.

| Mol | Chain | Residues | Atoms | | | | | AltConf | Trace |
|---|---|---|---|---|---|---|---|---|---|
| 17 | H | 50 | Total | C | N | O | S | 0 | 0 |
| | | | 384 | 247 | 68 | 68 | 1 | | |

- Molecule 18 is a protein called 50S RIBOSOMAL PROTEIN L11.

| Mol | Chain | Residues | Atoms | | | | | AltConf | Trace |
|---|---|---|---|---|---|---|---|---|---|
| 18 | I | 141 | Total | C | N | O | S | 0 | 0 |
| | | | 1032 | 651 | 179 | 196 | 6 | | |

- Molecule 19 is a protein called 50S RIBOSOMAL PROTEIN L13.

| Mol | Chain | Residues | Atoms | | | | | AltConf | Trace |
|---|---|---|---|---|---|---|---|---|---|
| 19 | J | 142 | Total | C | N | O | S | 0 | 0 |
| | | | 1129 | 714 | 212 | 199 | 4 | | |

- Molecule 20 is a protein called 50S RIBOSOMAL PROTEIN L14.

| Mol | Chain | Residues | Atoms | | | | | AltConf | Trace |
|---|---|---|---|---|---|---|---|---|---|
| 20 | K | 122 | Total | C | N | O | S | 0 | 0 |
| | | | 938 | 587 | 180 | 165 | 6 | | |

- Molecule 21 is a protein called 50S RIBOSOMAL PROTEIN L15.

| Mol | Chain | Residues | Atoms | | | | | AltConf | Trace |
|---|---|---|---|---|---|---|---|---|---|
| 21 | L | 143 | Total | C | N | O | S | 0 | 0 |
| | | | 1045 | 649 | 206 | 189 | 1 | | |

- Molecule 22 is a protein called 50S RIBOSOMAL PROTEIN L16.

| Mol | Chain | Residues | Atoms | | | | | AltConf | Trace |
|---|---|---|---|---|---|---|---|---|---|
| 22 | M | 136 | Total | C | N | O | S | 0 | 0 |
| | | | 1074 | 686 | 205 | 177 | 6 | | |

- Molecule 23 is a protein called 50S RIBOSOMAL PROTEIN L17.

| Mol | Chain | Residues | Atoms | | | | | AltConf | Trace |
|---|---|---|---|---|---|---|---|---|---|
| 23 | N | 120 | Total | C | N | O | S | 0 | 0 |
| | | | 960 | 593 | 196 | 166 | 5 | | |

- Molecule 24 is a protein called 50S RIBOSOMAL PROTEIN L18.

| Mol | Chain | Residues | Atoms | | | | AltConf | Trace |
|---|---|---|---|---|---|---|---|---|
| 24 | O | 116 | Total | C | N | O | 0 | 0 |
| | | | 892 | 552 | 178 | 162 | | |

- Molecule 25 is a protein called 50S RIBOSOMAL PROTEIN L19.

| Mol | Chain | Residues | Atoms | | | | | AltConf | Trace |
|---|---|---|---|---|---|---|---|---|---|
| 25 | P | 114 | Total | C | N | O | S | 0 | 0 |
| | | | 917 | 574 | 179 | 163 | 1 | | |

- Molecule 26 is a protein called 50S RIBOSOMAL PROTEIN L20.

| Mol | Chain | Residues | Atoms | | | | AltConf | Trace |
|---|---|---|---|---|---|---|---|---|
| 26 | Q | 117 | Total | C | N | O | 0 | 0 |
| | | | 947 | 604 | 192 | 151 | | |

- Molecule 27 is a protein called 50S RIBOSOMAL PROTEIN L21.

| Mol | Chain | Residues | Atoms | | | | | AltConf | Trace |
|---|---|---|---|---|---|---|---|---|---|
| 27 | R | 103 | Total | C | N | O | S | 0 | 0 |
| | | | 816 | 516 | 153 | 145 | 2 | | |

- Molecule 28 is a protein called 50S RIBOSOMAL PROTEIN L22.

| Mol | Chain | Residues | Atoms | | | | | AltConf | Trace |
|---|---|---|---|---|---|---|---|---|---|
| 28 | S | 110 | Total | C | N | O | S | 0 | 0 |
| | | | 857 | 532 | 166 | 156 | 3 | | |

- Molecule 29 is a protein called 50S RIBOSOMAL PROTEIN L23.

| Mol | Chain | Residues | Atoms | | | | | AltConf | Trace |
|---|---|---|---|---|---|---|---|---|---|
| 29 | T | 93 | Total | C | N | O | S | 0 | 0 |
| | | | 738 | 466 | 139 | 131 | 2 | | |

- Molecule 30 is a protein called 50S RIBOSOMAL PROTEIN L24.

| Mol | Chain | Residues | Atoms | | | | AltConf | Trace |
|---|---|---|---|---|---|---|---|---|
| 30 | U | 102 | Total | C | N | O | 0 | 0 |
| | | | 779 | 492 | 146 | 141 | | |

- Molecule 31 is a RNA chain called RNA.

| Mol | Chain | Residues | Atoms | | | | | AltConf | Trace |
|---|---|---|---|---|---|---|---|---|---|
| 31 | V | 77 | Total | C | N | O | P | 0 | 0 |
| | | | 1649 | 733 | 297 | 542 | 77 | | |

- Molecule 32 is a protein called 50S RIBOSOMAL PROTEIN L27.

| Mol | Chain | Residues | Atoms | | | | | AltConf | Trace |
|---|---|---|---|---|---|---|---|---|---|
| 32 | W | 79 | Total | C | N | O | S | 0 | 0 |
| | | | 596 | 367 | 120 | 108 | 1 | | |

- Molecule 33 is a protein called 50S RIBOSOMAL PROTEIN L28.

| Mol | Chain | Residues | Atoms | | | | | AltConf | Trace |
|---|---|---|---|---|---|---|---|---|---|
| 33 | X | 77 | Total | C | N | O | S | 0 | 0 |
| | | | 625 | 388 | 129 | 106 | 2 | | |

- Molecule 34 is a protein called 50S RIBOSOMAL PROTEIN L29.

| Mol | Chain | Residues | Atoms | | | | | AltConf | Trace |
|---|---|---|---|---|---|---|---|---|---|
| 34 | Y | 63 | Total | C | N | O | S | 0 | 0 |
| | | | 509 | 313 | 99 | 95 | 2 | | |

- Molecule 35 is a protein called 50S RIBOSOMAL PROTEIN L30.

| Mol | Chain | Residues | Atoms | | | | | AltConf | Trace |
|---|---|---|---|---|---|---|---|---|---|
| 35 | Z | 58 | Total | C | N | O | S | 0 | 0 |
| | | | 449 | 281 | 87 | 79 | 2 | | |

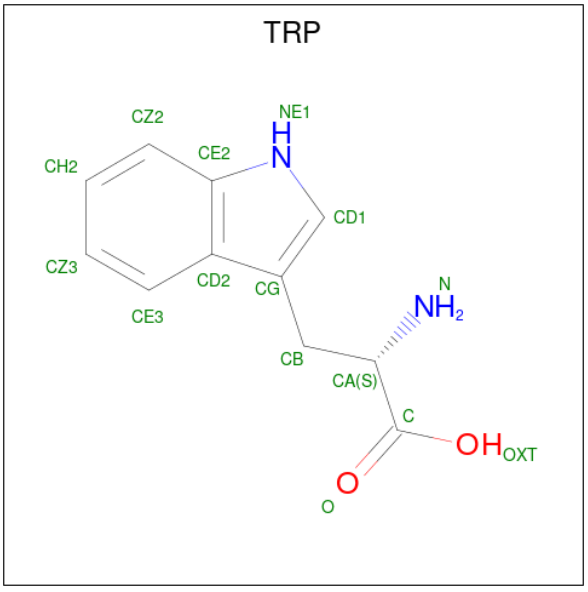
- Molecule 36 is MAGNESIUM ION (three-letter code: MG) (formula: Mg).

| Mol | Chain | Residues | Atoms | | AltConf |
|---|---|---|---|---|---|
| 36 | 4 | 1 | Total | Mg | 0 |
| | | | 1 | 1 | |
| 36 | A | 135 | Total | Mg | 0 |
| | | | 135 | 135 | |
| 36 | B | 4 | Total | Mg | 0 |
| | | | 4 | 4 | |
| 36 | C | 2 | Total | Mg | 0 |
| | | | 2 | 2 | |
| 36 | E | 1 | Total | Mg | 0 |
| | | | 1 | 1 | |

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

| Mol | Chain | Residues | Atoms | | AltConf |
|---|---|---|---|---|---|
| 37 | 4 | 1 | Total | Zn | 0 |
| | | | 1 | 1 | |

- Molecule 38 is TRYPTOPHAN (three-letter code: TRP) (formula: $C_{11}H_{12}N_2O_2$).



| Mol | Chain | Residues | Atoms | | | | | AltConf |
|---|---|---|---|---|---|---|---|---|
| 38 | 7 | 1 | Total | C | H | N | O | 0 |
| | | | 38 | 22 | 8 | 4 | 4 | |
| 38 | 7 | 1 | Total | C | H | N | O | 0 |
| | | | 38 | 22 | 8 | 4 | 4 | |

- Molecule 39 is water.

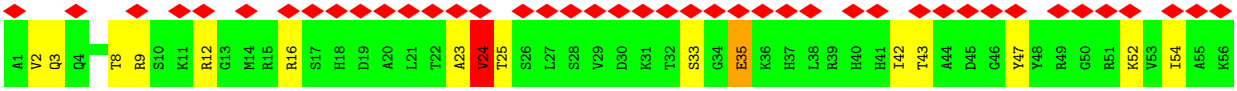
| Mol | Chain | Residues | Atoms | | AltConf |
|---|---|---|---|---|---|
| 39 | A | 416 | Total | O | 0 |
| | | | 416 | 416 | |
| 39 | B | 14 | Total | O | 0 |
| | | | 14 | 14 | |
| 39 | C | 2 | Total | O | 0 |
| | | | 2 | 2 | |
| 39 | D | 3 | Total | O | 0 |
| | | | 3 | 3 | |
| 39 | E | 2 | Total | O | 0 |
| | | | 2 | 2 | |
| 39 | L | 2 | Total | O | 0 |
| | | | 2 | 2 | |

# 3 Residue-property plots (i)

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

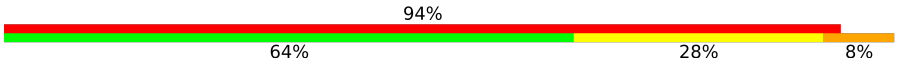
• Molecule 1: 50S RIBOSOMAL PROTEIN L32

Chain 0:


• Molecule 2: 50S RIBOSOMAL PROTEIN L33

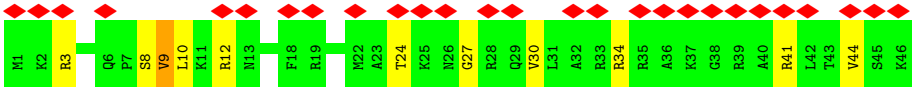
Chain 1:





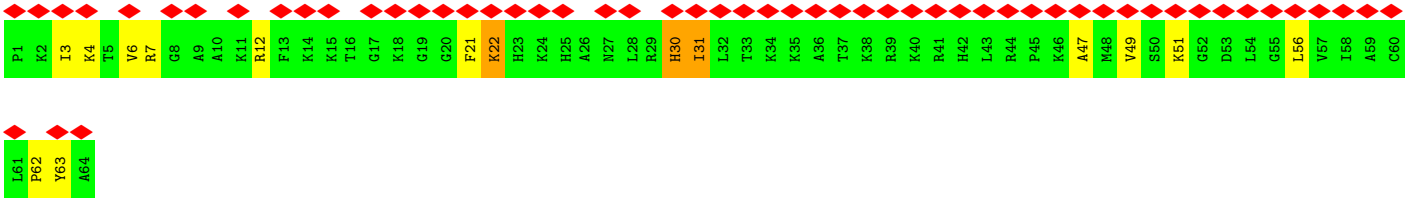
• Molecule 3: 50S RIBOSOMAL PROTEIN L34

Chain 2:

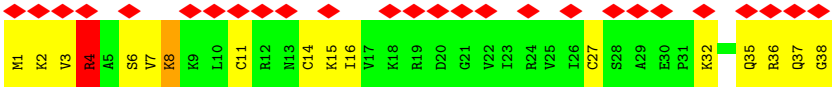

• Molecule 4: 50S RIBOSOMAL PROTEIN L35

Chain 3:

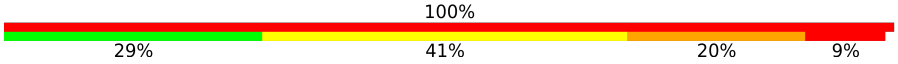



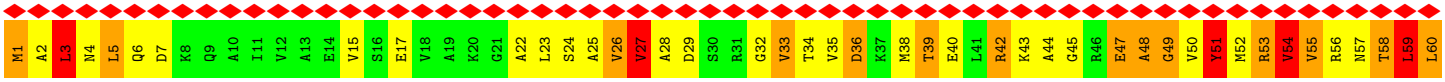

• Molecule 5: 50S RIBOSOMAL PROTEIN L36

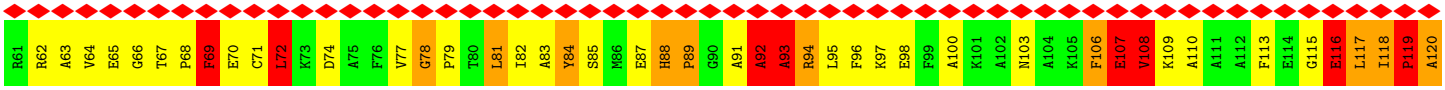
Chain 4:

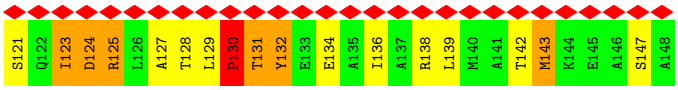



• Molecule 6: 50S RIBOSOMAL PROTEIN L10

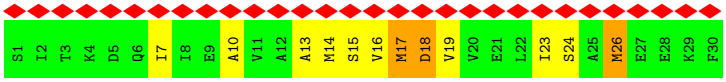


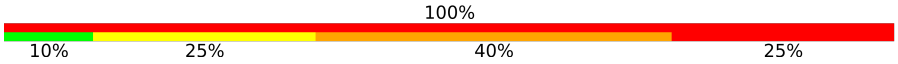




• Molecule 7: RIBOSOMAL L7 PROTEIN

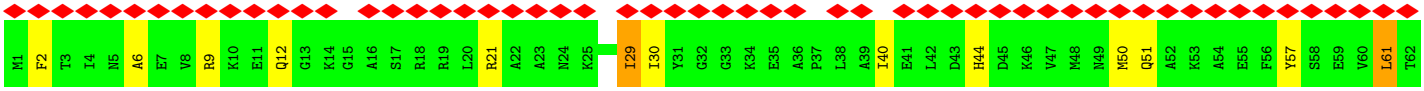



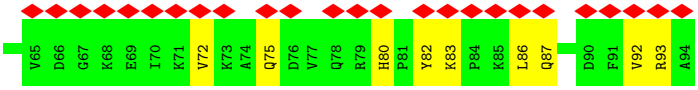

• Molecule 8: TRYPTOPHANASE



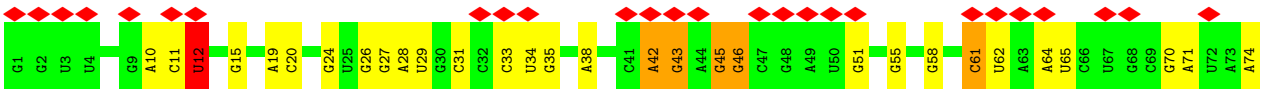


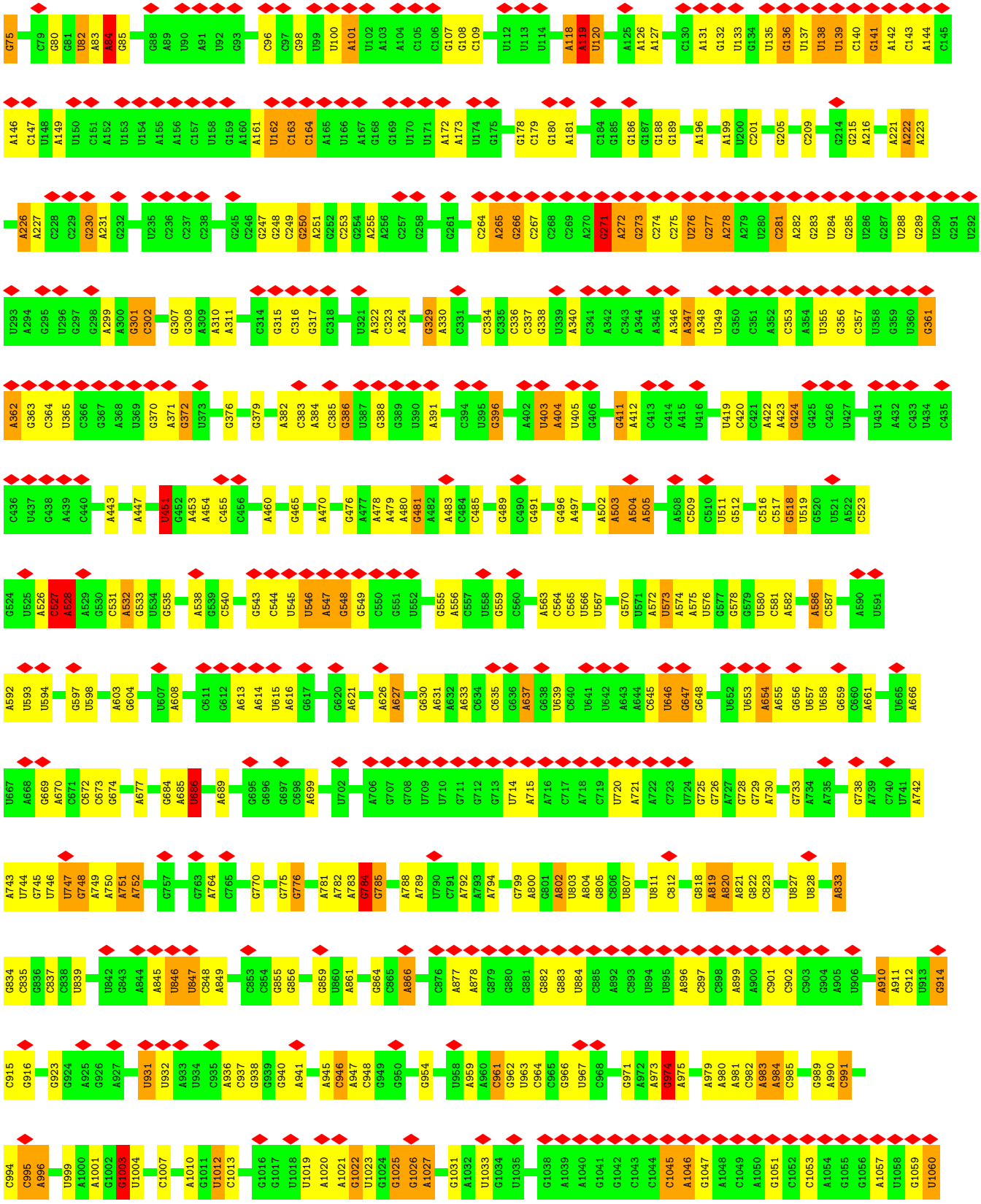
• Molecule 9: 50S RIBOSOMAL PROTEIN L25

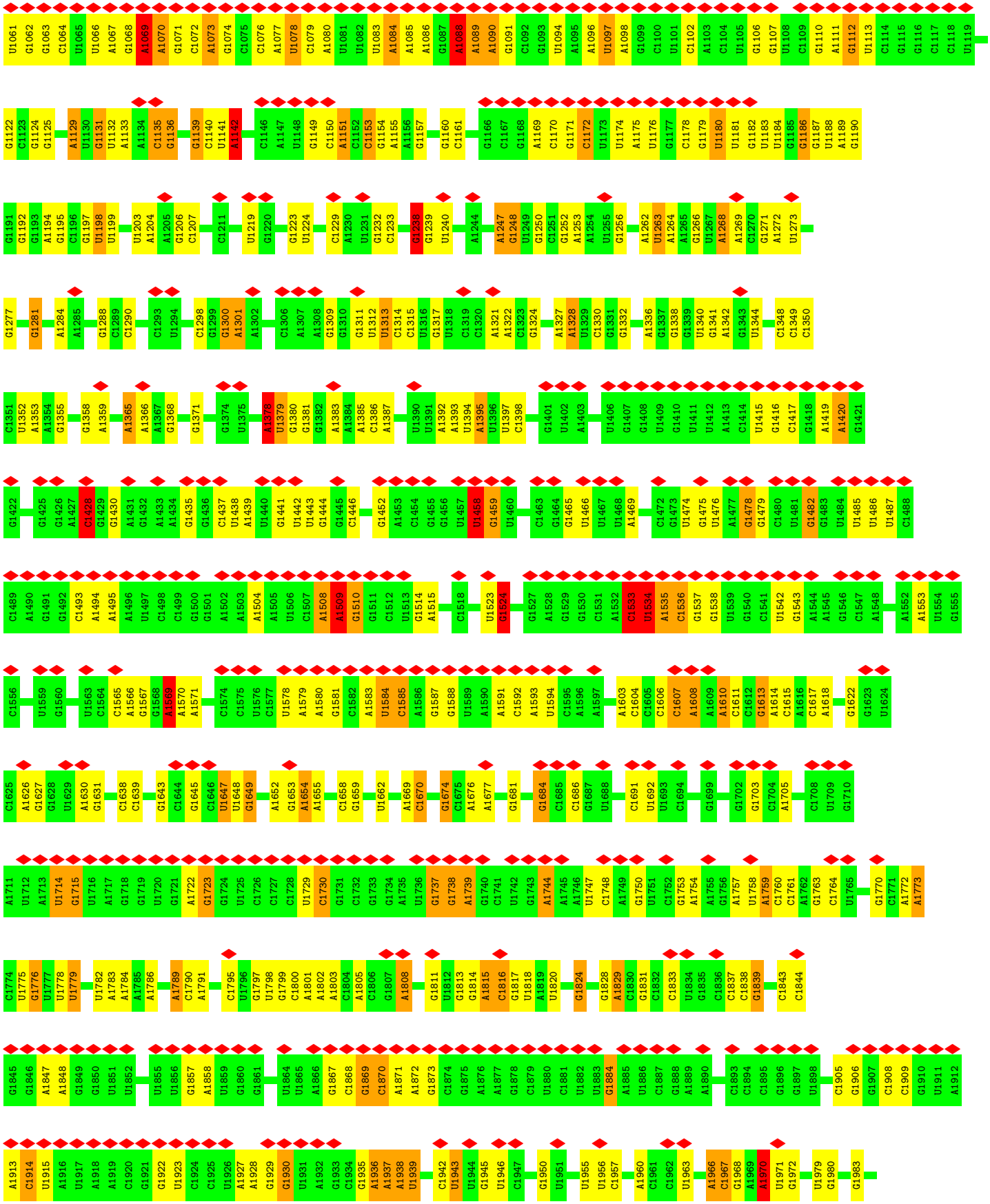




• Molecule 10: RRNA-23S RIBOSOMAL RNA

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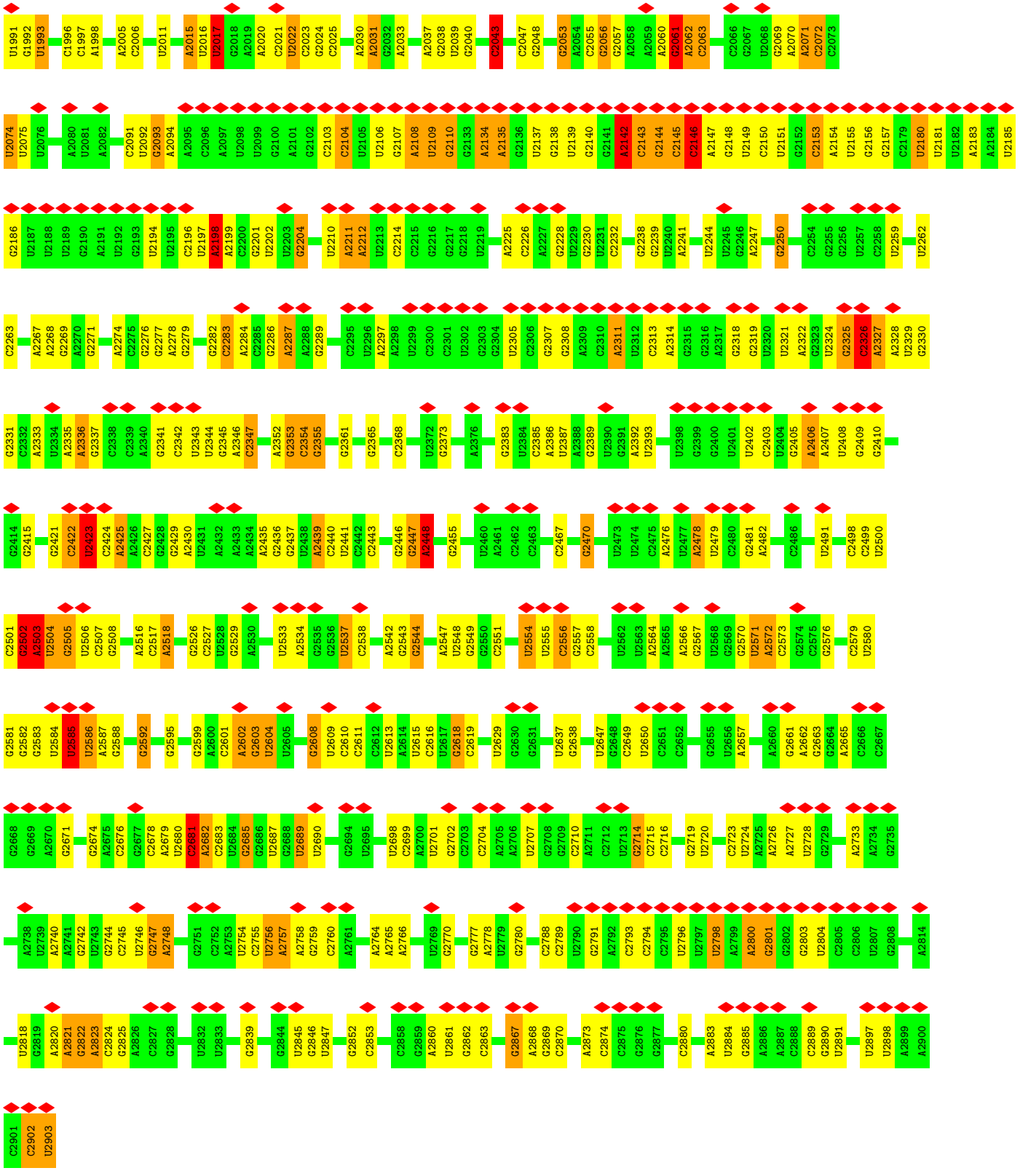
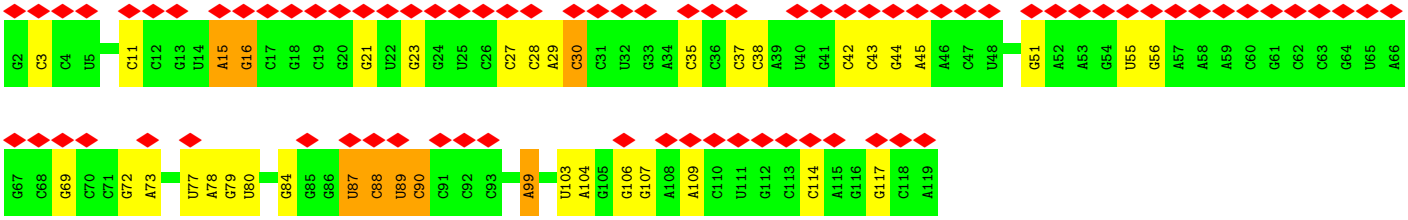
G1122 C1123 G1124 G1125 A1129 U1130 G1131 U1132 A1133 A1134 C1135 G1136 G1139 C1140 U1141 A1142 C1146 A1147 U1148 G1149 C1150 A1151 C1152 C1153 G1154 A1155 A1156 G1157 G1160 C1161 G1166 C1167 G1168 A1169 C1170 G1171 C1172 U1173 U1174 A1175 U1176 G1177 C1178 G1179 U1180 U1181 G1182 U1183 U1184 G1185 G1186 G1187 U1188 A1189 G1190
G1191 G1192 G1193 A1194 G1195 C1196 G1197 U1198 U1199 U1203 A1204 A1205 G1206 C1207 C1211 U1219 G1220 G1223 U1224 C1229 A1230 U1231 G1232 C1233 G1238 G1239 U1240 A1244 A1247 G1248 U1249 G1250 C1251 G1252 A1253 A1254 U1255 G1256 A1262 U1263 A1264 A1265 G1266 U1267 A1268 A1269 C1270 G1271 A1272 U1273
G1277 G1281 A1284 A1285 G1288 C1289 C1290 C1293 U1294 C1298 G1299 G1300 A1301 A1302 C1306 A1307 A1308 G1309 G1310 G1311 U1312 U1313 C1314 C1315 U1316 G1317 U1318 C1319 C1320 A1321 A1322 C1323 G1324 A1327 A1328 U1329 C1330 G1331 G1332 A1336 G1337 G1338 G1339 U1340 G1341 A1342 G1343 U1344 C1348 C1349 C1350
C1351 U1352 A1353 A1354 G1355 G1358 A1359 A1365 A1366 A1367 G1368 G1371 G1374 U1375 A1378 U1379 G1380 G1381 G1382 A1383 A1384 A1385 C1386 A1387 U1390 U1391 A1392 A1393 U1394 A1395 U1396 U1397 C1398 G1401 U1402 A1403 U1406 G1407 G1408 U1409 G1410 U1411 U1412 A1413 C1414 U1415 G1416 C1417 G1418 A1419 A1420 G1421
G1422 G1425 G1426 A1427 C1428 G1429 G1430 A1431 G1432 A1433 A1434 G1435 G1436 C1437 U1438 A1439 U1440 G1441 U1442 U1443 G1444 G1445 C1446 G1452 A1453 C1454 G1455 G1456 U1457 U1458 G1459 U1460 C1463 G1464 G1465 U1466 U1467 U1468 A1469 C1472 G1473 U1474 G1475 U1476 A1477 G1478 G1479 C1480 U1481 G1482 G1483 U1484 U1485 U1486 U1487 C1488
C1489 A1490 G1491 G1492 C1493 A1494 A1495 A1496 U1497 C1498 C1499 G1500 G1501 A1502 A1503 A1504 A1505 U1506 C1507 A1508 A1509 G1510 G1511 C1512 U1513 G1514 A1515 C1518 U1523 G1524 G1527 A1528 G1529 G1530 C1531 A1532 C1533 U1534 A1535 C1536 G1537 G1538 U1539 G1540 C1541 U1542 G1543 A1544 A1545 G1546 C1547 A1548 A1552 A1553 U1554 G1555
C1556 U1559 G1560 U1563 C1564 C1565 A1566 G1567 G1568 A1569 A1570 A1571 C1574 C1575 U1576 C1577 U1578 A1579 A1580 G1581 C1582 A1583 U1584 C1585 A1586 G1587 G1588 U1589 A1590 A1591 C1592 A1593 U1594 C1595 A1596 A1597 A1603 C1604 C1605 C1606 C1607 A1608 A1609 A1610 C1611 C1612 G1613 A1614 C1615 A1616 C1617 A1618 G1622 G1623 U1624
C1625 A1626 G1627 G1628 U1629 A1630 G1631 C1638 C1639 G1643 C1644 G1645 C1646 U1647 U1648 G1649 A1652 G1653 A1654 A1655 C1658 G1659 U1662 A1669 C1670 G1674 C1675 A1676 A1677 G1681 G1684 C1685 C1686 G1687 U1688 C1691 U1692 U1693 C1694 G1699 G1702 G1703 C1704 A1705 C1708 U1709 G1710
A1711 U1712 A1713 U1714 G1715 U1716 A1717 G1718 G1719 U1720 G1721 A1722 G1723 G1724 U1725 C1726 C1727 C1728 U1729 C1730 G1731 C1732 G1733 G1734 A1735 U1736 G1737 G1738 A1739 G1740 C1741 U1742 G1743 A1744 A1745 A1746 U1747 C1748 A1749 G1750 U1751 C1752 G1753 A1754 A1755 G1756 A1757 U1758 A1759 C1760 C1761 A1762 G1763 C1764 U1765 G1770 C1771 A1772 A1773
C1774 U1775 G1776 U1777 U1778 U1779 U1782 A1783 A1784 A1785 A1786 A1789 C1790 A1791 C1795 U1796 A1797 U1798 G1799 C1800 A1801 A1802 A1803 C1804 A1805 C1806 G1807 A1808 G1811 U1812 G1813 G1814 A1815 C1816 G1817 U1818 A1819 U1820 G1824 G1828 A1829 C1830 G1831 C1832 C1833 U1834 G1835 C1836 C1837 C1838 G1839 C1843 C1844
G1845 G1846 A1847 A1848 G1849 G1850 U1851 U1852 U1855 U1856 G1857 A1858 U1859 G1860 G1861 U1864 U1865 A1866 G1867 C1868 G1869 C1870 A1871 A1872 G1873 C1874 G1875 A1876 A1877 G1878 C1879 U1880 C1881 U1882 U1883 G1884 A1885 U1886 C1887 G1888 A1889 A1890 C1893 C1894 C1895 G1896 G1897 U1898 C1905 G1906 G1907 C1908 C1909 G1910 U1911 A1912
A1913 C1914 U1915 A1916 U1917 A1918 A1919 C1920 G1921 G1922 U1923 C1924 C1925 U1926 A1927 A1928 G1929 G1930 U1931 A1932 G1933 C1934 G1935 A1936 A1937 A1938 U1939 C1942 U1943 G1944 G1945 U1946 C1947 G1950 U1951 U1955 U1956 C1957 A1960 C1961 C1962 U1963 A1966 C1967 G1968 A1969 A1970 U1971 G1972 U1979 G1980 G1983



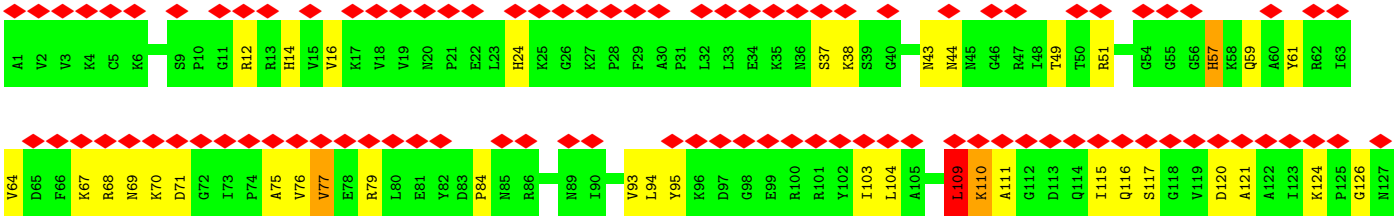
• Molecule 11: RRNA-5S RIBOSOMAL RNA

Chain B:



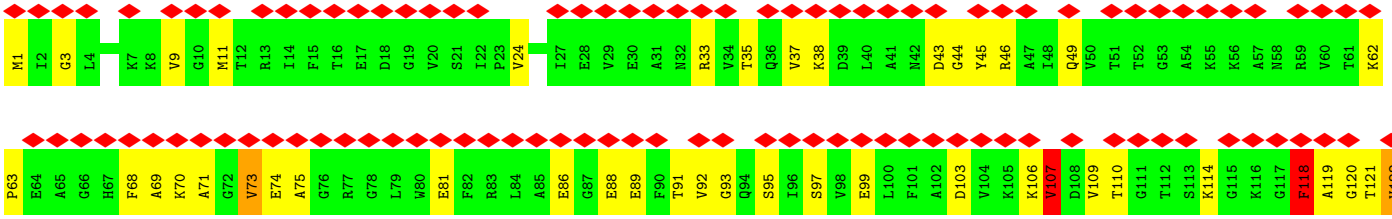

• Molecule 12: 50S RIBOSOMAL PROTEIN L2

Chain C:


• Molecule 13: 50S RIBOSOMAL PROTEIN L3

Chain D:

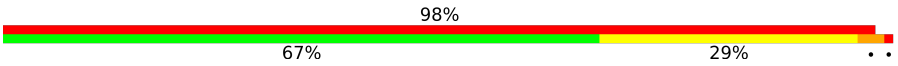



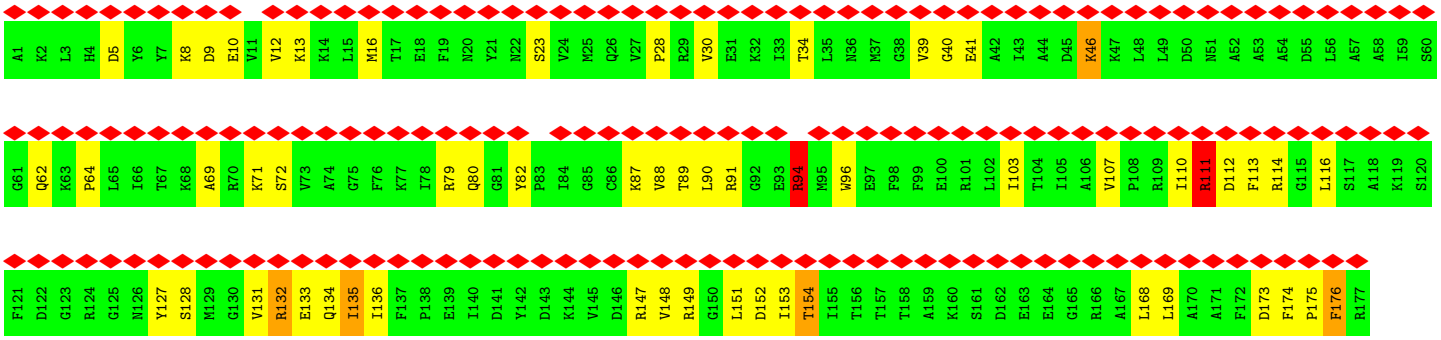

• Molecule 14: 50S RIBOSOMAL PROTEIN L4

Chain E:


• Molecule 15: 50S RIBOSOMAL PROTEIN L5

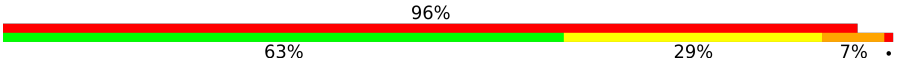
Chain F:

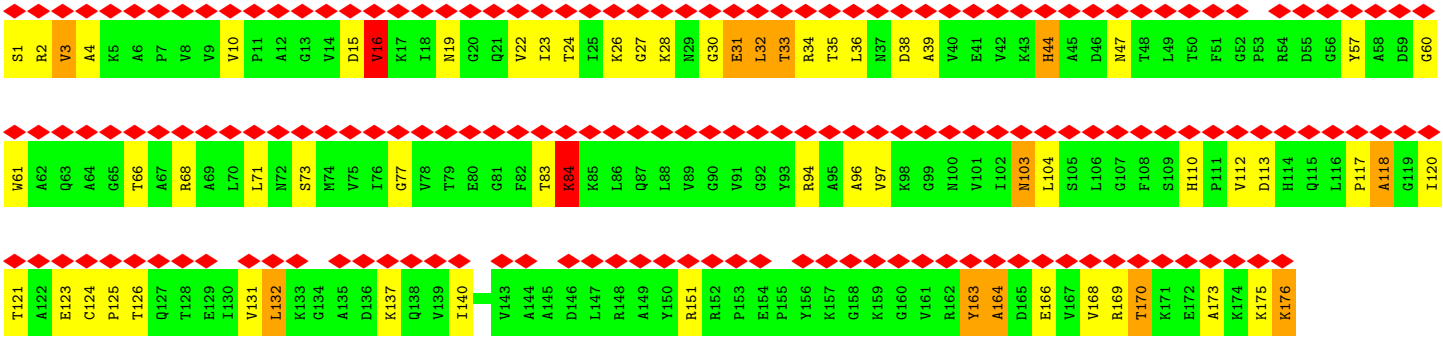



• Molecule 16: 50S RIBOSOMAL PROTEIN L6

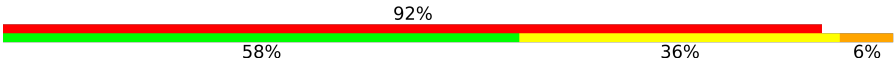
Chain G:



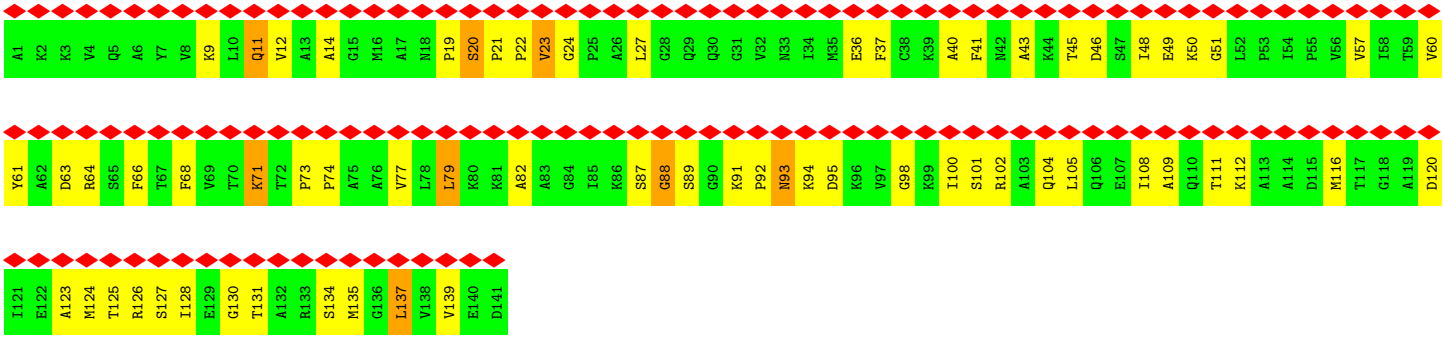

• Molecule 17: RIBOSOMAL PROTEIN L9

Chain H:



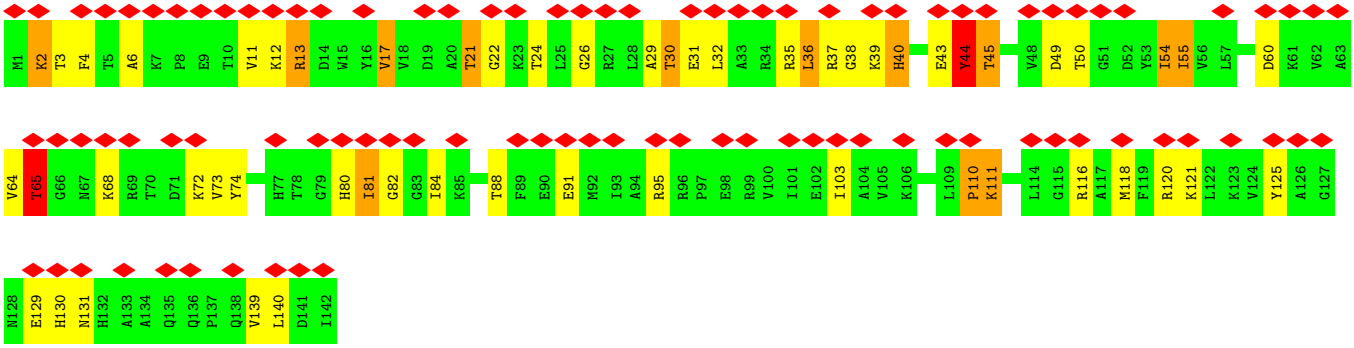

• Molecule 18: 50S RIBOSOMAL PROTEIN L11

Chain I:

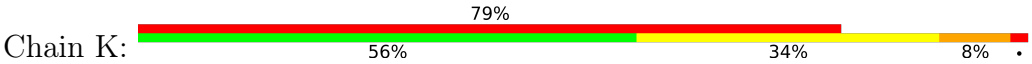

• Molecule 19: 50S RIBOSOMAL PROTEIN L13

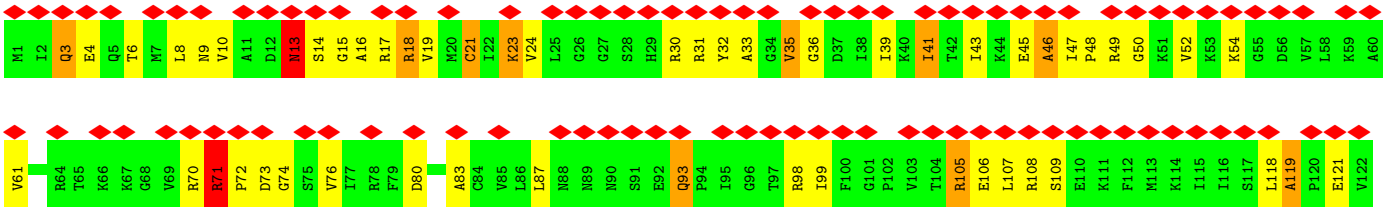
Chain J:


• Molecule 20: 50S RIBOSOMAL PROTEIN L14

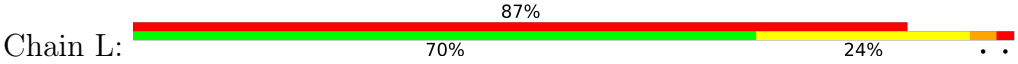
Chain K:

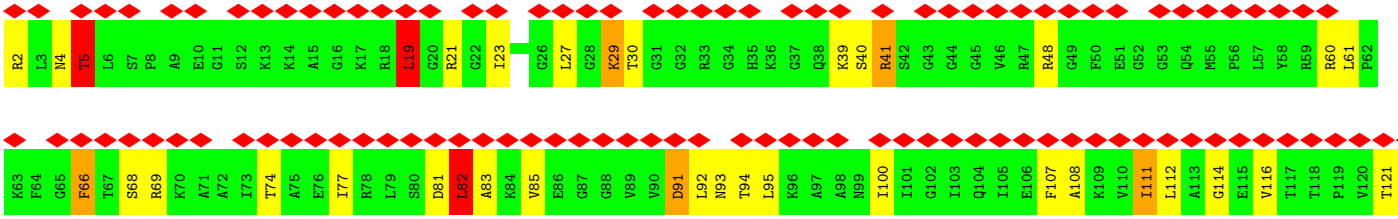


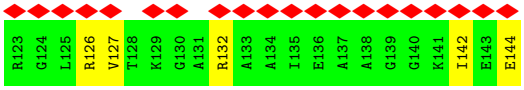




• Molecule 21: 50S RIBOSOMAL PROTEIN L15

Chain L:

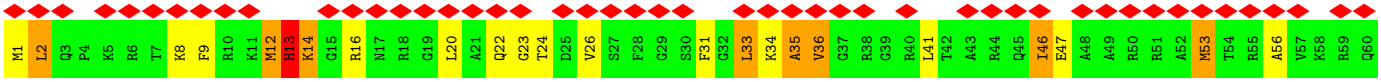


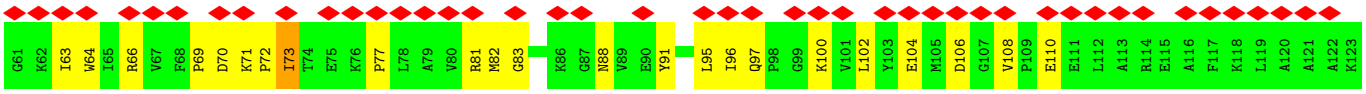



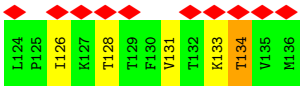



• Molecule 22: 50S RIBOSOMAL PROTEIN L16

Chain M:

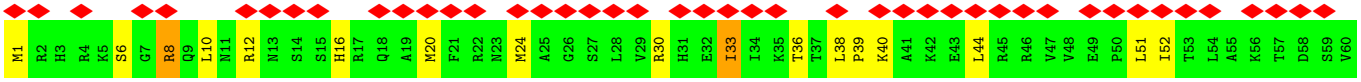



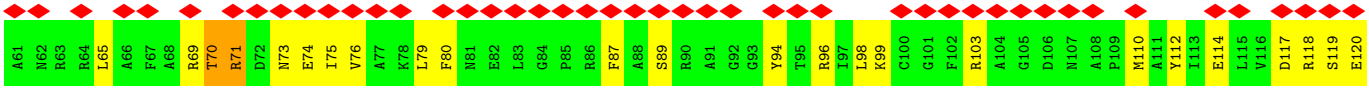




• Molecule 23: 50S RIBOSOMAL PROTEIN L17

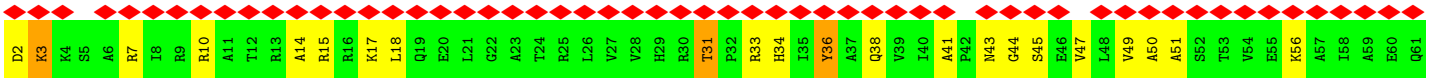
Chain N:

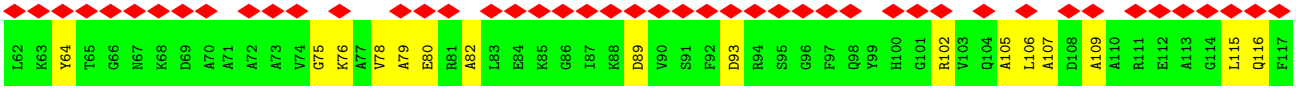




• Molecule 24: 50S RIBOSOMAL PROTEIN L18

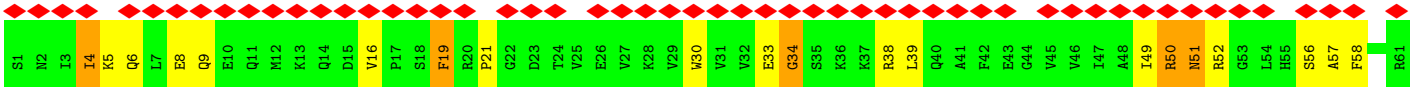
Chain O:

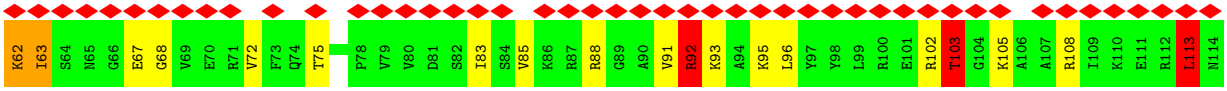




• Molecule 25: 50S RIBOSOMAL PROTEIN L19

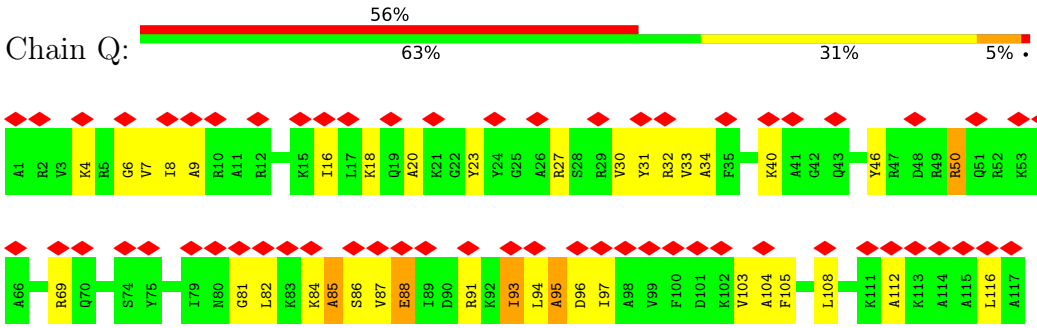
Chain P:

