# Full wwPDB X-ray Structure Validation Report ⓘ

Mar 20, 2026 – 04:13 AM UTC

| | | |
|---|---|---|
| PDB ID | : | 8CQW / pdb_00008cqw |
| Title | : | Crystal structure of the Candida albicans 80S ribosome in complex with Hygromycin B |
| Authors | : | Kolosova, O.; Zgadzay, Y.; Yusupov, M. |
| Deposited on | : | 2023-03-07 |
| Resolution | : | 3.05 Å(reported) |

This is a Full wwPDB X-ray Structure 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/XrayValidationReportHelp
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.

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

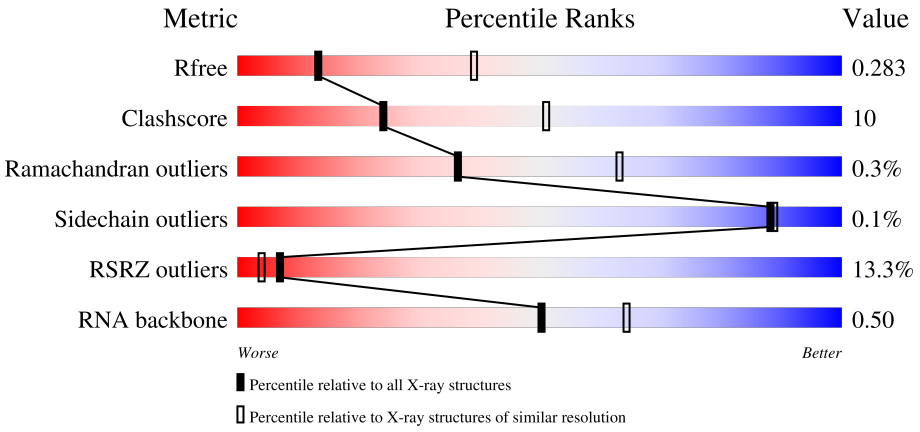
| | | |
|---|---|---|
| MolProbity | : | 4-5-2 with Phenix2.0 |
| Mogul | : | 2022.3.0, CSD as543be (2022) |
| Xtriage (Phenix) | : | 2.0 |
| EDS | : | 3.0 |
| Buster-report | : | wwPDB partial adaption of 1.1.7 (2018) |
| Percentile statistics | : | 20250101.v01 (using entries in the PDB archive January 1st 2025) |
| CCP4 | : | 9.0.010 (Gargrove) |
| Density-Fitness | : | 1.0.12 |
| Ideal geometry (proteins) | : | Engh & Huber (2001) |
| Ideal geometry (DNA, RNA) | : | Parkinson et al. (1996) |
| Validation Pipeline (wwPDB-VP) | : | 2.49 |

# 1 Overall quality at a glance (i)

The following experimental techniques were used to determine the structure:
*X-RAY DIFFRACTION*

The reported resolution of this entry is 3.05 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) | Similar resolution (#Entries, resolution range(Å)) |
|---|---|---|
| $R_{free}$ | 180053 | 2469 (3.10-3.02) |
| Clashscore | 190562 | 2569 (3.10-3.02) |
| Ramachandran outliers | 187476 | 2424 (3.10-3.02) |
| Sidechain outliers | 187428 | 2423 (3.10-3.02) |
| RSRZ outliers | 180081 | 2469 (3.10-3.02) |
| RNA backbone | 3983 | 1079 (3.30-2.82) |

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments of the lower 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 electron density. The numeric value is given above the bar.

| Mol | Chain | Length | Quality of chain |
|---|---|---|---|
| 1 | 1 | 3359 | 2% 47% 41% 8% |
| 1 | AS | 3359 | 3% 48% 38% 9% |
| 2 | 3 | 121 | 64% 34% |
| 2 | AT | 121 | % 69% 30% |

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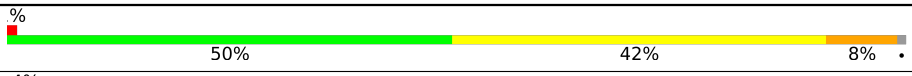
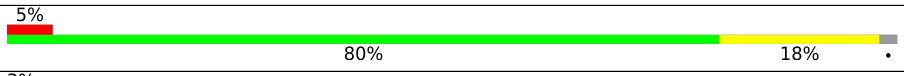
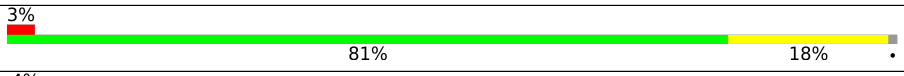
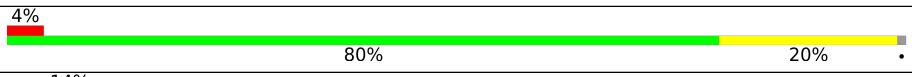
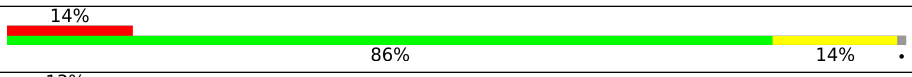
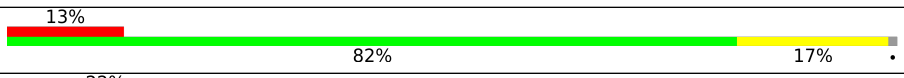
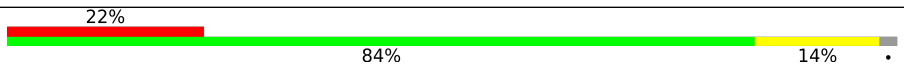
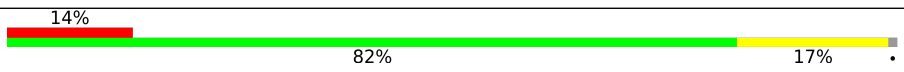
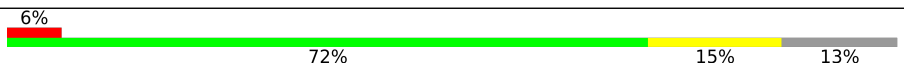
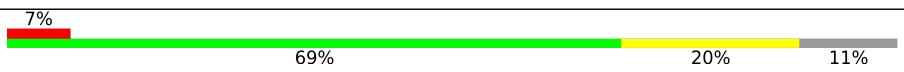
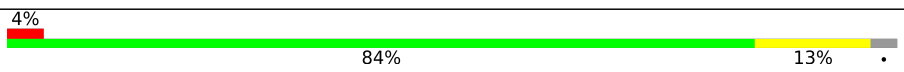
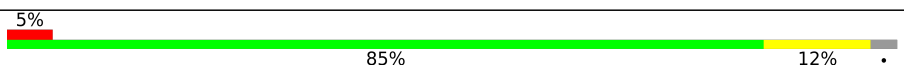
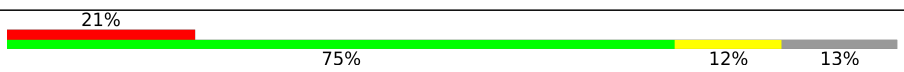
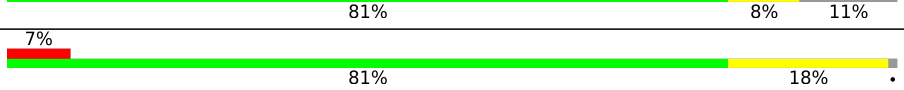
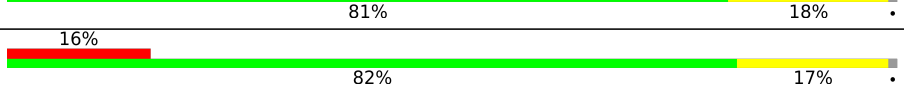
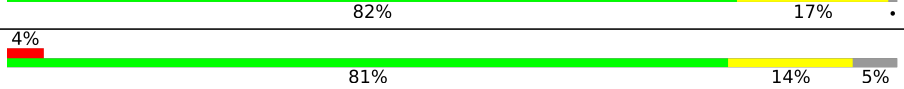
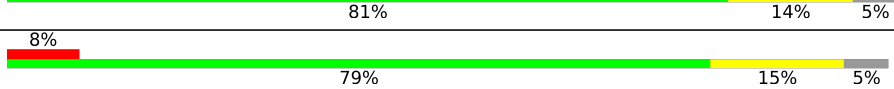
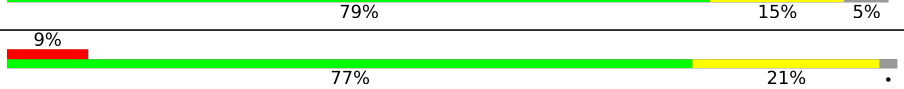
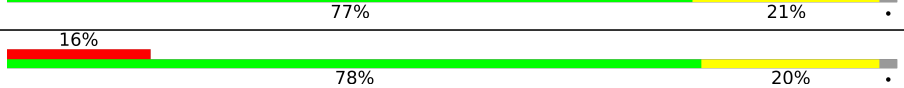
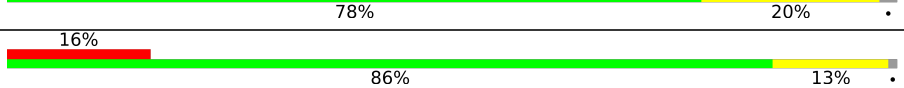
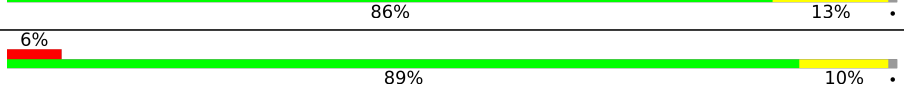
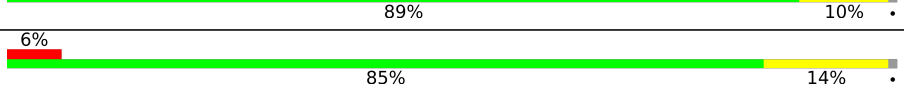
| Mol | Chain | Length | Quality of chain |
|---|---|---|---|
| 3 | 4 | 158 |   |
| 3 | AU | 158 | |
| 4 | AW | 254 | |
| 4 | j | 254 |   |
| 5 | AX | 389 |   |
| 5 | k | 389 |   |
| 6 | AY | 363 |   |
| 6 | l | 363 |   |
| 7 | AZ | 298 |   |
| 7 | m | 298 |   |
| 8 | BA | 176 |   |
| 8 | n | 176 |   |
| 9 | BB | 241 |   |
| 9 | o | 241 |   |
| 10 | BC | 262 |   |
| 10 | p | 262 | |
| 11 | BD | 191 |   |
| 11 | q | 191 |   |
| 12 | BE | 220 |   |
| 12 | r | 220 |   |
| 13 | BF | 174 |   |
| 13 | s | 174 |   |
| 14 | BG | 202 |   |
| 14 | t | 202 |   |
| 15 | BH | 131 |   |

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| Mol | Chain | Length | Quality of chain |
|---|---|---|---|
| 15 | u | 131 | 6% 83% 16% |
| 16 | BI | 204 | 23% 73% 27% |
| 16 | v | 204 | 10% 73% 26% |
| 17 | BJ | 200 | 4% 86% 14% |
| 17 | w | 200 | 6% 82% 18% |
| 18 | BK | 185 | 8% 82% 13% 5% |
| 18 | x | 185 | 7% 75% 19% 6% |
| 19 | BL | 186 | 5% 81% 18% |
| 19 | y | 186 | 24% 82% 18% |
| 20 | BM | 190 | 9% 78% 16% 6% |
| 20 | z | 190 | 3% 83% 11% 6% |
| 21 | 0 | 172 | 9% 80% 19% |
| 21 | BN | 172 | 5% 74% 24% |
| 22 | 2 | 160 | 12% 84% 15% |
| 22 | BO | 160 | 12% 82% 18% |
| 23 | 5 | 124 | 7% 66% 15% 18% |
| 23 | BP | 124 | 11% 57% 24% 18% |
| 24 | 6 | 137 | 4% 88% 8% |
| 24 | BQ | 137 | 5% 80% 16% |
| 25 | 7 | 155 | 8% 64% 12% 24% |
| 25 | BR | 155 | 10% 54% 10% 37% |
| 26 | 8 | 142 | 7% 70% 14% 15% |
| 26 | BS | 142 | 20% 70% 13% 16% |
| 27 | 9 | 127 | 20% 80% 20% |
| 27 | BT | 127 | 13% 77% 22% |

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| Mol | Chain | Length | Quality of chain |
|---|---|---|---|
| 28 | AA | 136 | 14% 78% 21% |
| 28 | BU | 136 | 15% 72% 27% |
| 29 | AB | 149 | 9% 79% 21% |
| 29 | BV | 149 | 16% 81% 19% |
| 30 | AC | 63 | 33% 81% 14% |
| 30 | BW | 63 | 21% 76% 21% |
| 31 | AD | 106 | 6% 74% 17% 9% |
| 31 | BX | 106 | 17% 72% 19% 9% |
| 32 | AE | 112 | 4% 79% 19% |
| 32 | BY | 112 | 7% 84% 14% |
| 33 | AF | 131 | 12% 79% 15% 5% |
| 33 | BZ | 131 | 5% 80% 15% 5% |
| 34 | AG | 107 | 13% 80% 19% |
| 34 | CA | 107 | 3% 87% 12% |
| 35 | AH | 122 | 14% 75% 17% 8% |
| 35 | CB | 122 | 25% 74% 18% 8% |
| 36 | AI | 120 | 11% 82% 18% |
| 36 | CC | 120 | 24% 75% 23% |
| 37 | AJ | 99 | 13% 87% 10% |
| 37 | CD | 99 | 21% 85% 13% |
| 38 | AK | 90 | 7% 72% 23% |
| 38 | CE | 90 | 14% 77% 19% |
| 39 | AL | 78 | 12% 86% 13% |
| 39 | CF | 78 | 21% 78% 21% |
| 40 | AM | 51 | 8% 75% 24% |

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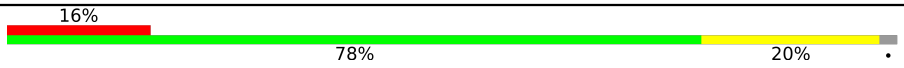
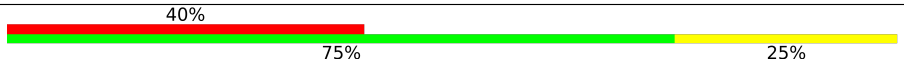
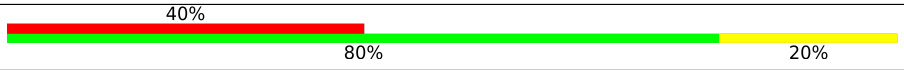
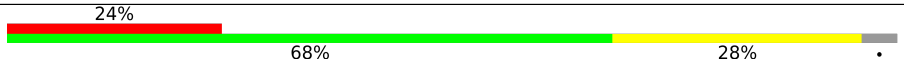
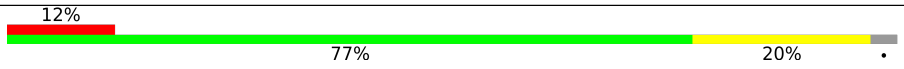
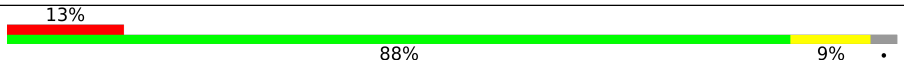
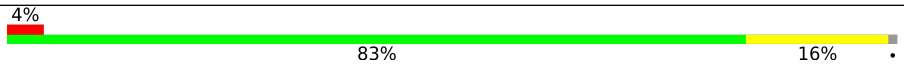
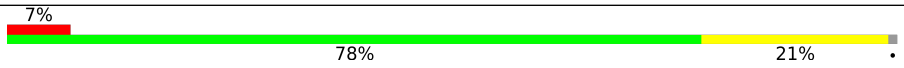
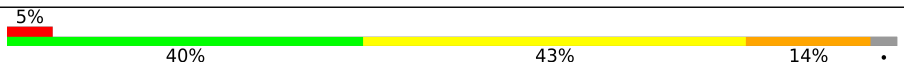
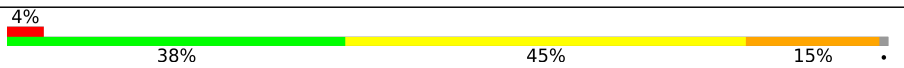
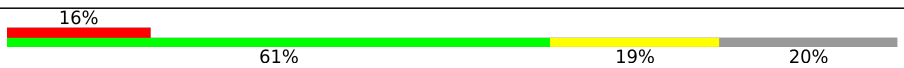
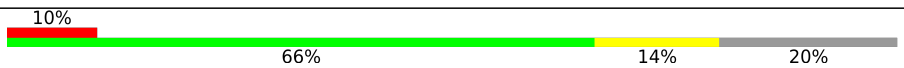
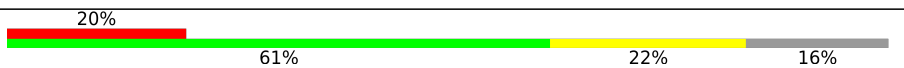
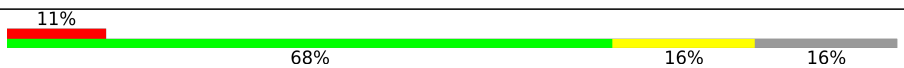
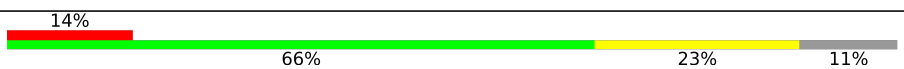
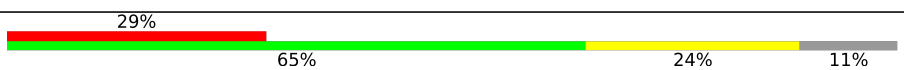
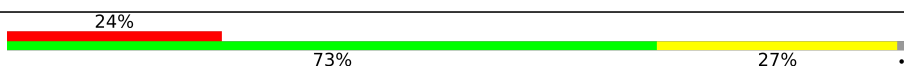
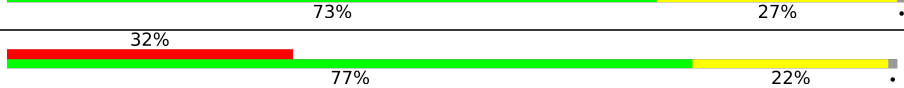
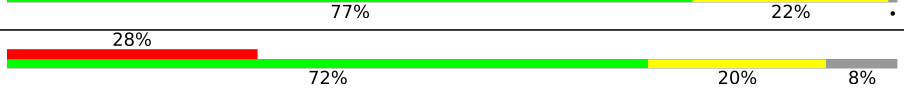
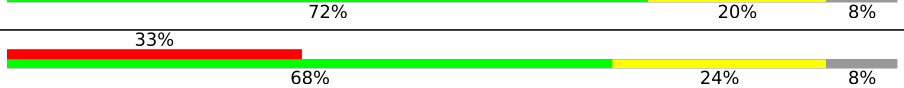
| Mol | Chain | Length | Quality of chain |
|---|---|---|---|
| 40 | CG | 51 |   |
| 41 | AN | 52 |   |
| 41 | CH | 52 | |
| 42 | AO | 25 |   |
| 42 | CI | 25 |   |
| 43 | AP | 106 |   |
| 43 | CJ | 106 |   |
| 44 | AQ | 92 |   |
| 44 | CK | 92 |   |
| 45 | CL | 267 | |
| 45 | i | 267 | |
| 46 | B | 1787 |   |
| 46 | CM | 1787 |   |
| 47 | C | 261 |   |
| 47 | CN | 261 |   |
| 48 | CO | 256 |   |
| 48 | D | 256 |   |
| 49 | CP | 249 | |
| 49 | E | 249 | |
| 50 | CQ | 251 |   |
| 50 | F | 251 |   |
| 51 | CR | 262 |   |
| 51 | G | 262 |   |
| 52 | CS | 225 |   |
| 52 | H | 225 |   |

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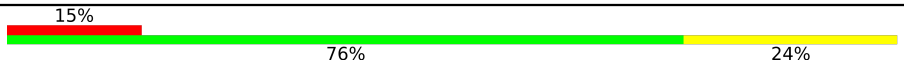
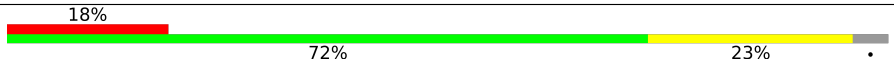
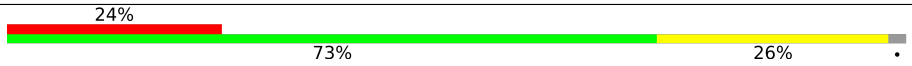
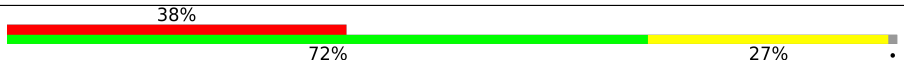
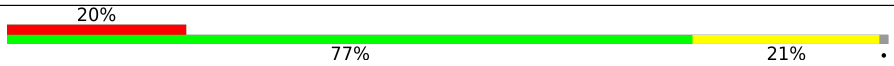
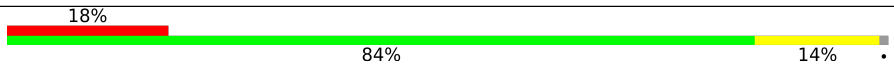
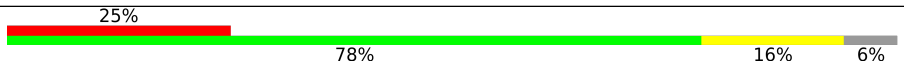
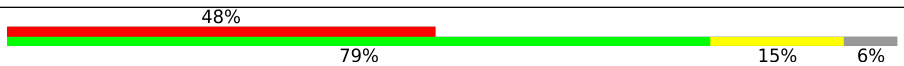
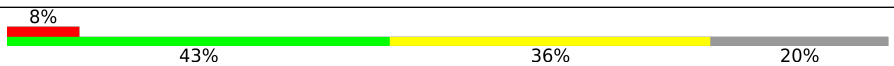
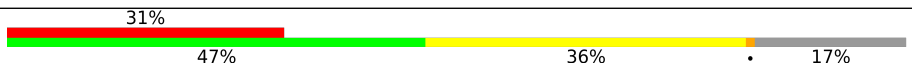
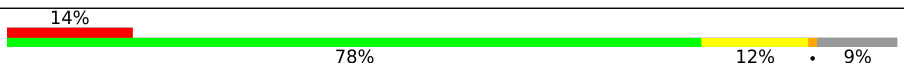
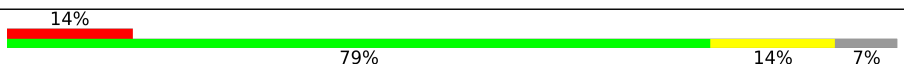
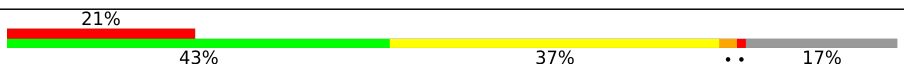
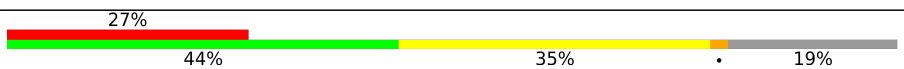
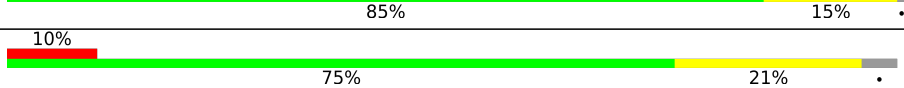
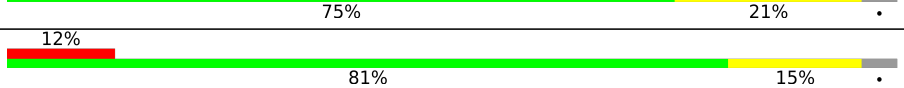
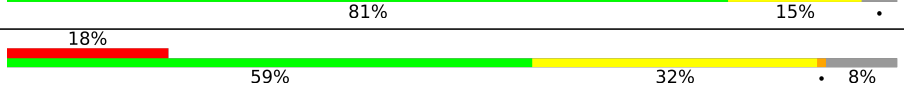
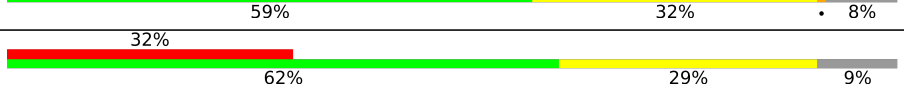
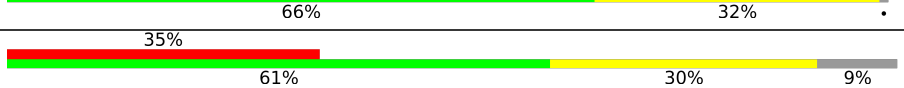
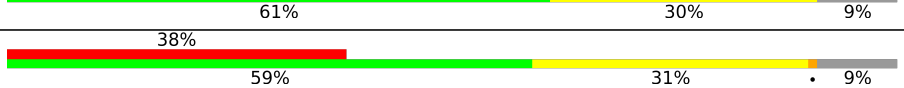
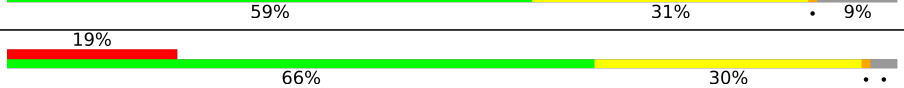
| Mol | Chain | Length | Quality of chain |
|---|---|---|---|
| 53 | CT | 236 |   |
| 53 | I | 236 |   |
| 54 | CU | 186 |   |
| 54 | J | 186 |   |
| 55 | CV | 206 |   |
| 55 | K | 206 |   |
| 56 | CW | 189 |   |
| 56 | L | 189 |   |
| 57 | CX | 118 |   |
| 57 | M | 118 |   |
| 58 | CY | 155 |   |
| 58 | N | 155 |   |
| 59 | CZ | 143 |   |
| 59 | O | 143 |   |
| 60 | DA | 151 | |
| 60 | P | 151 | |
| 61 | DB | 132 |   |
| 61 | Q | 132 |   |
| 62 | DC | 142 |   |
| 62 | R | 142 |   |
| 63 | DD | 142 | |
| 63 | S | 142 | |
| 64 | DE | 137 |   |
| 64 | T | 137 |   |
| 65 | DF | 145 |   |

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| Mol | Chain | Length | Quality of chain |
|---|---|---|---|
| 65 | U | 145 | 27% 73% 26% |
| 66 | DG | 145 | 28% 75% 22% |
| 66 | V | 145 | 33% 73% 24% |
| 67 | DH | 119 | 24% 59% 23% 18% |
| 67 | W | 119 | 33% 68% 18% 14% |
| 68 | DI | 87 | 8% 83% 17% |
| 68 | X | 87 | 14% 69% 31% |
| 69 | DJ | 130 | 21% 76% 23% |
| 69 | Y | 130 | 32% 80% 19% |
| 70 | DK | 145 | 17% 80% 19% |
| 70 | Z | 145 | 20% 78% 21% |
| 71 | DL | 135 | 12% 81% 16% |
| 71 | a | 135 | 24% 86% 13% |
| 72 | DM | 105 | 10% 52% 15% 32% |
| 72 | b | 105 | 12% 49% 20% 31% |
| 73 | DN | 119 | 15% 61% 20% 18% |
| 73 | c | 119 | 20% 68% 14% 18% |
| 74 | DO | 82 | 22% 85% 13% |
| 74 | d | 82 | 16% 88% 11% |
| 75 | DP | 67 | 13% 55% 36% 9% |
| 75 | e | 67 | 19% 61% 31% 7% |
| 76 | DQ | 56 | 21% 73% 23% |
| 76 | f | 56 | 30% 82% 16% |
| 77 | DR | 63 | 24% 63% 29% 8% |
| 77 | g | 63 | 25% 73% 22% 5% |

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| Mol | Chain | Length | Quality of chain |
|---|---|---|---|
| 78 | DS | 193 | 19% 19% 16% 64% |
| 78 | h | 193 | 15% 21% 15% 64% |
| 79 | AR | 317 | 27% 71% 27% |
| 79 | DT | 317 | 32% 63% 33% |
| 80 | P0 | 312 | 10% 24% 10% 66% |
| 80 | p0 | 312 | 12% 12% 12% 75% |
| 81 | 12 | 165 | 4% 18% 20% 62% |
| 82 | L1 | 217 | 13% 58% 41% |
| 82 | l1 | 217 | 24% 40% 56% |

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 |
|---|---|---|---|---|---|---|---|
| 83 | MG | 8 | 202 | - | - | - | X |

# 2 Entry composition

There are 87 unique types of molecules in this entry. The entry contains 408804 atoms, of which 0 are hydrogens and 0 are deuteriums.

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

- Molecule 1 is a RNA chain called 25S.

| Mol | Chain | Residues | Atoms | | | | | ZeroOcc | AltConf | Trace |
|---|---|---|---|---|---|---|---|---|---|---|
| 1 | 1 | 3208 | Total | C | N | O | P | 0 | 0 | 0 |
| | | | 68581 | 30637 | 12330 | 22406 | 3208 | | | |
| 1 | AS | 3227 | Total | C | N | O | P | 0 | 0 | 0 |
| | | | 68985 | 30817 | 12402 | 22539 | 3227 | | | |

- Molecule 2 is a RNA chain called 5S.

| Mol | Chain | Residues | Atoms | | | | | ZeroOcc | AltConf | Trace |
|---|---|---|---|---|---|---|---|---|---|---|
| 2 | 3 | 121 | Total | C | N | O | P | 0 | 0 | 0 |
| | | | 2579 | 1153 | 463 | 842 | 121 | | | |
| 2 | AT | 121 | Total | C | N | O | P | 0 | 0 | 0 |
| | | | 2579 | 1153 | 463 | 842 | 121 | | | |

- Molecule 3 is a RNA chain called 5.8S.

| Mol | Chain | Residues | Atoms | | | | | ZeroOcc | AltConf | Trace |
|---|---|---|---|---|---|---|---|---|---|---|
| 3 | 4 | 157 | Total | C | N | O | P | 0 | 0 | 0 |
| | | | 3333 | 1491 | 583 | 1102 | 157 | | | |
| 3 | AU | 157 | Total | C | N | O | P | 0 | 0 | 0 |
| | | | 3333 | 1491 | 583 | 1102 | 157 | | | |

- Molecule 4 is a protein called 60S ribosomal protein L2-B.

| Mol | Chain | Residues | Atoms | | | | | ZeroOcc | AltConf | Trace |
|---|---|---|---|---|---|---|---|---|---|---|
| 4 | j | 249 | Total | C | N | O | S | 0 | 0 | 0 |
| | | | 1888 | 1180 | 376 | 330 | 2 | | | |
| 4 | AW | 249 | Total | C | N | O | S | 0 | 0 | 0 |
| | | | 1888 | 1180 | 376 | 330 | 2 | | | |

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

| Mol | Chain | Residues | Atoms | | | | | ZeroOcc | AltConf | Trace |
|---|---|---|---|---|---|---|---|---|---|---|
| 5 | k | 386 | Total | C | N | O | S | 0 | 0 | 0 |
| | | | 3077 | 1950 | 582 | 538 | 7 | | | |
| 5 | AX | 386 | Total | C | N | O | S | 0 | 0 | 0 |
| | | | 3077 | 1950 | 582 | 538 | 7 | | | |

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

| Mol | Chain | Residues | Atoms | | | | | ZeroOcc | AltConf | Trace |
|---|---|---|---|---|---|---|---|---|---|---|
| 6 | l | 361 | Total | C | N | O | S | 0 | 0 | 0 |
| | | | 2751 | 1729 | 529 | 490 | 3 | | | |
| 6 | AY | 361 | Total | C | N | O | S | 0 | 0 | 0 |
| | | | 2751 | 1729 | 529 | 490 | 3 | | | |

- Molecule 7 is a protein called Uncharacterized protein CaJ7.0206.

| Mol | Chain | Residues | Atoms | | | | | ZeroOcc | AltConf | Trace |
|---|---|---|---|---|---|---|---|---|---|---|
| 7 | m | 296 | Total | C | N | O | S | 0 | 0 | 0 |
| | | | 2426 | 1544 | 422 | 458 | 2 | | | |
| 7 | AZ | 292 | Total | C | N | O | S | 0 | 0 | 0 |
| | | | 2394 | 1526 | 416 | 450 | 2 | | | |

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

| Mol | Chain | Residues | Atoms | | | | | ZeroOcc | AltConf | Trace |
|---|---|---|---|---|---|---|---|---|---|---|
| 8 | n | 157 | Total | C | N | O | S | 0 | 0 | 0 |
| | | | 1242 | 796 | 226 | 219 | 1 | | | |
| 8 | BA | 153 | Total | C | N | O | | 0 | 0 | 0 |
| | | | 1210 | 777 | 221 | 212 | | | | |

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

| Mol | Chain | Residues | Atoms | | | | | ZeroOcc | AltConf | Trace |
|---|---|---|---|---|---|---|---|---|---|---|
| 9 | o | 233 | Total | C | N | O | S | 0 | 0 | 0 |
| | | | 1876 | 1203 | 344 | 328 | 1 | | | |
| 9 | BB | 234 | Total | C | N | O | S | 0 | 0 | 0 |
| | | | 1885 | 1208 | 345 | 331 | 1 | | | |

- Molecule 10 is a protein called 60S ribosomal protein L8.

| Mol | Chain | Residues | Atoms | | | | | ZeroOcc | AltConf | Trace |
|---|---|---|---|---|---|---|---|---|---|---|
| 10 | p | 233 | Total | C | N | O | S | 0 | 0 | 0 |
| | | | 1805 | 1156 | 321 | 325 | 3 | | | |

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| Mol | Chain | Residues | Atoms | | | | | ZeroOcc | AltConf | Trace |
|---|---|---|---|---|---|---|---|---|---|---|
| 10 | BC | 229 | Total | C | N | O | S | 0 | 0 | 0 |
| | | | 1778 | 1140 | 316 | 319 | 3 | | | |

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

| Mol | Chain | Residues | Atoms | | | | | ZeroOcc | AltConf | Trace |
|---|---|---|---|---|---|---|---|---|---|---|
| 11 | q | 189 | Total | C | N | O | S | 0 | 0 | 0 |
| | | | 1510 | 953 | 275 | 278 | 4 | | | |
| 11 | BD | 190 | Total | C | N | O | S | 0 | 0 | 0 |
| | | | 1519 | 958 | 276 | 281 | 4 | | | |

- Molecule 12 is a protein called 60S ribosomal protein L10.

| Mol | Chain | Residues | Atoms | | | | | ZeroOcc | AltConf | Trace |
|---|---|---|---|---|---|---|---|---|---|---|
| 12 | r | 208 | Total | C | N | O | S | 0 | 0 | 0 |
| | | | 1689 | 1069 | 322 | 291 | 7 | | | |
| 12 | BE | 208 | Total | C | N | O | S | 0 | 0 | 0 |
| | | | 1689 | 1069 | 322 | 291 | 7 | | | |

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

| Mol | Chain | Residues | Atoms | | | | | ZeroOcc | AltConf | Trace |
|---|---|---|---|---|---|---|---|---|---|---|
| 13 | s | 171 | Total | C | N | O | S | 0 | 0 | 0 |
| | | | 1371 | 857 | 260 | 250 | 4 | | | |
| 13 | BF | 171 | Total | C | N | O | S | 0 | 0 | 0 |
| | | | 1371 | 857 | 260 | 250 | 4 | | | |

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

| Mol | Chain | Residues | Atoms | | | | ZeroOcc | AltConf | Trace |
|---|---|---|---|---|---|---|---|---|---|
| 14 | t | 200 | Total | C | N | O | 0 | 0 | 0 |
| | | | 1610 | 1009 | 318 | 283 | | | |
| 14 | BG | 200 | Total | C | N | O | 0 | 0 | 0 |
| | | | 1610 | 1009 | 318 | 283 | | | |

- Molecule 15 is a protein called 60S ribosomal protein L14-B.

| Mol | Chain | Residues | Atoms | | | | | ZeroOcc | AltConf | Trace |
|---|---|---|---|---|---|---|---|---|---|---|
| 15 | u | 130 | Total | C | N | O | S | 0 | 0 | 0 |
| | | | 1029 | 660 | 193 | 175 | 1 | | | |
| 15 | BH | 130 | Total | C | N | O | S | 0 | 0 | 0 |
| | | | 1029 | 660 | 193 | 175 | 1 | | | |

- Molecule 16 is a protein called 60S ribosomal protein L15-A.

| Mol | Chain | Residues | Atoms | | | | | ZeroOcc | AltConf | Trace |
|---|---|---|---|---|---|---|---|---|---|---|
| 16 | v | 203 | Total | C | N | O | S | 0 | 0 | 0 |
| | | | 1713 | 1075 | 356 | 280 | 2 | | | |
| 16 | BI | 203 | Total | C | N | O | S | 0 | 0 | 0 |
| | | | 1713 | 1075 | 356 | 280 | 2 | | | |

- Molecule 17 is a protein called Ribosomal protein L13.

| Mol | Chain | Residues | Atoms | | | | | ZeroOcc | AltConf | Trace |
|---|---|---|---|---|---|---|---|---|---|---|
| 17 | w | 199 | Total | C | N | O | S | 0 | 0 | 0 |
| | | | 1590 | 1025 | 294 | 269 | 2 | | | |
| 17 | BJ | 199 | Total | C | N | O | S | 0 | 0 | 0 |
| | | | 1590 | 1025 | 294 | 269 | 2 | | | |

- Molecule 18 is a protein called Ribosomal protein L22.

| Mol | Chain | Residues | Atoms | | | | ZeroOcc | AltConf | Trace |
|---|---|---|---|---|---|---|---|---|---|
| 18 | x | 173 | Total | C | N | O | 0 | 0 | 0 |
| | | | 1387 | 856 | 280 | 251 | | | |
| 18 | BK | 176 | Total | C | N | O | 0 | 0 | 0 |
| | | | 1406 | 868 | 284 | 254 | | | |

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

| Mol | Chain | Residues | Atoms | | | | ZeroOcc | AltConf | Trace |
|---|---|---|---|---|---|---|---|---|---|
| 19 | y | 185 | Total | C | N | O | 0 | 0 | 0 |
| | | | 1458 | 916 | 297 | 245 | | | |
| 19 | BL | 185 | Total | C | N | O | 0 | 0 | 0 |
| | | | 1458 | 916 | 297 | 245 | | | |

- Molecule 20 is a protein called 60S ribosomal protein L19-A.

| Mol | Chain | Residues | Atoms | | | | | ZeroOcc | AltConf | Trace |
|---|---|---|---|---|---|---|---|---|---|---|
| 20 | z | 179 | Total | C | N | O | S | 0 | 0 | 0 |
| | | | 1457 | 901 | 310 | 243 | 3 | | | |
| 20 | BM | 179 | Total | C | N | O | S | 0 | 0 | 0 |
| | | | 1457 | 901 | 310 | 243 | 3 | | | |

- Molecule 21 is a protein called 60S ribosomal protein L20.

| Mol | Chain | Residues | Atoms | | | | | ZeroOcc | AltConf | Trace |
|---|---|---|---|---|---|---|---|---|---|---|
| 21 | 0 | 170 | Total | C | N | O | S | 0 | 0 | 0 |
| | | | 1423 | 921 | 258 | 241 | 3 | | | |
| 21 | BN | 170 | Total | C | N | O | S | 0 | 0 | 0 |
| | | | 1423 | 921 | 258 | 241 | 3 | | | |

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

| Mol | Chain | Residues | Atoms | | | | | ZeroOcc | AltConf | Trace |
|---|---|---|---|---|---|---|---|---|---|---|
| 22 | 2 | 159 | Total | C | N | O | S | 0 | 0 | 0 |
| | | | 1262 | 798 | 241 | 221 | 2 | | | |
| 22 | BO | 159 | Total | C | N | O | S | 0 | 0 | 0 |
| | | | 1262 | 798 | 241 | 221 | 2 | | | |

- Molecule 23 is a protein called 60S ribosomal protein L22-B.

| Mol | Chain | Residues | Atoms | | | | ZeroOcc | AltConf | Trace |
|---|---|---|---|---|---|---|---|---|---|
| 23 | 5 | 102 | Total | C | N | O | 0 | 0 | 0 |
| | | | 826 | 536 | 137 | 153 | | | |
| 23 | BP | 102 | Total | C | N | O | 0 | 0 | 0 |
| | | | 826 | 536 | 137 | 153 | | | |

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

| Mol | Chain | Residues | Atoms | | | | | ZeroOcc | AltConf | Trace |
|---|---|---|---|---|---|---|---|---|---|---|
| 24 | 6 | 131 | Total | C | N | O | S | 0 | 0 | 0 |
| | | | 977 | 615 | 183 | 171 | 8 | | | |
| 24 | BQ | 131 | Total | C | N | O | S | 0 | 0 | 0 |
| | | | 977 | 615 | 183 | 171 | 8 | | | |

- Molecule 25 is a protein called 60S ribosomal protein L24-A.

| Mol | Chain | Residues | Atoms | | | | | ZeroOcc | AltConf | Trace |
|---|---|---|---|---|---|---|---|---|---|---|
| 25 | 7 | 118 | Total | C | N | O | S | 0 | 0 | 0 |
| | | | 945 | 591 | 192 | 161 | 1 | | | |
| 25 | BR | 98 | Total | C | N | O | S | 0 | 0 | 0 |
| | | | 801 | 501 | 162 | 137 | 1 | | | |

- Molecule 26 is a protein called 60S ribosomal protein L25.

| Mol | Chain | Residues | Atoms | | | | | ZeroOcc | AltConf | Trace |
|---|---|---|---|---|---|---|---|---|---|---|
| 26 | 8 | 120 | Total | C | N | O | S | 0 | 0 | 0 |
| | | | 965 | 616 | 173 | 175 | 1 | | | |

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| Mol | Chain | Residues | Atoms | | | | | ZeroOcc | AltConf | Trace |
|---|---|---|---|---|---|---|---|---|---|---|
| 26 | BS | 119 | Total<br>960 | C<br>613 | N<br>172 | O<br>174 | S<br>1 | 0 | 0 | 0 |

- Molecule 27 is a protein called Ribosomal protein L24.

| Mol | Chain | Residues | Atoms | | | | ZeroOcc | AltConf | Trace |
|---|---|---|---|---|---|---|---|---|---|
| 27 | 9 | 126 | Total<br>989 | C<br>618 | N<br>190 | O<br>181 | 0 | 0 | 0 |
| 27 | BT | 126 | Total<br>989 | C<br>618 | N<br>190 | O<br>181 | 0 | 0 | 0 |