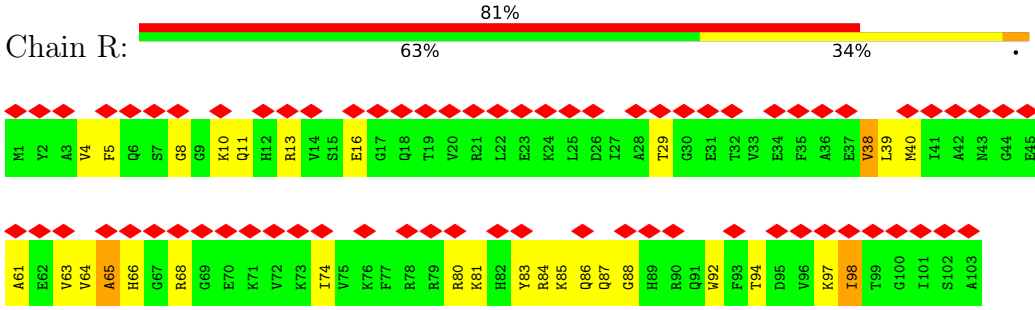
• Molecule 26: 50S RIBOSOMAL PROTEIN L20

Chain Q:



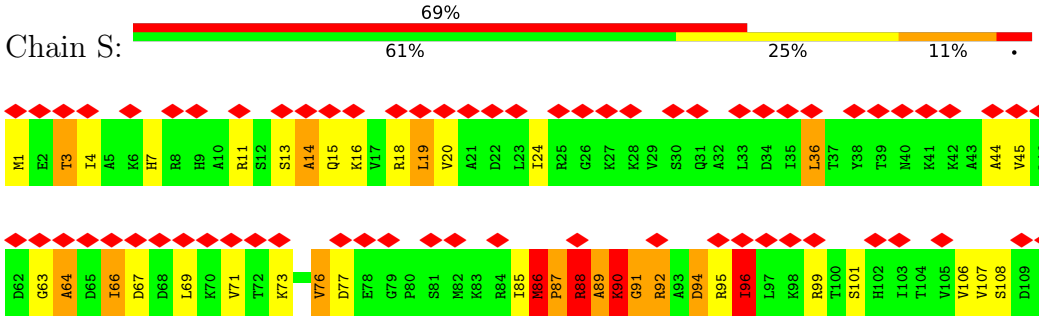

• Molecule 27: 50S RIBOSOMAL PROTEIN L21

Chain R:



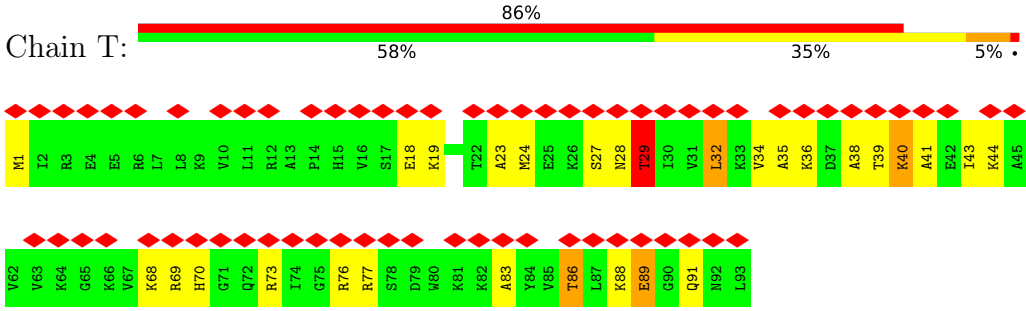

• Molecule 28: 50S RIBOSOMAL PROTEIN L22

Chain S:



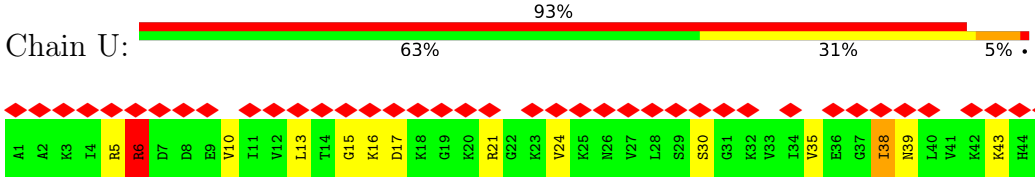

• Molecule 29: 50S RIBOSOMAL PROTEIN L23

Chain T:



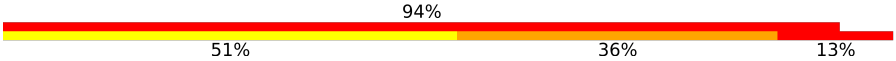

• Molecule 30: 50S RIBOSOMAL PROTEIN L24

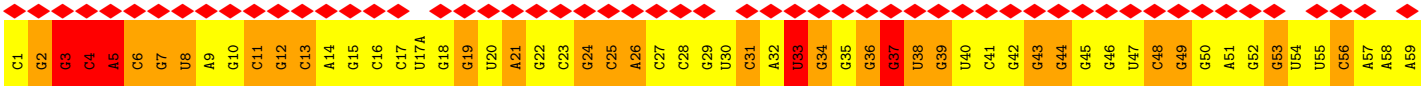
Chain U:




• Molecule 31: RNA

Chain V:

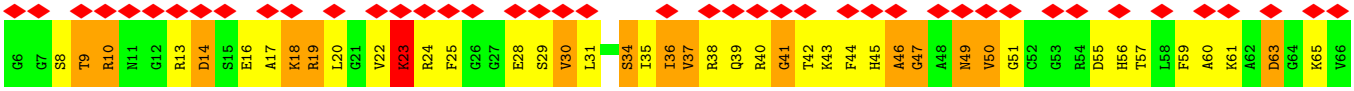




• Molecule 32: 50S RIBOSOMAL PROTEIN L27

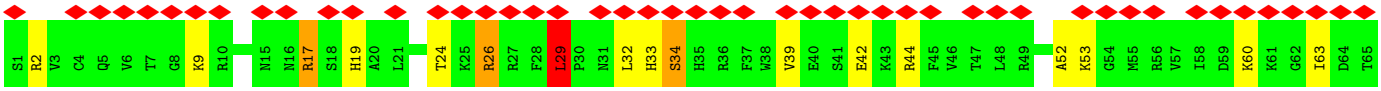
Chain W:

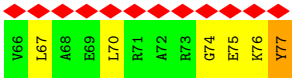





• Molecule 33: 50S RIBOSOMAL PROTEIN L28

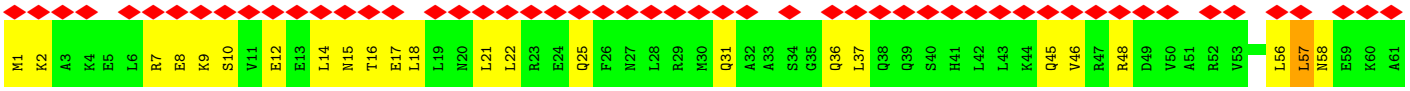
Chain X:


• Molecule 34: 50S RIBOSOMAL PROTEIN L29

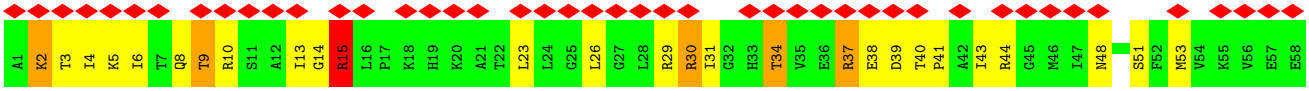
Chain Y:



• Molecule 35: 50S RIBOSOMAL PROTEIN L30

Chain Z:


A1
K2
T3
I4
K5
I6
T7
Q8
T9
R10
S11
A12
I13
G14
R15
L16
P17
K18
H19
K20
A21
T22
L23
L24
G25
L26
G27
L28
R29
R30
I31
G32
H33
T34
V35
E36
R37
E38
D39
T40
P41
A42
I43
R44
G45
M46
I47
M48
S51
F52
M53
V54
K55
V56
E57
E58

# 4 Experimental information (i)

| Property | Value | Source |
|---|---|---|
| EM reconstruction method | SINGLE PARTICLE | Depositor |
| Imposed symmetry | POINT, C1 | Depositor |
| Number of particles used | 72468 | Depositor |
| Resolution determination method | Not provided | |
| CTF correction method | MICROGRAPH | Depositor |
| Microscope | FEI TITAN KRIOS | Depositor |
| Voltage (kV) | 300 | Depositor |
| Electron dose ($e^-/Å^2$) | Not provided | |
| 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 | 3.354 | Depositor |
| Minimum map value | -2.711 | Depositor |
| Average map value | -0.001 | Depositor |
| Map value standard deviation | 0.183 | Depositor |
| Recommended contour level | 0.9 | Depositor |
| Map size (Å) | 404.80002, 404.80002, 404.80002 | wwPDB |
| Map dimensions | 368, 368, 368 | wwPDB |
| Map angles (°) | 90.0, 90.0, 90.0 | wwPDB |
| Pixel spacing (Å) | 1.1, 1.1, 1.1 | Depositor |

# 5 Model quality

## 5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: 5MU, MG, ZN

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 | 0 | 0.54 | 0/450 | 0.70 | 0/599 |
| 2 | 1 | 0.53 | 0/416 | 0.74 | 0/554 |
| 3 | 2 | 0.53 | 0/380 | 0.70 | 0/498 |
| 4 | 3 | 0.53 | 0/513 | 0.75 | 0/676 |
| 5 | 4 | 0.59 | 0/303 | 0.84 | 0/397 |
| 6 | 5 | 0.74 | 0/1131 | 1.32 | 26/1524 (1.7%) |
| 7 | 6 | 0.58 | 0/227 | 0.65 | 0/304 |
| 8 | 7 | 0.62 | 0/175 | 2.72 | 9/237 (3.8%) |
| 9 | 8 | 0.48 | 0/766 | 0.67 | 1/1025 (0.1%) |
| 10 | A | 0.81 | 19/68626 (0.0%) | 1.23 | 316/107056 (0.3%) |
| 11 | B | 0.66 | 0/2828 | 1.10 | 2/4410 (0.0%) |
| 12 | C | 0.54 | 0/2121 | 0.79 | 3/2852 (0.1%) |
| 13 | D | 0.57 | 0/1586 | 0.77 | 1/2134 (0.0%) |
| 14 | E | 0.53 | 0/1571 | 0.76 | 2/2113 (0.1%) |
| 15 | F | 0.50 | 0/1434 | 0.71 | 1/1926 (0.1%) |
| 16 | G | 0.55 | 0/1343 | 0.73 | 0/1816 |
| 17 | H | 0.53 | 0/389 | 0.73 | 0/523 |
| 18 | I | 0.62 | 0/1046 | 0.84 | 1/1410 (0.1%) |
| 19 | J | 0.63 | 1/1152 (0.1%) | 0.78 | 0/1551 |
| 20 | K | 0.65 | 1/947 (0.1%) | 0.77 | 0/1268 |
| 21 | L | 0.56 | 0/1054 | 0.79 | 2/1403 (0.1%) |
| 22 | M | 0.61 | 0/1093 | 0.77 | 0/1460 |
| 23 | N | 0.51 | 0/973 | 0.68 | 0/1301 |
| 24 | O | 0.46 | 0/902 | 0.70 | 0/1209 |
| 25 | P | 0.52 | 0/929 | 0.78 | 1/1242 (0.1%) |
| 26 | Q | 0.62 | 0/960 | 0.71 | 1/1278 (0.1%) |
| 27 | R | 0.61 | 1/829 (0.1%) | 0.76 | 0/1107 |
| 28 | S | 0.88 | 3/864 (0.3%) | 1.34 | 8/1156 (0.7%) |
| 29 | T | 0.55 | 0/744 | 0.85 | 1/994 (0.1%) |
| 30 | U | 0.56 | 0/787 | 0.78 | 0/1051 |
| 31 | V | 2.39 | 77/1820 (4.2%) | 2.84 | 254/2836 (9.0%) |
| 32 | W | 0.69 | 0/603 | 1.00 | 1/797 (0.1%) |

| Mol | Chain | Bond lengths | | Bond angles | |
|---|---|---|---|---|---|
| | | RMSZ | #\|Z\| >5 | RMSZ | #\|Z\| >5 |
| 33 | X | 0.50 | 0/635 | 0.79 | 1/848 (0.1%) |
| 34 | Y | 0.46 | 0/510 | 0.75 | 0/677 |
| 35 | Z | 0.54 | 0/453 | 0.84 | 1/605 (0.2%) |
| All | All | 0.81 | 102/100560 (0.1%) | 1.20 | 632/150837 (0.4%) |

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 |
|---|---|---|---|
| 6 | 5 | 0 | 1 |
| 8 | 7 | 0 | 4 |
| 12 | C | 0 | 1 |
| 13 | D | 0 | 1 |
| 19 | J | 0 | 1 |
| 20 | K | 0 | 1 |
| 28 | S | 0 | 3 |
| 31 | V | 0 | 13 |
| All | All | 0 | 25 |

All (102) bond length outliers are listed below:

| Mol | Chain | Res | Type | Atoms | Z | Observed(Å) | Ideal(Å) |
|---|---|---|---|---|---|---|---|
| 31 | V | 39 | G | N9-C4 | 15.38 | 1.50 | 1.38 |
| 31 | V | 69 | G | C6-N1 | 13.21 | 1.48 | 1.39 |
| 31 | V | 5 | A | C6-N1 | 12.91 | 1.44 | 1.35 |
| 31 | V | 39 | G | C2-N3 | 12.19 | 1.42 | 1.32 |
| 31 | V | 39 | G | N1-C2 | 11.42 | 1.46 | 1.37 |
| 31 | V | 5 | A | C6-N6 | 10.61 | 1.42 | 1.33 |
| 31 | V | 67 | G | N9-C4 | 10.41 | 1.46 | 1.38 |
| 31 | V | 67 | G | N7-C5 | 10.08 | 1.45 | 1.39 |
| 10 | A | 2602 | A | O3'-P | -10.05 | 1.49 | 1.61 |
| 31 | V | 37 | G | C2-N3 | 9.96 | 1.40 | 1.32 |
| 31 | V | 5 | A | N7-C5 | -9.68 | 1.33 | 1.39 |
| 31 | V | 70 | C | N1-C6 | 9.59 | 1.43 | 1.37 |
| 31 | V | 73 | A | N7-C5 | -9.48 | 1.33 | 1.39 |
| 31 | V | 1 | C | C2-N3 | 9.36 | 1.43 | 1.35 |
| 31 | V | 69 | G | N1-C2 | 8.94 | 1.45 | 1.37 |
| 31 | V | 7 | G | C8-N7 | -8.92 | 1.25 | 1.30 |
| 31 | V | 75 | C | N1-C6 | 8.64 | 1.42 | 1.37 |
| 10 | A | 984 | A | N9-C4 | -8.39 | 1.32 | 1.37 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(Å) | Ideal(Å) |
|---|---|---|---|---|---|---|---|
| 31 | V | 38 | U | C2'-C1' | -8.21 | 1.44 | 1.53 |
| 31 | V | 4 | C | C2-N3 | 8.17 | 1.42 | 1.35 |
| 31 | V | 70 | C | P-O5' | -8.07 | 1.51 | 1.59 |
| 31 | V | 32 | A | N9-C8 | 8.06 | 1.44 | 1.37 |
| 31 | V | 2 | G | C8-N7 | -7.99 | 1.26 | 1.30 |
| 31 | V | 73 | A | C5'-C4' | 7.93 | 1.60 | 1.51 |
| 31 | V | 76 | A | C5-C4 | -7.86 | 1.33 | 1.38 |
| 31 | V | 72 | G | C2'-C1' | -7.78 | 1.44 | 1.53 |
| 31 | V | 3 | G | O3'-P | -7.70 | 1.51 | 1.61 |
| 31 | V | 6 | C | C4-C5 | -7.62 | 1.36 | 1.43 |
| 31 | V | 72 | G | C2-N2 | 7.58 | 1.42 | 1.34 |
| 31 | V | 3 | G | N9-C4 | 7.54 | 1.44 | 1.38 |
| 31 | V | 33 | U | C4'-C3' | 7.43 | 1.61 | 1.53 |
| 31 | V | 32 | A | C4'-O4' | -7.18 | 1.36 | 1.45 |
| 31 | V | 13 | C | C4'-O4' | 7.09 | 1.54 | 1.45 |
| 31 | V | 75 | C | N3-C4 | 7.06 | 1.38 | 1.33 |
| 31 | V | 6 | C | C4-N4 | 6.79 | 1.40 | 1.33 |
| 31 | V | 76 | A | C6-N6 | 6.76 | 1.39 | 1.33 |
| 31 | V | 37 | G | C5-C4 | -6.65 | 1.33 | 1.38 |
| 10 | A | 528 | A | N9-C4 | -6.64 | 1.33 | 1.37 |
| 31 | V | 71 | C | C4'-O4' | 6.63 | 1.54 | 1.45 |
| 31 | V | 7 | G | N9-C8 | 6.57 | 1.42 | 1.37 |
| 31 | V | 3 | G | C2'-C1' | -6.55 | 1.46 | 1.53 |
| 10 | A | 1142 | A | N9-C4 | -6.53 | 1.33 | 1.37 |
| 31 | V | 32 | A | O3'-P | -6.47 | 1.53 | 1.61 |
| 31 | V | 38 | U | C4'-C3' | -6.46 | 1.46 | 1.53 |
| 31 | V | 68 | U | C4-O4 | -6.42 | 1.18 | 1.23 |
| 31 | V | 76 | A | C6-N1 | 6.33 | 1.40 | 1.35 |
| 31 | V | 34 | G | C3'-C2' | -6.33 | 1.45 | 1.52 |
| 31 | V | 5 | A | C2-N3 | 6.29 | 1.39 | 1.33 |
| 31 | V | 1 | C | C2-O2 | 6.24 | 1.30 | 1.24 |
| 10 | A | 1569 | A | N9-C4 | -6.22 | 1.34 | 1.37 |
| 31 | V | 76 | A | C8-N7 | -6.21 | 1.27 | 1.31 |
| 31 | V | 32 | A | N9-C4 | 6.18 | 1.41 | 1.37 |
| 31 | V | 2 | G | N9-C4 | 6.15 | 1.42 | 1.38 |
| 10 | A | 2504 | U | C4-O4 | 6.14 | 1.28 | 1.23 |
| 10 | A | 783 | A | N3-C4 | -6.07 | 1.31 | 1.34 |
| 10 | A | 783 | A | N9-C4 | -6.02 | 1.34 | 1.37 |
| 31 | V | 5 | A | N1-C2 | -5.91 | 1.29 | 1.34 |
| 31 | V | 5 | A | C5-C6 | 5.85 | 1.46 | 1.41 |
| 10 | A | 1073 | A | C5-C6 | 5.84 | 1.46 | 1.41 |
| 28 | S | 88 | ARG | CA-C | -5.81 | 1.37 | 1.52 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(Å) | Ideal(Å) |
|---|---|---|---|---|---|---|---|
| 10 | A | 2504 | U | N3-C4 | 5.79 | 1.43 | 1.38 |
| 31 | V | 69 | G | C8-N7 | -5.77 | 1.27 | 1.30 |
| 31 | V | 70 | C | O3'-P | 5.75 | 1.68 | 1.61 |
| 31 | V | 76 | A | N1-C2 | -5.74 | 1.29 | 1.34 |
| 31 | V | 2 | G | C4'-C3' | -5.71 | 1.46 | 1.52 |
| 31 | V | 7 | G | P-O5' | -5.71 | 1.54 | 1.59 |
| 31 | V | 6 | C | C3'-C2' | 5.67 | 1.59 | 1.52 |
| 19 | J | 44 | TYR | CD2-CE2 | -5.64 | 1.30 | 1.39 |
| 31 | V | 4 | C | C4'-C3' | 5.64 | 1.59 | 1.53 |
| 31 | V | 1 | C | C3'-C2' | -5.62 | 1.46 | 1.52 |
| 31 | V | 32 | A | C3'-C2' | 5.58 | 1.59 | 1.52 |
| 31 | V | 76 | A | N9-C4 | 5.56 | 1.41 | 1.37 |
| 31 | V | 69 | G | C5-C6 | -5.56 | 1.36 | 1.42 |
| 10 | A | 2504 | U | C2-N3 | 5.55 | 1.41 | 1.37 |
| 10 | A | 783 | A | N7-C5 | -5.53 | 1.35 | 1.39 |
| 31 | V | 68 | U | C2'-C1' | -5.50 | 1.47 | 1.53 |
| 31 | V | 38 | U | N1-C6 | 5.50 | 1.42 | 1.38 |
| 10 | A | 528 | A | N3-C4 | -5.49 | 1.31 | 1.34 |
| 31 | V | 4 | C | O4'-C1' | -5.46 | 1.34 | 1.41 |
| 10 | A | 1142 | A | C5-C6 | -5.44 | 1.36 | 1.41 |
| 31 | V | 67 | G | P-O5' | -5.41 | 1.54 | 1.59 |
| 31 | V | 72 | G | O3'-P | -5.39 | 1.54 | 1.61 |
| 31 | V | 36 | G | C4'-C3' | -5.38 | 1.47 | 1.52 |
| 27 | R | 86 | GLN | CB-CG | 5.38 | 1.67 | 1.52 |
| 31 | V | 67 | G | C5-C4 | -5.34 | 1.34 | 1.38 |
| 31 | V | 73 | A | N3-C4 | -5.32 | 1.31 | 1.34 |
| 28 | S | 86 | MET | CA-C | -5.25 | 1.39 | 1.52 |
| 31 | V | 37 | G | C2'-C1' | -5.25 | 1.47 | 1.53 |
| 20 | K | 21 | CYS | CB-SG | -5.24 | 1.73 | 1.81 |
| 10 | A | 2478 | A | N9-C4 | -5.20 | 1.34 | 1.37 |
| 31 | V | 70 | C | O4'-C1' | 5.20 | 1.48 | 1.41 |
| 10 | A | 2053 | G | C6-O6 | 5.16 | 1.28 | 1.24 |
| 10 | A | 783 | A | C5-C6 | -5.14 | 1.36 | 1.41 |
| 28 | S | 91 | GLY | C-O | -5.12 | 1.15 | 1.23 |
| 31 | V | 7 | G | C2'-C1' | -5.11 | 1.47 | 1.53 |
| 10 | A | 1321 | A | N9-C4 | 5.08 | 1.40 | 1.37 |
| 31 | V | 4 | C | C2-O2 | 5.05 | 1.28 | 1.24 |
| 31 | V | 4 | C | N1-C6 | -5.05 | 1.34 | 1.37 |
| 10 | A | 2015 | A | N3-C4 | -5.04 | 1.31 | 1.34 |
| 31 | V | 5 | A | C8-N7 | 5.03 | 1.35 | 1.31 |
| 31 | V | 7 | G | N3-C4 | 5.03 | 1.39 | 1.35 |
| 31 | V | 73 | A | C2-N3 | 5.00 | 1.38 | 1.33 |

All (632) bond angle outliers are listed below:

| Mol | Chain | Res | Type | Atoms | Z | Observed($^o$) | Ideal($^o$) |
|---|---|---|---|---|---|---|---|
| 28 | S | 86 | MET | C-N-CD | -30.06 | 54.48 | 120.60 |
| 31 | V | 73 | A | N1-C6-N6 | 22.84 | 132.30 | 118.60 |
| 10 | A | 1073 | A | N1-C6-N6 | -19.93 | 106.64 | 118.60 |
| 31 | V | 69 | G | N1-C6-O6 | 19.71 | 131.73 | 119.90 |
| 31 | V | 69 | G | C5-C6-O6 | -19.59 | 116.85 | 128.60 |
| 8 | 7 | 14 | ASN | N-CA-CB | 15.73 | 138.91 | 110.60 |
| 31 | V | 73 | A | C5-C6-N6 | -15.38 | 111.40 | 123.70 |
| 8 | 7 | 5 | HIS | CB-CA-C | 14.92 | 140.24 | 110.40 |
| 10 | A | 2608 | G | C4'-C3'-O3' | 14.21 | 141.42 | 113.00 |
| 10 | A | 1073 | A | C5-C6-N6 | 14.10 | 134.98 | 123.70 |
| 8 | 7 | 23 | ARG | O-C-N | 14.06 | 147.82 | 121.10 |
| 8 | 7 | 5 | HIS | N-CA-C | -14.01 | 73.17 | 111.00 |
| 10 | A | 2053 | G | N1-C6-O6 | 13.74 | 128.15 | 119.90 |
| 31 | V | 2 | G | N1-C6-O6 | 13.60 | 128.06 | 119.90 |
| 31 | V | 3 | G | C6-C5-N7 | -13.52 | 122.29 | 130.40 |
| 31 | V | 4 | C | N3-C4-N4 | 13.28 | 127.30 | 118.00 |
| 31 | V | 70 | C | O4'-C1'-N1 | 13.17 | 118.74 | 108.20 |
| 31 | V | 67 | G | N1-C6-O6 | 13.17 | 127.80 | 119.90 |
| 10 | A | 2504 | U | N3-C4-O4 | 13.00 | 128.50 | 119.40 |
| 8 | 7 | 23 | ARG | C-N-CD | 12.74 | 155.15 | 128.40 |
| 31 | V | 4 | C | C5-C4-N4 | -12.69 | 111.32 | 120.20 |
| 31 | V | 39 | G | C8-N9-C4 | -12.66 | 101.34 | 106.40 |
| 31 | V | 6 | C | C6-N1-C2 | -12.57 | 115.27 | 120.30 |
| 31 | V | 26 | A | N1-C6-N6 | 12.56 | 126.14 | 118.60 |
| 10 | A | 2585 | U | C4'-C3'-O3' | -12.52 | 83.11 | 109.40 |
| 8 | 7 | 14 | ASN | CB-CA-C | -12.40 | 85.61 | 110.40 |
| 31 | V | 21 | A | N1-C6-N6 | 12.31 | 125.98 | 118.60 |
| 31 | V | 51 | A | N1-C6-N6 | 12.31 | 125.98 | 118.60 |
| 31 | V | 5 | A | O4'-C1'-N9 | 12.29 | 118.03 | 108.20 |
| 31 | V | 14 | A | N1-C6-N6 | 12.27 | 125.96 | 118.60 |
| 31 | V | 9 | A | N1-C6-N6 | 12.26 | 125.95 | 118.60 |
| 10 | A | 984 | A | C2-N3-C4 | -12.10 | 104.55 | 110.60 |
| 31 | V | 57 | A | N1-C6-N6 | 12.04 | 125.82 | 118.60 |
| 31 | V | 7 | G | N3-C2-N2 | 12.03 | 128.32 | 119.90 |
| 31 | V | 58 | A | N1-C6-N6 | 11.84 | 125.70 | 118.60 |
| 10 | A | 961 | C | O5'-P-OP2 | -11.83 | 95.06 | 105.70 |
| 10 | A | 2053 | G | C6-C5-N7 | -11.60 | 123.44 | 130.40 |
| 31 | V | 72 | G | P-O3'-C3' | 11.52 | 133.53 | 119.70 |
| 31 | V | 32 | A | P-O3'-C3' | 11.47 | 133.47 | 119.70 |
| 31 | V | 59 | A | N1-C6-N6 | 11.46 | 125.47 | 118.60 |
| 10 | A | 1073 | A | C6-C5-N7 | 11.39 | 140.28 | 132.30 |
| 10 | A | 2053 | G | C5-C6-N1 | -11.34 | 105.83 | 111.50 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed($^o$) | Ideal($^o$) |
|---|---|---|---|---|---|---|---|
| 10 | A | 1073 | A | C4-C5-N7 | -11.26 | 105.07 | 110.70 |
| 10 | A | 751 | A | C4'-C3'-O3' | 11.22 | 135.44 | 113.00 |
| 31 | V | 69 | G | O4'-C1'-N9 | 11.19 | 117.15 | 108.20 |
| 31 | V | 67 | G | C5-C6-O6 | -11.00 | 122.00 | 128.60 |
| 31 | V | 6 | C | C5-C6-N1 | 10.95 | 126.47 | 121.00 |
| 31 | V | 5 | A | N1-C6-N6 | 10.94 | 125.17 | 118.60 |
| 8 | 7 | 16 | ASP | N-CA-CB | -10.85 | 91.07 | 110.60 |
| 10 | A | 783 | A | C5-N7-C8 | -10.72 | 98.54 | 103.90 |
| 10 | A | 2504 | U | C5-C6-N1 | 10.55 | 127.98 | 122.70 |
| 10 | A | 974 | G | C6-C5-N7 | -10.49 | 124.11 | 130.40 |
| 10 | A | 2586 | U | C4'-C3'-O3' | -10.43 | 87.49 | 109.40 |
| 10 | A | 2053 | G | C4-C5-C6 | 10.13 | 124.88 | 118.80 |
| 31 | V | 37 | G | N3-C4-C5 | -10.01 | 123.60 | 128.60 |
| 31 | V | 33 | U | P-O3'-C3' | 9.89 | 131.57 | 119.70 |
| 10 | A | 2504 | U | C6-N1-C2 | -9.85 | 115.09 | 121.00 |
| 31 | V | 53 | G | N1-C6-O6 | 9.79 | 125.77 | 119.90 |
| 10 | A | 974 | G | C4-C5-N7 | 9.78 | 114.71 | 110.80 |
| 31 | V | 34 | G | P-O5'-C5' | 9.76 | 136.52 | 120.90 |
| 31 | V | 4 | C | O4'-C1'-N1 | 9.74 | 115.99 | 108.20 |
| 31 | V | 7 | G | P-O3'-C3' | 9.69 | 131.33 | 119.70 |
| 10 | A | 783 | A | N7-C8-N9 | 9.65 | 118.62 | 113.80 |
| 6 | 5 | 92 | ALA | C-N-CA | 9.60 | 145.69 | 121.70 |
| 31 | V | 10 | G | N1-C6-O6 | 9.56 | 125.64 | 119.90 |
| 31 | V | 32 | A | N7-C8-N9 | -9.55 | 109.03 | 113.80 |
| 31 | V | 65 | U | P-O3'-C3' | 9.41 | 130.99 | 119.70 |
| 31 | V | 22 | G | N1-C6-O6 | 9.39 | 125.54 | 119.90 |
| 8 | 7 | 23 | ARG | CA-C-N | -9.35 | 90.93 | 117.10 |
| 10 | A | 1534 | U | C2-N1-C1' | 9.33 | 128.90 | 117.70 |
| 31 | V | 37 | G | C2-N3-C4 | 9.32 | 116.56 | 111.90 |
| 31 | V | 46 | G | N1-C6-O6 | 9.32 | 125.49 | 119.90 |
| 10 | A | 528 | A | C2-N3-C4 | -9.32 | 105.94 | 110.60 |
| 28 | S | 88 | ARG | N-CA-C | -9.28 | 85.94 | 111.00 |
| 10 | A | 1073 | A | C5-N7-C8 | 9.28 | 108.54 | 103.90 |
| 31 | V | 72 | G | O4'-C1'-N9 | 9.21 | 115.57 | 108.20 |
| 31 | V | 43 | G | N1-C6-O6 | 9.18 | 125.41 | 119.90 |
| 31 | V | 39 | G | N3-C4-C5 | -9.16 | 124.02 | 128.60 |
| 31 | V | 31 | C | O4'-C1'-N1 | 9.08 | 115.47 | 108.20 |
| 6 | 5 | 93 | ALA | C-N-CA | 9.07 | 144.38 | 121.70 |
| 31 | V | 50 | G | N1-C6-O6 | 9.00 | 125.30 | 119.90 |
| 31 | V | 39 | G | C6-C5-N7 | -8.97 | 125.02 | 130.40 |
| 31 | V | 15 | G | N1-C6-O6 | 8.96 | 125.28 | 119.90 |
| 31 | V | 24 | G | N1-C6-O6 | 8.87 | 125.22 | 119.90 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed($^o$) | Ideal($^o$) |
|---|---|---|---|---|---|---|---|
| 10 | A | 465 | G | C8-N9-C4 | -8.86 | 102.85 | 106.40 |
| 31 | V | 37 | G | O4'-C1'-N9 | 8.86 | 115.28 | 108.20 |
| 31 | V | 42 | G | N1-C6-O6 | 8.85 | 125.21 | 119.90 |
| 10 | A | 1950 | G | N1-C6-O6 | 8.84 | 125.21 | 119.90 |
| 31 | V | 74 | C | O4'-C1'-N1 | 8.83 | 115.26 | 108.20 |
| 10 | A | 783 | A | C8-N9-C4 | -8.82 | 102.27 | 105.80 |
| 31 | V | 29 | G | N1-C6-O6 | 8.79 | 125.17 | 119.90 |
| 10 | A | 2061 | G | C4'-C3'-O3' | -8.74 | 91.04 | 109.40 |
| 31 | V | 52 | G | N1-C6-O6 | 8.72 | 125.13 | 119.90 |
| 31 | V | 12 | G | N1-C6-O6 | 8.69 | 125.11 | 119.90 |
| 31 | V | 44 | G | N1-C6-O6 | 8.66 | 125.10 | 119.90 |
| 10 | A | 1073 | A | N9-C4-C5 | 8.65 | 109.26 | 105.80 |
| 10 | A | 2534 | A | N1-C6-N6 | 8.64 | 123.78 | 118.60 |
| 31 | V | 39 | G | O4'-C1'-N9 | 8.63 | 115.11 | 108.20 |
| 31 | V | 45 | G | N1-C6-O6 | 8.61 | 125.07 | 119.90 |
| 31 | V | 73 | A | C5'-C4'-C3' | 8.59 | 129.74 | 116.00 |
| 10 | A | 2074 | U | O5'-P-OP2 | -8.53 | 98.02 | 105.70 |
| 31 | V | 18 | G | N1-C6-O6 | 8.51 | 125.01 | 119.90 |
| 10 | A | 1533 | C | N1-C2-O2 | 8.51 | 124.01 | 118.90 |
| 31 | V | 2 | G | C5-C6-O6 | -8.48 | 123.51 | 128.60 |
| 10 | A | 1936 | A | C2-N3-C4 | -8.47 | 106.36 | 110.60 |
| 10 | A | 1533 | C | C2-N1-C1' | 8.46 | 128.10 | 118.80 |
| 10 | A | 974 | G | C4-N9-C1' | 8.43 | 137.46 | 126.50 |
| 10 | A | 2572 | A | N1-C6-N6 | 8.36 | 123.61 | 118.60 |
| 31 | V | 19 | G | N1-C6-O6 | 8.35 | 124.91 | 119.90 |
| 31 | V | 34 | G | OP1-P-OP2 | -8.35 | 107.07 | 119.60 |
| 31 | V | 3 | G | N1-C2-N3 | -8.35 | 118.89 | 123.90 |
| 10 | A | 1142 | A | C2-N3-C4 | -8.29 | 106.46 | 110.60 |
| 31 | V | 56 | C | O4'-C1'-N1 | 8.27 | 114.81 | 108.20 |
| 31 | V | 39 | G | C6-N1-C2 | -8.24 | 120.16 | 125.10 |
| 31 | V | 49 | G | N1-C6-O6 | 8.22 | 124.83 | 119.90 |
| 6 | 5 | 27 | VAL | CG1-CB-CG2 | 8.21 | 124.03 | 110.90 |
| 31 | V | 25 | C | O4'-C1'-N1 | 8.12 | 114.69 | 108.20 |
| 10 | A | 586 | A | O5'-P-OP1 | -8.08 | 98.42 | 105.70 |
| 31 | V | 53 | G | C5-C6-O6 | -8.07 | 123.76 | 128.60 |
| 31 | V | 61 | C | O4'-C1'-N1 | 8.06 | 114.65 | 108.20 |
| 10 | A | 1533 | C | C6-N1-C2 | -8.04 | 117.08 | 120.30 |
| 13 | D | 151 | THR | C-N-CD | 7.99 | 145.17 | 128.40 |
| 31 | V | 65 | U | O4'-C1'-N1 | 7.98 | 114.58 | 108.20 |
| 31 | V | 39 | G | C4-C5-C6 | 7.96 | 123.58 | 118.80 |
| 31 | V | 11 | C | O4'-C1'-N1 | 7.96 | 114.57 | 108.20 |
| 10 | A | 1795 | C | C6-N1-C2 | -7.94 | 117.12 | 120.30 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed($^o$) | Ideal($^o$) |
|---|---|---|---|---|---|---|---|
| 31 | V | 62 | C | O4'-C1'-N1 | 7.93 | 114.54 | 108.20 |
| 10 | A | 783 | A | C4-C5-N7 | 7.92 | 114.66 | 110.70 |
| 10 | A | 2609 | U | C5'-C4'-O4' | 7.92 | 118.61 | 109.10 |
| 10 | A | 2609 | U | O4'-C1'-N1 | 7.91 | 114.53 | 108.20 |
| 28 | S | 86 | MET | N-CA-C | -7.89 | 89.70 | 111.00 |
| 10 | A | 984 | A | N3-C4-C5 | 7.85 | 132.29 | 126.80 |
| 31 | V | 71 | C | O4'-C1'-N1 | 7.80 | 114.44 | 108.20 |
| 31 | V | 27 | C | O4'-C1'-N1 | 7.78 | 114.43 | 108.20 |
| 31 | V | 64 | C | O4'-C1'-N1 | 7.77 | 114.42 | 108.20 |
| 31 | V | 70 | C | N1-C2-O2 | 7.76 | 123.55 | 118.90 |
| 31 | V | 10 | G | C5-C6-O6 | -7.72 | 123.97 | 128.60 |
| 31 | V | 23 | C | O4'-C1'-N1 | 7.71 | 114.37 | 108.20 |
| 31 | V | 46 | G | C5-C6-O6 | -7.70 | 123.98 | 128.60 |
| 10 | A | 1478 | G | N1-C6-O6 | 7.70 | 124.52 | 119.90 |
| 10 | A | 2504 | U | N3-C4-C5 | -7.69 | 109.99 | 114.60 |
| 10 | A | 465 | G | N3-C4-C5 | -7.68 | 124.76 | 128.60 |
| 6 | 5 | 51 | TYR | C-N-CA | 7.68 | 140.90 | 121.70 |
| 10 | A | 2609 | U | P-O5'-C5' | 7.68 | 133.19 | 120.90 |
| 10 | A | 2053 | G | C4-N9-C1' | 7.67 | 136.47 | 126.50 |
| 6 | 5 | 49 | GLY | C-N-CA | 7.66 | 140.86 | 121.70 |
| 31 | V | 20 | U | O4'-C1'-N1 | 7.63 | 114.31 | 108.20 |
| 6 | 5 | 123 | ILE | CG1-CB-CG2 | 7.62 | 128.17 | 111.40 |
| 31 | V | 28 | C | O4'-C1'-N1 | 7.60 | 114.28 | 108.20 |
| 10 | A | 2146 | C | N3-C4-C5 | -7.60 | 118.86 | 121.90 |
| 10 | A | 974 | G | C8-N9-C1' | -7.60 | 117.13 | 127.00 |
| 10 | A | 2053 | G | C2-N3-C4 | -7.57 | 108.11 | 111.90 |
| 31 | V | 30 | U | O4'-C1'-N1 | 7.56 | 114.25 | 108.20 |
| 31 | V | 41 | C | O4'-C1'-N1 | 7.56 | 114.25 | 108.20 |
| 10 | A | 783 | A | N1-C6-N6 | 7.56 | 123.13 | 118.60 |
| 6 | 5 | 119 | PRO | C-N-CA | 7.54 | 140.56 | 121.70 |
| 14 | E | 44 | ARG | NE-CZ-NH1 | 7.51 | 124.06 | 120.30 |
| 32 | W | 76 | ARG | NE-CZ-NH1 | 7.48 | 124.04 | 120.30 |
| 10 | A | 1839 | G | N1-C6-O6 | 7.48 | 124.39 | 119.90 |
| 10 | A | 783 | A | C6-C5-N7 | -7.48 | 127.07 | 132.30 |
| 10 | A | 776 | G | C5-C6-O6 | 7.46 | 133.08 | 128.60 |
| 31 | V | 2 | G | C6-N1-C2 | 7.45 | 129.57 | 125.10 |
| 31 | V | 17 | C | O4'-C1'-N1 | 7.44 | 114.16 | 108.20 |
| 31 | V | 76 | A | C8-N9-C4 | -7.39 | 102.84 | 105.80 |
| 6 | 5 | 72 | LEU | C-N-CA | 7.36 | 140.09 | 121.70 |
| 31 | V | 22 | G | C5-C6-O6 | -7.36 | 124.19 | 128.60 |
| 31 | V | 43 | G | C5-C6-O6 | -7.35 | 124.19 | 128.60 |
| 10 | A | 1533 | C | N3-C2-O2 | -7.32 | 116.77 | 121.90 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed($^o$) | Ideal($^o$) |
|---|---|---|---|---|---|---|---|
| 10 | A | 2504 | U | C5-C4-O4 | -7.32 | 121.51 | 125.90 |
| 6 | 5 | 81 | LEU | CB-CG-CD2 | 7.29 | 123.39 | 111.00 |
| 31 | V | 3 | G | N3-C2-N2 | 7.28 | 125.00 | 119.90 |
| 10 | A | 1073 | A | O5'-P-OP2 | 7.28 | 119.43 | 110.70 |
| 10 | A | 974 | G | C5-N7-C8 | -7.27 | 100.67 | 104.30 |
| 31 | V | 3 | G | C2-N3-C4 | 7.24 | 115.52 | 111.90 |
| 10 | A | 1534 | U | C6-N1-C1' | -7.23 | 111.08 | 121.20 |
| 10 | A | 2447 | G | O5'-P-OP1 | -7.20 | 99.22 | 105.70 |
| 31 | V | 63 | U | O4'-C1'-N1 | 7.19 | 113.95 | 108.20 |
| 10 | A | 2501 | C | C2-N1-C1' | -7.19 | 110.89 | 118.80 |
| 10 | A | 2602 | A | C4'-C3'-O3' | -7.19 | 94.31 | 109.40 |
| 10 | A | 2053 | G | N1-C2-N3 | 7.17 | 128.20 | 123.90 |
| 10 | A | 1950 | G | C6-C5-N7 | -7.16 | 126.11 | 130.40 |
| 10 | A | 2053 | G | C8-N9-C1' | -7.15 | 117.70 | 127.00 |
| 31 | V | 15 | G | C5-C6-O6 | -7.15 | 124.31 | 128.60 |
| 6 | 5 | 28 | ALA | C-N-CA | 7.14 | 139.55 | 121.70 |
| 31 | V | 37 | G | C4-C5-C6 | 7.12 | 123.07 | 118.80 |
| 31 | V | 75 | C | N3-C4-C5 | -7.11 | 119.06 | 121.90 |
| 31 | V | 1 | C | N3-C4-N4 | 7.09 | 122.96 | 118.00 |
| 28 | S | 94 | ASP | N-CA-C | -7.09 | 91.87 | 111.00 |
| 10 | A | 2250 | G | C6-C5-N7 | -7.08 | 126.15 | 130.40 |
| 10 | A | 1142 | A | N1-C6-N6 | 7.07 | 122.84 | 118.60 |
| 10 | A | 776 | G | C5-C6-N1 | -7.05 | 107.98 | 111.50 |
| 31 | V | 66 | C | N3-C4-C5 | -7.05 | 119.08 | 121.90 |
| 31 | V | 8 | U | O4'-C1'-N1 | 7.04 | 113.84 | 108.20 |
| 6 | 5 | 47 | GLU | C-N-CA | 7.04 | 139.29 | 121.70 |
| 6 | 5 | 54 | VAL | CG1-CB-CG2 | 7.00 | 122.10 | 110.90 |
| 31 | V | 37 | G | N1-C2-N3 | -7.00 | 119.70 | 123.90 |
| 31 | V | 67 | G | C4-C5-C6 | 6.99 | 123.00 | 118.80 |
| 10 | A | 2423 | U | P-O3'-C3' | 6.99 | 128.09 | 119.70 |
| 31 | V | 7 | G | OP1-P-O3' | 6.97 | 120.54 | 105.20 |
| 31 | V | 7 | G | N1-C2-N3 | -6.97 | 119.72 | 123.90 |
| 10 | A | 2503 | A | C5-C6-N6 | -6.97 | 118.12 | 123.70 |
| 10 | A | 984 | A | N3-C4-N9 | -6.96 | 121.83 | 127.40 |
| 10 | A | 2448 | A | N1-C6-N6 | 6.96 | 122.78 | 118.60 |
| 10 | A | 802 | A | N1-C6-N6 | -6.96 | 114.42 | 118.60 |
| 31 | V | 50 | G | C5-C6-O6 | -6.96 | 124.42 | 128.60 |
| 31 | V | 2 | G | C6-C5-N7 | -6.95 | 126.23 | 130.40 |
| 28 | S | 91 | GLY | N-CA-C | -6.94 | 95.76 | 113.10 |
| 10 | A | 2602 | A | P-O3'-C3' | 6.93 | 128.02 | 119.70 |
| 10 | A | 1284 | A | O5'-P-OP2 | -6.92 | 99.47 | 105.70 |
| 31 | V | 37 | G | C8-N9-C4 | -6.90 | 103.64 | 106.40 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed($^o$) | Ideal($^o$) |
|---|---|---|---|---|---|---|---|
| 31 | V | 3 | G | O4'-C1'-N9 | 6.89 | 113.71 | 108.20 |
| 31 | V | 60 | U | O4'-C1'-N1 | 6.89 | 113.71 | 108.20 |
| 10 | A | 1378 | A | P-O3'-C3' | 6.89 | 127.96 | 119.70 |
| 10 | A | 1935 | G | O5'-P-OP2 | -6.89 | 99.50 | 105.70 |
| 28 | S | 90 | LYS | N-CA-C | -6.89 | 92.41 | 111.00 |
| 10 | A | 2250 | G | N1-C6-O6 | 6.88 | 124.03 | 119.90 |
| 31 | V | 67 | G | C6-C5-N7 | -6.88 | 126.27 | 130.40 |
| 10 | A | 2504 | U | C2-N1-C1' | 6.88 | 125.95 | 117.70 |
| 10 | A | 1839 | G | C6-C5-N7 | -6.87 | 126.28 | 130.40 |
| 10 | A | 1654 | A | O5'-P-OP1 | -6.85 | 99.53 | 105.70 |
| 10 | A | 974 | G | N1-C6-O6 | 6.83 | 124.00 | 119.90 |
| 10 | A | 2681 | C | C6-N1-C2 | 6.83 | 123.03 | 120.30 |
| 31 | V | 42 | G | C5-C6-O6 | -6.82 | 124.51 | 128.60 |
| 31 | V | 76 | A | N1-C6-N6 | 6.81 | 122.69 | 118.60 |
| 10 | A | 783 | A | C2-N3-C4 | -6.79 | 107.20 | 110.60 |
| 31 | V | 12 | G | C5-C6-O6 | -6.77 | 124.54 | 128.60 |
| 10 | A | 1192 | G | C8-N9-C4 | 6.76 | 109.10 | 106.40 |
| 10 | A | 503 | A | C8-N9-C4 | -6.76 | 103.10 | 105.80 |
| 31 | V | 14 | A | C4-C5-C6 | 6.76 | 120.38 | 117.00 |
| 8 | 7 | 23 | ARG | C-N-CA | -6.74 | 93.68 | 122.00 |
| 10 | A | 974 | G | N3-C4-N9 | 6.74 | 130.04 | 126.00 |
| 10 | A | 1815 | A | N9-C4-C5 | 6.74 | 108.50 | 105.80 |
| 10 | A | 12 | U | N3-C2-O2 | -6.73 | 117.49 | 122.20 |
| 10 | A | 974 | G | C5-C6-O6 | -6.73 | 124.56 | 128.60 |
| 21 | L | 19 | LEU | CA-CB-CG | 6.72 | 130.75 | 115.30 |
| 31 | V | 47 | U | O4'-C1'-N1 | 6.70 | 113.56 | 108.20 |
| 31 | V | 69 | G | N3-C4-C5 | 6.70 | 131.95 | 128.60 |
| 31 | V | 6 | C | C4'-C3'-C2' | -6.69 | 95.91 | 102.60 |
| 10 | A | 974 | G | N7-C8-N9 | 6.69 | 116.44 | 113.10 |
| 10 | A | 1311 | G | C8-N9-C4 | -6.69 | 103.72 | 106.40 |
| 31 | V | 52 | G | C5-C6-O6 | -6.69 | 124.59 | 128.60 |
| 31 | V | 29 | G | C5-C6-O6 | -6.68 | 124.59 | 128.60 |
| 10 | A | 2823 | A | C8-N9-C4 | -6.66 | 103.14 | 105.80 |
| 31 | V | 1 | C | O4'-C1'-N1 | 6.65 | 113.52 | 108.20 |
| 31 | V | 36 | G | P-O5'-C5' | -6.65 | 110.26 | 120.90 |
| 15 | F | 94 | ARG | NE-CZ-NH1 | 6.65 | 123.62 | 120.30 |
| 10 | A | 974 | G | N9-C4-C5 | -6.62 | 102.75 | 105.40 |
| 31 | V | 3 | G | N9-C4-C5 | -6.60 | 102.76 | 105.40 |
| 31 | V | 45 | G | C5-C6-O6 | -6.60 | 124.64 | 128.60 |
| 10 | A | 528 | A | N1-C6-N6 | 6.59 | 122.56 | 118.60 |
| 31 | V | 39 | G | N3-C4-N9 | 6.58 | 129.95 | 126.00 |
| 31 | V | 48 | C | O4'-C1'-N1 | 6.58 | 113.46 | 108.20 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed($^o$) | Ideal($^o$) |
|---|---|---|---|---|---|---|---|
| 12 | C | 233 | GLY | N-CA-C | -6.58 | 96.66 | 113.10 |
| 31 | V | 44 | G | C5-C6-O6 | -6.57 | 124.66 | 128.60 |
| 10 | A | 2146 | C | C2-N3-C4 | 6.55 | 123.18 | 119.90 |
| 10 | A | 670 | A | O4'-C1'-N9 | -6.54 | 102.97 | 108.20 |
| 31 | V | 24 | G | C5-C6-O6 | -6.53 | 124.68 | 128.60 |
| 31 | V | 69 | G | N9-C4-C5 | -6.51 | 102.80 | 105.40 |
| 31 | V | 40 | U | O4'-C1'-N1 | 6.49 | 113.39 | 108.20 |
| 6 | 5 | 147 | SER | C-N-CA | 6.48 | 137.90 | 121.70 |
| 6 | 5 | 84 | TYR | C-N-CA | 6.46 | 137.85 | 121.70 |
| 10 | A | 820 | A | O5'-P-OP1 | -6.46 | 99.88 | 105.70 |
| 10 | A | 1263 | U | N3-C4-C5 | -6.46 | 110.73 | 114.60 |
| 31 | V | 55 | U | O4'-C1'-N1 | 6.45 | 113.36 | 108.20 |
| 31 | V | 21 | A | C4-C5-C6 | 6.45 | 120.23 | 117.00 |
| 31 | V | 3 | G | P-O5'-C5' | -6.44 | 110.59 | 120.90 |
| 6 | 5 | 40 | GLU | C-N-CA | 6.43 | 137.77 | 121.70 |
| 31 | V | 72 | G | N3-C2-N2 | 6.42 | 124.39 | 119.90 |
| 31 | V | 19 | G | C5-C6-O6 | -6.41 | 124.76 | 128.60 |
| 31 | V | 69 | G | C5-N7-C8 | 6.40 | 107.50 | 104.30 |
| 31 | V | 6 | C | C2-N3-C4 | 6.39 | 123.10 | 119.90 |
| 10 | A | 2689 | U | C5-C4-O4 | 6.39 | 129.73 | 125.90 |
| 10 | A | 404 | A | P-O3'-C3' | 6.39 | 127.37 | 119.70 |
| 14 | E | 44 | ARG | NE-CZ-NH2 | -6.39 | 117.11 | 120.30 |
| 31 | V | 39 | G | N7-C8-N9 | 6.39 | 116.29 | 113.10 |
| 10 | A | 2551 | C | OP2-P-O3' | 6.37 | 119.22 | 105.20 |
| 31 | V | 6 | C | O4'-C1'-N1 | 6.37 | 113.30 | 108.20 |
| 6 | 5 | 50 | VAL | C-N-CA | 6.36 | 137.59 | 121.70 |
| 31 | V | 5 | A | C5'-C4'-C3' | 6.35 | 126.16 | 116.00 |
| 31 | V | 58 | A | C4-C5-C6 | 6.35 | 120.18 | 117.00 |
| 28 | S | 85 | ILE | O-C-N | -6.34 | 112.55 | 122.70 |
| 10 | A | 2770 | G | N1-C6-O6 | -6.34 | 116.09 | 119.90 |
| 31 | V | 2 | G | N1-C2-N3 | -6.34 | 120.10 | 123.90 |
| 31 | V | 9 | A | C4-C5-C6 | 6.34 | 120.17 | 117.00 |
| 10 | A | 2754 | U | N3-C4-O4 | 6.34 | 123.83 | 119.40 |
| 10 | A | 2142 | A | OP2-P-O3' | 6.33 | 119.13 | 105.20 |
| 28 | S | 94 | ASP | CB-CG-OD2 | 6.32 | 123.98 | 118.30 |
| 31 | V | 18 | G | C5-C6-O6 | -6.32 | 124.81 | 128.60 |
| 31 | V | 37 | G | N9-C4-C5 | 6.30 | 107.92 | 105.40 |
| 31 | V | 66 | C | P-O3'-C3' | 6.29 | 127.25 | 119.70 |
| 10 | A | 2267 | A | C8-N9-C4 | -6.28 | 103.29 | 105.80 |
| 10 | A | 1125 | G | N1-C6-O6 | 6.27 | 123.66 | 119.90 |
| 31 | V | 70 | C | P-O5'-C5' | 6.26 | 130.92 | 120.90 |
| 10 | A | 1839 | G | C5-C6-O6 | -6.26 | 124.84 | 128.60 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed($^o$) | Ideal($^o$) |
|---|---|---|---|---|---|---|---|
| 10 | A | 2447 | G | N1-C6-O6 | 6.25 | 123.65 | 119.90 |
| 10 | A | 1142 | A | N3-C4-C5 | 6.25 | 131.18 | 126.80 |
| 31 | V | 13 | C | N3-C4-N4 | 6.25 | 122.37 | 118.00 |
| 31 | V | 49 | G | C5-C6-O6 | -6.25 | 124.85 | 128.60 |
| 31 | V | 39 | G | C2'-C3'-O3' | 6.24 | 123.68 | 113.70 |
| 6 | 5 | 108 | VAL | CG1-CB-CG2 | 6.23 | 120.87 | 110.90 |
| 10 | A | 984 | A | N1-C6-N6 | 6.23 | 122.34 | 118.60 |
| 6 | 5 | 39 | THR | C-N-CA | 6.22 | 137.24 | 121.70 |
| 6 | 5 | 60 | LEU | CB-CG-CD1 | 6.20 | 121.55 | 111.00 |
| 10 | A | 748 | G | O4'-C1'-N9 | 6.20 | 113.16 | 108.20 |
| 31 | V | 66 | C | O4'-C1'-N1 | 6.20 | 113.16 | 108.20 |
| 31 | V | 26 | A | C4-C5-C6 | 6.19 | 120.09 | 117.00 |
| 31 | V | 44 | G | O4'-C1'-N9 | 6.19 | 113.15 | 108.20 |
| 31 | V | 2 | G | C5-C6-N1 | -6.18 | 108.41 | 111.50 |
| 31 | V | 57 | A | C4-C5-C6 | 6.18 | 120.09 | 117.00 |
| 12 | C | 109 | LEU | CA-CB-CG | 6.17 | 129.49 | 115.30 |
| 31 | V | 52 | G | O4'-C1'-N9 | 6.17 | 113.14 | 108.20 |
| 31 | V | 37 | G | C5-N7-C8 | 6.15 | 107.37 | 104.30 |
| 31 | V | 26 | A | C5-C6-N6 | -6.14 | 118.78 | 123.70 |
| 31 | V | 1 | C | C5-C4-N4 | -6.14 | 115.90 | 120.20 |
| 10 | A | 1003 | G | O5'-P-OP2 | -6.14 | 100.18 | 105.70 |
| 10 | A | 567 | U | N1-C2-O2 | -6.13 | 118.51 | 122.80 |
| 10 | A | 1142 | A | C5-N7-C8 | -6.13 | 100.84 | 103.90 |
| 10 | A | 2592 | G | O5'-P-OP2 | -6.13 | 100.19 | 105.70 |
| 10 | A | 1950 | G | C5-C6-O6 | -6.12 | 124.92 | 128.60 |
| 31 | V | 38 | U | C6-N1-C2 | -6.10 | 117.34 | 121.00 |
| 10 | A | 1815 | A | C8-N9-C4 | -6.10 | 103.36 | 105.80 |
| 10 | A | 1142 | A | C4-C5-N7 | 6.10 | 113.75 | 110.70 |
| 10 | A | 2241 | A | C8-N9-C4 | -6.09 | 103.37 | 105.80 |
| 31 | V | 21 | A | C5-C6-N6 | -6.08 | 118.84 | 123.70 |
| 10 | A | 784 | G | P-O3'-C3' | 6.07 | 126.99 | 119.70 |
| 6 | 5 | 59 | LEU | C-N-CA | 6.07 | 136.87 | 121.70 |
| 10 | A | 1328 | A | O5'-P-OP2 | -6.06 | 100.25 | 105.70 |
| 10 | A | 784 | G | O4'-C1'-N9 | -6.06 | 103.35 | 108.20 |
| 10 | A | 379 | G | N1-C6-O6 | 6.06 | 123.53 | 119.90 |
| 21 | L | 82 | LEU | CA-CB-CG | 6.05 | 129.22 | 115.30 |
| 31 | V | 74 | C | C3'-C2'-C1' | -6.05 | 96.66 | 101.50 |
| 10 | A | 2505 | G | O5'-P-OP2 | -6.04 | 100.26 | 105.70 |
| 10 | A | 1025 | G | P-O3'-C3' | 6.02 | 126.92 | 119.70 |
| 10 | A | 2250 | G | C4-C5-N7 | 6.01 | 113.20 | 110.80 |
| 31 | V | 76 | A | C1'-O4'-C4' | 6.00 | 114.70 | 109.90 |
| 10 | A | 548 | G | C8-N9-C4 | -5.99 | 104.00 | 106.40 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed($^o$) | Ideal($^o$) |
|---|---|---|---|---|---|---|---|
| 10 | A | 1069 | A | OP2-P-O3' | 5.99 | 118.38 | 105.20 |
| 31 | V | 59 | A | O4'-C1'-N9 | 5.99 | 112.99 | 108.20 |
| 10 | A | 1358 | G | C8-N9-C4 | -5.98 | 104.01 | 106.40 |
| 10 | A | 2554 | U | O5'-P-OP1 | -5.98 | 100.32 | 105.70 |
| 10 | A | 119 | A | O5'-P-OP2 | -5.97 | 100.32 | 105.70 |
| 10 | A | 1073 | A | N7-C8-N9 | -5.96 | 110.82 | 113.80 |
| 10 | A | 1428 | C | O5'-P-OP1 | -5.96 | 100.34 | 105.70 |
| 10 | A | 2534 | A | C4-C5-N7 | 5.96 | 113.68 | 110.70 |
| 31 | V | 49 | G | O4'-C1'-N9 | 5.95 | 112.96 | 108.20 |
| 10 | A | 2250 | G | C5-N7-C8 | -5.95 | 101.33 | 104.30 |
| 31 | V | 70 | C | C5-C4-N4 | -5.94 | 116.04 | 120.20 |
| 31 | V | 51 | A | C5-C6-N6 | -5.94 | 118.94 | 123.70 |
| 10 | A | 1670 | C | N1-C2-O2 | -5.93 | 115.34 | 118.90 |
| 6 | 5 | 53 | ARG | C-N-CA | 5.92 | 136.50 | 121.70 |
| 10 | A | 1509 | A | O4'-C1'-N9 | 5.92 | 112.93 | 108.20 |
| 31 | V | 75 | C | C2-N3-C4 | 5.91 | 122.86 | 119.90 |
| 31 | V | 3 | G | N3-C4-N9 | 5.90 | 129.54 | 126.00 |
| 10 | A | 1779 | U | N3-C4-O4 | -5.89 | 115.27 | 119.40 |
| 10 | A | 528 | A | C5-C6-N1 | -5.89 | 114.75 | 117.70 |
| 10 | A | 2715 | C | C6-N1-C2 | 5.89 | 122.66 | 120.30 |
| 10 | A | 2747 | G | OP2-P-O3' | 5.89 | 118.16 | 105.20 |
| 10 | A | 2043 | C | C6-N1-C2 | -5.89 | 117.94 | 120.30 |
| 10 | A | 527 | C | P-O3'-C3' | 5.89 | 126.77 | 119.70 |
| 31 | V | 29 | G | O4'-C1'-N9 | 5.87 | 112.89 | 108.20 |
| 31 | V | 36 | G | O5'-C5'-C4' | 5.86 | 122.84 | 111.70 |
| 10 | A | 964 | C | O5'-P-OP2 | -5.86 | 100.43 | 105.70 |
| 31 | V | 51 | A | C4-C5-C6 | 5.85 | 119.93 | 117.00 |
| 31 | V | 68 | U | C6-N1-C2 | -5.85 | 117.49 | 121.00 |
| 10 | A | 1094 | U | N3-C4-C5 | -5.85 | 111.09 | 114.60 |
| 10 | A | 1837 | C | O5'-P-OP1 | -5.84 | 100.44 | 105.70 |
| 31 | V | 76 | A | N7-C8-N9 | 5.84 | 116.72 | 113.80 |
| 31 | V | 32 | A | C5-N7-C8 | 5.83 | 106.81 | 103.90 |
| 31 | V | 70 | C | N3-C2-O2 | -5.83 | 117.82 | 121.90 |
| 31 | V | 9 | A | C5-C6-N6 | -5.82 | 119.04 | 123.70 |
| 31 | V | 16 | C | N3-C4-N4 | 5.82 | 122.07 | 118.00 |
| 10 | A | 2448 | A | C6-C5-N7 | -5.80 | 128.24 | 132.30 |
| 10 | A | 516 | C | O5'-P-OP1 | -5.80 | 100.48 | 105.70 |
| 31 | V | 59 | A | C4-C5-C6 | 5.79 | 119.89 | 117.00 |
| 10 | A | 2241 | A | N9-C4-C5 | 5.79 | 108.11 | 105.80 |
| 10 | A | 2447 | G | C5-C6-O6 | -5.79 | 125.13 | 128.60 |
| 31 | V | 16 | C | O4'-C1'-N1 | 5.79 | 112.83 | 108.20 |
| 31 | V | 2 | G | N7-C8-N9 | 5.78 | 115.99 | 113.10 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed($^o$) | Ideal($^o$) |
|---|---|---|---|---|---|---|---|
| 31 | V | 14 | A | C5-C6-N6 | -5.77 | 119.08 | 123.70 |
| 31 | V | 42 | G | O4'-C1'-N9 | 5.75 | 112.80 | 108.20 |
| 10 | A | 1088 | A | O4'-C1'-N9 | -5.74 | 103.61 | 108.20 |
| 31 | V | 48 | C | N3-C4-N4 | 5.74 | 122.02 | 118.00 |
| 10 | A | 1645 | G | N3-C4-C5 | -5.72 | 125.74 | 128.60 |
| 31 | V | 7 | G | N3-C4-C5 | -5.72 | 125.74 | 128.60 |
| 10 | A | 1247 | A | P-O3'-C3' | 5.72 | 126.56 | 119.70 |
| 10 | A | 1606 | C | C2-N3-C4 | -5.72 | 117.04 | 119.90 |
| 10 | A | 2604 | U | N3-C4-O4 | -5.72 | 115.40 | 119.40 |
| 31 | V | 27 | C | N3-C4-N4 | 5.72 | 122.00 | 118.00 |
| 6 | 5 | 117 | LEU | C-N-CA | 5.71 | 135.99 | 121.70 |
| 31 | V | 26 | A | O4'-C1'-N9 | 5.71 | 112.77 | 108.20 |
| 10 | A | 2719 | G | N1-C6-O6 | 5.70 | 123.32 | 119.90 |
| 31 | V | 16 | C | N3-C4-C5 | -5.69 | 119.62 | 121.90 |
| 10 | A | 1069 | A | C8-N9-C4 | -5.69 | 103.53 | 105.80 |
| 10 | A | 2501 | C | N3-C4-C5 | 5.68 | 124.17 | 121.90 |
| 10 | A | 2719 | G | C5-C6-N1 | -5.68 | 108.66 | 111.50 |
| 10 | A | 866 | A | N1-C6-N6 | 5.68 | 122.01 | 118.60 |
| 10 | A | 2271 | G | C5-C6-O6 | -5.68 | 125.19 | 128.60 |
| 31 | V | 45 | G | O4'-C1'-N9 | 5.67 | 112.74 | 108.20 |
| 10 | A | 2534 | A | C5-N7-C8 | -5.67 | 101.06 | 103.90 |
| 10 | A | 1066 | U | N3-C2-O2 | -5.67 | 118.23 | 122.20 |
| 31 | V | 7 | G | P-O5'-C5' | 5.67 | 129.97 | 120.90 |
| 10 | A | 1263 | U | C6-N1-C2 | -5.66 | 117.61 | 121.00 |
| 10 | A | 1789 | A | O5'-P-OP1 | -5.65 | 100.61 | 105.70 |
| 31 | V | 61 | C | N3-C4-N4 | 5.65 | 121.95 | 118.00 |
| 10 | A | 626 | A | N1-C6-N6 | 5.65 | 121.99 | 118.60 |
| 10 | A | 1153 | C | N1-C2-O2 | -5.65 | 115.51 | 118.90 |
| 31 | V | 57 | A | C5-C6-N6 | -5.64 | 119.19 | 123.70 |
| 31 | V | 62 | C | N3-C4-N4 | 5.62 | 121.93 | 118.00 |
| 10 | A | 271 | G | OP1-P-O3' | 5.61 | 117.55 | 105.20 |
| 31 | V | 31 | C | N3-C4-N4 | 5.60 | 121.92 | 118.00 |
| 10 | A | 1207 | C | C6-N1-C2 | -5.60 | 118.06 | 120.30 |
| 31 | V | 76 | A | OP1-P-OP2 | -5.60 | 111.20 | 119.60 |
| 10 | A | 1979 | U | C6-N1-C2 | -5.59 | 117.64 | 121.00 |
| 10 | A | 1509 | A | P-O3'-C3' | 5.59 | 126.41 | 119.70 |
| 31 | V | 3 | G | C4-C5-C6 | 5.59 | 122.16 | 118.80 |
| 10 | A | 1534 | U | C5-C6-N1 | 5.58 | 125.49 | 122.70 |
| 31 | V | 12 | G | O4'-C1'-N9 | 5.58 | 112.66 | 108.20 |
| 31 | V | 69 | G | C6-N1-C2 | -5.57 | 121.76 | 125.10 |
| 10 | A | 1611 | C | N1-C2-O2 | -5.57 | 115.56 | 118.90 |
| 31 | V | 48 | C | N3-C4-C5 | -5.56 | 119.67 | 121.90 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed($^o$) | Ideal($^o$) |
|---|---|---|---|---|---|---|---|
| 10 | A | 1073 | A | C4-N9-C1' | -5.56 | 116.30 | 126.30 |
| 10 | A | 1198 | U | O5'-P-OP2 | -5.56 | 100.70 | 105.70 |
| 31 | V | 22 | G | O4'-C1'-N9 | 5.56 | 112.65 | 108.20 |
| 10 | A | 2586 | U | O5'-C5'-C4' | 5.55 | 122.25 | 111.70 |
| 10 | A | 2146 | C | C6-N1-C2 | -5.55 | 118.08 | 120.30 |
| 10 | A | 2053 | G | N3-C2-N2 | -5.54 | 116.02 | 119.90 |
| 31 | V | 58 | A | C5-C6-N1 | -5.54 | 114.93 | 117.70 |
| 10 | A | 989 | G | O4'-C1'-N9 | 5.54 | 112.63 | 108.20 |
| 10 | A | 2544 | G | C6-C5-N7 | -5.54 | 127.08 | 130.40 |
| 31 | V | 43 | G | O4'-C1'-N9 | 5.54 | 112.63 | 108.20 |
| 31 | V | 41 | C | N3-C4-N4 | 5.54 | 121.88 | 118.00 |
| 10 | A | 2439 | A | N1-C6-N6 | 5.53 | 121.92 | 118.60 |
| 10 | A | 1069 | A | O4'-C1'-N9 | 5.53 | 112.62 | 108.20 |
| 31 | V | 57 | A | O4'-C1'-N9 | 5.53 | 112.62 | 108.20 |
| 10 | A | 209 | C | C6-N1-C2 | 5.52 | 122.51 | 120.30 |
| 31 | V | 25 | C | N3-C4-C5 | -5.52 | 119.69 | 121.90 |
| 31 | V | 28 | C | N3-C4-N4 | 5.52 | 121.87 | 118.00 |
| 10 | A | 2326 | C | C5-C4-N4 | -5.52 | 116.33 | 120.20 |
| 10 | A | 1157 | G | N1-C6-O6 | 5.52 | 123.21 | 119.90 |
| 10 | A | 2353 | G | N1-C6-O6 | -5.52 | 116.59 | 119.90 |
| 31 | V | 23 | C | N3-C4-N4 | 5.51 | 121.86 | 118.00 |
| 31 | V | 62 | C | N3-C4-C5 | -5.50 | 119.70 | 121.90 |
| 10 | A | 2544 | G | N1-C6-O6 | 5.50 | 123.20 | 119.90 |
| 31 | V | 33 | U | O3'-P-O5' | 5.50 | 114.44 | 104.00 |
| 31 | V | 28 | C | N3-C4-C5 | -5.49 | 119.70 | 121.90 |
| 31 | V | 23 | C | N3-C4-C5 | -5.49 | 119.70 | 121.90 |
| 31 | V | 14 | A | C5-C6-N1 | -5.49 | 114.96 | 117.70 |
| 10 | A | 2685 | G | C5-C6-N1 | -5.48 | 108.76 | 111.50 |
| 31 | V | 25 | C | N3-C4-N4 | 5.48 | 121.84 | 118.00 |
| 10 | A | 84 | A | N1-C6-N6 | -5.47 | 115.32 | 118.60 |
| 31 | V | 17 | C | N3-C4-N4 | 5.47 | 121.83 | 118.00 |
| 31 | V | 31 | C | N3-C4-C5 | -5.46 | 119.71 | 121.90 |
| 31 | V | 50 | G | O4'-C1'-N9 | 5.46 | 112.57 | 108.20 |
| 10 | A | 2689 | U | N3-C4-O4 | -5.46 | 115.58 | 119.40 |
| 10 | A | 2355 | G | C8-N9-C4 | 5.46 | 108.58 | 106.40 |
| 10 | A | 2604 | U | C5-C4-O4 | 5.46 | 129.17 | 125.90 |
| 10 | A | 29 | U | OP2-P-O3' | 5.46 | 117.20 | 105.20 |
| 10 | A | 55 | G | C5-C6-O6 | -5.46 | 125.33 | 128.60 |
| 10 | A | 451 | U | O4'-C1'-N1 | 5.45 | 112.56 | 108.20 |
| 10 | A | 1125 | G | C6-C5-N7 | -5.45 | 127.13 | 130.40 |
| 31 | V | 57 | A | C5-C6-N1 | -5.45 | 114.98 | 117.70 |
| 10 | A | 1129 | A | O5'-P-OP1 | -5.45 | 100.80 | 105.70 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed($^o$) | Ideal($^o$) |
|---|---|---|---|---|---|---|---|
| 10 | A | 2446 | G | OP2-P-O3' | 5.45 | 117.18 | 105.20 |
| 11 | B | 80 | U | N1-C2-N3 | 5.44 | 118.17 | 114.90 |
| 10 | A | 1355 | G | C8-N9-C4 | -5.44 | 104.22 | 106.40 |
| 10 | A | 1027 | A | O4'-C1'-N9 | -5.44 | 103.85 | 108.20 |
| 10 | A | 1824 | G | N9-C4-C5 | 5.44 | 107.57 | 105.40 |
| 31 | V | 70 | C | N3-C4-C5 | 5.43 | 124.07 | 121.90 |
| 10 | A | 1192 | G | N9-C4-C5 | -5.42 | 103.23 | 105.40 |
| 10 | A | 2271 | G | N1-C6-O6 | 5.42 | 123.15 | 119.90 |
| 10 | A | 672 | C | N1-C2-O2 | 5.42 | 122.15 | 118.90 |
| 31 | V | 58 | A | C5-C6-N6 | -5.42 | 119.36 | 123.70 |
| 10 | A | 2609 | U | N1-C1'-C2' | 5.42 | 121.04 | 114.00 |
| 31 | V | 7 | G | C1'-O4'-C4' | 5.42 | 114.23 | 109.90 |
| 31 | V | 11 | C | N3-C4-C5 | -5.41 | 119.73 | 121.90 |
| 10 | A | 598 | U | OP2-P-O3' | 5.41 | 117.10 | 105.20 |
| 10 | A | 1190 | G | C5-N7-C8 | -5.41 | 101.60 | 104.30 |
| 10 | A | 2244 | U | C5-C4-O4 | -5.41 | 122.66 | 125.90 |
| 10 | A | 532 | A | C8-N9-C4 | -5.40 | 103.64 | 105.80 |
| 10 | A | 1533 | C | C5-C6-N1 | 5.39 | 123.70 | 121.00 |
| 10 | A | 2723 | C | C6-N1-C2 | -5.39 | 118.14 | 120.30 |
| 31 | V | 9 | A | C5-C6-N1 | -5.39 | 115.01 | 117.70 |
| 10 | A | 984 | A | C5-C6-N1 | -5.39 | 115.01 | 117.70 |
| 10 | A | 1073 | A | C8-N9-C1' | 5.38 | 137.38 | 127.70 |
| 10 | A | 1565 | C | C6-N1-C2 | -5.38 | 118.15 | 120.30 |
| 31 | V | 73 | A | C2'-C3'-O3' | 5.38 | 122.30 | 113.70 |
| 25 | P | 113 | LEU | CA-CB-CG | 5.37 | 127.66 | 115.30 |
| 10 | A | 250 | G | O5'-P-OP2 | -5.37 | 100.87 | 105.70 |
| 10 | A | 1229 | C | C6-N1-C2 | 5.37 | 122.45 | 120.30 |
| 10 | A | 1950 | G | C8-N9-C1' | -5.36 | 120.03 | 127.00 |
| 10 | A | 2153 | C | O4'-C1'-N1 | 5.36 | 112.49 | 108.20 |
| 10 | A | 2037 | A | N9-C4-C5 | 5.36 | 107.94 | 105.80 |
| 10 | A | 2263 | C | N3-C4-C5 | -5.36 | 119.76 | 121.90 |
| 10 | A | 2353 | G | C2-N3-C4 | 5.35 | 114.58 | 111.90 |
| 10 | A | 991 | C | C6-N1-C2 | -5.35 | 118.16 | 120.30 |
| 10 | A | 837 | C | N1-C2-O2 | -5.35 | 115.69 | 118.90 |
| 10 | A | 2015 | A | N1-C6-N6 | -5.34 | 115.39 | 118.60 |
| 10 | A | 1420 | A | O4'-C1'-N9 | 5.34 | 112.47 | 108.20 |
| 31 | V | 53 | G | O4'-C1'-N9 | 5.33 | 112.47 | 108.20 |
| 31 | V | 61 | C | N3-C4-C5 | -5.33 | 119.77 | 121.90 |
| 10 | A | 1025 | G | N3-C4-C5 | -5.33 | 125.94 | 128.60 |
| 10 | A | 677 | A | OP1-P-O3' | 5.33 | 116.92 | 105.20 |
| 6 | 5 | 131 | THR | N-CA-C | -5.33 | 96.62 | 111.00 |
| 10 | A | 2571 | U | C2-N1-C1' | -5.33 | 111.31 | 117.70 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed($^o$) | Ideal($^o$) |
|---|---|---|---|---|---|---|---|
| 10 | A | 1684 | G | N3-C4-C5 | -5.32 | 125.94 | 128.60 |
| 6 | 5 | 50 | VAL | CG1-CB-CG2 | 5.32 | 119.41 | 110.90 |
| 31 | V | 59 | A | C5-C6-N6 | -5.32 | 119.45 | 123.70 |
| 31 | V | 68 | U | C1'-O4'-C4' | 5.31 | 114.15 | 109.90 |
| 31 | V | 56 | C | N3-C4-C5 | -5.31 | 119.78 | 121.90 |
| 31 | V | 64 | C | N3-C4-N4 | 5.30 | 121.71 | 118.00 |
| 10 | A | 518 | G | O5'-P-OP1 | -5.29 | 100.94 | 105.70 |
| 31 | V | 15 | G | O4'-C1'-N9 | 5.29 | 112.43 | 108.20 |
| 31 | V | 51 | A | O4'-C1'-N9 | 5.29 | 112.43 | 108.20 |
| 10 | A | 1311 | G | N7-C8-N9 | 5.29 | 115.75 | 113.10 |
| 31 | V | 2 | G | N9-C4-C5 | -5.29 | 103.28 | 105.40 |
| 10 | A | 2071 | A | OP2-P-O3' | 5.29 | 116.83 | 105.20 |
| 31 | V | 9 | A | O4'-C1'-N9 | 5.29 | 112.43 | 108.20 |
| 10 | A | 1430 | G | N1-C6-O6 | 5.28 | 123.07 | 119.90 |
| 10 | A | 2704 | C | C6-N1-C2 | 5.28 | 122.41 | 120.30 |
| 10 | A | 2250 | G | C2-N3-C4 | -5.28 | 109.26 | 111.90 |
| 31 | V | 41 | C | N3-C4-C5 | -5.28 | 119.79 | 121.90 |
| 10 | A | 748 | G | C4-C5-N7 | -5.28 | 108.69 | 110.80 |
| 10 | A | 1458 | U | P-O3'-C3' | 5.28 | 126.03 | 119.70 |
| 10 | A | 1759 | A | N1-C6-N6 | 5.27 | 121.77 | 118.60 |
| 26 | Q | 63 | ARG | NE-CZ-NH2 | -5.26 | 117.67 | 120.30 |
| 31 | V | 51 | A | C5-C6-N1 | -5.26 | 115.07 | 117.70 |
| 10 | A | 2470 | G | OP2-P-O3' | 5.26 | 116.77 | 105.20 |
| 6 | 5 | 50 | VAL | CA-CB-CG1 | 5.26 | 118.79 | 110.90 |
| 10 | A | 776 | G | C4-N9-C1' | 5.26 | 133.34 | 126.50 |
| 10 | A | 1524 | G | C8-N9-C4 | -5.26 | 104.30 | 106.40 |
| 10 | A | 1970 | A | C8-N9-C4 | -5.26 | 103.70 | 105.80 |
| 10 | A | 2618 | G | C5-C6-N1 | -5.26 | 108.87 | 111.50 |
| 10 | A | 548 | G | N3-C4-C5 | -5.25 | 125.97 | 128.60 |
| 10 | A | 2368 | C | C6-N1-C2 | 5.25 | 122.40 | 120.30 |
| 10 | A | 916 | G | C6-C5-N7 | -5.25 | 127.25 | 130.40 |
| 10 | A | 1131 | G | OP1-P-O3' | 5.25 | 116.76 | 105.20 |
| 10 | A | 1446 | C | C6-N1-C2 | -5.25 | 118.20 | 120.30 |
| 10 | A | 2501 | C | C6-N1-C1' | 5.25 | 127.10 | 120.80 |
| 35 | Z | 15 | ARG | NE-CZ-NH1 | 5.25 | 122.93 | 120.30 |
| 10 | A | 404 | A | C8-N9-C4 | -5.25 | 103.70 | 105.80 |
| 31 | V | 59 | A | C5-C6-N1 | -5.25 | 115.08 | 117.70 |
| 31 | V | 26 | A | C5-C6-N1 | -5.25 | 115.08 | 117.70 |
| 10 | A | 1936 | A | N3-C4-C5 | 5.24 | 130.47 | 126.80 |
| 31 | V | 10 | G | O4'-C1'-N9 | 5.24 | 112.39 | 108.20 |
| 10 | A | 1206 | G | N3-C4-C5 | -5.24 | 125.98 | 128.60 |
| 10 | A | 1350 | C | C6-N1-C2 | 5.24 | 122.40 | 120.30 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed($^o$) | Ideal($^o$) |
|---|---|---|---|---|---|---|---|
| 31 | V | 6 | C | N3-C4-C5 | -5.24 | 119.80 | 121.90 |
| 31 | V | 13 | C | C1'-O4'-C4' | -5.24 | 105.71 | 109.90 |
| 33 | X | 29 | LEU | CA-CB-CG | 5.24 | 127.35 | 115.30 |
| 10 | A | 1264 | A | O5'-P-OP1 | -5.24 | 100.99 | 105.70 |
| 10 | A | 733 | G | C8-N9-C4 | -5.23 | 104.31 | 106.40 |
| 10 | A | 2250 | G | N7-C8-N9 | 5.22 | 115.71 | 113.10 |
| 10 | A | 1355 | G | N3-C2-N2 | -5.22 | 116.25 | 119.90 |
| 10 | A | 1943 | U | C5-C4-O4 | 5.21 | 129.03 | 125.90 |
| 10 | A | 940 | G | N1-C6-O6 | 5.20 | 123.02 | 119.90 |
| 10 | A | 2503 | A | N1-C6-N6 | 5.20 | 121.72 | 118.60 |
| 10 | A | 1831 | G | C8-N9-C4 | -5.20 | 104.32 | 106.40 |
| 10 | A | 2537 | U | C5-C4-O4 | 5.20 | 129.02 | 125.90 |
| 31 | V | 7 | G | C2-N3-C4 | 5.19 | 114.50 | 111.90 |
| 10 | A | 833 | A | C8-N9-C4 | -5.18 | 103.73 | 105.80 |
| 31 | V | 7 | G | N7-C8-N9 | -5.18 | 110.51 | 113.10 |
| 10 | A | 2602 | A | O4'-C1'-N9 | 5.17 | 112.33 | 108.20 |
| 10 | A | 119 | A | P-O3'-C3' | 5.17 | 125.90 | 119.70 |
| 10 | A | 1238 | G | O5'-P-OP2 | -5.17 | 101.05 | 105.70 |
| 11 | B | 114 | C | C5-C4-N4 | -5.17 | 116.58 | 120.20 |
| 10 | A | 2518 | A | N1-C6-N6 | 5.16 | 121.70 | 118.60 |
| 10 | A | 807 | U | N3-C4-O4 | 5.16 | 123.01 | 119.40 |
| 10 | A | 2534 | A | C5-C6-N6 | -5.16 | 119.57 | 123.70 |
| 6 | 5 | 130 | PRO | CA-N-CD | -5.15 | 104.29 | 111.50 |
| 10 | A | 699 | A | N1-C6-N6 | 5.14 | 121.69 | 118.60 |
| 10 | A | 2825 | G | N3-C4-N9 | 5.14 | 129.09 | 126.00 |
| 10 | A | 2603 | G | O4'-C4'-C3' | 5.14 | 110.21 | 106.10 |
| 10 | A | 1639 | C | C6-N1-C2 | 5.14 | 122.36 | 120.30 |
| 10 | A | 186 | G | N3-C4-C5 | 5.13 | 131.16 | 128.60 |
| 31 | V | 56 | C | N3-C4-N4 | 5.13 | 121.59 | 118.00 |
| 31 | V | 24 | G | O4'-C1'-N9 | 5.12 | 112.30 | 108.20 |
| 10 | A | 1928 | A | N1-C6-N6 | 5.12 | 121.67 | 118.60 |
| 31 | V | 17 | C | N3-C4-C5 | -5.12 | 119.85 | 121.90 |
| 10 | A | 2282 | G | C8-N9-C4 | -5.11 | 104.36 | 106.40 |
| 31 | V | 71 | C | C2-N3-C4 | 5.11 | 122.46 | 119.90 |
| 9 | 8 | 61 | LEU | CA-CB-CG | 5.11 | 127.05 | 115.30 |
| 10 | A | 1395 | A | O4'-C1'-N9 | 5.11 | 112.28 | 108.20 |
| 31 | V | 5 | A | C5-C6-N6 | -5.10 | 119.62 | 123.70 |
| 10 | A | 1534 | U | N1-C2-O2 | 5.10 | 126.37 | 122.80 |
| 10 | A | 1025 | G | C8-N9-C4 | -5.09 | 104.36 | 106.40 |
| 10 | A | 1795 | C | N3-C4-C5 | -5.09 | 119.86 | 121.90 |
| 31 | V | 64 | C | N3-C4-C5 | -5.09 | 119.86 | 121.90 |
| 31 | V | 32 | A | N1-C6-N6 | 5.09 | 121.66 | 118.60 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed($^o$) | Ideal($^o$) |
|---|---|---|---|---|---|---|---|
| 10 | A | 465 | G | C4-C5-C6 | 5.09 | 121.85 | 118.80 |
| 10 | A | 1659 | G | N3-C4-C5 | 5.09 | 131.15 | 128.60 |
| 10 | A | 2198 | A | O4'-C1'-N9 | 5.09 | 112.27 | 108.20 |
| 10 | A | 2422 | C | N1-C2-O2 | 5.09 | 121.95 | 118.90 |
| 10 | A | 2443 | C | N3-C4-N4 | 5.09 | 121.56 | 118.00 |
| 10 | A | 454 | A | O5'-P-OP2 | -5.08 | 101.12 | 105.70 |
| 10 | A | 403 | U | P-O3'-C3' | 5.08 | 125.80 | 119.70 |
| 10 | A | 2015 | A | N9-C4-C5 | 5.08 | 107.83 | 105.80 |
| 10 | A | 1779 | U | C5-C6-N1 | -5.08 | 120.16 | 122.70 |
| 10 | A | 1122 | G | N3-C4-N9 | -5.07 | 122.96 | 126.00 |
| 10 | A | 2443 | C | C6-N1-C2 | -5.07 | 118.27 | 120.30 |
| 10 | A | 2537 | U | N1-C2-N3 | 5.07 | 117.94 | 114.90 |
| 10 | A | 1533 | C | C6-N1-C1' | -5.07 | 114.72 | 120.80 |
| 31 | V | 7 | G | N1-C2-N2 | -5.05 | 111.65 | 116.20 |
| 31 | V | 17(A) | U | O4'-C1'-N1 | 5.05 | 112.24 | 108.20 |
| 10 | A | 1606 | C | P-O3'-C3' | 5.05 | 125.76 | 119.70 |
| 18 | I | 79 | LEU | CA-CB-CG | 5.05 | 126.92 | 115.30 |
| 10 | A | 2448 | A | C5-C6-N6 | -5.05 | 119.66 | 123.70 |
| 10 | A | 984 | A | N1-C2-N3 | 5.05 | 131.82 | 129.30 |
| 10 | A | 1538 | G | N3-C4-C5 | 5.04 | 131.12 | 128.60 |
| 31 | V | 21 | A | C5-C6-N1 | -5.04 | 115.18 | 117.70 |
| 31 | V | 21 | A | O4'-C1'-N9 | 5.04 | 112.24 | 108.20 |
| 10 | A | 776 | G | C4-C5-C6 | 5.04 | 121.83 | 118.80 |
| 10 | A | 55 | G | N1-C6-O6 | 5.04 | 122.92 | 119.90 |
| 31 | V | 5 | A | C5-C6-N1 | -5.04 | 115.18 | 117.70 |
| 10 | A | 376 | G | C6-C5-N7 | -5.04 | 127.38 | 130.40 |
| 10 | A | 686 | U | C2-N1-C1' | -5.04 | 111.65 | 117.70 |
| 31 | V | 4 | C | C4'-C3'-C2' | -5.03 | 97.57 | 102.60 |
| 29 | T | 29 | THR | N-CA-C | 5.03 | 124.58 | 111.00 |
| 10 | A | 2502 | G | N3-C4-C5 | -5.03 | 126.09 | 128.60 |
| 10 | A | 2551 | C | O5'-P-OP1 | -5.03 | 101.18 | 105.70 |
| 31 | V | 38 | U | N3-C2-O2 | 5.03 | 125.72 | 122.20 |
| 10 | A | 2017 | U | N3-C4-O4 | 5.02 | 122.92 | 119.40 |
| 10 | A | 2822 | G | C6-C5-N7 | -5.02 | 127.39 | 130.40 |
| 10 | A | 1358 | G | N7-C8-N9 | 5.02 | 115.61 | 113.10 |
| 10 | A | 2455 | G | O5'-P-OP2 | -5.02 | 101.19 | 105.70 |
| 12 | C | 155 | ARG | CG-CD-NE | 5.02 | 122.33 | 111.80 |
| 10 | A | 752 | A | C8-N9-C1' | 5.01 | 136.73 | 127.70 |
| 10 | A | 1314 | C | C2-N1-C1' | 5.01 | 124.31 | 118.80 |
| 10 | A | 2439 | A | C4-C5-N7 | 5.01 | 113.21 | 110.70 |
| 10 | A | 1659 | G | C2-N3-C4 | -5.01 | 109.39 | 111.90 |
| 10 | A | 2015 | A | C5-C6-N6 | 5.01 | 127.71 | 123.70 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed($^o$) | Ideal($^o$) |
|---|---|---|---|---|---|---|---|
| 31 | V | 3 | G | C5-C6-N1 | -5.01 | 109.00 | 111.50 |
| 10 | A | 1649 | G | O5'-P-OP1 | -5.01 | 101.19 | 105.70 |

There are no chirality outliers.

All (25) planarity outliers are listed below:

| Mol | Chain | Res | Type | Group |
|---|---|---|---|---|
| 6 | 5 | 130 | PRO | Peptide |
| 8 | 7 | 15 | ILE | Peptide |
| 8 | 7 | 21 | ASP | Peptide |
| 8 | 7 | 23 | ARG | Sidechain |
| 8 | 7 | 6 | ILE | Peptide |
| 12 | C | 233 | GLY | Peptide |
| 13 | D | 9 | VAL | Peptide |
| 19 | J | 110 | PRO | Peptide |
| 20 | K | 71 | ARG | Peptide |
| 28 | S | 86 | MET | Mainchain |
| 28 | S | 88 | ARG | Peptide |
| 28 | S | 89 | ALA | Peptide |
| 31 | V | 13 | C | Sidechain |
| 31 | V | 3 | G | Sidechain |
| 31 | V | 33 | U | Sidechain |
| 31 | V | 37 | G | Sidechain |
| 31 | V | 39 | G | Sidechain |
| 31 | V | 4 | C | Sidechain |
| 31 | V | 5 | A | Sidechain |
| 31 | V | 66 | C | Sidechain |
| 31 | V | 67 | G | Sidechain |
| 31 | V | 69 | G | Sidechain |
| 31 | V | 70 | C | Sidechain |
| 31 | V | 71 | C | Sidechain |
| 31 | V | 75 | C | Sidechain |

## 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 | 0 | 444 | 0 | 461 | 19 | 0 |
| 2 | 1 | 409 | 0 | 440 | 15 | 0 |
| 3 | 2 | 377 | 0 | 418 | 9 | 0 |
| 4 | 3 | 504 | 0 | 574 | 10 | 0 |
| 5 | 4 | 302 | 0 | 340 | 16 | 0 |
| 6 | 5 | 1117 | 0 | 1155 | 121 | 0 |
| 7 | 6 | 227 | 0 | 237 | 7 | 0 |
| 8 | 7 | 170 | 0 | 166 | 94 | 0 |
| 9 | 8 | 753 | 0 | 780 | 14 | 0 |
| 10 | A | 61274 | 0 | 30816 | 828 | 0 |
| 11 | B | 2529 | 0 | 1281 | 21 | 0 |
| 12 | C | 2082 | 0 | 2157 | 54 | 0 |
| 13 | D | 1565 | 0 | 1616 | 47 | 0 |
| 14 | E | 1552 | 0 | 1619 | 41 | 0 |
| 15 | F | 1410 | 0 | 1445 | 45 | 0 |
| 16 | G | 1323 | 0 | 1374 | 38 | 0 |
| 17 | H | 384 | 0 | 405 | 13 | 0 |
| 18 | I | 1032 | 0 | 1088 | 51 | 0 |
| 19 | J | 1129 | 0 | 1162 | 53 | 0 |
| 20 | K | 938 | 0 | 1012 | 38 | 0 |
| 21 | L | 1045 | 0 | 1117 | 36 | 0 |
| 22 | M | 1074 | 0 | 1157 | 29 | 0 |
| 23 | N | 960 | 0 | 1000 | 30 | 0 |
| 24 | O | 892 | 0 | 923 | 20 | 0 |
| 25 | P | 917 | 0 | 965 | 40 | 0 |
| 26 | Q | 947 | 0 | 1022 | 51 | 0 |
| 27 | R | 816 | 0 | 839 | 35 | 0 |
| 28 | S | 857 | 0 | 922 | 53 | 0 |
| 29 | T | 738 | 0 | 807 | 35 | 0 |
| 30 | U | 779 | 0 | 834 | 26 | 0 |
| 31 | V | 1649 | 0 | 832 | 49 | 0 |
| 32 | W | 596 | 0 | 610 | 79 | 0 |
| 33 | X | 625 | 0 | 655 | 18 | 0 |
| 34 | Y | 509 | 0 | 543 | 13 | 0 |
| 35 | Z | 449 | 0 | 491 | 18 | 0 |
| 36 | 4 | 1 | 0 | 0 | 0 | 0 |
| 36 | A | 135 | 0 | 0 | 0 | 0 |
| 36 | B | 4 | 0 | 0 | 0 | 0 |
| 36 | C | 2 | 0 | 0 | 0 | 0 |
| 36 | E | 1 | 0 | 0 | 0 | 0 |
| 37 | 4 | 1 | 0 | 0 | 0 | 0 |
| 38 | 7 | 30 | 8 | 18 | 24 | 0 |
| 39 | A | 416 | 0 | 0 | 78 | 0 |

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| Mol | Chain | Non-H | H(model) | H(added) | Clashes | Symm-Clashes |
|---|---|---|---|---|---|---|
| 39 | B | 14 | 0 | 0 | 1 | 0 |
| 39 | C | 2 | 0 | 0 | 0 | 0 |
| 39 | D | 3 | 0 | 0 | 0 | 0 |
| 39 | E | 2 | 0 | 0 | 0 | 0 |
| 39 | L | 2 | 0 | 0 | 0 | 0 |
| All | All | 92987 | 8 | 61281 | 1782 | 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 12.