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

| Mol | Chain | Residues | Atoms | | | | | ZeroOcc | AltConf | Trace |
|---|---|---|---|---|---|---|---|---|---|---|
| 28 | AA | 135 | Total<br>1087 | C<br>705 | N<br>197 | O<br>183 | S<br>2 | 0 | 0 | 0 |
| 28 | BU | 135 | Total<br>1087 | C<br>705 | N<br>197 | O<br>183 | S<br>2 | 0 | 0 | 0 |

- Molecule 29 is a protein called 60S ribosomal protein L28.

| Mol | Chain | Residues | Atoms | | | | | ZeroOcc | AltConf | Trace |
|---|---|---|---|---|---|---|---|---|---|---|
| 29 | AB | 148 | Total<br>1170 | C<br>741 | N<br>231 | O<br>197 | S<br>1 | 0 | 0 | 0 |
| 29 | BV | 148 | Total<br>1170 | C<br>741 | N<br>231 | O<br>197 | S<br>1 | 0 | 0 | 0 |

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

| Mol | Chain | Residues | Atoms | | | | ZeroOcc | AltConf | Trace |
|---|---|---|---|---|---|---|---|---|---|
| 30 | AC | 62 | Total<br>493 | C<br>307 | N<br>105 | O<br>81 | 0 | 0 | 0 |
| 30 | BW | 61 | Total<br>488 | C<br>304 | N<br>104 | O<br>80 | 0 | 0 | 0 |

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

| Mol | Chain | Residues | Atoms | | | | | ZeroOcc | AltConf | Trace |
|---|---|---|---|---|---|---|---|---|---|---|
| 31 | AD | 96 | Total<br>729 | C<br>469 | N<br>121 | O<br>137 | S<br>2 | 0 | 0 | 0 |
| 31 | BX | 96 | Total<br>729 | C<br>469 | N<br>121 | O<br>137 | S<br>2 | 0 | 0 | 0 |

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

| Mol | Chain | Residues | Atoms | | | | | ZeroOcc | AltConf | Trace |
|---|---|---|---|---|---|---|---|---|---|---|
| 32 | AE | 110 | Total | C | N | O | S | 0 | 0 | 0 |
| | | | 894 | 565 | 168 | 159 | 2 | | | |
| 32 | BY | 110 | Total | C | N | O | S | 0 | 0 | 0 |
| | | | 894 | 565 | 168 | 159 | 2 | | | |

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

| Mol | Chain | Residues | Atoms | | | | | ZeroOcc | AltConf | Trace |
|---|---|---|---|---|---|---|---|---|---|---|
| 33 | AF | 124 | Total | C | N | O | S | 0 | 0 | 0 |
| | | | 1000 | 638 | 194 | 167 | 1 | | | |
| 33 | BZ | 124 | Total | C | N | O | S | 0 | 0 | 0 |
| | | | 1004 | 641 | 195 | 167 | 1 | | | |

- Molecule 34 is a protein called 60S ribosomal protein L33-A.

| Mol | Chain | Residues | Atoms | | | | | ZeroOcc | AltConf | Trace |
|---|---|---|---|---|---|---|---|---|---|---|
| 34 | AG | 106 | Total | C | N | O | S | 0 | 0 | 0 |
| | | | 847 | 543 | 161 | 142 | 1 | | | |
| 34 | CA | 106 | Total | C | N | O | S | 0 | 0 | 0 |
| | | | 847 | 543 | 161 | 142 | 1 | | | |

- Molecule 35 is a protein called 60S ribosomal protein L34-B.

| Mol | Chain | Residues | Atoms | | | | | ZeroOcc | AltConf | Trace |
|---|---|---|---|---|---|---|---|---|---|---|
| 35 | AH | 112 | Total | C | N | O | S | 0 | 0 | 0 |
| | | | 887 | 547 | 182 | 154 | 4 | | | |
| 35 | CB | 112 | Total | C | N | O | S | 0 | 0 | 0 |
| | | | 887 | 547 | 182 | 154 | 4 | | | |

- Molecule 36 is a protein called Ribosomal protein L29.

| Mol | Chain | Residues | Atoms | | | | | ZeroOcc | AltConf | Trace |
|---|---|---|---|---|---|---|---|---|---|---|
| 36 | AI | 120 | Total | C | N | O | S | 0 | 0 | 0 |
| | | | 992 | 629 | 195 | 167 | 1 | | | |
| 36 | CC | 118 | Total | C | N | O | | 0 | 0 | 0 |
| | | | 979 | 621 | 193 | 165 | | | | |

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

| Mol | Chain | Residues | Atoms | | | | | ZeroOcc | AltConf | Trace |
|---|---|---|---|---|---|---|---|---|---|---|
| 37 | AJ | 97 | Total | C | N | O | S | 0 | 0 | 0 |
| | | | 758 | 471 | 156 | 130 | 1 | | | |
| 37 | CD | 97 | Total | C | N | O | S | 0 | 0 | 0 |
| | | | 758 | 471 | 156 | 130 | 1 | | | |

- Molecule 38 is a protein called 60S ribosomal protein L37-B.

| Mol | Chain | Residues | Atoms | | | | | ZeroOcc | AltConf | Trace |
|---|---|---|---|---|---|---|---|---|---|---|
| 38 | AK | 86 | Total | C | N | O | S | 0 | 0 | 0 |
| | | | 677 | 413 | 148 | 110 | 6 | | | |
| 38 | CE | 86 | Total | C | N | O | S | 0 | 0 | 0 |
| | | | 677 | 413 | 148 | 110 | 6 | | | |

- Molecule 39 is a protein called 60S ribosomal protein L38.

| Mol | Chain | Residues | Atoms | | | | ZeroOcc | AltConf | Trace |
|---|---|---|---|---|---|---|---|---|---|
| 39 | AL | 77 | Total | C | N | O | 0 | 0 | 0 |
| | | | 617 | 393 | 115 | 109 | | | |
| 39 | CF | 77 | Total | C | N | O | 0 | 0 | 0 |
| | | | 617 | 393 | 115 | 109 | | | |

- Molecule 40 is a protein called 60S ribosomal protein L39.

| Mol | Chain | Residues | Atoms | | | | ZeroOcc | AltConf | Trace |
|---|---|---|---|---|---|---|---|---|---|
| 40 | AM | 50 | Total | C | N | O | 0 | 0 | 0 |
| | | | 438 | 275 | 97 | 66 | | | |
| 40 | CG | 50 | Total | C | N | O | 0 | 0 | 0 |
| | | | 438 | 275 | 97 | 66 | | | |

- Molecule 41 is a protein called 60S ribosomal protein L40-B.

| Mol | Chain | Residues | Atoms | | | | | ZeroOcc | AltConf | Trace |
|---|---|---|---|---|---|---|---|---|---|---|
| 41 | AN | 52 | Total | C | N | O | S | 0 | 0 | 0 |
| | | | 419 | 260 | 86 | 67 | 6 | | | |
| 41 | CH | 51 | Total | C | N | O | S | 0 | 0 | 0 |
| | | | 411 | 255 | 85 | 66 | 5 | | | |

- Molecule 42 is a protein called 60S ribosomal protein L41.

| Mol | Chain | Residues | Atoms | | | | | ZeroOcc | AltConf | Trace |
|---|---|---|---|---|---|---|---|---|---|---|
| 42 | AO | 25 | Total | C | N | O | S | 0 | 0 | 0 |
| | | | 236 | 144 | 63 | 28 | 1 | | | |

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| Mol | Chain | Residues | Atoms | | | | | ZeroOcc | AltConf | Trace |
|---|---|---|---|---|---|---|---|---|---|---|
| 42 | CI | 24 | Total | C | N | O | S | 0 | 0 | 0 |
| | | | 227 | 138 | 61 | 27 | 1 | | | |

- Molecule 43 is a protein called 60S ribosomal protein L42-B.

| Mol | Chain | Residues | Atoms | | | | | ZeroOcc | AltConf | Trace |
|---|---|---|---|---|---|---|---|---|---|---|
| 43 | AP | 103 | Total | C | N | O | S | 0 | 0 | 0 |
| | | | 828 | 521 | 165 | 137 | 5 | | | |
| 43 | CJ | 103 | Total | C | N | O | S | 0 | 0 | 0 |
| | | | 828 | 521 | 165 | 137 | 5 | | | |

- Molecule 44 is a protein called 60S ribosomal protein L43-A.

| Mol | Chain | Residues | Atoms | | | | | ZeroOcc | AltConf | Trace |
|---|---|---|---|---|---|---|---|---|---|---|
| 44 | AQ | 91 | Total | C | N | O | S | 0 | 0 | 0 |
| | | | 698 | 430 | 140 | 124 | 4 | | | |
| 44 | CK | 91 | Total | C | N | O | S | 0 | 0 | 0 |
| | | | 698 | 430 | 140 | 124 | 4 | | | |

- Molecule 45 is a protein called 60S ribosomal protein CAALFM_C304810CA.

| Mol | Chain | Residues | Atoms | | | | ZeroOcc | AltConf | Trace |
|---|---|---|---|---|---|---|---|---|---|
| 45 | i | 120 | Total | C | N | O | 0 | 0 | 0 |
| | | | 922 | 558 | 165 | 199 | | | |
| 45 | CL | 121 | Total | C | N | O | 0 | 0 | 0 |
| | | | 931 | 563 | 166 | 202 | | | |

- Molecule 46 is a RNA chain called 18S.

| Mol | Chain | Residues | Atoms | | | | | ZeroOcc | AltConf | Trace |
|---|---|---|---|---|---|---|---|---|---|---|
| 46 | B | 1741 | Total | C | N | O | P | 0 | 0 | 0 |
| | | | 37113 | 16590 | 6583 | 12199 | 1741 | | | |
| 46 | CM | 1765 | Total | C | N | O | P | 0 | 0 | 0 |
| | | | 37621 | 16818 | 6670 | 12368 | 1765 | | | |

- Molecule 47 is a protein called 40S ribosomal protein S0.

| Mol | Chain | Residues | Atoms | | | | | ZeroOcc | AltConf | Trace |
|---|---|---|---|---|---|---|---|---|---|---|
| 47 | C | 208 | Total | C | N | O | S | 0 | 0 | 0 |
| | | | 1627 | 1041 | 284 | 297 | 5 | | | |
| 47 | CN | 208 | Total | C | N | O | S | 0 | 0 | 0 |
| | | | 1627 | 1041 | 284 | 297 | 5 | | | |

- Molecule 48 is a protein called 40S ribosomal protein S1.

| Mol | Chain | Residues | Atoms | | | | | ZeroOcc | AltConf | Trace |
|---|---|---|---|---|---|---|---|---|---|---|
| 48 | D | 214 | Total | C | N | O | S | 0 | 0 | 0 |
| | | | 1724 | 1094 | 313 | 313 | 4 | | | |
| 48 | CO | 214 | Total | C | N | O | S | 0 | 0 | 0 |
| | | | 1724 | 1094 | 313 | 313 | 4 | | | |

- Molecule 49 is a protein called Ribosomal protein S5.

| Mol | Chain | Residues | Atoms | | | | | ZeroOcc | AltConf | Trace |
|---|---|---|---|---|---|---|---|---|---|---|
| 49 | E | 217 | Total | C | N | O | S | 0 | 0 | 0 |
| | | | 1629 | 1039 | 289 | 296 | 5 | | | |
| 49 | CP | 217 | Total | C | N | O | S | 0 | 0 | 0 |
| | | | 1629 | 1039 | 289 | 296 | 5 | | | |

- Molecule 50 is a protein called Ribosomal protein S3.

| Mol | Chain | Residues | Atoms | | | | | ZeroOcc | AltConf | Trace |
|---|---|---|---|---|---|---|---|---|---|---|
| 50 | F | 223 | Total | C | N | O | S | 0 | 0 | 0 |
| | | | 1707 | 1087 | 311 | 305 | 4 | | | |
| 50 | CQ | 223 | Total | C | N | O | S | 0 | 0 | 0 |
| | | | 1707 | 1087 | 311 | 305 | 4 | | | |

- Molecule 51 is a protein called 40S ribosomal protein S4.

| Mol | Chain | Residues | Atoms | | | | | ZeroOcc | AltConf | Trace |
|---|---|---|---|---|---|---|---|---|---|---|
| 51 | G | 259 | Total | C | N | O | S | 0 | 0 | 0 |
| | | | 2051 | 1304 | 385 | 357 | 5 | | | |
| 51 | CR | 260 | Total | C | N | O | S | 0 | 0 | 0 |
| | | | 2055 | 1306 | 386 | 358 | 5 | | | |

- Molecule 52 is a protein called Ribosomal protein S7.

| Mol | Chain | Residues | Atoms | | | | | ZeroOcc | AltConf | Trace |
|---|---|---|---|---|---|---|---|---|---|---|
| 52 | H | 206 | Total | C | N | O | S | 0 | 0 | 0 |
| | | | 1614 | 1008 | 301 | 301 | 4 | | | |
| 52 | CS | 206 | Total | C | N | O | S | 0 | 0 | 0 |
| | | | 1614 | 1008 | 301 | 301 | 4 | | | |

- Molecule 53 is a protein called 40S ribosomal protein S6.

| Mol | Chain | Residues | Atoms | | | | | ZeroOcc | AltConf | Trace |
|---|---|---|---|---|---|---|---|---|---|---|
| 53 | I | 226 | Total | C | N | O | S | 0 | 0 | 0 |
| | | | 1820 | 1133 | 351 | 330 | 6 | | | |
| 53 | CT | 236 | Total | C | N | O | S | 0 | 0 | 0 |
| | | | 1904 | 1184 | 369 | 345 | 6 | | | |

- Molecule 54 is a protein called 40S ribosomal protein S7.

| Mol | Chain | Residues | Atoms | | | | ZeroOcc | AltConf | Trace |
|---|---|---|---|---|---|---|---|---|---|
| 54 | J | 184 | Total | C | N | O | 0 | 0 | 0 |
| | | | 1485 | 950 | 268 | 267 | | | |
| 54 | CU | 183 | Total | C | N | O | 0 | 0 | 0 |
| | | | 1475 | 944 | 265 | 266 | | | |

- Molecule 55 is a protein called 40S ribosomal protein S8.

| Mol | Chain | Residues | Atoms | | | | | ZeroOcc | AltConf | Trace |
|---|---|---|---|---|---|---|---|---|---|---|
| 55 | K | 203 | Total | C | N | O | S | 0 | 0 | 0 |
| | | | 1579 | 973 | 322 | 283 | 1 | | | |
| 55 | CV | 203 | Total | C | N | O | S | 0 | 0 | 0 |
| | | | 1579 | 973 | 322 | 283 | 1 | | | |

- Molecule 56 is a protein called Ribosomal protein S4.

| Mol | Chain | Residues | Atoms | | | | | ZeroOcc | AltConf | Trace |
|---|---|---|---|---|---|---|---|---|---|---|
| 56 | L | 178 | Total | C | N | O | S | 0 | 0 | 0 |
| | | | 1453 | 918 | 286 | 248 | 1 | | | |
| 56 | CW | 178 | Total | C | N | O | S | 0 | 0 | 0 |
| | | | 1453 | 918 | 286 | 248 | 1 | | | |

- Molecule 57 is a protein called 40S ribosomal protein S10-A.

| Mol | Chain | Residues | Atoms | | | | | ZeroOcc | AltConf | Trace |
|---|---|---|---|---|---|---|---|---|---|---|
| 57 | M | 98 | Total | C | N | O | S | 0 | 0 | 0 |
| | | | 817 | 531 | 135 | 150 | 1 | | | |
| 57 | CX | 94 | Total | C | N | O | S | 0 | 0 | 0 |
| | | | 791 | 515 | 131 | 144 | 1 | | | |

- Molecule 58 is a protein called 40S ribosomal protein S11A.

| Mol | Chain | Residues | Atoms | | | | | ZeroOcc | AltConf | Trace |
|---|---|---|---|---|---|---|---|---|---|---|
| 58 | N | 144 | Total | C | N | O | S | 0 | 0 | 0 |
| | | | 1150 | 734 | 215 | 198 | 3 | | | |

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| Mol | Chain | Residues | Atoms | | | | | ZeroOcc | AltConf | Trace |
|---|---|---|---|---|---|---|---|---|---|---|
| 58 | CY | 141 | Total | C | N | O | S | 0 | 0 | 0 |
| | | | 1129 | 722 | 212 | 192 | 3 | | | |

- Molecule 59 is a protein called 40S ribosomal protein S12.

| Mol | Chain | Residues | Atoms | | | | | ZeroOcc | AltConf | Trace |
|---|---|---|---|---|---|---|---|---|---|---|
| 59 | O | 116 | Total | C | N | O | S | 0 | 0 | 0 |
| | | | 885 | 550 | 158 | 172 | 5 | | | |
| 59 | CZ | 119 | Total | C | N | O | S | 0 | 0 | 0 |
| | | | 913 | 566 | 163 | 179 | 5 | | | |

- Molecule 60 is a protein called 40S ribosomal protein S13.

| Mol | Chain | Residues | Atoms | | | | | ZeroOcc | AltConf | Trace |
|---|---|---|---|---|---|---|---|---|---|---|
| 60 | P | 150 | Total | C | N | O | S | 0 | 0 | 0 |
| | | | 1187 | 757 | 219 | 210 | 1 | | | |
| 60 | DA | 150 | Total | C | N | O | S | 0 | 0 | 0 |
| | | | 1187 | 757 | 219 | 210 | 1 | | | |

- Molecule 61 is a protein called 40S ribosomal protein S14-A.

| Mol | Chain | Residues | Atoms | | | | | ZeroOcc | AltConf | Trace |
|---|---|---|---|---|---|---|---|---|---|---|
| 61 | Q | 127 | Total | C | N | O | S | 0 | 0 | 0 |
| | | | 942 | 579 | 186 | 174 | 3 | | | |
| 61 | DB | 127 | Total | C | N | O | S | 0 | 0 | 0 |
| | | | 942 | 579 | 186 | 174 | 3 | | | |

- Molecule 62 is a protein called 40S ribosomal protein S15.

| Mol | Chain | Residues | Atoms | | | | | ZeroOcc | AltConf | Trace |
|---|---|---|---|---|---|---|---|---|---|---|
| 62 | R | 129 | Total | C | N | O | S | 0 | 0 | 0 |
| | | | 1018 | 649 | 185 | 177 | 7 | | | |
| 62 | DC | 130 | Total | C | N | O | S | 0 | 0 | 0 |
| | | | 1029 | 655 | 189 | 178 | 7 | | | |

- Molecule 63 is a protein called 40S ribosomal protein S16.

| Mol | Chain | Residues | Atoms | | | | | ZeroOcc | AltConf | Trace |
|---|---|---|---|---|---|---|---|---|---|---|
| 63 | S | 140 | Total | C | N | O | S | 0 | 0 | 0 |
| | | | 1091 | 700 | 198 | 192 | 1 | | | |
| 63 | DD | 140 | Total | C | N | O | S | 0 | 0 | 0 |
| | | | 1091 | 700 | 198 | 192 | 1 | | | |

- Molecule 64 is a protein called 40S ribosomal protein S17-B.

| Mol | Chain | Residues | Atoms | | | | | ZeroOcc | AltConf | Trace |
|---|---|---|---|---|---|---|---|---|---|---|
| 64 | T | 124 | Total | C | N | O | S | 0 | 0 | 0 |
| | | | 997 | 628 | 183 | 185 | 1 | | | |
| 64 | DE | 124 | Total | C | N | O | S | 0 | 0 | 0 |
| | | | 997 | 628 | 183 | 185 | 1 | | | |

- Molecule 65 is a protein called 40S ribosomal protein S18-B.

| Mol | Chain | Residues | Atoms | | | | | ZeroOcc | AltConf | Trace |
|---|---|---|---|---|---|---|---|---|---|---|
| 65 | U | 144 | Total | C | N | O | S | 0 | 0 | 0 |
| | | | 1187 | 744 | 233 | 207 | 3 | | | |
| 65 | DF | 141 | Total | C | N | O | S | 0 | 0 | 0 |
| | | | 1161 | 727 | 227 | 204 | 3 | | | |

- Molecule 66 is a protein called 40S ribosomal protein S19-A.

| Mol | Chain | Residues | Atoms | | | | | ZeroOcc | AltConf | Trace |
|---|---|---|---|---|---|---|---|---|---|---|
| 66 | V | 141 | Total | C | N | O | S | 0 | 0 | 0 |
| | | | 1100 | 689 | 210 | 200 | 1 | | | |
| 66 | DG | 141 | Total | C | N | O | S | 0 | 0 | 0 |
| | | | 1100 | 689 | 210 | 200 | 1 | | | |

- Molecule 67 is a protein called Ribosomal protein S10.

| Mol | Chain | Residues | Atoms | | | | | ZeroOcc | AltConf | Trace |
|---|---|---|---|---|---|---|---|---|---|---|
| 67 | W | 102 | Total | C | N | O | S | 0 | 0 | 0 |
| | | | 808 | 509 | 150 | 147 | 2 | | | |
| 67 | DH | 97 | Total | C | N | O | S | 0 | 0 | 0 |
| | | | 763 | 481 | 140 | 140 | 2 | | | |

- Molecule 68 is a protein called 40S ribosomal protein S21.

| Mol | Chain | Residues | Atoms | | | | | ZeroOcc | AltConf | Trace |
|---|---|---|---|---|---|---|---|---|---|---|
| 68 | X | 87 | Total | C | N | O | S | 0 | 0 | 0 |
| | | | 676 | 415 | 126 | 133 | 2 | | | |
| 68 | DI | 87 | Total | C | N | O | S | 0 | 0 | 0 |
| | | | 676 | 415 | 126 | 133 | 2 | | | |

- Molecule 69 is a protein called 40S ribosomal protein S22-A.

| Mol | Chain | Residues | Atoms | | | | | ZeroOcc | AltConf | Trace |
|---|---|---|---|---|---|---|---|---|---|---|
| 69 | Y | 129 | Total | C | N | O | S | 0 | 0 | 0 |
| | | | 1032 | 655 | 191 | 183 | 3 | | | |
| 69 | DJ | 129 | Total | C | N | O | S | 0 | 0 | 0 |
| | | | 1032 | 655 | 191 | 183 | 3 | | | |

- Molecule 70 is a protein called Ribosomal protein S23 (S12).

| Mol | Chain | Residues | Atoms | | | | | ZeroOcc | AltConf | Trace |
|---|---|---|---|---|---|---|---|---|---|---|
| 70 | Z | 143 | Total | C | N | O | S | 0 | 0 | 0 |
| | | | 1110 | 701 | 219 | 188 | 2 | | | |
| 70 | DK | 143 | Total | C | N | O | S | 0 | 0 | 0 |
| | | | 1110 | 701 | 219 | 188 | 2 | | | |

- Molecule 71 is a protein called 40S ribosomal protein S24.

| Mol | Chain | Residues | Atoms | | | | ZeroOcc | AltConf | Trace |
|---|---|---|---|---|---|---|---|---|---|
| 71 | a | 134 | Total | C | N | O | 0 | 0 | 0 |
| | | | 1086 | 677 | 218 | 191 | | | |
| 71 | DL | 132 | Total | C | N | O | 0 | 0 | 0 |
| | | | 1072 | 670 | 216 | 186 | | | |

- Molecule 72 is a protein called 40S ribosomal protein S25.

| Mol | Chain | Residues | Atoms | | | | ZeroOcc | AltConf | Trace |
|---|---|---|---|---|---|---|---|---|---|
| 72 | b | 72 | Total | C | N | O | 0 | 0 | 0 |
| | | | 578 | 369 | 103 | 106 | | | |
| 72 | DM | 71 | Total | C | N | O | 0 | 0 | 0 |
| | | | 570 | 365 | 102 | 103 | | | |

- Molecule 73 is a protein called 40S ribosomal protein S26.

| Mol | Chain | Residues | Atoms | | | | | ZeroOcc | AltConf | Trace |
|---|---|---|---|---|---|---|---|---|---|---|
| 73 | c | 98 | Total | C | N | O | S | 0 | 0 | 0 |
| | | | 779 | 482 | 163 | 128 | 6 | | | |
| 73 | DN | 97 | Total | C | N | O | S | 0 | 0 | 0 |
| | | | 770 | 477 | 161 | 126 | 6 | | | |

- Molecule 74 is a protein called 40S ribosomal protein S27.

| Mol | Chain | Residues | Atoms | | | | | ZeroOcc | AltConf | Trace |
|---|---|---|---|---|---|---|---|---|---|---|
| 74 | d | 81 | Total | C | N | O | S | 0 | 0 | 0 |
| | | | 614 | 383 | 110 | 114 | 7 | | | |

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| Mol | Chain | Residues | Atoms | | | | | ZeroOcc | AltConf | Trace |
|---|---|---|---|---|---|---|---|---|---|---|
| 74 | DO | 81 | Total | C | N | O | S | 0 | 0 | 0 |
| | | | 614 | 383 | 110 | 114 | 7 | | | |

- Molecule 75 is a protein called 40S ribosomal protein S28-B.

| Mol | Chain | Residues | Atoms | | | | | ZeroOcc | AltConf | Trace |
|---|---|---|---|---|---|---|---|---|---|---|
| 75 | e | 62 | Total | C | N | O | S | 0 | 0 | 0 |
| | | | 487 | 299 | 98 | 88 | 2 | | | |
| 75 | DP | 61 | Total | C | N | O | S | 0 | 0 | 0 |
| | | | 476 | 293 | 94 | 87 | 2 | | | |

- Molecule 76 is a protein called 40S ribosomal protein S29A.

| Mol | Chain | Residues | Atoms | | | | | ZeroOcc | AltConf | Trace |
|---|---|---|---|---|---|---|---|---|---|---|
| 76 | f | 55 | Total | C | N | O | S | 0 | 0 | 0 |
| | | | 454 | 281 | 94 | 75 | 4 | | | |
| 76 | DQ | 54 | Total | C | N | O | S | 0 | 0 | 0 |
| | | | 449 | 278 | 93 | 74 | 4 | | | |

- Molecule 77 is a protein called 40S ribosomal protein S30.

| Mol | Chain | Residues | Atoms | | | | | ZeroOcc | AltConf | Trace |
|---|---|---|---|---|---|---|---|---|---|---|
| 77 | g | 60 | Total | C | N | O | S | 0 | 0 | 0 |
| | | | 474 | 297 | 96 | 79 | 2 | | | |
| 77 | DR | 58 | Total | C | N | O | S | 0 | 0 | 0 |
| | | | 461 | 289 | 93 | 77 | 2 | | | |

- Molecule 78 is a protein called Ubiquitin-40S ribosomal protein S31 fusion protein.

| Mol | Chain | Residues | Atoms | | | | | ZeroOcc | AltConf | Trace |
|---|---|---|---|---|---|---|---|---|---|---|
| 78 | h | 70 | Total | C | N | O | S | 0 | 0 | 0 |
| | | | 574 | 362 | 113 | 93 | 6 | | | |
| 78 | DS | 70 | Total | C | N | O | S | 0 | 0 | 0 |
| | | | 574 | 362 | 113 | 93 | 6 | | | |

- Molecule 79 is a protein called Guanine nucleotide-binding protein subunit beta-like protein.

| Mol | Chain | Residues | Atoms | | | | | ZeroOcc | AltConf | Trace |
|---|---|---|---|---|---|---|---|---|---|---|
| 79 | AR | 311 | Total | C | N | O | S | 0 | 0 | 0 |
| | | | 2398 | 1519 | 412 | 462 | 5 | | | |
| 79 | DT | 306 | Total | C | N | O | S | 0 | 0 | 0 |
| | | | 2357 | 1494 | 402 | 456 | 5 | | | |

- Molecule 80 is a protein called 60S acidic ribosomal protein P0.

| Mol | Chain | Residues | Atoms | | | | | ZeroOcc | AltConf | Trace |
|---|---|---|---|---|---|---|---|---|---|---|
| 80 | P0 | 107 | Total 845 | C 542 | N 150 | O 150 | S 3 | 0 | 0 | 0 |
| 80 | p0 | 79 | Total 635 | C 404 | N 114 | O 115 | S 2 | 0 | 0 | 0 |

- Molecule 81 is a protein called 60S ribosomal protein L12-A.

| Mol | Chain | Residues | Atoms | | | | | ZeroOcc | AltConf | Trace |
|---|---|---|---|---|---|---|---|---|---|---|
| 81 | 12 | 63 | Total 480 | C 297 | N 85 | O 96 | S 2 | 0 | 0 | 0 |

- Molecule 82 is a protein called Ribosomal protein.

| Mol | Chain | Residues | Atoms | | | | | ZeroOcc | AltConf | Trace |
|---|---|---|---|---|---|---|---|---|---|---|
| 82 | L1 | 217 | Total 1711 | C 1096 | N 294 | O 312 | S 9 | 0 | 0 | 0 |
| 82 | l1 | 217 | Total 1711 | C 1096 | N 294 | O 312 | S 9 | 0 | 0 | 0 |

- Molecule 83 is MAGNESIUM ION (CCD ID: MG) (formula: Mg).

| Mol | Chain | Residues | Atoms | | ZeroOcc | AltConf |
|---|---|---|---|---|---|---|
| 83 | 1 | 530 | Total 530 | Mg 530 | 0 | 0 |
| 83 | 3 | 14 | Total 14 | Mg 14 | 0 | 0 |
| 83 | 4 | 12 | Total 12 | Mg 12 | 0 | 0 |
| 83 | j | 3 | Total 3 | Mg 3 | 0 | 0 |
| 83 | k | 4 | Total 4 | Mg 4 | 0 | 0 |
| 83 | o | 3 | Total 3 | Mg 3 | 0 | 0 |
| 83 | r | 2 | Total 2 | Mg 2 | 0 | 0 |
| 83 | s | 1 | Total 1 | Mg 1 | 0 | 0 |
| 83 | u | 2 | Total 2 | Mg 2 | 0 | 0 |

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| Mol | Chain | Residues | Atoms | ZeroOcc | AltConf |
|---|---|---|---|---|---|
| 83 | v | 3 | Total Mg<br>3 3 | 0 | 0 |
| 83 | w | 3 | Total Mg<br>3 3 | 0 | 0 |
| 83 | x | 3 | Total Mg<br>3 3 | 0 | 0 |
| 83 | y | 1 | Total Mg<br>1 1 | 0 | 0 |
| 83 | 0 | 5 | Total Mg<br>5 5 | 0 | 0 |
| 83 | 2 | 3 | Total Mg<br>3 3 | 0 | 0 |
| 83 | 5 | 1 | Total Mg<br>1 1 | 0 | 0 |
| 83 | 6 | 3 | Total Mg<br>3 3 | 0 | 0 |
| 83 | 8 | 2 | Total Mg<br>2 2 | 0 | 0 |
| 83 | 9 | 2 | Total Mg<br>2 2 | 0 | 0 |
| 83 | AB | 2 | Total Mg<br>2 2 | 0 | 0 |
| 83 | AC | 1 | Total Mg<br>1 1 | 0 | 0 |
| 83 | AD | 1 | Total Mg<br>1 1 | 0 | 0 |
| 83 | AE | 2 | Total Mg<br>2 2 | 0 | 0 |
| 83 | AF | 1 | Total Mg<br>1 1 | 0 | 0 |
| 83 | AG | 2 | Total Mg<br>2 2 | 0 | 0 |
| 83 | AH | 2 | Total Mg<br>2 2 | 0 | 0 |
| 83 | AJ | 1 | Total Mg<br>1 1 | 0 | 0 |
| 83 | AK | 1 | Total Mg<br>1 1 | 0 | 0 |
| 83 | AM | 1 | Total Mg<br>1 1 | 0 | 0 |
| 83 | AP | 2 | Total Mg<br>2 2 | 0 | 0 |

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| Mol | Chain | Residues | Atoms | ZeroOcc | AltConf |
|---|---|---|---|---|---|
| 83 | B | 152 | Total Mg<br>152 152 | 0 | 0 |
| 83 | D | 1 | Total Mg<br>1 1 | 0 | 0 |
| 83 | G | 2 | Total Mg<br>2 2 | 0 | 0 |
| 83 | I | 2 | Total Mg<br>2 2 | 0 | 0 |
| 83 | J | 1 | Total Mg<br>1 1 | 0 | 0 |
| 83 | K | 1 | Total Mg<br>1 1 | 0 | 0 |
| 83 | L | 1 | Total Mg<br>1 1 | 0 | 0 |
| 83 | Q | 1 | Total Mg<br>1 1 | 0 | 0 |
| 83 | R | 1 | Total Mg<br>1 1 | 0 | 0 |
| 83 | V | 1 | Total Mg<br>1 1 | 0 | 0 |
| 83 | Y | 3 | Total Mg<br>3 3 | 0 | 0 |
| 83 | Z | 2 | Total Mg<br>2 2 | 0 | 0 |
| 83 | a | 1 | Total Mg<br>1 1 | 0 | 0 |
| 83 | f | 1 | Total Mg<br>1 1 | 0 | 0 |
| 83 | AR | 1 | Total Mg<br>1 1 | 0 | 0 |
| 83 | AS | 278 | Total Mg<br>278 278 | 0 | 0 |
| 83 | AT | 9 | Total Mg<br>9 9 | 0 | 0 |
| 83 | AU | 2 | Total Mg<br>2 2 | 0 | 0 |
| 83 | AW | 4 | Total Mg<br>4 4 | 0 | 0 |
| 83 | BB | 2 | Total Mg<br>2 2 | 0 | 0 |
| 83 | BE | 2 | Total Mg<br>2 2 | 0 | 0 |

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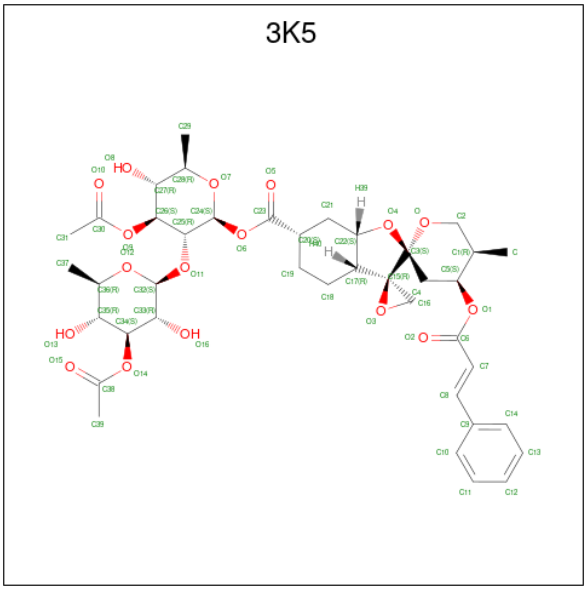
| Mol | Chain | Residues | Atoms | ZeroOcc | AltConf |
|---|---|---|---|---|---|
| 83 | BF | 1 | Total Mg<br>1 1 | 0 | 0 |
| 83 | BH | 1 | Total Mg<br>1 1 | 0 | 0 |
| 83 | BJ | 3 | Total Mg<br>3 3 | 0 | 0 |
| 83 | BK | 1 | Total Mg<br>1 1 | 0 | 0 |
| 83 | BN | 1 | Total Mg<br>1 1 | 0 | 0 |
| 83 | BQ | 1 | Total Mg<br>1 1 | 0 | 0 |
| 83 | BV | 1 | Total Mg<br>1 1 | 0 | 0 |
| 83 | BZ | 2 | Total Mg<br>2 2 | 0 | 0 |
| 83 | CA | 1 | Total Mg<br>1 1 | 0 | 0 |
| 83 | CJ | 1 | Total Mg<br>1 1 | 0 | 0 |
| 83 | CK | 1 | Total Mg<br>1 1 | 0 | 0 |
| 83 | CL | 3 | Total Mg<br>3 3 | 0 | 0 |
| 83 | CM | 102 | Total Mg<br>102 102 | 0 | 0 |
| 83 | CO | 1 | Total Mg<br>1 1 | 0 | 0 |
| 83 | CP | 1 | Total Mg<br>1 1 | 0 | 0 |
| 83 | CQ | 1 | Total Mg<br>1 1 | 0 | 0 |
| 83 | DA | 1 | Total Mg<br>1 1 | 0 | 0 |
| 83 | DB | 3 | Total Mg<br>3 3 | 0 | 0 |
| 83 | DG | 2 | Total Mg<br>2 2 | 0 | 0 |
| 83 | DQ | 1 | Total Mg<br>1 1 | 0 | 0 |

- Molecule 84 is 3-O-acetyl-2-O-(3-O-acetyl-6-deoxy-beta-D-glucopyranosyl)-6-deoxy-1-O-{[(2R,2'S,3a'R,4''S,5''R,6'S,7a'S)-5''-methyl-4''-{[(2E)-3-phenylprop-2-enoyl]oxy}decahydrodispiro[oxirane-2,3'-[1]benzofuran-2',2''-pyran]-6'-yl]carbonyl}-beta-D-glucopyranose (CCD ID:

3K5) (formula: $C_{40}H_{52}O_{17}$).




| Mol | Chain | Residues | Atoms | ZeroOcc | AltConf |
|---|---|---|---|---|---|
| 84 | 1 | 1 | Total C O<br>57 40 17 | 0 | 0 |
| 84 | AS | 1 | Total C O<br>57 40 17 | 0 | 0 |

- Molecule 85 is ZINC ION (CCD ID: ZN) (formula: Zn).

| Mol | Chain | Residues | Atoms | ZeroOcc | AltConf |
|---|---|---|---|---|---|
| 85 | AH | 1 | Total Zn<br>1 1 | 0 | 0 |
| 85 | AK | 1 | Total Zn<br>1 1 | 0 | 0 |
| 85 | AN | 1 | Total Zn<br>1 1 | 0 | 0 |
| 85 | AP | 1 | Total Zn<br>1 1 | 0 | 0 |
| 85 | AQ | 1 | Total Zn<br>1 1 | 0 | 0 |
| 85 | c | 1 | Total Zn<br>1 1 | 0 | 0 |
| 85 | d | 1 | Total Zn<br>1 1 | 0 | 0 |
| 85 | f | 1 | Total Zn<br>1 1 | 0 | 0 |
| 85 | h | 1 | Total Zn<br>1 1 | 0 | 0 |

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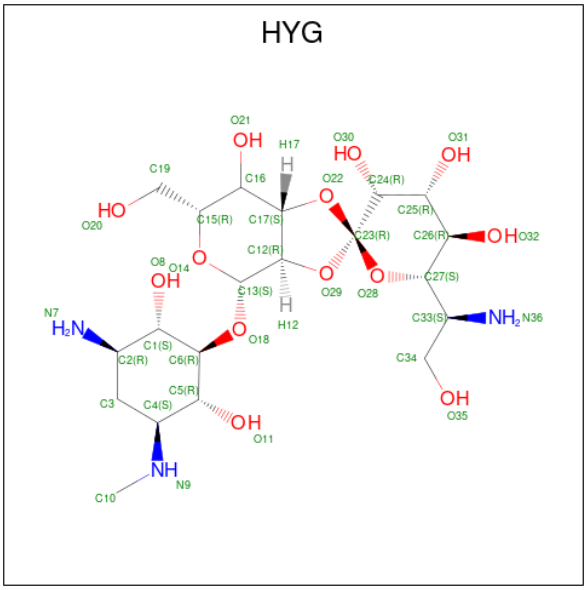
| Mol | Chain | Residues | Atoms | ZeroOcc | AltConf |
|---|---|---|---|---|---|
| 85 | CB | 1 | Total Zn<br>1 1 | 0 | 0 |
| 85 | CE | 1 | Total Zn<br>1 1 | 0 | 0 |
| 85 | CH | 1 | Total Zn<br>1 1 | 0 | 0 |
| 85 | CJ | 1 | Total Zn<br>1 1 | 0 | 0 |
| 85 | CK | 1 | Total Zn<br>1 1 | 0 | 0 |
| 85 | DN | 1 | Total Zn<br>1 1 | 0 | 0 |
| 85 | DQ | 1 | Total Zn<br>1 1 | 0 | 0 |
| 85 | DS | 1 | Total Zn<br>1 1 | 0 | 0 |

- Molecule 86 is HYGROMYCIN B (CCD ID: HYG) (formula: $C_{20}H_{37}N_3O_{13}$) (labeled as "Ligand of Interest" by depositor).




| Mol | Chain | Residues | Atoms | ZeroOcc | AltConf |
|---|---|---|---|---|---|
| 86 | B | 1 | Total C N O<br>36 20 3 13 | 0 | 0 |
| 86 | CM | 1 | Total C N O<br>36 20 3 13 | 0 | 0 |

- Molecule 87 is water.