All (1782) 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) |
|---|---|---|---|
| 8:7:11:LYS:CE | 28:S:91:GLY:HA3 | 1.51 | 1.40 |
| 8:7:7:CYS:SG | 28:S:95:ARG:NH2 | 2.05 | 1.29 |
| 15:F:79:ARG:NH2 | 31:V:56:C:O2 | 1.62 | 1.27 |
| 8:7:14:ASN:O | 8:7:15:ILE:HD13 | 1.35 | 1.25 |
| 10:A:1923:U:H5" | 31:V:24:G:O2' | 1.04 | 1.19 |
| 10:A:912:C:OP1 | 22:M:8:LYS:NZ | 1.79 | 1.13 |
| 8:7:6:ILE:HG13 | 8:7:7:CYS:N | 1.57 | 1.10 |
| 8:7:11:LYS:HE3 | 28:S:91:GLY:HA3 | 1.13 | 1.10 |
| 10:A:1923:U:C5' | 31:V:24:G:O2' | 1.98 | 1.09 |
| 28:S:88:ARG:NH1 | 28:S:94:ASP:OD2 | 1.84 | 1.09 |
| 8:7:15:ILE:HD11 | 38:7:1002:TRP:HZ3 | 1.18 | 1.07 |
| 15:F:79:ARG:NH2 | 31:V:56:C:C2 | 2.25 | 1.05 |
| 6:5:71:CYS:HB3 | 6:5:117:LEU:HD12 | 1.33 | 1.04 |
| 8:7:21:ASP:HB2 | 38:7:1001:TRP:N | 1.72 | 1.04 |
| 8:7:15:ILE:CD1 | 38:7:1002:TRP:CZ3 | 2.40 | 1.03 |
| 8:7:15:ILE:CD1 | 38:7:1002:TRP:HZ3 | 1.72 | 1.02 |
| 6:5:26:VAL:HG21 | 6:5:115:GLY:H | 1.23 | 1.01 |
| 10:A:1782:U:C2' | 10:A:2608:G:O2' | 2.09 | 1.00 |
| 6:5:3:LEU:O | 6:5:7:ASP:OD1 | 1.79 | 1.00 |
| 8:7:7:CYS:O | 8:7:8:VAL:CG2 | 2.10 | 1.00 |
| 8:7:6:ILE:CG1 | 8:7:7:CYS:H | 1.72 | 1.00 |
| 8:7:15:ILE:HD11 | 38:7:1002:TRP:CZ3 | 1.95 | 0.99 |
| 10:A:1782:U:H2' | 10:A:2608:G:O2' | 1.62 | 0.98 |
| 8:7:14:ASN:HB3 | 8:7:15:ILE:HD13 | 1.43 | 0.98 |
| 10:A:1923:U:H5" | 31:V:24:G:C2' | 1.92 | 0.97 |
| 8:7:16:ASP:O | 8:7:17:ASN:HB2 | 1.65 | 0.96 |
| 8:7:11:LYS:HE2 | 28:S:91:GLY:HA3 | 1.46 | 0.95 |
| 8:7:6:ILE:HG13 | 8:7:7:CYS:H | 0.81 | 0.94 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 10:A:1909:C:H4' | 31:V:11:C:H4' | 1.49 | 0.94 |
| 8:7:15:ILE:HG13 | 38:7:1002:TRP:CE3 | 2.03 | 0.94 |
| 10:A:576:U:OP1 | 39:A:3661:HOH:O | 1.85 | 0.94 |
| 6:5:117:LEU:CD2 | 6:5:120:ALA:HA | 1.97 | 0.93 |
| 3:2:3:ARG:NH2 | 10:A:752:A:P | 2.42 | 0.93 |
| 8:7:11:LYS:CE | 28:S:91:GLY:CA | 2.45 | 0.92 |
| 10:A:1154:G:OP2 | 26:Q:57:ARG:NH1 | 2.03 | 0.92 |
| 8:7:19:ILE:O | 8:7:20:VAL:HG23 | 1.69 | 0.92 |
| 10:A:1248:G:OP2 | 14:E:44:ARG:NH2 | 2.03 | 0.92 |
| 6:5:71:CYS:HB3 | 6:5:117:LEU:CD1 | 1.98 | 0.91 |
| 6:5:71:CYS:CB | 6:5:117:LEU:HD12 | 2.00 | 0.91 |
| 10:A:1923:U:H5" | 31:V:24:G:HO2' | 1.32 | 0.91 |
| 8:7:22:HIS:C | 8:7:23:ARG:HG3 | 1.91 | 0.90 |
| 10:A:2279:G:N7 | 32:W:10:ARG:NH2 | 2.20 | 0.90 |
| 8:7:7:CYS:O | 8:7:8:VAL:HG22 | 1.70 | 0.90 |
| 10:A:2062:A:H2' | 10:A:2063:C:C5 | 2.06 | 0.89 |
| 8:7:14:ASN:HB3 | 8:7:15:ILE:CD1 | 2.02 | 0.89 |
| 6:5:24:SER:HB2 | 6:5:116:GLU:HG2 | 1.54 | 0.89 |
| 11:B:43:C:O2 | 15:F:91:ARG:NH1 | 2.04 | 0.89 |
| 10:A:1922:G:O2' | 31:V:25:C:H1' | 1.73 | 0.89 |
| 8:7:14:ASN:O | 8:7:15:ILE:CD1 | 2.20 | 0.89 |
| 8:7:14:ASN:OD1 | 14:E:61:ARG:CZ | 2.19 | 0.89 |
| 30:U:98:ASN:O | 30:U:100:GLU:N | 2.06 | 0.88 |
| 6:5:71:CYS:CB | 6:5:117:LEU:CD1 | 2.50 | 0.88 |
| 8:7:19:ILE:HD12 | 38:7:1001:TRP:CD1 | 2.08 | 0.88 |
| 10:A:996:A:OP2 | 26:Q:91:ARG:NH2 | 2.07 | 0.87 |
| 10:A:1336:A:OP2 | 29:T:68:LYS:NZ | 2.06 | 0.87 |
| 10:A:2608:G:H8 | 10:A:2608:G:H5" | 1.38 | 0.86 |
| 8:7:7:CYS:SG | 8:7:7:CYS:O | 2.34 | 0.86 |
| 29:T:39:THR:O | 29:T:41:ALA:N | 2.09 | 0.86 |
| 8:7:19:ILE:C | 8:7:20:VAL:HG23 | 1.93 | 0.86 |
| 10:A:2611:C:OP2 | 39:A:3536:HOH:O | 1.93 | 0.86 |
| 8:7:15:ILE:HG13 | 38:7:1002:TRP:CZ3 | 2.13 | 0.84 |
| 8:7:18:LYS:HE3 | 10:A:746:U:O2 | 1.78 | 0.84 |
| 6:5:71:CYS:HA | 6:5:117:LEU:HD13 | 1.60 | 0.84 |
| 8:7:14:ASN:OD1 | 14:E:61:ARG:NH2 | 2.11 | 0.84 |
| 8:7:19:ILE:HD12 | 38:7:1001:TRP:HD1 | 1.40 | 0.84 |
| 10:A:1723:G:O6 | 10:A:1737:G:O2' | 1.94 | 0.84 |
| 10:A:981:A:OP1 | 39:A:3588:HOH:O | 1.95 | 0.83 |
| 10:A:1909:C:O4' | 31:V:11:C:O2' | 1.95 | 0.83 |
| 10:A:2608:G:H5" | 10:A:2608:G:C8 | 2.12 | 0.83 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 10:A:1069:A:N3 | 10:A:1073:A:N6 | 2.25 | 0.83 |
| 10:A:1922:G:O3' | 31:V:25:C:H4' | 1.79 | 0.83 |
| 10:A:2585:U:O2' | 10:A:2586:U:H5' | 1.78 | 0.83 |
| 6:5:33:VAL:N | 6:5:36:ASP:OD2 | 2.12 | 0.82 |
| 6:5:103:ASN:ND2 | 6:5:107:GLU:O | 2.13 | 0.82 |
| 12:C:196:ASN:O | 12:C:198:GLU:N | 2.12 | 0.82 |
| 10:A:1923:U:OP1 | 31:V:25:C:H5' | 1.79 | 0.82 |
| 6:5:71:CYS:HA | 6:5:117:LEU:CD1 | 2.09 | 0.82 |
| 6:5:77:VAL:C | 6:5:79:PRO:HD2 | 2.00 | 0.81 |
| 28:S:91:GLY:O | 28:S:92:ARG:HG2 | 1.80 | 0.81 |
| 10:A:945:A:OP2 | 39:A:3342:HOH:O | 1.98 | 0.81 |
| 10:A:1783:A:OP1 | 39:A:3689:HOH:O | 1.98 | 0.81 |
| 10:A:1647:U:OP2 | 39:A:3416:HOH:O | 1.98 | 0.81 |
| 10:A:526:A:OP1 | 39:A:3246:HOH:O | 1.97 | 0.81 |
| 24:O:34:HIS:O | 24:O:102:ARG:NH2 | 2.14 | 0.81 |
| 10:A:991:C:OP2 | 39:A:3593:HOH:O | 1.97 | 0.81 |
| 25:P:50:ARG:HB3 | 25:P:57:ALA:H | 1.43 | 0.81 |
| 10:A:2608:G:H8 | 10:A:2608:G:C5' | 1.93 | 0.81 |
| 10:A:504:A:O2' | 10:A:505:A:OP1 | 1.98 | 0.80 |
| 10:A:1371:G:N7 | 39:A:3398:HOH:O | 2.13 | 0.80 |
| 8:7:21:ASP:CB | 38:7:1001:TRP:N | 2.44 | 0.80 |
| 10:A:1908:C:O2' | 31:V:12:G:H5' | 1.80 | 0.80 |
| 10:A:1268:A:OP1 | 39:A:3373:HOH:O | 1.99 | 0.80 |
| 10:A:1012:U:OP2 | 26:Q:69:ARG:NH2 | 2.14 | 0.80 |
| 10:A:1614:A:C6 | 28:S:87:PRO:HB3 | 2.17 | 0.80 |
| 10:A:2448:A:OP2 | 39:A:3677:HOH:O | 2.00 | 0.79 |
| 28:S:88:ARG:HD2 | 28:S:94:ASP:OD1 | 1.83 | 0.79 |
| 10:A:1799:G:OP2 | 12:C:269:ARG:NH2 | 2.16 | 0.79 |
| 6:5:33:VAL:HG12 | 6:5:34:THR:H | 1.48 | 0.79 |
| 6:5:43:LYS:NZ | 6:5:98:GLU:OE1 | 2.16 | 0.79 |
| 6:5:91:ALA:C | 6:5:93:ALA:H | 1.87 | 0.78 |
| 10:A:2720:U:OP1 | 25:P:52:ARG:NH2 | 2.15 | 0.78 |
| 10:A:1509:A:O2' | 10:A:1510:G:OP2 | 2.01 | 0.78 |
| 10:A:975:A:OP2 | 39:A:3584:HOH:O | 2.00 | 0.78 |
| 34:Y:18:LEU:O | 34:Y:22:LEU:N | 2.17 | 0.78 |
| 20:K:105:ARG:NH1 | 20:K:106:GLU:OE2 | 2.16 | 0.78 |
| 8:7:15:ILE:CG1 | 38:7:1002:TRP:CZ3 | 2.66 | 0.78 |
| 8:7:22:HIS:CD2 | 10:A:2503:A:H8 | 2.01 | 0.78 |
| 10:A:1782:U:O2 | 10:A:2608:G:O2' | 2.02 | 0.77 |
| 6:5:117:LEU:HD23 | 6:5:120:ALA:HA | 1.64 | 0.77 |
| 10:A:946:C:OP2 | 39:A:3342:HOH:O | 2.02 | 0.77 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 10:A:2025:C:OP2 | 39:A:3471:HOH:O | 2.03 | 0.77 |
| 6:5:35:VAL:HA | 6:5:38:MET:SD | 2.24 | 0.77 |
| 10:A:2062:A:H2' | 10:A:2063:C:C6 | 2.19 | 0.77 |
| 13:D:184:ARG:NH2 | 25:P:6:GLN:OE1 | 2.17 | 0.77 |
| 6:5:71:CYS:CA | 6:5:117:LEU:CD1 | 2.62 | 0.77 |
| 8:7:16:ASP:O | 8:7:17:ASN:CB | 2.34 | 0.76 |
| 3:2:3:ARG:NH2 | 10:A:752:A:OP2 | 2.18 | 0.76 |
| 8:7:19:ILE:HD13 | 10:A:2610:C:H5' | 1.66 | 0.76 |
| 8:7:7:CYS:O | 8:7:8:VAL:HG23 | 1.85 | 0.76 |
| 10:A:526:A:OP1 | 39:A:3248:HOH:O | 2.03 | 0.76 |
| 12:C:68:ARG:NH2 | 12:C:126:GLY:O | 2.18 | 0.76 |
| 12:C:69:ASN:O | 12:C:71:ASP:N | 2.18 | 0.76 |
| 8:7:14:ASN:O | 8:7:15:ILE:HG23 | 1.86 | 0.75 |
| 10:A:1187:G:OP1 | 27:R:85:LYS:NZ | 2.20 | 0.75 |
| 10:A:1380:G:OP2 | 39:A:3741:HOH:O | 2.03 | 0.75 |
| 10:A:2331:G:O2' | 32:W:39:GLN:O | 2.04 | 0.75 |
| 10:A:2588:G:OP2 | 39:A:3540:HOH:O | 2.04 | 0.75 |
| 8:7:18:LYS:O | 8:7:19:ILE:HG22 | 1.87 | 0.75 |
| 10:A:2579:C:OP1 | 39:A:3537:HOH:O | 2.05 | 0.75 |
| 10:A:1922:G:O2' | 31:V:25:C:C1' | 2.35 | 0.75 |
| 8:7:7:CYS:C | 8:7:8:VAL:HG23 | 2.07 | 0.74 |
| 6:5:131:THR:O | 6:5:134:GLU:N | 2.20 | 0.74 |
| 5:4:11:CYS:SG | 5:4:14:CYS:N | 2.60 | 0.74 |
| 11:B:23:G:O6 | 39:B:1307:HOH:O | 2.05 | 0.74 |
| 10:A:2006:C:OP1 | 39:A:3373:HOH:O | 2.04 | 0.74 |
| 6:5:1:MET:SD | 6:5:2:ALA:N | 2.58 | 0.74 |
| 10:A:1186:G:OP2 | 39:A:3592:HOH:O | 2.04 | 0.74 |
| 13:D:91:THR:O | 13:D:93:GLY:N | 2.21 | 0.74 |
| 10:A:1342:A:O2' | 10:A:1344:U:OP2 | 2.04 | 0.74 |
| 10:A:2707:U:O2 | 23:N:71:ARG:NH2 | 2.20 | 0.74 |
| 10:A:990:A:OP2 | 39:A:3591:HOH:O | 2.06 | 0.74 |
| 10:A:1153:C:OP2 | 39:A:3354:HOH:O | 2.04 | 0.74 |
| 10:A:2503:A:OP1 | 39:A:3661:HOH:O | 2.04 | 0.74 |
| 6:5:57:ASN:O | 6:5:59:LEU:N | 2.21 | 0.73 |
| 10:A:572:A:OP2 | 27:R:80:ARG:NH2 | 2.21 | 0.73 |
| 10:A:1782:U:C2 | 10:A:2586:U:O4 | 2.41 | 0.73 |
| 10:A:1782:U:N3 | 10:A:2586:U:N3 | 2.35 | 0.73 |
| 10:A:2056:G:OP2 | 39:A:3482:HOH:O | 2.06 | 0.73 |
| 19:J:43:GLU:O | 19:J:45:THR:N | 2.22 | 0.73 |
| 8:7:11:LYS:HE3 | 28:S:91:GLY:CA | 2.07 | 0.72 |
| 10:A:1970:A:OP2 | 39:A:3467:HOH:O | 2.07 | 0.72 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 10:A:1998:A:OP2 | 13:D:141:ARG:NH2 | 2.21 | 0.72 |
| 10:A:2062:A:H2' | 10:A:2063:C:H5 | 1.55 | 0.72 |
| 5:4:2:LYS:NZ | 10:A:2478:A:OP2 | 2.23 | 0.72 |
| 8:7:15:ILE:CG1 | 38:7:1002:TRP:HZ3 | 2.03 | 0.72 |
| 16:G:22:VAL:HG12 | 16:G:36:LEU:CD1 | 2.19 | 0.72 |
| 6:5:106:PHE:O | 6:5:108:VAL:N | 2.22 | 0.71 |
| 10:A:1439:A:OP2 | 39:A:3624:HOH:O | 2.07 | 0.71 |
| 10:A:1922:G:HO2' | 31:V:25:C:C2' | 2.00 | 0.71 |
| 8:7:22:HIS:CB | 10:A:2062:A:H61 | 2.03 | 0.71 |
| 10:A:981:A:OP1 | 39:A:3586:HOH:O | 2.08 | 0.71 |
| 10:A:621:A:OP2 | 39:A:3292:HOH:O | 2.08 | 0.71 |
| 10:A:1776:G:OP2 | 39:A:3448:HOH:O | 2.09 | 0.71 |
| 10:A:1993:U:H4' | 13:D:133:THR:HG21 | 1.73 | 0.71 |
| 10:A:2353:G:H1' | 32:W:30:VAL:HG12 | 1.72 | 0.71 |
| 25:P:5:LYS:NZ | 25:P:9:GLN:OE1 | 2.23 | 0.70 |
| 10:A:2057:G:OP2 | 39:A:3482:HOH:O | 2.08 | 0.70 |
| 10:A:1010:A:OP2 | 39:A:3769:HOH:O | 2.08 | 0.70 |
| 10:A:1805:A:N3 | 12:C:49:THR:OG1 | 2.24 | 0.70 |
| 10:A:1938:A:OP2 | 39:A:3721:HOH:O | 2.09 | 0.70 |
| 10:A:1604:C:OP1 | 39:A:3403:HOH:O | 2.09 | 0.70 |
| 10:A:2324:U:H3' | 10:A:2325:G:H5" | 1.74 | 0.70 |
| 15:F:116:LEU:N | 15:F:176:PHE:O | 2.24 | 0.70 |
| 10:A:1799:G:O2' | 12:C:179:GLU:OE2 | 2.07 | 0.70 |
| 10:A:1332:G:OP1 | 39:A:3752:HOH:O | 2.09 | 0.70 |
| 10:A:587:C:OP2 | 21:L:21:ARG:NH2 | 2.25 | 0.70 |
| 10:A:1782:U:N3 | 10:A:2586:U:C4 | 2.59 | 0.70 |
| 10:A:161:A:H3' | 10:A:162:U:H5" | 1.72 | 0.69 |
| 10:A:971:G:OP2 | 10:A:974:G:N2 | 2.25 | 0.69 |
| 10:A:512:G:N7 | 39:A:3758:HOH:O | 2.25 | 0.69 |
| 10:A:2091:C:O2 | 33:X:33:HIS:NE2 | 2.26 | 0.69 |
| 10:A:2247:A:OP1 | 39:A:3500:HOH:O | 2.10 | 0.69 |
| 35:Z:8:GLN:O | 35:Z:10:ARG:N | 2.25 | 0.69 |
| 8:7:19:ILE:HG23 | 8:7:20:VAL:HG22 | 1.73 | 0.69 |
| 10:A:2269:G:OP1 | 39:A:3504:HOH:O | 2.11 | 0.69 |
| 13:D:149:ASN:OD1 | 13:D:150:GLN:N | 2.26 | 0.69 |
| 22:M:66:ARG:NH1 | 22:M:104:GLU:OE2 | 2.26 | 0.68 |
| 6:5:25:ALA:O | 6:5:26:VAL:HG13 | 1.94 | 0.68 |
| 8:7:15:ILE:HG13 | 38:7:1002:TRP:HE3 | 1.59 | 0.68 |
| 6:5:117:LEU:HD22 | 6:5:120:ALA:HA | 1.76 | 0.68 |
| 10:A:42:A:C2' | 10:A:43:G:H5' | 2.24 | 0.68 |
| 10:A:948:C:O2 | 10:A:984:A:O2' | 2.12 | 0.68 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 32:W:30:VAL:HG13 | 32:W:30:VAL:O | 1.92 | 0.68 |
| 10:A:301:G:OP2 | 30:U:81:ARG:NH2 | 2.26 | 0.67 |
| 10:A:1782:U:O2 | 10:A:2586:U:O4 | 2.11 | 0.67 |
| 10:A:2602:A:H4' | 10:A:2603:G:H5' | 1.74 | 0.67 |
| 21:L:93:ASN:O | 21:L:95:LEU:N | 2.27 | 0.67 |
| 8:7:22:HIS:CD2 | 10:A:2503:A:C8 | 2.82 | 0.67 |
| 10:A:1614:A:N6 | 28:S:87:PRO:HB3 | 2.10 | 0.67 |
| 20:K:76:VAL:HB | 25:P:72:VAL:HG22 | 1.76 | 0.67 |
| 10:A:1936:A:N6 | 10:A:1963:U:O2 | 2.26 | 0.67 |
| 6:5:26:VAL:O | 6:5:27:VAL:HB | 1.93 | 0.67 |
| 8:7:19:ILE:HG23 | 8:7:20:VAL:CG2 | 2.25 | 0.67 |
| 10:A:324:A:N6 | 10:A:338:G:O2' | 2.27 | 0.67 |
| 10:A:1820:U:OP1 | 12:C:176:ARG:NH1 | 2.27 | 0.67 |
| 11:B:73:A:C4 | 11:B:104:A:C2 | 2.82 | 0.67 |
| 18:I:100:ILE:HB | 18:I:139:VAL:HA | 1.76 | 0.67 |
| 10:A:2615:U:OP1 | 39:A:3738:HOH:O | 2.12 | 0.67 |
| 20:K:18:ARG:HB2 | 20:K:45:GLU:HB2 | 1.77 | 0.66 |
| 10:A:1658:C:OP1 | 39:A:3647:HOH:O | 2.11 | 0.66 |
| 19:J:4:PHE:N | 19:J:44:TYR:OH | 2.28 | 0.66 |
| 10:A:120:U:OP1 | 39:A:3220:HOH:O | 2.12 | 0.66 |
| 10:A:1417:C:HO2' | 10:A:1587:G:HO2' | 1.43 | 0.66 |
| 10:A:2602:A:O2' | 31:V:74:C:OP1 | 2.12 | 0.66 |
| 10:A:819:A:OP2 | 10:A:1187:G:N2 | 2.23 | 0.66 |
| 28:S:88:ARG:HB3 | 28:S:88:ARG:CZ | 2.26 | 0.66 |
| 32:W:37:VAL:HG12 | 32:W:38:ARG:H | 1.61 | 0.66 |
| 6:5:24:SER:CB | 6:5:116:GLU:HG2 | 2.24 | 0.66 |
| 21:L:93:ASN:OD1 | 21:L:94:THR:N | 2.28 | 0.66 |
| 6:5:39:THR:HA | 6:5:42:ARG:HD2 | 1.78 | 0.66 |
| 8:7:21:ASP:O | 8:7:23:ARG:N | 2.29 | 0.65 |
| 10:A:2062:A:OP2 | 39:A:3490:HOH:O | 2.14 | 0.65 |
| 10:A:363:G:H2' | 10:A:364:C:C6 | 2.31 | 0.65 |
| 19:J:6:ALA:HB3 | 19:J:45:THR:HG21 | 1.78 | 0.65 |
| 8:7:7:CYS:C | 8:7:8:VAL:CG2 | 2.61 | 0.65 |
| 8:7:11:LYS:HE2 | 28:S:91:GLY:CA | 2.17 | 0.65 |
| 8:7:15:ILE:CG1 | 38:7:1002:TRP:CE3 | 2.78 | 0.65 |
| 20:K:71:ARG:HB3 | 20:K:72:PRO:HD3 | 1.78 | 0.65 |
| 10:A:1908:C:O2' | 31:V:12:G:C5' | 2.45 | 0.65 |
| 10:A:1482:G:H1' | 10:A:1509:A:H61 | 1.62 | 0.65 |
| 10:A:1670:C:OP1 | 39:A:3432:HOH:O | 2.14 | 0.65 |
| 10:A:1199:U:H5' | 26:Q:4:LYS:HE3 | 1.79 | 0.64 |
| 10:A:999:U:OP2 | 39:A:3355:HOH:O | 2.15 | 0.64 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 10:A:1669:A:OP2 | 39:A:3713:HOH:O | 2.15 | 0.64 |
| 16:G:38:ASP:N | 16:G:38:ASP:OD1 | 2.29 | 0.64 |
| 23:N:118:ARG:O | 23:N:120:GLU:N | 2.30 | 0.64 |
| 10:A:2602:A:H2' | 31:V:74:C:H5" | 1.80 | 0.64 |
| 16:G:1:SER:O | 16:G:3:VAL:N | 2.31 | 0.64 |
| 12:C:43:ASN:OD1 | 12:C:44:ASN:N | 2.30 | 0.64 |
| 18:I:73:PRO:O | 18:I:112:LYS:NZ | 2.31 | 0.64 |
| 25:P:4:ILE:O | 25:P:6:GLN:N | 2.31 | 0.64 |
| 28:S:18:ARG:O | 28:S:19:LEU:HB2 | 1.98 | 0.64 |
| 10:A:1617:C:OP1 | 39:A:3417:HOH:O | 2.15 | 0.64 |
| 10:A:2142:A:H4' | 10:A:2143:C:OP2 | 1.96 | 0.64 |
| 10:A:2608:G:C8 | 10:A:2608:G:C5' | 2.76 | 0.64 |
| 25:P:50:ARG:HG3 | 25:P:57:ALA:O | 1.97 | 0.64 |
| 32:W:35:ILE:O | 32:W:37:VAL:N | 2.31 | 0.63 |
| 19:J:44:TYR:HB2 | 26:Q:63:ARG:HB3 | 1.79 | 0.63 |
| 14:E:58:LYS:NZ | 14:E:70:SER:O | 2.31 | 0.63 |
| 10:A:1385:A:H1' | 10:A:1386:C:C6 | 2.34 | 0.63 |
| 11:B:87:U:H3' | 11:B:88:C:H5' | 1.80 | 0.63 |
| 30:U:73:ASN:ND2 | 30:U:80:ASP:OD2 | 2.31 | 0.63 |
| 10:A:42:A:H2' | 10:A:43:G:H5' | 1.80 | 0.63 |
| 25:P:50:ARG:CB | 25:P:57:ALA:H | 2.11 | 0.63 |
| 29:T:32:LEU:H | 29:T:83:ALA:HB3 | 1.63 | 0.63 |
| 1:0:42:ILE:HD11 | 23:N:98:LEU:HB3 | 1.79 | 0.63 |
| 10:A:546:U:O2' | 10:A:547:A:H4' | 1.99 | 0.63 |
| 10:A:1614:A:N1 | 28:S:87:PRO:HB3 | 2.13 | 0.63 |
| 10:A:2062:A:O2' | 10:A:2063:C:H6 | 1.82 | 0.63 |
| 10:A:2588:G:OP2 | 39:A:3538:HOH:O | 2.15 | 0.63 |
| 28:S:88:ARG:HG2 | 28:S:88:ARG:HH11 | 1.64 | 0.63 |
| 8:7:19:ILE:HG13 | 8:7:20:VAL:H | 1.63 | 0.62 |
| 6:5:129:LEU:O | 6:5:131:THR:N | 2.26 | 0.62 |
| 10:A:1567:G:H5' | 12:C:57:HIS:CD2 | 2.35 | 0.62 |
| 28:S:88:ARG:HG2 | 28:S:94:ASP:OD2 | 1.99 | 0.62 |
| 10:A:1813:G:H1' | 12:C:49:THR:HG21 | 1.81 | 0.62 |
| 8:7:19:ILE:C | 8:7:20:VAL:CG2 | 2.66 | 0.62 |
| 10:A:2061:G:OP2 | 39:A:3489:HOH:O | 2.16 | 0.62 |
| 18:I:108:ILE:O | 18:I:111:THR:OG1 | 2.17 | 0.62 |
| 30:U:15:GLY:O | 30:U:17:ASP:N | 2.32 | 0.62 |
| 10:A:923:G:H1' | 32:W:23:LYS:HD3 | 1.81 | 0.62 |
| 10:A:1922:G:O2' | 31:V:25:C:C2' | 2.47 | 0.62 |
| 10:A:1938:A:OP2 | 39:A:3719:HOH:O | 2.16 | 0.62 |
| 10:A:2346:A:H3' | 10:A:2347:C:C5' | 2.29 | 0.62 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 10:A:2011:U:OP2 | 28:S:16:LYS:NZ | 2.31 | 0.62 |
| 8:7:21:ASP:OD2 | 38:7:1001:TRP:CZ3 | 2.53 | 0.62 |
| 10:A:861:A:N3 | 11:B:79:G:O2' | 2.27 | 0.62 |
| 18:I:131:THR:O | 18:I:134:SER:OG | 2.16 | 0.62 |
| 10:A:163:C:O2' | 10:A:164:C:O5' | 2.17 | 0.61 |
| 10:A:1922:G:O3' | 31:V:25:C:C4' | 2.47 | 0.61 |
| 24:O:76:LYS:NZ | 24:O:80:GLU:OE2 | 2.29 | 0.61 |
| 23:N:73:ASN:HA | 23:N:76:VAL:HG12 | 1.81 | 0.61 |
| 6:5:27:VAL:HG13 | 6:5:83:ALA:HB3 | 1.83 | 0.61 |
| 6:5:29:ASP:HA | 6:5:108:VAL:HG11 | 1.82 | 0.61 |
| 10:A:2062:A:HO2' | 10:A:2063:C:H6 | 1.49 | 0.61 |
| 10:A:856:G:H21 | 32:W:19:ARG:NH2 | 1.97 | 0.61 |
| 10:A:1248:G:N7 | 14:E:46:GLN:NE2 | 2.48 | 0.61 |
| 5:4:36:ARG:HG2 | 5:4:37:GLN:H | 1.66 | 0.61 |
| 19:J:6:ALA:CB | 19:J:45:THR:HG21 | 2.31 | 0.61 |
| 10:A:963:U:OP2 | 39:A:3353:HOH:O | 2.16 | 0.61 |
| 10:A:1803:A:O3' | 12:C:256:THR:OG1 | 2.19 | 0.61 |
| 7:6:18:ASP:OD1 | 7:6:18:ASP:N | 2.32 | 0.60 |
| 32:W:55:ASP:O | 32:W:57:THR:N | 2.34 | 0.60 |
| 10:A:511:U:OP2 | 39:A:3759:HOH:O | 2.15 | 0.60 |
| 10:A:1359:A:OP1 | 39:A:3608:HOH:O | 2.16 | 0.60 |
| 18:I:100:ILE:HG22 | 18:I:101:SER:N | 2.15 | 0.60 |
| 23:N:98:LEU:O | 23:N:112:TYR:N | 2.34 | 0.60 |
| 10:A:2353:G:N3 | 32:W:30:VAL:CG1 | 2.65 | 0.60 |
| 13:D:118:PHE:HD1 | 13:D:119:ALA:H | 1.49 | 0.60 |
| 32:W:63:ASP:OD1 | 32:W:63:ASP:N | 2.35 | 0.60 |
| 10:A:983:A:C6 | 10:A:984:A:C2 | 2.90 | 0.60 |
| 10:A:1828:G:OP2 | 39:A:3793:HOH:O | 2.16 | 0.60 |
| 12:C:16:VAL:N | 12:C:203:VAL:HG12 | 2.17 | 0.60 |
| 24:O:89:ASP:HA | 24:O:116:GLN:HB3 | 1.84 | 0.60 |
| 29:T:19:LYS:O | 29:T:23:ALA:N | 2.35 | 0.60 |
| 10:A:480:A:OP2 | 30:U:43:LYS:NZ | 2.34 | 0.60 |
| 10:A:616:A:H4' | 14:E:101:TYR:CE2 | 2.36 | 0.59 |
| 10:A:1262:A:OP2 | 28:S:99:ARG:NH2 | 2.35 | 0.59 |
| 30:U:38:ILE:CG2 | 30:U:39:ASN:N | 2.64 | 0.59 |
| 10:A:1782:U:C4 | 10:A:2586:U:N3 | 2.70 | 0.59 |
| 8:7:22:HIS:HB2 | 10:A:2062:A:H61 | 1.67 | 0.59 |
| 10:A:1338:G:O2' | 29:T:18:GLU:OE2 | 2.20 | 0.59 |
| 10:A:1782:U:O2' | 10:A:2608:G:O2' | 2.21 | 0.59 |
| 6:5:26:VAL:HG21 | 6:5:115:GLY:N | 2.06 | 0.59 |
| 8:7:19:ILE:HA | 38:7:1001:TRP:CD1 | 2.38 | 0.59 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 10:A:2062:A:C2' | 10:A:2063:C:C6 | 2.85 | 0.59 |
| 10:A:800:A:OP1 | 39:A:3321:HOH:O | 2.17 | 0.59 |
| 10:A:635:C:OP2 | 21:L:126:ARG:NH2 | 2.35 | 0.59 |
| 18:I:92:PRO:O | 18:I:94:LYS:N | 2.36 | 0.59 |
| 24:O:105:ALA:O | 24:O:107:ALA:N | 2.35 | 0.59 |
| 6:5:15:VAL:HG22 | 6:5:66:GLY:HA3 | 1.84 | 0.59 |
| 10:A:1922:G:O2' | 31:V:25:C:O2' | 1.73 | 0.59 |
| 10:A:2800:A:H3' | 10:A:2801:G:C5' | 2.32 | 0.59 |
| 14:E:168:ASP:OD2 | 14:E:170:ARG:NH1 | 2.36 | 0.59 |
| 18:I:93:ASN:ND2 | 18:I:135:MET:O | 2.35 | 0.59 |
| 8:7:22:HIS:HB3 | 10:A:2062:A:H61 | 1.66 | 0.59 |
| 22:M:41:LEU:HD11 | 22:M:126:ILE:HD13 | 1.85 | 0.59 |
| 8:7:22:HIS:O | 8:7:23:ARG:HG3 | 2.03 | 0.59 |
| 10:A:276:U:O2' | 10:A:278:A:N7 | 2.34 | 0.59 |
| 10:A:673:C:OP1 | 14:E:49:ARG:NH1 | 2.36 | 0.59 |
| 10:A:1131:G:OP1 | 19:J:82:GLY:HA2 | 2.02 | 0.59 |
| 29:T:35:ALA:HB3 | 29:T:38:ALA:HB2 | 1.85 | 0.58 |
| 32:W:51:GLY:HA3 | 32:W:59:PHE:CZ | 2.38 | 0.58 |
| 8:7:19:ILE:O | 8:7:20:VAL:CG2 | 2.47 | 0.58 |
| 26:Q:84:LYS:O | 26:Q:86:SER:N | 2.36 | 0.58 |
| 10:A:370:G:OP2 | 39:A:3553:HOH:O | 2.16 | 0.58 |
| 10:A:1654:A:O2' | 13:D:118:PHE:CG | 2.55 | 0.58 |
| 10:A:1359:A:OP1 | 39:A:3611:HOH:O | 2.17 | 0.58 |
| 10:A:1386:C:H2' | 10:A:1387:A:C8 | 2.39 | 0.58 |
| 10:A:2780:G:OP2 | 19:J:120:ARG:NE | 2.33 | 0.58 |
| 12:C:77:VAL:HG23 | 12:C:111:ALA:HA | 1.85 | 0.58 |
| 10:A:2499:C:O2 | 39:A:3524:HOH:O | 2.13 | 0.58 |
| 26:Q:63:ARG:NH1 | 26:Q:95:ALA:O | 2.36 | 0.58 |
| 10:A:370:G:O2' | 10:A:424:G:OP1 | 2.15 | 0.58 |
| 10:A:1076:C:H2' | 10:A:1077:A:O4' | 2.04 | 0.58 |
| 18:I:37:PHE:O | 18:I:41:PHE:HB3 | 2.04 | 0.58 |
| 25:P:63:ILE:HA | 25:P:68:GLY:HA2 | 1.85 | 0.58 |
| 6:5:45:GLY:HA2 | 6:5:49:GLY:HA2 | 1.86 | 0.58 |
| 10:A:1930:G:O2' | 10:A:1968:G:O6 | 2.17 | 0.57 |
| 10:A:2579:C:OP1 | 39:A:3535:HOH:O | 2.18 | 0.57 |
| 32:W:51:GLY:HA3 | 32:W:59:PHE:CE1 | 2.38 | 0.57 |
| 26:Q:81:GLY:O | 26:Q:85:ALA:N | 2.37 | 0.57 |
| 10:A:2548:U:O2 | 20:K:23:LYS:NZ | 2.37 | 0.57 |
| 32:W:39:GLN:HG2 | 32:W:41:GLY:H | 1.69 | 0.57 |
| 10:A:802:A:OP1 | 39:A:3327:HOH:O | 2.17 | 0.57 |
| 10:A:1076:C:H1' | 18:I:93:ASN:HB3 | 1.86 | 0.57 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 25:P:50:ARG:HB3 | 25:P:57:ALA:N | 2.17 | 0.57 |
| 10:A:2502:G:OP2 | 39:A:3488:HOH:O | 2.18 | 0.57 |
| 10:A:2517:C:C6 | 10:A:2542:A:N7 | 2.73 | 0.57 |
| 32:W:9:THR:OG1 | 32:W:10:ARG:N | 2.31 | 0.57 |
| 32:W:28:GLU:HB3 | 32:W:31:LEU:HD21 | 1.86 | 0.57 |
| 32:W:76:ARG:HH11 | 32:W:76:ARG:CG | 2.17 | 0.57 |
| 6:5:3:LEU:CD1 | 6:5:5:LEU:HG | 2.35 | 0.57 |
| 10:A:27:G:O2' | 10:A:28:A:OP2 | 2.19 | 0.57 |
| 10:A:1773:A:N7 | 10:A:1829:A:H1' | 2.20 | 0.57 |
| 25:P:58:PHE:CD1 | 25:P:75:THR:HG22 | 2.40 | 0.57 |
| 10:A:422:A:C2 | 10:A:423:A:C4 | 2.92 | 0.57 |
| 10:A:1019:U:H3 | 10:A:1142:A:H62 | 1.53 | 0.57 |
| 26:Q:105:PHE:O | 26:Q:108:LEU:N | 2.38 | 0.57 |
| 10:A:2331:G:O2' | 10:A:2336:A:N1 | 2.38 | 0.57 |
| 6:5:62:ARG:NH2 | 10:A:1106:G:OP1 | 2.35 | 0.56 |
| 24:O:2:ASP:OD1 | 24:O:3:LYS:N | 2.39 | 0.56 |
| 33:X:32:LEU:O | 33:X:33:HIS:ND1 | 2.39 | 0.56 |
| 6:5:132:TYR:CZ | 7:6:23:ILE:HD11 | 2.40 | 0.56 |
| 10:A:1923:U:H5' | 31:V:25:C:O4' | 2.04 | 0.56 |
| 10:A:2439:A:N6 | 31:V:76:A:OP1 | 2.39 | 0.56 |
| 14:E:150:THR:HG21 | 14:E:153:LEU:HA | 1.87 | 0.56 |
| 29:T:54:GLU:HG3 | 29:T:88:LYS:HB2 | 1.86 | 0.56 |
| 10:A:85:G:OP2 | 30:U:6:ARG:HG3 | 2.06 | 0.56 |
| 10:A:1676:A:OP2 | 39:A:3755:HOH:O | 2.18 | 0.56 |
| 10:A:1936:A:H2 | 10:A:1943:U:C5 | 2.23 | 0.56 |
| 28:S:88:ARG:HH11 | 28:S:88:ARG:CG | 2.17 | 0.56 |
| 3:2:3:ARG:HH22 | 10:A:752:A:P | 2.29 | 0.56 |
| 10:A:1315:C:OP2 | 39:A:3750:HOH:O | 2.18 | 0.56 |
| 26:Q:63:ARG:HH22 | 26:Q:95:ALA:C | 2.08 | 0.56 |
| 1:0:2:VAL:HG22 | 10:A:2015:A:C2 | 2.41 | 0.56 |
| 6:5:81:LEU:HA | 10:A:1107:G:H4' | 1.88 | 0.56 |
| 13:D:118:PHE:O | 13:D:120:GLY:N | 2.36 | 0.56 |
| 10:A:910:A:N6 | 10:A:2277:G:O2' | 2.36 | 0.56 |
| 10:A:1353:A:C8 | 10:A:1378:A:N6 | 2.73 | 0.56 |
| 10:A:2681:C:OP2 | 13:D:114:LYS:NZ | 2.33 | 0.56 |
| 12:C:14:HIS:O | 12:C:203:VAL:HG11 | 2.05 | 0.56 |
| 20:K:121:GLU:OE2 | 25:P:62:LYS:NZ | 2.36 | 0.56 |
| 8:7:14:ASN:C | 8:7:15:ILE:CG1 | 2.74 | 0.56 |
| 8:7:19:ILE:HA | 38:7:1001:TRP:NE1 | 2.20 | 0.56 |
| 6:5:56:ARG:O | 6:5:57:ASN:ND2 | 2.39 | 0.56 |
| 10:A:1324:G:C4 | 10:A:1328:A:N6 | 2.74 | 0.56 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 19:J:81:ILE:HG13 | 19:J:82:GLY:N | 2.21 | 0.56 |
| 5:4:36:ARG:NH1 | 10:A:2742:G:OP1 | 2.38 | 0.55 |
| 6:5:58:THR:CG2 | 10:A:1107:G:H5" | 2.36 | 0.55 |
| 10:A:2355:G:H4' | 32:W:20:LEU:HD13 | 1.88 | 0.55 |
| 10:A:2757:A:N1 | 16:G:66:THR:HG21 | 2.21 | 0.55 |
| 15:F:151:LEU:HD12 | 15:F:152:ASP:N | 2.21 | 0.55 |
| 27:R:39:LEU:O | 27:R:49:ILE:HG23 | 2.07 | 0.55 |
| 2:1:8:ILE:HD11 | 2:1:24:LYS:N | 2.21 | 0.55 |
| 10:A:100:U:H4' | 10:A:101:A:O5' | 2.06 | 0.55 |
| 10:A:1482:G:C6 | 10:A:1508:A:C2 | 2.94 | 0.55 |
| 10:A:443:A:N7 | 14:E:40:ARG:HD3 | 2.21 | 0.55 |
| 21:L:85:VAL:CG2 | 21:L:94:THR:HG22 | 2.36 | 0.55 |
| 25:P:33:GLU:HB2 | 25:P:38:ARG:HH21 | 1.71 | 0.55 |
| 28:S:89:ALA:HA | 28:S:90:LYS:O | 2.07 | 0.55 |
| 6:5:64:VAL:O | 6:5:68:PRO:HD2 | 2.07 | 0.55 |
| 6:5:129:LEU:C | 6:5:131:THR:H | 2.10 | 0.55 |
| 18:I:116:MET:SD | 18:I:124:MET:HE2 | 2.46 | 0.55 |
| 10:A:283:G:C2 | 10:A:284:U:H1' | 2.41 | 0.55 |
| 32:W:18:LYS:HG3 | 32:W:19:ARG:N | 2.21 | 0.55 |
| 10:A:163:C:O2' | 10:A:164:C:P | 2.65 | 0.55 |
| 10:A:1397:U:OP2 | 10:A:1398:C:N4 | 2.34 | 0.55 |
| 18:I:100:ILE:HD11 | 18:I:137:LEU:HG | 1.88 | 0.55 |
| 10:A:1909:C:H4' | 31:V:11:C:C4' | 2.30 | 0.55 |
| 10:A:2698:U:H2' | 10:A:2699:C:H6 | 1.72 | 0.55 |
| 35:Z:5:LYS:H | 35:Z:5:LYS:HD2 | 1.72 | 0.55 |
| 10:A:686:U:H2' | 10:A:788:A:N1 | 2.21 | 0.55 |
| 10:A:834:G:C6 | 10:A:835:C:C4 | 2.95 | 0.55 |
| 19:J:17:VAL:HG23 | 19:J:139:VAL:HA | 1.88 | 0.55 |
| 29:T:59:ASN:O | 29:T:83:ALA:O | 2.24 | 0.55 |
| 6:5:44:ALA:O | 6:5:49:GLY:N | 2.40 | 0.55 |
| 10:A:31:C:OP1 | 39:A:3696:HOH:O | 2.18 | 0.55 |
| 10:A:1001:A:OP2 | 39:A:3726:HOH:O | 2.18 | 0.55 |
| 6:5:129:LEU:HB3 | 6:5:130:PRO:HD2 | 1.89 | 0.55 |
| 10:A:1458:U:H4' | 10:A:1459:G:O5' | 2.07 | 0.55 |
| 10:A:2335:A:C6 | 10:A:2337:G:H1' | 2.42 | 0.55 |
| 12:C:68:ARG:CD | 12:C:103:ILE:HD11 | 2.37 | 0.55 |
| 23:N:30:ARG:NH1 | 23:N:74:GLU:OE2 | 2.40 | 0.55 |
| 10:A:811:U:C4 | 21:L:21:ARG:NH1 | 2.74 | 0.54 |
| 10:A:1759:A:HO2' | 10:A:2714:G:HO2' | 1.49 | 0.54 |
| 10:A:1824:G:N3 | 12:C:251:THR:HG21 | 2.21 | 0.54 |
| 10:A:1936:A:N6 | 10:A:1963:U:H3 | 2.05 | 0.54 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 18:I:135:MET:HB3 | 18:I:137:LEU:HD22 | 1.88 | 0.54 |
| 20:K:43:ILE:CD1 | 20:K:52:VAL:HB | 2.37 | 0.54 |
| 1:0:2:VAL:HG11 | 10:A:2016:U:H1' | 1.89 | 0.54 |
| 8:7:15:ILE:CD1 | 38:7:1002:TRP:CE3 | 2.90 | 0.54 |
| 10:A:565:C:O3' | 39:A:3329:HOH:O | 2.18 | 0.54 |
| 10:A:1909:C:C4' | 31:V:11:C:O2' | 2.55 | 0.54 |
| 29:T:32:LEU:N | 29:T:83:ALA:HB3 | 2.21 | 0.54 |
| 10:A:784:G:O2' | 10:A:785:G:OP2 | 2.15 | 0.54 |
| 13:D:107:VAL:CG2 | 13:D:203:VAL:HG23 | 2.37 | 0.54 |
| 25:P:50:ARG:CG | 25:P:57:ALA:O | 2.55 | 0.54 |
| 26:Q:91:ARG:NH1 | 27:R:10:LYS:HB3 | 2.23 | 0.54 |
| 6:5:60:LEU:O | 6:5:64:VAL:HB | 2.08 | 0.54 |
| 10:A:674:G:H1' | 14:E:69:ARG:HE | 1.72 | 0.54 |
| 10:A:877:A:C2 | 10:A:899:A:C2 | 2.96 | 0.54 |
| 10:A:2585:U:O2 | 10:A:2585:U:H2' | 2.06 | 0.54 |
| 27:R:49:ILE:HB | 27:R:51:VAL:O | 2.08 | 0.54 |
| 28:S:73:LYS:HB3 | 28:S:106:VAL:HB | 1.90 | 0.54 |
| 10:A:277:G:O2' | 10:A:278:A:OP2 | 2.25 | 0.54 |
| 10:A:855:G:H1' | 32:W:23:LYS:HE3 | 1.89 | 0.54 |
| 10:A:1786:A:H1' | 10:A:1938:A:N6 | 2.22 | 0.54 |
| 30:U:38:ILE:HG22 | 30:U:39:ASN:H | 1.73 | 0.54 |
| 6:5:43:LYS:HZ3 | 6:5:98:GLU:HB2 | 1.72 | 0.54 |
| 10:A:265:A:H4' | 10:A:266:G:OP1 | 2.07 | 0.54 |
| 10:A:1772:A:N1 | 10:A:1980:G:C6 | 2.76 | 0.54 |
| 10:A:2680:U:H5' | 13:D:194:PRO:HA | 1.88 | 0.54 |
| 30:U:21:ARG:CZ | 30:U:72:PHE:CE2 | 2.90 | 0.54 |
| 9:8:80:HIS:HD2 | 9:8:83:LYS:N | 2.05 | 0.54 |
| 18:I:98:GLY:HA3 | 18:I:137:LEU:HB3 | 1.90 | 0.54 |
| 25:P:4:ILE:HG22 | 25:P:5:LYS:H | 1.72 | 0.54 |
| 27:R:49:ILE:HG22 | 27:R:54:VAL:HG13 | 1.89 | 0.54 |
| 1:0:12:ARG:NH1 | 10:A:1263:U:OP1 | 2.41 | 0.54 |
| 6:5:58:THR:HB | 6:5:82:ILE:HB | 1.89 | 0.54 |
| 10:A:84:A:P | 30:U:5:ARG:NH1 | 2.81 | 0.54 |
| 10:A:1754:A:H4' | 25:P:102:ARG:NH2 | 2.22 | 0.54 |
| 15:F:103:ILE:HG23 | 15:F:175:PRO:HD3 | 1.90 | 0.54 |
| 21:L:77:ILE:CD1 | 21:L:108:ALA:HB1 | 2.38 | 0.54 |
| 8:7:12:TRP:O | 8:7:13:PHE:O | 2.26 | 0.54 |
| 10:A:1535:A:H4' | 10:A:1536:C:OP2 | 2.08 | 0.54 |
| 6:5:4:ASN:O | 6:5:6:GLN:N | 2.41 | 0.53 |
| 10:A:1080:A:H1' | 18:I:127:SER:HA | 1.91 | 0.53 |
| 10:A:1187:G:H5" | 27:R:83:TYR:CE2 | 2.43 | 0.53 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 10:A:1750:G:O2' | 10:A:2860:A:N1 | 2.37 | 0.53 |
| 30:U:35:VAL:HB | 30:U:38:ILE:HG21 | 1.90 | 0.53 |
| 6:5:23:LEU:HG | 6:5:24:SER:N | 2.22 | 0.53 |
| 13:D:106:LYS:HB3 | 13:D:206:ALA:HB3 | 1.89 | 0.53 |
| 6:5:54:VAL:HA | 6:5:84:TYR:O | 2.08 | 0.53 |
| 10:A:1779:U:H5 | 10:A:1784:A:N7 | 2.06 | 0.53 |
| 13:D:120:GLY:HA2 | 13:D:162:ALA:CB | 2.38 | 0.53 |
| 20:K:80:ASP:HB2 | 25:P:67:GLU:HG3 | 1.90 | 0.53 |
| 5:4:1:MET:N | 10:A:2526:G:N3 | 2.57 | 0.53 |
| 10:A:954:G:OP2 | 22:M:16:ARG:NH2 | 2.42 | 0.53 |
| 10:A:1069:A:C4 | 10:A:1073:A:N7 | 2.77 | 0.53 |
| 10:A:411:G:OP2 | 10:A:2406:A:O2' | 2.25 | 0.53 |
| 10:A:2415:G:H4' | 21:L:66:PHE:HB2 | 1.90 | 0.53 |
| 16:G:84:LYS:HB3 | 16:G:132:LEU:O | 2.09 | 0.53 |
| 29:T:50:LEU:C | 29:T:52:GLU:H | 2.11 | 0.53 |
| 29:T:50:LEU:HD12 | 29:T:50:LEU:H | 1.74 | 0.53 |
| 32:W:37:VAL:HG13 | 32:W:55:ASP:C | 2.29 | 0.53 |
| 8:7:22:HIS:HD2 | 10:A:2503:A:H8 | 1.52 | 0.53 |
| 10:A:396:G:OP2 | 33:X:9:LYS:NZ | 2.40 | 0.53 |
| 10:A:1614:A:N6 | 28:S:91:GLY:HA2 | 2.23 | 0.53 |
| 19:J:32:LEU:HD22 | 19:J:54:ILE:HD12 | 1.90 | 0.53 |
| 22:M:33:LEU:HD22 | 22:M:128:THR:HB | 1.90 | 0.53 |
| 26:Q:93:ILE:O | 26:Q:96:ASP:N | 2.39 | 0.53 |
| 32:W:13:ARG:HG2 | 32:W:14:ASP:H | 1.74 | 0.53 |
| 10:A:729:G:H2' | 10:A:1775:U:H1' | 1.91 | 0.53 |
| 10:A:2211:A:O2' | 10:A:2212:A:OP1 | 2.25 | 0.53 |
| 10:A:2425:A:H5" | 10:A:2427:C:O4' | 2.09 | 0.53 |
| 10:A:2405:G:O2' | 10:A:2406:A:OP1 | 2.26 | 0.53 |
| 10:A:2547:A:H2' | 10:A:2548:U:C6 | 2.43 | 0.53 |
| 10:A:2602:A:H4' | 10:A:2603:G:C5' | 2.39 | 0.53 |
| 16:G:84:LYS:HG3 | 16:G:132:LEU:H | 1.73 | 0.53 |
| 19:J:39:LYS:HA | 19:J:43:GLU:HB2 | 1.91 | 0.53 |
| 20:K:107:LEU:O | 20:K:109:SER:N | 2.38 | 0.53 |
| 10:A:1378:A:O2' | 10:A:1380:G:N7 | 2.27 | 0.53 |
| 32:W:46:ALA:HB3 | 32:W:80:SER:HB3 | 1.91 | 0.53 |
| 10:A:2533:U:OP1 | 10:A:2665:A:O2' | 2.20 | 0.53 |
| 23:N:73:ASN:HA | 23:N:76:VAL:CG1 | 2.39 | 0.53 |
| 26:Q:31:TYR:O | 26:Q:34:ALA:N | 2.42 | 0.53 |
| 26:Q:81:GLY:HA2 | 26:Q:116:LEU:CD1 | 2.38 | 0.53 |
| 10:A:2232:C:P | 33:X:26:ARG:HH22 | 2.33 | 0.52 |
| 20:K:10:VAL:HG11 | 20:K:16:ALA:HB3 | 1.90 | 0.52 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 24:O:31:THR:HG22 | 24:O:34:HIS:H | 1.74 | 0.52 |
| 6:5:25:ALA:HB3 | 6:5:85:SER:OG | 2.09 | 0.52 |
| 10:A:299:A:OP2 | 39:A:3547:HOH:O | 2.18 | 0.52 |
| 10:A:384:A:H2' | 10:A:385:C:H5' | 1.90 | 0.52 |
| 10:A:947:A:HO2' | 10:A:984:A:H2 | 1.58 | 0.52 |
| 10:A:1288:G:C4 | 10:A:1327:A:C2 | 2.98 | 0.52 |
| 10:A:1738:G:O2' | 10:A:1739:A:O5' | 2.25 | 0.52 |
| 10:A:2092:U:H4' | 10:A:2093:G:O5' | 2.09 | 0.52 |
| 10:A:2297:A:N1 | 10:A:2321:U:H5 | 2.07 | 0.52 |
| 8:7:24:PRO:HG2 | 31:V:76:A:O3' | 2.09 | 0.52 |
| 10:A:2134:A:HO2' | 10:A:2135:A:H8 | 1.55 | 0.52 |
| 20:K:70:ARG:HD3 | 20:K:76:VAL:HG22 | 1.90 | 0.52 |
| 10:A:1509:A:HO2' | 10:A:1510:G:P | 2.29 | 0.52 |
| 10:A:2502:G:H5' | 10:A:2503:A:H5" | 1.92 | 0.52 |
| 10:A:1332:G:OP1 | 39:A:3750:HOH:O | 2.18 | 0.52 |
| 10:A:1715:G:N2 | 10:A:1744:A:OP2 | 2.36 | 0.52 |
| 1:0:2:VAL:CG1 | 10:A:2016:U:H1' | 2.40 | 0.52 |
| 10:A:1417:C:O2' | 10:A:1587:G:O2' | 2.19 | 0.52 |
| 19:J:55:ILE:HD11 | 19:J:130:HIS:CG | 2.45 | 0.52 |
| 26:Q:63:ARG:HH12 | 26:Q:96:ASP:CA | 2.22 | 0.52 |
| 10:A:38:A:O2' | 14:E:43:THR:HA | 2.09 | 0.52 |
| 34:Y:56:LEU:O | 34:Y:58:ASN:N | 2.39 | 0.52 |
| 6:5:118:ILE:HB | 6:5:119:PRO:CD | 2.39 | 0.52 |
| 10:A:2313:C:H5" | 15:F:87:LYS:HD3 | 1.92 | 0.52 |
| 27:R:61:ALA:HB2 | 27:R:98:ILE:HA | 1.92 | 0.52 |
| 29:T:69:ARG:CG | 29:T:70:HIS:H | 2.23 | 0.52 |
| 30:U:82:VAL:HG12 | 30:U:83:GLY:N | 2.25 | 0.52 |
| 6:5:25:ALA:O | 6:5:116:GLU:OE1 | 2.28 | 0.52 |
| 8:7:14:ASN:OD1 | 14:E:61:ARG:NH1 | 2.41 | 0.52 |
| 10:A:1776:G:OP2 | 39:A:3446:HOH:O | 2.19 | 0.52 |
| 16:G:83:THR:HA | 16:G:84:LYS:CE | 2.39 | 0.52 |
| 35:Z:48:ASN:O | 35:Z:51:SER:OG | 2.27 | 0.52 |
| 5:4:3:VAL:HG23 | 5:4:4:ARG:H | 1.74 | 0.52 |
| 6:5:43:LYS:NZ | 6:5:98:GLU:HB2 | 2.24 | 0.52 |
| 6:5:81:LEU:HD23 | 6:5:82:ILE:N | 2.24 | 0.52 |
| 8:7:15:ILE:HD12 | 38:7:1002:TRP:CZ3 | 2.41 | 0.52 |
| 10:A:273:G:N2 | 10:A:365:U:C2 | 2.77 | 0.52 |
| 10:A:1069:A:C5 | 10:A:1073:A:N7 | 2.77 | 0.52 |
| 10:A:2053:G:H1 | 10:A:2616:C:H42 | 1.57 | 0.52 |
| 29:T:44:LYS:HG3 | 29:T:55:VAL:HG11 | 1.90 | 0.52 |
| 2:1:20:TYR:HH | 10:A:2347:C:HO2' | 1.56 | 0.51 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 10:A:489:G:N7 | 28:S:49:LYS:NZ | 2.58 | 0.51 |
| 10:A:1328:A:H2' | 10:A:1330:C:C5 | 2.45 | 0.51 |
| 32:W:8:SER:O | 32:W:9:THR:HG22 | 2.10 | 0.51 |
| 32:W:37:VAL:HB | 32:W:38:ARG:HH11 | 1.74 | 0.51 |
| 10:A:1277:G:C5' | 23:N:20:MET:HE2 | 2.40 | 0.51 |
| 10:A:2039:U:H2' | 10:A:2040:G:C8 | 2.45 | 0.51 |
| 12:C:255:LYS:O | 12:C:257:ARG:N | 2.43 | 0.51 |
| 19:J:39:LYS:HA | 19:J:43:GLU:HG3 | 1.91 | 0.51 |
| 25:P:33:GLU:CD | 25:P:34:GLY:N | 2.63 | 0.51 |
| 25:P:50:ARG:CD | 25:P:51:ASN:N | 2.72 | 0.51 |
| 29:T:50:LEU:O | 29:T:52:GLU:N | 2.42 | 0.51 |
| 6:5:36:ASP:O | 6:5:39:THR:OG1 | 2.26 | 0.51 |
| 10:A:460:A:C2 | 10:A:470:A:C4 | 2.99 | 0.51 |
| 10:A:2803:G:H2' | 10:A:2804:U:C6 | 2.45 | 0.51 |
| 13:D:151:THR:HG22 | 13:D:152:PRO:HD3 | 1.92 | 0.51 |
| 17:H:41:LYS:HA | 17:H:44:ILE:HG12 | 1.93 | 0.51 |
| 22:M:73:ILE:HG21 | 22:M:91:TYR:CZ | 2.45 | 0.51 |
| 26:Q:94:LEU:C | 26:Q:96:ASP:H | 2.14 | 0.51 |
| 10:A:2584:U:O5' | 10:A:2584:U:H6 | 1.94 | 0.51 |
| 13:D:62:LYS:HB2 | 13:D:63:PRO:HD3 | 1.92 | 0.51 |
| 22:M:8:LYS:HE3 | 22:M:9:PHE:CE2 | 2.45 | 0.51 |
| 6:5:94:ARG:O | 6:5:97:LYS:N | 2.43 | 0.51 |
| 10:A:1753:G:OP1 | 25:P:92:ARG:NE | 2.38 | 0.51 |
| 10:A:2387:U:O2' | 32:W:38:ARG:NH2 | 2.43 | 0.51 |
| 15:F:132:ARG:O | 15:F:133:GLU:HB3 | 2.10 | 0.51 |
| 10:A:856:G:H21 | 32:W:19:ARG:HH22 | 1.58 | 0.51 |
| 10:A:974:G:H8 | 10:A:990:A:H62 | 1.58 | 0.51 |
| 10:A:1394:U:H4' | 10:A:1603:A:H4' | 1.92 | 0.51 |
| 10:A:1647:U:OP2 | 39:A:3418:HOH:O | 2.19 | 0.51 |
| 10:A:2062:A:C2' | 10:A:2063:C:H6 | 2.24 | 0.51 |
| 31:V:33:U:C4 | 31:V:35:G:OP2 | 2.63 | 0.51 |
| 35:Z:6:ILE:O | 35:Z:34:THR:HA | 2.10 | 0.51 |
| 9:8:9:ARG:NH2 | 9:8:12:GLN:HA | 2.26 | 0.51 |
| 10:A:26:G:C6 | 10:A:27:G:N1 | 2.79 | 0.51 |
| 10:A:1783:A:N1 | 10:A:2587:A:H2' | 2.25 | 0.51 |
| 10:A:1797:G:O2' | 12:C:256:THR:CG2 | 2.59 | 0.51 |
| 18:I:109:ALA:HB2 | 18:I:128:ILE:HG13 | 1.93 | 0.51 |
| 19:J:44:TYR:O | 19:J:45:THR:HB | 2.11 | 0.51 |
| 23:N:20:MET:HE1 | 23:N:40:LYS:HE2 | 1.93 | 0.51 |
| 24:O:36:TYR:N | 24:O:36:TYR:CD1 | 2.78 | 0.51 |
| 32:W:76:ARG:HH11 | 32:W:76:ARG:HG2 | 1.76 | 0.51 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 35:Z:41:PRO:HA | 35:Z:44:ARG:HB3 | 1.93 | 0.51 |
| 6:5:3:LEU:HD12 | 6:5:5:LEU:H | 1.76 | 0.51 |
| 20:K:9:ASN:O | 20:K:83:ALA:HA | 2.11 | 0.51 |
| 22:M:20:LEU:HD22 | 22:M:20:LEU:N | 2.26 | 0.51 |
| 10:A:945:A:C5 | 10:A:2448:A:C2 | 2.98 | 0.51 |
| 10:A:954:G:O2' | 10:A:2274:A:N1 | 2.41 | 0.51 |
| 10:A:2063:C:O2 | 10:A:2063:C:H2' | 2.10 | 0.51 |
| 19:J:81:ILE:CG1 | 19:J:82:GLY:N | 2.74 | 0.51 |
| 32:W:16:GLU:O | 32:W:17:ALA:HB3 | 2.10 | 0.51 |
| 10:A:1816:C:C5 | 12:C:61:TYR:CE2 | 2.98 | 0.51 |
| 10:A:1869:G:H3' | 10:A:1870:C:H5" | 1.94 | 0.51 |
| 10:A:2094:A:C2 | 10:A:2196:C:C2 | 2.99 | 0.51 |
| 16:G:16:VAL:HG21 | 16:G:44:HIS:CD2 | 2.46 | 0.51 |
| 21:L:81:ASP:O | 21:L:83:ALA:N | 2.41 | 0.51 |
| 21:L:91:ASP:OD1 | 21:L:92:LEU:N | 2.43 | 0.51 |
| 35:Z:30:ARG:HB3 | 35:Z:30:ARG:HH11 | 1.76 | 0.51 |
| 2:1:33:LEU:N | 2:1:51:ALA:HB3 | 2.25 | 0.50 |
| 8:7:19:ILE:HD13 | 10:A:2610:C:C5' | 2.39 | 0.50 |
| 9:8:44:HIS:HE1 | 9:8:86:LEU:H | 1.59 | 0.50 |
| 9:8:51:GLN:OE1 | 9:8:57:TYR:OH | 2.28 | 0.50 |
| 10:A:2314:A:OP1 | 15:F:87:LYS:NZ | 2.44 | 0.50 |
| 13:D:193:VAL:HG21 | 13:D:201:LEU:HD21 | 1.93 | 0.50 |
| 15:F:71:LYS:HD3 | 15:F:72:SER:N | 2.26 | 0.50 |
| 22:M:53:MET:HE3 | 22:M:63:ILE:HD13 | 1.93 | 0.50 |
| 26:Q:94:LEU:C | 26:Q:96:ASP:N | 2.65 | 0.50 |
| 28:S:86:MET:SD | 28:S:96:ILE:HG21 | 2.51 | 0.50 |
| 2:1:4:ILE:HG23 | 2:1:5:ARG:H | 1.76 | 0.50 |
| 10:A:654:A:H3' | 10:A:654:A:N3 | 2.26 | 0.50 |
| 14:E:148:ILE:HA | 14:E:187:VAL:HB | 1.93 | 0.50 |
| 20:K:19:VAL:CG1 | 20:K:41:ILE:HG12 | 2.40 | 0.50 |
| 10:A:2329:U:H2' | 10:A:2330:G:C8 | 2.47 | 0.50 |
| 13:D:91:THR:O | 13:D:91:THR:OG1 | 2.28 | 0.50 |
| 23:N:52:ILE:HB | 23:N:94:TYR:CD2 | 2.46 | 0.50 |
| 26:Q:65:ASN:OD1 | 26:Q:69:ARG:NH1 | 2.42 | 0.50 |
| 26:Q:91:ARG:HE | 26:Q:93:ILE:CG2 | 2.25 | 0.50 |
| 29:T:89:GLU:O | 29:T:91:GLN:N | 2.41 | 0.50 |
| 6:5:55:VAL:HG13 | 10:A:1084:A:H5' | 1.93 | 0.50 |
| 10:A:223:A:C5 | 10:A:422:A:C8 | 3.00 | 0.50 |
| 10:A:1203:U:O2' | 21:L:4:ASN:OD1 | 2.28 | 0.50 |
| 10:A:1300:G:H4' | 10:A:1301:A:H5' | 1.92 | 0.50 |
| 10:A:1778:U:H2' | 10:A:1784:A:N6 | 2.27 | 0.50 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 10:A:2571:U:O2' | 13:D:151:THR:CG2 | 2.60 | 0.50 |
| 3:2:34:ARG:NH1 | 3:2:41:ARG:O | 2.45 | 0.50 |
| 10:A:1437:C:H2' | 10:A:1438:U:C6 | 2.46 | 0.50 |
| 10:A:1475:G:O2' | 10:A:1514:G:O6 | 2.30 | 0.50 |
| 10:A:1533:C:H2' | 10:A:1534:U:C6 | 2.46 | 0.50 |
| 16:G:96:ALA:HB3 | 16:G:103:ASN:HB2 | 1.93 | 0.50 |
| 18:I:48:ILE:HG13 | 18:I:49:GLU:H | 1.77 | 0.50 |
| 10:A:27:G:N2 | 10:A:512:G:H1' | 2.26 | 0.50 |
| 10:A:139:U:O2' | 29:T:1:MET:HA | 2.12 | 0.50 |
| 10:A:141:G:N1 | 29:T:1:MET:O | 2.44 | 0.50 |
| 10:A:189:G:O6 | 10:A:205:G:O2' | 2.19 | 0.50 |
| 10:A:322:A:H5' | 10:A:340:A:H1' | 1.94 | 0.50 |
| 10:A:565:C:H2' | 10:A:566:U:O4' | 2.11 | 0.50 |
| 10:A:750:A:OP1 | 10:A:1615:C:N4 | 2.40 | 0.50 |
| 22:M:35:ALA:O | 22:M:36:VAL:HB | 2.11 | 0.50 |
| 5:4:7:VAL:O | 5:4:35:GLN:NE2 | 2.42 | 0.50 |
| 10:A:2352:A:C6 | 32:W:30:VAL:HG11 | 2.47 | 0.50 |
| 11:B:55:U:O3' | 15:F:23:SER:OG | 2.21 | 0.50 |
| 21:L:19:LEU:HB2 | 21:L:27:LEU:HB3 | 1.94 | 0.50 |
| 28:S:13:SER:O | 28:S:14:ALA:CB | 2.60 | 0.50 |
| 3:2:27:GLY:O | 3:2:30:VAL:HB | 2.11 | 0.50 |
| 10:A:1022:G:C5 | 10:A:1140:C:C4 | 3.00 | 0.50 |
| 10:A:1533:C:C2 | 10:A:1534:U:C4 | 2.99 | 0.50 |
| 10:A:1808:A:O2' | 33:X:2:ARG:NH2 | 2.45 | 0.50 |
| 10:A:2354:C:H4' | 32:W:31:LEU:HD22 | 1.92 | 0.50 |
| 12:C:256:THR:OG1 | 12:C:256:THR:O | 2.28 | 0.50 |
| 18:I:36:GLU:HB3 | 18:I:66:PHE:CE1 | 2.46 | 0.50 |
| 20:K:13:ASN:O | 20:K:15:GLY:N | 2.43 | 0.50 |
| 8:7:11:LYS:NZ | 28:S:91:GLY:HA3 | 2.22 | 0.50 |
| 10:A:118:A:N3 | 10:A:178:G:H1' | 2.27 | 0.50 |
| 10:A:1923:U:C5' | 31:V:24:G:C2' | 2.76 | 0.50 |
| 10:A:2074:U:H2' | 10:A:2075:U:C6 | 2.46 | 0.50 |
| 13:D:148:GLN:OE1 | 13:D:148:GLN:N | 2.45 | 0.50 |
| 14:E:112:LEU:HD13 | 14:E:186:VAL:HG11 | 1.94 | 0.50 |
| 16:G:73:SER:O | 16:G:77:GLY:N | 2.45 | 0.50 |
| 22:M:106:ASP:O | 22:M:108:VAL:N | 2.44 | 0.50 |
| 27:R:39:LEU:HA | 27:R:49:ILE:HG21 | 1.92 | 0.50 |
| 10:A:1654:A:H2' | 10:A:1655:A:H8 | 1.76 | 0.49 |
| 16:G:30:GLY:O | 16:G:32:LEU:N | 2.38 | 0.49 |
| 28:S:20:VAL:HG11 | 28:S:44:ALA:HA | 1.93 | 0.49 |
| 10:A:391:A:C6 | 10:A:411:G:C2 | 3.00 | 0.49 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 10:A:1179:G:H2' | 10:A:1180:U:O4' | 2.12 | 0.49 |
| 6:5:138:ARG:NH2 | 7:6:26:MET:HA | 2.28 | 0.49 |
| 10:A:1607:C:H4' | 10:A:1608:A:O5' | 2.13 | 0.49 |
| 10:A:1782:U:H2' | 10:A:2608:G:HO2' | 1.72 | 0.49 |
| 10:A:2061:G:H21 | 10:A:2062:A:H2 | 1.59 | 0.49 |
| 10:A:2504:U:O5' | 10:A:2504:U:H6 | 1.94 | 0.49 |
| 10:A:2701:U:H3' | 10:A:2702:G:C5' | 2.42 | 0.49 |
| 26:Q:63:ARG:NH1 | 26:Q:96:ASP:HA | 2.28 | 0.49 |
| 34:Y:8:GLU:O | 34:Y:12:GLU:HB2 | 2.12 | 0.49 |
| 6:5:4:ASN:C | 6:5:6:GLN:H | 2.16 | 0.49 |
| 10:A:1474:U:H2' | 10:A:1475:G:H5' | 1.95 | 0.49 |
| 10:A:1730:C:OP1 | 10:A:1730:C:H4' | 2.12 | 0.49 |
| 10:A:443:A:C5 | 14:E:40:ARG:HD3 | 2.47 | 0.49 |
| 10:A:564:C:O2 | 10:A:578:G:N2 | 2.46 | 0.49 |
| 10:A:748:G:OP2 | 28:S:88:ARG:HB2 | 2.12 | 0.49 |
| 10:A:2211:A:O2' | 10:A:2212:A:P | 2.70 | 0.49 |
| 13:D:151:THR:CG2 | 13:D:152:PRO:HD3 | 2.42 | 0.49 |
| 14:E:32:VAL:HG23 | 14:E:178:VAL:HG12 | 1.95 | 0.49 |
| 23:N:96:ARG:NH1 | 23:N:114:GLU:OE2 | 2.44 | 0.49 |
| 4:3:4:LYS:NZ | 10:A:253:C:OP2 | 2.38 | 0.49 |
| 8:7:21:ASP:OD2 | 38:7:1001:TRP:CE3 | 2.66 | 0.49 |
| 10:A:308:G:O2' | 10:A:329:G:N2 | 2.46 | 0.49 |
| 18:I:123:ALA:HA | 18:I:126:ARG:CZ | 2.43 | 0.49 |
| 24:O:51:ALA:HB3 | 24:O:78:VAL:HG13 | 1.95 | 0.49 |
| 33:X:70:LEU:O | 33:X:75:GLU:N | 2.45 | 0.49 |
| 6:5:95:LEU:HD22 | 6:5:95:LEU:H | 1.77 | 0.49 |
| 10:A:923:G:H1' | 32:W:23:LYS:CD | 2.43 | 0.49 |
| 10:A:995:C:O2 | 19:J:3:THR:HG23 | 2.13 | 0.49 |
| 10:A:1908:C:HO2' | 31:V:12:G:H5' | 1.74 | 0.49 |
| 28:S:24:ILE:HG22 | 28:S:71:VAL:HG11 | 1.95 | 0.49 |
| 29:T:54:GLU:CG | 29:T:88:LYS:HB2 | 2.42 | 0.49 |
| 4:3:30:HIS:HD2 | 10:A:2421:G:N7 | 2.10 | 0.49 |
| 10:A:1567:G:H2' | 12:C:84:PRO:HG3 | 1.95 | 0.49 |
| 10:A:2062:A:C2' | 10:A:2062:A:N3 | 2.76 | 0.49 |
| 18:I:60:VAL:HG22 | 18:I:66:PHE:HB3 | 1.95 | 0.49 |
| 19:J:21:THR:HG22 | 19:J:22:GLY:N | 2.27 | 0.49 |
| 31:V:6:C:H2' | 31:V:7:G:H8 | 1.78 | 0.49 |
| 10:A:479:A:C2 | 10:A:480:A:C4 | 3.01 | 0.49 |
| 10:A:1417:C:N3 | 10:A:1581:G:N2 | 2.60 | 0.49 |
| 10:A:2228:G:H22 | 33:X:33:HIS:HE2 | 1.61 | 0.49 |
| 17:H:9:VAL:O | 17:H:13:GLY:N | 2.46 | 0.49 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 18:I:135:MET:HB3 | 18:I:137:LEU:CD2 | 2.43 | 0.49 |
| 25:P:91:VAL:O | 25:P:92:ARG:HG2 | 2.12 | 0.49 |
| 35:Z:26:LEU:O | 35:Z:37:ARG:NH1 | 2.44 | 0.49 |
| 6:5:51:TYR:C | 6:5:51:TYR:CD1 | 2.86 | 0.49 |
| 10:A:1022:G:C6 | 10:A:1140:C:C4 | 3.01 | 0.49 |
| 15:F:110:ILE:O | 15:F:112:ASP:N | 2.46 | 0.49 |
| 28:S:88:ARG:NH1 | 28:S:88:ARG:HB3 | 2.28 | 0.49 |
| 1:0:24:VAL:O | 1:0:25:THR:OG1 | 2.30 | 0.48 |
| 3:2:10:LEU:HD23 | 10:A:770:G:H5" | 1.95 | 0.48 |
| 8:7:21:ASP:O | 8:7:22:HIS:C | 2.51 | 0.48 |
| 10:A:999:U:OP2 | 39:A:3356:HOH:O | 2.19 | 0.48 |
| 10:A:2109:U:H2' | 10:A:2110:G:H5' | 1.93 | 0.48 |
| 10:A:2330:G:C2 | 10:A:2386:A:C2 | 3.01 | 0.48 |
| 30:U:85:ARG:HD3 | 30:U:86:PHE:N | 2.28 | 0.48 |
| 10:A:1844:C:O3' | 12:C:255:LYS:NZ | 2.43 | 0.48 |
| 10:A:1922:G:H4' | 31:V:25:C:O2' | 2.13 | 0.48 |
| 10:A:2016:U:H2' | 10:A:2017:U:C6 | 2.48 | 0.48 |
| 10:A:2393:U:H5' | 21:L:60:ARG:O | 2.13 | 0.48 |
| 10:A:2583:G:H3' | 10:A:2584:U:C5 | 2.47 | 0.48 |
| 13:D:68:PHE:C | 13:D:73:VAL:HG12 | 2.33 | 0.48 |
| 15:F:10:GLU:O | 15:F:12:VAL:N | 2.44 | 0.48 |
| 16:G:15:ASP:O | 16:G:16:VAL:HG13 | 2.12 | 0.48 |
| 18:I:89:SER:OG | 18:I:135:MET:SD | 2.68 | 0.48 |
| 32:W:49:ASN:HA | 32:W:61:LYS:HB2 | 1.94 | 0.48 |
| 6:5:4:ASN:C | 6:5:6:GLN:N | 2.66 | 0.48 |
| 10:A:107:G:H2' | 10:A:108:G:H8 | 1.78 | 0.48 |
| 10:A:301:G:H1' | 10:A:302:C:C6 | 2.48 | 0.48 |
| 10:A:1327:A:N6 | 10:A:1328:A:C2 | 2.81 | 0.48 |
| 10:A:1485:U:H2' | 10:A:1486:U:C6 | 2.49 | 0.48 |
| 15:F:79:ARG:HB3 | 15:F:82:TYR:CZ | 2.48 | 0.48 |
| 27:R:49:ILE:HD12 | 27:R:52:PRO:HA | 1.95 | 0.48 |
| 29:T:34:VAL:CG2 | 29:T:34:VAL:O | 2.61 | 0.48 |
| 32:W:9:THR:HG23 | 32:W:10:ARG:HD3 | 1.95 | 0.48 |
| 1:0:2:VAL:CG2 | 10:A:2015:A:C2 | 2.96 | 0.48 |
| 4:3:51:LYS:NZ | 10:A:938:G:OP2 | 2.33 | 0.48 |
| 10:A:1996:C:OP1 | 20:K:31:ARG:NE | 2.46 | 0.48 |
| 25:P:105:LYS:HA | 25:P:108:ARG:HD2 | 1.95 | 0.48 |
| 32:W:49:ASN:ND2 | 32:W:49:ASN:C | 2.66 | 0.48 |
| 10:A:250:G:C6 | 10:A:251:A:C6 | 3.01 | 0.48 |
| 10:A:1069:A:C1' | 10:A:1073:A:H62 | 2.27 | 0.48 |
| 10:A:1268:A:OP1 | 39:A:3374:HOH:O | 2.20 | 0.48 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 10:A:1778:U:H2' | 10:A:1784:A:H62 | 1.78 | 0.48 |
| 28:S:88:ARG:HG2 | 28:S:94:ASP:CG | 2.34 | 0.48 |
| 5:4:6:SER:HB2 | 10:A:1031:G:H4' | 1.95 | 0.48 |
| 6:5:58:THR:HG23 | 10:A:1107:G:H5" | 1.94 | 0.48 |
| 10:A:528:A:C2 | 10:A:2043:C:H4' | 2.49 | 0.48 |
| 10:A:747:U:O2' | 28:S:88:ARG:NE | 2.47 | 0.48 |
| 10:A:846:U:HO2' | 10:A:847:U:P | 2.36 | 0.48 |
| 10:A:856:G:O2' | 32:W:22:VAL:HG23 | 2.14 | 0.48 |
| 10:A:973:A:P | 27:R:81:LYS:HZ3 | 2.36 | 0.48 |
| 10:A:2581:G:C2 | 10:A:2610:C:C6 | 3.02 | 0.48 |
| 16:G:104:LEU:HB2 | 16:G:112:VAL:HG21 | 1.96 | 0.48 |
| 18:I:40:ALA:O | 18:I:43:ALA:HB3 | 2.14 | 0.48 |
| 22:M:1:MET:O | 22:M:2:LEU:CB | 2.62 | 0.48 |
| 5:4:2:LYS:HZ1 | 10:A:2478:A:P | 2.35 | 0.48 |
| 10:A:1199:U:H5' | 26:Q:4:LYS:CE | 2.42 | 0.48 |
| 12:C:225:ASN:HB3 | 12:C:226:PRO:HD2 | 1.96 | 0.48 |
| 15:F:79:ARG:HB3 | 15:F:82:TYR:CE1 | 2.48 | 0.48 |
| 16:G:84:LYS:HG3 | 16:G:132:LEU:N | 2.28 | 0.48 |
| 19:J:32:LEU:CD2 | 19:J:54:ILE:HD12 | 2.44 | 0.48 |
| 4:3:63:TYR:HH | 10:A:592:A:HO2' | 1.61 | 0.48 |
| 6:5:39:THR:HA | 6:5:42:ARG:CD | 2.43 | 0.48 |
| 6:5:68:PRO:HA | 6:5:72:LEU:HD11 | 1.94 | 0.48 |
| 10:A:749:A:C6 | 10:A:1618:A:C2 | 3.01 | 0.48 |
| 10:A:1135:C:N4 | 10:A:1139:G:C6 | 2.82 | 0.48 |
| 10:A:1348:C:H2' | 10:A:1349:C:H5' | 1.96 | 0.48 |
| 10:A:1760:C:H2' | 10:A:1761:C:O4' | 2.14 | 0.48 |
| 10:A:2406:A:C2 | 21:L:69:ARG:NH2 | 2.82 | 0.48 |
| 10:A:2800:A:H3' | 10:A:2801:G:H5" | 1.96 | 0.48 |
| 14:E:164:LEU:HB3 | 14:E:167:VAL:CG1 | 2.44 | 0.48 |
| 18:I:14:ALA:HB3 | 18:I:51:GLY:H | 1.79 | 0.48 |
| 25:P:19:PHE:N | 25:P:19:PHE:CD1 | 2.82 | 0.48 |
| 27:R:68:ARG:HD3 | 27:R:92:TRP:CZ2 | 2.49 | 0.48 |
| 34:Y:56:LEU:O | 34:Y:57:LEU:HB3 | 2.14 | 0.48 |
| 6:5:51:TYR:HD1 | 6:5:52:MET:N | 2.12 | 0.48 |
| 8:7:14:ASN:O | 8:7:15:ILE:CG1 | 2.61 | 0.48 |
| 10:A:11:C:C3' | 10:A:12:U:H5' | 2.44 | 0.48 |
| 10:A:580:U:H2' | 10:A:581:C:H6 | 1.79 | 0.48 |
| 10:A:983:A:N6 | 10:A:984:A:C2 | 2.82 | 0.48 |
| 10:A:2867:G:O2' | 10:A:2868:A:OP2 | 2.28 | 0.48 |
| 16:G:23:ILE:HG21 | 16:G:71:LEU:HD11 | 1.95 | 0.48 |
| 19:J:44:TYR:CD1 | 26:Q:63:ARG:HG2 | 2.49 | 0.48 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 32:W:18:LYS:CG | 32:W:19:ARG:N | 2.77 | 0.48 |
| 6:5:15:VAL:HG22 | 6:5:66:GLY:CA | 2.44 | 0.48 |
| 8:7:11:LYS:NZ | 10:A:1614:A:C5 | 2.81 | 0.48 |
| 8:7:14:ASN:C | 8:7:15:ILE:HG12 | 2.34 | 0.48 |
| 10:A:1923:U:H5" | 31:V:24:G:H2' | 1.90 | 0.48 |
| 10:A:2425:A:C5' | 10:A:2427:C:O4' | 2.62 | 0.48 |
| 10:A:2747:G:O2' | 16:G:66:THR:HG22 | 2.14 | 0.48 |
| 18:I:100:ILE:HD13 | 18:I:137:LEU:HD12 | 1.96 | 0.48 |
| 10:A:725:G:C6 | 10:A:726:G:N1 | 2.82 | 0.47 |
| 10:A:1799:G:C5 | 12:C:175:LEU:HD23 | 2.49 | 0.47 |
| 10:A:1814:G:C6 | 10:A:1815:A:N6 | 2.82 | 0.47 |
| 10:A:2678:C:H2' | 10:A:2679:A:O4' | 2.14 | 0.47 |
| 15:F:79:ARG:CZ | 31:V:56:C:C2 | 2.87 | 0.47 |
| 21:L:82:LEU:CD1 | 21:L:116:VAL:HG23 | 2.44 | 0.47 |
| 32:W:44:PHE:HD1 | 32:W:45:HIS:CE1 | 2.32 | 0.47 |
| 6:5:110:ALA:HB1 | 6:5:113:PHE:CZ | 2.49 | 0.47 |
| 10:A:983:A:N6 | 10:A:984:A:N1 | 2.62 | 0.47 |
| 10:A:2862:G:C5 | 10:A:2863:C:C5 | 3.02 | 0.47 |
| 12:C:232:GLY:H | 12:C:241:LYS:HE3 | 1.79 | 0.47 |
| 15:F:64:PRO:HA | 15:F:88:VAL:HG22 | 1.95 | 0.47 |
| 20:K:13:ASN:O | 20:K:14:SER:OG | 2.29 | 0.47 |
| 22:M:34:LYS:HD2 | 22:M:131:VAL:HG11 | 1.95 | 0.47 |
| 31:V:6:C:H2' | 31:V:7:G:C8 | 2.49 | 0.47 |
| 31:V:34:G:C2 | 31:V:35:G:C4 | 3.02 | 0.47 |
| 32:W:39:GLN:HG2 | 32:W:40:ARG:N | 2.28 | 0.47 |
| 33:X:70:LEU:O | 33:X:74:GLY:N | 2.46 | 0.47 |
| 6:5:23:LEU:H | 6:5:87:GLU:HB2 | 1.79 | 0.47 |
| 6:5:100:ALA:HB2 | 6:5:125:ARG:HE | 1.79 | 0.47 |
| 10:A:391:A:C5 | 10:A:411:G:C2 | 3.02 | 0.47 |
| 10:A:2230:G:O3' | 33:X:29:LEU:HD23 | 2.14 | 0.47 |
| 26:Q:63:ARG:HH22 | 26:Q:96:ASP:N | 2.12 | 0.47 |
| 27:R:66:HIS:CG | 27:R:94:THR:HG22 | 2.50 | 0.47 |
| 29:T:29:THR:OG1 | 29:T:86:THR:N | 2.43 | 0.47 |
| 35:Z:38:GLU:O | 35:Z:43:ILE:HG12 | 2.13 | 0.47 |
| 6:5:54:VAL:HG22 | 6:5:83:ALA:HB1 | 1.97 | 0.47 |
| 6:5:60:LEU:HD23 | 6:5:78:GLY:HA3 | 1.96 | 0.47 |
| 6:5:71:CYS:CA | 6:5:117:LEU:HD13 | 2.31 | 0.47 |
| 6:5:123:ILE:HG12 | 6:5:124:ASP:N | 2.30 | 0.47 |
| 10:A:2902:C:C2' | 10:A:2903:U:O5' | 2.63 | 0.47 |
| 17:H:8:LYS:O | 17:H:9:VAL:HB | 2.15 | 0.47 |
| 20:K:30:ARG:NH1 | 20:K:32:TYR:O | 2.45 | 0.47 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 10:A:1088:A:HO2' | 10:A:1089:A:P | 2.37 | 0.47 |
| 10:A:2335:A:C5 | 10:A:2337:G:C4 | 3.02 | 0.47 |
| 10:A:2355:G:H4' | 32:W:20:LEU:CD1 | 2.44 | 0.47 |
| 18:I:19:PRO:CG | 18:I:23:VAL:HG23 | 2.45 | 0.47 |
| 19:J:43:GLU:O | 19:J:45:THR:HG22 | 2.13 | 0.47 |
| 26:Q:91:ARG:HH21 | 26:Q:93:ILE:HD13 | 1.80 | 0.47 |
| 28:S:63:GLY:O | 28:S:64:ALA:CB | 2.62 | 0.47 |
| 10:A:451:U:C2 | 10:A:453:A:N7 | 2.83 | 0.47 |
| 10:A:478:A:C6 | 10:A:480:A:C6 | 3.03 | 0.47 |
| 13:D:38:LYS:NZ | 13:D:81:GLU:OE2 | 2.26 | 0.47 |
| 13:D:174:SER:OG | 13:D:175:LEU:N | 2.46 | 0.47 |
| 16:G:22:VAL:HG23 | 16:G:22:VAL:O | 2.14 | 0.47 |
| 21:L:68:SER:O | 21:L:69:ARG:HB3 | 2.15 | 0.47 |
| 29:T:54:GLU:N | 29:T:54:GLU:OE1 | 2.48 | 0.47 |
| 32:W:9:THR:HG23 | 32:W:10:ARG:N | 2.30 | 0.47 |
| 6:5:110:ALA:HB1 | 6:5:113:PHE:CE1 | 2.49 | 0.47 |
| 6:5:127:ALA:O | 6:5:129:LEU:N | 2.48 | 0.47 |
| 8:7:19:ILE:HG13 | 8:7:20:VAL:N | 2.30 | 0.47 |
| 9:8:2:PHE:HB3 | 9:8:50:MET:HE1 | 1.97 | 0.47 |
| 9:8:80:HIS:HD2 | 9:8:83:LYS:H | 1.62 | 0.47 |
| 10:A:996:A:H4' | 26:Q:91:ARG:NE | 2.29 | 0.47 |
| 10:A:1817:G:H2' | 10:A:1818:U:H5' | 1.97 | 0.47 |
| 10:A:2346:A:H3' | 10:A:2347:C:H5" | 1.96 | 0.47 |
| 10:A:2701:U:H3' | 10:A:2702:G:H5" | 1.96 | 0.47 |
| 10:A:2839:G:N2 | 10:A:2880:C:C4 | 2.82 | 0.47 |
| 10:A:2889:C:N4 | 10:A:2890:G:C6 | 2.83 | 0.47 |
| 16:G:112:VAL:HG23 | 16:G:113:ASP:N | 2.28 | 0.47 |
| 18:I:14:ALA:HB1 | 18:I:45:THR:HG23 | 1.97 | 0.47 |
| 28:S:88:ARG:NH1 | 28:S:88:ARG:CG | 2.73 | 0.47 |
| 30:U:38:ILE:CG2 | 30:U:39:ASN:H | 2.28 | 0.47 |
| 32:W:23:LYS:HE2 | 32:W:24:ARG:H | 1.79 | 0.47 |
| 33:X:39:VAL:HG22 | 33:X:44:ARG:O | 2.13 | 0.47 |
| 33:X:67:LEU:HD23 | 33:X:70:LEU:HD12 | 1.96 | 0.47 |
| 10:A:1079:C:O2 | 18:I:130:GLY:HA3 | 2.15 | 0.47 |
| 10:A:1327:A:H2' | 10:A:1328:A:O4' | 2.14 | 0.47 |
| 10:A:1474:U:C2' | 10:A:1475:G:H5' | 2.44 | 0.47 |
| 10:A:2601:C:O5' | 10:A:2601:C:H6 | 1.97 | 0.47 |
| 15:F:5:ASP:OD1 | 15:F:8:LYS:NZ | 2.46 | 0.47 |
| 20:K:24:VAL:HG13 | 20:K:33:ALA:HB2 | 1.95 | 0.47 |
| 22:M:46:ILE:HD13 | 22:M:47:GLU:N | 2.30 | 0.47 |
| 32:W:18:LYS:HA | 32:W:36:ILE:HG13 | 1.95 | 0.47 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 32:W:28:GLU:O | 32:W:30:VAL:N | 2.48 | 0.47 |
| 32:W:72:GLY:N | 32:W:73:PRO:CD | 2.78 | 0.47 |
| 1:0:9:ARG:NH1 | 10:A:517:C:OP2 | 2.48 | 0.47 |
| 2:1:4:ILE:HD11 | 2:1:27:ARG:HB2 | 1.96 | 0.47 |
| 10:A:221:A:N1 | 10:A:265:A:O2' | 2.45 | 0.47 |
| 10:A:1392:A:N6 | 10:A:1393:A:N6 | 2.63 | 0.47 |
| 10:A:1939:U:O2 | 10:A:1967:C:H4' | 2.15 | 0.47 |
| 10:A:2210:U:H4' | 10:A:2211:A:H5' | 1.97 | 0.47 |
| 12:C:265:PHE:N | 12:C:265:PHE:CD1 | 2.82 | 0.47 |
| 15:F:69:ALA:N | 15:F:82:TYR:O | 2.47 | 0.47 |
| 18:I:120:ASP:O | 18:I:123:ALA:N | 2.46 | 0.47 |
| 21:L:23:ILE:HD12 | 27:R:84:ARG:CZ | 2.45 | 0.47 |
| 32:W:9:THR:CG2 | 32:W:10:ARG:HD3 | 2.44 | 0.47 |
| 32:W:47:GLY:H | 32:W:80:SER:HB3 | 1.80 | 0.47 |
| 4:3:21:PHE:O | 4:3:22:LYS:O | 2.33 | 0.47 |
| 10:A:587:C:P | 21:L:21:ARG:NH2 | 2.88 | 0.47 |
| 10:A:657:U:H2' | 10:A:658:U:C6 | 2.50 | 0.47 |
| 10:A:1198:U:O3' | 26:Q:4:LYS:HE3 | 2.15 | 0.47 |
| 10:A:2587:A:O5' | 10:A:2587:A:H8 | 1.97 | 0.47 |
| 13:D:148:GLN:HB2 | 13:D:152:PRO:HG2 | 1.97 | 0.47 |
| 13:D:169:ARG:O | 13:D:170:VAL:HG13 | 2.15 | 0.47 |
| 15:F:134:GLN:O | 15:F:136:ILE:N | 2.47 | 0.47 |
| 19:J:36:LEU:O | 19:J:121:LYS:NZ | 2.39 | 0.47 |
| 19:J:84:ILE:HG23 | 19:J:84:ILE:O | 2.15 | 0.47 |
| 28:S:24:ILE:HD11 | 28:S:36:LEU:HD13 | 1.96 | 0.47 |
| 3:2:3:ARG:NH2 | 10:A:752:A:OP1 | 2.48 | 0.46 |
| 10:A:630:G:N2 | 10:A:633:A:OP2 | 2.37 | 0.46 |
| 10:A:995:C:N4 | 19:J:2:LYS:HB3 | 2.29 | 0.46 |
| 10:A:1161:C:H1' | 27:R:8:GLY:O | 2.15 | 0.46 |
| 10:A:1219:U:OP2 | 26:Q:18:LYS:NZ | 2.46 | 0.46 |
| 10:A:1738:G:HO2' | 10:A:1739:A:P | 2.38 | 0.46 |
| 11:B:29:A:H2' | 11:B:30:C:C6 | 2.50 | 0.46 |
| 12:C:246:PRO:HG2 | 12:C:247:TRP:CZ3 | 2.50 | 0.46 |
| 21:L:19:LEU:HD23 | 21:L:19:LEU:C | 2.35 | 0.46 |
| 6:5:77:VAL:O | 6:5:79:PRO:HD2 | 2.13 | 0.46 |
| 16:G:123:GLU:HG2 | 16:G:124:CYS:N | 2.30 | 0.46 |
| 22:M:22:GLN:O | 22:M:24:THR:N | 2.48 | 0.46 |
| 25:P:72:VAL:HG23 | 25:P:72:VAL:O | 2.15 | 0.46 |
| 29:T:61:LEU:C | 29:T:61:LEU:HD12 | 2.35 | 0.46 |
| 30:U:73:ASN:HA | 30:U:95:PHE:CE2 | 2.50 | 0.46 |
| 6:5:15:VAL:HG21 | 6:5:66:GLY:HA2 | 1.96 | 0.46 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 10:A:479:A:H4' | 10:A:480:A:OP1 | 2.15 | 0.46 |
| 10:A:923:G:N3 | 32:W:23:LYS:HD2 | 2.31 | 0.46 |
| 10:A:2436:G:C2 | 10:A:2437:G:C8 | 3.04 | 0.46 |
| 12:C:75:ALA:HB2 | 12:C:95:TYR:HA | 1.97 | 0.46 |
| 33:X:39:VAL:HG21 | 33:X:42:GLU:HB2 | 1.96 | 0.46 |
| 5:4:8:LYS:NZ | 10:A:2467:C:OP1 | 2.48 | 0.46 |
| 6:5:68:PRO:HA | 6:5:72:LEU:CG | 2.46 | 0.46 |
| 10:A:504:A:HO2' | 10:A:505:A:P | 2.29 | 0.46 |
| 10:A:523:C:H5" | 10:A:540:C:O2' | 2.15 | 0.46 |
| 10:A:1567:G:C2' | 12:C:84:PRO:HG3 | 2.46 | 0.46 |
| 10:A:2478:A:H2' | 10:A:2479:U:H5' | 1.98 | 0.46 |
| 10:A:2649:C:H2' | 10:A:2650:U:C6 | 2.50 | 0.46 |
| 10:A:2897:U:H2' | 10:A:2898:U:C6 | 2.51 | 0.46 |
| 11:B:51:G:OP2 | 24:O:64:TYR:HD2 | 1.98 | 0.46 |
| 15:F:39:VAL:HG13 | 15:F:40:GLY:N | 2.31 | 0.46 |
| 19:J:12:LYS:O | 19:J:13:ARG:CB | 2.64 | 0.46 |
| 27:R:64:VAL:HG21 | 27:R:97:LYS:HB2 | 1.97 | 0.46 |
| 31:V:26:A:H61 | 31:V:44:G:H1 | 1.64 | 0.46 |
| 32:W:17:ALA:O | 32:W:18:LYS:CB | 2.64 | 0.46 |
| 10:A:227:A:O2' | 10:A:2407:A:O2' | 2.19 | 0.46 |
| 10:A:419:U:H2' | 10:A:420:C:C6 | 2.50 | 0.46 |
| 10:A:947:A:O2' | 10:A:984:A:H2 | 1.98 | 0.46 |
| 12:C:67:LYS:HG2 | 12:C:150:GLY:HA2 | 1.97 | 0.46 |
| 12:C:93:VAL:HG12 | 12:C:94:LEU:N | 2.31 | 0.46 |
| 16:G:163:TYR:O | 16:G:164:ALA:HB2 | 2.15 | 0.46 |
| 18:I:24:GLY:O | 18:I:27:LEU:HG | 2.16 | 0.46 |
| 19:J:37:ARG:HA | 19:J:118:MET:CE | 2.45 | 0.46 |
| 20:K:24:VAL:CG1 | 20:K:30:ARG:HD3 | 2.45 | 0.46 |
| 27:R:49:ILE:HG22 | 27:R:53:PHE:C | 2.36 | 0.46 |
| 10:A:959:A:H62 | 22:M:82:MET:CE | 2.28 | 0.46 |
| 10:A:1057:A:C6 | 10:A:1086:A:C2 | 3.04 | 0.46 |
| 10:A:1090:A:C2 | 10:A:1102:C:H1' | 2.50 | 0.46 |
| 10:A:1478:G:C2 | 10:A:1479:G:N7 | 2.83 | 0.46 |
| 10:A:2318:G:C6 | 10:A:2319:G:C6 | 3.03 | 0.46 |
| 10:A:2365:G:H4' | 32:W:59:PHE:CZ | 2.51 | 0.46 |
| 16:G:23:ILE:HD12 | 16:G:23:ILE:H | 1.81 | 0.46 |
| 18:I:125:THR:O | 18:I:128:ILE:N | 2.48 | 0.46 |
| 25:P:50:ARG:HG2 | 25:P:57:ALA:N | 2.30 | 0.46 |
| 5:4:36:ARG:O | 5:4:37:GLN:C | 2.54 | 0.46 |
| 6:5:88:HIS:CB | 6:5:89:PRO:HD3 | 2.44 | 0.46 |
| 10:A:1248:G:C5 | 14:E:46:GLN:NE2 | 2.84 | 0.46 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 10:A:1313:U:H2' | 10:A:1610:A:C2 | 2.51 | 0.46 |
| 10:A:1509:A:C4 | 10:A:1510:G:C8 | 3.04 | 0.46 |
| 10:A:2740:A:C6 | 10:A:2764:A:C8 | 3.04 | 0.46 |
| 10:A:2793:C:H2' | 10:A:2794:C:C6 | 2.50 | 0.46 |
| 15:F:131:VAL:HG22 | 15:F:151:LEU:H | 1.80 | 0.46 |
| 17:H:21:VAL:CG2 | 17:H:25:TYR:CD2 | 2.98 | 0.46 |
| 17:H:40:THR:C | 17:H:42:LYS:H | 2.19 | 0.46 |
| 32:W:60:ALA:HA | 32:W:81:ILE:HD12 | 1.97 | 0.46 |
| 35:Z:39:ASP:OD2 | 35:Z:44:ARG:NH2 | 2.46 | 0.46 |
| 2:1:16:THR:HG21 | 2:1:41:VAL:HG13 | 1.97 | 0.46 |
| 6:5:33:VAL:HG12 | 6:5:34:THR:N | 2.26 | 0.46 |
| 6:5:48:ALA:HB3 | 6:5:51:TYR:HB3 | 1.98 | 0.46 |
| 6:5:71:CYS:HA | 6:5:117:LEU:HD11 | 1.96 | 0.46 |
| 9:8:80:HIS:CD2 | 9:8:83:LYS:HB2 | 2.51 | 0.46 |
| 10:A:627:A:C6 | 10:A:637:A:C8 | 3.04 | 0.46 |
| 10:A:1936:A:C2 | 10:A:1943:U:C5 | 3.03 | 0.46 |
| 10:A:2326:C:H4' | 10:A:2327:A:OP1 | 2.16 | 0.46 |
| 11:B:37:C:C5 | 11:B:38:C:C4 | 3.04 | 0.46 |
| 15:F:30:VAL:CG1 | 15:F:96:TRP:CH2 | 2.99 | 0.46 |
| 29:T:69:ARG:CD | 29:T:70:HIS:H | 2.28 | 0.46 |
| 32:W:30:VAL:HG23 | 32:W:60:ALA:O | 2.15 | 0.46 |
| 1:0:42:ILE:HD11 | 23:N:98:LEU:CB | 2.46 | 0.46 |
| 10:A:11:C:H2' | 10:A:12:U:H5' | 1.98 | 0.46 |
| 10:A:1060:U:H3 | 10:A:1088:A:H2 | 1.64 | 0.46 |
| 10:A:2024:G:C4 | 10:A:2040:G:N2 | 2.84 | 0.46 |
| 20:K:98:ARG:HA | 20:K:118:LEU:HD23 | 1.97 | 0.46 |
| 1:0:8:THR:HG21 | 10:A:2021:C:P | 2.56 | 0.46 |
| 1:0:42:ILE:H | 1:0:42:ILE:HD12 | 1.80 | 0.46 |
| 8:7:14:ASN:C | 8:7:15:ILE:HD13 | 2.22 | 0.46 |
| 14:E:44:ARG:HG3 | 14:E:44:ARG:HH11 | 1.80 | 0.46 |
| 14:E:187:VAL:O | 14:E:188:MET:HB3 | 2.16 | 0.46 |
| 19:J:12:LYS:O | 19:J:13:ARG:HB2 | 2.15 | 0.46 |
| 29:T:29:THR:HB | 29:T:86:THR:HG22 | 1.98 | 0.46 |
| 1:0:3:GLN:HA | 10:A:2615:U:C2 | 2.51 | 0.45 |
| 8:7:14:ASN:O | 8:7:15:ILE:CG2 | 2.62 | 0.45 |
| 10:A:751:A:C6 | 10:A:789:A:C5 | 3.04 | 0.45 |
| 15:F:113:PHE:HE1 | 15:F:116:LEU:HD13 | 1.81 | 0.45 |
| 15:F:147:ARG:HG3 | 15:F:148:VAL:N | 2.30 | 0.45 |
| 17:H:31:VAL:HB | 17:H:32:PRO:CD | 2.46 | 0.45 |
| 18:I:61:TYR:N | 18:I:61:TYR:CD1 | 2.82 | 0.45 |
| 20:K:99:ILE:HG21 | 20:K:119:ALA:HB2 | 1.98 | 0.45 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 23:N:103:ARG:CZ | 23:N:110:MET:CE | 2.95 | 0.45 |
| 27:R:68:ARG:HD3 | 27:R:92:TRP:CE2 | 2.50 | 0.45 |
| 35:Z:3:THR:HA | 35:Z:37:ARG:O | 2.16 | 0.45 |
| 6:5:110:ALA:O | 6:5:113:PHE:N | 2.46 | 0.45 |
| 10:A:728:G:H4' | 12:C:12:ARG:HD3 | 1.98 | 0.45 |
| 10:A:1569:A:N6 | 10:A:1570:A:C6 | 2.84 | 0.45 |
| 10:A:1662:U:O2 | 10:A:2687:U:H4' | 2.17 | 0.45 |
| 13:D:193:VAL:HB | 13:D:194:PRO:HD2 | 1.98 | 0.45 |
| 17:H:14:SER:OG | 17:H:17:ASP:CG | 2.55 | 0.45 |
| 18:I:57:VAL:HG23 | 18:I:71:LYS:CE | 2.46 | 0.45 |
| 18:I:137:LEU:HD23 | 18:I:137:LEU:H | 1.81 | 0.45 |
| 6:5:71:CYS:CA | 6:5:117:LEU:HD11 | 2.43 | 0.45 |
| 6:5:100:ALA:HB3 | 6:5:125:ARG:HD2 | 1.98 | 0.45 |
| 10:A:118:A:C8 | 10:A:119:A:C8 | 3.04 | 0.45 |
| 10:A:666:A:H4' | 21:L:48:ARG:HD2 | 1.99 | 0.45 |
| 10:A:1141:U:H4' | 10:A:1142:A:O4' | 2.17 | 0.45 |
| 10:A:1171:G:C6 | 10:A:1172:C:C4 | 3.04 | 0.45 |
| 10:A:1936:A:N6 | 10:A:1963:U:C2 | 2.84 | 0.45 |
| 10:A:2108:A:C2' | 10:A:2109:U:O5' | 2.64 | 0.45 |
| 16:G:118:ALA:O | 16:G:120:ILE:N | 2.41 | 0.45 |
| 18:I:100:ILE:CG2 | 18:I:101:SER:N | 2.79 | 0.45 |
| 26:Q:4:LYS:NZ | 26:Q:7:VAL:CG1 | 2.79 | 0.45 |
| 26:Q:91:ARG:HH21 | 26:Q:93:ILE:HG21 | 1.81 | 0.45 |
| 32:W:19:ARG:CZ | 32:W:22:VAL:HB | 2.46 | 0.45 |
| 2:1:33:LEU:N | 2:1:51:ALA:CB | 2.80 | 0.45 |
| 6:5:63:ALA:HB3 | 6:5:84:TYR:CE2 | 2.52 | 0.45 |
| 10:A:271:G:H4' | 10:A:272:A:OP1 | 2.17 | 0.45 |
| 10:A:1542:U:H2' | 10:A:1543:G:O4' | 2.16 | 0.45 |
| 10:A:1593:A:H2' | 10:A:1594:U:O4' | 2.17 | 0.45 |
| 10:A:2144:G:H3' | 10:A:2144:G:N3 | 2.30 | 0.45 |
| 10:A:2862:G:C6 | 10:A:2863:C:C4 | 3.04 | 0.45 |
| 11:B:11:C:O2' | 11:B:15:A:N6 | 2.50 | 0.45 |
| 12:C:163:ILE:HG23 | 12:C:171:VAL:CG1 | 2.47 | 0.45 |
| 14:E:154:ASP:OD1 | 14:E:154:ASP:N | 2.50 | 0.45 |
| 23:N:70:THR:HB | 23:N:75:ILE:CD1 | 2.46 | 0.45 |
| 25:P:21:PRO:HD3 | 25:P:49:ILE:HD12 | 1.98 | 0.45 |
| 31:V:70:C:H2' | 31:V:71:C:H5' | 1.98 | 0.45 |
| 10:A:281:C:H2' | 10:A:282:A:C8 | 2.51 | 0.45 |
| 26:Q:91:ARG:HH12 | 27:R:10:LYS:HB3 | 1.82 | 0.45 |
| 26:Q:103:VAL:HG23 | 26:Q:104:ALA:N | 2.32 | 0.45 |
| 32:W:39:GLN:HG3 | 32:W:42:THR:H | 1.81 | 0.45 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 35:Z:5:LYS:HD2 | 35:Z:5:LYS:N | 2.32 | 0.45 |
| 10:A:855:G:H21 | 32:W:23:LYS:HG2 | 1.82 | 0.45 |
| 10:A:1482:G:H1' | 10:A:1509:A:N6 | 2.30 | 0.45 |
| 10:A:1686:C:C2 | 10:A:1703:G:C2 | 3.05 | 0.45 |
| 10:A:1992:G:OP1 | 39:A:3420:HOH:O | 2.20 | 0.45 |
| 10:A:2353:G:N3 | 32:W:30:VAL:HG12 | 2.32 | 0.45 |
| 10:A:2852:G:C6 | 10:A:2853:C:N3 | 2.84 | 0.45 |
| 12:C:24:HIS:NE2 | 12:C:79:ARG:NH1 | 2.65 | 0.45 |
| 20:K:98:ARG:HA | 20:K:118:LEU:CD2 | 2.47 | 0.45 |
| 29:T:29:THR:CB | 29:T:86:THR:H | 2.29 | 0.45 |
| 2:1:8:ILE:HG21 | 2:1:51:ALA:HA | 1.98 | 0.45 |
| 10:A:635:C:O2' | 10:A:639:U:OP1 | 2.34 | 0.45 |
| 10:A:1838:C:H4' | 10:A:1839:G:C8 | 2.51 | 0.45 |
| 10:A:2343:U:O2' | 10:A:2373:G:O2' | 2.28 | 0.45 |
| 10:A:2481:G:HO2' | 10:A:2482:A:H8 | 1.64 | 0.45 |
| 19:J:44:TYR:HD1 | 26:Q:63:ARG:HG2 | 1.81 | 0.45 |
| 19:J:49:ASP:OD1 | 19:J:121:LYS:NZ | 2.32 | 0.45 |
| 21:L:132:ARG:HG3 | 21:L:142:ILE:HD12 | 1.98 | 0.45 |
| 23:N:33:ILE:CD1 | 23:N:118:ARG:NE | 2.80 | 0.45 |
| 25:P:50:ARG:CB | 25:P:57:ALA:N | 2.78 | 0.45 |
| 28:S:88:ARG:HD2 | 28:S:94:ASP:CG | 2.35 | 0.45 |
| 1:0:3:GLN:NE2 | 10:A:2016:U:O2 | 2.46 | 0.45 |
| 2:1:4:ILE:HG23 | 2:1:5:ARG:N | 2.32 | 0.45 |
| 4:3:12:ARG:HD3 | 21:L:61:LEU:O | 2.16 | 0.45 |
| 6:5:136:ILE:HG13 | 6:5:139:LEU:HD12 | 1.98 | 0.45 |
| 10:A:593:U:H2' | 10:A:594:U:C6 | 2.51 | 0.45 |
| 10:A:792:A:C6 | 10:A:2440:C:C6 | 3.05 | 0.45 |
| 10:A:1186:G:P | 39:A:3593:HOH:O | 2.75 | 0.45 |
| 10:A:1340:U:H4' | 10:A:1341:G:OP2 | 2.17 | 0.45 |
| 10:A:2262:U:H4' | 10:A:2328:A:C2 | 2.52 | 0.45 |
| 12:C:38:LYS:NZ | 12:C:57:HIS:O | 2.39 | 0.45 |
| 13:D:121:THR:O | 13:D:122:VAL:HB | 2.17 | 0.45 |
| 26:Q:4:LYS:NZ | 26:Q:7:VAL:HG11 | 2.31 | 0.45 |
| 31:V:2:G:C6 | 31:V:3:G:C5 | 3.05 | 0.45 |
| 32:W:19:ARG:C | 32:W:19:ARG:CD | 2.85 | 0.45 |
| 2:1:6:GLU:OE1 | 2:1:52:LYS:CE | 2.64 | 0.45 |
| 10:A:33:C:O2 | 10:A:447:A:N6 | 2.50 | 0.45 |
| 10:A:278:A:N1 | 10:A:362:A:C8 | 2.85 | 0.45 |
| 10:A:979:A:H2' | 10:A:982:C:H42 | 1.82 | 0.45 |
| 13:D:1:MET:HG2 | 13:D:205:PRO:HG3 | 1.98 | 0.45 |
| 14:E:119:ILE:HG13 | 14:E:119:ILE:O | 2.16 | 0.45 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 16:G:83:THR:C | 16:G:84:LYS:HD3 | 2.37 | 0.45 |
| 19:J:44:TYR:O | 19:J:45:THR:CB | 2.64 | 0.45 |
| 21:L:85:VAL:HG22 | 21:L:94:THR:HG22 | 1.97 | 0.45 |
| 28:S:1:MET:O | 28:S:108:SER:HB2 | 2.16 | 0.45 |
| 34:Y:45:GLN:O | 34:Y:46:VAL:HB | 2.17 | 0.45 |
| 10:A:247:G:H4' | 10:A:386:G:C5 | 2.51 | 0.45 |
| 10:A:288:U:H2' | 10:A:289:G:C8 | 2.52 | 0.45 |
| 10:A:820:A:H2' | 10:A:821:A:O4' | 2.16 | 0.45 |
| 10:A:1150:C:H2' | 10:A:1151:A:O5' | 2.17 | 0.45 |
| 10:A:2103:C:H2' | 10:A:2104:C:C5' | 2.47 | 0.45 |
| 10:A:2745:C:C4 | 10:A:2746:U:C4 | 3.05 | 0.45 |
| 13:D:44:GLY:HA3 | 13:D:45:TYR:HD1 | 1.82 | 0.45 |
| 25:P:91:VAL:HG11 | 25:P:96:LEU:HD21 | 1.98 | 0.45 |
| 10:A:597:G:C2 | 10:A:661:A:C2 | 3.04 | 0.44 |
| 10:A:2407:A:C2 | 10:A:2408:U:C2 | 3.05 | 0.44 |
| 10:A:2564:A:C2 | 10:A:2647:U:H4' | 2.53 | 0.44 |
| 10:A:2758:A:H2' | 10:A:2759:G:H5' | 1.99 | 0.44 |
| 10:A:2846:G:H2' | 10:A:2847:U:O4' | 2.17 | 0.44 |
| 13:D:70:LYS:O | 13:D:71:ALA:HB3 | 2.16 | 0.44 |
| 14:E:147:LEU:HB3 | 14:E:186:VAL:HG23 | 2.00 | 0.44 |
| 19:J:55:ILE:HD11 | 19:J:130:HIS:CD2 | 2.51 | 0.44 |
| 20:K:10:VAL:HG21 | 20:K:17:ARG:H | 1.81 | 0.44 |
| 26:Q:7:VAL:HG13 | 26:Q:8:ILE:N | 2.32 | 0.44 |
| 31:V:36:G:H2' | 31:V:37:G:O4' | 2.17 | 0.44 |
| 4:3:3:ILE:HG21 | 4:3:62:PRO:HG3 | 1.98 | 0.44 |
| 10:A:85:G:OP1 | 30:U:6:ARG:N | 2.49 | 0.44 |
| 10:A:973:A:O4' | 10:A:1188:U:C6 | 2.70 | 0.44 |
| 10:A:980:A:C6 | 10:A:981:A:N1 | 2.86 | 0.44 |
| 10:A:1428:C:C5 | 10:A:1569:A:H5" | 2.52 | 0.44 |
| 10:A:2180:U:C2 | 10:A:2181:U:C5 | 3.06 | 0.44 |
| 13:D:3:GLY:HA3 | 13:D:204:LYS:HG2 | 1.99 | 0.44 |
| 14:E:160:ALA:O | 14:E:161:ALA:HB3 | 2.18 | 0.44 |
| 24:O:79:ALA:O | 24:O:82:ALA:N | 2.49 | 0.44 |
| 29:T:48:GLN:O | 29:T:52:GLU:HA | 2.17 | 0.44 |
| 4:3:31:ILE:O | 4:3:31:ILE:HG13 | 2.17 | 0.44 |
| 6:5:125:ARG:CZ | 6:5:125:ARG:HA | 2.47 | 0.44 |
| 10:A:336:C:N3 | 10:A:337:C:C5 | 2.86 | 0.44 |
| 10:A:748:G:OP2 | 28:S:88:ARG:CB | 2.66 | 0.44 |
| 10:A:994:C:H1' | 27:R:10:LYS:CE | 2.47 | 0.44 |
| 10:A:996:A:H4' | 26:Q:91:ARG:CD | 2.47 | 0.44 |
| 10:A:1181:U:H2' | 10:A:1182:G:C8 | 2.52 | 0.44 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 10:A:2683:C:O2 | 20:K:70:ARG:NH2 | 2.38 | 0.44 |
| 15:F:128:SER:HA | 15:F:154:THR:HA | 1.99 | 0.44 |
| 16:G:175:LYS:HA | 16:G:176:LYS:HA | 1.79 | 0.44 |
| 20:K:61:VAL:HG22 | 20:K:87:LEU:HD11 | 1.98 | 0.44 |
| 9:8:80:HIS:CD2 | 9:8:82:TYR:H | 2.35 | 0.44 |
| 10:A:799:G:C6 | 10:A:800:A:C6 | 3.05 | 0.44 |
| 10:A:819:A:C4 | 10:A:1189:A:C2 | 3.06 | 0.44 |
| 10:A:2062:A:O2' | 10:A:2063:C:O5' | 2.31 | 0.44 |
| 10:A:2283:C:C2 | 10:A:2389:G:C2 | 3.06 | 0.44 |
| 12:C:76:VAL:HG22 | 12:C:76:VAL:O | 2.17 | 0.44 |
| 12:C:265:PHE:N | 12:C:265:PHE:HD1 | 2.15 | 0.44 |
| 13:D:69:ALA:HA | 13:D:73:VAL:CG1 | 2.47 | 0.44 |
| 13:D:86:GLU:CD | 13:D:86:GLU:N | 2.69 | 0.44 |
| 15:F:127:TYR:O | 15:F:128:SER:CB | 2.65 | 0.44 |
| 22:M:26:VAL:HB | 22:M:133:LYS:HA | 2.00 | 0.44 |
| 25:P:58:PHE:CE1 | 25:P:75:THR:HG22 | 2.51 | 0.44 |
| 30:U:73:ASN:O | 30:U:74:ALA:HB3 | 2.18 | 0.44 |
| 31:V:34:G:H2' | 31:V:35:G:C8 | 2.53 | 0.44 |
| 10:A:61:C:H2' | 10:A:62:U:H5' | 2.00 | 0.44 |
| 10:A:1252:G:C2 | 26:Q:32:ARG:HG2 | 2.52 | 0.44 |
| 10:A:1387:A:H5' | 10:A:1469:A:H1' | 2.00 | 0.44 |
| 10:A:1523:U:O2' | 10:A:1524:G:H5' | 2.18 | 0.44 |
| 10:A:2326:C:C6 | 10:A:2326:C:H3' | 2.52 | 0.44 |
| 16:G:24:THR:HG23 | 16:G:34:ARG:HG2 | 1.99 | 0.44 |
| 17:H:8:LYS:O | 17:H:13:GLY:HA2 | 2.16 | 0.44 |
| 18:I:45:THR:O | 18:I:48:ILE:HG13 | 2.17 | 0.44 |
| 20:K:118:LEU:O | 20:K:119:ALA:HB3 | 2.17 | 0.44 |
| 21:L:122:VAL:CG1 | 21:L:142:ILE:HG12 | 2.47 | 0.44 |
| 25:P:102:ARG:O | 25:P:103:THR:HG22 | 2.17 | 0.44 |
| 27:R:64:VAL:O | 27:R:65:ALA:HB3 | 2.18 | 0.44 |
| 29:T:40:LYS:HG2 | 29:T:58:VAL:HG22 | 1.99 | 0.44 |
| 30:U:53:GLN:N | 30:U:54:PRO:CD | 2.80 | 0.44 |
| 31:V:34:G:C6 | 31:V:35:G:C6 | 3.05 | 0.44 |
| 5:4:6:SER:HB2 | 10:A:1031:G:C4' | 2.47 | 0.44 |
| 6:5:15:VAL:CG2 | 6:5:66:GLY:HA2 | 2.47 | 0.44 |
| 8:7:17:ASN:O | 38:7:1002:TRP:CG | 2.70 | 0.44 |
| 10:A:132:G:C2' | 10:A:133:U:H5' | 2.48 | 0.44 |
| 10:A:315:G:H2' | 10:A:316:C:C6 | 2.52 | 0.44 |
| 10:A:545:U:H2' | 10:A:546:U:O3' | 2.18 | 0.44 |
| 10:A:764:A:C6 | 10:A:781:A:C2 | 3.06 | 0.44 |
| 10:A:1045:C:C3' | 10:A:1046:A:H5' | 2.48 | 0.44 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 10:A:1443:U:H2' | 10:A:1444:G:C8 | 2.53 | 0.44 |
| 10:A:1737:G:H5" | 10:A:1738:G:OP2 | 2.17 | 0.44 |
| 10:A:1867:G:C5 | 10:A:1868:C:C5 | 3.05 | 0.44 |
| 10:A:2902:C:H2' | 10:A:2903:U:O5' | 2.18 | 0.44 |
| 15:F:134:GLN:OE1 | 15:F:149:ARG:HB3 | 2.18 | 0.44 |
| 18:I:109:ALA:CB | 18:I:128:ILE:HG13 | 2.48 | 0.44 |
| 24:O:43:ASN:O | 24:O:45:SER:N | 2.50 | 0.44 |
| 8:7:14:ASN:C | 8:7:15:ILE:CD1 | 2.85 | 0.44 |
| 10:A:222:A:N6 | 10:A:231:A:C2 | 2.86 | 0.44 |
| 10:A:684:G:C2 | 10:A:794:A:C2 | 3.06 | 0.44 |
| 10:A:800:A:OP1 | 39:A:3324:HOH:O | 2.21 | 0.44 |