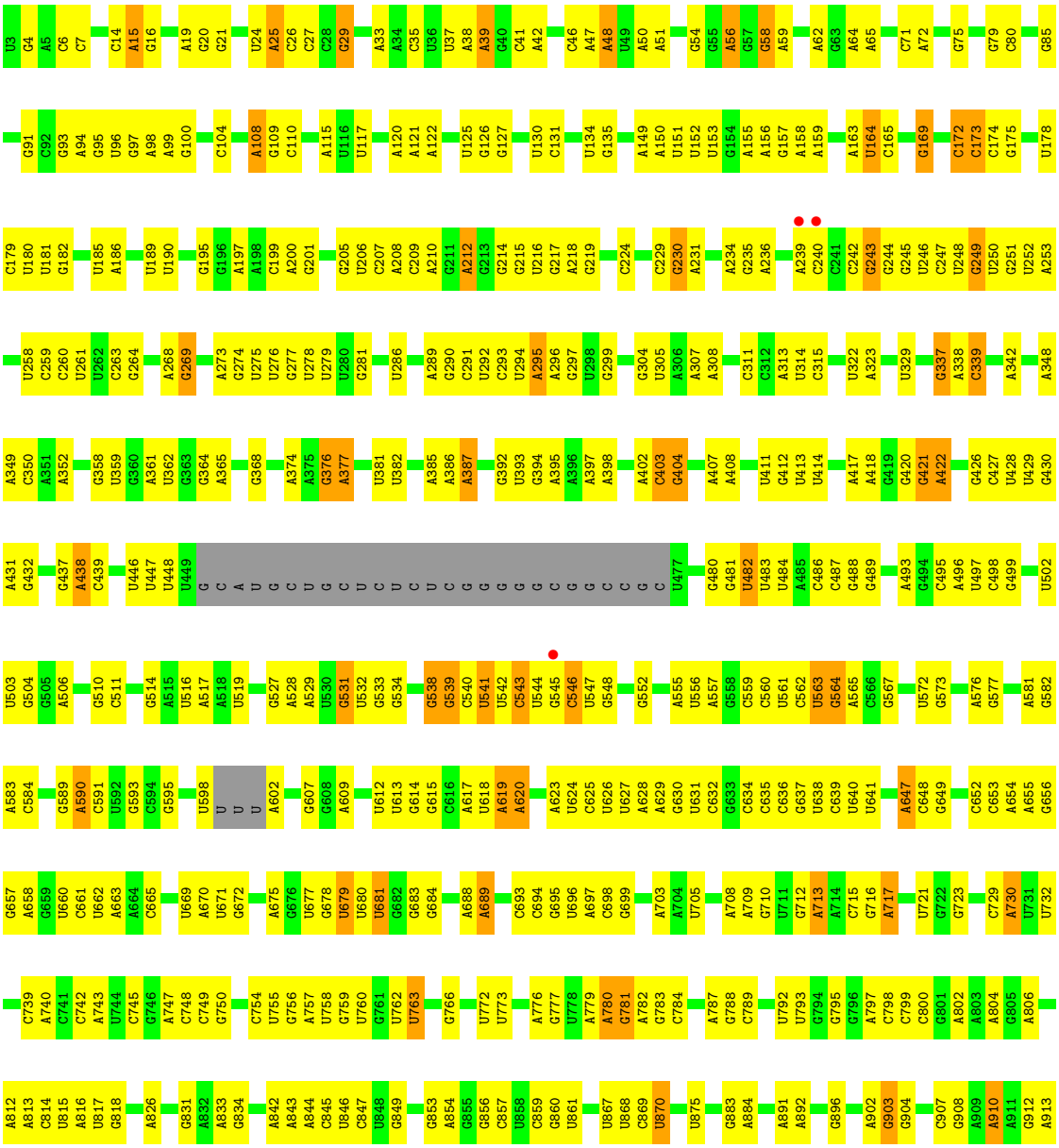
| Mol | Chain | Residues | Atoms | ZeroOcc | AltConf |
|---|---|---|---|---|---|
| 87 | 1 | 9 | Total O<br>9 9 | 0 | 0 |
| 87 | 4 | 3 | Total O<br>3 3 | 0 | 0 |
| 87 | B | 6 | Total O<br>6 6 | 0 | 0 |
| 87 | AS | 12 | Total O<br>12 12 | 0 | 0 |

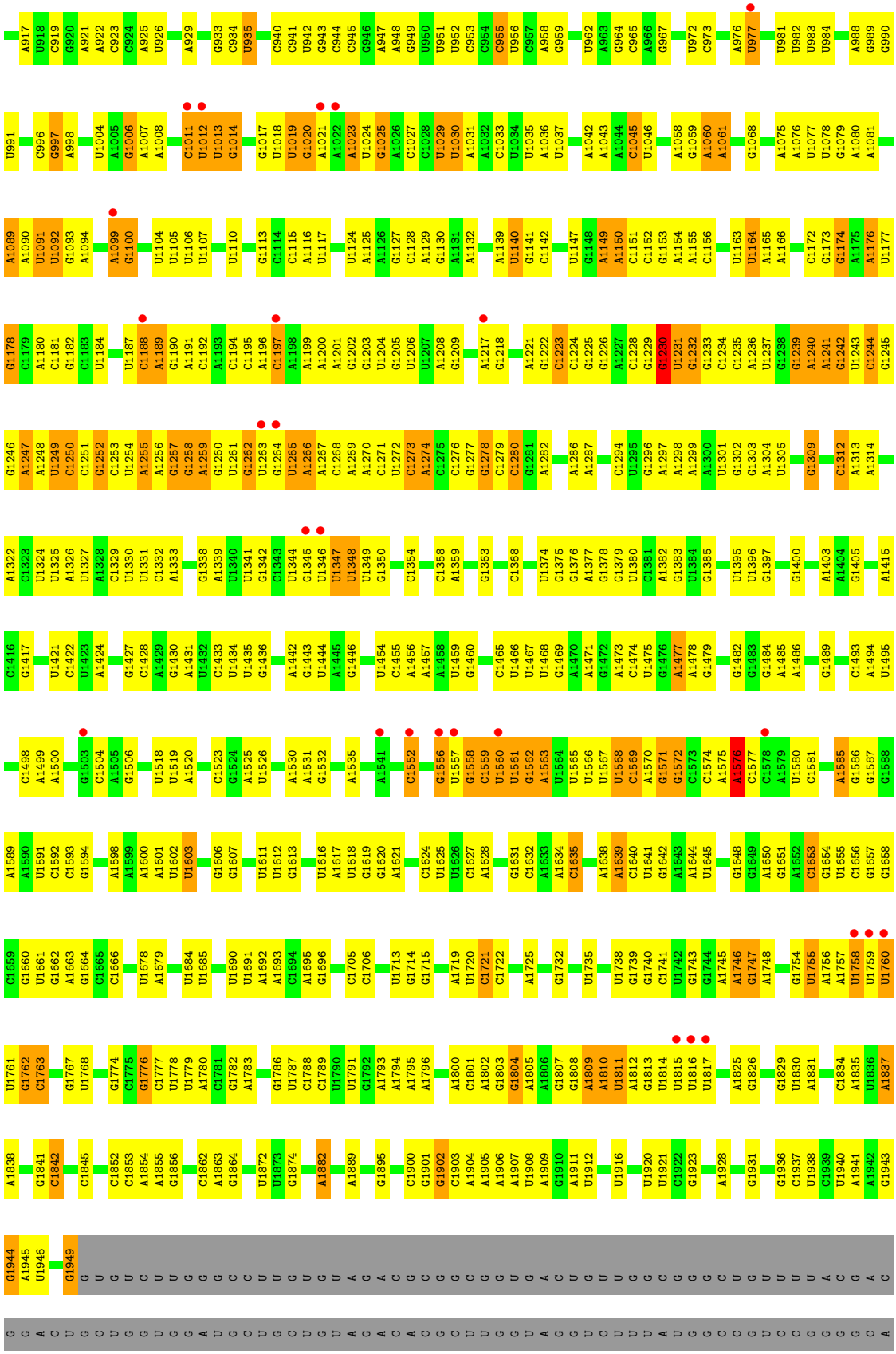
# 3 Residue-property plots (i)

These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron 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 dot above a residue indicates a poor fit to the electron density (RSRZ > 2). Stretches of 2 or more consecutive residues without any outlier are shown as a green connector. Residues present in the sample, but not in the model, are shown in grey.

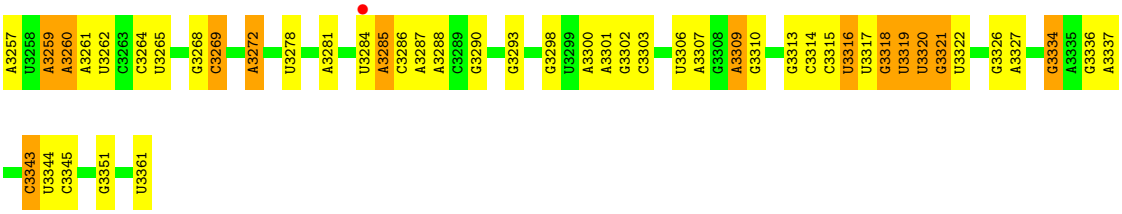
- Molecule 1: 25S

Chain 1:



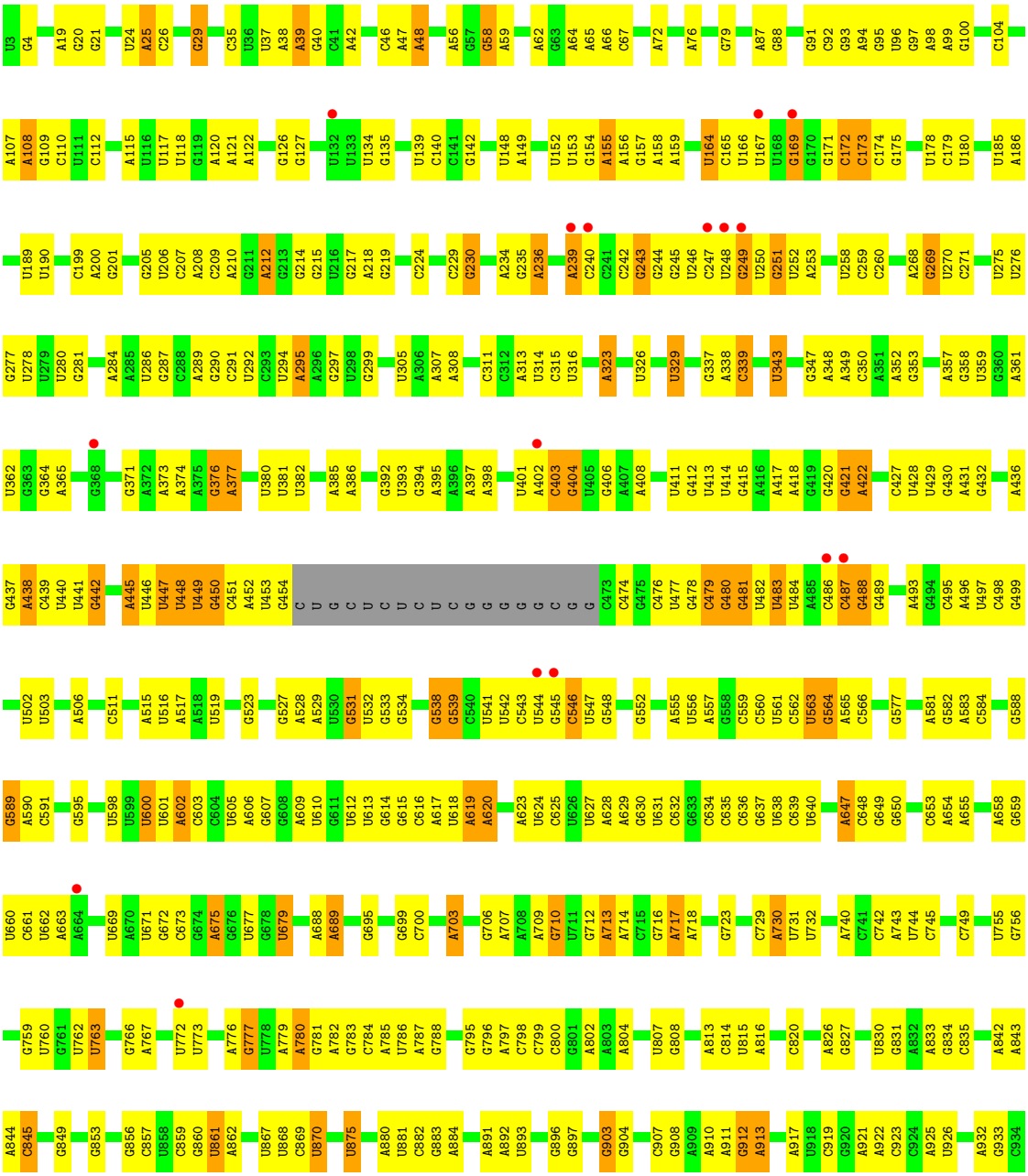


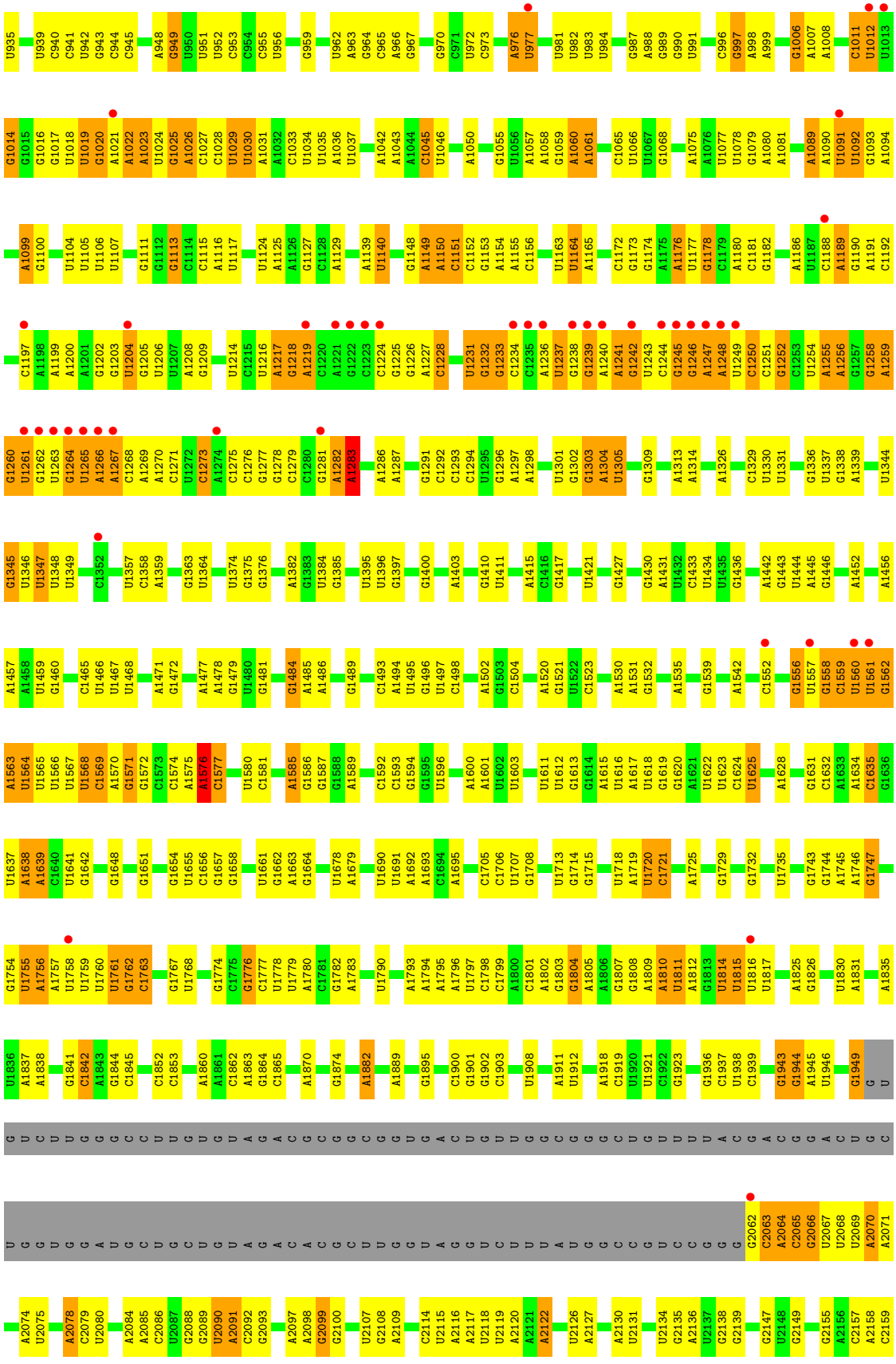
C G U2067 U2068 U2069 A2070 A2071 C2072 A2077 A2078 C2079 U2080 A2084 A2085 C2086 U2087 G2088 G2089 U2090 A2091 C2092 G2093 A2098 G2099 G2100 U2107 G2108 A2109 C2110 U2111 U2115 A2116 A2117 U2118 U2119 A2122 A2125 U2126 A2127 G2128 C2129 A2130 U2131 A2136 U2137 G2138 G2139 G2147 U2148 G2149
G2155 A2156 C2157 A2158 C2159 G2163 U2164 U2167 U2171 G2172 C2173 C2174 C2175 A2176 G2177 C2182 U2183 G2184 A2185 A2186 U2187 G2188 A2191 A2192 U2195 G2196 A2197 A2198 G2199 A2200 A2201 A2202 C2205 A2206 A2207 A2210 A2211 G2216 A2220 A2221 A2222 C2223 G2227 U2232 A2233 A2234 C2235 U2236
A2237 U2238 G2239 A2240 C2241 U2242 C2243 U2244 C2245 G2250 G2251 A2259 U2260 U2270 U2276 G2285 C2286 A2287 U2288 G2289 A2290 A2291 U2292 G2293 U2296 U2297 C2308 C2309 U2312 G2313 U2314 U2322 A2323 C2324 U2325 A2326 A2330 G2331 A2334 A2335 A2336 A2339 C2340 A2341 G2342 C2343 C2344 A2345
A2346 G2347 G2348 A2351 C2352 G2353 G2354 G2355 C2361 A2362 G2363 U2366 C2367 A2368 G2369 C2370 G2371 G2372 G2373 G2374 A2375 A2380 G2381 A2382 C2383 C2384 C2385 U2386 U2389 G2390 A2391 G2392 C2393 U2394 U2395 G2396 A2397 C2398 U2399 C2400 U2401 A2402 G2403 U2404 U2405 U2406 G2407 A2408 C2409 A2410 U2411 U2412 G2413 A2418
A2419 G2420 A2421 C2422 A2423 G2426 A2427 G2428 G2429 G2430 U2431 G2432 U2433 A2434 G2435 A2436 A2437 U2438 A2439 A2440 G2441 U2442 G2443 G2444 G2445 A2446 G2447 C2448 U2449 U2450 C2451 G2452 G C G2455 C2456 C2457 G2458 G2459 U2460 A2464 U A C2467 C2468 A2469 C2470 U2471 A2472 C2473 C2474 U2475 C2476 U2477 A2478 U2479 A2480 G2481
U2482 U2483 U2484 U2485 A2489 U2492 A2493 A2497 A2498 U2499 A2502 G2503 G2511 G2512 A2513 G2514 G2515 U2516 C2517 A2518 A2519 A2520 C2521 A2525 C2526 G2527 U2528 U2529 C2530 G2533 U2536 U2537 A2538 C2545 U2546 G2547 G2551 A2552 U2553 C2554 G2557 G2558 A2565 C2566 G2578 G2579
U2583 U2584 U2585 G2586 G2587 C2588 U2589 G2590 A2598 U2601 A2608 A2609 C2610 G2611 A2614 A2615 C2618 G2621 U2622 G2623 U2624 C2625 C2626 U2627 A2628 A2629 G2630 G2631 G2632 G2633 G2634 A2635 C2636 U2637 C2638 G2641 G2642 A2643 G2644 A2645 A2646 G2649 A2650 A2651 U2655 C2656 C2657 A2658 G2659 U2660 A2661
G2662 A2663 A2664 C2665 A2666 A2667 A2668 A2669 G2670 A2676 A2677 G2678 U2679 C2680 C2681 C2682 G2686 A2687 U2690 U2691 U2694 A2699 G2700 U2701 C2709 C2713 G2717 A2718 A2719 A2720 G2721 U2724 G2725 U2729 G2733 A2734 U2735 C2736 C2737 U2738 U2739 U2740 A2741 G2742 U2743 C2744 C2745 G2749
G2750 U2753 U2754 C2766 U2767 G2768 A2771 G2772 A2773 A2774 C2782 A2785 G2786 A2789 U2790 A2791 G2796 C2797 G2802 U2807 C2808 C2812 G2813 U2814 U2815 C2816 A2817 G2820 C2824 A2825 U2826 U2827 G2828 C2829 U2830 U2831 U2832 U2833 A2836 C2839 U2840 G2843 A2844 U2847
G2850 C2851 U2852 C2853 U2854 U2855 C2856 C2857 U2858 A2859 U2860 C2861 C2866 G2867 A2868 A2869 G2870 C2871 A2872 G2873 A2874 A2875 U2876 U2877 G2886 U2887 U2888 U2895 U2896 C2899 C2900 C2901 A2902 C2903 U2907 A2908 G2909 G2910 G2911 A2912 A2913 C2914 G2915 U2916 G2919 C2920 U2921 G2922 G2923 G2924 U2925 U2926
C2932 G2933 U2934 C2935 G2936 U2937 G2938 A2939 G2940 A2941 C2942 A2943 U2946 U2947 A2954 C2955 C2956 C2957 U2958 A2959 C2960 U2961 G2962 G2969 A2972 U2973 C2974 A2978 U2979 A2980 G2981 A2984 U2985 U2986 G2987 A2988 A2989 U2992 U2995 A2996 A3005 C3006 U3010 U3013 U3014 C3015 A3016 G3017 A3018
U3019 A3020 A3021 U3022 U3023 G3024 G3025 U3026 U3027 U3028 G3031 C3035 U3036 G3037 U3038 C3039 A3042 U3043 C3044 A3045 G3046 G3047 A3050 C3051 G3052 C3056 G3057 A3058 A3059 G3060 C3061 U3062 A3063 C3064 C3065 A3066 U3067 C3068 G3073 U3077 A3078 C3082 U3083 G3084 A3085 A3086 C3089 C3090 U3091 C3092 U3093
A3094 A3101 A3102 U3103 C3104 C3105 G3108 C3109 U3110 A3111 G3112 A3113 A3114 C3115 U3124 U3125 U3126 U3127 G3128 U3132 G3133 C3134 A3135 C3136 A3137 U3138 U3139 G3143 A3144 U3145 G3146 G3147 A3148 U3149 A3150 C3151 G3152 A3153 A3154 A3157 G3158 A3159 C3160 U3161 U3162 U3163 U3164 U3165 A3166 G3167 C3171 U3172
C3176 C3177 A3178 U3179 C3182 A3183 G3184 G3185 C3190 A3191 A3192 C3193 G3194 G3195 U3196 G3197 C3198 G3199 G3207 A3208 A3209 A3210 G3211 G3212 C3213 U3214 U3215 U3216 G3217 U3218 G3219 C3220 G3221 U3224 G3225 G3228 G3229 U3234 A3235 A3238 A3239 U3240 G3241 A3244 A3245 C3246 C3252 G3253 G3254 G3255 G3256



• Molecule 1: 25S

Chain AS:

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G1014 G1015 G1016 G1017 U1018 U1019 G1020 A1021 A1022 A1023 U1024 G1025 A1026 C1027 C1028 U1029 U1030 A1031 A1032 C1033 U1034 U1035 A1036 U1037 A1042 A1043 A1044 C1045 U1046 A1050 G1055 U1056 A1057 A1058 G1059 A1060 A1061 C1065 U1066 U1067 G1068 A1075 A1076 U1077 U1078 G1079 A1080 A1081 A1089 A1090 U1091 U1092 G1093 A1094
A1099 G1100 U1104 U1105 U1106 U1107 G1111 G1112 G1113 C1114 C1115 A1116 U1117 U1124 A1125 A1126 G1127 C1128 A1129 A1139 U1140 G1148 A1149 A1150 C1151 C1152 G1153 A1154 A1155 C1156 U1163 U1164 A1165 C1172 G1173 G1174 A1175 A1176 U1177 G1178 C1179 A1180 C1181 G1182 A1186 U1187 C1188 A1189 G1190 A1191 C1192
C1197 A1198 A1199 A1200 A1201 G1202 G1203 U1204 G1205 U1206 U1207 A1208 G1209 U1214 C1215 U1216 A1217 G1218 A1219 C1220 A1221 G1222 C1223 C1224 G1225 G1226 A1227 C1228 U1231 G1232 G1233 C1234 C1235 A1236 U1237 G1238 G1239 A1240 A1241 G1242 U1243 C1244 G1245 G1246 A1247 A1248 U1249 C1250 C1251 G1252 C1253 U1254 A1255 A1256 G1257 G1258 A1259
G1260 U1261 G1262 U1263 G1264 U1265 A1266 A1267 C1268 A1269 A1270 C1271 U1272 C1273 A1274 C1275 C1276 G1277 G1278 C1279 C1280 G1281 A1282 A1283 A1286 A1287 G1291 C1292 C1293 C1294 U1295 G1296 A1297 A1298 U1301 G1302 G1303 A1304 U1305 G1309 A1313 A1314 A1326 C1329 U1330 U1331 G1336 U1337 G1338 A1339 U1344
G1345 U1346 U1347 U1348 U1349 C1352 U1357 C1358 A1359 G1363 U1364 U1374 G1375 G1376 A1382 G1383 U1384 G1385 U1395 U1396 G1397 G1400 A1403 G1410 U1411 A1415 C1416 G1417 U1421 G1427 G1430 A1431 U1432 C1433 U1434 U1435 G1436 A1442 G1443 U1444 A1445 G1446 A1452 A1456
A1457 A1458 U1459 G1460 C1465 U1466 U1467 U1468 A1471 G1472 A1477 A1478 G1479 U1480 G1481 G1484 A1485 A1486 G1489 C1493 A1494 U1495 G1496 U1497 C1498 A1502 G1503 C1504 A1520 G1521 U1522 C1523 A1530 A1531 G1532 A1535 G1539 A1542 C1552 G1556 U1557 G1558 C1559 U1560 U1561 G1562
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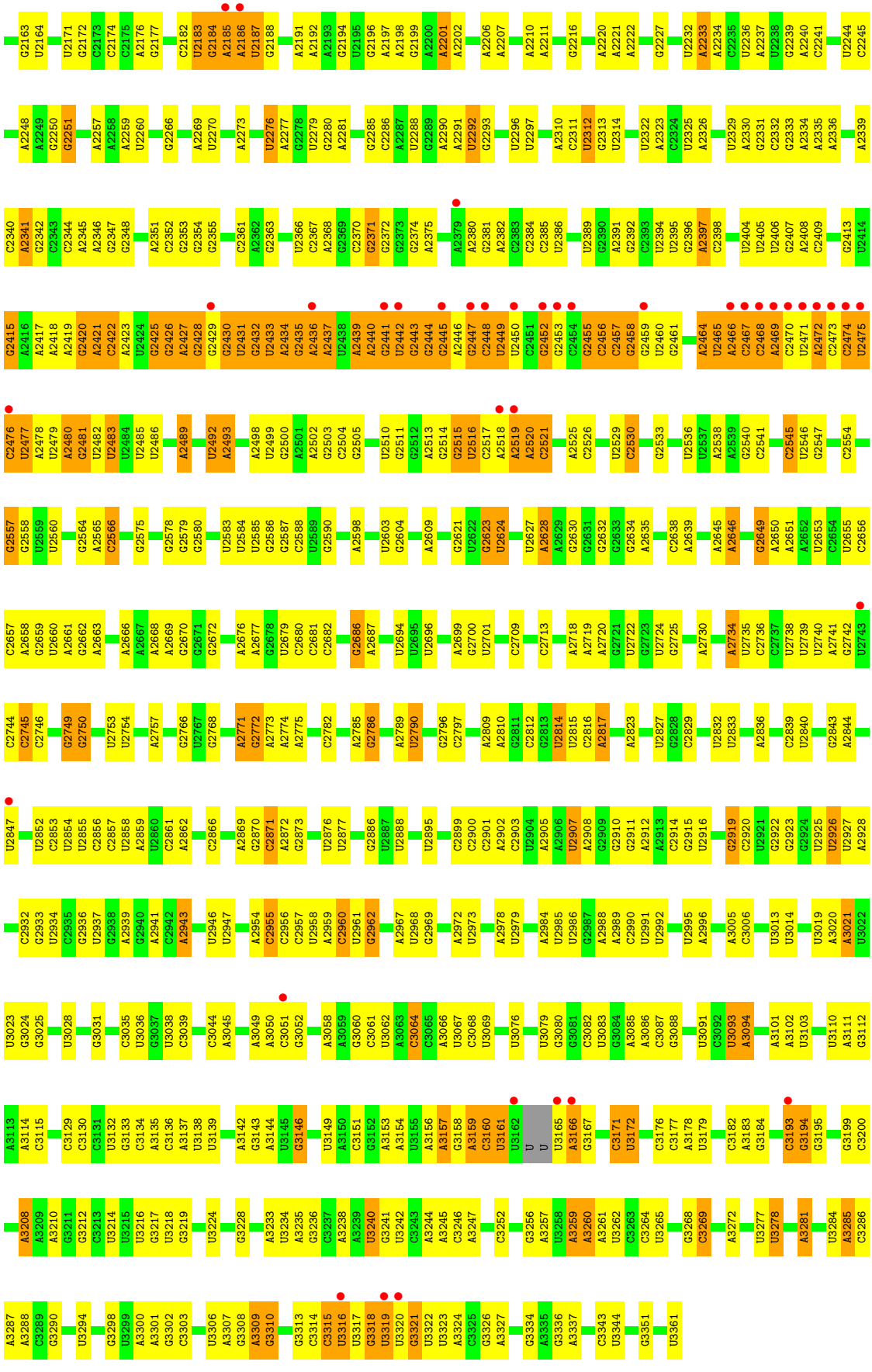

• Molecule 2: 5S

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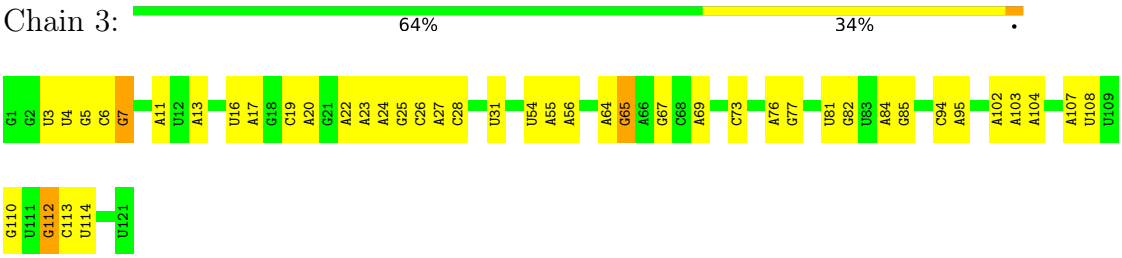


• Molecule 2: 5S

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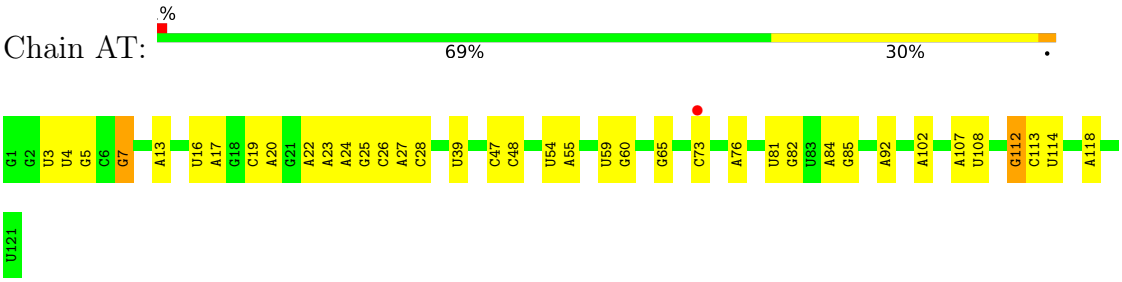
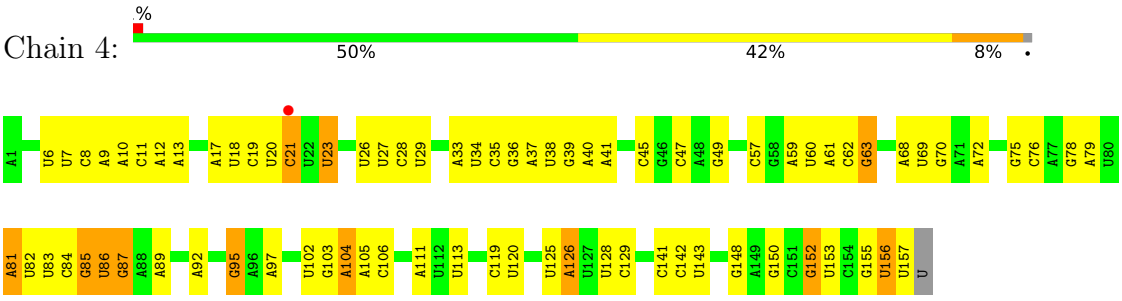



• Molecule 3: 5.8S

Chain 4:




• Molecule 3: 5.8S

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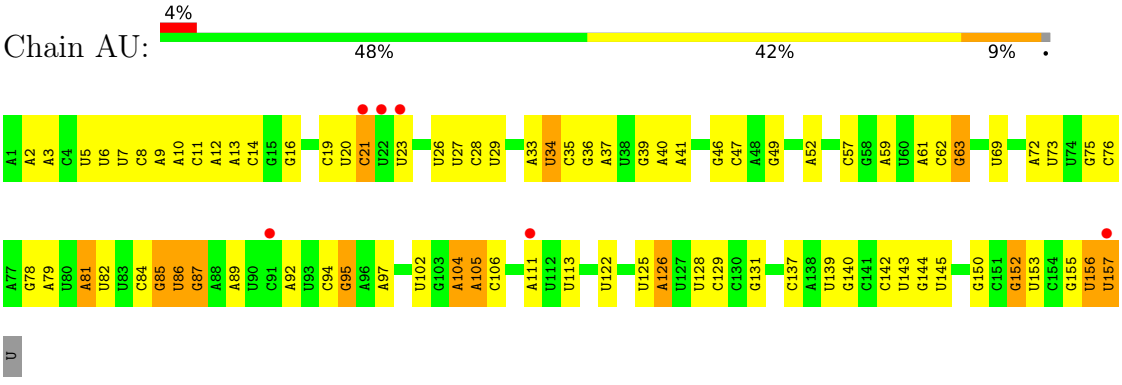
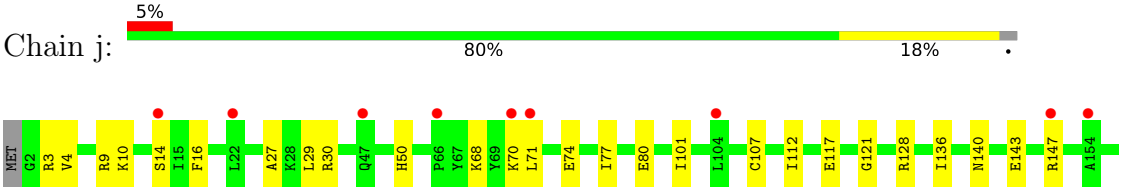
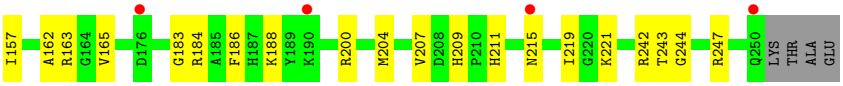



• Molecule 4: 60S ribosomal protein L2-B

Chain j:






• Molecule 4: 60S ribosomal protein L2-B

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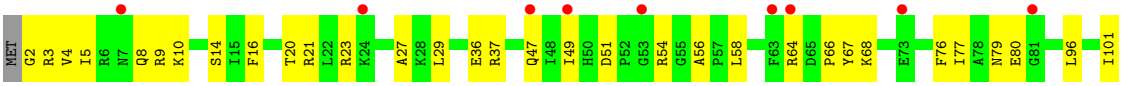
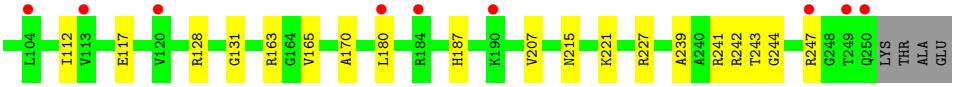
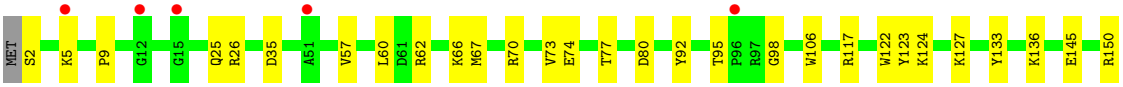
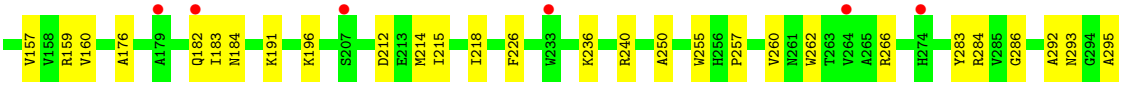


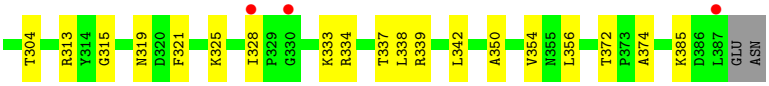




• Molecule 5: 60S ribosomal protein L3

Chain k:

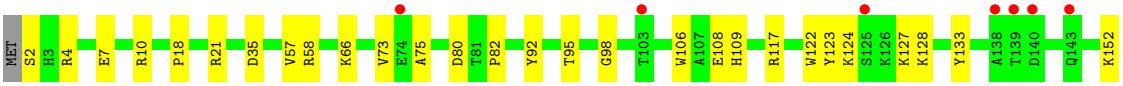


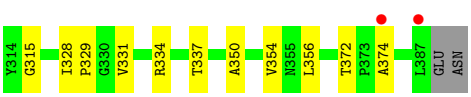




• Molecule 5: 60S ribosomal protein L3

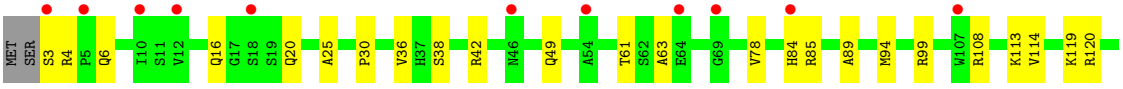
Chain AX:

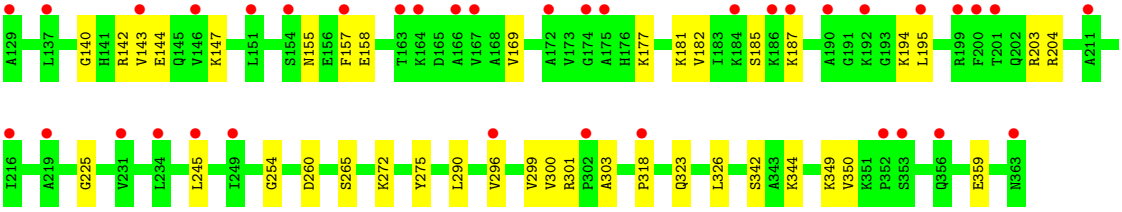




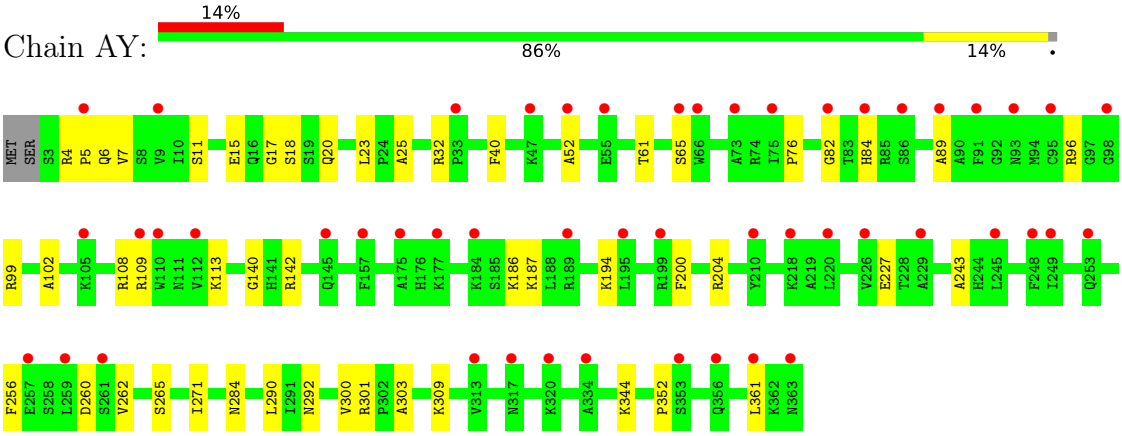

• Molecule 6: 60S ribosomal protein L4-B

Chain l:

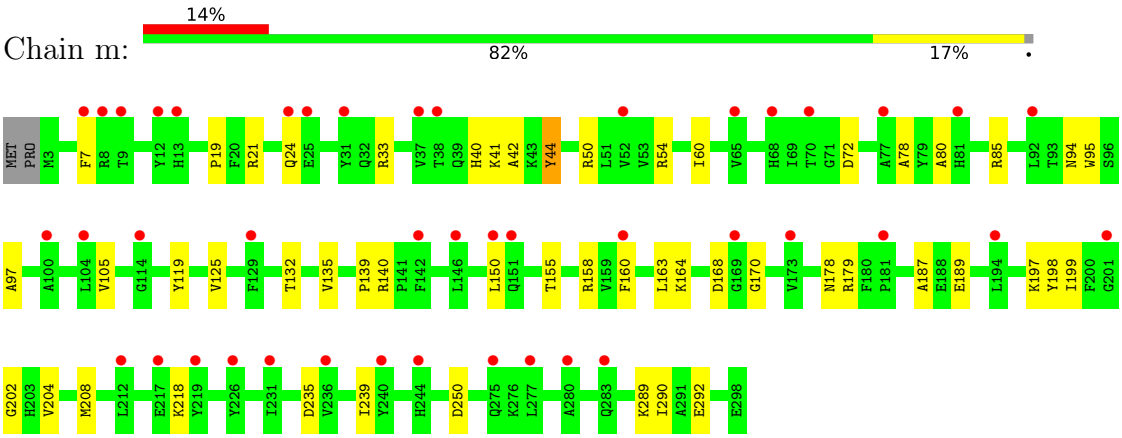




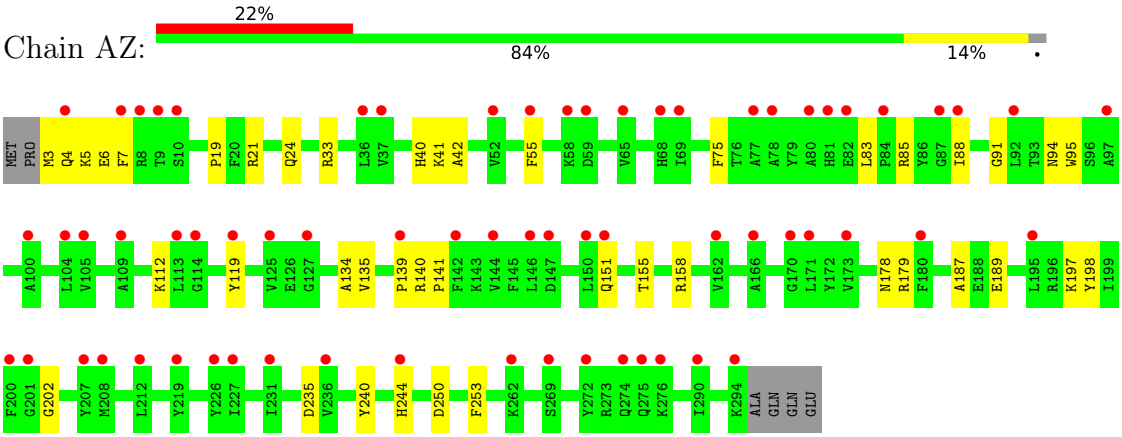

• Molecule 6: 60S ribosomal protein L4-B




• Molecule 7: Uncharacterized protein CaJ7.0206

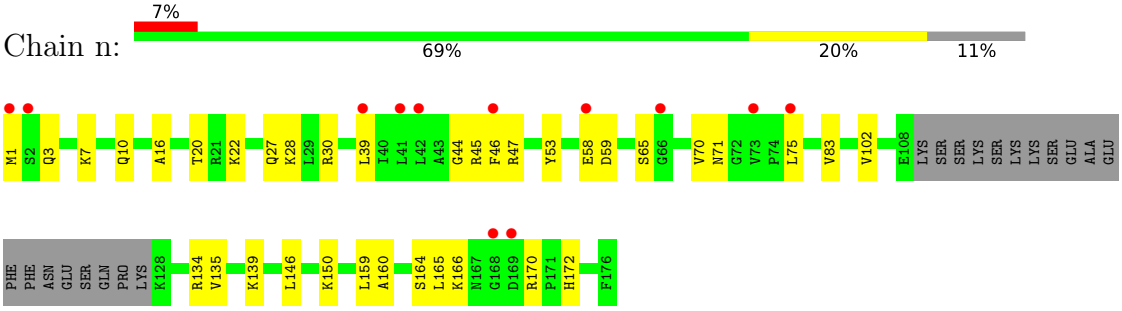



• Molecule 7: Uncharacterized protein CaJ7.0206



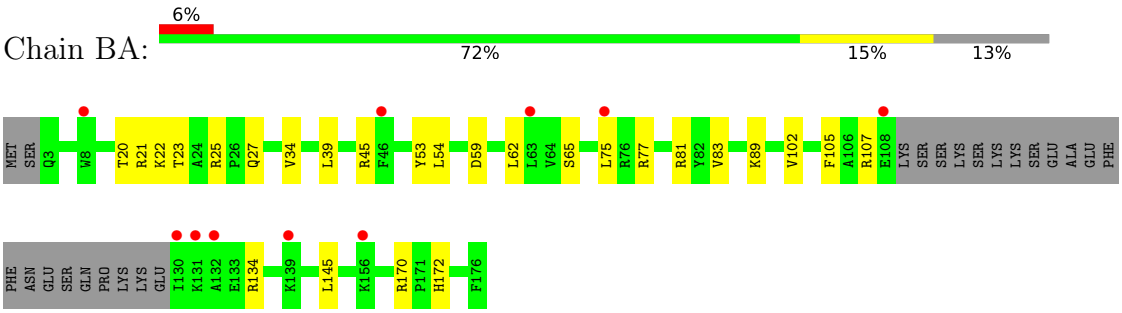
• Molecule 8: 60S ribosomal protein L6

Chain n:



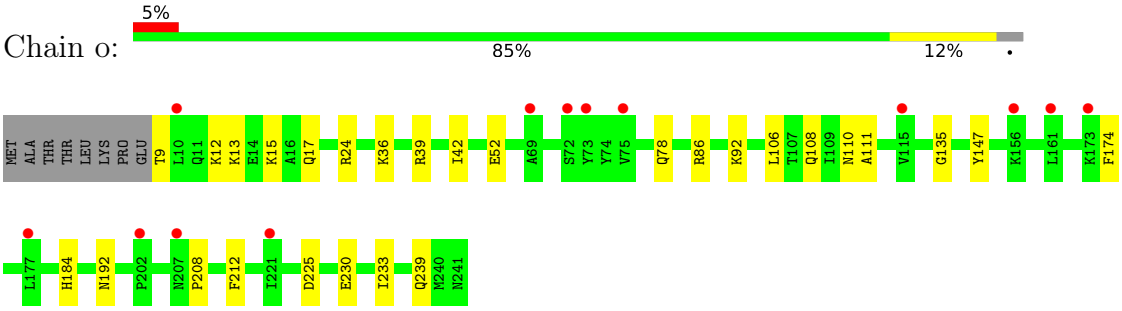

• Molecule 8: 60S ribosomal protein L6

Chain BA:



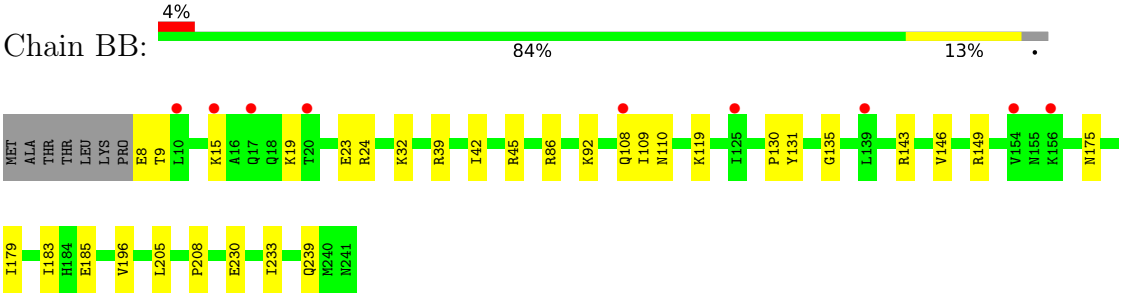

• Molecule 9: 60S ribosomal protein L7-A

Chain o:



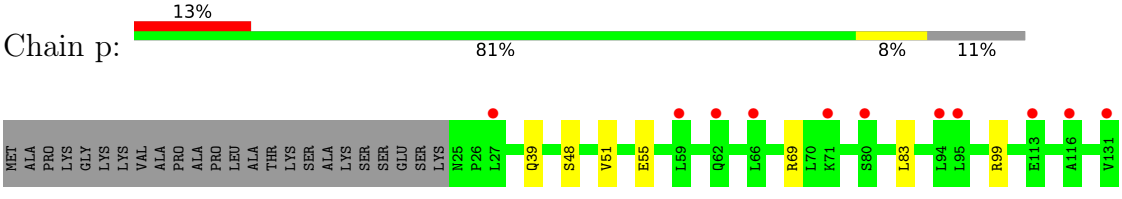

• Molecule 9: 60S ribosomal protein L7-A

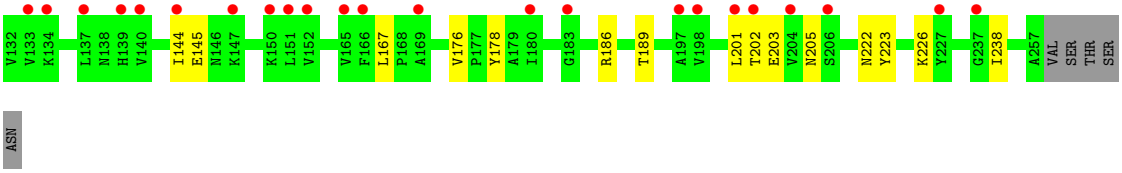
Chain BB:



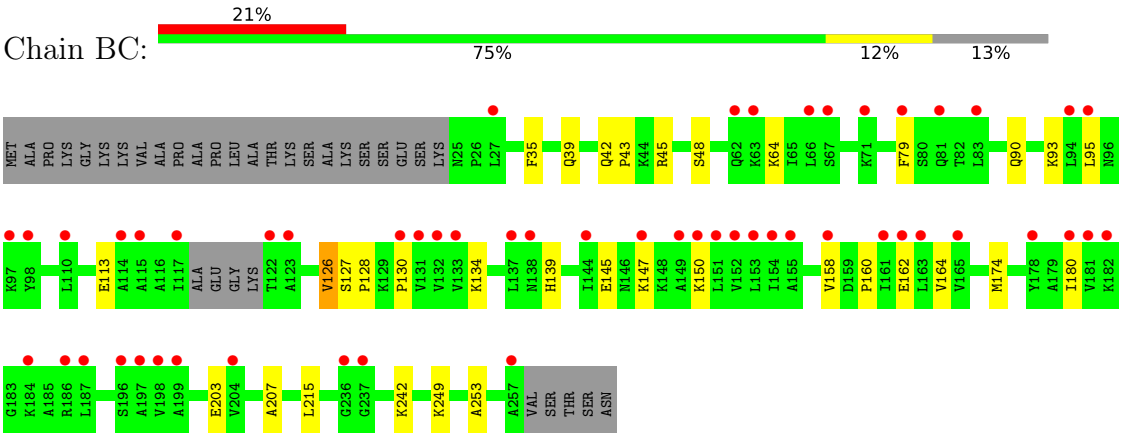

• Molecule 10: 60S ribosomal protein L8

Chain p:

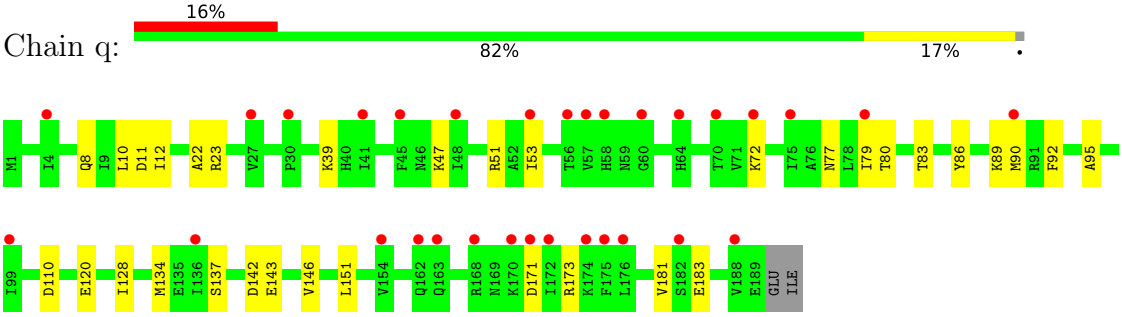




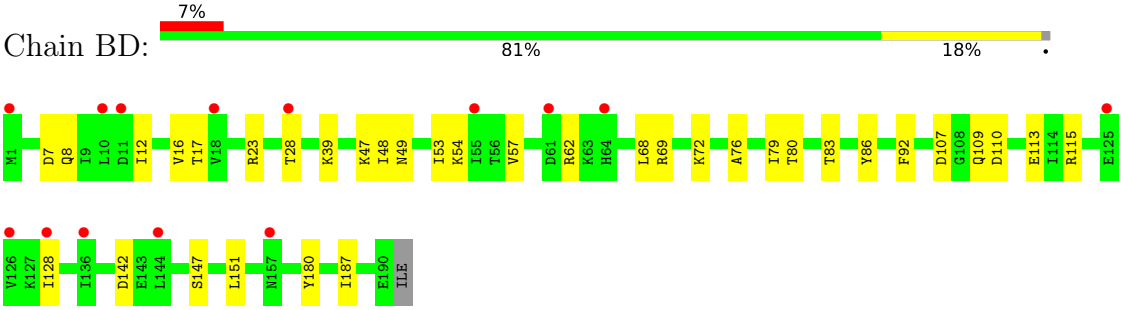

• Molecule 10: 60S ribosomal protein L8



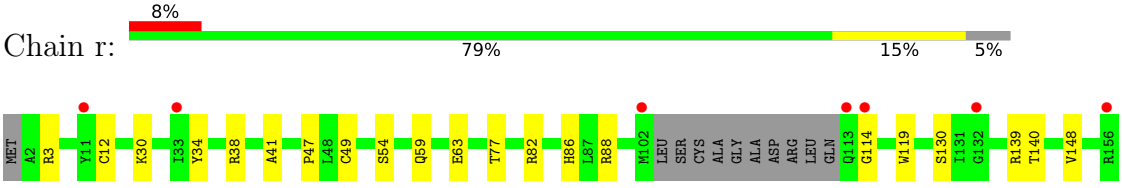

• Molecule 11: 60S ribosomal protein L9-B

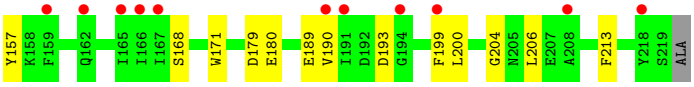



• Molecule 11: 60S ribosomal protein L9-B



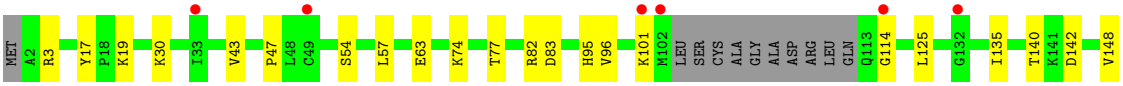

• Molecule 12: 60S ribosomal protein L10

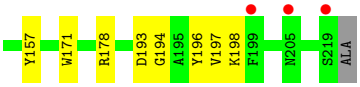





• Molecule 12: 60S ribosomal protein L10

Chain BE:




• Molecule 13: 60S ribosomal protein L11-B

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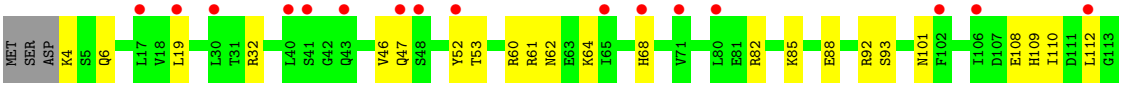


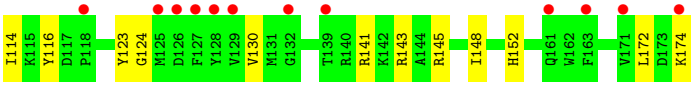


• Molecule 13: 60S ribosomal protein L11-B

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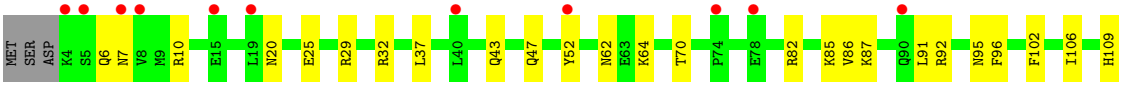


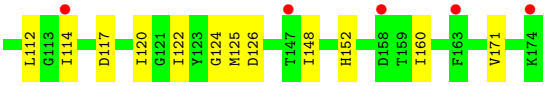


• Molecule 14: 60S ribosomal protein L13

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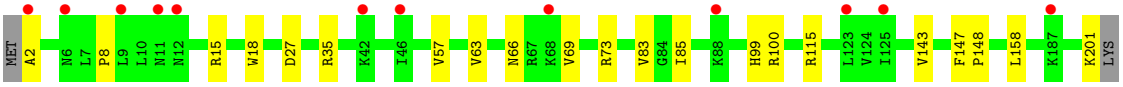


• Molecule 14: 60S ribosomal protein L13

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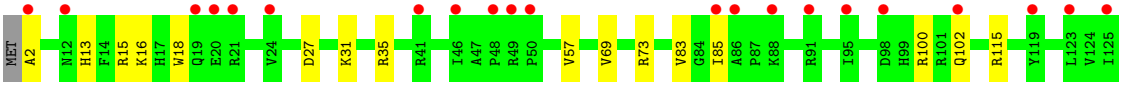
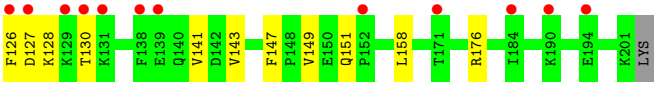
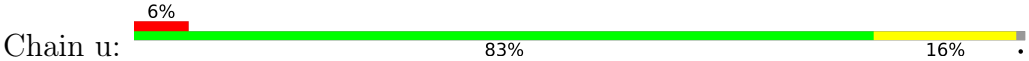
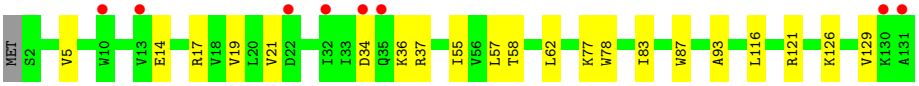


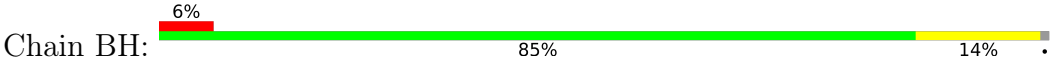


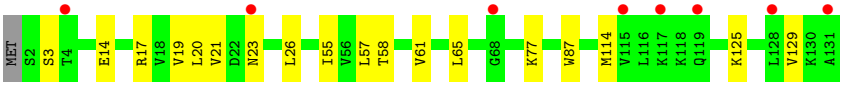

• Molecule 15: 60S ribosomal protein L14-B



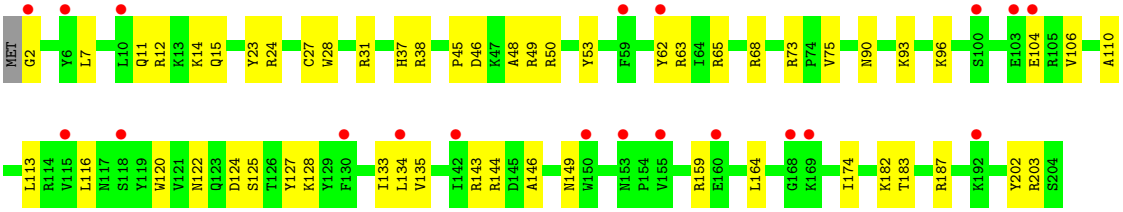




• Molecule 15: 60S ribosomal protein L14-B

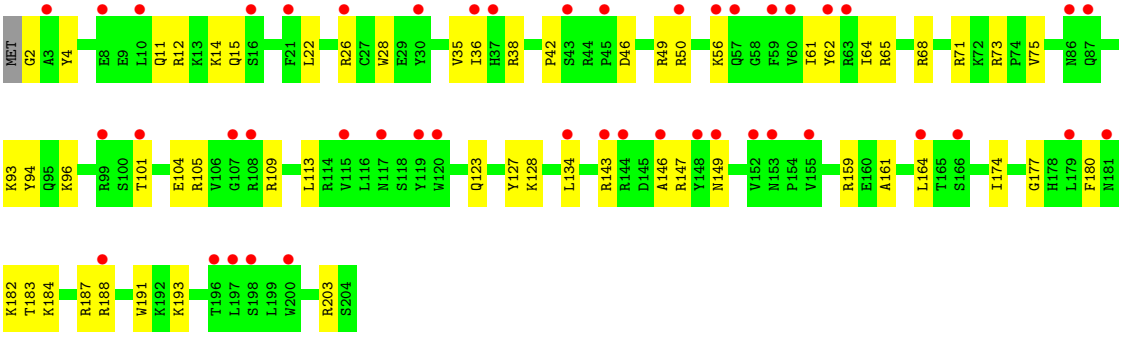


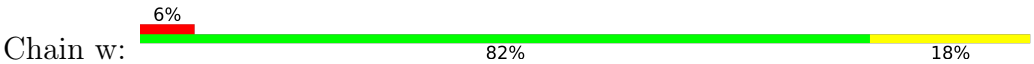

• Molecule 16: 60S ribosomal protein L15-A

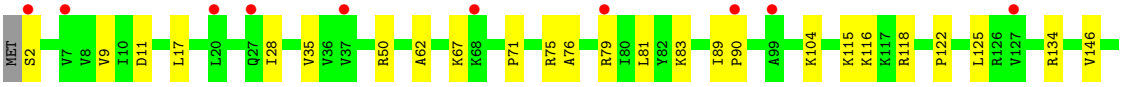


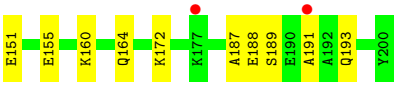

• Molecule 16: 60S ribosomal protein L15-A




• Molecule 17: Ribosomal protein L13

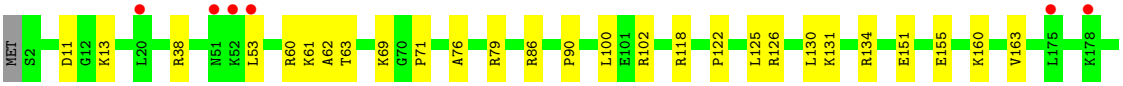




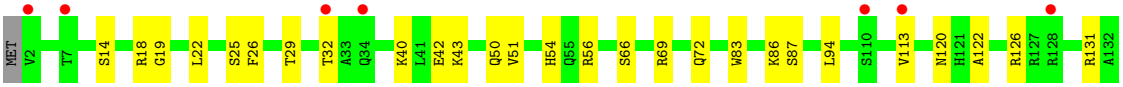

• Molecule 17: Ribosomal protein L13

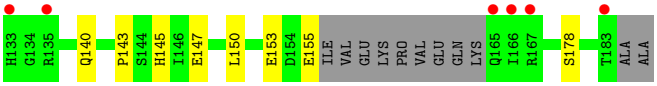
Chain BJ:



• Molecule 18: Ribosomal protein L22

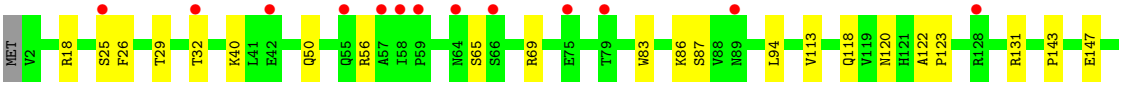
Chain x:

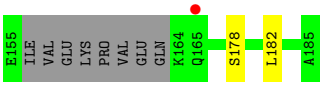



• Molecule 18: Ribosomal protein L22

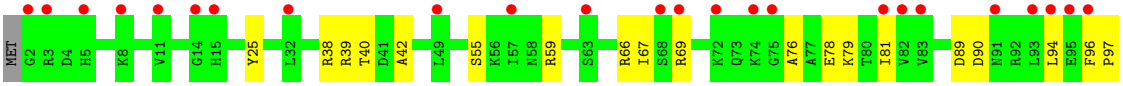
Chain BK:

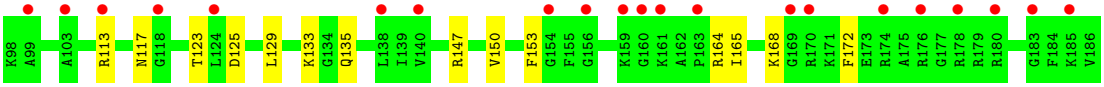



• Molecule 19: 60S ribosomal protein L18-A

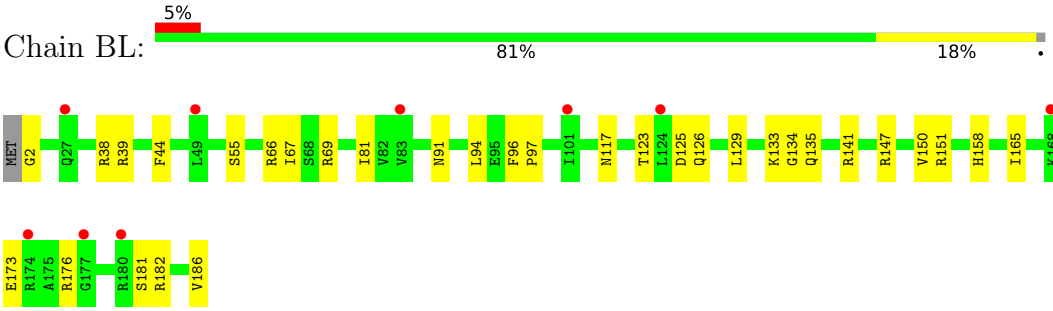
Chain y:



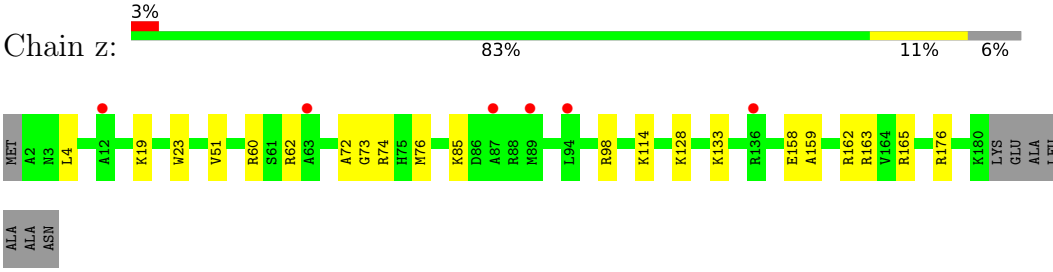

• Molecule 19: 60S ribosomal protein L18-A

Chain BL:



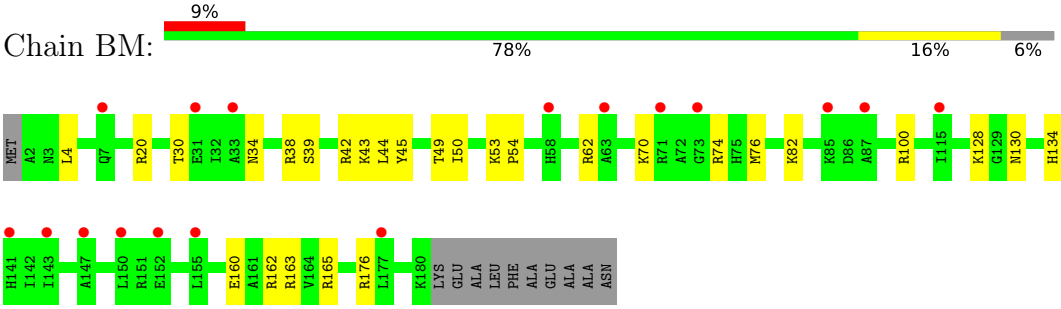

• Molecule 20: 60S ribosomal protein L19-A

Chain z:



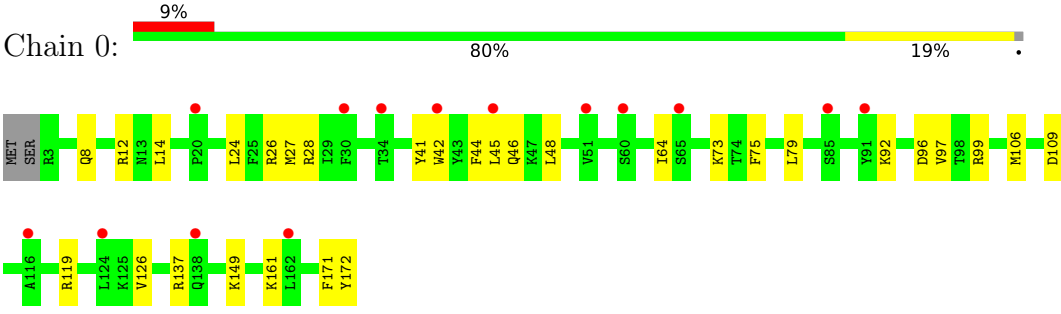

• Molecule 20: 60S ribosomal protein L19-A

Chain BM:



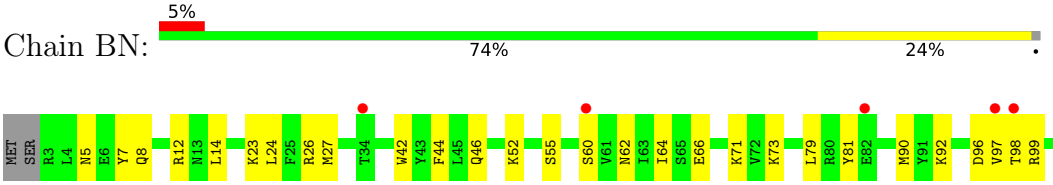

• Molecule 21: 60S ribosomal protein L20

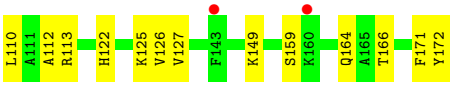
Chain 0:



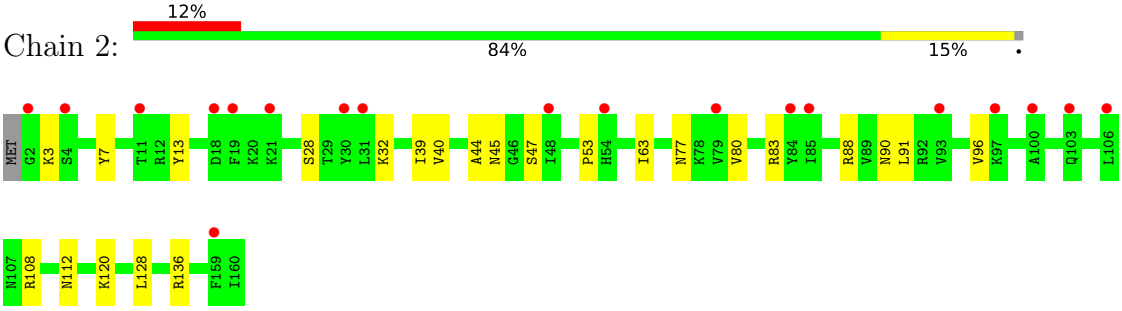

• Molecule 21: 60S ribosomal protein L20

Chain BN:

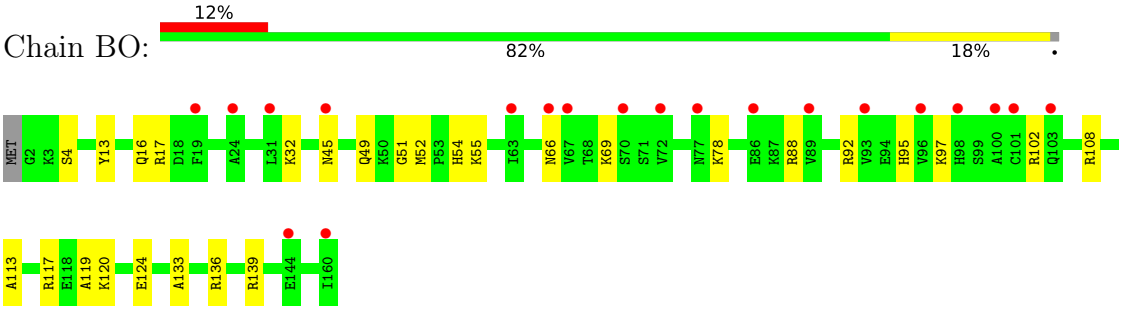




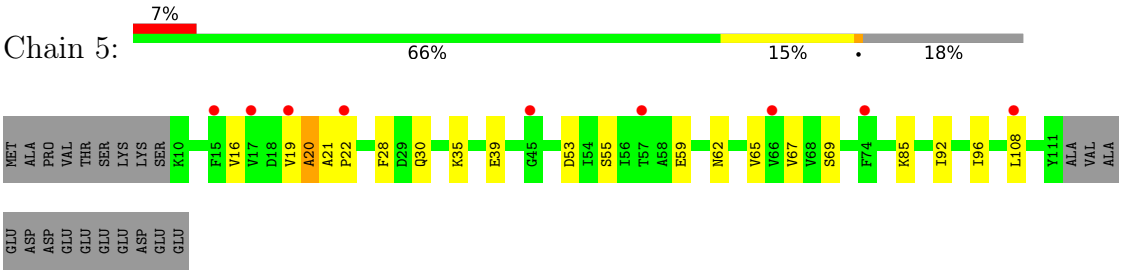

• Molecule 22: 60S ribosomal protein L21-A



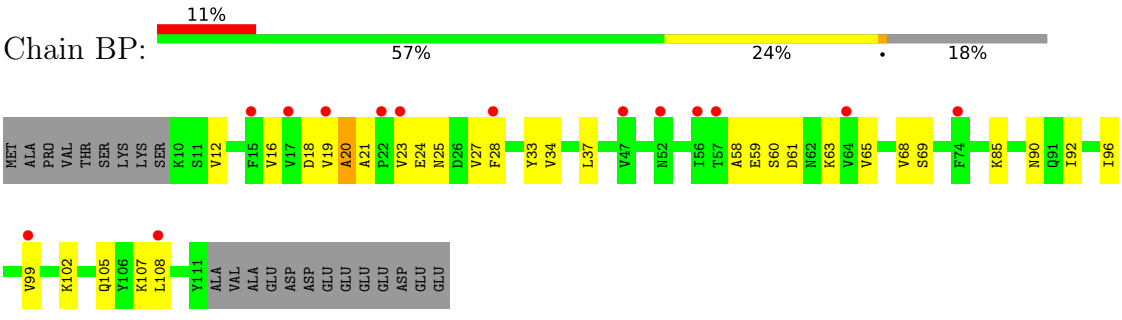

• Molecule 22: 60S ribosomal protein L21-A



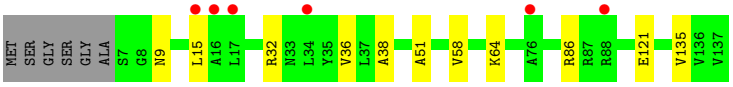

• Molecule 23: 60S ribosomal protein L22-B




• Molecule 23: 60S ribosomal protein L22-B

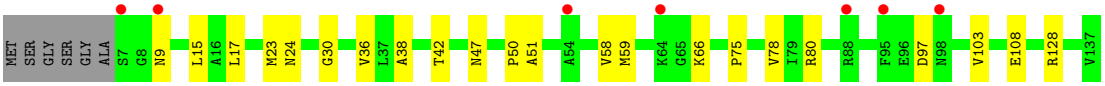



• Molecule 24: 60S ribosomal protein L23-A



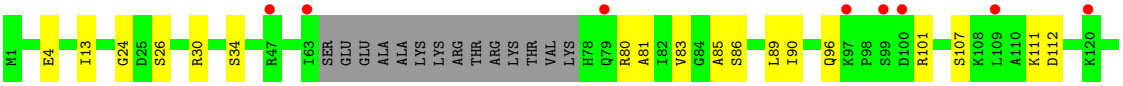

• Molecule 24: 60S ribosomal protein L23-A

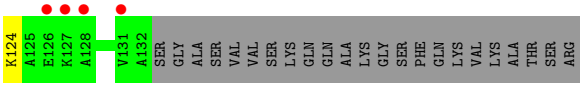
Chain BQ:




• Molecule 25: 60S ribosomal protein L24-A

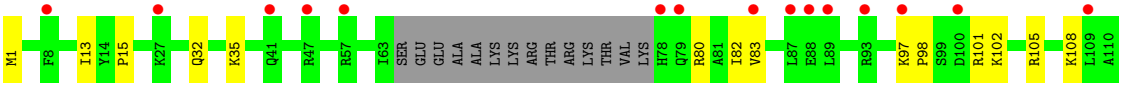
Chain 7:

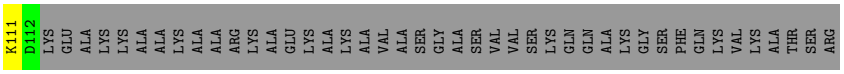



• Molecule 25: 60S ribosomal protein L24-A

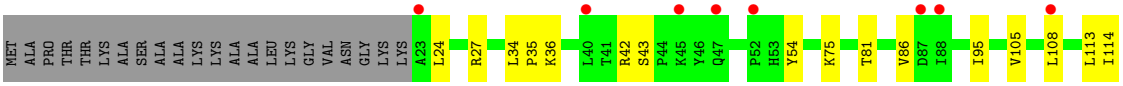
Chain BR:

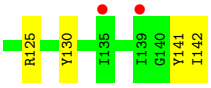



• Molecule 26: 60S ribosomal protein L25

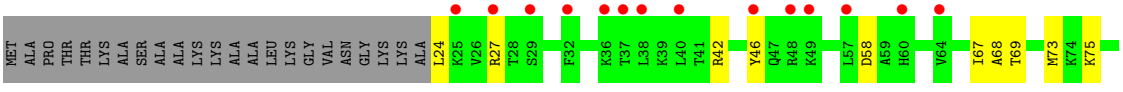
Chain 8:

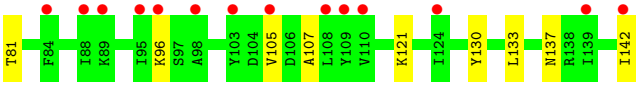



• Molecule 26: 60S ribosomal protein L25

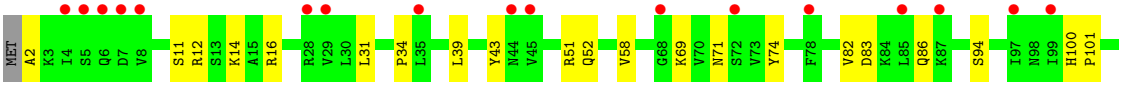
Chain BS:

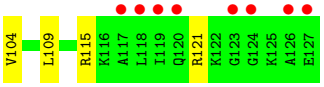





• Molecule 27: Ribosomal protein L24

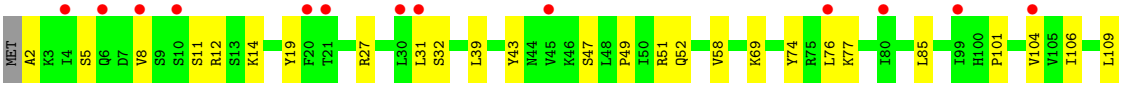
Chain 9:

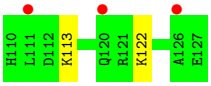



• Molecule 27: Ribosomal protein L24

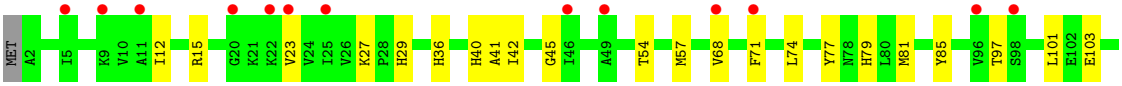
Chain BT:

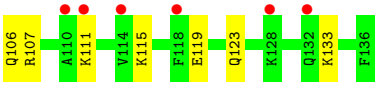



• Molecule 28: 60S ribosomal protein L27

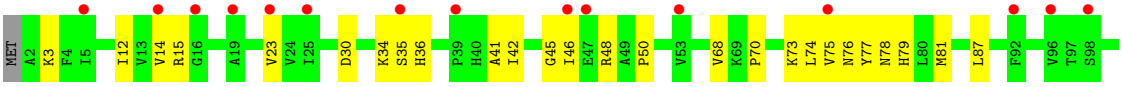
Chain AA:

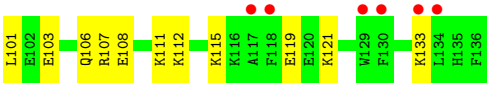



• Molecule 28: 60S ribosomal protein L27

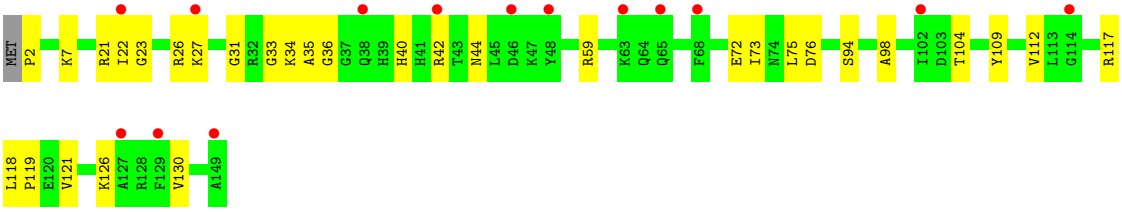
Chain BU:



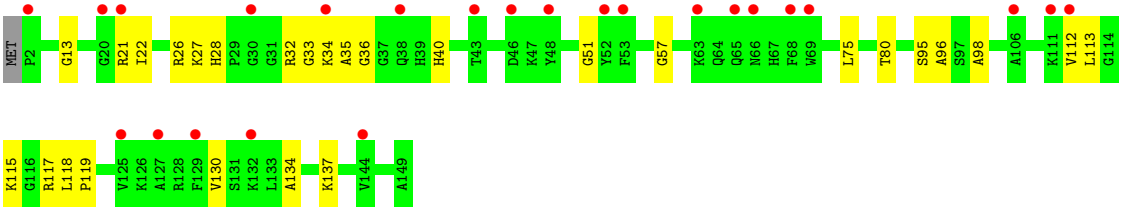

• Molecule 29: 60S ribosomal protein L28

Chain AB:



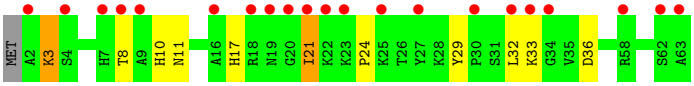

• Molecule 29: 60S ribosomal protein L28

Chain BV:



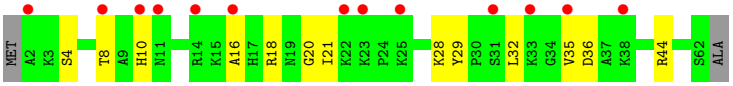

• Molecule 30: 60S ribosomal protein L29

Chain AC:



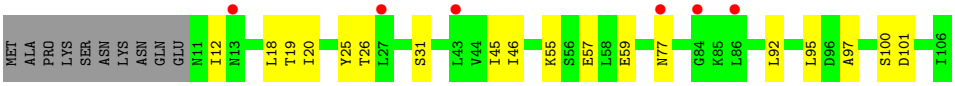

• Molecule 30: 60S ribosomal protein L29

Chain BW:



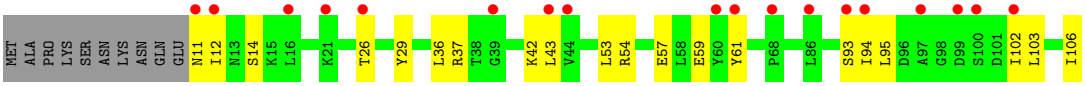

• Molecule 31: 60S ribosomal protein L30

Chain AD:



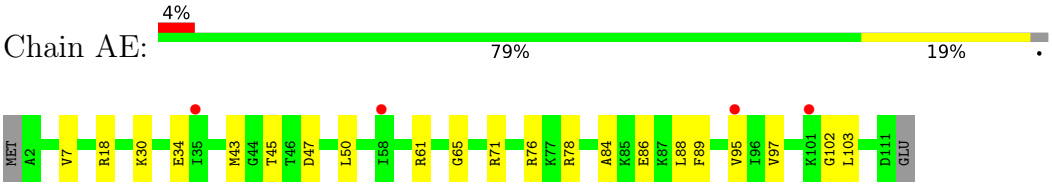

• Molecule 31: 60S ribosomal protein L30

Chain BX:



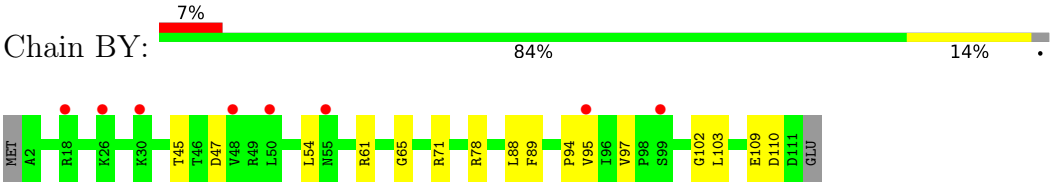

• Molecule 32: 60S ribosomal protein L31-B

Chain AE:



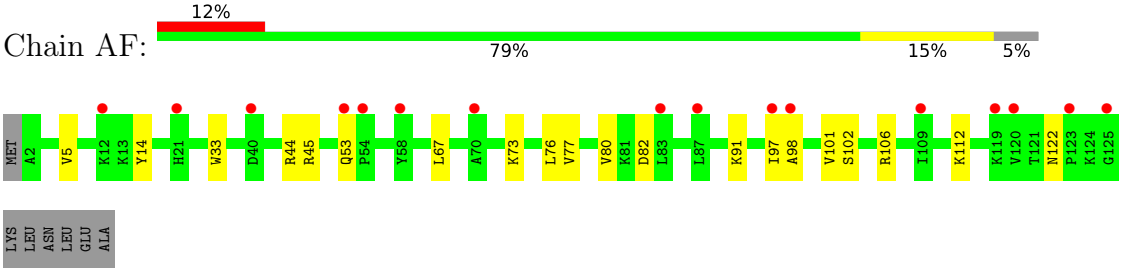

• Molecule 32: 60S ribosomal protein L31-B

Chain BY:



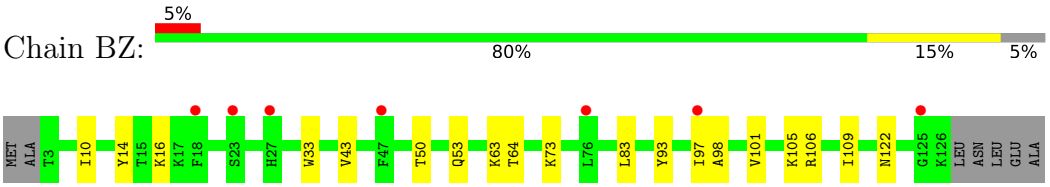

• Molecule 33: 60S ribosomal protein L32

Chain AF:



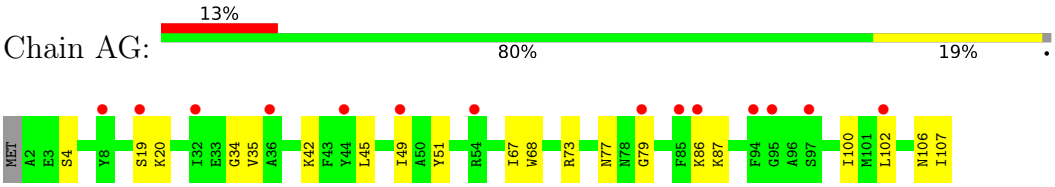

• Molecule 33: 60S ribosomal protein L32

Chain BZ:



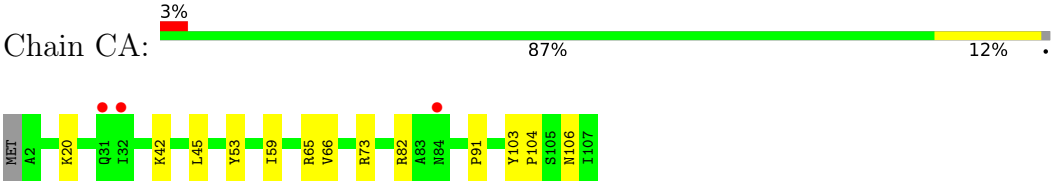

• Molecule 34: 60S ribosomal protein L33-A

Chain AG:



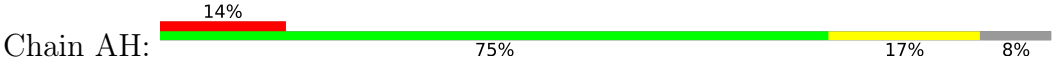

• Molecule 34: 60S ribosomal protein L33-A

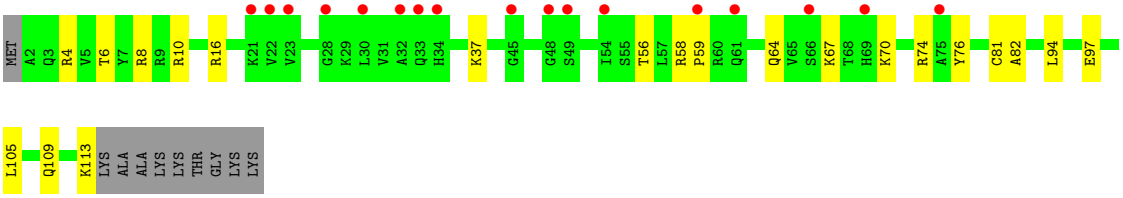
Chain CA:



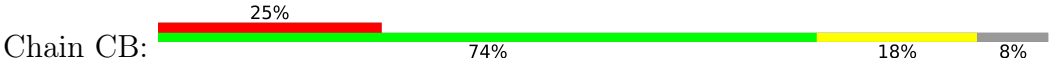

• Molecule 35: 60S ribosomal protein L34-B

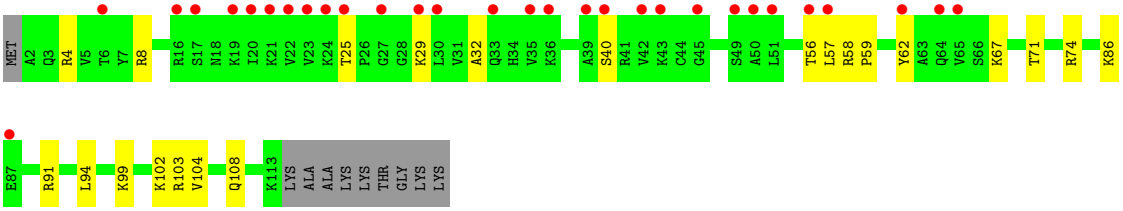
Chain AH:



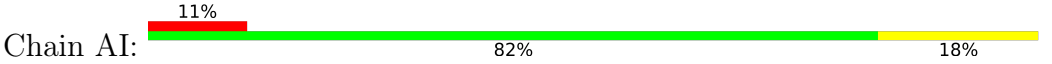


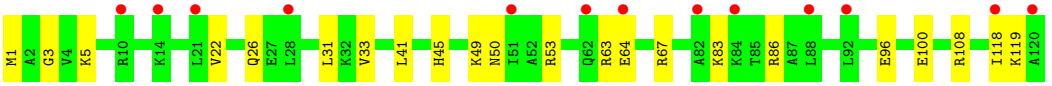

• Molecule 35: 60S ribosomal protein L34-B



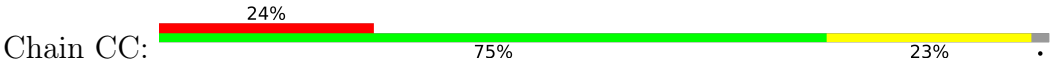



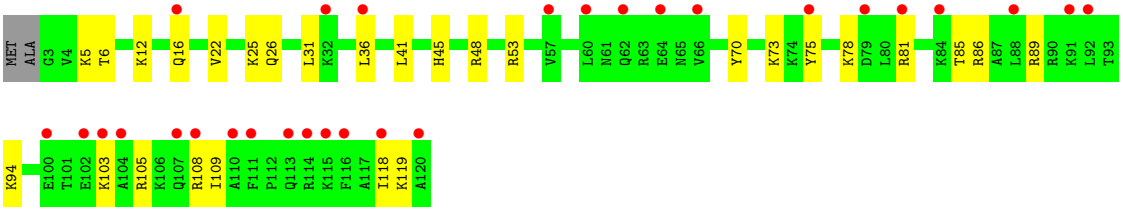

• Molecule 36: Ribosomal protein L29



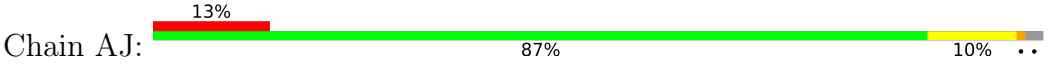



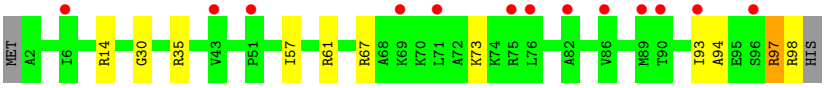

• Molecule 36: Ribosomal protein L29



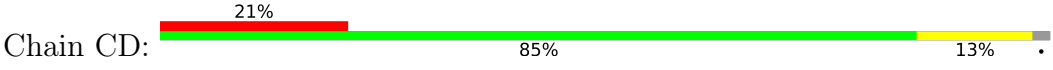



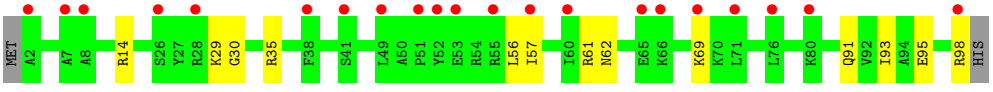

• Molecule 37: 60S ribosomal protein L36



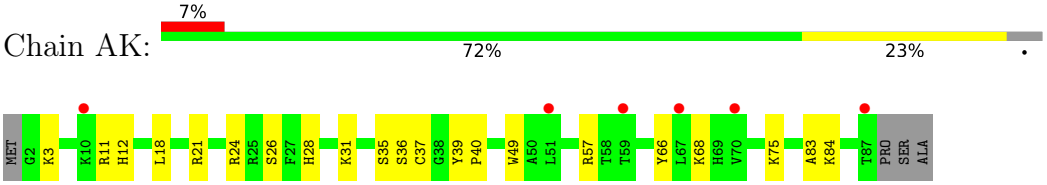

• Molecule 37: 60S ribosomal protein L36



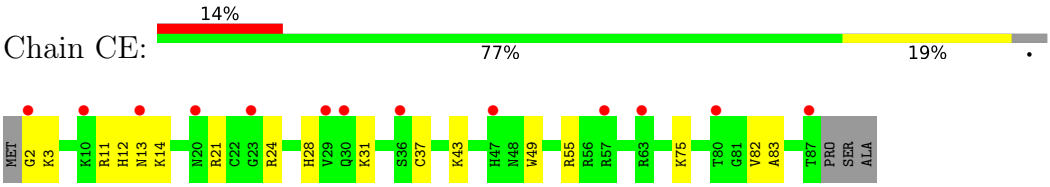
• Molecule 38: 60S ribosomal protein L37-B

Chain AK:



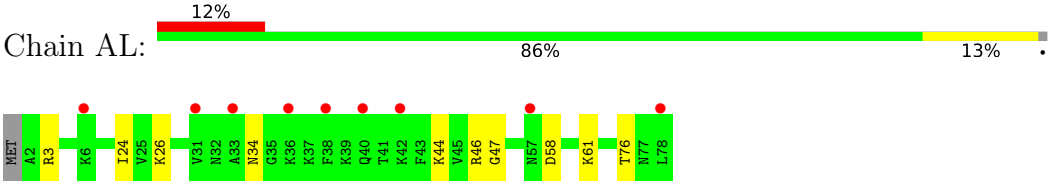

• Molecule 38: 60S ribosomal protein L37-B

Chain CE:



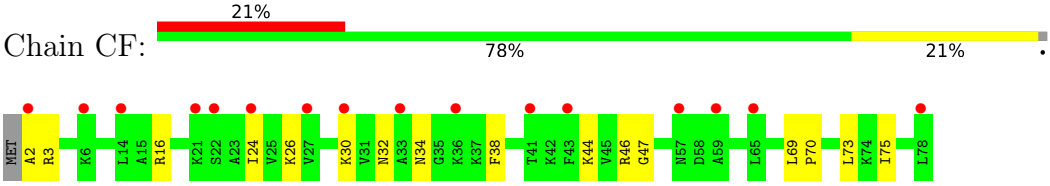

• Molecule 39: 60S ribosomal protein L38

Chain AL:



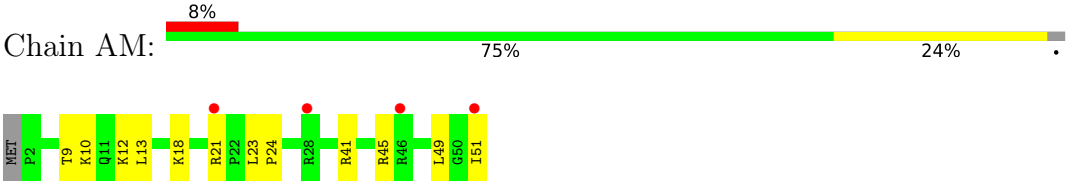

• Molecule 39: 60S ribosomal protein L38

Chain CF:



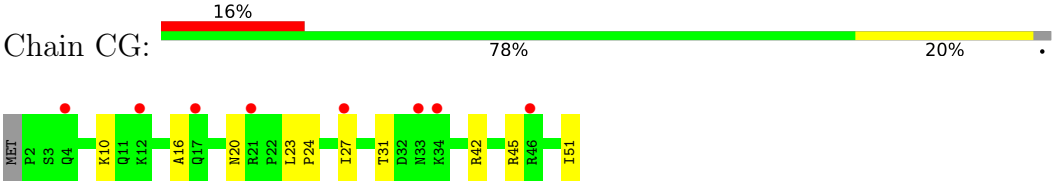

• Molecule 40: 60S ribosomal protein L39

Chain AM:




• Molecule 40: 60S ribosomal protein L39

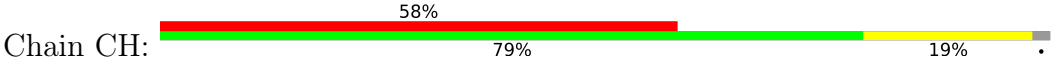
Chain CG:

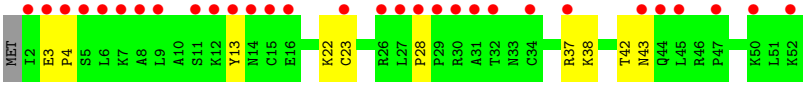



• Molecule 41: 60S ribosomal protein L40-B

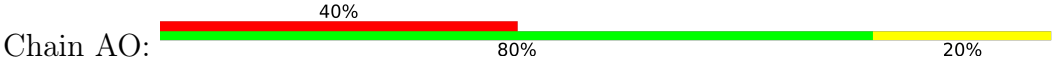
Chain AN:

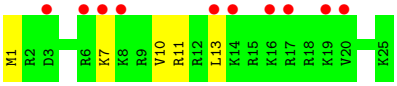
• Molecule 41: 60S ribosomal protein L40-B



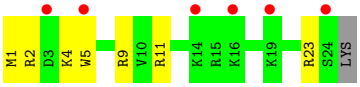




• Molecule 42: 60S ribosomal protein L41

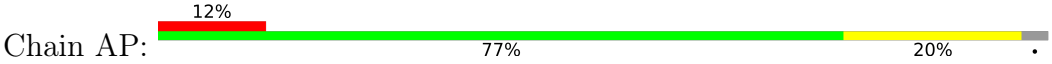


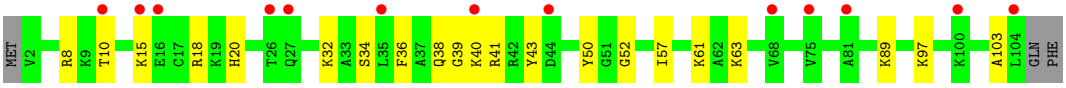




• Molecule 42: 60S ribosomal protein L41

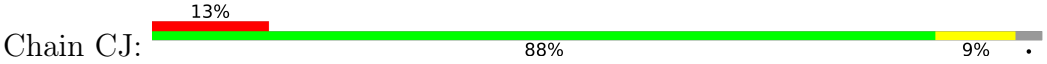


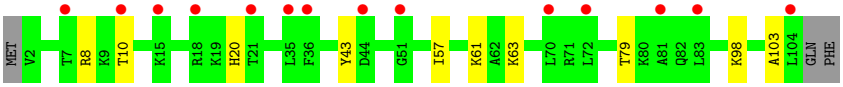

• Molecule 43: 60S ribosomal protein L42-B



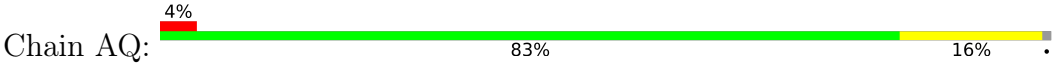




• Molecule 43: 60S ribosomal protein L42-B



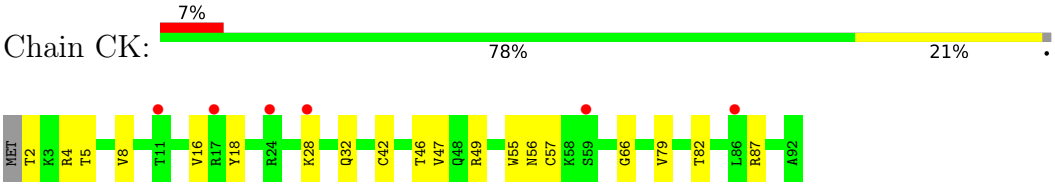




• Molecule 44: 60S ribosomal protein L43-A



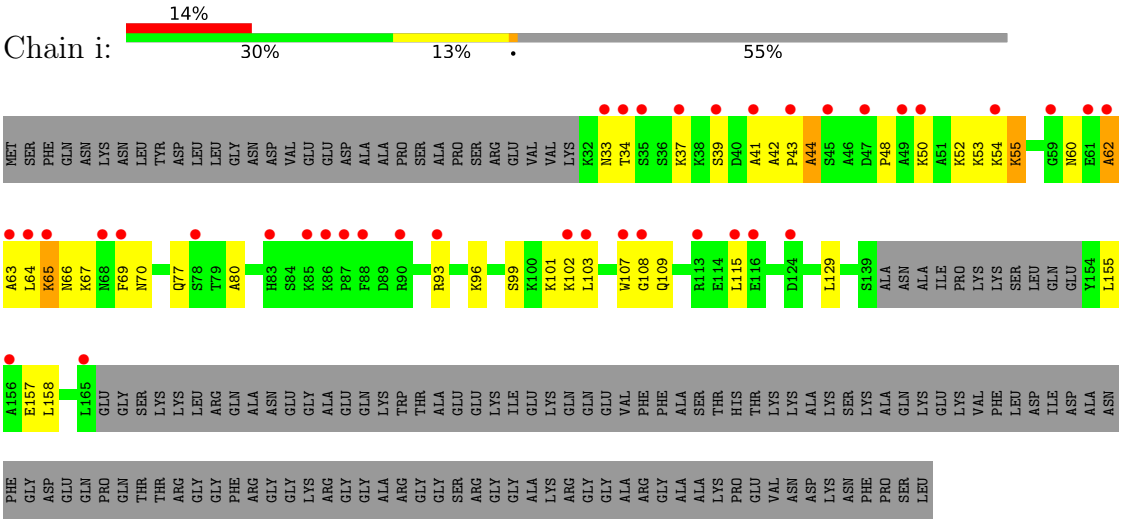
• Molecule 44: 60S ribosomal protein L43-A

Chain CK:



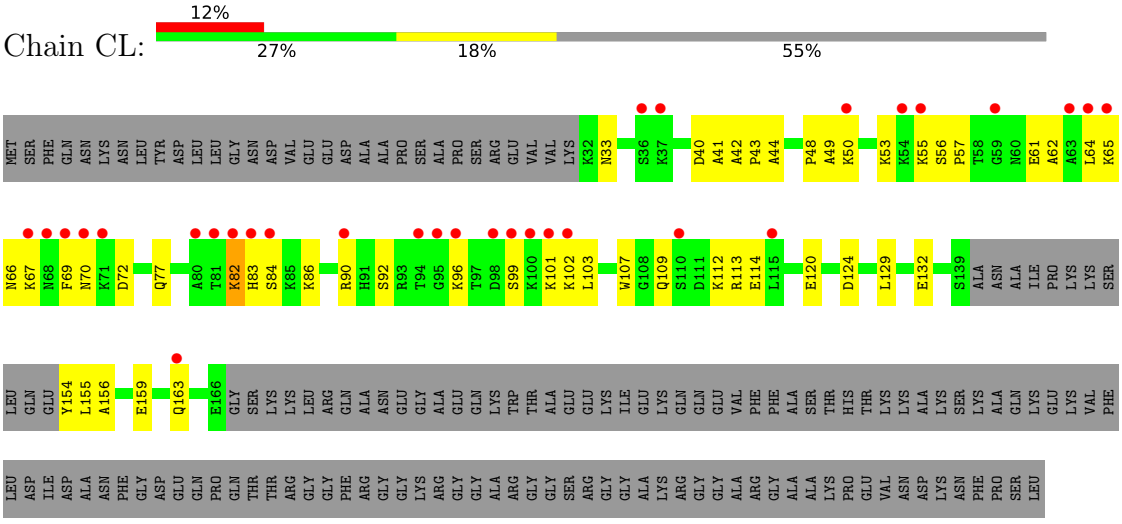

• Molecule 45: 60S ribosomal protein CAALFM_C304810CA

Chain i:



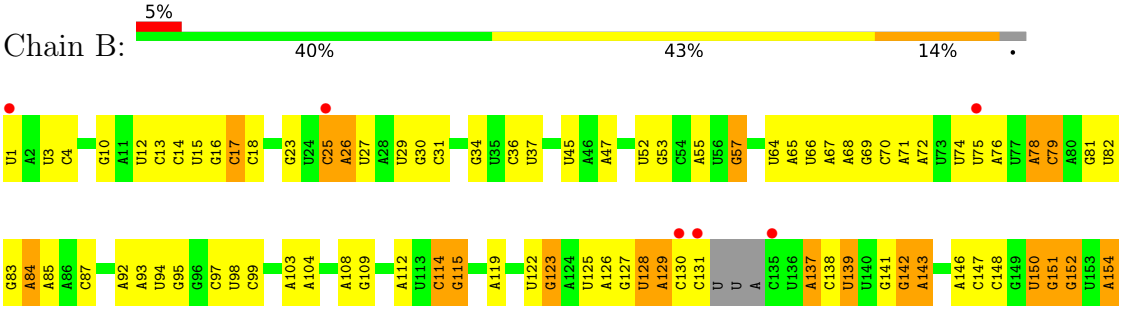

• Molecule 45: 60S ribosomal protein CAALFM_C304810CA

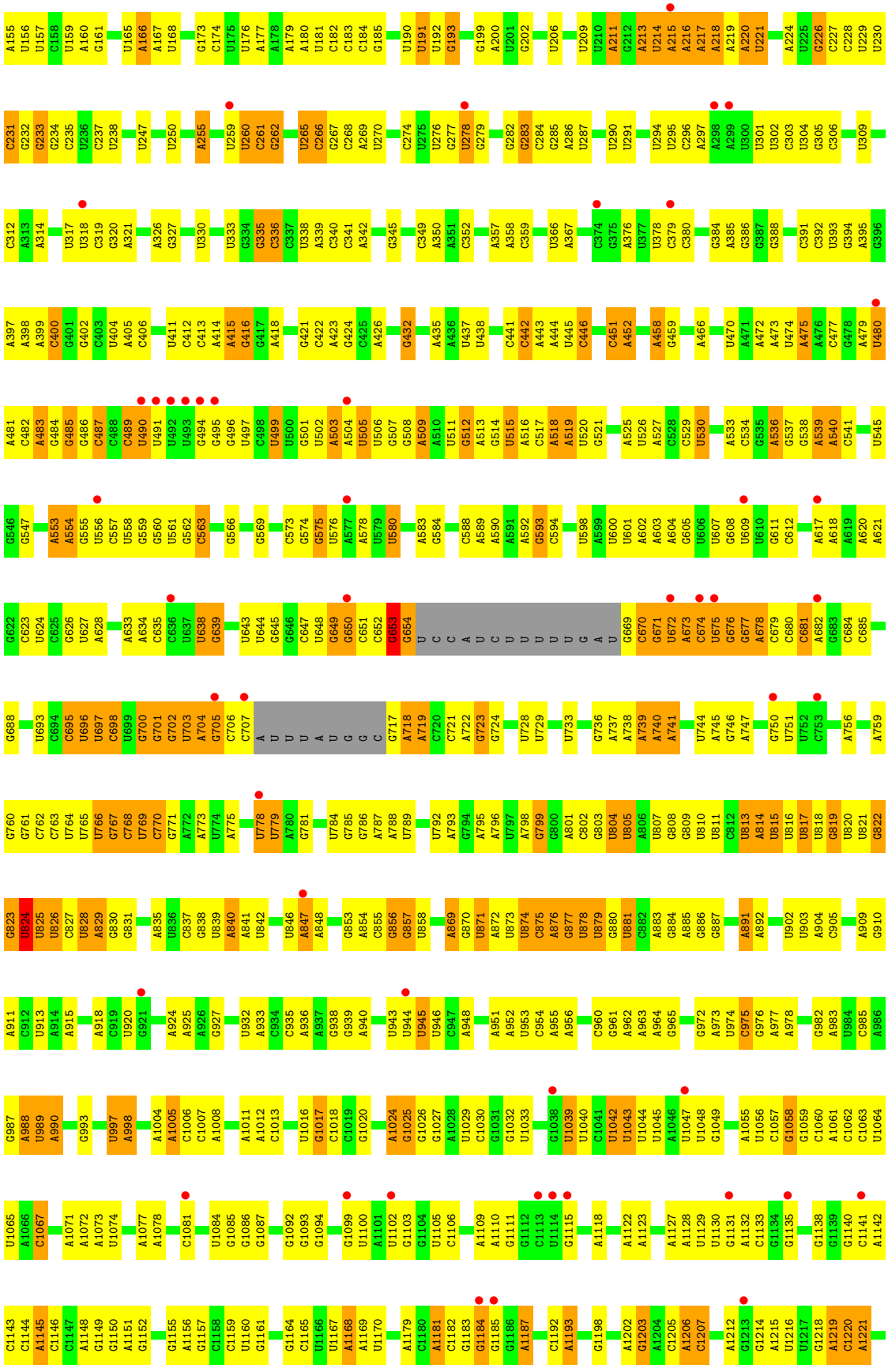
Chain CL:

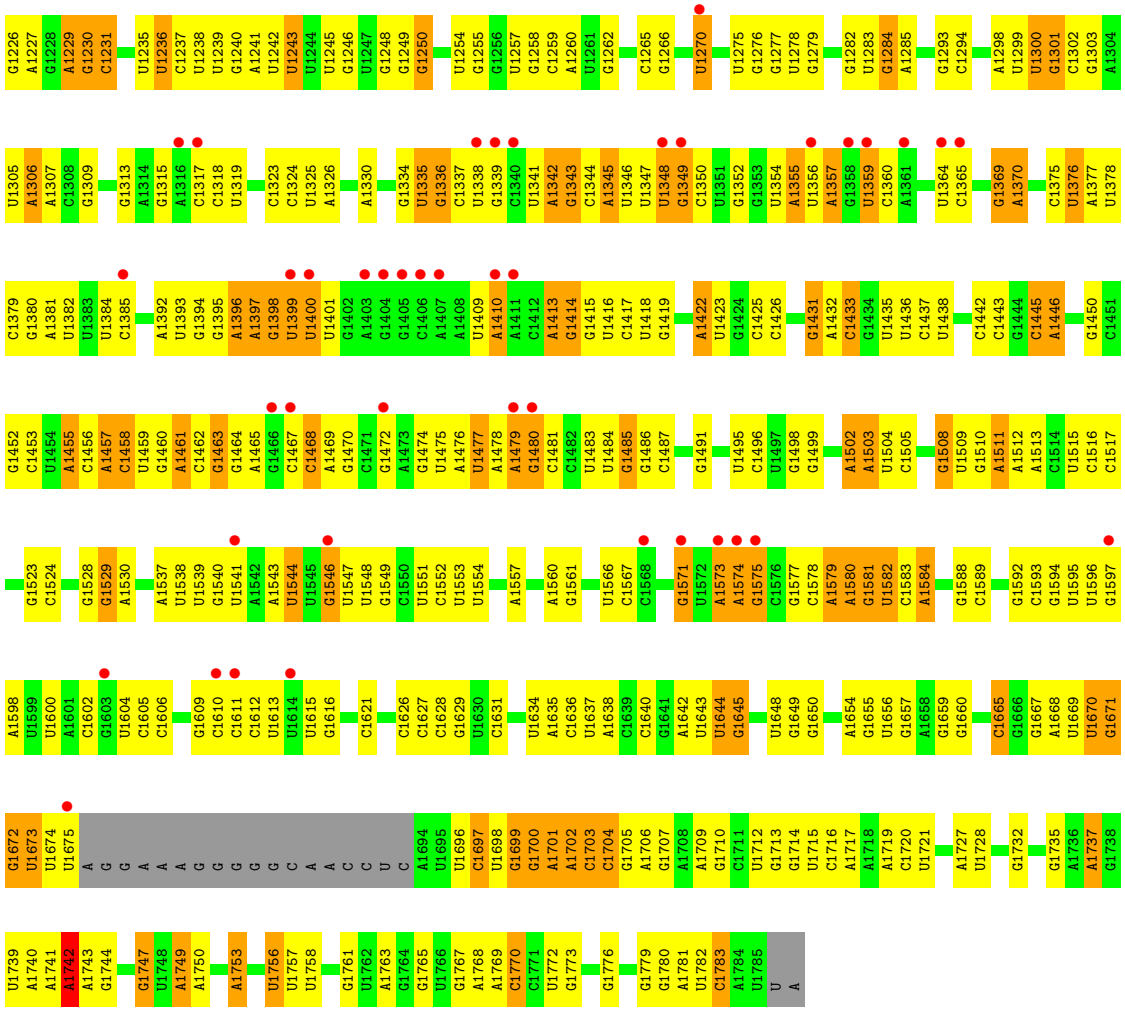



• Molecule 46: 18S

Chain B:

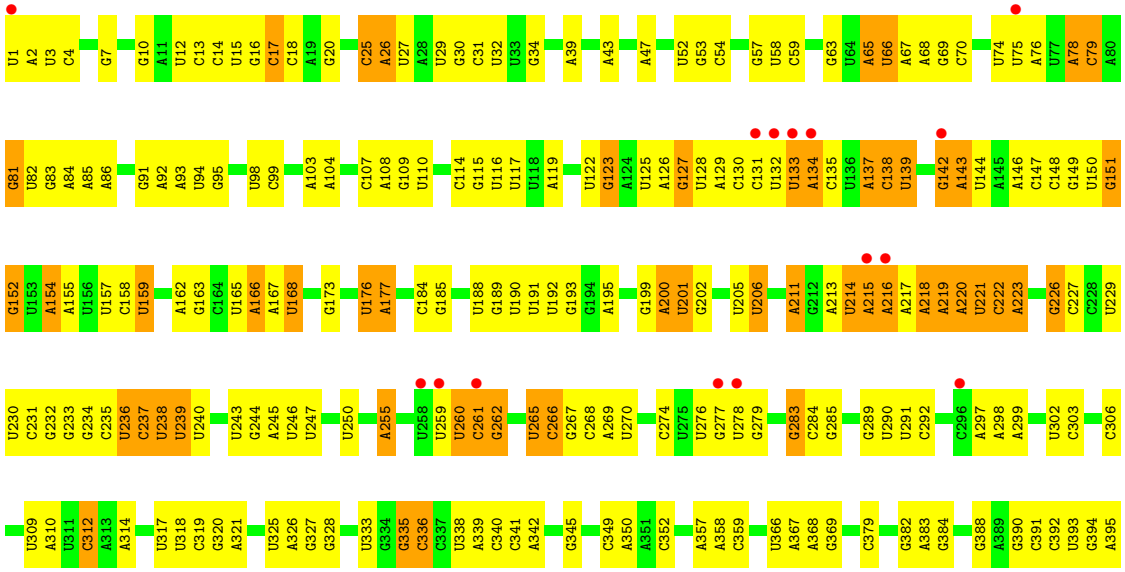


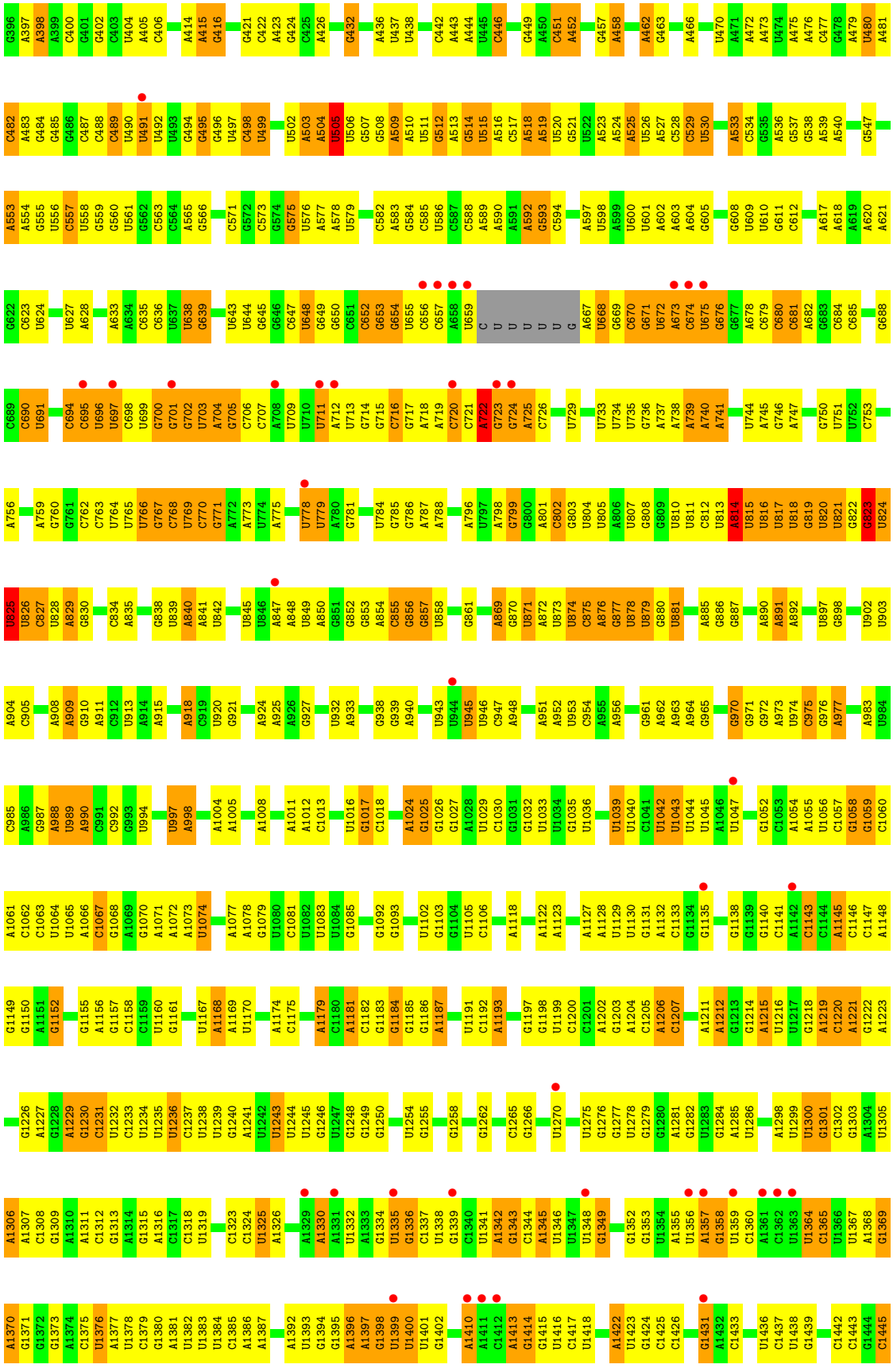


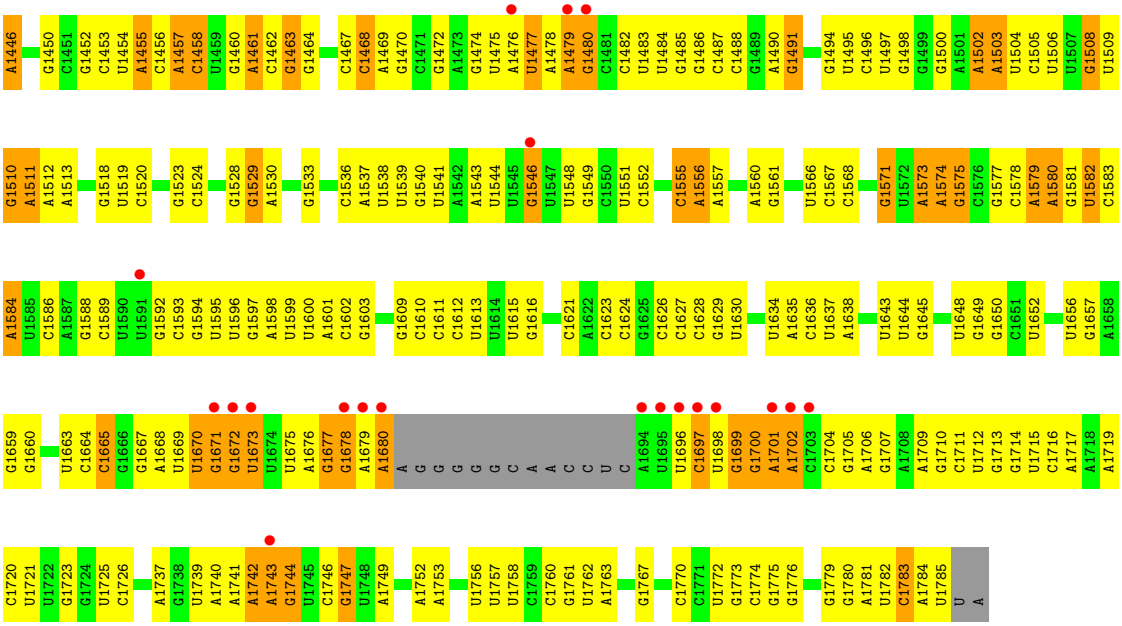


• Molecule 46: 18S

Chain CM:

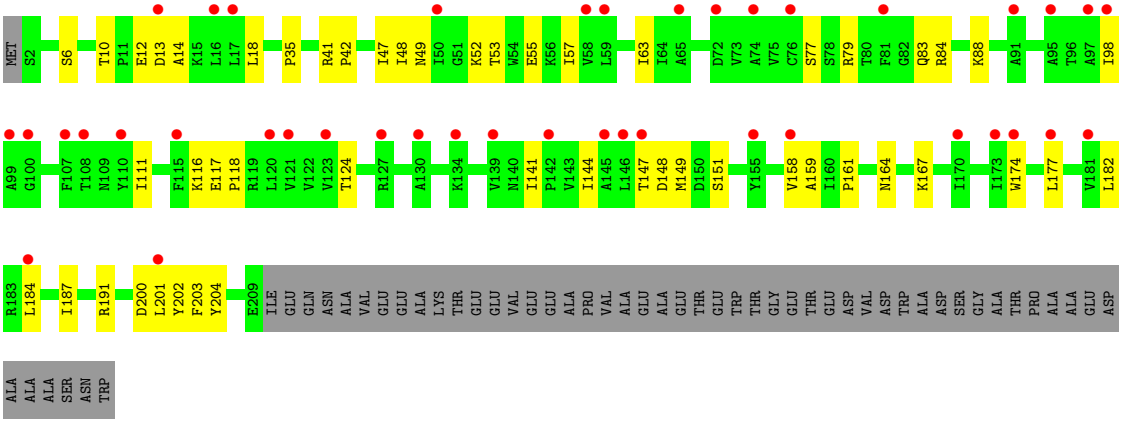






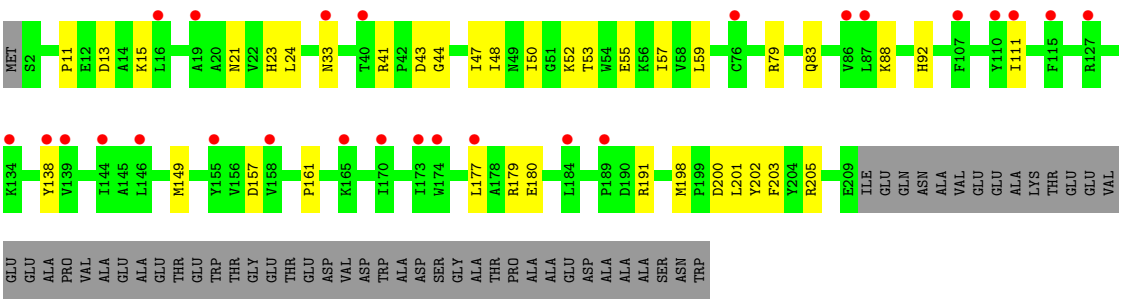
• Molecule 47: 40S ribosomal protein S0

Chain C:



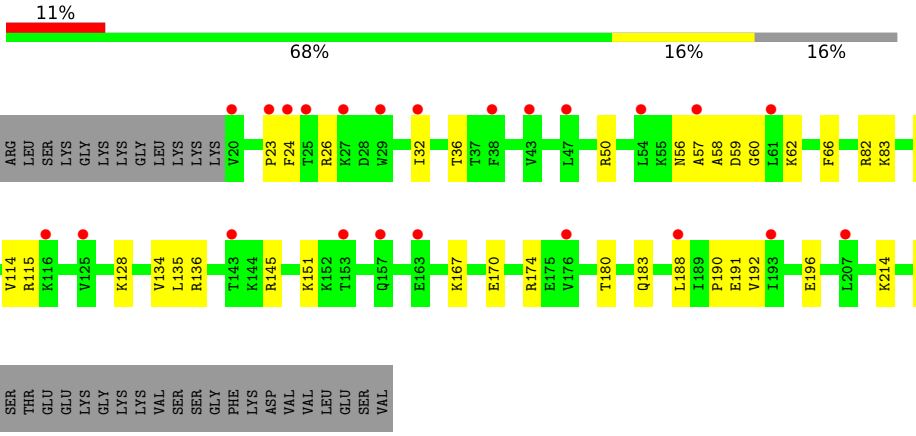
• Molecule 47: 40S ribosomal protein S0

Chain CN:



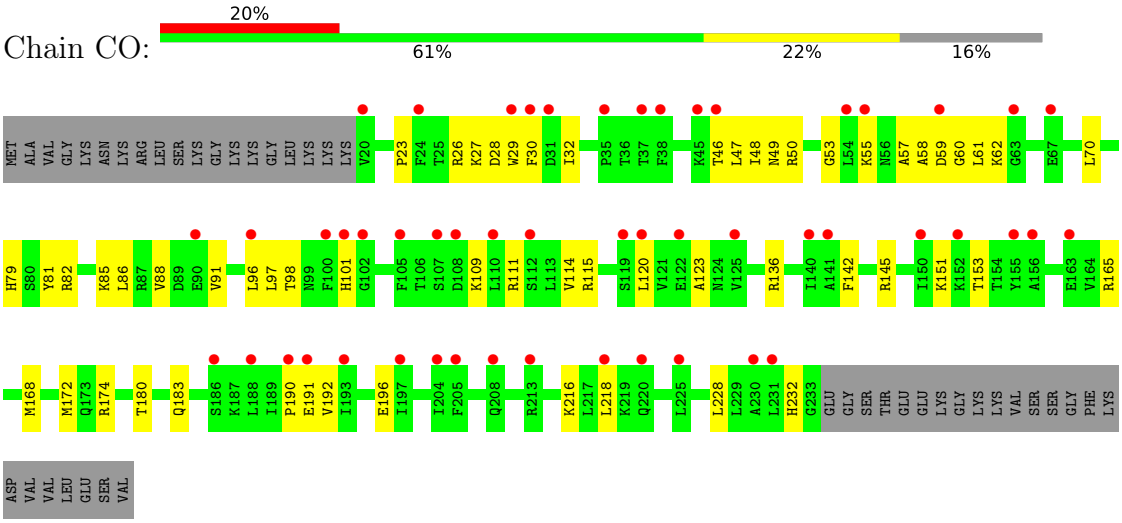
• Molecule 48: 40S ribosomal protein S1

Chain D:



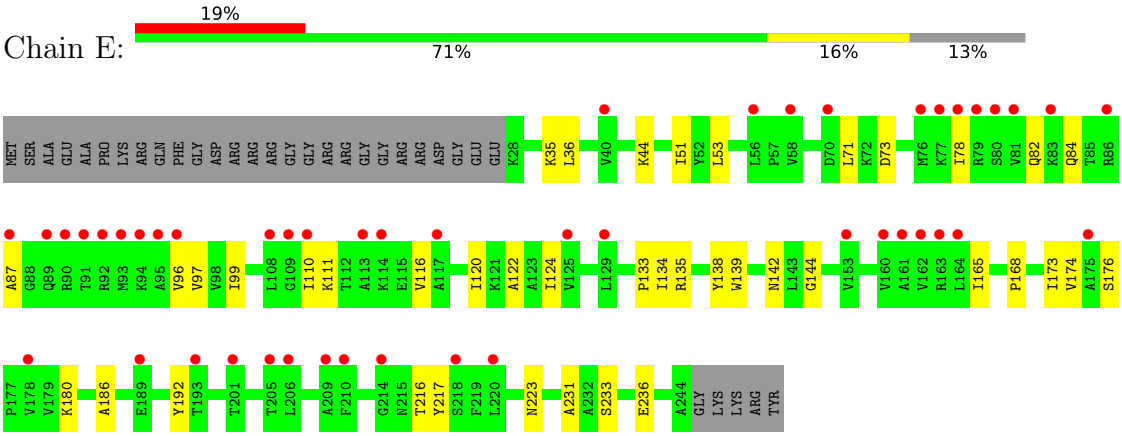

• Molecule 48: 40S ribosomal protein S1

Chain CO:



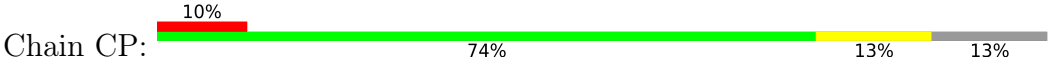

• Molecule 49: Ribosomal protein S5

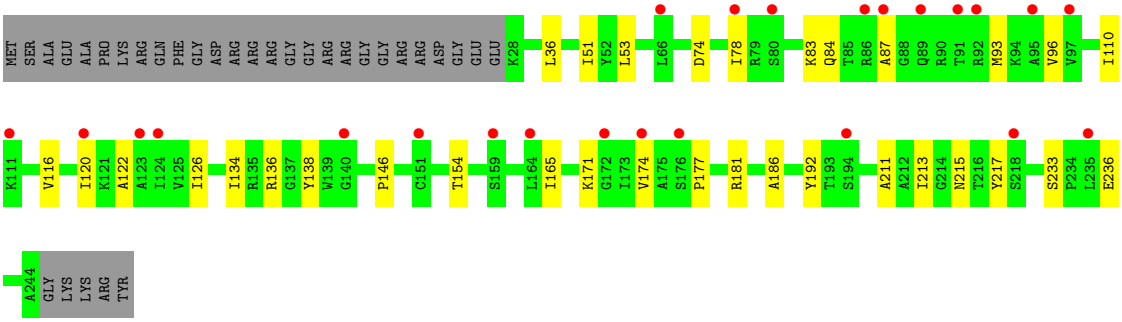
Chain E:




• Molecule 49: Ribosomal protein S5

Chain CP:

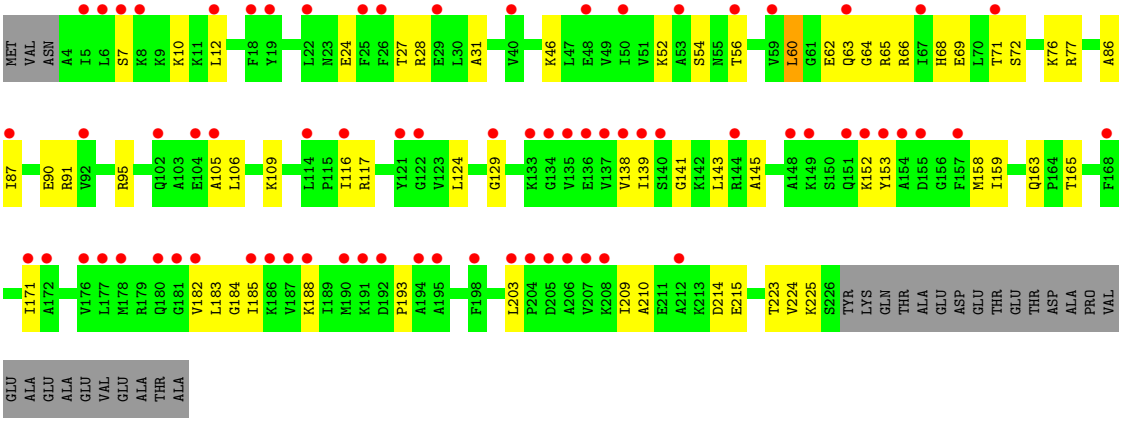






• Molecule 50: Ribosomal protein S3

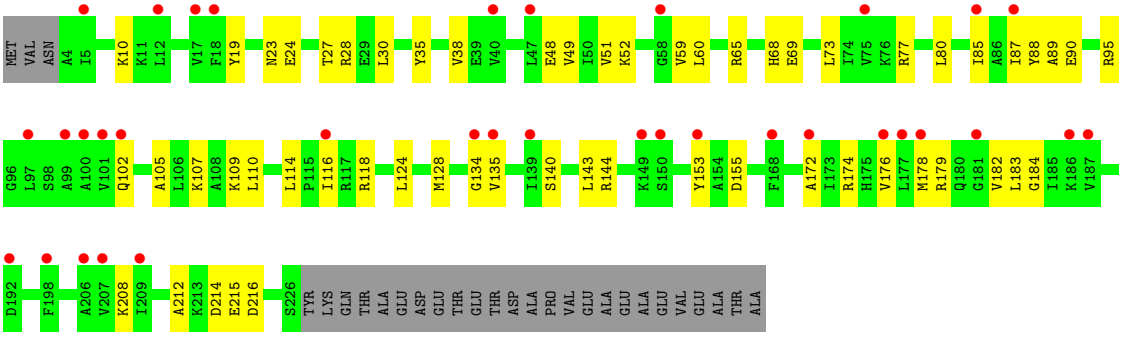
Chain F:





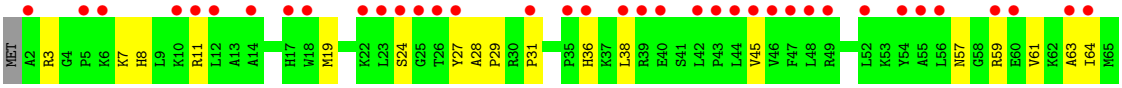
• Molecule 50: Ribosomal protein S3

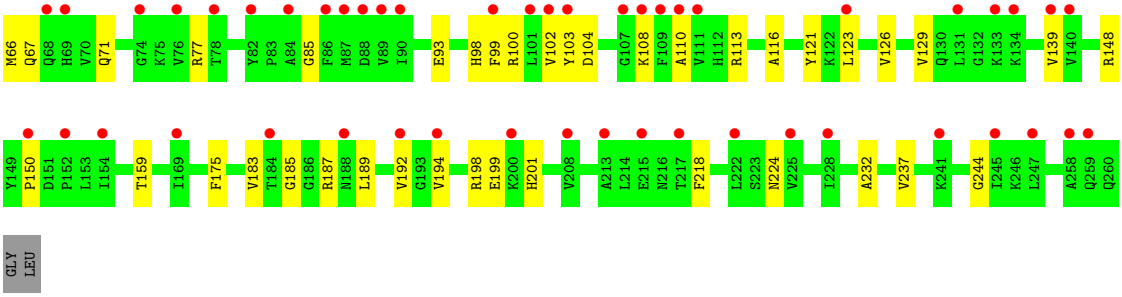
Chain CQ:



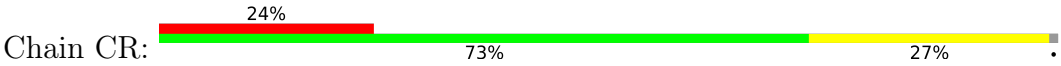
• Molecule 51: 40S ribosomal protein S4

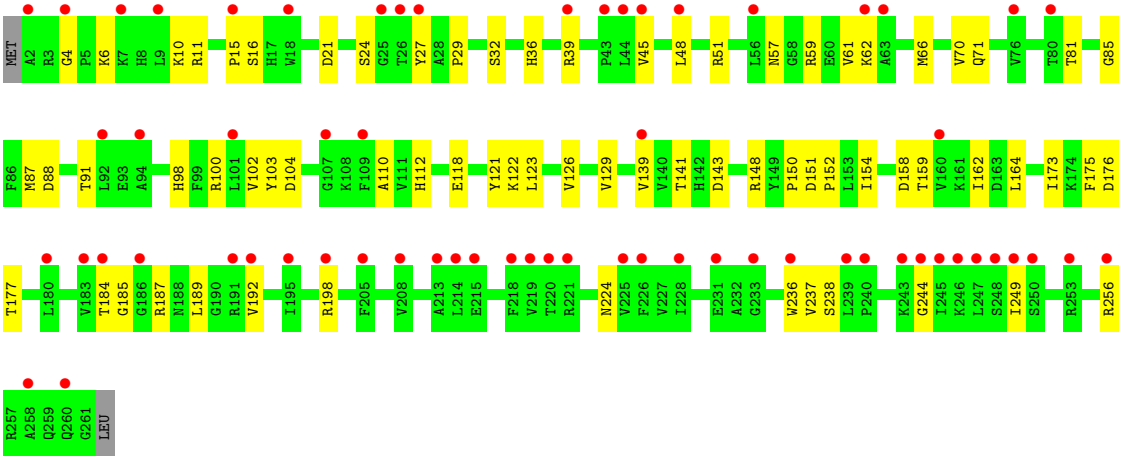
Chain G:



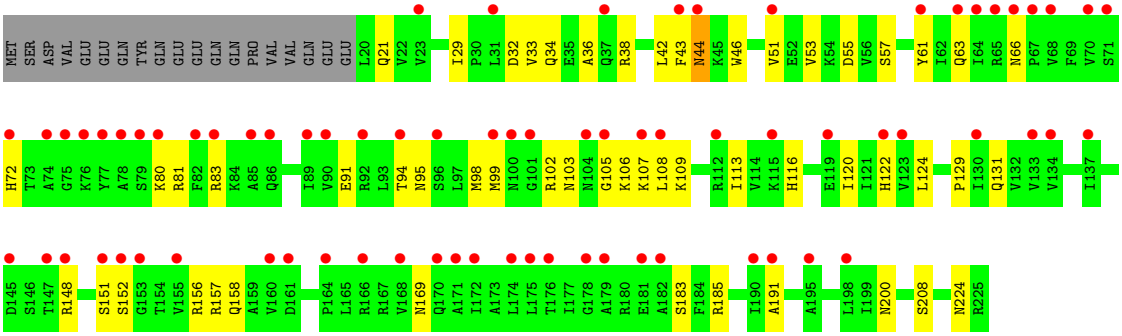



• Molecule 51: 40S ribosomal protein S4

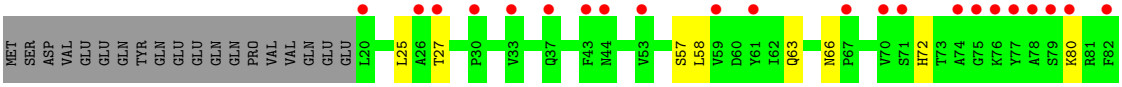


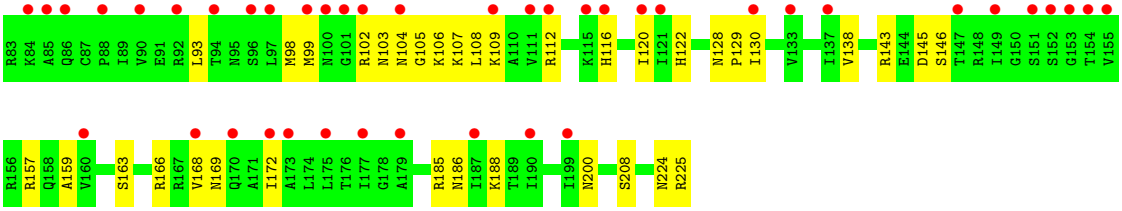




• Molecule 52: Ribosomal protein S7



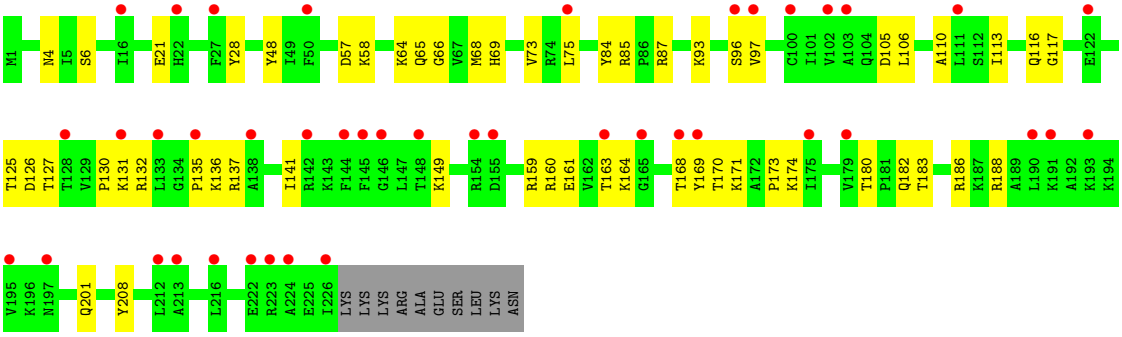

• Molecule 52: Ribosomal protein S7





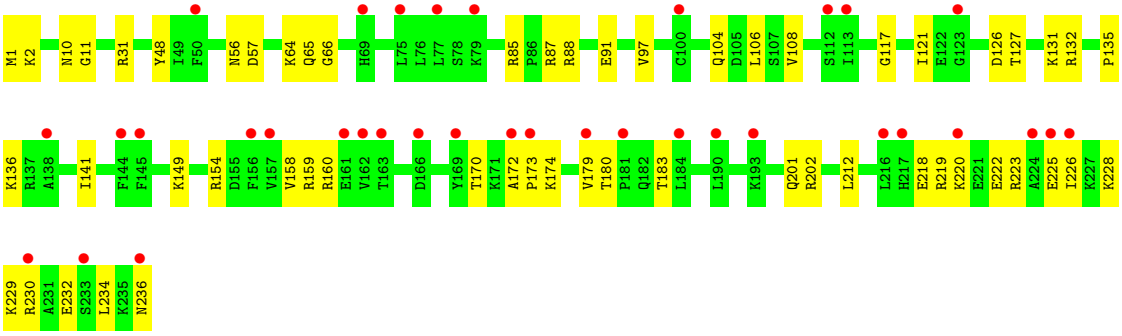

• Molecule 53: 40S ribosomal protein S6

Chain I:



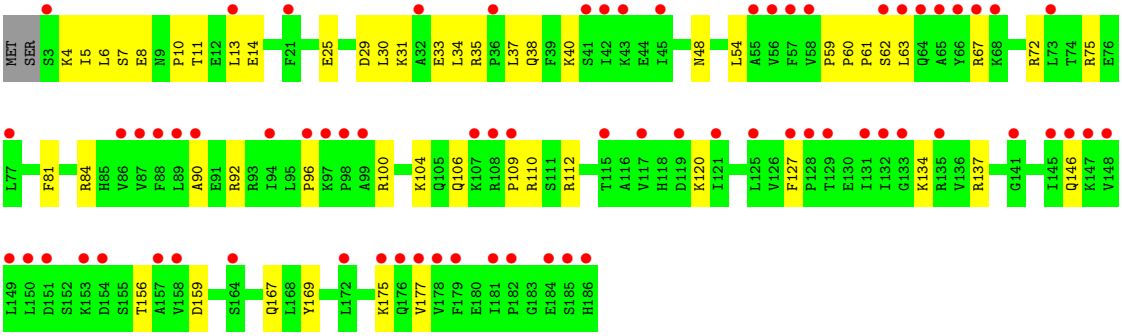

• Molecule 53: 40S ribosomal protein S6

Chain CT:



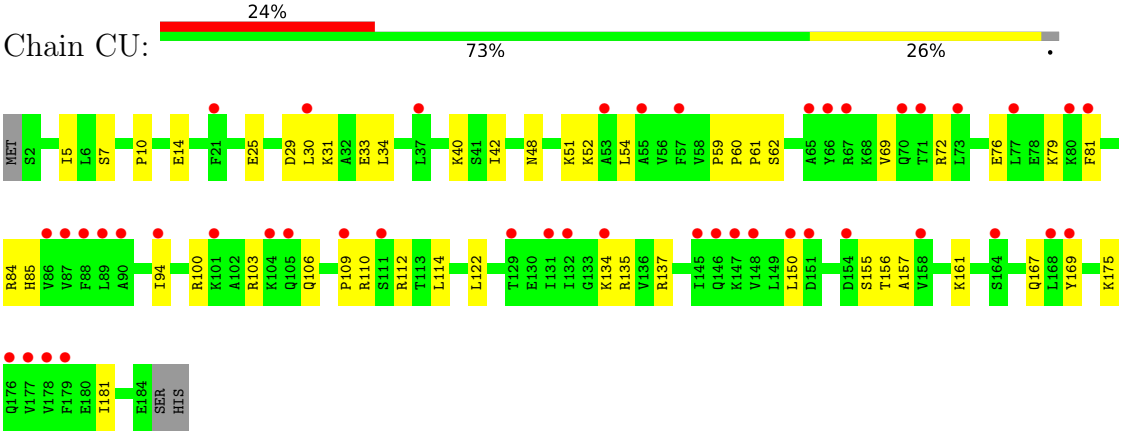

• Molecule 54: 40S ribosomal protein S7

Chain J:



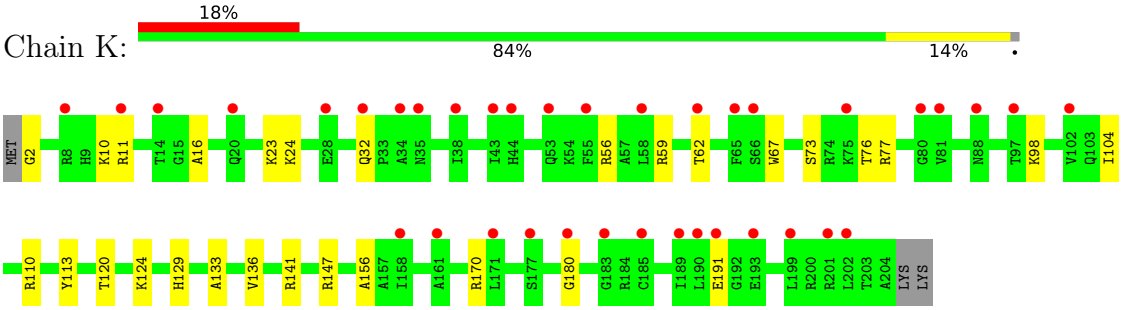
• Molecule 54: 40S ribosomal protein S7

Chain CU:



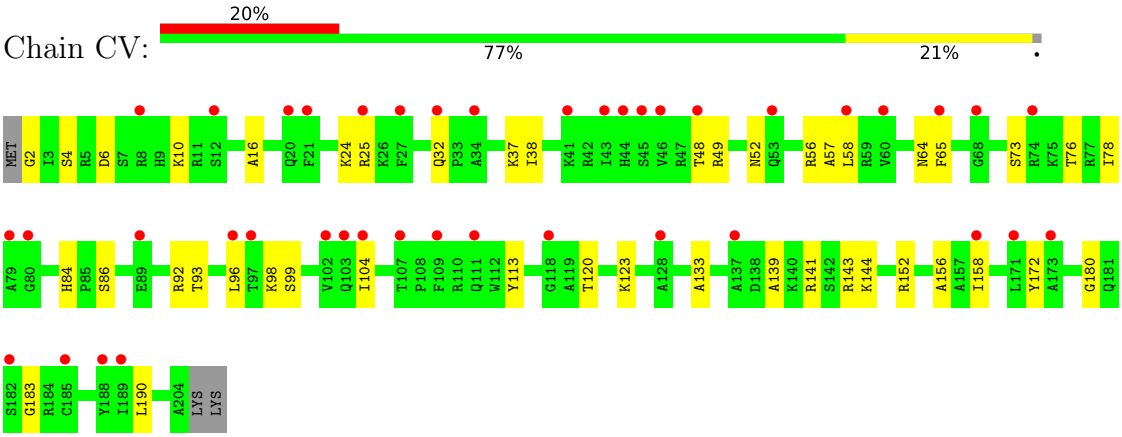

• Molecule 55: 40S ribosomal protein S8

Chain K:



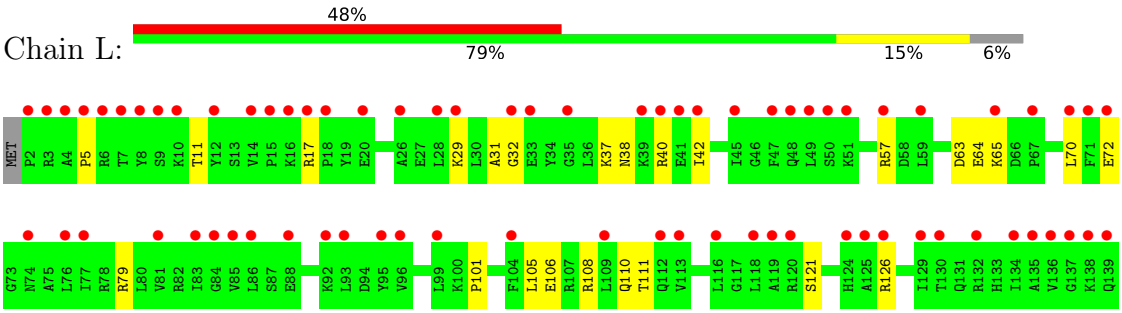

• Molecule 55: 40S ribosomal protein S8

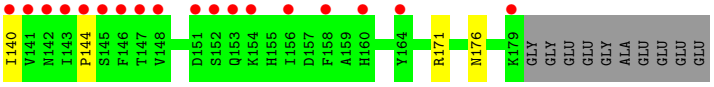
Chain CV:



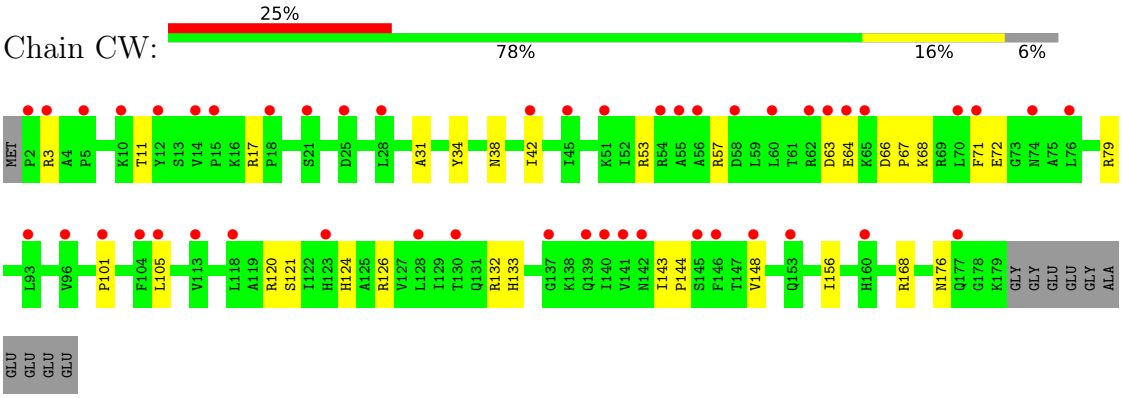

• Molecule 56: Ribosomal protein S4

Chain L:

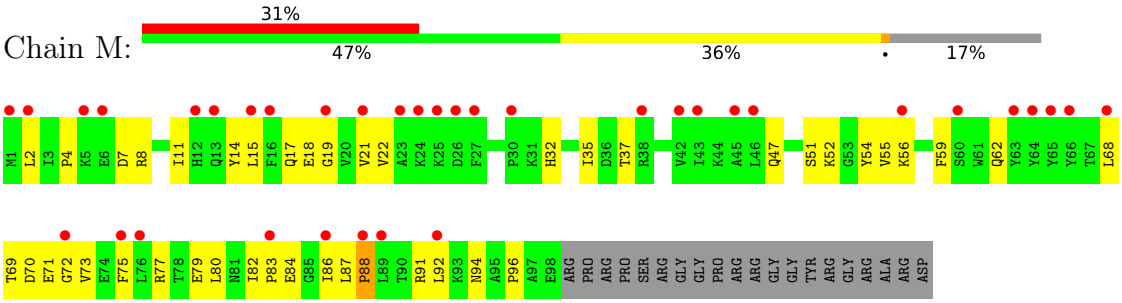




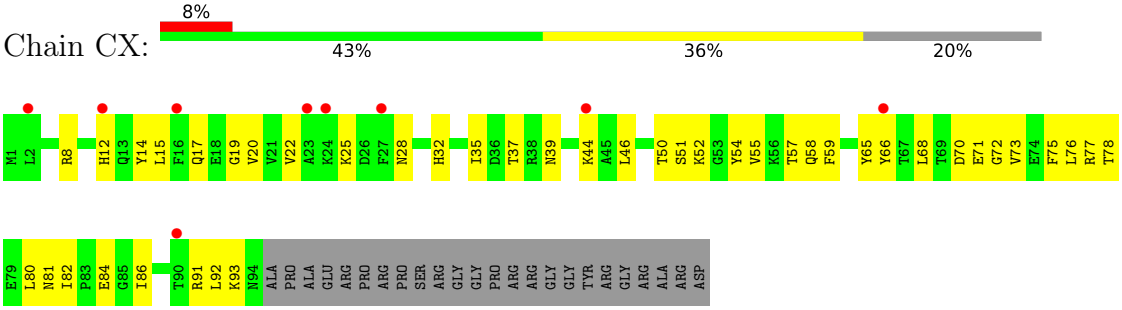

• Molecule 56: Ribosomal protein S4



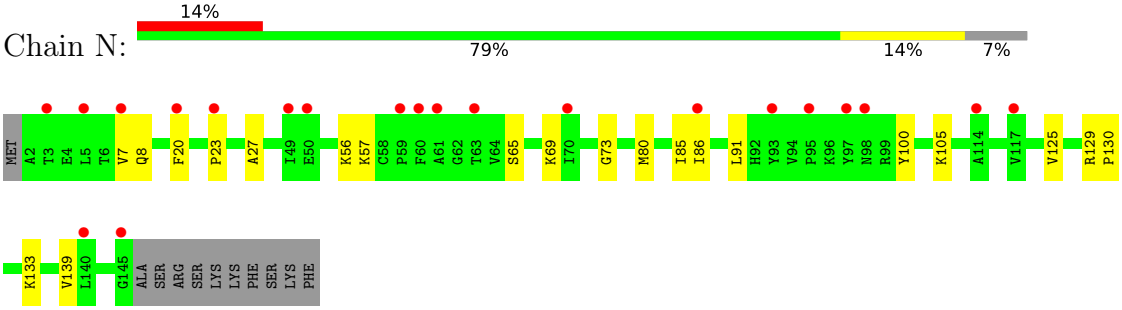

• Molecule 57: 40S ribosomal protein S10-A




• Molecule 57: 40S ribosomal protein S10-A

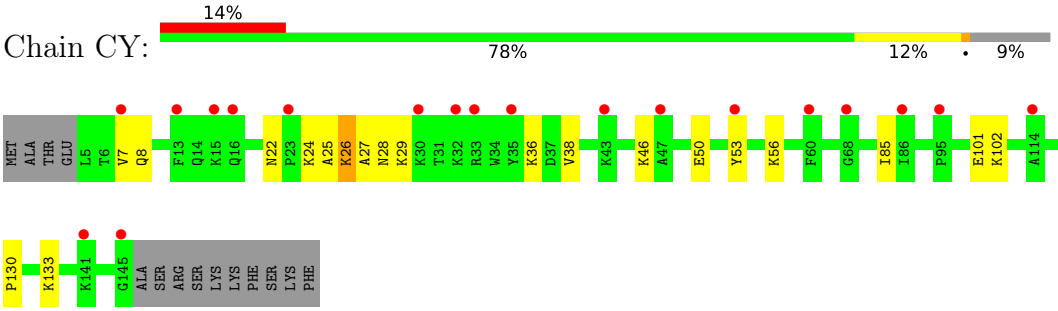



• Molecule 58: 40S ribosomal protein S11A



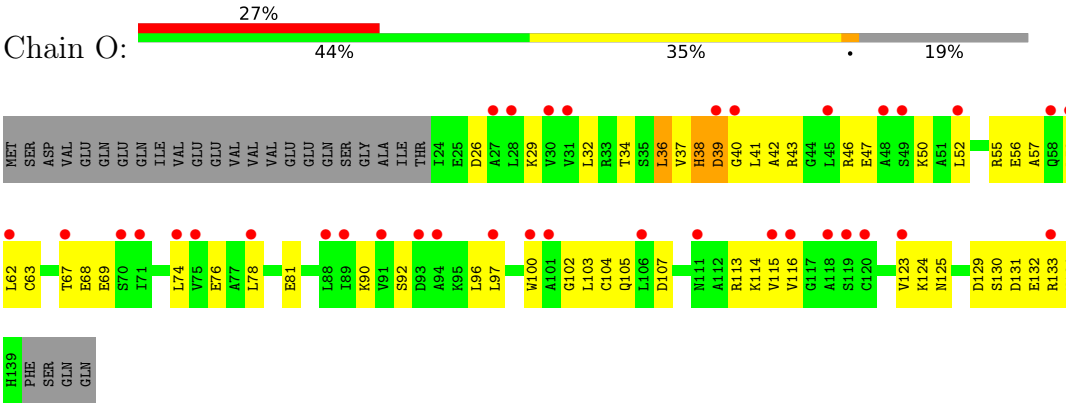

• Molecule 58: 40S ribosomal protein S11A

Chain CY:



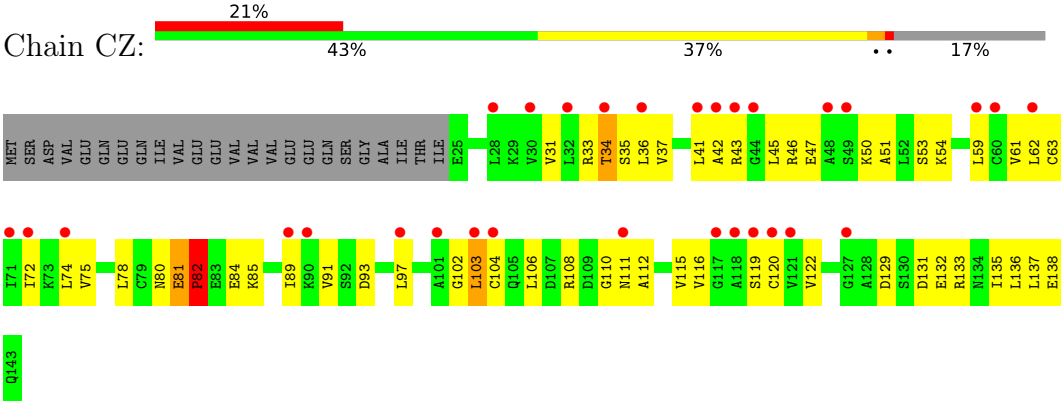

• Molecule 59: 40S ribosomal protein S12

Chain O:



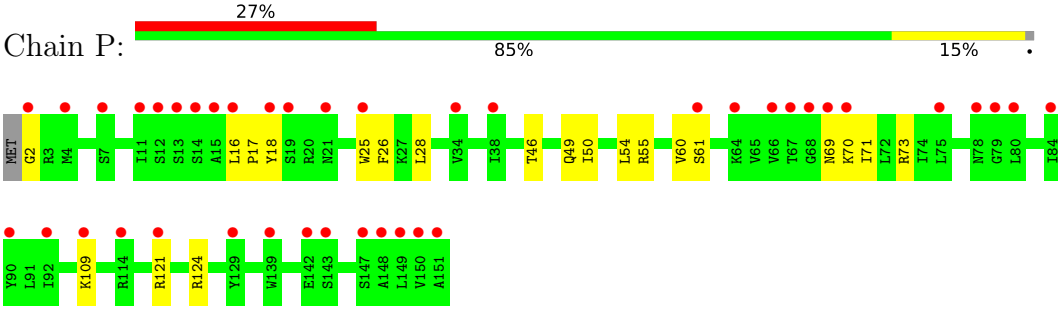

• Molecule 59: 40S ribosomal protein S12

Chain CZ:



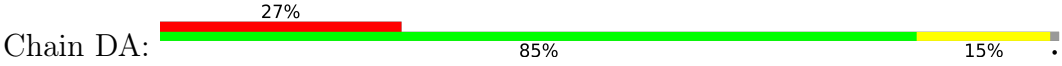

• Molecule 60: 40S ribosomal protein S13

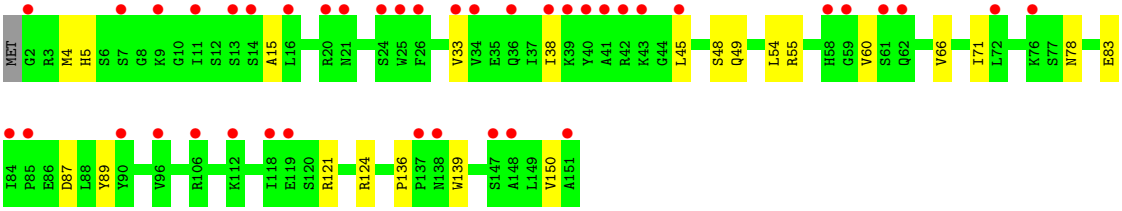
Chain P:




• Molecule 60: 40S ribosomal protein S13

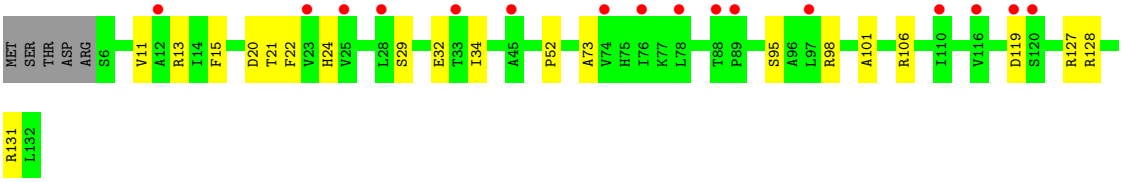
Chain DA:





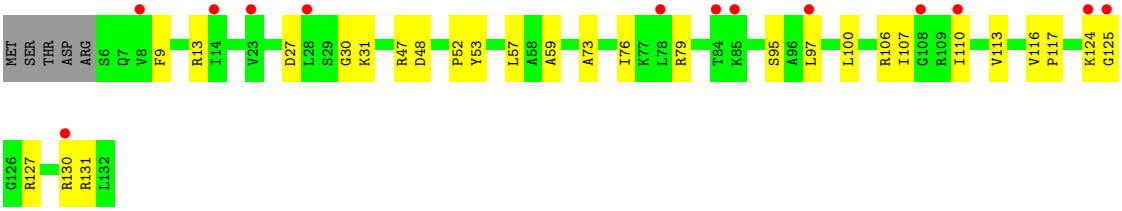

• Molecule 61: 40S ribosomal protein S14-A

Chain Q:



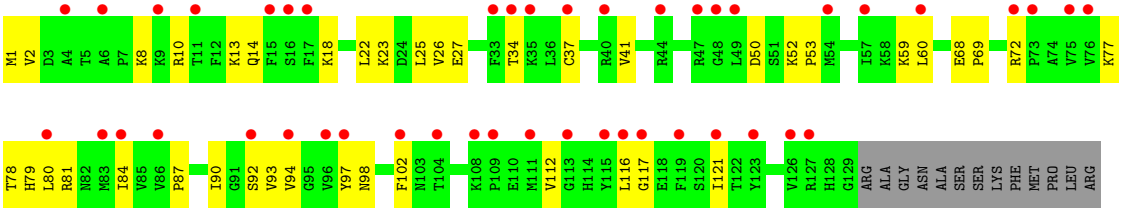

• Molecule 61: 40S ribosomal protein S14-A

Chain DB:



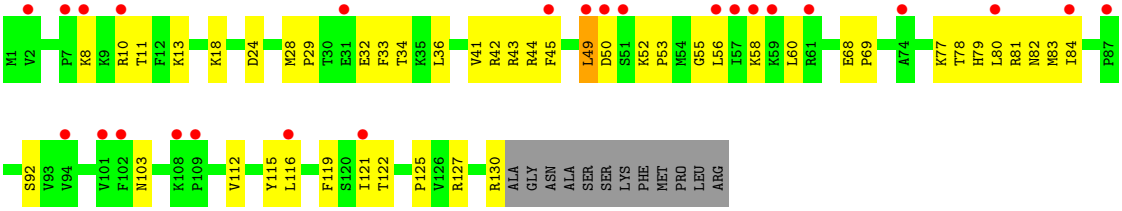

• Molecule 62: 40S ribosomal protein S15

Chain R:



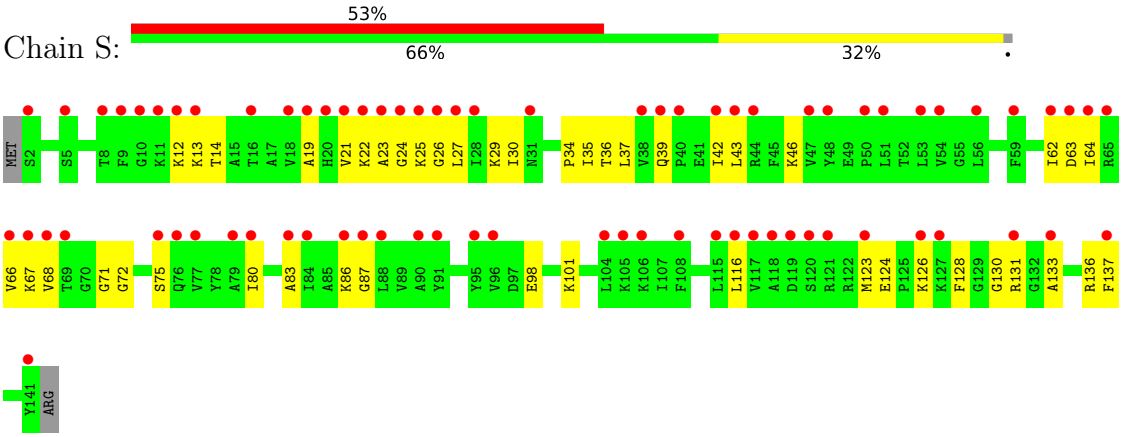

• Molecule 62: 40S ribosomal protein S15

Chain DC:



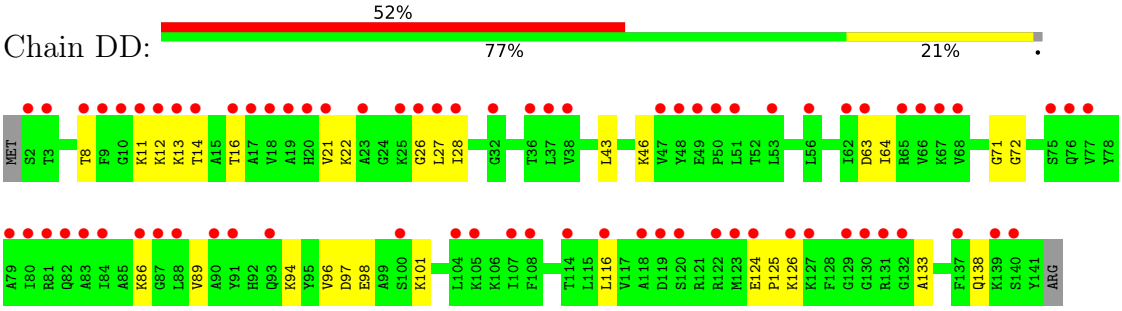
• Molecule 63: 40S ribosomal protein S16

Chain S:



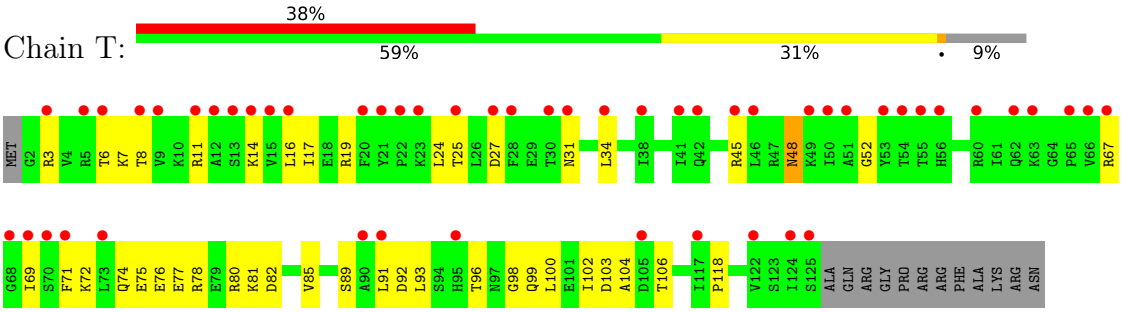

• Molecule 63: 40S ribosomal protein S16

Chain DD:



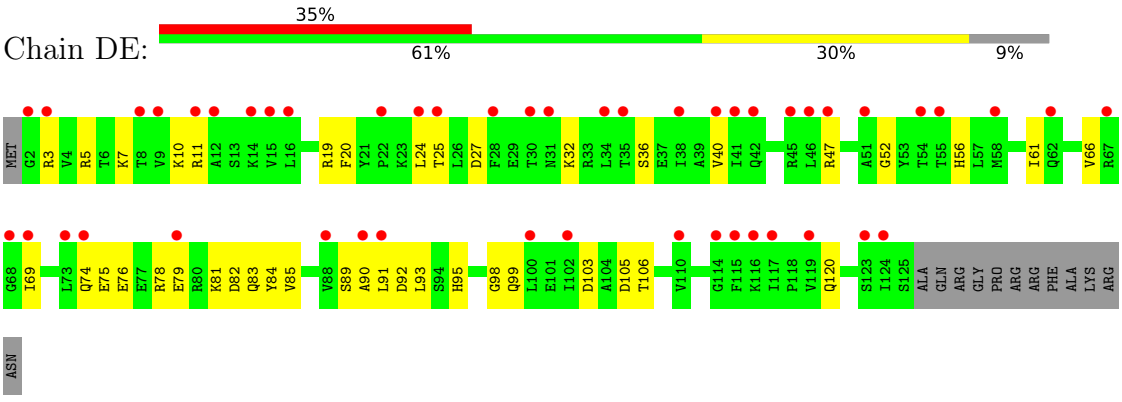

• Molecule 64: 40S ribosomal protein S17-B

Chain T:



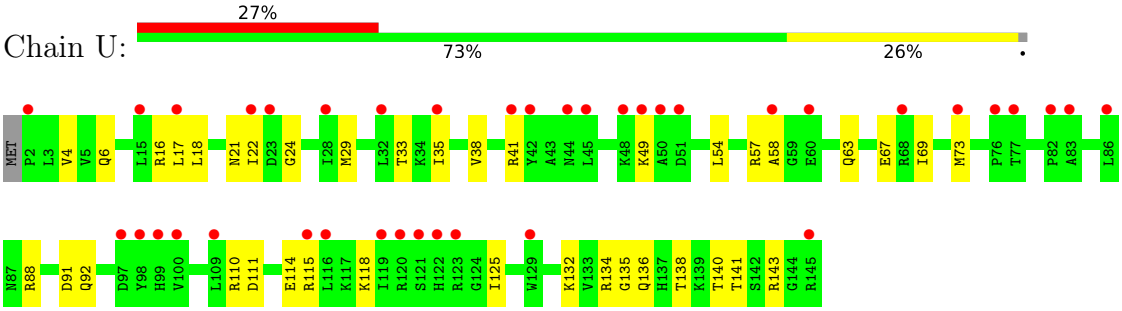

• Molecule 64: 40S ribosomal protein S17-B

Chain DE:



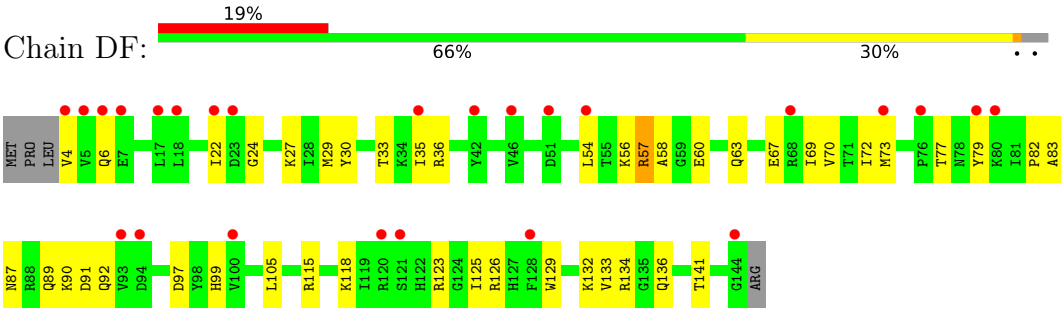

• Molecule 65: 40S ribosomal protein S18-B

Chain U:



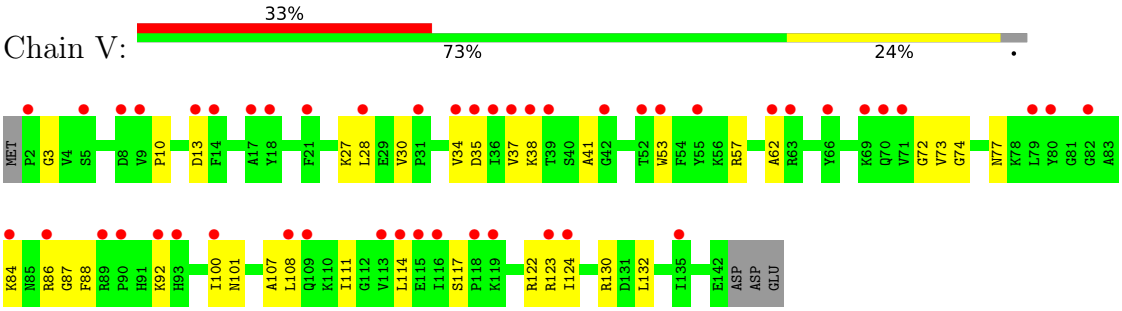

• Molecule 65: 40S ribosomal protein S18-B

Chain DF:



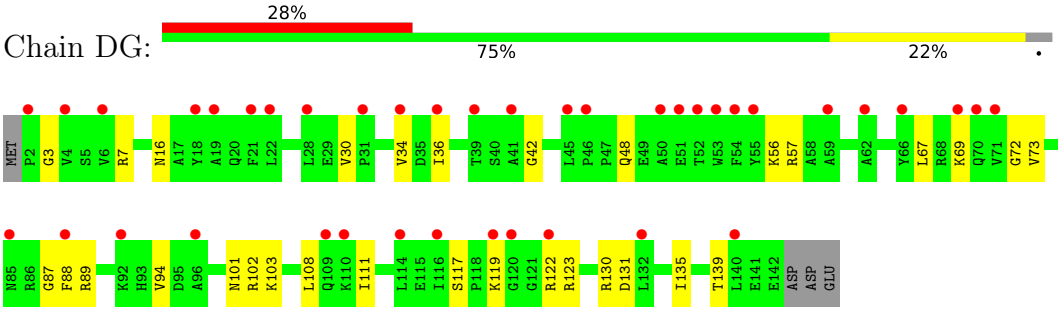

• Molecule 66: 40S ribosomal protein S19-A

Chain V:



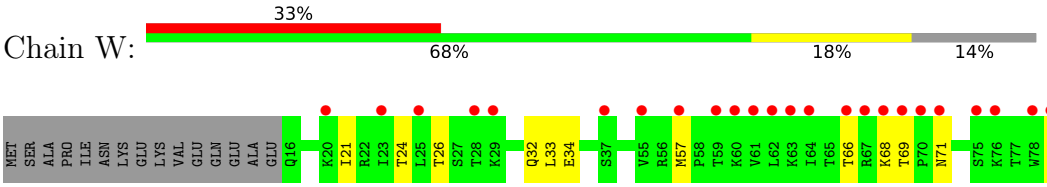

• Molecule 66: 40S ribosomal protein S19-A

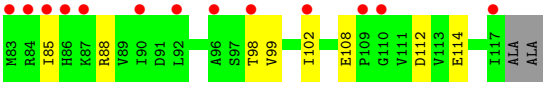
Chain DG:




• Molecule 67: Ribosomal protein S10

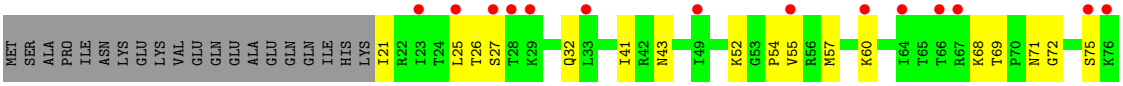
Chain W:

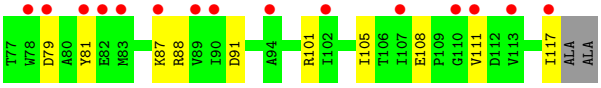





• Molecule 67: Ribosomal protein S10

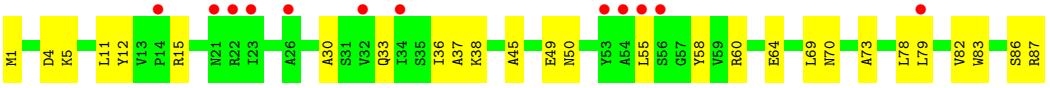
Chain DH:



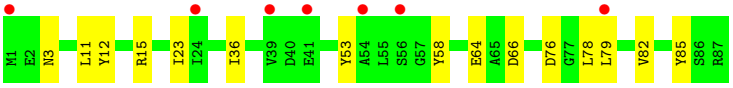

• Molecule 68: 40S ribosomal protein S21

Chain X:



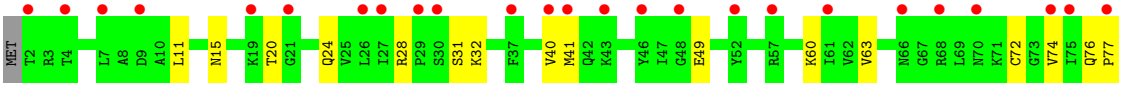

• Molecule 68: 40S ribosomal protein S21

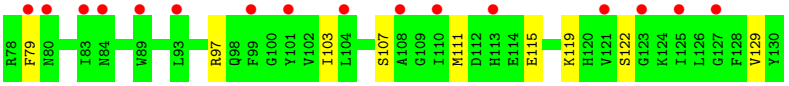
Chain DI:




• Molecule 69: 40S ribosomal protein S22-A

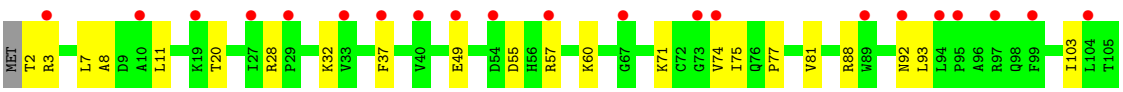
Chain Y:

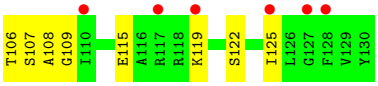



• Molecule 69: 40S ribosomal protein S22-A

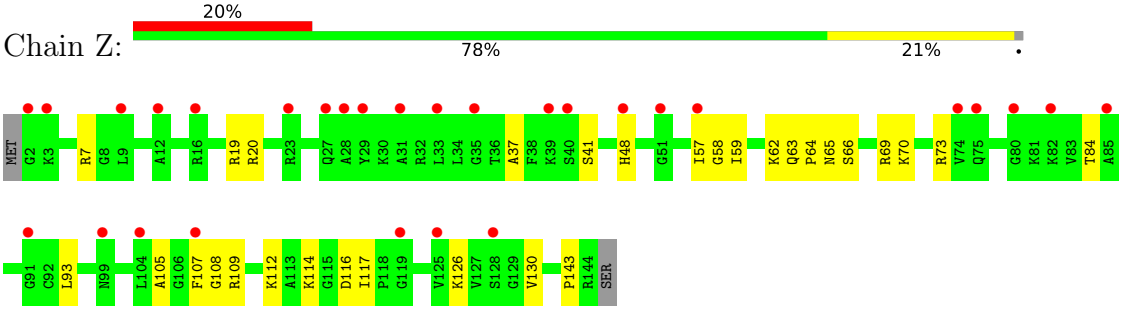
Chain DJ:



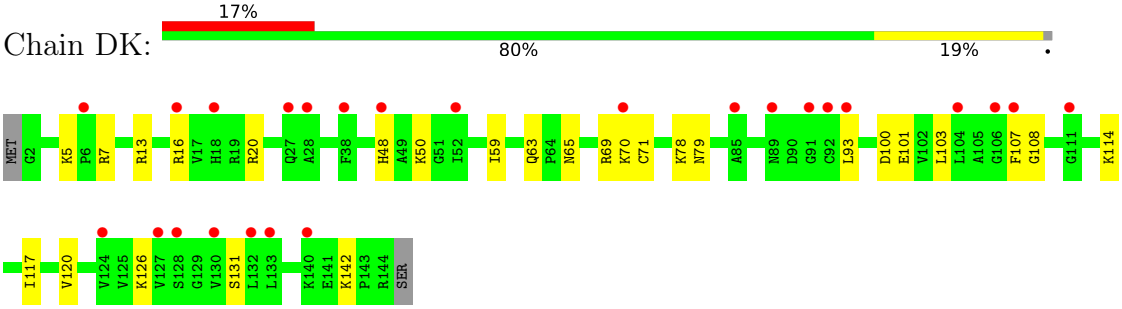
• Molecule 70: Ribosomal protein S23 (S12)

Chain Z:



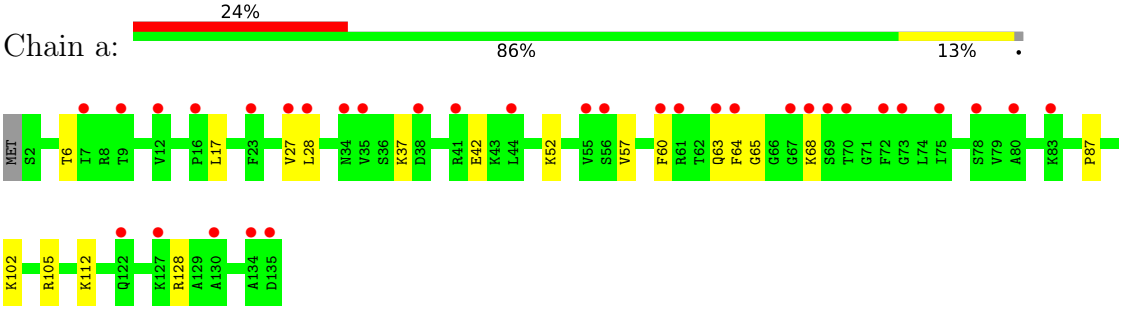

• Molecule 70: Ribosomal protein S23 (S12)

Chain DK:



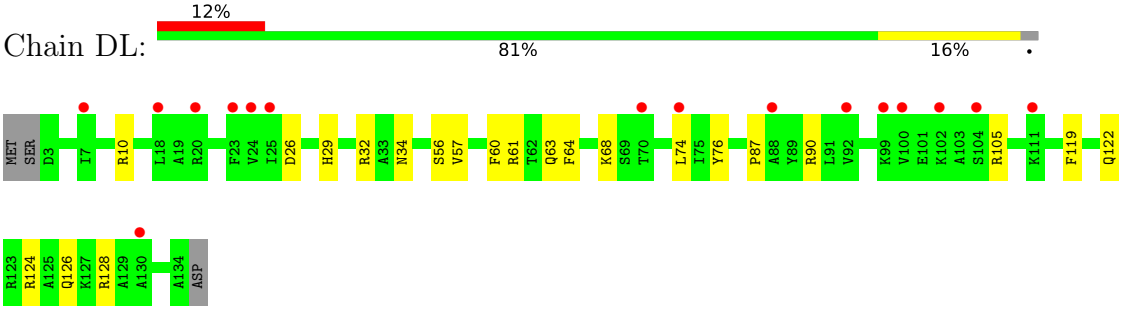

• Molecule 71: 40S ribosomal protein S24

Chain a:



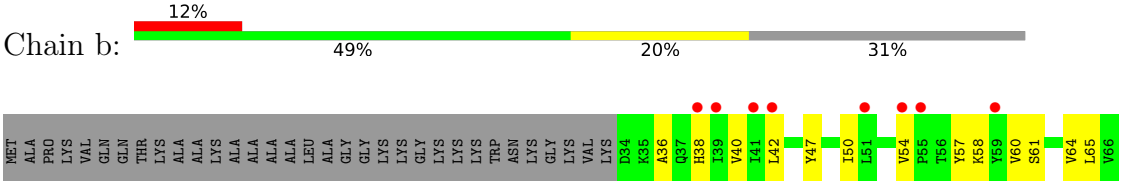

• Molecule 71: 40S ribosomal protein S24

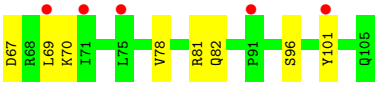
Chain DL:




• Molecule 72: 40S ribosomal protein S25

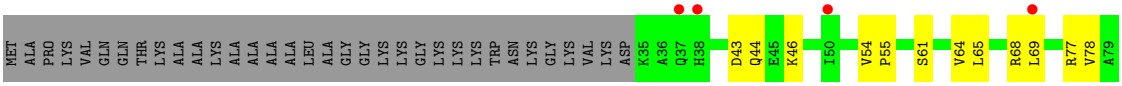
Chain b:

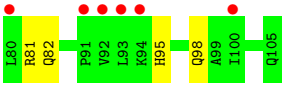





• Molecule 72: 40S ribosomal protein S25

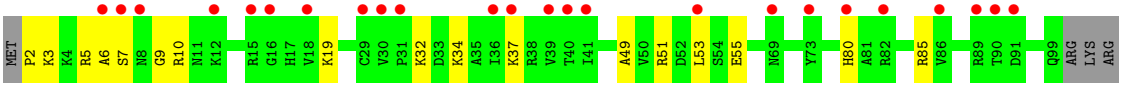
Chain DM:



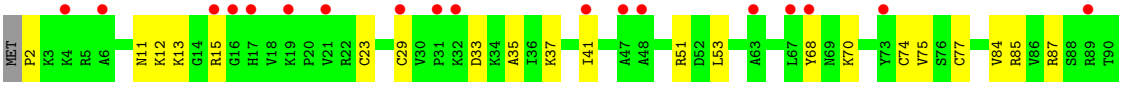

• Molecule 73: 40S ribosomal protein S26

Chain c:



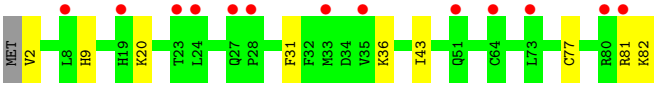
• Molecule 73: 40S ribosomal protein S26

Chain DN:



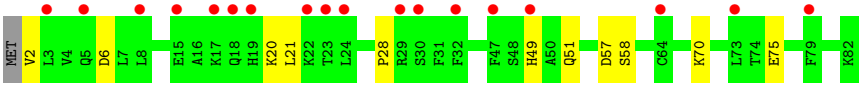
• Molecule 74: 40S ribosomal protein S27

Chain d:



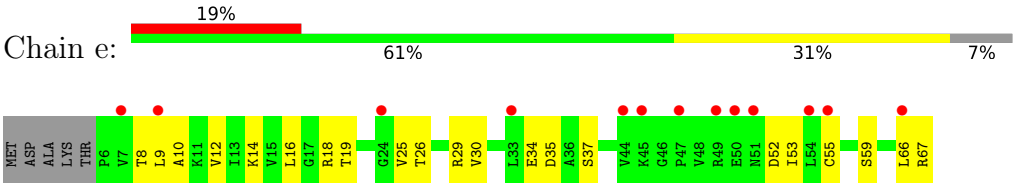

• Molecule 74: 40S ribosomal protein S27

Chain DO:



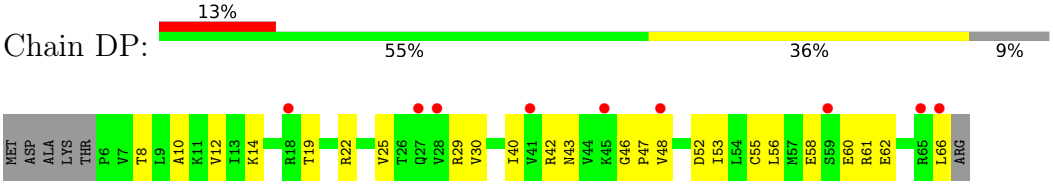
• Molecule 75: 40S ribosomal protein S28-B

Chain e:



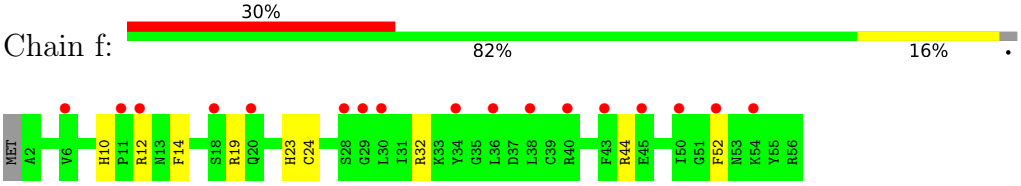

• Molecule 75: 40S ribosomal protein S28-B

Chain DP:



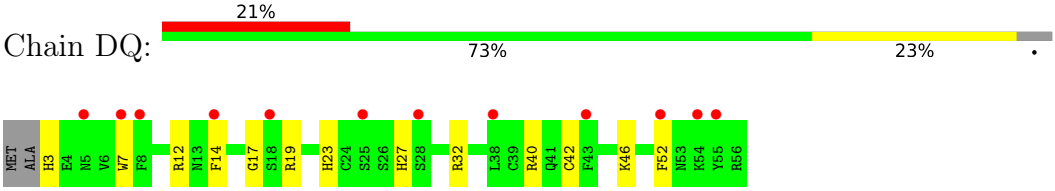

• Molecule 76: 40S ribosomal protein S29A

Chain f:



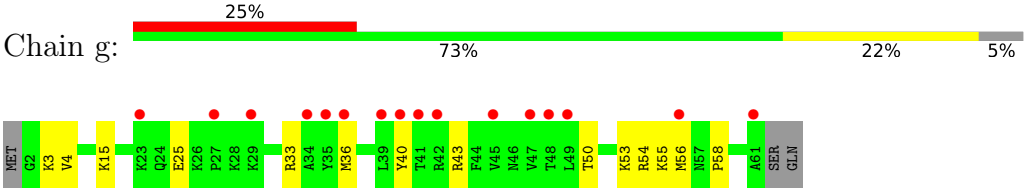

• Molecule 76: 40S ribosomal protein S29A

Chain DQ:



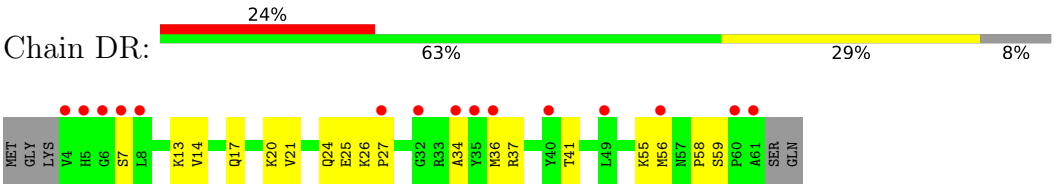

• Molecule 77: 40S ribosomal protein S30

Chain g:



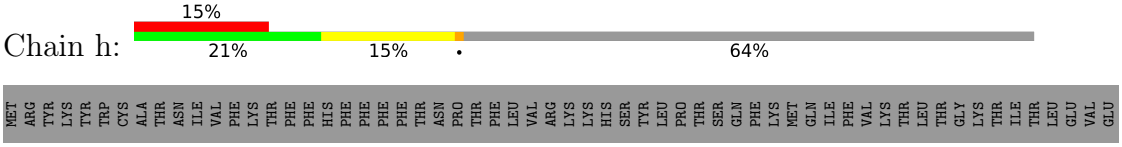

• Molecule 77: 40S ribosomal protein S30

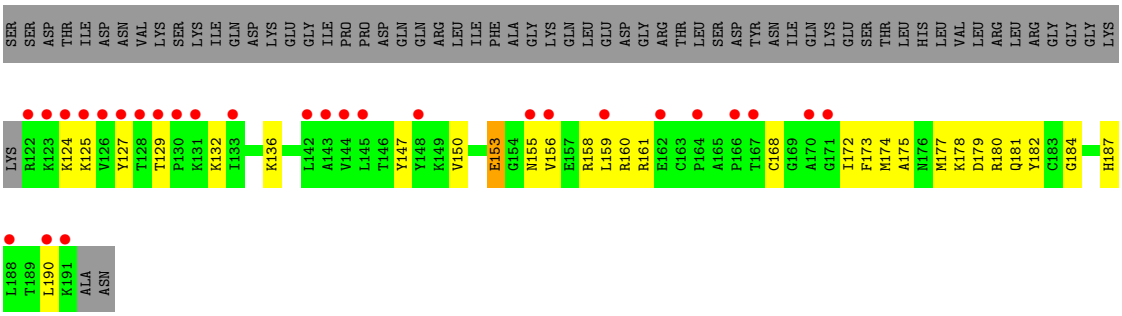
Chain DR:




• Molecule 78: Ubiquitin-40S ribosomal protein S31 fusion protein

Chain h:

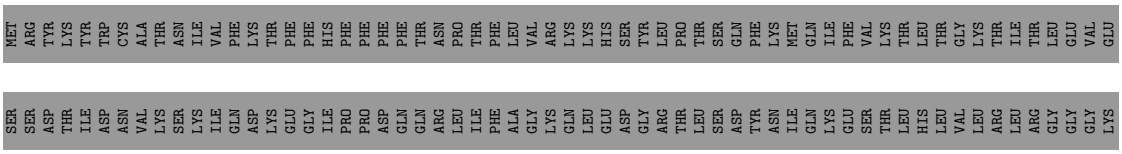


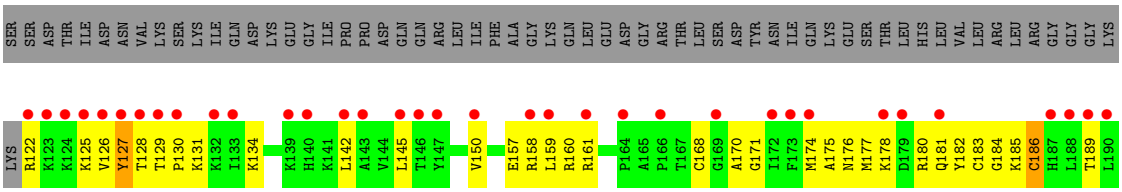




• Molecule 78: Ubiquitin-40S ribosomal protein S31 fusion protein

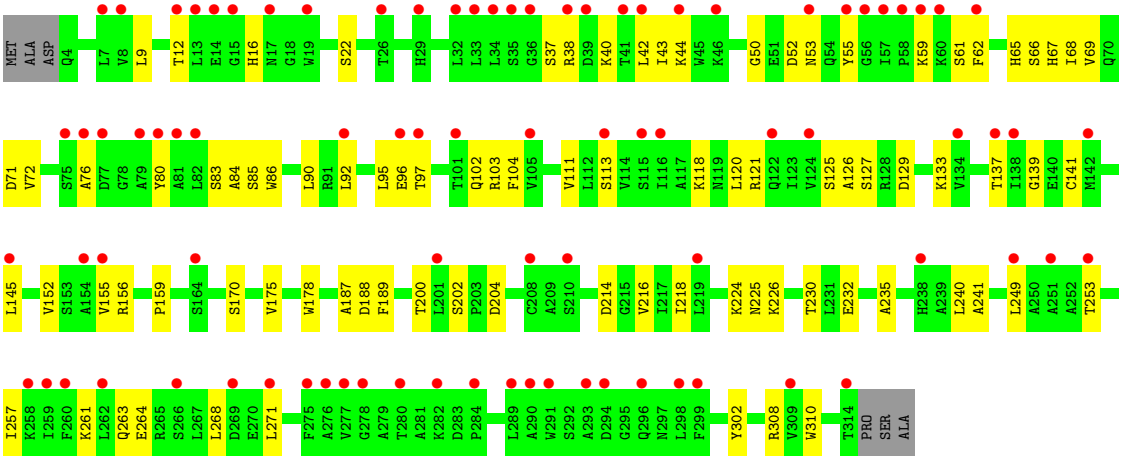
Chain DS:





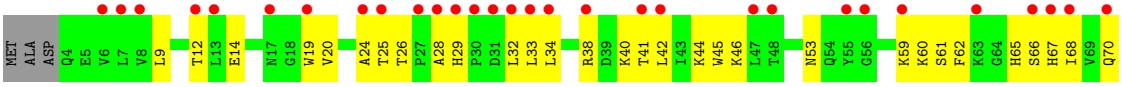
• Molecule 79: Guanine nucleotide-binding protein subunit beta-like protein

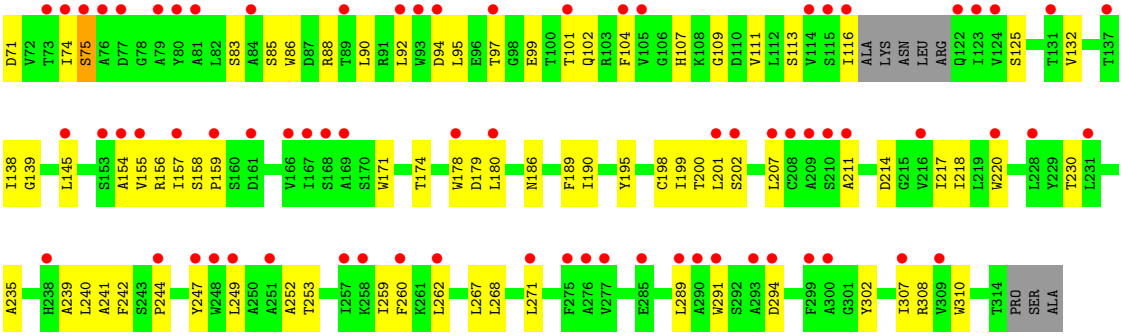
Chain AR:



• Molecule 79: Guanine nucleotide-binding protein subunit beta-like protein

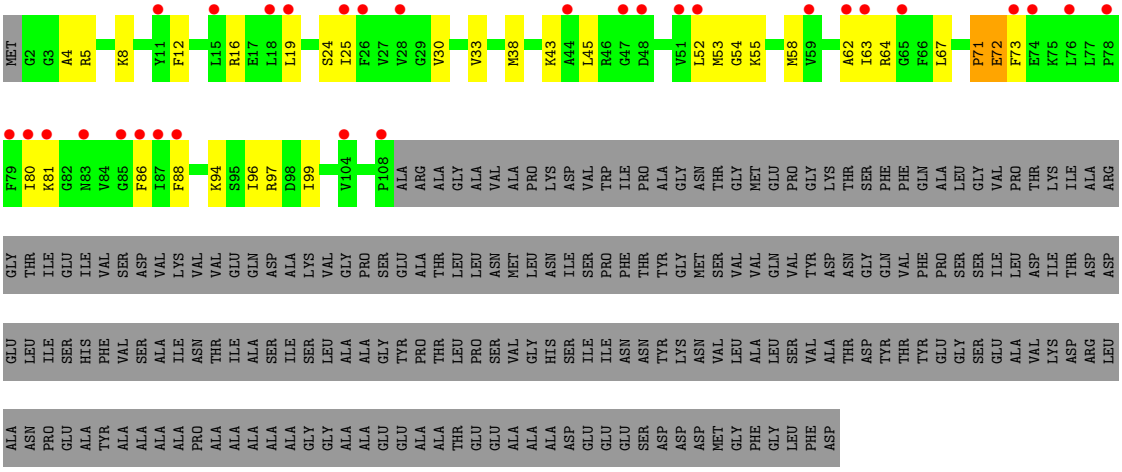
Chain DT:





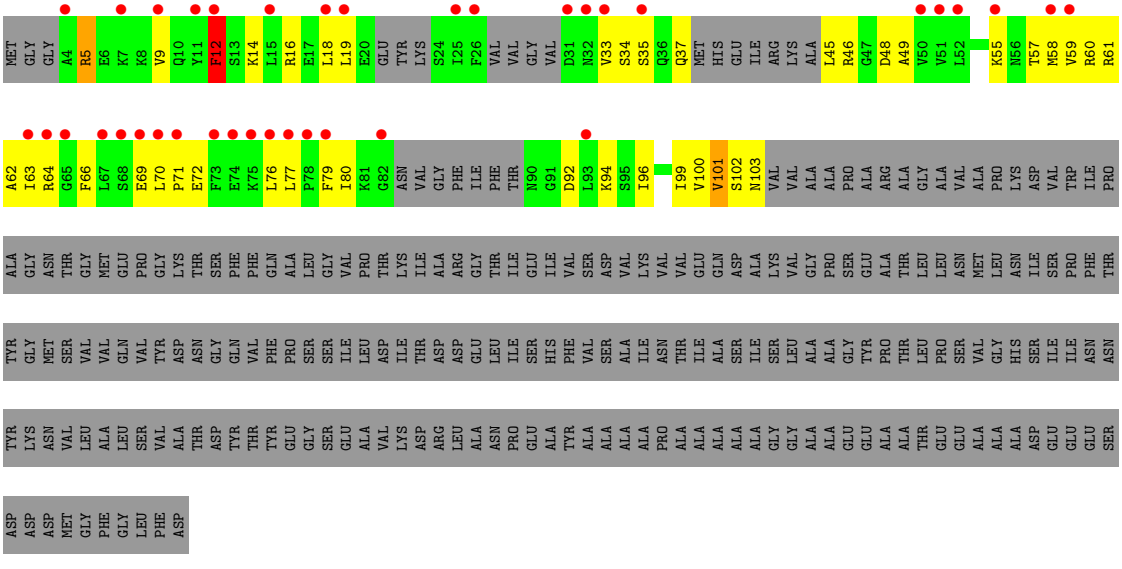

• Molecule 80: 60S acidic ribosomal protein P0

Chain P0:



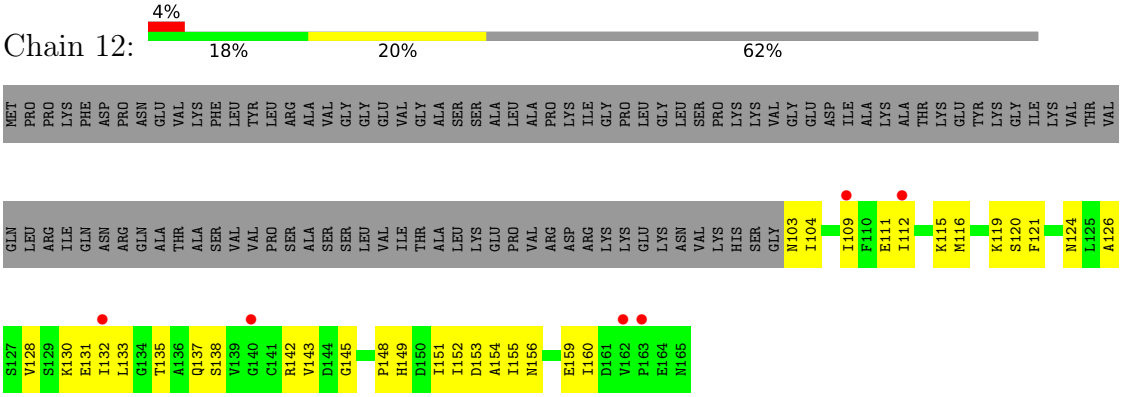

• Molecule 80: 60S acidic ribosomal protein P0

Chain p0:



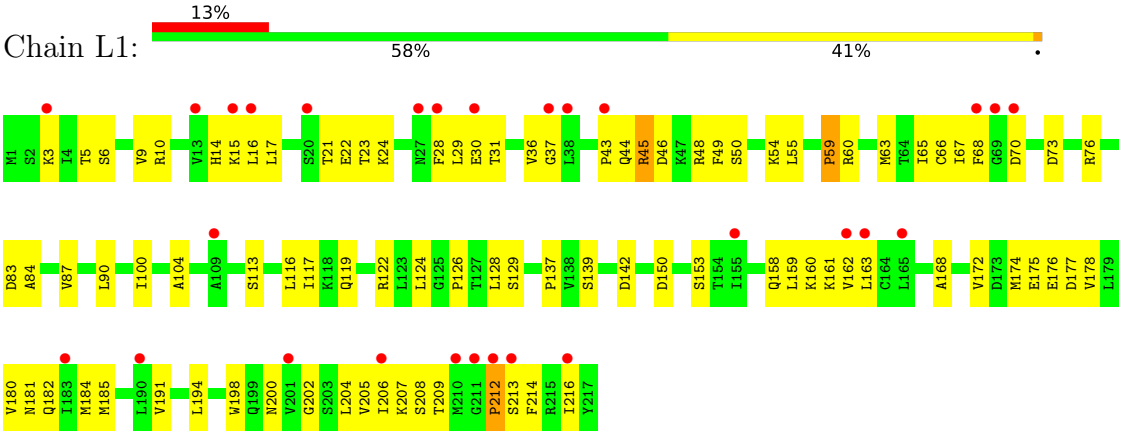
• Molecule 81: 60S ribosomal protein L12-A

Chain 12:



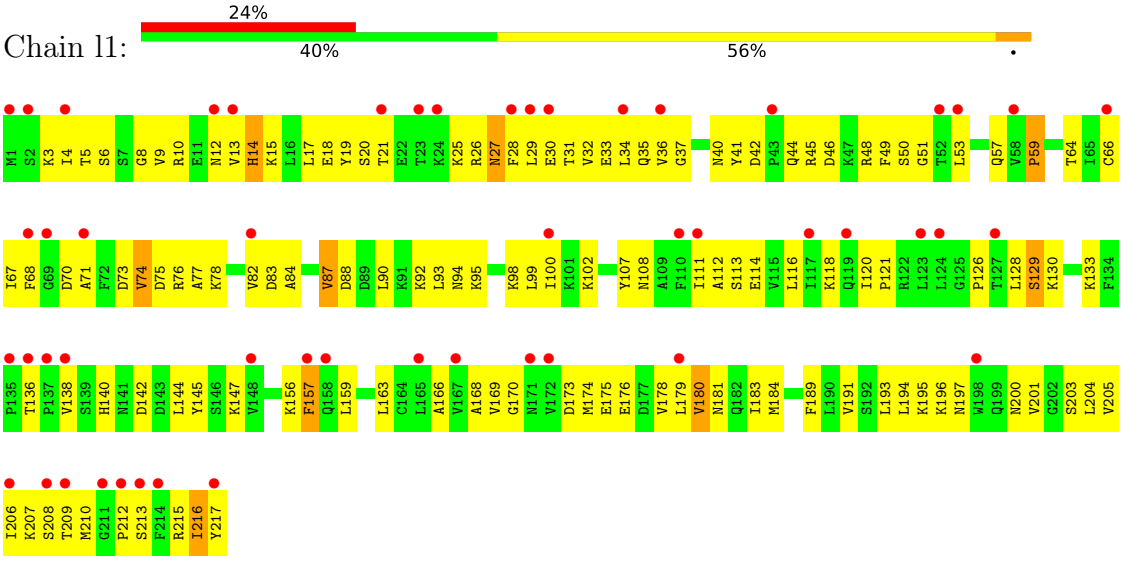

• Molecule 82: Ribosomal protein

Chain L1:




• Molecule 82: Ribosomal protein

Chain l1:



# 4 Data and refinement statistics (i)

| Property | Value | Source |
|---|---|---|
| Space group | P 1 21 1 | Depositor |
| Cell constants<br>a, b, c, $\alpha$, $\beta$, $\gamma$ | 298.81Å 292.84Å 450.18Å<br>90.00° 100.11° 90.00° | Depositor |
| Resolution (Å) | 163.72 – 3.05<br>163.72 – 3.05 | Depositor<br>EDS |
| % Data completeness<br>(in resolution range) | 99.1 (163.72-3.05)<br>89.6 (163.72-3.05) | Depositor<br>EDS |
| $R_{merge}$ | 0.84 | Depositor |
| $R_{sym}$ | (Not available) | Depositor |
| $< I/\sigma(I) >$ [1] | 1.00 (at 3.07Å) | Xtriage |
| Refinement program | PHENIX (1.19rc4_4035: ???) | Depositor |
| R, $R_{free}$ | 0.283 , 0.307<br>(Not available) , 0.283 | Depositor<br>DCC |
| $R_{free}$ test set | 2000 reflections (0.14%) | wwPDB-VP |
| Wilson B-factor (Å$^2$) | 50.5 | Xtriage |
| Anisotropy | 0.070 | Xtriage |
| Bulk solvent $k_{sol}$(e/Å$^3$), $B_{sol}$(Å$^2$) | 0.27 , 40.9 | EDS |
| L-test for twinning[2] | $< \|L\| > = 0.40$, $< L^2 > = 0.23$ | Xtriage |
| Estimated twinning fraction | No twinning to report. | Xtriage |
| $F_o$,$F_c$ correlation | 0.85 | EDS |
| Total number of atoms | 408804 | wwPDB-VP |
| Average B, all atoms (Å$^2$) | 87.0 | wwPDB-VP |

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 1.31% of the height of the origin peak. No significant pseudotranslation is detected.*

[1] Intensities estimated from amplitudes.

[2] Theoretical values of $< |L| >$, $< L^2 >$ for acentric reflections are 0.5, 0.333 respectively for untwinned datasets, and 0.375, 0.2 for perfectly twinned datasets.