| 10:A:980:A:C4 | 10:A:1136:G:O4' | 2.70 | 0.44 |
| 10:A:1197:G:H2' | 10:A:1198:U:H6 | 1.83 | 0.44 |
| 10:A:2747:G:O6 | 10:A:2755:C:H5" | 2.18 | 0.44 |
| 11:B:90:C:H6 | 11:B:90:C:H5" | 1.83 | 0.44 |
| 15:F:107:VAL:HG11 | 15:F:116:LEU:HD21 | 1.99 | 0.44 |
| 16:G:104:LEU:HB2 | 16:G:112:VAL:CG2 | 2.47 | 0.44 |
| 20:K:80:ASP:CB | 25:P:67:GLU:HG3 | 2.47 | 0.44 |
| 21:L:111:ILE:N | 21:L:111:ILE:HD12 | 2.33 | 0.44 |
| 30:U:6:ARG:O | 30:U:24:VAL:HB | 2.17 | 0.44 |
| 32:W:19:ARG:NH2 | 32:W:22:VAL:HG21 | 2.33 | 0.44 |
| 4:3:31:ILE:O | 4:3:31:ILE:CG1 | 2.66 | 0.44 |
| 6:5:129:LEU:CB | 6:5:130:PRO:HD2 | 2.47 | 0.44 |
| 10:A:277:G:H2' | 10:A:361:G:O6 | 2.17 | 0.44 |
| 10:A:476:G:H4' | 10:A:502:A:N1 | 2.33 | 0.44 |
| 10:A:855:G:H21 | 32:W:23:LYS:CG | 2.31 | 0.44 |
| 11:B:27:C:C5 | 11:B:28:C:C5 | 3.06 | 0.44 |
| 12:C:109:LEU:HD23 | 12:C:110:LYS:H | 1.83 | 0.44 |
| 13:D:35:THR:N | 13:D:49:GLN:O | 2.41 | 0.44 |
| 13:D:110:THR:HG23 | 13:D:171:THR:HG22 | 2.00 | 0.44 |
| 16:G:60:GLY:O | 16:G:61:TRP:HB2 | 2.17 | 0.44 |
| 19:J:30:THR:HG22 | 19:J:31:GLU:N | 2.31 | 0.44 |
| 21:L:2:ARG:HA | 21:L:5:THR:CG2 | 2.48 | 0.44 |
| 26:Q:91:ARG:HH11 | 27:R:11:GLN:H | 1.64 | 0.44 |
| 28:S:18:ARG:HG3 | 28:S:76:VAL:HG13 | 1.98 | 0.44 |
| 29:T:69:ARG:HG3 | 29:T:70:HIS:H | 1.83 | 0.44 |
| 31:V:37:G:C2 | 31:V:38:U:H1' | 2.53 | 0.44 |
| 10:A:247:G:N7 | 10:A:249:C:C2 | 2.86 | 0.44 |
| 10:A:818:G:H5' | 10:A:839:U:OP1 | 2.18 | 0.44 |
| 10:A:1171:G:N2 | 10:A:1179:G:C4 | 2.86 | 0.44 |
| 10:A:2276:G:P | 22:M:83:GLY:O | 2.76 | 0.44 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 10:A:2788:C:H2' | 10:A:2789:C:C6 | 2.53 | 0.44 |
| 13:D:73:VAL:HG23 | 13:D:74:GLU:H | 1.83 | 0.44 |
| 15:F:72:SER:HB2 | 15:F:80:GLN:HB2 | 1.99 | 0.44 |
| 24:O:15:ARG:NE | 24:O:93:ASP:OD2 | 2.44 | 0.44 |
| 32:W:19:ARG:HA | 32:W:34:SER:HA | 2.00 | 0.44 |
| 32:W:24:ARG:HD3 | 32:W:65:LYS:HG2 | 2.00 | 0.44 |
| 8:7:17:ASN:HA | 38:7:1002:TRP:CE3 | 2.52 | 0.43 |
| 9:8:29:ILE:HD13 | 9:8:30:ILE:N | 2.33 | 0.43 |
| 10:A:580:U:O3' | 26:Q:30:VAL:HG13 | 2.18 | 0.43 |
| 10:A:581:C:H2' | 10:A:582:A:C8 | 2.54 | 0.43 |
| 10:A:1071:G:H1' | 10:A:1089:A:C5 | 2.53 | 0.43 |
| 10:A:2283:C:H5" | 10:A:2389:G:O2' | 2.18 | 0.43 |
| 11:B:78:A:H2' | 11:B:79:G:O4' | 2.18 | 0.43 |
| 12:C:180:MET:O | 12:C:267:VAL:N | 2.43 | 0.43 |
| 14:E:42:GLY:O | 14:E:43:THR:OG1 | 2.35 | 0.43 |
| 16:G:123:GLU:HG2 | 16:G:125:PRO:HD3 | 2.01 | 0.43 |
| 18:I:100:ILE:HD11 | 18:I:137:LEU:CG | 2.48 | 0.43 |
| 19:J:44:TYR:O | 19:J:44:TYR:CD2 | 2.71 | 0.43 |
| 19:J:80:HIS:O | 19:J:82:GLY:N | 2.50 | 0.43 |
| 22:M:13:HIS:O | 22:M:14:LYS:CB | 2.66 | 0.43 |
| 22:M:102:LEU:N | 22:M:102:LEU:HD12 | 2.32 | 0.43 |
| 24:O:41:ALA:O | 24:O:44:GLY:N | 2.41 | 0.43 |
| 26:Q:27:ARG:HA | 26:Q:33:VAL:HG12 | 1.99 | 0.43 |
| 29:T:69:ARG:CG | 29:T:70:HIS:N | 2.81 | 0.43 |
| 35:Z:15:ARG:HG2 | 35:Z:15:ARG:HH11 | 1.82 | 0.43 |
| 8:7:13:PHE:CG | 8:7:14:ASN:N | 2.83 | 0.43 |
| 10:A:201:C:OP1 | 33:X:17:ARG:NH2 | 2.51 | 0.43 |
| 10:A:1923:U:C5' | 31:V:24:G:H2' | 2.48 | 0.43 |
| 10:A:2307:G:N2 | 10:A:2311:A:C8 | 2.85 | 0.43 |
| 10:A:2682:A:C8 | 13:D:11:MET:HG3 | 2.53 | 0.43 |
| 15:F:94:ARG:HH11 | 15:F:94:ARG:CG | 2.31 | 0.43 |
| 17:H:8:LYS:O | 17:H:9:VAL:CB | 2.66 | 0.43 |
| 18:I:91:LYS:HB2 | 18:I:95:ASP:HB2 | 2.00 | 0.43 |
| 21:L:112:LEU:HD23 | 21:L:114:GLY:H | 1.83 | 0.43 |
| 28:S:66:ILE:HD13 | 28:S:67:ASP:N | 2.32 | 0.43 |
| 6:5:51:TYR:CE1 | 6:5:52:MET:HG2 | 2.53 | 0.43 |
| 8:7:15:ILE:CG1 | 8:7:16:ASP:H | 2.30 | 0.43 |
| 10:A:720:U:H2' | 10:A:721:A:C8 | 2.53 | 0.43 |
| 10:A:742:A:H2' | 10:A:743:A:C8 | 2.53 | 0.43 |
| 10:A:948:C:H1' | 10:A:984:A:O2' | 2.17 | 0.43 |
| 10:A:962:G:P | 39:A:3352:HOH:O | 2.77 | 0.43 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 10:A:1223:G:P | 27:R:68:ARG:HH21 | 2.41 | 0.43 |
| 10:A:1779:U:C5 | 10:A:1784:A:N7 | 2.86 | 0.43 |
| 10:A:2134:A:O2' | 10:A:2135:A:O4' | 2.36 | 0.43 |
| 10:A:2602:A:O2' | 31:V:74:C:P | 2.76 | 0.43 |
| 11:B:51:G:H5" | 24:O:64:TYR:CD2 | 2.52 | 0.43 |
| 18:I:40:ALA:O | 18:I:68:PHE:CZ | 2.71 | 0.43 |
| 26:Q:91:ARG:HH11 | 27:R:11:GLN:N | 2.16 | 0.43 |
| 32:W:17:ALA:O | 32:W:18:LYS:HB2 | 2.18 | 0.43 |
| 6:5:87:GLU:OE2 | 6:5:95:LEU:HD23 | 2.18 | 0.43 |
| 7:6:13:ALA:HB1 | 7:6:17:MET:CE | 2.49 | 0.43 |
| 10:A:1003:G:N2 | 10:A:1004:U:C2 | 2.86 | 0.43 |
| 10:A:1171:G:H1 | 10:A:1178:C:H42 | 1.66 | 0.43 |
| 10:A:1441:G:H2' | 10:A:1442:U:C6 | 2.53 | 0.43 |
| 10:A:1584:U:H2' | 10:A:1585:C:H5' | 1.99 | 0.43 |
| 10:A:2043:C:OP1 | 10:A:2777:G:O2' | 2.24 | 0.43 |
| 10:A:2197:U:O2 | 10:A:2198:A:O2' | 2.21 | 0.43 |
| 10:A:2335:A:N6 | 10:A:2337:G:H1' | 2.33 | 0.43 |
| 10:A:2603:G:H2' | 10:A:2604:U:O4' | 2.18 | 0.43 |
| 12:C:24:HIS:CE1 | 12:C:79:ARG:HH11 | 2.36 | 0.43 |
| 20:K:35:VAL:HG12 | 20:K:36:GLY:N | 2.34 | 0.43 |
| 23:N:38:LEU:HB3 | 23:N:39:PRO:CD | 2.48 | 0.43 |
| 32:W:37:VAL:HG11 | 32:W:55:ASP:HB2 | 1.99 | 0.43 |
| 1:0:42:ILE:HG22 | 1:0:43:THR:O | 2.19 | 0.43 |
| 6:5:17:GLU:OE2 | 6:5:53:ARG:NH1 | 2.51 | 0.43 |
| 6:5:88:HIS:CB | 6:5:89:PRO:CD | 2.97 | 0.43 |
| 9:8:75:GLN:HB2 | 9:8:92:VAL:CG2 | 2.48 | 0.43 |
| 10:A:172:A:H2' | 10:A:173:A:C8 | 2.53 | 0.43 |
| 10:A:822:G:H2' | 10:A:823:C:H6 | 1.83 | 0.43 |
| 10:A:959:A:H62 | 22:M:82:MET:HE1 | 1.84 | 0.43 |
| 10:A:1494:A:C2 | 10:A:1495:A:C4 | 3.06 | 0.43 |
| 10:A:1536:C:H1' | 10:A:1537:G:N2 | 2.34 | 0.43 |
| 10:A:1638:C:H4' | 10:A:2710:C:O2 | 2.19 | 0.43 |
| 10:A:2031:A:C6 | 10:A:2498:C:H1' | 2.53 | 0.43 |
| 10:A:2094:A:P | 17:H:22:LYS:HD2 | 2.59 | 0.43 |
| 10:A:2108:A:H2' | 10:A:2109:U:O5' | 2.17 | 0.43 |
| 10:A:2517:C:C5 | 10:A:2542:A:C5 | 3.06 | 0.43 |
| 15:F:134:GLN:HG2 | 15:F:135:ILE:N | 2.34 | 0.43 |
| 18:I:87:SER:OG | 18:I:88:GLY:N | 2.43 | 0.43 |
| 20:K:72:PRO:O | 20:K:74:GLY:N | 2.43 | 0.43 |
| 32:W:18:LYS:N | 32:W:36:ILE:HG13 | 2.33 | 0.43 |
| 33:X:67:LEU:HD22 | 33:X:77:TYR:CE1 | 2.53 | 0.43 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 8:7:22:HIS:C | 8:7:23:ARG:CG | 2.75 | 0.43 |
| 10:A:479:A:N3 | 10:A:481:G:H5" | 2.34 | 0.43 |
| 10:A:936:A:H2' | 10:A:937:C:C6 | 2.54 | 0.43 |
| 10:A:1439:A:C2 | 10:A:1553:A:C4 | 3.06 | 0.43 |
| 10:A:1914:C:H2' | 10:A:1915:U:O4' | 2.18 | 0.43 |
| 12:C:16:VAL:H | 12:C:203:VAL:HG12 | 1.83 | 0.43 |
| 14:E:44:ARG:HH11 | 14:E:44:ARG:CG | 2.31 | 0.43 |
| 23:N:70:THR:HB | 23:N:75:ILE:HD11 | 2.00 | 0.43 |
| 32:W:24:ARG:HD3 | 32:W:65:LYS:CD | 2.48 | 0.43 |
| 32:W:37:VAL:HB | 32:W:38:ARG:NH1 | 2.34 | 0.43 |
| 32:W:49:ASN:ND2 | 32:W:50:VAL:N | 2.67 | 0.43 |
| 2:1:8:ILE:CD1 | 2:1:24:LYS:HG2 | 2.48 | 0.43 |
| 6:5:54:VAL:O | 6:5:55:VAL:C | 2.57 | 0.43 |
| 10:A:348:A:C5 | 10:A:349:U:C5 | 3.07 | 0.43 |
| 10:A:1322:A:OP1 | 28:S:11:ARG:NE | 2.38 | 0.43 |
| 10:A:1782:U:O2 | 10:A:2608:G:C2' | 2.66 | 0.43 |
| 10:A:1942:C:OP2 | 10:A:1943:U:O2' | 2.28 | 0.43 |
| 10:A:2698:U:H2' | 10:A:2699:C:C6 | 2.51 | 0.43 |
| 19:J:44:TYR:HA | 26:Q:59:LEU:CD2 | 2.48 | 0.43 |
| 22:M:8:LYS:CE | 22:M:9:PHE:CE2 | 3.02 | 0.43 |
| 23:N:8:ARG:HB3 | 23:N:10:LEU:CD2 | 2.48 | 0.43 |
| 9:8:72:VAL:HG12 | 9:8:93:ARG:HA | 2.01 | 0.43 |
| 10:A:226:A:C6 | 10:A:227:A:C6 | 3.07 | 0.43 |
| 10:A:323:C:OP1 | 10:A:338:G:N2 | 2.51 | 0.43 |
| 10:A:975:A:C5 | 10:A:990:A:N7 | 2.86 | 0.43 |
| 10:A:1232:G:C5 | 10:A:1233:C:C5 | 3.06 | 0.43 |
| 10:A:1239:G:H2' | 10:A:1240:U:O4' | 2.19 | 0.43 |
| 10:A:1281:G:C2 | 10:A:1290:C:C2 | 3.07 | 0.43 |
| 10:A:1485:U:H2' | 10:A:1486:U:H6 | 1.83 | 0.43 |
| 10:A:1857:G:C2 | 10:A:1884:G:N3 | 2.86 | 0.43 |
| 10:A:2508:G:N1 | 10:A:2582:G:O6 | 2.52 | 0.43 |
| 10:A:2584:U:O2' | 10:A:2585:U:C5 | 2.72 | 0.43 |
| 16:G:39:ALA:HB2 | 16:G:57:TYR:CD2 | 2.54 | 0.43 |
| 26:Q:86:SER:O | 27:R:51:VAL:HA | 2.18 | 0.43 |
| 34:Y:56:LEU:HD22 | 34:Y:56:LEU:H | 1.84 | 0.43 |
| 5:4:36:ARG:HG2 | 5:4:37:GLN:N | 2.34 | 0.43 |
| 10:A:356:G:C6 | 10:A:357:C:C4 | 3.07 | 0.43 |
| 10:A:646:U:H3' | 10:A:647:G:H5" | 1.99 | 0.43 |
| 10:A:744:U:H2' | 10:A:745:G:O4' | 2.19 | 0.43 |
| 10:A:1224:U:H4' | 27:R:88:GLY:O | 2.18 | 0.43 |
| 10:A:2070:A:H2' | 10:A:2071:A:O4' | 2.19 | 0.43 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 10:A:2344:U:H4' | 10:A:2345:G:OP1 | 2.17 | 0.43 |
| 10:A:2423:U:H5' | 10:A:2423:U:H6 | 1.83 | 0.43 |
| 11:B:78:A:C2 | 11:B:99:A:C4 | 3.06 | 0.43 |
| 11:B:106:G:H2' | 11:B:107:G:O4' | 2.19 | 0.43 |
| 13:D:45:TYR:N | 13:D:45:TYR:CD1 | 2.86 | 0.43 |
| 14:E:52:VAL:HG11 | 14:E:81:GLY:HA3 | 2.01 | 0.43 |
| 14:E:187:VAL:O | 14:E:188:MET:CB | 2.67 | 0.43 |
| 23:N:117:ASP:O | 23:N:118:ARG:C | 2.56 | 0.43 |
| 26:Q:4:LYS:HZ3 | 26:Q:7:VAL:CG1 | 2.32 | 0.43 |
| 27:R:74:ILE:HB | 27:R:87:GLN:O | 2.18 | 0.43 |
| 28:S:88:ARG:CZ | 28:S:88:ARG:CB | 2.92 | 0.43 |
| 32:W:39:GLN:HG2 | 32:W:41:GLY:N | 2.34 | 0.43 |
| 6:5:142:THR:OG1 | 6:5:143:MET:N | 2.52 | 0.43 |
| 10:A:545:U:H6 | 10:A:545:U:O5' | 2.02 | 0.43 |
| 10:A:945:A:C4 | 10:A:2448:A:C2 | 3.07 | 0.43 |
| 10:A:1096:A:H2' | 10:A:1097:U:H5" | 2.01 | 0.43 |
| 10:A:1204:A:C2 | 10:A:1240:U:N3 | 2.87 | 0.43 |
| 10:A:1476:U:C5 | 10:A:1514:G:C2 | 3.07 | 0.43 |
| 10:A:1747:U:H2' | 10:A:1748:C:C6 | 2.54 | 0.43 |
| 10:A:2274:A:C5 | 10:A:2276:G:C8 | 3.07 | 0.43 |
| 10:A:2595:G:N1 | 10:A:2599:G:C6 | 2.87 | 0.43 |
| 10:A:2657:A:C2 | 10:A:2665:A:C4 | 3.06 | 0.43 |
| 13:D:124:ARG:HA | 13:D:165:MET:SD | 2.58 | 0.43 |
| 15:F:62:GLN:NE2 | 15:F:89:THR:O | 2.46 | 0.43 |
| 18:I:93:ASN:HB2 | 18:I:135:MET:SD | 2.59 | 0.43 |
| 19:J:88:THR:HG22 | 19:J:91:GLU:CG | 2.49 | 0.43 |
| 19:J:110:PRO:HB2 | 19:J:111:LYS:HG3 | 2.00 | 0.43 |
| 29:T:70:HIS:HB3 | 29:T:73:ARG:O | 2.19 | 0.43 |
| 32:W:36:ILE:HG22 | 32:W:36:ILE:O | 2.18 | 0.43 |
| 32:W:44:PHE:O | 32:W:78:PHE:HA | 2.19 | 0.43 |
| 34:Y:1:MET:H3 | 34:Y:2:LYS:HD2 | 1.84 | 0.43 |
| 6:5:67:THR:C | 6:5:69:PHE:N | 2.73 | 0.42 |
| 6:5:71:CYS:SG | 6:5:117:LEU:HD12 | 2.58 | 0.42 |
| 10:A:570:G:C4 | 10:A:2030:A:N7 | 2.87 | 0.42 |
| 10:A:1188:U:H4' | 27:R:81:LYS:O | 2.19 | 0.42 |
| 10:A:2516:A:N6 | 10:A:2517:C:N4 | 2.67 | 0.42 |
| 10:A:2661:G:C6 | 10:A:2662:A:C2 | 3.06 | 0.42 |
| 12:C:16:VAL:N | 12:C:203:VAL:CG1 | 2.82 | 0.42 |
| 16:G:36:LEU:HD22 | 16:G:36:LEU:N | 2.33 | 0.42 |
| 18:I:46:ASP:HA | 18:I:50:LYS:HD2 | 2.00 | 0.42 |
| 18:I:82:ALA:HB1 | 18:I:108:ILE:HG21 | 2.00 | 0.42 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 2:1:7:LYS:NZ | 10:A:2421:G:P | 2.92 | 0.42 |
| 3:2:12:ARG:HH21 | 3:2:44:VAL:HG11 | 1.82 | 0.42 |
| 6:5:71:CYS:HB3 | 6:5:74:ASP:OD2 | 2.18 | 0.42 |
| 10:A:274:C:H2' | 10:A:275:C:O4' | 2.19 | 0.42 |
| 10:A:301:G:H2' | 10:A:334:C:H2' | 2.01 | 0.42 |
| 10:A:528:A:P | 19:J:116:ARG:HH21 | 2.42 | 0.42 |
| 10:A:573:U:O2' | 10:A:574:A:H3' | 2.19 | 0.42 |
| 10:A:1465:G:H2' | 10:A:1466:U:O4' | 2.19 | 0.42 |
| 10:A:2062:A:N3 | 10:A:2063:C:C6 | 2.87 | 0.42 |
| 10:A:2287:A:C8 | 10:A:2289:G:C8 | 3.08 | 0.42 |
| 10:A:2602:A:H8 | 31:V:74:C:OP2 | 2.03 | 0.42 |
| 10:A:2661:G:H2' | 10:A:2662:A:O4' | 2.19 | 0.42 |
| 11:B:72:G:N2 | 11:B:103:U:C5 | 2.86 | 0.42 |
| 13:D:118:PHE:HZ | 23:N:1:MET:HB2 | 1.85 | 0.42 |
| 14:E:12:LEU:HD12 | 14:E:193:VAL:HG11 | 2.01 | 0.42 |
| 21:L:2:ARG:HA | 21:L:5:THR:HG21 | 2.01 | 0.42 |
| 23:N:103:ARG:HD3 | 23:N:110:MET:HE3 | 2.00 | 0.42 |
| 25:P:58:PHE:HD1 | 25:P:75:THR:HG22 | 1.83 | 0.42 |
| 30:U:38:ILE:HG23 | 30:U:39:ASN:N | 2.33 | 0.42 |
| 6:5:17:GLU:HA | 6:5:88:HIS:CE1 | 2.54 | 0.42 |
| 10:A:959:A:N6 | 22:M:82:MET:CE | 2.82 | 0.42 |
| 10:A:1966:A:N3 | 10:A:2592:G:O2' | 2.47 | 0.42 |
| 10:A:2755:C:O2' | 10:A:2756:U:H2' | 2.19 | 0.42 |
| 13:D:120:GLY:HA2 | 13:D:162:ALA:HA | 2.00 | 0.42 |
| 14:E:158:PHE:HD2 | 14:E:159:LEU:HD12 | 1.83 | 0.42 |
| 15:F:103:ILE:HG21 | 15:F:173:ASP:HB2 | 2.01 | 0.42 |
| 30:U:35:VAL:O | 30:U:38:ILE:HB | 2.19 | 0.42 |
| 34:Y:14:LEU:HA | 34:Y:17:GLU:HB3 | 2.01 | 0.42 |
| 35:Z:15:ARG:HD3 | 35:Z:53:MET:SD | 2.59 | 0.42 |
| 6:5:3:LEU:HD12 | 6:5:5:LEU:N | 2.35 | 0.42 |
| 10:A:1298:C:C2 | 10:A:1643:G:N2 | 2.88 | 0.42 |
| 10:A:1378:A:C4 | 10:A:1380:G:N7 | 2.87 | 0.42 |
| 10:A:1770:G:C6 | 10:A:1983:G:C6 | 3.07 | 0.42 |
| 10:A:1782:U:N3 | 10:A:2587:A:C6 | 2.87 | 0.42 |
| 10:A:2022:U:OP1 | 39:A:3657:HOH:O | 2.20 | 0.42 |
| 10:A:2071:A:H2' | 10:A:2072:C:C6 | 2.54 | 0.42 |
| 10:A:2557:G:H2' | 10:A:2558:C:C6 | 2.54 | 0.42 |
| 10:A:2748:A:H1' | 16:G:66:THR:CG2 | 2.49 | 0.42 |
| 10:A:2803:G:H2' | 10:A:2804:U:H6 | 1.84 | 0.42 |
| 13:D:149:ASN:CG | 13:D:150:GLN:H | 2.21 | 0.42 |
| 15:F:111:ARG:NE | 15:F:111:ARG:HA | 2.34 | 0.42 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 19:J:38:GLY:O | 19:J:43:GLU:HB2 | 2.19 | 0.42 |
| 23:N:24:MET:HE2 | 23:N:44:LEU:HD22 | 2.02 | 0.42 |
| 24:O:31:THR:HG22 | 24:O:34:HIS:N | 2.33 | 0.42 |
| 26:Q:60:TRP:CE2 | 26:Q:93:ILE:HB | 2.54 | 0.42 |
| 26:Q:94:LEU:CD1 | 27:R:13:ARG:HB2 | 2.49 | 0.42 |
| 28:S:89:ALA:O | 28:S:90:LYS:HG3 | 2.19 | 0.42 |
| 32:W:42:THR:HG22 | 32:W:43:LYS:HZ2 | 1.83 | 0.42 |
| 6:5:47:GLU:HG2 | 6:5:95:LEU:HD21 | 2.00 | 0.42 |
| 7:6:15:SER:OG | 7:6:16:VAL:N | 2.53 | 0.42 |
| 10:A:146:A:H2' | 10:A:147:C:C6 | 2.54 | 0.42 |
| 10:A:1238:G:O2' | 10:A:1239:G:H5' | 2.19 | 0.42 |
| 10:A:2039:U:H2' | 10:A:2040:G:H8 | 1.82 | 0.42 |
| 10:A:2392:A:OP2 | 10:A:2422:C:N4 | 2.50 | 0.42 |
| 14:E:51:GLU:OE2 | 14:E:88:ARG:NH2 | 2.45 | 0.42 |
| 16:G:35:THR:HG22 | 16:G:36:LEU:N | 2.33 | 0.42 |
| 20:K:3:GLN:HG3 | 20:K:4:GLU:N | 2.34 | 0.42 |
| 29:T:76:ARG:HG3 | 29:T:77:ARG:N | 2.34 | 0.42 |
| 33:X:52:ALA:O | 33:X:53:LYS:CB | 2.67 | 0.42 |
| 35:Z:39:ASP:CG | 35:Z:44:ARG:HH21 | 2.23 | 0.42 |
| 2:1:18:HIS:CE1 | 2:1:40:PRO:HD3 | 2.54 | 0.42 |
| 10:A:1312:U:H4' | 10:A:1313:U:O5' | 2.20 | 0.42 |
| 10:A:1937:A:N7 | 10:A:1939:U:H2' | 2.35 | 0.42 |
| 10:A:1956:U:H2' | 10:A:1957:C:H5' | 2.01 | 0.42 |
| 10:A:2047:C:O2' | 10:A:2048:G:H5' | 2.19 | 0.42 |
| 10:A:2352:A:N1 | 32:W:30:VAL:HG21 | 2.35 | 0.42 |
| 10:A:2823:A:C5 | 10:A:2824:C:C5 | 3.07 | 0.42 |
| 10:A:2845:U:H5" | 25:P:51:ASN:O | 2.20 | 0.42 |
| 14:E:188:MET:HE3 | 14:E:196:VAL:HG21 | 2.02 | 0.42 |
| 16:G:1:SER:O | 16:G:4:ALA:N | 2.48 | 0.42 |
| 19:J:43:GLU:O | 19:J:44:TYR:C | 2.58 | 0.42 |
| 23:N:12:ARG:CZ | 23:N:20:MET:HE1 | 2.50 | 0.42 |
| 24:O:14:ALA:O | 24:O:17:LYS:N | 2.52 | 0.42 |
| 29:T:34:VAL:O | 29:T:34:VAL:HG22 | 2.20 | 0.42 |
| 30:U:84:PHE:O | 30:U:85:ARG:HB3 | 2.19 | 0.42 |
| 34:Y:31:GLN:HG2 | 34:Y:36:GLN:HB2 | 2.01 | 0.42 |
| 4:3:22:LYS:HA | 4:3:47:ALA:O | 2.19 | 0.42 |
| 6:5:22:ALA:N | 6:5:87:GLU:O | 2.53 | 0.42 |
| 6:5:51:TYR:CD1 | 6:5:52:MET:HG2 | 2.55 | 0.42 |
| 6:5:131:THR:HA | 6:5:134:GLU:CG | 2.50 | 0.42 |
| 10:A:84:A:N1 | 10:A:98:G:O2' | 2.30 | 0.42 |
| 10:A:272:A:HO2' | 10:A:273:G:H8 | 1.65 | 0.42 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 10:A:518:G:H2' | 10:A:519:U:C6 | 2.55 | 0.42 |
| 10:A:1112:G:C5 | 10:A:1113:U:C5 | 3.07 | 0.42 |
| 10:A:1183:U:H2' | 10:A:1184:U:C6 | 2.55 | 0.42 |
| 10:A:1814:G:C6 | 10:A:1815:A:C6 | 3.08 | 0.42 |
| 10:A:2674:G:H4' | 20:K:30:ARG:HG3 | 2.02 | 0.42 |
| 13:D:133:THR:HG23 | 13:D:134:HIS:N | 2.34 | 0.42 |
| 15:F:28:PRO:HB2 | 15:F:168:LEU:HD22 | 2.02 | 0.42 |
| 18:I:9:LYS:HB3 | 18:I:71:LYS:NZ | 2.34 | 0.42 |
| 19:J:11:VAL:HG11 | 19:J:50:THR:HA | 2.01 | 0.42 |
| 20:K:47:ILE:HG13 | 20:K:48:PRO:HD2 | 2.00 | 0.42 |
| 23:N:8:ARG:HB3 | 23:N:10:LEU:HD22 | 2.01 | 0.42 |
| 27:R:16:GLU:HA | 27:R:98:ILE:HG22 | 2.01 | 0.42 |
| 10:A:1010:A:OP2 | 39:A:3767:HOH:O | 2.20 | 0.42 |
| 10:A:1084:A:C6 | 10:A:1085:A:C6 | 3.08 | 0.42 |
| 10:A:1607:C:H42 | 10:A:1622:G:P | 2.43 | 0.42 |
| 10:A:1909:C:C1' | 31:V:11:C:O2' | 2.68 | 0.42 |
| 11:B:16:G:C5 | 11:B:69:G:C2 | 3.07 | 0.42 |
| 15:F:94:ARG:HH11 | 15:F:94:ARG:HB2 | 1.84 | 0.42 |
| 15:F:107:VAL:HG13 | 15:F:110:ILE:HD12 | 2.02 | 0.42 |
| 20:K:39:ILE:HD12 | 20:K:41:ILE:HD11 | 2.02 | 0.42 |
| 26:Q:6:GLY:HA2 | 26:Q:9:ALA:HB3 | 2.02 | 0.42 |
| 26:Q:82:LEU:HD12 | 26:Q:112:ALA:HB2 | 2.02 | 0.42 |
| 27:R:80:ARG:O | 27:R:81:LYS:HD3 | 2.20 | 0.42 |
| 34:Y:21:LEU:HA | 34:Y:25:GLN:HB3 | 2.01 | 0.42 |
| 8:7:17:ASN:O | 38:7:1002:TRP:CD2 | 2.73 | 0.42 |
| 10:A:126:A:C6 | 10:A:127:A:N1 | 2.88 | 0.42 |
| 10:A:479:A:C2 | 10:A:480:A:C5 | 3.08 | 0.42 |
| 10:A:685:A:C2 | 10:A:689:A:C6 | 3.08 | 0.42 |
| 10:A:833:A:OP1 | 21:L:39:LYS:HE3 | 2.19 | 0.42 |
| 10:A:1691:C:C4 | 10:A:1692:U:C4 | 3.08 | 0.42 |
| 10:A:1782:U:C1' | 10:A:2608:G:O2' | 2.66 | 0.42 |
| 10:A:2637:U:C2' | 10:A:2638:G:H5' | 2.50 | 0.42 |
| 10:A:2821:A:C2 | 10:A:2822:G:C4 | 3.08 | 0.42 |
| 11:B:89:U:H3' | 11:B:90:C:C5' | 2.49 | 0.42 |
| 13:D:24:VAL:HA | 13:D:191:GLY:H | 1.85 | 0.42 |
| 16:G:137:LYS:HA | 16:G:140:ILE:HG22 | 2.02 | 0.42 |
| 26:Q:20:ALA:HA | 26:Q:23:TYR:CE2 | 2.54 | 0.42 |
| 27:R:5:PHE:HB3 | 27:R:59:ILE:HD12 | 2.01 | 0.42 |
| 27:R:38:VAL:O | 27:R:53:PHE:HA | 2.20 | 0.42 |
| 28:S:96:ILE:O | 28:S:96:ILE:HG13 | 2.20 | 0.42 |
| 29:T:29:THR:HB | 29:T:86:THR:HA | 2.01 | 0.42 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 32:W:60:ALA:CB | 32:W:81:ILE:CD1 | 2.98 | 0.42 |
| 2:1:5:ARG:CZ | 2:1:24:LYS:HA | 2.49 | 0.42 |
| 6:5:67:THR:CG2 | 6:5:72:LEU:HA | 2.49 | 0.42 |
| 6:5:108:VAL:HG12 | 6:5:109:LYS:N | 2.35 | 0.42 |
| 8:7:17:ASN:ND2 | 8:7:17:ASN:C | 2.73 | 0.42 |
| 8:7:22:HIS:O | 8:7:23:ARG:O | 2.37 | 0.42 |
| 10:A:75:G:H4' | 34:Y:48:ARG:NH2 | 2.34 | 0.42 |
| 10:A:179:C:C2 | 10:A:180:G:C8 | 3.08 | 0.42 |
| 10:A:996:A:C5 | 10:A:1160:G:C2 | 3.08 | 0.42 |
| 10:A:1194:A:C2' | 10:A:1195:G:O5' | 2.68 | 0.42 |
| 10:A:1394:U:OP1 | 39:A:3405:HOH:O | 2.22 | 0.42 |
| 10:A:1789:A:H2' | 10:A:1790:C:O4' | 2.20 | 0.42 |
| 12:C:184:GLU:O | 12:C:185:ALA:HB3 | 2.20 | 0.42 |
| 12:C:203:VAL:O | 12:C:205:GLY:N | 2.53 | 0.42 |
| 18:I:11:GLN:OE1 | 18:I:11:GLN:N | 2.43 | 0.42 |
| 19:J:4:PHE:HB3 | 19:J:44:TYR:CE2 | 2.55 | 0.42 |
| 19:J:81:ILE:CG1 | 19:J:82:GLY:H | 2.33 | 0.42 |
| 24:O:75:GLY:HA3 | 24:O:109:ALA:HB3 | 2.00 | 0.42 |
| 27:R:74:ILE:HD12 | 27:R:74:ILE:N | 2.34 | 0.42 |
| 28:S:18:ARG:HG3 | 28:S:76:VAL:CG1 | 2.50 | 0.42 |
| 28:S:59:GLU:HA | 28:S:64:ALA:CB | 2.50 | 0.42 |
| 8:7:19:ILE:HD12 | 8:7:19:ILE:HA | 1.89 | 0.41 |
| 10:A:109:C:H4' | 10:A:348:A:H4' | 2.02 | 0.41 |
| 10:A:864:G:OP2 | 22:M:22:GLN:NE2 | 2.52 | 0.41 |
| 10:A:2526:G:C5 | 10:A:2527:C:C5 | 3.08 | 0.41 |
| 16:G:26:LYS:CG | 16:G:27:GLY:N | 2.83 | 0.41 |
| 19:J:4:PHE:O | 19:J:44:TYR:OH | 2.35 | 0.41 |
| 19:J:64:VAL:HG13 | 19:J:65:THR:N | 2.35 | 0.41 |
| 23:N:12:ARG:HB3 | 23:N:16:HIS:HB3 | 2.02 | 0.41 |
| 24:O:49:VAL:HG12 | 24:O:50:ALA:N | 2.35 | 0.41 |
| 25:P:92:ARG:CG | 25:P:92:ARG:O | 2.68 | 0.41 |
| 31:V:3:G:C2 | 31:V:71:C:C2 | 3.08 | 0.41 |
| 35:Z:13:ILE:HG22 | 35:Z:14:GLY:N | 2.34 | 0.41 |
| 6:5:27:VAL:O | 6:5:83:ALA:N | 2.52 | 0.41 |
| 10:A:201:C:O2' | 10:A:251:A:N1 | 2.38 | 0.41 |
| 10:A:555:G:O2' | 10:A:556:A:OP2 | 2.31 | 0.41 |
| 10:A:653:U:H5 | 10:A:654:A:C2 | 2.38 | 0.41 |
| 10:A:1591:A:H2' | 10:A:1592:C:C6 | 2.55 | 0.41 |
| 10:A:1936:A:C2 | 10:A:1943:U:H5 | 2.38 | 0.41 |
| 10:A:1945:G:C6 | 10:A:1946:U:C4 | 3.09 | 0.41 |
| 10:A:2576:G:H3' | 10:A:2576:G:N3 | 2.35 | 0.41 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 16:G:31:GLU:O | 16:G:33:THR:N | 2.52 | 0.41 |
| 17:H:39:ALA:HB1 | 17:H:44:ILE:HG22 | 2.01 | 0.41 |
| 19:J:60:ASP:OD1 | 19:J:60:ASP:N | 2.52 | 0.41 |
| 25:P:92:ARG:HH11 | 25:P:92:ARG:HB2 | 1.85 | 0.41 |
| 6:5:108:VAL:CG1 | 6:5:109:LYS:N | 2.82 | 0.41 |
| 10:A:1078:U:H5" | 10:A:1079:C:OP1 | 2.20 | 0.41 |
| 10:A:1338:G:O2' | 10:A:1393:A:N1 | 2.44 | 0.41 |
| 10:A:1378:A:H4' | 10:A:1379:U:OP1 | 2.20 | 0.41 |
| 10:A:1509:A:H1' | 10:A:1510:G:O5' | 2.20 | 0.41 |
| 10:A:1647:U:P | 10:A:1647:U:H3' | 2.60 | 0.41 |
| 10:A:1843:C:H5' | 12:C:250:GLN:NE2 | 2.36 | 0.41 |
| 10:A:2409:G:H2' | 10:A:2410:G:O4' | 2.20 | 0.41 |
| 14:E:79:ARG:HG2 | 14:E:80:SER:N | 2.35 | 0.41 |
| 18:I:20:SER:HB3 | 18:I:21:PRO:HD3 | 2.01 | 0.41 |
| 19:J:35:ARG:HG2 | 19:J:40:HIS:HD2 | 1.84 | 0.41 |
| 20:K:13:ASN:O | 20:K:14:SER:CB | 2.67 | 0.41 |
| 20:K:15:GLY:O | 20:K:46:ALA:HA | 2.20 | 0.41 |
| 25:P:30:TRP:CE3 | 25:P:39:LEU:HD12 | 2.56 | 0.41 |
| 27:R:61:ALA:HB1 | 27:R:98:ILE:H | 1.84 | 0.41 |
| 35:Z:4:ILE:HD13 | 35:Z:44:ARG:NH2 | 2.35 | 0.41 |
| 1:0:12:ARG:HD2 | 1:0:16:ARG:NH2 | 2.36 | 0.41 |
| 1:0:42:ILE:HD12 | 23:N:99:LYS:O | 2.20 | 0.41 |
| 10:A:19:A:H2' | 10:A:20:C:O4' | 2.20 | 0.41 |
| 10:A:633:A:OP1 | 21:L:68:SER:OG | 2.34 | 0.41 |
| 10:A:803:U:C4 | 10:A:804:A:N7 | 2.88 | 0.41 |
| 10:A:966:G:C6 | 10:A:967:U:C4 | 3.07 | 0.41 |
| 10:A:1722:A:C2 | 10:A:1739:A:N3 | 2.89 | 0.41 |
| 10:A:1923:U:H5' | 31:V:25:C:C1' | 2.50 | 0.41 |
| 10:A:2543:G:C6 | 10:A:2544:G:C6 | 3.08 | 0.41 |
| 10:A:2580:U:C5 | 10:A:2581:G:C6 | 3.08 | 0.41 |
| 11:B:117:G:OP1 | 24:O:56:LYS:NZ | 2.49 | 0.41 |
| 12:C:172:THR:HG22 | 12:C:182:LYS:HG2 | 2.02 | 0.41 |
| 14:E:134:LEU:CD2 | 14:E:161:ALA:HB2 | 2.50 | 0.41 |
| 18:I:100:ILE:CD1 | 18:I:137:LEU:HD12 | 2.50 | 0.41 |
| 19:J:65:THR:HG22 | 19:J:68:LYS:NZ | 2.36 | 0.41 |
| 22:M:53:MET:CE | 22:M:63:ILE:HG21 | 2.50 | 0.41 |
| 28:S:89:ALA:O | 28:S:90:LYS:CG | 2.69 | 0.41 |
| 32:W:24:ARG:HH11 | 32:W:65:LYS:HG2 | 1.85 | 0.41 |
| 5:4:32:LYS:HD3 | 10:A:2478:A:H5' | 2.02 | 0.41 |
| 6:5:33:VAL:HB | 6:5:36:ASP:OD1 | 2.20 | 0.41 |
| 8:7:19:ILE:O | 38:7:1002:TRP:HD1 | 2.03 | 0.41 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 8:7:19:ILE:CG1 | 8:7:20:VAL:H | 2.32 | 0.41 |
| 9:8:21:ARG:NH1 | 11:B:77:U:OP1 | 2.54 | 0.41 |
| 10:A:347:A:C2 | 10:A:348:A:C4 | 3.09 | 0.41 |
| 10:A:372:G:C4 | 33:X:60:LYS:HE2 | 2.54 | 0.41 |
| 10:A:669:G:N3 | 10:A:669:G:C2' | 2.83 | 0.41 |
| 10:A:1019:U:H3 | 10:A:1142:A:N6 | 2.17 | 0.41 |
| 10:A:1579:A:H2' | 10:A:1580:A:C8 | 2.56 | 0.41 |
| 10:A:1681:G:N2 | 10:A:1763:G:OP2 | 2.45 | 0.41 |
| 10:A:2204:G:OP2 | 12:C:146:LYS:NZ | 2.34 | 0.41 |
| 10:A:2478:A:C2' | 10:A:2479:U:H5' | 2.51 | 0.41 |
| 10:A:2586:U:H2' | 10:A:2587:A:C8 | 2.55 | 0.41 |
| 10:A:2676:C:P | 20:K:31:ARG:HH12 | 2.43 | 0.41 |
| 12:C:143:VAL:HB | 12:C:153:LEU:HB2 | 2.02 | 0.41 |
| 13:D:88:GLU:O | 13:D:89:GLU:HG3 | 2.21 | 0.41 |
| 15:F:151:LEU:CD1 | 15:F:153:ILE:HG23 | 2.51 | 0.41 |
| 20:K:13:ASN:N | 20:K:13:ASN:OD1 | 2.48 | 0.41 |
| 23:N:79:LEU:O | 23:N:80:PHE:HB2 | 2.19 | 0.41 |
| 26:Q:63:ARG:HH12 | 26:Q:96:ASP:HA | 1.86 | 0.41 |
| 9:8:6:ALA:HB1 | 9:8:40:ILE:CG2 | 2.50 | 0.41 |
| 10:A:138:U:H5' | 10:A:139:U:C5' | 2.51 | 0.41 |
| 10:A:580:U:H2' | 10:A:581:C:C6 | 2.54 | 0.41 |
| 10:A:749:A:C5 | 10:A:1618:A:C2 | 3.09 | 0.41 |
| 10:A:1179:G:C6 | 10:A:1180:U:C4 | 3.08 | 0.41 |
| 10:A:1301:A:H2' | 10:A:1301:A:N3 | 2.35 | 0.41 |
| 10:A:1494:A:C6 | 10:A:1495:A:C5 | 3.08 | 0.41 |
| 10:A:2555:U:C5 | 10:A:2556:C:C2 | 3.09 | 0.41 |
| 10:A:2796:U:C4 | 10:A:2798:U:C5 | 3.08 | 0.41 |
| 14:E:129:PRO:HG3 | 14:E:156:ASN:OD1 | 2.21 | 0.41 |
| 15:F:46:LYS:H | 15:F:46:LYS:HD3 | 1.86 | 0.41 |
| 15:F:111:ARG:HA | 15:F:111:ARG:CZ | 2.51 | 0.41 |
| 30:U:10:VAL:HG12 | 30:U:71:ILE:HA | 2.01 | 0.41 |
| 10:A:58:G:N2 | 10:A:70:G:C4 | 2.89 | 0.41 |
| 10:A:635:C:P | 21:L:126:ARG:HH21 | 2.44 | 0.41 |
| 10:A:1268:A:H2' | 10:A:1269:A:O4' | 2.20 | 0.41 |
| 10:A:1365:A:N6 | 10:A:1366:A:C6 | 2.89 | 0.41 |
| 10:A:1365:A:OP1 | 33:X:2:ARG:NE | 2.48 | 0.41 |
| 10:A:1714:U:H5' | 10:A:1715:G:H5' | 2.02 | 0.41 |
| 14:E:187:VAL:HG12 | 14:E:188:MET:N | 2.36 | 0.41 |
| 15:F:112:ASP:N | 15:F:112:ASP:OD1 | 2.54 | 0.41 |
| 21:L:40:SER:O | 21:L:41:ARG:CB | 2.67 | 0.41 |
| 22:M:63:ILE:HG22 | 22:M:64:TRP:N | 2.36 | 0.41 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 22:M:64:TRP:HZ3 | 22:M:106:ASP:HB2 | 1.86 | 0.41 |
| 23:N:87:PHE:O | 23:N:89:SER:N | 2.54 | 0.41 |
| 30:U:98:ASN:ND2 | 30:U:100:GLU:OE1 | 2.53 | 0.41 |
| 32:W:19:ARG:NH1 | 32:W:22:VAL:CG2 | 2.83 | 0.41 |
| 34:Y:12:GLU:O | 34:Y:15:ASN:HB2 | 2.21 | 0.41 |
| 35:Z:2:LYS:CB | 35:Z:39:ASP:HB3 | 2.51 | 0.41 |
| 8:7:19:ILE:HG23 | 8:7:20:VAL:HG23 | 2.01 | 0.41 |
| 10:A:84:A:P | 30:U:5:ARG:HH12 | 2.42 | 0.41 |
| 10:A:1069:A:C2' | 10:A:1070:A:OP2 | 2.68 | 0.41 |
| 10:A:1392:A:C6 | 10:A:1393:A:C6 | 3.09 | 0.41 |
| 10:A:2145:C:N3 | 10:A:2146:C:N3 | 2.69 | 0.41 |
| 10:A:2201:G:C6 | 10:A:2202:U:C4 | 3.08 | 0.41 |
| 10:A:2581:G:C4 | 10:A:2610:C:C5 | 3.09 | 0.41 |
| 10:A:2685:G:H1 | 10:A:2724:U:H3 | 1.68 | 0.41 |
| 10:A:2727:A:C6 | 10:A:2728:U:O4 | 2.73 | 0.41 |
| 12:C:77:VAL:HG23 | 12:C:77:VAL:O | 2.20 | 0.41 |
| 19:J:4:PHE:CD2 | 19:J:44:TYR:CE2 | 3.08 | 0.41 |
| 19:J:26:GLY:HA2 | 19:J:29:ALA:HB3 | 2.02 | 0.41 |
| 19:J:88:THR:HG23 | 19:J:91:GLU:H | 1.86 | 0.41 |
| 29:T:69:ARG:HG3 | 29:T:70:HIS:N | 2.36 | 0.41 |
| 3:2:9:VAL:HG13 | 10:A:1309:G:OP1 | 2.21 | 0.41 |
| 10:A:307:G:N2 | 10:A:310:A:C8 | 2.89 | 0.41 |
| 10:A:527:C:H4' | 10:A:528:A:O5' | 2.21 | 0.41 |
| 10:A:528:A:H2 | 10:A:2043:C:H5' | 1.85 | 0.41 |
| 10:A:659:G:H4' | 14:E:95:LYS:HD3 | 2.02 | 0.41 |
| 10:A:866:A:N7 | 10:A:914:G:C6 | 2.88 | 0.41 |
| 10:A:996:A:C6 | 10:A:1160:G:C2 | 3.08 | 0.41 |
| 10:A:1063:G:H2' | 10:A:1064:C:O4' | 2.20 | 0.41 |
| 10:A:1096:A:N6 | 10:A:1097:U:C4 | 2.89 | 0.41 |
| 10:A:1486:U:H2' | 10:A:1487:U:C6 | 2.55 | 0.41 |
| 10:A:1509:A:O2' | 10:A:1510:G:P | 2.76 | 0.41 |
| 10:A:1587:G:C4 | 10:A:1588:G:C8 | 3.09 | 0.41 |
| 10:A:1613:G:O6 | 10:A:1617:C:H2' | 2.21 | 0.41 |
| 10:A:1630:A:H2' | 10:A:1631:G:H5' | 2.03 | 0.41 |
| 10:A:1970:A:OP2 | 39:A:3464:HOH:O | 2.21 | 0.41 |
| 10:A:2259:U:H1' | 10:A:2427:C:C2 | 2.56 | 0.41 |
| 10:A:2341:G:H2' | 10:A:2342:C:C6 | 2.56 | 0.41 |
| 10:A:2581:G:C2 | 10:A:2610:C:C5 | 3.09 | 0.41 |
| 10:A:2583:G:N7 | 10:A:2584:U:C4 | 2.89 | 0.41 |
| 10:A:2618:G:C6 | 10:A:2619:C:C4 | 3.09 | 0.41 |
| 10:A:2681:C:C2 | 10:A:2724:U:O4 | 2.74 | 0.41 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 10:A:2766:A:N3 | 10:A:2766:A:H2' | 2.36 | 0.41 |
| 12:C:16:VAL:HB | 12:C:203:VAL:HG12 | 2.02 | 0.41 |
| 15:F:169:LEU:O | 15:F:174:PHE:HB2 | 2.21 | 0.41 |
| 18:I:104:GLN:O | 18:I:105:LEU:CB | 2.69 | 0.41 |
| 23:N:24:MET:CE | 23:N:36:THR:HG21 | 2.51 | 0.41 |
| 25:P:50:ARG:CD | 25:P:56:SER:HB3 | 2.51 | 0.41 |
| 28:S:63:GLY:O | 28:S:64:ALA:HB3 | 2.21 | 0.41 |
| 28:S:69:LEU:HG | 28:S:107:VAL:HG22 | 2.03 | 0.41 |
| 32:W:19:ARG:HG2 | 32:W:19:ARG:HH11 | 1.86 | 0.41 |
| 1:0:16:ARG:CZ | 28:S:15:GLN:NE2 | 2.84 | 0.41 |
| 5:4:38:GLY:OXT | 10:A:1124:G:H1' | 2.21 | 0.41 |
| 10:A:45:G:C5' | 10:A:46:G:H5' | 2.51 | 0.41 |
| 10:A:485:C:C2 | 10:A:496:G:N2 | 2.88 | 0.41 |
| 10:A:528:A:H2 | 10:A:2043:C:C5' | 2.33 | 0.41 |
| 10:A:608:A:C8 | 10:A:621:A:N6 | 2.89 | 0.41 |
| 10:A:996:A:C5 | 10:A:1160:G:N2 | 2.89 | 0.41 |
| 10:A:1381:G:H1' | 10:A:1571:A:N1 | 2.35 | 0.41 |
| 10:A:1638:C:H5" | 10:A:2710:C:O2' | 2.21 | 0.41 |
| 10:A:2038:G:H2' | 10:A:2039:U:O4' | 2.21 | 0.41 |
| 10:A:2103:C:H2' | 10:A:2104:C:H5" | 2.02 | 0.41 |
| 10:A:2180:U:N3 | 10:A:2181:U:C5 | 2.89 | 0.41 |
| 10:A:2447:G:C5 | 10:A:2500:U:C5 | 3.09 | 0.41 |
| 10:A:2537:U:C4 | 10:A:2538:C:N4 | 2.89 | 0.41 |
| 10:A:2869:G:C6 | 10:A:2870:C:C4 | 3.09 | 0.41 |
| 20:K:19:VAL:HG13 | 20:K:41:ILE:HG12 | 2.02 | 0.41 |
| 21:L:29:LYS:HG2 | 21:L:30:THR:N | 2.36 | 0.41 |
| 21:L:127:VAL:HG11 | 21:L:142:ILE:HG21 | 2.03 | 0.41 |
| 23:N:51:LEU:HD21 | 23:N:70:THR:CG2 | 2.51 | 0.41 |
| 26:Q:46:TYR:CZ | 26:Q:50:ARG:NH2 | 2.89 | 0.41 |
| 32:W:19:ARG:NH1 | 32:W:19:ARG:HG2 | 2.36 | 0.41 |
| 6:5:47:GLU:CG | 6:5:95:LEU:HD21 | 2.51 | 0.40 |
| 10:A:901:C:C4 | 10:A:902:C:C4 | 3.09 | 0.40 |
| 10:A:1669:A:O2' | 10:A:2549:G:OP1 | 2.36 | 0.40 |
| 10:A:2134:A:C8 | 10:A:2134:A:OP2 | 2.75 | 0.40 |
| 10:A:2570:G:H2' | 10:A:2571:U:O4' | 2.21 | 0.40 |
| 13:D:68:PHE:CE2 | 13:D:75:ALA:HB1 | 2.56 | 0.40 |
| 14:E:109:LEU:O | 14:E:112:LEU:N | 2.54 | 0.40 |
| 15:F:10:GLU:HG2 | 15:F:13:LYS:HD3 | 2.02 | 0.40 |
| 16:G:10:VAL:HG22 | 16:G:47:ASN:C | 2.41 | 0.40 |
| 17:H:24:GLY:O | 17:H:28:ASN:HB2 | 2.21 | 0.40 |
| 18:I:74:PRO:HG2 | 18:I:77:VAL:HB | 2.02 | 0.40 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 19:J:43:GLU:O | 19:J:45:THR:CG2 | 2.70 | 0.40 |
| 22:M:12:MET:HE3 | 22:M:71:LYS:HG3 | 2.03 | 0.40 |
| 28:S:88:ARG:CD | 28:S:94:ASP:OD2 | 2.70 | 0.40 |
| 29:T:24:MET:HG3 | 29:T:29:THR:CG2 | 2.51 | 0.40 |
| 30:U:13:LEU:HD11 | 30:U:70:ALA:HB2 | 2.03 | 0.40 |
| 32:W:22:VAL:O | 32:W:23:LYS:HG3 | 2.22 | 0.40 |
| 1:0:47:TYR:CE1 | 1:0:52:LYS:HD3 | 2.57 | 0.40 |
| 5:4:32:LYS:CD | 10:A:2478:A:H5' | 2.51 | 0.40 |
| 6:5:23:LEU:HD22 | 6:5:92:ALA:O | 2.21 | 0.40 |
| 6:5:106:PHE:CG | 6:5:107:GLU:N | 2.87 | 0.40 |
| 6:5:131:THR:HA | 6:5:134:GLU:HG3 | 2.03 | 0.40 |
| 6:5:132:TYR:HE1 | 7:6:19:VAL:HG13 | 1.85 | 0.40 |
| 7:6:7:ILE:HA | 7:6:10:ALA:HB3 | 2.02 | 0.40 |
| 8:7:14:ASN:CG | 14:E:61:ARG:NH2 | 2.74 | 0.40 |
| 10:A:848:C:H2' | 10:A:849:A:C8 | 2.56 | 0.40 |
| 10:A:2583:G:C5 | 10:A:2584:U:C4 | 3.09 | 0.40 |
| 10:A:2780:G:P | 19:J:120:ARG:HE | 2.44 | 0.40 |
| 14:E:178:VAL:HG23 | 14:E:179:SER:N | 2.36 | 0.40 |
| 21:L:77:ILE:HD13 | 21:L:108:ALA:HB1 | 2.02 | 0.40 |
| 25:P:33:GLU:HB2 | 25:P:38:ARG:NH2 | 2.35 | 0.40 |
| 6:5:88:HIS:HB3 | 6:5:89:PRO:HD3 | 2.03 | 0.40 |
| 8:7:24:PRO:HB2 | 31:V:76:A:O3' | 2.21 | 0.40 |
| 9:8:44:HIS:CE1 | 9:8:86:LEU:H | 2.39 | 0.40 |
| 10:A:24:G:H1' | 28:S:77:ASP:HB3 | 2.04 | 0.40 |
| 10:A:45:G:H5' | 10:A:46:G:H5' | 2.03 | 0.40 |
| 10:A:230:G:N2 | 10:A:231:A:C4 | 2.90 | 0.40 |
| 10:A:483:A:N7 | 10:A:497:A:H2 | 2.20 | 0.40 |
| 10:A:580:U:O3' | 26:Q:30:VAL:CG1 | 2.70 | 0.40 |
| 10:A:1570:A:C6 | 10:A:1571:A:C6 | 3.09 | 0.40 |
| 10:A:1684:G:C2 | 10:A:1705:A:C2 | 3.10 | 0.40 |
| 10:A:1905:C:N4 | 10:A:1930:G:C2 | 2.89 | 0.40 |
| 10:A:2447:G:C4 | 10:A:2500:U:C5 | 3.09 | 0.40 |
| 12:C:158:GLY:H | 12:C:194:VAL:HG22 | 1.86 | 0.40 |
| 18:I:19:PRO:HG2 | 18:I:24:GLY:H | 1.85 | 0.40 |
| 31:V:72:G:C3' | 31:V:73:A:H5" | 2.51 | 0.40 |
| 32:W:39:GLN:OE1 | 32:W:43:LYS:HB2 | 2.21 | 0.40 |
| 1:0:33:SER:OG | 1:0:35:GLU:HG3 | 2.21 | 0.40 |
| 2:1:35:LEU:HD22 | 2:1:35:LEU:N | 2.37 | 0.40 |
| 8:7:11:LYS:H | 8:7:11:LYS:HG3 | 1.72 | 0.40 |
| 10:A:64:A:C6 | 10:A:65:U:C4 | 3.10 | 0.40 |
| 10:A:82:U:H2' | 10:A:83:A:C8 | 2.57 | 0.40 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 10:A:136:G:H1 | 10:A:143:C:H42 | 1.69 | 0.40 |
| 10:A:911:A:C5 | 22:M:9:PHE:CE2 | 3.10 | 0.40 |
| 10:A:1007:C:OP1 | 19:J:37:ARG:NH1 | 2.54 | 0.40 |
| 10:A:1149:G:H2' | 10:A:1150:C:C6 | 2.57 | 0.40 |
| 10:A:1494:A:C6 | 10:A:1495:A:C6 | 3.08 | 0.40 |
| 10:A:1655:A:N6 | 10:A:2005:A:H1' | 2.37 | 0.40 |
| 10:A:2070:A:C2 | 10:A:2071:A:C4 | 3.09 | 0.40 |
| 12:C:68:ARG:NE | 12:C:128:THR:OG1 | 2.55 | 0.40 |
| 15:F:148:VAL:HG23 | 15:F:149:ARG:N | 2.36 | 0.40 |
| 18:I:14:ALA:HB1 | 18:I:45:THR:CG2 | 2.52 | 0.40 |
| 24:O:7:ARG:HA | 24:O:10:ARG:NH1 | 2.36 | 0.40 |
| 25:P:4:ILE:HG22 | 25:P:8:GLU:HG3 | 2.04 | 0.40 |
| 25:P:88:ARG:HH22 | 25:P:113:LEU:HA | 1.86 | 0.40 |
| 6:5:59:LEU:HD23 | 6:5:62:ARG:HE | 1.85 | 0.40 |
| 6:5:129:LEU:C | 6:5:131:THR:N | 2.73 | 0.40 |
| 8:7:15:ILE:CG1 | 8:7:16:ASP:N | 2.84 | 0.40 |
| 10:A:301:G:C6 | 10:A:317:G:C6 | 3.09 | 0.40 |
| 10:A:535:G:C6 | 10:A:559:G:C6 | 3.09 | 0.40 |
| 10:A:931:U:OP1 | 35:Z:29:ARG:NH2 | 2.55 | 0.40 |
| 10:A:1022:G:C5 | 10:A:1140:C:N4 | 2.89 | 0.40 |
| 10:A:1026:G:H2' | 10:A:1027:A:C8 | 2.55 | 0.40 |
| 10:A:1068:G:H3' | 10:A:1069:A:H5" | 2.03 | 0.40 |
| 10:A:1674:G:N2 | 10:A:1677:A:N1 | 2.69 | 0.40 |
| 10:A:1798:U:OP1 | 12:C:255:LYS:O | 2.40 | 0.40 |
| 10:A:2103:C:N4 | 10:A:2186:G:H1 | 2.19 | 0.40 |
| 10:A:2740:A:N6 | 10:A:2764:A:C8 | 2.90 | 0.40 |
| 12:C:115:ILE:HG22 | 12:C:116:GLN:N | 2.36 | 0.40 |
| 13:D:46:ARG:CZ | 13:D:46:ARG:HB3 | 2.50 | 0.40 |
| 16:G:19:ASN:O | 16:G:22:VAL:HG22 | 2.21 | 0.40 |
| 17:H:27:ARG:NH2 | 33:X:63:ILE:HG13 | 2.36 | 0.40 |
| 21:L:74:THR:HG22 | 21:L:107:PHE:HB2 | 2.03 | 0.40 |
| 34:Y:2:LYS:HD2 | 34:Y:2:LYS:N | 2.36 | 0.40 |

There are no symmetry-related clashes.

## 5.3 Torsion angles (i)

### 5.3.1 Protein backbone (i)

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

entries.

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

| Mol | Chain | Analysed | Favoured | Allowed | Outliers | Percentiles |
|---|---|---|---|---|---|---|
| 1 | 0 | 54/56 (96%) | 43 (80%) | 7 (13%) | 4 (7%) | 1 16 |
| 2 | 1 | 48/50 (96%) | 42 (88%) | 3 (6%) | 3 (6%) | 1 20 |
| 3 | 2 | 44/46 (96%) | 41 (93%) | 3 (7%) | 0 | 100 100 |
| 4 | 3 | 62/64 (97%) | 53 (86%) | 7 (11%) | 2 (3%) | 4 32 |
| 5 | 4 | 36/38 (95%) | 29 (81%) | 4 (11%) | 3 (8%) | 1 13 |
| 6 | 5 | 146/148 (99%) | 77 (53%) | 41 (28%) | 28 (19%) | 0 2 |
| 7 | 6 | 28/30 (93%) | 20 (71%) | 7 (25%) | 1 (4%) | 3 30 |
| 8 | 7 | 18/20 (90%) | 7 (39%) | 1 (6%) | 10 (56%) | 0 0 |
| 9 | 8 | 92/94 (98%) | 81 (88%) | 11 (12%) | 0 | 100 100 |
| 12 | C | 269/271 (99%) | 211 (78%) | 43 (16%) | 15 (6%) | 2 21 |
| 13 | D | 207/209 (99%) | 163 (79%) | 30 (14%) | 14 (7%) | 1 18 |
| 14 | E | 199/201 (99%) | 162 (81%) | 27 (14%) | 10 (5%) | 2 23 |
| 15 | F | 175/177 (99%) | 141 (81%) | 30 (17%) | 4 (2%) | 6 38 |
| 16 | G | 174/176 (99%) | 127 (73%) | 30 (17%) | 17 (10%) | 0 10 |
| 17 | H | 48/50 (96%) | 29 (60%) | 14 (29%) | 5 (10%) | 0 9 |
| 18 | I | 139/141 (99%) | 97 (70%) | 33 (24%) | 9 (6%) | 1 19 |
| 19 | J | 140/142 (99%) | 113 (81%) | 18 (13%) | 9 (6%) | 1 20 |
| 20 | K | 120/122 (98%) | 95 (79%) | 15 (12%) | 10 (8%) | 1 13 |
| 21 | L | 141/143 (99%) | 104 (74%) | 32 (23%) | 5 (4%) | 3 31 |
| 22 | M | 134/136 (98%) | 107 (80%) | 16 (12%) | 11 (8%) | 1 13 |
| 23 | N | 118/120 (98%) | 101 (86%) | 16 (14%) | 1 (1%) | 19 57 |
| 24 | O | 114/116 (98%) | 95 (83%) | 18 (16%) | 1 (1%) | 17 54 |
| 25 | P | 112/114 (98%) | 86 (77%) | 17 (15%) | 9 (8%) | 1 14 |
| 26 | Q | 115/117 (98%) | 99 (86%) | 12 (10%) | 4 (4%) | 3 31 |
| 27 | R | 101/103 (98%) | 83 (82%) | 15 (15%) | 3 (3%) | 4 33 |
| 28 | S | 108/110 (98%) | 90 (83%) | 10 (9%) | 8 (7%) | 1 16 |
| 29 | T | 91/93 (98%) | 57 (63%) | 24 (26%) | 10 (11%) | 0 8 |
| 30 | U | 100/102 (98%) | 74 (74%) | 16 (16%) | 10 (10%) | 0 9 |
| 32 | W | 77/79 (98%) | 39 (51%) | 21 (27%) | 17 (22%) | 0 1 |

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| Mol | Chain | Analysed | Favoured | Allowed | Outliers | Percentiles |
|---|---|---|---|---|---|---|
| 33 | X | 75/77 (97%) | 64 (85%) | 8 (11%) | 3 (4%) | 3 28 |
| 34 | Y | 61/63 (97%) | 39 (64%) | 18 (30%) | 4 (7%) | 1 19 |
| 35 | Z | 56/58 (97%) | 46 (82%) | 8 (14%) | 2 (4%) | 3 30 |
| All | All | 3402/3466 (98%) | 2615 (77%) | 555 (16%) | 232 (7%) | 2 18 |

All (232) Ramachandran outliers are listed below:

| Mol | Chain | Res | Type |
|---|---|---|---|
| 1 | 0 | 23 | ALA |
| 4 | 3 | 22 | LYS |
| 5 | 4 | 8 | LYS |
| 6 | 5 | 27 | VAL |
| 6 | 5 | 48 | ALA |
| 6 | 5 | 54 | VAL |
| 6 | 5 | 55 | VAL |
| 6 | 5 | 58 | THR |
| 6 | 5 | 69 | PHE |
| 6 | 5 | 93 | ALA |
| 6 | 5 | 107 | GLU |
| 6 | 5 | 108 | VAL |
| 6 | 5 | 120 | ALA |
| 6 | 5 | 124 | ASP |
| 6 | 5 | 130 | PRO |
| 8 | 7 | 8 | VAL |
| 8 | 7 | 13 | PHE |
| 8 | 7 | 15 | ILE |
| 8 | 7 | 17 | ASN |
| 8 | 7 | 19 | ILE |
| 12 | C | 70 | LYS |
| 12 | C | 104 | LEU |
| 12 | C | 121 | ALA |
| 12 | C | 140 | VAL |
| 13 | D | 43 | ASP |
| 13 | D | 73 | VAL |
| 13 | D | 170 | VAL |
| 14 | E | 79 | ARG |
| 15 | F | 111 | ARG |
| 16 | G | 2 | ARG |
| 16 | G | 16 | VAL |
| 16 | G | 28 | LYS |
| 16 | G | 31 | GLU |

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| Mol | Chain | Res | Type |
|---|---|---|---|
| 16 | G | 84 | LYS |
| 16 | G | 164 | ALA |
| 16 | G | 168 | VAL |
| 17 | H | 3 | VAL |
| 19 | J | 13 | ARG |
| 19 | J | 21 | THR |
| 19 | J | 44 | TYR |
| 19 | J | 45 | THR |
| 19 | J | 81 | ILE |
| 19 | J | 125 | TYR |
| 21 | L | 66 | PHE |
| 22 | M | 14 | LYS |
| 22 | M | 77 | PRO |
| 23 | N | 119 | SER |
| 25 | P | 50 | ARG |
| 25 | P | 51 | ASN |
| 25 | P | 93 | LYS |
| 28 | S | 3 | THR |
| 28 | S | 14 | ALA |
| 28 | S | 64 | ALA |
| 28 | S | 87 | PRO |
| 29 | T | 27 | SER |
| 29 | T | 29 | THR |
| 29 | T | 40 | LYS |
| 30 | U | 6 | ARG |
| 30 | U | 87 | GLU |
| 30 | U | 92 | VAL |
| 30 | U | 98 | ASN |
| 30 | U | 99 | SER |
| 32 | W | 9 | THR |
| 32 | W | 18 | LYS |
| 32 | W | 29 | SER |
| 32 | W | 36 | ILE |
| 32 | W | 56 | HIS |
| 35 | Z | 9 | THR |
| 1 | 0 | 35 | GLU |
| 2 | 1 | 4 | ILE |
| 2 | 1 | 50 | GLU |
| 6 | 5 | 3 | LEU |
| 6 | 5 | 33 | VAL |
| 6 | 5 | 88 | HIS |
| 6 | 5 | 92 | ALA |

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| Mol | Chain | Res | Type |
|---|---|---|---|
| 6 | 5 | 116 | GLU |
| 6 | 5 | 119 | PRO |
| 8 | 7 | 20 | VAL |
| 12 | C | 37 | SER |
| 12 | C | 77 | VAL |
| 12 | C | 238 | ASN |
| 12 | C | 256 | THR |
| 13 | D | 92 | VAL |
| 13 | D | 99 | GLU |
| 13 | D | 107 | VAL |
| 13 | D | 118 | PHE |
| 15 | F | 135 | ILE |
| 15 | F | 176 | PHE |
| 16 | G | 169 | ARG |
| 17 | H | 9 | VAL |
| 17 | H | 16 | GLY |
| 18 | I | 20 | SER |
| 18 | I | 79 | LEU |
| 19 | J | 111 | LYS |
| 20 | K | 35 | VAL |
| 20 | K | 71 | ARG |
| 21 | L | 111 | ILE |
| 22 | M | 2 | LEU |
| 22 | M | 36 | VAL |
| 22 | M | 56 | ALA |
| 27 | R | 65 | ALA |
| 28 | S | 19 | LEU |
| 28 | S | 96 | ILE |
| 29 | T | 36 | LYS |
| 29 | T | 49 | LYS |
| 30 | U | 51 | LEU |
| 32 | W | 14 | ASP |
| 32 | W | 47 | GLY |
| 32 | W | 50 | VAL |
| 32 | W | 74 | LYS |
| 34 | Y | 37 | LEU |
| 2 | 1 | 51 | ALA |
| 5 | 4 | 4 | ARG |
| 6 | 5 | 5 | LEU |
| 6 | 5 | 78 | GLY |
| 6 | 5 | 118 | ILE |
| 7 | 6 | 14 | MET |

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| Mol | Chain | Res | Type |
|---|---|---|---|
| 8 | 7 | 21 | ASP |
| 12 | C | 110 | LYS |
| 13 | D | 95 | SER |
| 13 | D | 109 | VAL |
| 13 | D | 192 | ALA |
| 14 | E | 7 | ASP |
| 14 | E | 70 | SER |
| 14 | E | 123 | LYS |
| 16 | G | 32 | LEU |
| 16 | G | 117 | PRO |
| 16 | G | 170 | THR |
| 17 | H | 10 | ALA |
| 18 | I | 11 | GLN |
| 20 | K | 13 | ASN |
| 20 | K | 46 | ALA |
| 20 | K | 93 | GLN |
| 22 | M | 69 | PRO |
| 24 | O | 3 | LYS |
| 25 | P | 113 | LEU |
| 27 | R | 98 | ILE |
| 28 | S | 92 | ARG |
| 29 | T | 28 | ASN |
| 30 | U | 85 | ARG |
| 30 | U | 101 | THR |
| 32 | W | 34 | SER |
| 33 | X | 17 | ARG |
| 33 | X | 34 | SER |
| 35 | Z | 34 | THR |
| 1 | 0 | 54 | ILE |
| 5 | 4 | 16 | ILE |
| 6 | 5 | 89 | PRO |
| 8 | 7 | 7 | CYS |
| 8 | 7 | 16 | ASP |
| 12 | C | 59 | GLN |
| 12 | C | 197 | ALA |
| 13 | D | 169 | ARG |
| 13 | D | 175 | LEU |
| 15 | F | 132 | ARG |
| 16 | G | 33 | THR |
| 16 | G | 173 | ALA |
| 18 | I | 64 | ARG |
| 19 | J | 74 | TYR |

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| Mol | Chain | Res | Type |
|---|---|---|---|
| 20 | K | 119 | ALA |
| 21 | L | 29 | LYS |
| 22 | M | 23 | GLY |
| 22 | M | 134 | THR |
| 25 | P | 4 | ILE |
| 25 | P | 103 | THR |
| 26 | Q | 87 | VAL |
| 26 | Q | 88 | GLU |
| 26 | Q | 95 | ALA |
| 28 | S | 90 | LYS |
| 29 | T | 51 | PHE |
| 29 | T | 55 | VAL |
| 32 | W | 37 | VAL |
| 33 | X | 76 | LYS |
| 34 | Y | 7 | ARG |
| 6 | 5 | 36 | ASP |
| 6 | 5 | 72 | LEU |
| 6 | 5 | 128 | THR |
| 8 | 7 | 23 | ARG |
| 12 | C | 64 | VAL |
| 12 | C | 120 | ASP |
| 12 | C | 196 | ASN |
| 13 | D | 183 | GLU |
| 14 | E | 46 | GLN |
| 14 | E | 96 | VAL |
| 16 | G | 97 | VAL |
| 16 | G | 163 | TYR |
| 16 | G | 166 | GLU |
| 18 | I | 12 | VAL |
| 18 | I | 71 | LYS |
| 19 | J | 65 | THR |
| 20 | K | 49 | ARG |
| 20 | K | 108 | ARG |
| 21 | L | 5 | THR |
| 21 | L | 41 | ARG |
| 22 | M | 35 | ALA |
| 22 | M | 73 | ILE |
| 25 | P | 34 | GLY |
| 25 | P | 92 | ARG |
| 26 | Q | 85 | ALA |
| 29 | T | 86 | THR |
| 29 | T | 89 | GLU |

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| Mol | Chain | Res | Type |
|---|---|---|---|
| 30 | U | 88 | ASP |
| 32 | W | 10 | ARG |
| 32 | W | 46 | ALA |
| 34 | Y | 9 | LYS |
| 6 | 5 | 59 | LEU |
| 6 | 5 | 94 | ARG |
| 14 | E | 83 | VAL |
| 14 | E | 153 | LEU |
| 16 | G | 118 | ALA |
| 17 | H | 14 | SER |
| 18 | I | 93 | ASN |
| 20 | K | 6 | THR |
| 20 | K | 50 | GLY |
| 22 | M | 13 | HIS |
| 27 | R | 40 | MET |
| 30 | U | 16 | LYS |
| 32 | W | 23 | LYS |
| 32 | W | 76 | ARG |
| 32 | W | 78 | PHE |
| 25 | P | 63 | ILE |
| 32 | W | 41 | GLY |
| 6 | 5 | 32 | GLY |
| 14 | E | 148 | ILE |
| 34 | Y | 62 | GLY |
| 4 | 3 | 6 | VAL |
| 12 | C | 232 | GLY |
| 13 | D | 122 | VAL |
| 18 | I | 22 | PRO |
| 18 | I | 88 | GLY |
| 1 | 0 | 24 | VAL |
| 14 | E | 71 | GLY |

### 5.3.2 Protein sidechains (i)

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

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

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| Mol | Chain | Analysed | Rotameric | Outliers | Percentiles |
|---|---|---|---|---|---|

| Mol | Chain | Analysed | Rotameric | Outliers | Percentiles |
|---|---|---|---|---|---|
| 1 | 0 | 47/47 (100%) | 46 (98%) | 1 (2%) | 53 74 |
| 2 | 1 | 45/45 (100%) | 42 (93%) | 3 (7%) | 16 47 |
| 3 | 2 | 38/38 (100%) | 35 (92%) | 3 (8%) | 12 42 |
| 4 | 3 | 51/51 (100%) | 46 (90%) | 5 (10%) | 8 33 |
| 5 | 4 | 34/34 (100%) | 31 (91%) | 3 (9%) | 10 38 |
| 6 | 5 | 112/112 (100%) | 93 (83%) | 19 (17%) | 2 14 |
| 7 | 6 | 26/26 (100%) | 22 (85%) | 4 (15%) | 2 17 |
| 8 | 7 | 20/20 (100%) | 15 (75%) | 5 (25%) | 0 4 |
| 9 | 8 | 78/78 (100%) | 75 (96%) | 3 (4%) | 33 61 |
| 12 | C | 216/216 (100%) | 202 (94%) | 14 (6%) | 17 48 |
| 13 | D | 164/164 (100%) | 151 (92%) | 13 (8%) | 12 42 |
| 14 | E | 165/165 (100%) | 146 (88%) | 19 (12%) | 5 27 |
| 15 | F | 148/148 (100%) | 138 (93%) | 10 (7%) | 16 47 |
| 16 | G | 137/137 (100%) | 122 (89%) | 15 (11%) | 6 29 |
| 17 | H | 40/40 (100%) | 39 (98%) | 1 (2%) | 47 70 |
| 18 | I | 109/109 (100%) | 105 (96%) | 4 (4%) | 34 62 |
| 19 | J | 116/116 (100%) | 100 (86%) | 16 (14%) | 3 22 |
| 20 | K | 103/103 (100%) | 92 (89%) | 11 (11%) | 6 30 |
| 21 | L | 102/102 (100%) | 95 (93%) | 7 (7%) | 15 46 |
| 22 | M | 109/109 (100%) | 93 (85%) | 16 (15%) | 3 19 |
| 23 | N | 100/100 (100%) | 93 (93%) | 7 (7%) | 15 46 |
| 24 | O | 86/86 (100%) | 78 (91%) | 8 (9%) | 9 35 |
| 25 | P | 99/99 (100%) | 91 (92%) | 8 (8%) | 11 41 |
| 26 | Q | 89/89 (100%) | 81 (91%) | 8 (9%) | 9 37 |
| 27 | R | 84/84 (100%) | 78 (93%) | 6 (7%) | 14 45 |
| 28 | S | 93/93 (100%) | 83 (89%) | 10 (11%) | 6 30 |
| 29 | T | 80/80 (100%) | 78 (98%) | 2 (2%) | 47 70 |
| 30 | U | 83/83 (100%) | 77 (93%) | 6 (7%) | 14 45 |
| 32 | W | 59/59 (100%) | 53 (90%) | 6 (10%) | 7 31 |
| 33 | X | 67/67 (100%) | 61 (91%) | 6 (9%) | 9 37 |

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| Mol | Chain | Analysed | Rotameric | Outliers | Percentiles |
|---|---|---|---|---|---|
| 34 | Y | 55/55 (100%) | 52 (94%) | 3 (6%) | 21 53 |
| 35 | Z | 48/48 (100%) | 40 (83%) | 8 (17%) | 2 15 |
| All | All | 2803/2803 (100%) | 2553 (91%) | 250 (9%) | 13 38 |

All (250) residues with a non-rotameric sidechain are listed below:

| Mol | Chain | Res | Type |
|---|---|---|---|
| 1 | 0 | 24 | VAL |
| 2 | 1 | 8 | ILE |
| 2 | 1 | 35 | LEU |
| 2 | 1 | 47 | ILE |
| 3 | 2 | 8 | SER |
| 3 | 2 | 9 | VAL |
| 3 | 2 | 24 | THR |
| 4 | 3 | 7 | ARG |
| 4 | 3 | 30 | HIS |
| 4 | 3 | 31 | ILE |
| 4 | 3 | 49 | VAL |
| 4 | 3 | 56 | LEU |
| 5 | 4 | 4 | ARG |
| 5 | 4 | 15 | LYS |
| 5 | 4 | 27 | CYS |
| 6 | 5 | 1 | MET |
| 6 | 5 | 3 | LEU |
| 6 | 5 | 26 | VAL |
| 6 | 5 | 42 | ARG |
| 6 | 5 | 51 | TYR |
| 6 | 5 | 54 | VAL |
| 6 | 5 | 59 | LEU |
| 6 | 5 | 65 | GLU |
| 6 | 5 | 69 | PHE |
| 6 | 5 | 70 | GLU |
| 6 | 5 | 96 | PHE |
| 6 | 5 | 106 | PHE |
| 6 | 5 | 107 | GLU |
| 6 | 5 | 116 | GLU |
| 6 | 5 | 121 | SER |
| 6 | 5 | 125 | ARG |
| 6 | 5 | 130 | PRO |
| 6 | 5 | 132 | TYR |
| 6 | 5 | 143 | MET |

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| Mol | Chain | Res | Type |
|---|---|---|---|
| 7 | 6 | 17 | MET |
| 7 | 6 | 18 | ASP |
| 7 | 6 | 24 | SER |
| 7 | 6 | 26 | MET |
| 8 | 7 | 11 | LYS |
| 8 | 7 | 13 | PHE |
| 8 | 7 | 15 | ILE |
| 8 | 7 | 21 | ASP |
| 8 | 7 | 23 | ARG |
| 9 | 8 | 29 | ILE |
| 9 | 8 | 61 | LEU |
| 9 | 8 | 87 | GLN |
| 12 | C | 51 | ARG |
| 12 | C | 57 | HIS |
| 12 | C | 109 | LEU |
| 12 | C | 117 | SER |
| 12 | C | 124 | LYS |
| 12 | C | 129 | LEU |
| 12 | C | 142 | ASN |
| 12 | C | 155 | ARG |
| 12 | C | 166 | ARG |
| 12 | C | 176 | ARG |
| 12 | C | 194 | VAL |
| 12 | C | 212 | TRP |
| 12 | C | 251 | THR |
| 12 | C | 270 | ARG |
| 13 | D | 33 | ARG |
| 13 | D | 37 | VAL |
| 13 | D | 97 | SER |
| 13 | D | 103 | ASP |
| 13 | D | 107 | VAL |
| 13 | D | 118 | PHE |
| 13 | D | 124 | ARG |
| 13 | D | 170 | VAL |
| 13 | D | 171 | THR |
| 13 | D | 177 | VAL |
| 13 | D | 183 | GLU |
| 13 | D | 201 | LEU |
| 13 | D | 203 | VAL |
| 14 | E | 5 | LEU |
| 14 | E | 12 | LEU |
| 14 | E | 21 | ARG |

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| Mol | Chain | Res | Type |
|---|---|---|---|
| 14 | E | 40 | ARG |
| 14 | E | 44 | ARG |
| 14 | E | 65 | THR |
| 14 | E | 69 | ARG |
| 14 | E | 70 | SER |
| 14 | E | 78 | TRP |
| 14 | E | 88 | ARG |
| 14 | E | 109 | LEU |
| 14 | E | 113 | VAL |
| 14 | E | 118 | LEU |
| 14 | E | 120 | VAL |
| 14 | E | 126 | VAL |
| 14 | E | 131 | THR |
| 14 | E | 149 | ILE |
| 14 | E | 167 | VAL |
| 14 | E | 171 | ASP |
| 15 | F | 9 | ASP |
| 15 | F | 16 | MET |
| 15 | F | 34 | THR |
| 15 | F | 41 | GLU |
| 15 | F | 46 | LYS |
| 15 | F | 90 | LEU |
| 15 | F | 94 | ARG |
| 15 | F | 111 | ARG |
| 15 | F | 114 | ARG |
| 15 | F | 154 | THR |
| 16 | G | 3 | VAL |
| 16 | G | 16 | VAL |
| 16 | G | 44 | HIS |
| 16 | G | 68 | ARG |
| 16 | G | 84 | LYS |
| 16 | G | 94 | ARG |
| 16 | G | 103 | ASN |
| 16 | G | 110 | HIS |
| 16 | G | 121 | THR |
| 16 | G | 126 | THR |
| 16 | G | 131 | VAL |
| 16 | G | 132 | LEU |
| 16 | G | 151 | ARG |
| 16 | G | 170 | THR |
| 16 | G | 176 | LYS |
| 17 | H | 3 | VAL |

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| Mol | Chain | Res | Type |
|---|---|---|---|
| 18 | I | 23 | VAL |
| 18 | I | 63 | ASP |
| 18 | I | 102 | ARG |
| 18 | I | 137 | LEU |
| 19 | J | 2 | LYS |
| 19 | J | 17 | VAL |
| 19 | J | 24 | THR |
| 19 | J | 30 | THR |
| 19 | J | 36 | LEU |
| 19 | J | 40 | HIS |
| 19 | J | 54 | ILE |
| 19 | J | 55 | ILE |
| 19 | J | 65 | THR |
| 19 | J | 72 | LYS |
| 19 | J | 73 | VAL |
| 19 | J | 95 | ARG |
| 19 | J | 103 | ILE |
| 19 | J | 129 | GLU |
| 19 | J | 131 | ASN |
| 19 | J | 140 | LEU |
| 20 | K | 3 | GLN |
| 20 | K | 8 | LEU |
| 20 | K | 13 | ASN |
| 20 | K | 18 | ARG |
| 20 | K | 21 | CYS |
| 20 | K | 23 | LYS |
| 20 | K | 41 | ILE |
| 20 | K | 54 | LYS |
| 20 | K | 73 | ASP |
| 20 | K | 93 | GLN |
| 20 | K | 105 | ARG |
| 21 | L | 5 | THR |
| 21 | L | 19 | LEU |
| 21 | L | 82 | LEU |
| 21 | L | 91 | ASP |
| 21 | L | 100 | ILE |
| 21 | L | 121 | THR |
| 21 | L | 144 | GLU |
| 22 | M | 12 | MET |
| 22 | M | 13 | HIS |
| 22 | M | 31 | PHE |
| 22 | M | 33 | LEU |

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| Mol | Chain | Res | Type |
|---|---|---|---|
| 22 | M | 46 | ILE |
| 22 | M | 53 | MET |
| 22 | M | 70 | ASP |
| 22 | M | 72 | PRO |
| 22 | M | 81 | ARG |
| 22 | M | 88 | ASN |
| 22 | M | 95 | LEU |
| 22 | M | 96 | ILE |
| 22 | M | 97 | GLN |
| 22 | M | 100 | LYS |
| 22 | M | 110 | GLU |
| 22 | M | 134 | THR |
| 23 | N | 6 | SER |
| 23 | N | 8 | ARG |
| 23 | N | 33 | ILE |
| 23 | N | 65 | LEU |
| 23 | N | 69 | ARG |
| 23 | N | 70 | THR |
| 23 | N | 71 | ARG |
| 24 | O | 18 | LEU |
| 24 | O | 31 | THR |
| 24 | O | 33 | ARG |
| 24 | O | 36 | TYR |
| 24 | O | 38 | GLN |
| 24 | O | 47 | VAL |
| 24 | O | 106 | LEU |
| 24 | O | 115 | LEU |
| 25 | P | 16 | VAL |
| 25 | P | 19 | PHE |
| 25 | P | 62 | LYS |
| 25 | P | 83 | ILE |
| 25 | P | 85 | VAL |
| 25 | P | 92 | ARG |
| 25 | P | 95 | LYS |
| 25 | P | 103 | THR |
| 26 | Q | 16 | ILE |
| 26 | Q | 40 | LYS |
| 26 | Q | 50 | ARG |
| 26 | Q | 59 | LEU |
| 26 | Q | 63 | ARG |
| 26 | Q | 88 | GLU |
| 26 | Q | 93 | ILE |

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| Mol | Chain | Res | Type |
|---|---|---|---|
| 26 | Q | 97 | ILE |
| 27 | R | 4 | VAL |
| 27 | R | 29 | THR |
| 27 | R | 38 | VAL |
| 27 | R | 46 | GLU |
| 27 | R | 48 | LYS |
| 27 | R | 63 | VAL |
| 28 | S | 3 | THR |
| 28 | S | 4 | ILE |
| 28 | S | 7 | HIS |
| 28 | S | 36 | LEU |
| 28 | S | 45 | VAL |
| 28 | S | 66 | ILE |
| 28 | S | 76 | VAL |
| 28 | S | 88 | ARG |
| 28 | S | 96 | ILE |
| 28 | S | 101 | SER |
| 29 | T | 32 | LEU |
| 29 | T | 43 | ILE |
| 30 | U | 6 | ARG |
| 30 | U | 30 | SER |
| 30 | U | 38 | ILE |
| 30 | U | 61 | GLU |
| 30 | U | 86 | PHE |
| 30 | U | 92 | VAL |
| 32 | W | 19 | ARG |
| 32 | W | 23 | LYS |
| 32 | W | 25 | PHE |
| 32 | W | 30 | VAL |
| 32 | W | 49 | ASN |
| 32 | W | 63 | ASP |
| 33 | X | 19 | HIS |
| 33 | X | 24 | THR |
| 33 | X | 26 | ARG |
| 33 | X | 29 | LEU |
| 33 | X | 34 | SER |
| 33 | X | 77 | TYR |
| 34 | Y | 10 | SER |
| 34 | Y | 16 | THR |
| 34 | Y | 57 | LEU |
| 35 | Z | 2 | LYS |
| 35 | Z | 9 | THR |

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| Mol | Chain | Res | Type |
|---|---|---|---|
| 35 | Z | 15 | ARG |
| 35 | Z | 23 | LEU |
| 35 | Z | 30 | ARG |
| 35 | Z | 31 | ILE |
| 35 | Z | 37 | ARG |
| 35 | Z | 40 | THR |

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (9) such sidechains are listed below:

| Mol | Chain | Res | Type |
|---|---|---|---|
| 4 | 3 | 30 | HIS |
| 8 | 7 | 17 | ASN |
| 8 | 7 | 22 | HIS |
| 9 | 8 | 44 | HIS |
| 9 | 8 | 80 | HIS |
| 15 | F | 4 | HIS |
| 15 | F | 26 | GLN |
| 24 | O | 34 | HIS |
| 34 | Y | 41 | HIS |

### 5.3.3 RNA

| Mol | Chain | Analysed | Backbone Outliers | Pucker Outliers |
|---|---|---|---|---|
| 10 | A | 2850/2854 (99%) | 453 (15%) | 40 (1%) |
| 11 | B | 117/118 (99%) | 17 (14%) | 0 |
| 31 | V | 76/77 (98%) | 15 (19%) | 0 |
| All | All | 3043/3049 (99%) | 485 (15%) | 40 (1%) |

All (485) RNA backbone outliers are listed below:

| Mol | Chain | Res | Type |
|---|---|---|---|
| 10 | A | 10 | A |
| 10 | A | 12 | U |
| 10 | A | 15 | G |
| 10 | A | 34 | U |
| 10 | A | 35 | G |
| 10 | A | 42 | A |
| 10 | A | 43 | G |
| 10 | A | 45 | G |
| 10 | A | 46 | G |

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| Mol | Chain | Res | Type |
|---|---|---|---|
| 10 | A | 51 | G |
| 10 | A | 61 | C |
| 10 | A | 71 | A |
| 10 | A | 74 | A |
| 10 | A | 75 | G |
| 10 | A | 80 | G |
| 10 | A | 82 | U |
| 10 | A | 84 | A |
| 10 | A | 96 | C |
| 10 | A | 101 | A |
| 10 | A | 118 | A |
| 10 | A | 119 | A |
| 10 | A | 120 | U |
| 10 | A | 131 | A |
| 10 | A | 135 | U |
| 10 | A | 136 | G |
| 10 | A | 137 | U |
| 10 | A | 138 | U |
| 10 | A | 139 | U |
| 10 | A | 140 | C |
| 10 | A | 141 | G |
| 10 | A | 142 | A |
| 10 | A | 144 | A |
| 10 | A | 149 | A |
| 10 | A | 162 | U |
| 10 | A | 163 | C |
| 10 | A | 164 | C |
| 10 | A | 181 | A |
| 10 | A | 188 | G |
| 10 | A | 196 | A |
| 10 | A | 199 | A |
| 10 | A | 215 | G |
| 10 | A | 216 | A |
| 10 | A | 222 | A |
| 10 | A | 226 | A |
| 10 | A | 230 | G |
| 10 | A | 248 | G |
| 10 | A | 255 | A |
| 10 | A | 264 | C |
| 10 | A | 265 | A |
| 10 | A | 266 | G |
| 10 | A | 267 | C |

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| Mol | Chain | Res | Type |
|---|---|---|---|
| 10 | A | 272 | A |
| 10 | A | 273 | G |
| 10 | A | 276 | U |
| 10 | A | 277 | G |
| 10 | A | 278 | A |
| 10 | A | 281 | C |
| 10 | A | 285 | G |
| 10 | A | 302 | C |
| 10 | A | 311 | A |
| 10 | A | 329 | G |
| 10 | A | 330 | A |
| 10 | A | 346 | A |
| 10 | A | 347 | A |
| 10 | A | 353 | C |
| 10 | A | 355 | U |
| 10 | A | 361 | G |
| 10 | A | 362 | A |
| 10 | A | 371 | A |
| 10 | A | 372 | G |
| 10 | A | 382 | A |
| 10 | A | 383 | C |
| 10 | A | 386 | G |
| 10 | A | 388 | G |
| 10 | A | 396 | G |
| 10 | A | 404 | A |
| 10 | A | 405 | U |
| 10 | A | 411 | G |
| 10 | A | 412 | A |
| 10 | A | 424 | G |
| 10 | A | 451 | U |
| 10 | A | 455 | C |
| 10 | A | 481 | G |
| 10 | A | 491 | G |
| 10 | A | 503 | A |
| 10 | A | 504 | A |
| 10 | A | 505 | A |
| 10 | A | 509 | C |
| 10 | A | 528 | A |
| 10 | A | 531 | C |
| 10 | A | 532 | A |
| 10 | A | 533 | G |
| 10 | A | 538 | A |

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| Mol | Chain | Res | Type |
|---|---|---|---|
| 10 | A | 543 | G |
| 10 | A | 544 | C |
| 10 | A | 546 | U |
| 10 | A | 547 | A |
| 10 | A | 548 | G |
| 10 | A | 549 | G |
| 10 | A | 563 | A |
| 10 | A | 573 | U |
| 10 | A | 575 | A |
| 10 | A | 586 | A |
| 10 | A | 603 | A |
| 10 | A | 604 | G |
| 10 | A | 613 | A |
| 10 | A | 614 | A |
| 10 | A | 615 | U |
| 10 | A | 627 | A |
| 10 | A | 631 | A |
| 10 | A | 637 | A |
| 10 | A | 645 | C |
| 10 | A | 646 | U |
| 10 | A | 647 | G |
| 10 | A | 648 | G |
| 10 | A | 654 | A |
| 10 | A | 655 | A |
| 10 | A | 656 | G |
| 10 | A | 686 | U |
| 10 | A | 714 | U |
| 10 | A | 715 | A |
| 10 | A | 730 | A |
| 10 | A | 738 | G |
| 10 | A | 747 | U |
| 10 | A | 775 | G |
| 10 | A | 776 | G |
| 10 | A | 782 | A |
| 10 | A | 784 | G |
| 10 | A | 785 | G |
| 10 | A | 805 | G |
| 10 | A | 812 | C |
| 10 | A | 819 | A |
| 10 | A | 827 | U |
| 10 | A | 828 | U |
| 10 | A | 845 | A |

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| Mol | Chain | Res | Type |
|---|---|---|---|
| 10 | A | 846 | U |
| 10 | A | 847 | U |
| 10 | A | 859 | G |
| 10 | A | 878 | A |
| 10 | A | 883 | G |
| 10 | A | 884 | U |
| 10 | A | 896 | A |
| 10 | A | 897 | C |
| 10 | A | 910 | A |
| 10 | A | 914 | G |
| 10 | A | 915 | C |
| 10 | A | 932 | U |
| 10 | A | 941 | A |
| 10 | A | 946 | C |
| 10 | A | 961 | C |
| 10 | A | 974 | G |
| 10 | A | 983 | A |
| 10 | A | 985 | C |
| 10 | A | 995 | C |
| 10 | A | 996 | A |
| 10 | A | 1003 | G |
| 10 | A | 1012 | U |
| 10 | A | 1013 | C |
| 10 | A | 1021 | A |
| 10 | A | 1022 | G |
| 10 | A | 1023 | U |
| 10 | A | 1025 | G |
| 10 | A | 1026 | G |
| 10 | A | 1033 | U |
| 10 | A | 1045 | C |
| 10 | A | 1046 | A |
| 10 | A | 1047 | G |
| 10 | A | 1051 | G |
| 10 | A | 1053 | C |
| 10 | A | 1059 | G |
| 10 | A | 1060 | U |
| 10 | A | 1061 | U |
| 10 | A | 1062 | G |
| 10 | A | 1067 | A |
| 10 | A | 1069 | A |
| 10 | A | 1070 | A |
| 10 | A | 1072 | C |

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| Mol | Chain | Res | Type |
|---|---|---|---|
| 10 | A | 1074 | G |
| 10 | A | 1078 | U |
| 10 | A | 1083 | U |
| 10 | A | 1084 | A |
| 10 | A | 1088 | A |
| 10 | A | 1089 | A |
| 10 | A | 1090 | A |
| 10 | A | 1091 | G |
| 10 | A | 1097 | U |
| 10 | A | 1098 | A |
| 10 | A | 1110 | G |
| 10 | A | 1111 | A |
| 10 | A | 1112 | G |
| 10 | A | 1129 | A |
| 10 | A | 1132 | U |
| 10 | A | 1133 | A |
| 10 | A | 1135 | C |
| 10 | A | 1136 | G |
| 10 | A | 1139 | G |
| 10 | A | 1142 | A |
| 10 | A | 1151 | A |
| 10 | A | 1155 | A |
| 10 | A | 1169 | A |
| 10 | A | 1170 | C |
| 10 | A | 1172 | C |
| 10 | A | 1174 | U |
| 10 | A | 1175 | A |
| 10 | A | 1176 | U |
| 10 | A | 1180 | U |
| 10 | A | 1186 | G |
| 10 | A | 1238 | G |
| 10 | A | 1248 | G |
| 10 | A | 1250 | G |
| 10 | A | 1253 | A |
| 10 | A | 1256 | G |
| 10 | A | 1266 | G |
| 10 | A | 1268 | A |
| 10 | A | 1271 | G |
| 10 | A | 1272 | A |
| 10 | A | 1273 | U |
| 10 | A | 1281 | G |
| 10 | A | 1300 | G |

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| Mol | Chain | Res | Type |
|---|---|---|---|
| 10 | A | 1301 | A |
| 10 | A | 1313 | U |
| 10 | A | 1317 | G |
| 10 | A | 1352 | U |
| 10 | A | 1365 | A |
| 10 | A | 1368 | G |
| 10 | A | 1378 | A |
| 10 | A | 1379 | U |
| 10 | A | 1383 | A |
| 10 | A | 1395 | A |
| 10 | A | 1415 | U |
| 10 | A | 1416 | G |
| 10 | A | 1419 | A |
| 10 | A | 1420 | A |
| 10 | A | 1428 | C |
| 10 | A | 1435 | G |
| 10 | A | 1452 | G |
| 10 | A | 1459 | G |
| 10 | A | 1482 | G |
| 10 | A | 1493 | C |
| 10 | A | 1504 | A |
| 10 | A | 1508 | A |
| 10 | A | 1510 | G |
| 10 | A | 1515 | A |
| 10 | A | 1524 | G |
| 10 | A | 1533 | C |
| 10 | A | 1534 | U |
| 10 | A | 1535 | A |
| 10 | A | 1536 | C |
| 10 | A | 1566 | A |
| 10 | A | 1569 | A |
| 10 | A | 1578 | U |
| 10 | A | 1583 | A |
| 10 | A | 1584 | U |
| 10 | A | 1585 | C |
| 10 | A | 1607 | C |
| 10 | A | 1608 | A |
| 10 | A | 1610 | A |
| 10 | A | 1613 | G |
| 10 | A | 1627 | G |
| 10 | A | 1647 | U |
| 10 | A | 1648 | U |

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| Mol | Chain | Res | Type |
|---|---|---|---|
| 10 | A | 1649 | G |
| 10 | A | 1652 | A |
| 10 | A | 1653 | G |
| 10 | A | 1674 | G |
| 10 | A | 1714 | U |
| 10 | A | 1715 | G |
| 10 | A | 1723 | G |
| 10 | A | 1729 | U |
| 10 | A | 1730 | C |
| 10 | A | 1737 | G |
| 10 | A | 1738 | G |
| 10 | A | 1739 | A |
| 10 | A | 1744 | A |
| 10 | A | 1758 | U |
| 10 | A | 1764 | C |
| 10 | A | 1773 | A |
| 10 | A | 1776 | G |
| 10 | A | 1791 | A |
| 10 | A | 1800 | C |
| 10 | A | 1801 | A |
| 10 | A | 1802 | A |
| 10 | A | 1808 | A |
| 10 | A | 1811 | G |
| 10 | A | 1816 | C |
| 10 | A | 1829 | A |
| 10 | A | 1833 | C |
| 10 | A | 1847 | A |
| 10 | A | 1848 | A |
| 10 | A | 1858 | A |
| 10 | A | 1869 | G |
| 10 | A | 1870 | C |
| 10 | A | 1871 | A |
| 10 | A | 1872 | A |
| 10 | A | 1873 | G |
| 10 | A | 1884 | G |
| 10 | A | 1906 | G |
| 10 | A | 1913 | A |
| 10 | A | 1914 | C |
| 10 | A | 1927 | A |
| 10 | A | 1929 | G |
| 10 | A | 1930 | G |
| 10 | A | 1937 | A |

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| Mol | Chain | Res | Type |
|---|---|---|---|
| 10 | A | 1938 | A |
| 10 | A | 1955 | U |
| 10 | A | 1960 | A |
| 10 | A | 1966 | A |
| 10 | A | 1967 | C |
| 10 | A | 1970 | A |
| 10 | A | 1971 | U |
| 10 | A | 1972 | G |
| 10 | A | 1991 | U |
| 10 | A | 1993 | U |
| 10 | A | 1997 | C |
| 10 | A | 2017 | U |
| 10 | A | 2020 | A |
| 10 | A | 2022 | U |
| 10 | A | 2023 | C |
| 10 | A | 2031 | A |
| 10 | A | 2033 | A |
| 10 | A | 2043 | C |
| 10 | A | 2055 | C |
| 10 | A | 2056 | G |
| 10 | A | 2060 | A |
| 10 | A | 2061 | G |
| 10 | A | 2062 | A |
| 10 | A | 2063 | C |
| 10 | A | 2069 | G |
| 10 | A | 2072 | C |
| 10 | A | 2093 | G |
| 10 | A | 2104 | C |
| 10 | A | 2106 | U |
| 10 | A | 2107 | G |
| 10 | A | 2108 | A |
| 10 | A | 2109 | U |
| 10 | A | 2110 | G |
| 10 | A | 2134 | A |
| 10 | A | 2135 | A |
| 10 | A | 2137 | U |
| 10 | A | 2138 | G |
| 10 | A | 2139 | U |
| 10 | A | 2140 | G |
| 10 | A | 2142 | A |
| 10 | A | 2143 | C |
| 10 | A | 2144 | G |

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| Mol | Chain | Res | Type |
|---|---|---|---|
| 10 | A | 2145 | C |
| 10 | A | 2146 | C |
| 10 | A | 2147 | A |
| 10 | A | 2148 | G |
| 10 | A | 2149 | U |
| 10 | A | 2150 | C |
| 10 | A | 2151 | U |
| 10 | A | 2153 | C |
| 10 | A | 2154 | A |
| 10 | A | 2155 | U |
| 10 | A | 2156 | G |
| 10 | A | 2157 | G |
| 10 | A | 2180 | U |
| 10 | A | 2183 | A |
| 10 | A | 2185 | U |
| 10 | A | 2194 | U |
| 10 | A | 2198 | A |
| 10 | A | 2199 | A |
| 10 | A | 2204 | G |
| 10 | A | 2211 | A |
| 10 | A | 2212 | A |
| 10 | A | 2214 | C |
| 10 | A | 2225 | A |
| 10 | A | 2226 | C |
| 10 | A | 2238 | G |
| 10 | A | 2239 | G |
| 10 | A | 2250 | G |
| 10 | A | 2268 | A |
| 10 | A | 2278 | A |
| 10 | A | 2283 | C |
| 10 | A | 2284 | A |
| 10 | A | 2286 | G |
| 10 | A | 2287 | A |
| 10 | A | 2305 | U |
| 10 | A | 2308 | G |
| 10 | A | 2311 | A |
| 10 | A | 2322 | A |
| 10 | A | 2325 | G |
| 10 | A | 2327 | A |
| 10 | A | 2333 | A |
| 10 | A | 2336 | A |
| 10 | A | 2347 | C |

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| Mol | Chain | Res | Type |
|---|---|---|---|
| 10 | A | 2354 | C |
| 10 | A | 2361 | G |
| 10 | A | 2383 | G |
| 10 | A | 2385 | C |
| 10 | A | 2402 | U |
| 10 | A | 2403 | C |
| 10 | A | 2406 | A |
| 10 | A | 2423 | U |
| 10 | A | 2424 | C |
| 10 | A | 2425 | A |
| 10 | A | 2429 | G |
| 10 | A | 2430 | A |
| 10 | A | 2435 | A |
| 10 | A | 2441 | U |
| 10 | A | 2448 | A |
| 10 | A | 2470 | G |
| 10 | A | 2476 | A |
| 10 | A | 2491 | U |
| 10 | A | 2502 | G |
| 10 | A | 2503 | A |
| 10 | A | 2505 | G |
| 10 | A | 2506 | U |
| 10 | A | 2507 | C |
| 10 | A | 2518 | A |
| 10 | A | 2529 | G |
| 10 | A | 2554 | U |
| 10 | A | 2556 | C |
| 10 | A | 2566 | A |
| 10 | A | 2567 | G |
| 10 | A | 2572 | A |
| 10 | A | 2573 | C |
| 10 | A | 2585 | U |
| 10 | A | 2613 | U |
| 10 | A | 2629 | U |
| 10 | A | 2663 | G |
| 10 | A | 2671 | G |
| 10 | A | 2681 | C |
| 10 | A | 2682 | A |
| 10 | A | 2689 | U |
| 10 | A | 2690 | U |
| 10 | A | 2714 | G |
| 10 | A | 2716 | C |

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| Mol | Chain | Res | Type |
|---|---|---|---|
| 10 | A | 2726 | A |
| 10 | A | 2733 | A |
| 10 | A | 2744 | G |
| 10 | A | 2748 | A |
| 10 | A | 2757 | A |
| 10 | A | 2760 | C |
| 10 | A | 2765 | A |
| 10 | A | 2778 | A |
| 10 | A | 2791 | G |
| 10 | A | 2798 | U |
| 10 | A | 2800 | A |
| 10 | A | 2801 | G |
| 10 | A | 2818 | U |
| 10 | A | 2820 | A |
| 10 | A | 2821 | A |
| 10 | A | 2861 | U |
| 10 | A | 2867 | G |
| 10 | A | 2873 | A |
| 10 | A | 2874 | C |
| 10 | A | 2883 | A |
| 10 | A | 2884 | U |
| 10 | A | 2885 | G |
| 10 | A | 2891 | U |
| 10 | A | 2903 | U |
| 11 | B | 3 | C |
| 11 | B | 15 | A |
| 11 | B | 16 | G |
| 11 | B | 21 | G |
| 11 | B | 30 | C |
| 11 | B | 35 | C |
| 11 | B | 42 | C |
| 11 | B | 44 | G |
| 11 | B | 45 | A |
| 11 | B | 56 | G |
| 11 | B | 84 | G |
| 11 | B | 87 | U |
| 11 | B | 88 | C |
| 11 | B | 89 | U |
| 11 | B | 90 | C |
| 11 | B | 99 | A |
| 11 | B | 109 | A |
| 31 | V | 4 | C |

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| Mol | Chain | Res | Type |
|---|---|---|---|
| 31 | V | 5 | A |
| 31 | V | 8 | U |
| 31 | V | 19 | G |
| 31 | V | 21 | A |
| 31 | V | 31 | C |
| 31 | V | 33 | U |
| 31 | V | 43 | G |
| 31 | V | 48 | C |
| 31 | V | 49 | G |
| 31 | V | 53 | G |
| 31 | V | 67 | G |
| 31 | V | 71 | C |
| 31 | V | 73 | A |
| 31 | V | 76 | A |

All (40) RNA pucker outliers are listed below:

| Mol | Chain | Res | Type |
|---|---|---|---|
| 10 | A | 119 | A |
| 10 | A | 271 | G |
| 10 | A | 277 | G |
| 10 | A | 301 | G |
| 10 | A | 403 | U |
| 10 | A | 404 | A |
| 10 | A | 503 | A |
| 10 | A | 527 | C |
| 10 | A | 613 | A |
| 10 | A | 655 | A |
| 10 | A | 784 | G |
| 10 | A | 827 | U |
| 10 | A | 846 | U |
| 10 | A | 882 | G |
| 10 | A | 931 | U |
| 10 | A | 1020 | A |
| 10 | A | 1025 | G |
| 10 | A | 1069 | A |
| 10 | A | 1088 | A |
| 10 | A | 1110 | G |
| 10 | A | 1247 | A |
| 10 | A | 1378 | A |
| 10 | A | 1458 | U |
| 10 | A | 1509 | A |

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| Mol | Chain | Res | Type |
|---|---|---|---|
| 10 | A | 1535 | A |
| 10 | A | 1626 | A |
| 10 | A | 1738 | G |
| 10 | A | 1757 | A |
| 10 | A | 1847 | A |
| 10 | A | 1870 | C |
| 10 | A | 1939 | U |
| 10 | A | 2108 | A |
| 10 | A | 2142 | A |
| 10 | A | 2211 | A |
| 10 | A | 2286 | G |
| 10 | A | 2326 | C |
| 10 | A | 2423 | U |
| 10 | A | 2756 | U |
| 10 | A | 2873 | A |
| 10 | A | 2902 | C |

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

1 non-standard protein/DNA/RNA residue is modelled in this entry.

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

| Mol | Type | Chain | Res | Link | Bond lengths | | | Bond angles | | |
|---|---|---|---|---|---|---|---|---|---|---|
| | | | | | Counts | RMSZ | $\#\|Z\| > 2$ | Counts | RMSZ | $\#\|Z\| > 2$ |
| 31 | 5MU | V | 54 | 31 | 18,21,23 | 0.64 | 0 | 26,30,35 | 0.73 | 1 (3%) |

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

| Mol | Type | Chain | Res | Link | Chirals | Torsions | Rings |
|---|---|---|---|---|---|---|---|
| 31 | 5MU | V | 54 | 31 | - | 0/7/25/26 | 0/2/2/2 |

There are no bond length outliers.

All (1) bond angle outliers are listed below:

| Mol | Chain | Res | Type | Atoms | Z | Observed($^o$) | Ideal($^o$) |
|---|---|---|---|---|---|---|---|
| 31 | V | 54 | 5MU | O4'-C1'-N1 | 2.43 | 113.91 | 108.36 |

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

No monomer is involved in short contacts.

## 5.5 Carbohydrates (i)

There are no monosaccharides in this entry.

## 5.6 Ligand geometry (i)

Of 146 ligands modelled in this entry, 144 are monoatomic - leaving 2 for Mogul analysis.

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

| Mol | Type | Chain | Res | Link | Bond lengths | | | Bond angles | | |
|---|---|---|---|---|---|---|---|---|---|---|
| | | | | | Counts | RMSZ | $\#\|Z\| > 2$ | Counts | RMSZ | $\#\|Z\| > 2$ |
| 38 | TRP | 7 | 1001 | - | 14,16,16 | 0.84 | 1 (7%) | 16,22,22 | 1.15 | 2 (12%) |
| 38 | TRP | 7 | 1002 | - | 14,16,16 | 0.84 | 1 (7%) | 16,22,22 | 1.16 | 2 (12%) |

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

| Mol | Type | Chain | Res | Link | Chirals | Torsions | Rings |
|---|---|---|---|---|---|---|---|
| 38 | TRP | 7 | 1001 | - | - | 0/7/8/8 | 0/2/2/2 |
| 38 | TRP | 7 | 1002 | - | - | 4/7/8/8 | 0/2/2/2 |

All (2) bond length outliers are listed below:

| Mol | Chain | Res | Type | Atoms | Z | Observed(Å) | Ideal(Å) |
|---|---|---|---|---|---|---|---|
| 38 | 7 | 1002 | TRP | OXT-C | -2.13 | 1.23 | 1.30 |
| 38 | 7 | 1001 | TRP | OXT-C | -2.11 | 1.23 | 1.30 |

All (4) bond angle outliers are listed below:

| Mol | Chain | Res | Type | Atoms | Z | Observed($^o$) | Ideal($^o$) |
|---|---|---|---|---|---|---|---|
| 38 | 7 | 1001 | TRP | OXT-C-O | -2.72 | 117.91 | 124.09 |
| 38 | 7 | 1002 | TRP | OXT-C-O | -2.65 | 118.07 | 124.09 |
| 38 | 7 | 1001 | TRP | OXT-C-CA | 2.24 | 121.00 | 113.38 |
| 38 | 7 | 1002 | TRP | OXT-C-CA | 2.22 | 120.95 | 113.38 |

There are no chirality outliers.

All (4) torsion outliers are listed below:

| Mol | Chain | Res | Type | Atoms |
|---|---|---|---|---|
| 38 | 7 | 1002 | TRP | C-CA-CB-CG |
| 38 | 7 | 1002 | TRP | N-CA-CB-CG |
| 38 | 7 | 1002 | TRP | OXT-C-CA-CB |
| 38 | 7 | 1002 | TRP | O-C-CA-CB |

There are no ring outliers.

2 monomers are involved in 24 short contacts:

| Mol | Chain | Res | Type | Clashes | Symm-Clashes |
|---|---|---|---|---|---|
| 38 | 7 | 1001 | TRP | 8 | 0 |
| 38 | 7 | 1002 | TRP | 16 | 0 |

## 5.7 Other polymers (i)

There are no such residues in this entry.

## 5.8 Polymer linkage issues (i)

The following chains have linkage breaks:

| Mol | Chain | Number of breaks |
|---|---|---|
| 10 | A | 3 |

All chain breaks are listed below:

| Model | Chain | Residue-1 | Atom-1 | Residue-2 | Atom-2 | Distance (Å) |
|---|---|---|---|---|---|---|
| 1 | A | 2157:G | O3' | 2179:C | P | 44.42 |
| 1 | A | 2110:G | O3' | 2133:G | P | 30.78 |
| 1 | A | 885:C | O3' | 892:A | P | 11.37 |

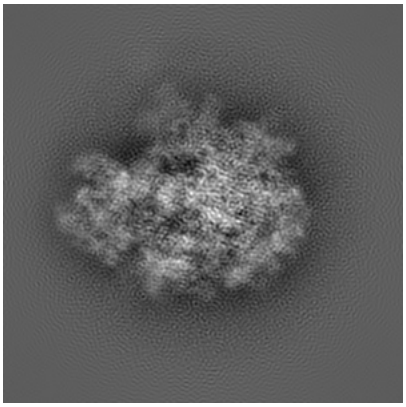
# 6 Map visualisation

This section contains visualisations of the EMDB entry EMD-2773. These allow visual inspection of the internal detail of the map and identification of artifacts.

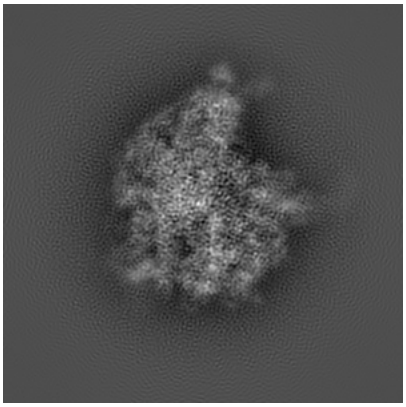
No raw map or half-maps were deposited for this entry and therefore no images, graphs, etc. pertaining to the raw map can be shown.

## 6.1 Orthogonal projections

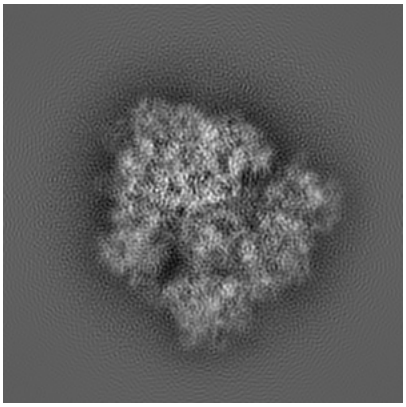
### 6.1.1 Primary map



X



Y

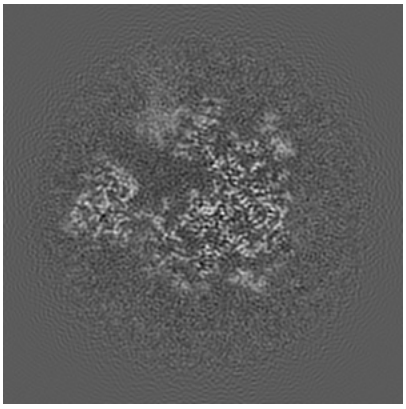


Z

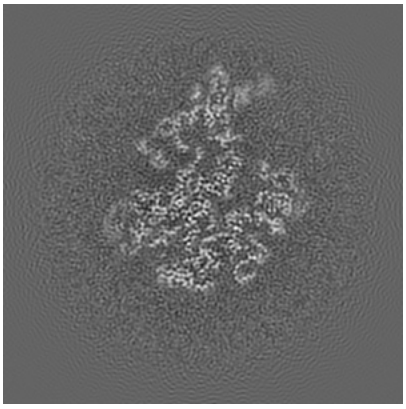
The images above show the map projected in three orthogonal directions.

## 6.2 Central slices

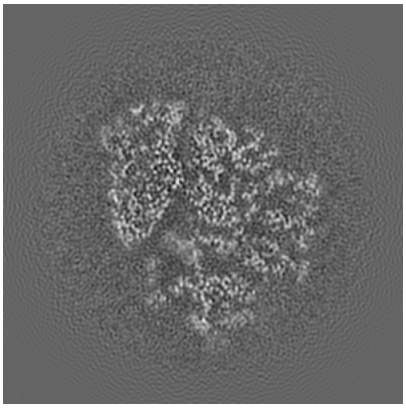
### 6.2.1 Primary map



X Index: 184



Y Index: 184

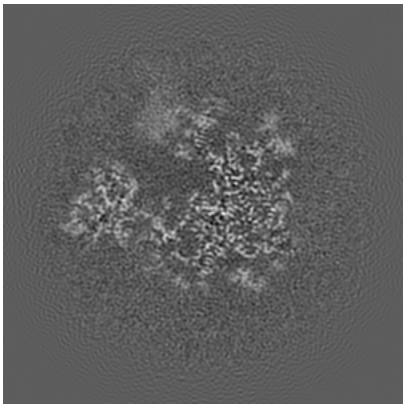


Z Index: 184

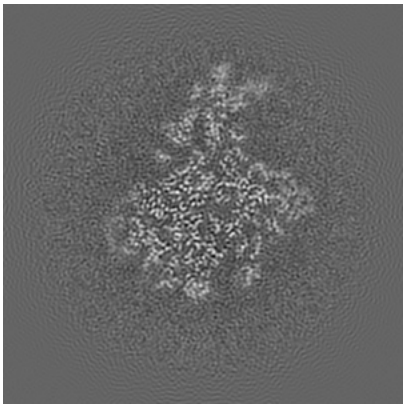
The images above show central slices of the map in three orthogonal directions.

## 6.3 Largest variance slices (i)

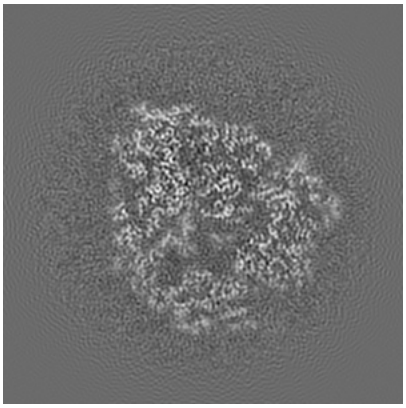
### 6.3.1 Primary map



X Index: 183



Y Index: 190



Z Index: 192

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

## 6.4 Orthogonal surface views (i)

### 6.4.1 Primary map

X

Y

Z

The images above show the 3D surface view of the map at the recommended contour level 0.9. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

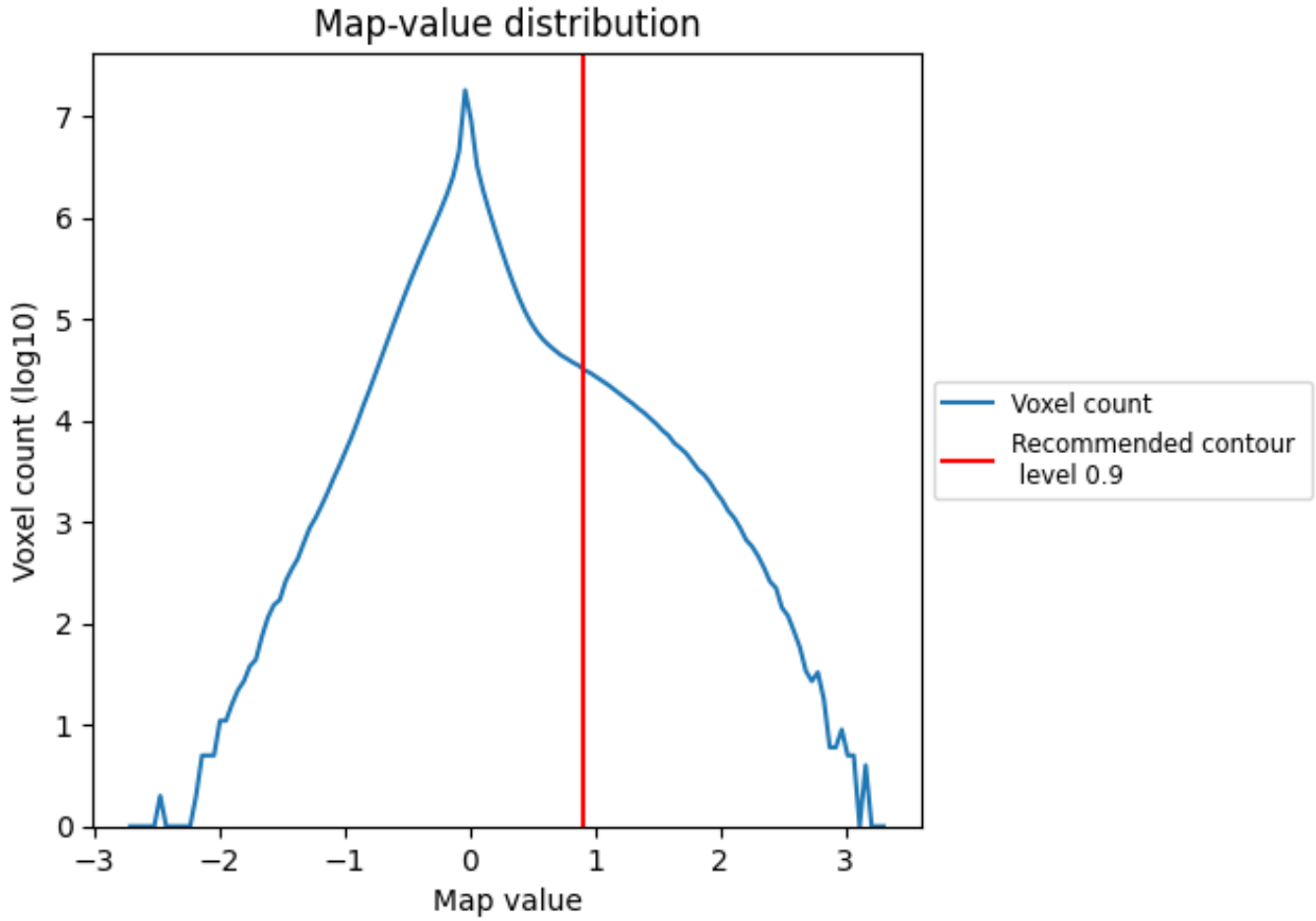
## 6.5 Mask visualisation (i)

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

# 7 Map analysis

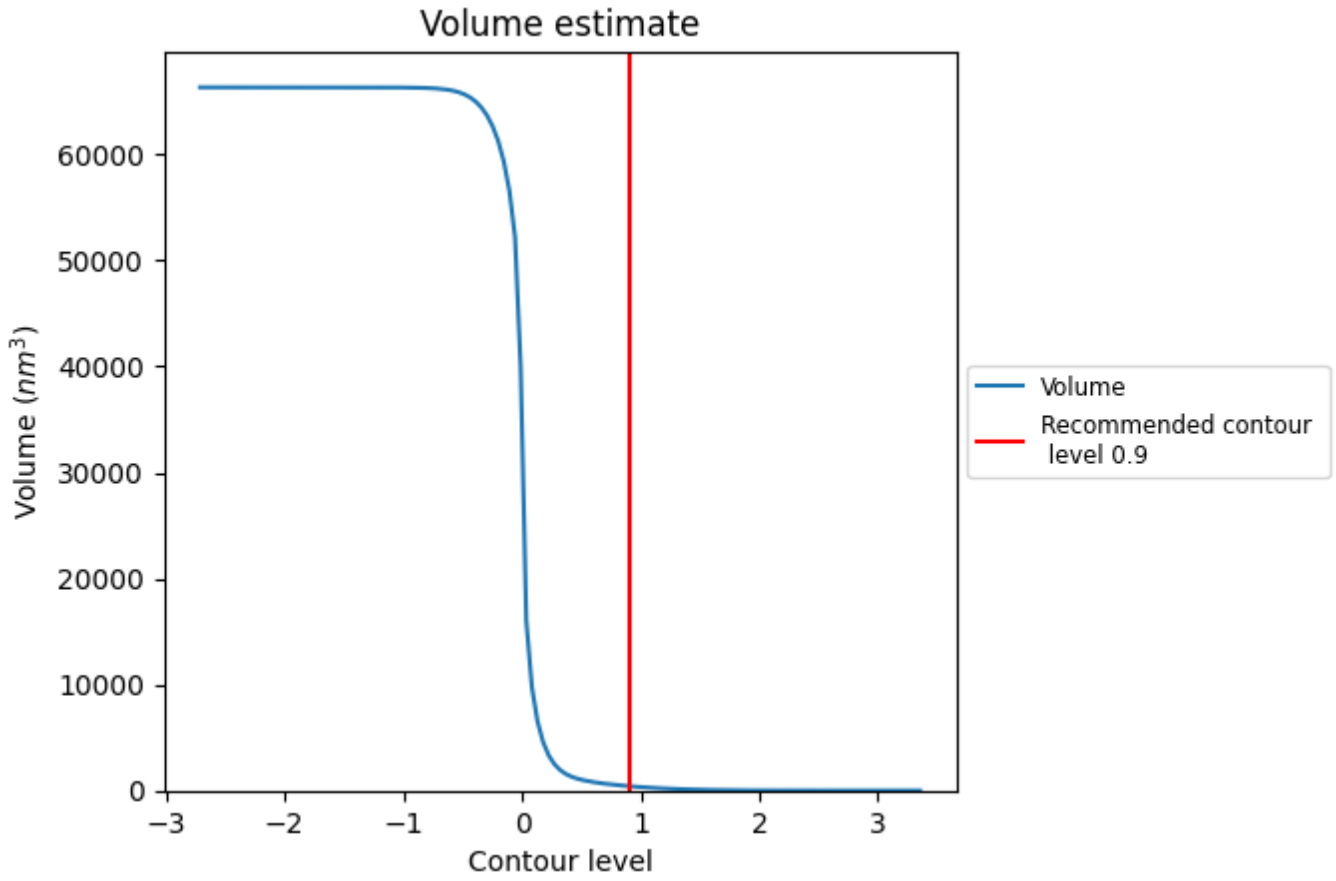
This section contains the results of statistical analysis of the map.

## 7.1 Map-value distribution




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.

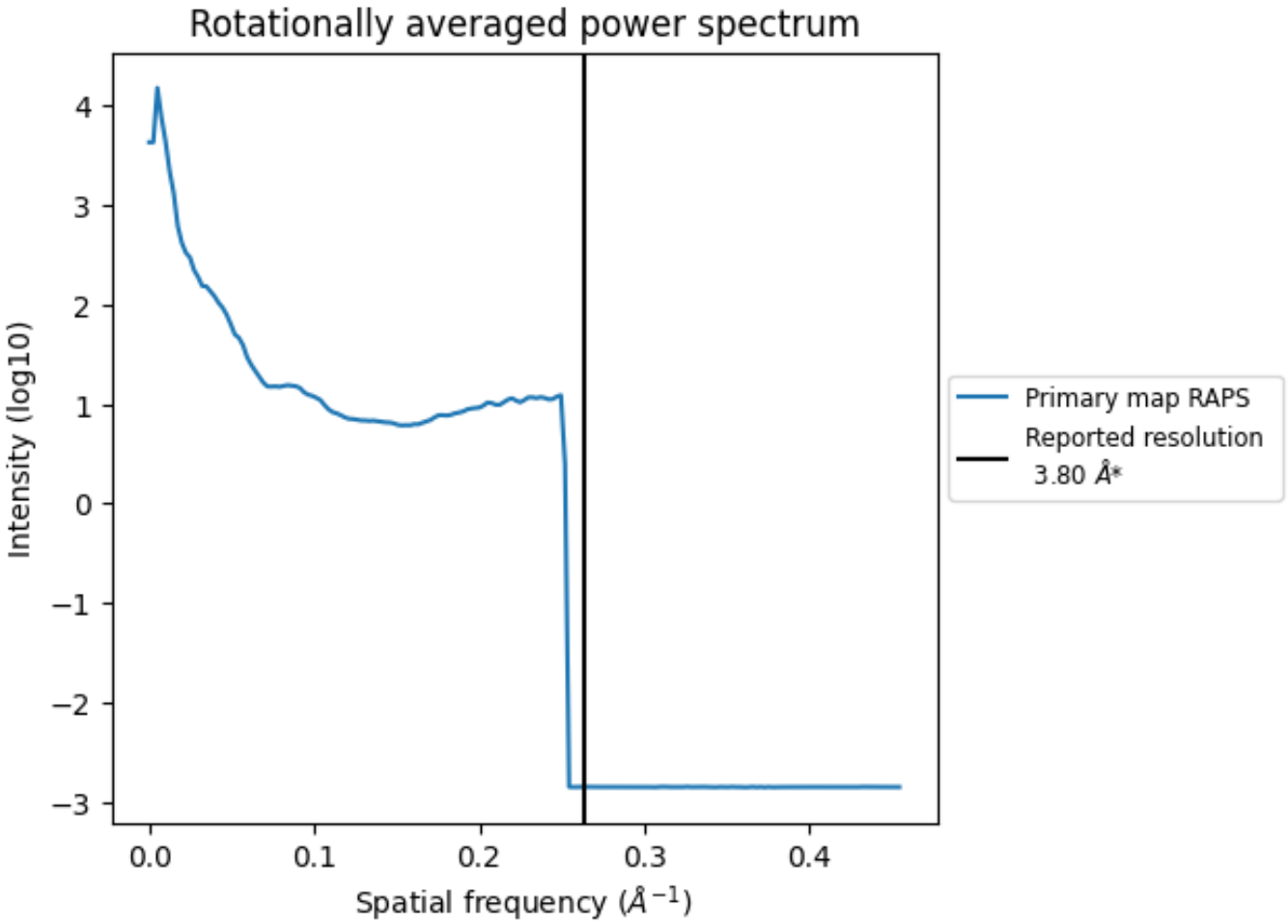
## 7.2 Volume estimate




The volume at the recommended contour level is 416 $nm^3$; this corresponds to an approximate mass of 376 kDa.

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

## 7.3 Rotationally averaged power spectrum (i)




*Reported resolution corresponds to spatial frequency of 0.263 Å$^{-1}$

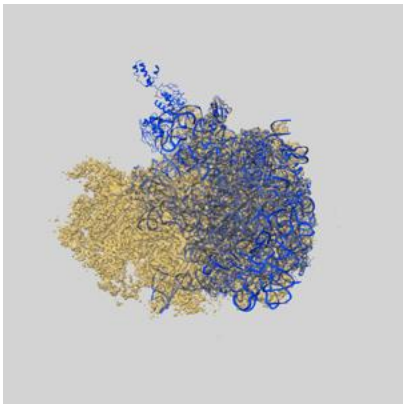
# 8 Fourier-Shell correlation (i)

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

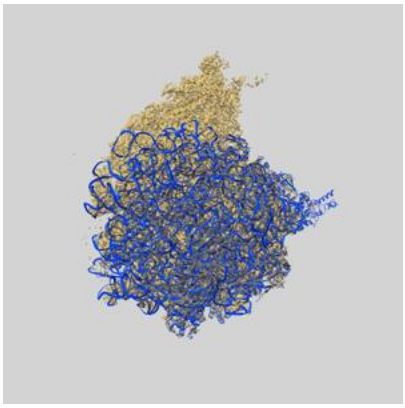
# 9 Map-model fit

This section contains information regarding the fit between EMDB map EMD-2773 and PDB model 4UY8. Per-residue inclusion information can be found in section 3 on page 12.

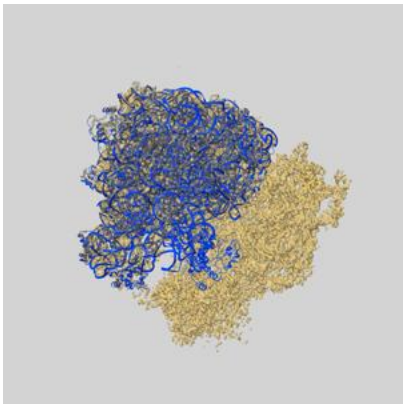
## 9.1 Map-model overlay



X



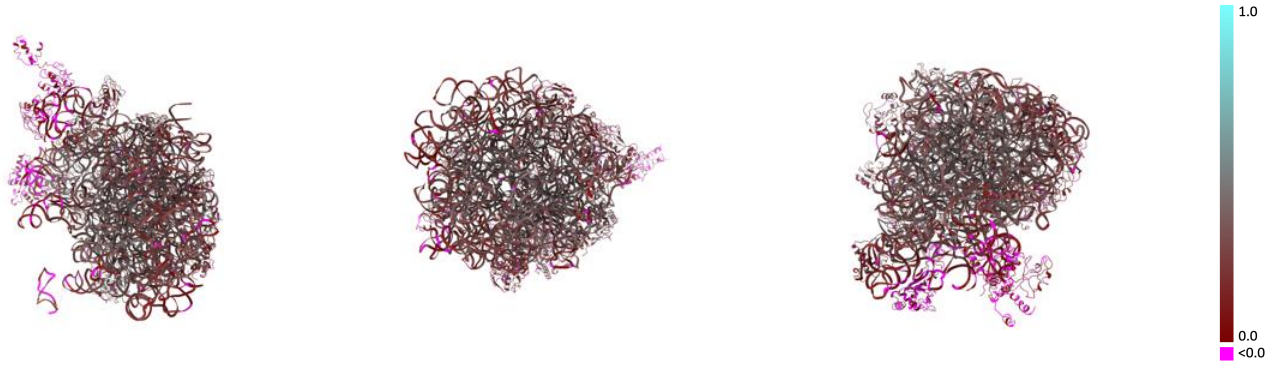
Y



Z

The images above show the 3D surface view of the map at the recommended contour level 0.9 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.

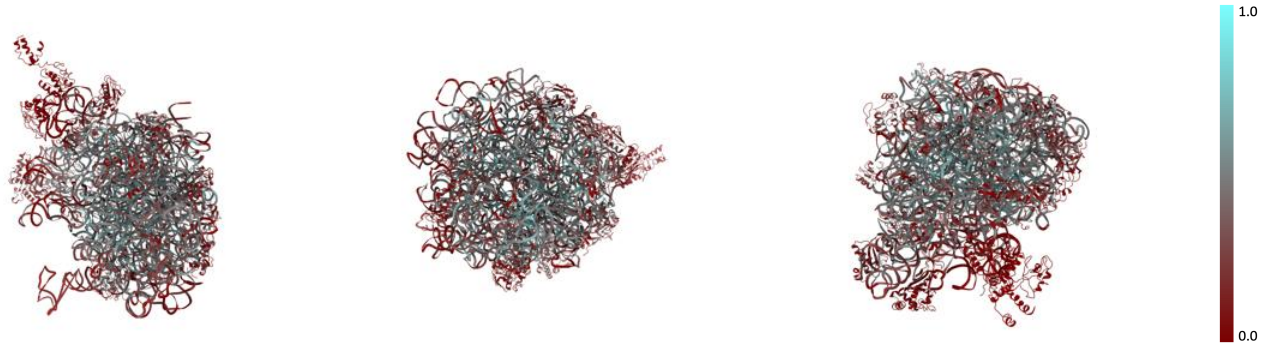
## 9.2 Q-score mapped to coordinate model




X Y Z

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

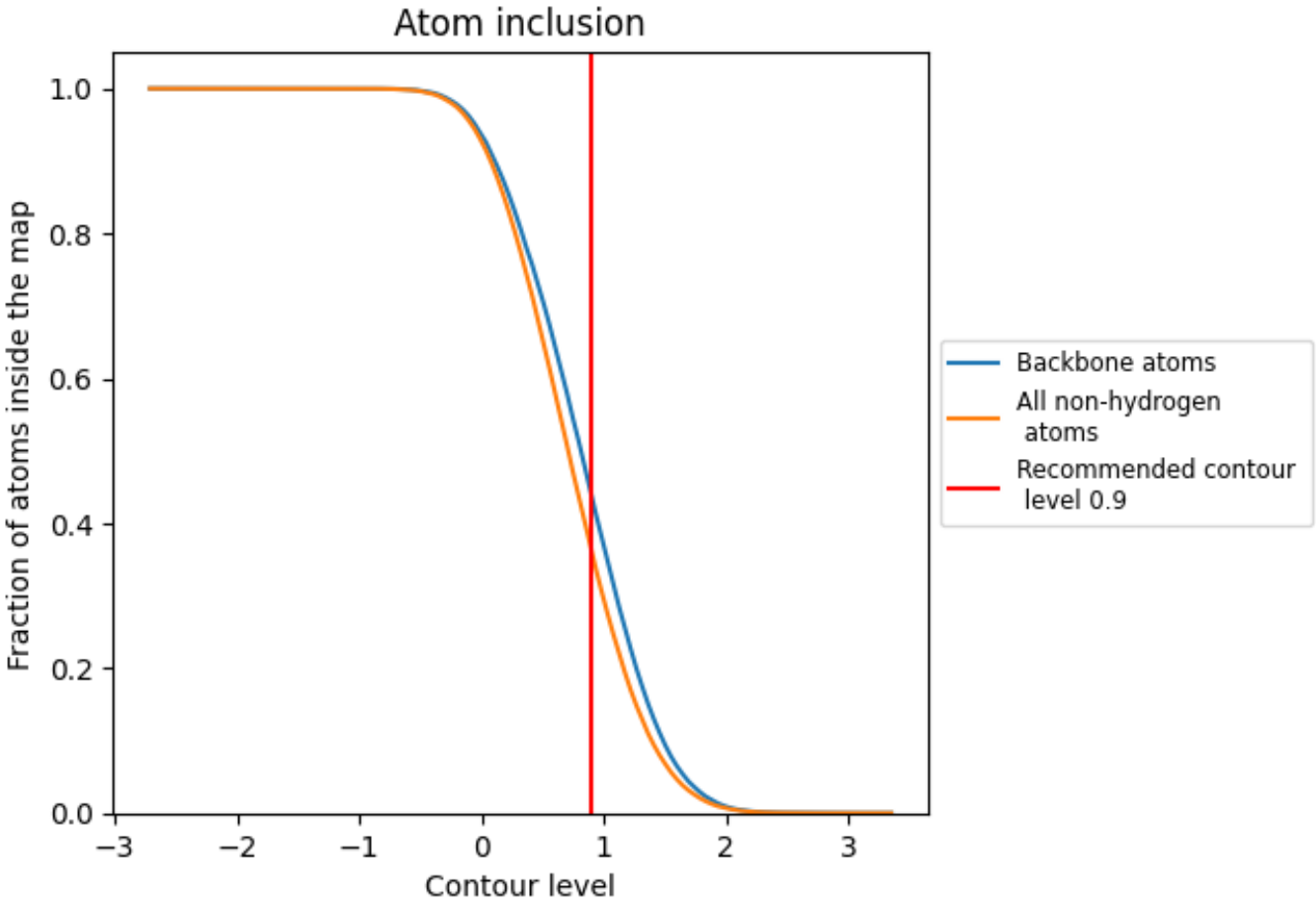
## 9.3 Atom inclusion mapped to coordinate model




X Y Z

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 (0.9).

## 9.4 Atom inclusion (i)




At the recommended contour level, 44% of all backbone atoms, 36% 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 (0.9) and Q-score for the entire model and for each chain.

| Chain | Atom inclusion | Q-score |
|---|---|---|
| All | 0.3629 | 0.2860 |
| 0 | 0.2827 | 0.3180 |
| 1 | 0.0973 | 0.2320 |
| 2 | 0.3549 | 0.3680 |
| 3 | 0.2444 | 0.3350 |
| 4 | 0.3061 | 0.3400 |
| 5 | 0.0018 | 0.0150 |
| 6 | 0.0000 | 0.0280 |
| 7 | 0.0103 | 0.4110 |
| 8 | 0.1992 | 0.2970 |
| A | 0.4362 | 0.3060 |
| B | 0.3427 | 0.2070 |
| C | 0.3023 | 0.3600 |
| D | 0.2568 | 0.3000 |
| E | 0.2078 | 0.2730 |
| F | 0.0641 | -0.0250 |
| G | 0.1049 | 0.2230 |
| H | 0.1293 | 0.2250 |
| I | 0.0029 | 0.0570 |
| J | 0.3409 | 0.3360 |
| K | 0.2464 | 0.2790 |
| L | 0.1969 | 0.2570 |
| M | 0.2841 | 0.3370 |
| N | 0.2831 | 0.2800 |
| O | 0.1703 | 0.1830 |
| P | 0.1847 | 0.2070 |
| Q | 0.3866 | 0.3430 |
| R | 0.2748 | 0.3380 |
| S | 0.3158 | 0.3620 |
| T | 0.2036 | 0.2620 |
| U | 0.1682 | 0.2830 |
| V | 0.1662 | 0.1640 |
| W | 0.2655 | 0.2670 |
| X | 0.2479 | 0.3210 |
| Y | 0.1791 | 0.2650 |
| Z | 0.2677 | 0.3130 |