# 5 Model quality

## 5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: 3K5, HYG, ZN, MG

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

| Mol | Chain | Bond lengths | | Bond angles | |
|---|---|---|---|---|---|
| | | RMSZ | #$\|Z\|>5$ | RMSZ | #$\|Z\|>5$ |
| 1 | 1 | 0.18 | 0/76756 | 0.44 | 8/119655 (0.0%) |
| 1 | AS | 0.17 | 0/77209 | 0.42 | 3/120366 (0.0%) |
| 2 | 3 | 0.15 | 0/2884 | 0.32 | 0/4492 |
| 2 | AT | 0.15 | 0/2884 | 0.32 | 0/4492 |
| 3 | 4 | 0.15 | 0/3724 | 0.38 | 1/5798 (0.0%) |
| 3 | AU | 0.15 | 0/3724 | 0.38 | 1/5798 (0.0%) |
| 4 | AW | 0.14 | 0/1922 | 0.36 | 0/2581 |
| 4 | j | 0.17 | 0/1922 | 0.41 | 0/2581 |
| 5 | AX | 0.15 | 0/3145 | 0.40 | 0/4231 |
| 5 | k | 0.16 | 0/3145 | 0.42 | 0/4231 |
| 6 | AY | 0.14 | 0/2799 | 0.38 | 0/3777 |
| 6 | l | 0.16 | 0/2799 | 0.42 | 0/3777 |
| 7 | AZ | 0.14 | 0/2447 | 0.36 | 0/3294 |
| 7 | m | 0.16 | 0/2479 | 0.43 | 0/3337 |
| 8 | BA | 0.14 | 0/1231 | 0.38 | 0/1662 |
| 8 | n | 0.15 | 0/1263 | 0.38 | 0/1703 |
| 9 | BB | 0.14 | 0/1918 | 0.35 | 0/2575 |
| 9 | o | 0.16 | 0/1909 | 0.38 | 0/2563 |
| 10 | BC | 0.27 | 0/1807 | 0.51 | 0/2434 |
| 10 | p | 0.17 | 0/1835 | 0.42 | 0/2472 |
| 11 | BD | 0.15 | 0/1537 | 0.39 | 0/2067 |
| 11 | q | 0.17 | 0/1528 | 0.42 | 0/2055 |
| 12 | BE | 0.17 | 0/1724 | 0.42 | 0/2314 |
| 12 | r | 0.22 | 0/1724 | 0.42 | 0/2314 |
| 13 | BF | 0.15 | 0/1390 | 0.40 | 0/1861 |
| 13 | s | 0.17 | 0/1390 | 0.44 | 0/1861 |
| 14 | BG | 0.17 | 0/1637 | 0.42 | 0/2195 |
| 14 | t | 0.16 | 0/1637 | 0.40 | 0/2195 |
| 15 | BH | 0.14 | 0/1044 | 0.38 | 0/1407 |
| 15 | u | 0.18 | 0/1044 | 0.40 | 0/1407 |
| 16 | BI | 0.14 | 0/1753 | 0.39 | 0/2347 |
| 16 | v | 0.17 | 0/1753 | 0.39 | 0/2347 |

| Mol | Chain | Bond lengths | | Bond angles | |
|---|---|---|---|---|---|
| | | RMSZ | #\|Z\| >5 | RMSZ | #\|Z\| >5 |
| 17 | BJ | 0.17 | 0/1620 | 0.40 | 0/2167 |
| 17 | w | 0.16 | 0/1620 | 0.39 | 0/2167 |
| 18 | BK | 0.15 | 0/1429 | 0.38 | 0/1920 |
| 18 | x | 0.14 | 0/1410 | 0.38 | 0/1895 |
| 19 | BL | 0.14 | 0/1482 | 0.34 | 0/1985 |
| 19 | y | 0.14 | 0/1482 | 0.37 | 0/1985 |
| 20 | BM | 0.14 | 0/1475 | 0.40 | 0/1961 |
| 20 | z | 0.16 | 0/1475 | 0.37 | 0/1961 |
| 21 | 0 | 0.15 | 0/1457 | 0.39 | 0/1962 |
| 21 | BN | 0.15 | 0/1457 | 0.36 | 0/1962 |
| 22 | 2 | 0.18 | 0/1285 | 0.44 | 0/1723 |
| 22 | BO | 0.15 | 0/1285 | 0.38 | 0/1723 |
| 23 | 5 | 0.31 | 0/841 | 0.50 | 0/1133 |
| 23 | BP | 0.16 | 0/841 | 0.47 | 0/1133 |
| 24 | 6 | 0.14 | 0/993 | 0.38 | 0/1339 |
| 24 | BQ | 0.14 | 0/993 | 0.38 | 0/1339 |
| 25 | 7 | 0.14 | 0/958 | 0.30 | 0/1267 |
| 25 | BR | 0.13 | 0/814 | 0.28 | 0/1079 |
| 26 | 8 | 0.14 | 0/981 | 0.36 | 0/1326 |
| 26 | BS | 0.11 | 0/976 | 0.32 | 0/1319 |
| 27 | 9 | 0.13 | 0/999 | 0.34 | 0/1334 |
| 27 | BT | 0.12 | 0/999 | 0.36 | 0/1334 |
| 28 | AA | 0.13 | 0/1112 | 0.34 | 0/1488 |
| 28 | BU | 0.13 | 0/1112 | 0.36 | 0/1488 |
| 29 | AB | 0.14 | 0/1199 | 0.38 | 0/1607 |
| 29 | BV | 0.16 | 0/1199 | 0.36 | 0/1607 |
| 30 | AC | 0.19 | 0/503 | 0.56 | 0/668 |
| 30 | BW | 0.15 | 0/498 | 0.38 | 0/661 |
| 31 | AD | 0.13 | 0/738 | 0.32 | 0/994 |
| 31 | BX | 0.12 | 0/738 | 0.38 | 0/994 |
| 32 | AE | 0.14 | 0/907 | 0.40 | 0/1219 |
| 32 | BY | 0.15 | 0/907 | 0.43 | 0/1219 |
| 33 | AF | 0.15 | 0/1021 | 0.37 | 0/1368 |
| 33 | BZ | 0.14 | 0/1025 | 0.40 | 0/1372 |
| 34 | AG | 0.13 | 0/866 | 0.35 | 0/1165 |
| 34 | CA | 0.20 | 0/866 | 0.38 | 0/1165 |
| 35 | AH | 0.14 | 0/896 | 0.39 | 0/1195 |
| 35 | CB | 0.13 | 0/896 | 0.39 | 0/1195 |
| 36 | AI | 0.14 | 0/1003 | 0.37 | 0/1336 |
| 36 | CC | 0.13 | 0/990 | 0.37 | 0/1319 |
| 37 | AJ | 0.34 | 0/763 | 0.56 | 1/1012 (0.1%) |
| 37 | CD | 0.12 | 0/763 | 0.37 | 0/1012 |
| 38 | AK | 0.15 | 0/690 | 0.39 | 0/916 |

| Mol | Chain | Bond lengths | | Bond angles | |
|---|---|---|---|---|---|
| | | RMSZ | #\|Z\| >5 | RMSZ | #\|Z\| >5 |
| 38 | CE | 0.18 | 0/690 | 0.38 | 0/916 |
| 39 | AL | 0.12 | 0/623 | 0.35 | 0/831 |
| 39 | CF | 0.17 | 0/623 | 0.46 | 0/831 |
| 40 | AM | 0.14 | 0/447 | 0.32 | 0/594 |
| 40 | CG | 0.15 | 0/447 | 0.42 | 0/594 |
| 41 | AN | 0.27 | 0/425 | 0.57 | 0/563 |
| 41 | CH | 0.26 | 0/417 | 0.54 | 0/553 |
| 42 | AO | 0.23 | 0/237 | 0.42 | 0/304 |
| 42 | CI | 0.15 | 0/228 | 0.37 | 0/293 |
| 43 | AP | 0.16 | 0/840 | 0.39 | 0/1110 |
| 43 | CJ | 0.17 | 0/840 | 0.36 | 0/1110 |
| 44 | AQ | 0.16 | 0/705 | 0.39 | 0/940 |
| 44 | CK | 0.13 | 0/705 | 0.37 | 0/940 |
| 45 | CL | 0.33 | 0/942 | 0.78 | 0/1258 |
| 45 | i | 0.41 | 0/933 | 0.90 | 3/1246 (0.2%) |
| 46 | B | 0.19 | 0/41511 | 0.46 | 11/64681 (0.0%) |
| 46 | CM | 0.19 | 0/42081 | 0.46 | 12/65573 (0.0%) |
| 47 | C | 0.12 | 0/1666 | 0.34 | 0/2273 |
| 47 | CN | 0.14 | 0/1666 | 0.39 | 0/2273 |
| 48 | CO | 0.17 | 0/1750 | 0.45 | 0/2354 |
| 48 | D | 0.13 | 0/1750 | 0.36 | 0/2354 |
| 49 | CP | 0.16 | 0/1657 | 0.38 | 0/2248 |
| 49 | E | 0.13 | 0/1657 | 0.34 | 0/2248 |
| 50 | CQ | 0.19 | 0/1731 | 0.53 | 0/2324 |
| 50 | F | 0.16 | 0/1731 | 0.48 | 1/2324 (0.0%) |
| 51 | CR | 0.15 | 0/2096 | 0.37 | 0/2822 |
| 51 | G | 0.13 | 0/2092 | 0.36 | 0/2817 |
| 52 | CS | 0.18 | 0/1631 | 0.40 | 0/2199 |
| 52 | H | 0.34 | 0/1631 | 0.55 | 0/2199 |
| 53 | CT | 0.14 | 0/1929 | 0.42 | 0/2571 |
| 53 | I | 0.13 | 0/1845 | 0.37 | 0/2464 |
| 54 | CU | 0.34 | 0/1499 | 0.47 | 0/2016 |
| 54 | J | 0.15 | 0/1510 | 0.39 | 0/2031 |
| 55 | CV | 0.15 | 0/1606 | 0.38 | 0/2150 |
| 55 | K | 0.16 | 0/1606 | 0.38 | 0/2150 |
| 56 | CW | 0.13 | 0/1478 | 0.35 | 0/1978 |
| 56 | L | 0.13 | 0/1478 | 0.35 | 0/1978 |
| 57 | CX | 0.20 | 0/809 | 0.55 | 0/1092 |
| 57 | M | 0.19 | 0/836 | 0.63 | 0/1130 |
| 58 | CY | 0.16 | 0/1154 | 0.38 | 0/1553 |
| 58 | N | 0.15 | 0/1175 | 0.40 | 0/1582 |
| 59 | CZ | 0.25 | 0/921 | 0.88 | 5/1240 (0.4%) |
| 59 | O | 0.35 | 0/892 | 0.93 | 3/1203 (0.2%) |

| Mol | Chain | Bond lengths | | Bond angles | |
|---|---|---|---|---|---|
| | | RMSZ | #\|Z\| >5 | RMSZ | #\|Z\| >5 |
| 60 | DA | 0.14 | 0/1210 | 0.37 | 0/1631 |
| 60 | P | 0.13 | 0/1210 | 0.35 | 0/1631 |
| 61 | DB | 0.15 | 0/953 | 0.41 | 0/1279 |
| 61 | Q | 0.35 | 0/953 | 0.53 | 0/1279 |
| 62 | DC | 0.19 | 0/1049 | 0.55 | 1/1409 (0.1%) |
| 62 | R | 0.20 | 0/1038 | 0.52 | 0/1395 |
| 63 | DD | 0.15 | 0/1109 | 0.41 | 0/1486 |
| 63 | S | 0.36 | 0/1109 | 0.67 | 2/1486 (0.1%) |
| 64 | DE | 0.18 | 0/1009 | 0.55 | 0/1354 |
| 64 | T | 0.20 | 0/1009 | 0.52 | 0/1354 |
| 65 | DF | 0.24 | 0/1178 | 0.52 | 0/1579 |
| 65 | U | 0.16 | 0/1205 | 0.43 | 0/1615 |
| 66 | DG | 0.16 | 0/1120 | 0.43 | 0/1508 |
| 66 | V | 0.17 | 0/1120 | 0.49 | 0/1508 |
| 67 | DH | 0.16 | 0/772 | 0.45 | 0/1045 |
| 67 | W | 0.15 | 0/818 | 0.41 | 0/1106 |
| 68 | DI | 0.18 | 0/683 | 0.48 | 0/918 |
| 68 | X | 0.15 | 0/683 | 0.39 | 0/918 |
| 69 | DJ | 0.16 | 0/1049 | 0.40 | 0/1412 |
| 69 | Y | 0.14 | 0/1049 | 0.34 | 0/1412 |
| 70 | DK | 0.16 | 0/1128 | 0.43 | 0/1505 |
| 70 | Z | 0.16 | 0/1128 | 0.49 | 0/1505 |
| 71 | DL | 0.13 | 0/1086 | 0.35 | 0/1447 |
| 71 | a | 0.14 | 0/1100 | 0.34 | 0/1466 |
| 72 | DM | 0.16 | 0/577 | 0.47 | 0/778 |
| 72 | b | 0.15 | 0/585 | 0.37 | 0/789 |
| 73 | DN | 0.14 | 0/782 | 0.39 | 0/1048 |
| 73 | c | 0.16 | 0/791 | 0.40 | 0/1060 |
| 74 | DO | 0.15 | 0/624 | 0.44 | 0/843 |
| 74 | d | 0.13 | 0/624 | 0.38 | 0/843 |
| 75 | DP | 0.15 | 0/478 | 0.52 | 0/640 |
| 75 | e | 0.13 | 0/489 | 0.43 | 0/654 |
| 76 | DQ | 0.21 | 0/461 | 0.47 | 0/613 |
| 76 | f | 0.14 | 0/466 | 0.40 | 0/620 |
| 77 | DR | 0.29 | 0/469 | 0.74 | 0/626 |
| 77 | g | 0.22 | 0/482 | 0.49 | 0/642 |
| 78 | DS | 0.38 | 0/585 | 0.88 | 2/778 (0.3%) |
| 78 | h | 0.40 | 0/585 | 0.75 | 0/778 |
| 79 | AR | 0.14 | 0/2451 | 0.38 | 0/3337 |
| 79 | DT | 0.19 | 0/2409 | 0.52 | 0/3280 |
| 80 | P0 | 0.17 | 0/857 | 0.44 | 0/1148 |
| 80 | p0 | 0.45 | 0/638 | 0.88 | 1/845 (0.1%) |
| 81 | 12 | 0.20 | 0/486 | 0.53 | 0/653 |

| Mol | Chain | Bond lengths | | Bond angles | |
|---|---|---|---|---|---|
| | | RMSZ | #\|Z\| >5 | RMSZ | #\|Z\| >5 |
| 82 | L1 | 0.21 | 0/1737 | 0.43 | 0/2335 |
| 82 | l1 | 0.35 | 0/1737 | 0.60 | 0/2335 |
| All | All | 0.18 | 0/437098 | 0.44 | 55/641006 (0.0%) |

There are no bond length outliers.

All (55) bond angle outliers are listed below:

| Mol | Chain | Res | Type | Atoms | Z | Observed($^o$) | Ideal($^o$) |
|---|---|---|---|---|---|---|---|
| 46 | CM | 823 | G | C4'-C3'-O3' | 9.09 | 123.04 | 109.40 |
| 1 | 1 | 3163 | U | OP1-P-O3' | -8.86 | 81.41 | 108.00 |
| 1 | 1 | 3163 | U | OP2-P-O3' | -8.22 | 83.34 | 108.00 |
| 46 | B | 653 | G | O5'-P-OP2 | -7.93 | 84.20 | 108.00 |
| 1 | 1 | 1653 | C | C3'-C2'-O2' | -7.60 | 103.20 | 114.60 |
| 46 | B | 1703 | C | C4'-C3'-O3' | 7.58 | 120.77 | 109.40 |
| 46 | CM | 823 | G | P-O5'-C5' | -7.36 | 109.86 | 120.90 |
| 45 | i | 65 | LYS | N-CA-C | -7.09 | 106.53 | 114.62 |
| 46 | B | 1742 | A | O4'-C1'-N9 | 7.06 | 119.08 | 108.50 |
| 46 | B | 700 | G | P-O5'-C5' | 7.01 | 131.41 | 120.90 |
| 63 | S | 24 | GLY | N-CA-C | 7.00 | 119.43 | 110.20 |
| 46 | CM | 1672 | G | O3'-P-O5' | 6.69 | 114.03 | 104.00 |
| 59 | CZ | 81 | GLU | C-N-CD | -6.61 | 97.88 | 125.00 |
| 1 | AS | 1247 | A | O3'-P-O5' | 6.59 | 113.89 | 104.00 |
| 59 | O | 39 | ASP | N-CA-C | -6.54 | 103.78 | 113.72 |
| 1 | AS | 1576 | A | O4'-C1'-N9 | 6.52 | 118.28 | 108.50 |
| 62 | DC | 49 | LEU | CB-CA-C | -6.38 | 107.41 | 116.34 |
| 1 | 1 | 1576 | A | O4'-C1'-N9 | 6.29 | 117.94 | 108.50 |
| 46 | CM | 725 | A | O5'-C5'-C4' | -6.24 | 102.15 | 111.50 |
| 78 | DS | 130 | PRO | CA-C-N | 6.07 | 129.49 | 120.87 |
| 78 | DS | 130 | PRO | C-N-CA | 6.07 | 129.49 | 120.87 |
| 46 | B | 1703 | C | C3'-C2'-O2' | -5.90 | 105.75 | 114.60 |
| 45 | i | 62 | ALA | N-CA-C | -5.85 | 106.77 | 112.97 |
| 59 | CZ | 82 | PRO | CA-C-N | 5.82 | 132.66 | 121.54 |
| 59 | CZ | 82 | PRO | C-N-CA | 5.82 | 132.66 | 121.54 |
| 46 | CM | 970 | G | O3'-P-O5' | 5.81 | 112.72 | 104.00 |
| 1 | 1 | 446 | U | O3'-P-O5' | -5.78 | 95.34 | 104.00 |
| 46 | CM | 725 | A | C5'-C4'-C3' | -5.74 | 107.39 | 116.00 |
| 63 | S | 42 | ILE | CB-CG1-CD1 | -5.68 | 101.86 | 113.80 |
| 37 | AJ | 97 | ARG | CA-C-O | -5.66 | 114.84 | 121.07 |
| 46 | B | 653 | G | O5'-P-OP1 | 5.54 | 124.63 | 108.00 |
| 80 | p0 | 12 | PHE | CA-CB-CG | 5.52 | 119.32 | 113.80 |
| 46 | B | 1742 | A | C4-N9-C1' | -5.45 | 109.94 | 126.30 |
| 46 | CM | 1672 | G | C5'-C4'-C3' | -5.45 | 107.83 | 116.00 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed($^o$) | Ideal($^o$) |
|---|---|---|---|---|---|---|---|
| 46 | B | 1742 | A | C8-N9-C1' | 5.41 | 143.94 | 127.70 |
| 46 | CM | 823 | G | N9-C1'-C2' | -5.37 | 105.95 | 114.00 |
| 59 | O | 42 | ALA | CA-C-N | -5.32 | 112.75 | 122.38 |
| 59 | O | 42 | ALA | C-N-CA | -5.32 | 112.75 | 122.38 |
| 46 | B | 824 | U | P-O5'-C5' | -5.29 | 112.96 | 120.90 |
| 50 | F | 60 | LEU | CA-CB-CG | 5.28 | 134.78 | 116.30 |
| 46 | CM | 825 | U | P-O3'-C3' | 5.26 | 128.09 | 120.20 |
| 3 | 4 | 21 | C | N1-C1'-C2' | 5.24 | 119.86 | 112.00 |
| 1 | AS | 1283 | A | P-O5'-C5' | 5.20 | 128.70 | 120.90 |
| 46 | CM | 814 | A | P-O3'-C3' | 5.16 | 127.94 | 120.20 |
| 1 | 1 | 1653 | C | C2'-C3'-O3' | -5.15 | 101.78 | 109.50 |
| 45 | i | 66 | ASN | N-CA-C | -5.15 | 107.51 | 112.97 |
| 46 | B | 1284 | G | P-O5'-C5' | 5.13 | 128.60 | 120.90 |
| 3 | AU | 21 | C | N1-C1'-C2' | 5.10 | 119.65 | 112.00 |
| 46 | CM | 505 | U | P-O3'-C3' | 5.09 | 127.84 | 120.20 |
| 59 | CZ | 111 | ASN | CA-C-N | 5.09 | 131.26 | 121.54 |
| 59 | CZ | 111 | ASN | C-N-CA | 5.09 | 131.26 | 121.54 |
| 1 | 1 | 2637 | U | C4'-C3'-O3' | -5.08 | 101.78 | 109.40 |
| 1 | 1 | 1230 | G | O4'-C1'-N9 | 5.07 | 116.11 | 108.50 |
| 46 | CM | 722 | A | O3'-P-O5' | -5.07 | 96.40 | 104.00 |
| 46 | B | 824 | U | O4'-C1'-N1 | -5.02 | 100.98 | 108.50 |

There are no chirality outliers.

There are no planarity outliers.

## 5.2 Too-close contacts (i)

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

| Mol | Chain | Non-H | H(model) | H(added) | Clashes | Symm-Clashes |
|---|---|---|---|---|---|---|
| 1 | 1 | 68581 | 0 | 34467 | 1209 | 0 |
| 1 | AS | 68985 | 0 | 34671 | 1173 | 0 |
| 2 | 3 | 2579 | 0 | 1304 | 35 | 0 |
| 2 | AT | 2579 | 0 | 1304 | 27 | 0 |
| 3 | 4 | 3333 | 0 | 1684 | 70 | 0 |
| 3 | AU | 3333 | 0 | 1684 | 66 | 0 |
| 4 | AW | 1888 | 0 | 1962 | 44 | 0 |
| 4 | j | 1888 | 0 | 1962 | 44 | 0 |

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| Mol | Chain | Non-H | H(model) | H(added) | Clashes | Symm-Clashes |
|---|---|---|---|---|---|---|
| 5 | AX | 3077 | 0 | 3166 | 56 | 0 |
| 5 | k | 3077 | 0 | 3166 | 64 | 0 |
| 6 | AY | 2751 | 0 | 2879 | 38 | 0 |
| 6 | l | 2751 | 0 | 2879 | 54 | 0 |
| 7 | AZ | 2394 | 0 | 2361 | 35 | 0 |
| 7 | m | 2426 | 0 | 2389 | 37 | 0 |
| 8 | BA | 1210 | 0 | 1285 | 23 | 0 |
| 8 | n | 1242 | 0 | 1321 | 28 | 0 |
| 9 | BB | 1885 | 0 | 1977 | 20 | 0 |
| 9 | o | 1876 | 0 | 1971 | 20 | 0 |
| 10 | BC | 1778 | 0 | 1897 | 23 | 0 |
| 10 | p | 1805 | 0 | 1925 | 15 | 0 |
| 11 | BD | 1519 | 0 | 1588 | 28 | 0 |
| 11 | q | 1510 | 0 | 1582 | 23 | 0 |
| 12 | BE | 1689 | 0 | 1731 | 19 | 0 |
| 12 | r | 1689 | 0 | 1731 | 26 | 0 |
| 13 | BF | 1371 | 0 | 1410 | 26 | 0 |
| 13 | s | 1371 | 0 | 1410 | 25 | 0 |
| 14 | BG | 1610 | 0 | 1686 | 23 | 0 |
| 14 | t | 1610 | 0 | 1686 | 20 | 0 |
| 15 | BH | 1029 | 0 | 1116 | 24 | 0 |
| 15 | u | 1029 | 0 | 1116 | 22 | 0 |
| 16 | BI | 1713 | 0 | 1764 | 47 | 0 |
| 16 | v | 1713 | 0 | 1763 | 46 | 0 |
| 17 | BJ | 1590 | 0 | 1705 | 19 | 0 |
| 17 | w | 1590 | 0 | 1705 | 26 | 0 |
| 18 | BK | 1406 | 0 | 1431 | 19 | 0 |
| 18 | x | 1387 | 0 | 1408 | 25 | 0 |
| 19 | BL | 1458 | 0 | 1556 | 28 | 0 |
| 19 | y | 1458 | 0 | 1556 | 28 | 0 |
| 20 | BM | 1457 | 0 | 1564 | 31 | 0 |
| 20 | z | 1457 | 0 | 1564 | 27 | 0 |
| 21 | 0 | 1423 | 0 | 1480 | 30 | 0 |
| 21 | BN | 1423 | 0 | 1480 | 29 | 0 |
| 22 | 2 | 1262 | 0 | 1314 | 17 | 0 |
| 22 | BO | 1262 | 0 | 1314 | 22 | 0 |
| 23 | 5 | 826 | 0 | 843 | 13 | 0 |
| 23 | BP | 826 | 0 | 843 | 22 | 0 |
| 24 | 6 | 977 | 0 | 1026 | 9 | 0 |
| 24 | BQ | 977 | 0 | 1026 | 13 | 0 |
| 25 | 7 | 945 | 0 | 1010 | 15 | 0 |
| 25 | BR | 801 | 0 | 840 | 15 | 0 |

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| Mol | Chain | Non-H | H(model) | H(added) | Clashes | Symm-Clashes |
|---|---|---|---|---|---|---|
| 26 | 8 | 965 | 0 | 1019 | 19 | 0 |
| 26 | BS | 960 | 0 | 1014 | 13 | 0 |
| 27 | 9 | 989 | 0 | 1064 | 21 | 0 |
| 27 | BT | 989 | 0 | 1064 | 20 | 0 |
| 28 | AA | 1087 | 0 | 1154 | 19 | 0 |
| 28 | BU | 1087 | 0 | 1154 | 26 | 0 |
| 29 | AB | 1170 | 0 | 1203 | 30 | 0 |
| 29 | BV | 1170 | 0 | 1203 | 27 | 0 |
| 30 | AC | 493 | 0 | 520 | 10 | 0 |
| 30 | BW | 488 | 0 | 515 | 10 | 0 |
| 31 | AD | 729 | 0 | 775 | 13 | 0 |
| 31 | BX | 729 | 0 | 775 | 15 | 0 |
| 32 | AE | 894 | 0 | 941 | 18 | 0 |
| 32 | BY | 894 | 0 | 941 | 10 | 0 |
| 33 | AF | 1000 | 0 | 1069 | 13 | 0 |
| 33 | BZ | 1004 | 0 | 1077 | 13 | 0 |
| 34 | AG | 847 | 0 | 893 | 17 | 0 |
| 34 | CA | 847 | 0 | 893 | 10 | 0 |
| 35 | AH | 887 | 0 | 947 | 19 | 0 |
| 35 | CB | 887 | 0 | 947 | 20 | 0 |
| 36 | AI | 992 | 0 | 1093 | 19 | 0 |
| 36 | CC | 979 | 0 | 1076 | 22 | 0 |
| 37 | AJ | 758 | 0 | 838 | 10 | 0 |
| 37 | CD | 758 | 0 | 838 | 11 | 0 |
| 38 | AK | 677 | 0 | 697 | 16 | 0 |
| 38 | CE | 677 | 0 | 696 | 17 | 0 |
| 39 | AL | 617 | 0 | 675 | 7 | 0 |
| 39 | CF | 617 | 0 | 675 | 14 | 0 |
| 40 | AM | 438 | 0 | 475 | 10 | 0 |
| 40 | CG | 438 | 0 | 475 | 9 | 0 |
| 41 | AN | 419 | 0 | 460 | 11 | 0 |
| 41 | CH | 411 | 0 | 448 | 6 | 0 |
| 42 | AO | 236 | 0 | 285 | 5 | 0 |
| 42 | CI | 227 | 0 | 272 | 7 | 0 |
| 43 | AP | 828 | 0 | 893 | 22 | 0 |
| 43 | CJ | 828 | 0 | 893 | 11 | 0 |
| 44 | AQ | 698 | 0 | 734 | 13 | 0 |
| 44 | CK | 698 | 0 | 734 | 17 | 0 |
| 45 | CL | 931 | 0 | 908 | 50 | 0 |
| 45 | i | 922 | 0 | 902 | 39 | 0 |
| 46 | B | 37113 | 0 | 18673 | 824 | 0 |
| 46 | CM | 37621 | 0 | 18927 | 896 | 0 |

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| Mol | Chain | Non-H | H(model) | H(added) | Clashes | Symm-Clashes |
|---|---|---|---|---|---|---|
| 47 | C | 1627 | 0 | 1644 | 37 | 0 |
| 47 | CN | 1627 | 0 | 1644 | 30 | 0 |
| 48 | CO | 1724 | 0 | 1805 | 48 | 0 |
| 48 | D | 1724 | 0 | 1805 | 30 | 0 |
| 49 | CP | 1629 | 0 | 1728 | 30 | 0 |
| 49 | E | 1629 | 0 | 1728 | 32 | 0 |
| 50 | CQ | 1707 | 0 | 1807 | 56 | 0 |
| 50 | F | 1707 | 0 | 1807 | 45 | 0 |
| 51 | CR | 2055 | 0 | 2137 | 51 | 0 |
| 51 | G | 2051 | 0 | 2134 | 43 | 0 |
| 52 | CS | 1614 | 0 | 1688 | 39 | 0 |
| 52 | H | 1614 | 0 | 1688 | 47 | 0 |
| 53 | CT | 1904 | 0 | 1994 | 53 | 0 |
| 53 | I | 1820 | 0 | 1896 | 44 | 0 |
| 54 | CU | 1475 | 0 | 1567 | 37 | 0 |
| 54 | J | 1485 | 0 | 1574 | 37 | 0 |
| 55 | CV | 1579 | 0 | 1602 | 38 | 0 |
| 55 | K | 1579 | 0 | 1602 | 26 | 0 |
| 56 | CW | 1453 | 0 | 1532 | 32 | 0 |
| 56 | L | 1453 | 0 | 1532 | 25 | 0 |
| 57 | CX | 791 | 0 | 805 | 44 | 0 |
| 57 | M | 817 | 0 | 828 | 39 | 0 |
| 58 | CY | 1129 | 0 | 1183 | 15 | 0 |
| 58 | N | 1150 | 0 | 1201 | 17 | 0 |
| 59 | CZ | 913 | 0 | 934 | 49 | 0 |
| 59 | O | 885 | 0 | 915 | 47 | 0 |
| 60 | DA | 1187 | 0 | 1249 | 17 | 0 |
| 60 | P | 1187 | 0 | 1249 | 18 | 0 |
| 61 | DB | 942 | 0 | 981 | 26 | 0 |
| 61 | Q | 942 | 0 | 981 | 15 | 0 |
| 62 | DC | 1029 | 0 | 1078 | 36 | 0 |
| 62 | R | 1018 | 0 | 1065 | 38 | 0 |
| 63 | DD | 1091 | 0 | 1155 | 26 | 0 |
| 63 | S | 1091 | 0 | 1155 | 42 | 0 |
| 64 | DE | 997 | 0 | 1053 | 37 | 0 |
| 64 | T | 997 | 0 | 1053 | 36 | 0 |
| 65 | DF | 1161 | 0 | 1205 | 33 | 0 |
| 65 | U | 1187 | 0 | 1237 | 31 | 0 |
| 66 | DG | 1100 | 0 | 1114 | 26 | 0 |
| 66 | V | 1100 | 0 | 1114 | 29 | 0 |
| 67 | DH | 763 | 0 | 824 | 20 | 0 |
| 67 | W | 808 | 0 | 871 | 17 | 0 |

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| Mol | Chain | Non-H | H(model) | H(added) | Clashes | Symm-Clashes |
|---|---|---|---|---|---|---|
| 68 | DI | 676 | 0 | 677 | 17 | 0 |
| 68 | X | 676 | 0 | 677 | 22 | 0 |
| 69 | DJ | 1032 | 0 | 1066 | 27 | 0 |
| 69 | Y | 1032 | 0 | 1066 | 19 | 0 |
| 70 | DK | 1110 | 0 | 1182 | 24 | 0 |
| 70 | Z | 1110 | 0 | 1181 | 26 | 0 |
| 71 | DL | 1072 | 0 | 1123 | 19 | 0 |
| 71 | a | 1086 | 0 | 1132 | 16 | 0 |
| 72 | DM | 570 | 0 | 609 | 15 | 0 |
| 72 | b | 578 | 0 | 613 | 16 | 0 |
| 73 | DN | 770 | 0 | 825 | 24 | 0 |
| 73 | c | 779 | 0 | 832 | 15 | 0 |
| 74 | DO | 614 | 0 | 630 | 10 | 0 |
| 74 | d | 614 | 0 | 627 | 7 | 0 |
| 75 | DP | 476 | 0 | 510 | 22 | 0 |
| 75 | e | 487 | 0 | 523 | 15 | 0 |
| 76 | DQ | 449 | 0 | 427 | 12 | 0 |
| 76 | f | 454 | 0 | 432 | 10 | 0 |
| 77 | DR | 461 | 0 | 499 | 17 | 0 |
| 77 | g | 474 | 0 | 515 | 15 | 0 |
| 78 | DS | 574 | 0 | 606 | 34 | 0 |
| 78 | h | 574 | 0 | 606 | 30 | 0 |
| 79 | AR | 2398 | 0 | 2374 | 60 | 0 |
| 79 | DT | 2357 | 0 | 2325 | 81 | 0 |
| 80 | P0 | 845 | 0 | 884 | 34 | 0 |
| 80 | p0 | 635 | 0 | 663 | 37 | 0 |
| 81 | 12 | 480 | 0 | 477 | 31 | 0 |
| 82 | L1 | 1711 | 0 | 1817 | 66 | 0 |
| 82 | l1 | 1711 | 0 | 1817 | 117 | 0 |
| 83 | 0 | 5 | 0 | 0 | 0 | 0 |
| 83 | 1 | 530 | 0 | 0 | 0 | 0 |
| 83 | 2 | 3 | 0 | 0 | 0 | 0 |
| 83 | 3 | 14 | 0 | 0 | 0 | 0 |
| 83 | 4 | 12 | 0 | 0 | 0 | 0 |
| 83 | 5 | 1 | 0 | 0 | 0 | 0 |
| 83 | 6 | 3 | 0 | 0 | 0 | 0 |
| 83 | 8 | 2 | 0 | 0 | 0 | 0 |
| 83 | 9 | 2 | 0 | 0 | 0 | 0 |
| 83 | AB | 2 | 0 | 0 | 0 | 0 |
| 83 | AC | 1 | 0 | 0 | 0 | 0 |
| 83 | AD | 1 | 0 | 0 | 0 | 0 |
| 83 | AE | 2 | 0 | 0 | 0 | 0 |

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| Mol | Chain | Non-H | H(model) | H(added) | Clashes | Symm-Clashes |
|---|---|---|---|---|---|---|
| 83 | AF | 1 | 0 | 0 | 0 | 0 |
| 83 | AG | 2 | 0 | 0 | 0 | 0 |
| 83 | AH | 2 | 0 | 0 | 0 | 0 |
| 83 | AJ | 1 | 0 | 0 | 0 | 0 |
| 83 | AK | 1 | 0 | 0 | 0 | 0 |
| 83 | AM | 1 | 0 | 0 | 0 | 0 |
| 83 | AP | 2 | 0 | 0 | 0 | 0 |
| 83 | AR | 1 | 0 | 0 | 0 | 0 |
| 83 | AS | 278 | 0 | 0 | 0 | 0 |
| 83 | AT | 9 | 0 | 0 | 0 | 0 |
| 83 | AU | 2 | 0 | 0 | 0 | 0 |
| 83 | AW | 4 | 0 | 0 | 0 | 0 |
| 83 | B | 152 | 0 | 0 | 0 | 0 |
| 83 | BB | 2 | 0 | 0 | 0 | 0 |
| 83 | BE | 2 | 0 | 0 | 0 | 0 |
| 83 | BF | 1 | 0 | 0 | 0 | 0 |
| 83 | BH | 1 | 0 | 0 | 0 | 0 |
| 83 | BJ | 3 | 0 | 0 | 0 | 0 |
| 83 | BK | 1 | 0 | 0 | 0 | 0 |
| 83 | BN | 1 | 0 | 0 | 0 | 0 |
| 83 | BQ | 1 | 0 | 0 | 0 | 0 |
| 83 | BV | 1 | 0 | 0 | 0 | 0 |
| 83 | BZ | 2 | 0 | 0 | 0 | 0 |
| 83 | CA | 1 | 0 | 0 | 0 | 0 |
| 83 | CJ | 1 | 0 | 0 | 0 | 0 |
| 83 | CK | 1 | 0 | 0 | 0 | 0 |
| 83 | CL | 3 | 0 | 0 | 0 | 0 |
| 83 | CM | 102 | 0 | 0 | 0 | 0 |
| 83 | CO | 1 | 0 | 0 | 0 | 0 |
| 83 | CP | 1 | 0 | 0 | 0 | 0 |
| 83 | CQ | 1 | 0 | 0 | 0 | 0 |
| 83 | D | 1 | 0 | 0 | 0 | 0 |
| 83 | DA | 1 | 0 | 0 | 0 | 0 |
| 83 | DB | 3 | 0 | 0 | 0 | 0 |
| 83 | DG | 2 | 0 | 0 | 0 | 0 |
| 83 | DQ | 1 | 0 | 0 | 0 | 0 |
| 83 | G | 2 | 0 | 0 | 0 | 0 |
| 83 | I | 2 | 0 | 0 | 0 | 0 |
| 83 | J | 1 | 0 | 0 | 0 | 0 |
| 83 | K | 1 | 0 | 0 | 0 | 0 |
| 83 | L | 1 | 0 | 0 | 0 | 0 |
| 83 | Q | 1 | 0 | 0 | 0 | 0 |

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| Mol | Chain | Non-H | H(model) | H(added) | Clashes | Symm-Clashes |
|---|---|---|---|---|---|---|
| 83 | R | 1 | 0 | 0 | 0 | 0 |
| 83 | V | 1 | 0 | 0 | 0 | 0 |
| 83 | Y | 3 | 0 | 0 | 0 | 0 |
| 83 | Z | 2 | 0 | 0 | 0 | 0 |
| 83 | a | 1 | 0 | 0 | 0 | 0 |
| 83 | f | 1 | 0 | 0 | 0 | 0 |
| 83 | j | 3 | 0 | 0 | 0 | 0 |
| 83 | k | 4 | 0 | 0 | 0 | 0 |
| 83 | o | 3 | 0 | 0 | 0 | 0 |
| 83 | r | 2 | 0 | 0 | 0 | 0 |
| 83 | s | 1 | 0 | 0 | 0 | 0 |
| 83 | u | 2 | 0 | 0 | 0 | 0 |
| 83 | v | 3 | 0 | 0 | 0 | 0 |
| 83 | w | 3 | 0 | 0 | 0 | 0 |
| 83 | x | 3 | 0 | 0 | 0 | 0 |
| 83 | y | 1 | 0 | 0 | 0 | 0 |
| 84 | 1 | 57 | 0 | 52 | 7 | 0 |
| 84 | AS | 57 | 0 | 52 | 8 | 0 |
| 85 | AH | 1 | 0 | 0 | 0 | 0 |
| 85 | AK | 1 | 0 | 0 | 0 | 0 |
| 85 | AN | 1 | 0 | 0 | 0 | 0 |
| 85 | AP | 1 | 0 | 0 | 0 | 0 |
| 85 | AQ | 1 | 0 | 0 | 0 | 0 |
| 85 | CB | 1 | 0 | 0 | 0 | 0 |
| 85 | CE | 1 | 0 | 0 | 0 | 0 |
| 85 | CH | 1 | 0 | 0 | 0 | 0 |
| 85 | CJ | 1 | 0 | 0 | 0 | 0 |
| 85 | CK | 1 | 0 | 0 | 0 | 0 |
| 85 | DN | 1 | 0 | 0 | 0 | 0 |
| 85 | DQ | 1 | 0 | 0 | 0 | 0 |
| 85 | DS | 1 | 0 | 0 | 0 | 0 |
| 85 | c | 1 | 0 | 0 | 0 | 0 |
| 85 | d | 1 | 0 | 0 | 0 | 0 |
| 85 | f | 1 | 0 | 0 | 0 | 0 |
| 85 | h | 1 | 0 | 0 | 0 | 0 |
| 86 | B | 36 | 0 | 36 | 0 | 0 |
| 86 | CM | 36 | 0 | 36 | 2 | 0 |
| 87 | 1 | 9 | 0 | 0 | 1 | 0 |
| 87 | 4 | 3 | 0 | 0 | 1 | 0 |
| 87 | AS | 12 | 0 | 0 | 0 | 0 |
| 87 | B | 6 | 0 | 0 | 0 | 0 |
| All | All | 408804 | 0 | 304392 | 7016 | 0 |

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

All (7016) 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) |
|---|---|---|---|
| 46:B:671:G:H3' | 46:B:672:U:H5' | 1.35 | 1.08 |
| 1:1:1233:G:H1 | 1:1:1247:A:N6 | 1.49 | 1.07 |
| 48:D:180:THR:HG22 | 48:D:183:GLN:OE1 | 1.61 | 0.99 |
| 48:CO:57:ALA:O | 48:CO:61:LEU:HD13 | 1.63 | 0.97 |
| 54:CU:25:GLU:HB2 | 54:CU:31:LYS:HG3 | 1.47 | 0.97 |
| 1:AS:185:U:H3 | 1:AS:229:C:H42 | 1.13 | 0.96 |
| 1:AS:538:G:H1 | 1:AS:547:U:H3 | 0.97 | 0.96 |
| 46:CM:694:C:H3' | 46:CM:695:C:H5" | 1.48 | 0.95 |
| 1:AS:1870:A:N7 | 20:BM:20:ARG:NH2 | 2.17 | 0.93 |
| 66:V:117:SER:HB2 | 66:V:123:ARG:HB2 | 1.49 | 0.93 |
| 1:AS:1014:G:H1 | 1:AS:1030:U:H3 | 1.01 | 0.92 |
| 1:AS:447:U:H2' | 1:AS:448:U:H5" | 1.52 | 0.91 |
| 46:B:961:G:H1 | 46:B:1008:A:HO2' | 0.90 | 0.90 |
| 82:l1:26:ARG:NH1 | 82:l1:210:MET:SD | 2.45 | 0.89 |
| 46:CM:218:A:H3' | 46:CM:219:A:H5" | 1.54 | 0.89 |
| 46:B:880:G:H1 | 46:B:902:U:H3 | 1.20 | 0.89 |
| 65:U:140:THR:HA | 65:U:143:ARG:HH21 | 1.37 | 0.89 |
| 80:p0:57:THR:HA | 80:p0:60:ARG:HD2 | 1.52 | 0.89 |
| 35:AH:58:ARG:HD3 | 35:AH:59:PRO:HD2 | 1.55 | 0.88 |
| 46:B:701:G:H2' | 46:B:702:G:H2' | 1.53 | 0.88 |
| 1:AS:2836:A:H5" | 12:BE:114:GLY:HA2 | 1.56 | 0.88 |
| 79:DT:42:LEU:HB2 | 79:DT:62:PHE:HB2 | 1.54 | 0.87 |
| 82:l1:53:LEU:HB3 | 82:l1:189:PHE:HZ | 1.40 | 0.87 |
| 20:z:165:ARG:CD | 46:B:835:A:H5' | 2.05 | 0.87 |
| 82:l1:59:PRO:HB3 | 82:l1:169:VAL:HB | 1.53 | 0.87 |
| 35:CB:58:ARG:HD3 | 35:CB:59:PRO:HD2 | 1.54 | 0.86 |
| 46:CM:701:G:H5' | 53:CT:230:ARG:HH12 | 1.38 | 0.86 |
| 55:CV:139:ALA:HB3 | 55:CV:141:ARG:HH12 | 1.40 | 0.86 |
| 46:CM:1410:A:H2' | 49:CP:87:ALA:HB3 | 1.58 | 0.86 |
| 50:CQ:215:GLU:HG3 | 50:CQ:216:ASP:H | 1.41 | 0.86 |
| 46:B:1042:U:H3' | 46:B:1043:U:H2' | 1.58 | 0.85 |
| 46:B:512:G:H1 | 46:B:541:C:H5 | 1.22 | 0.85 |
| 1:1:1231:U:H4' | 1:1:1232:G:H5' | 1.58 | 0.85 |
| 1:AS:617:A:H5' | 1:AS:619:A:H1' | 1.58 | 0.85 |
| 45:CL:82:LYS:HD2 | 45:CL:83:HIS:H | 1.39 | 0.85 |
| 54:CU:81:PHE:HB3 | 54:CU:84:ARG:HD2 | 1.57 | 0.85 |
| 78:DS:157:GLU:HG2 | 78:DS:159:LEU:HG | 1.58 | 0.85 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 1:AS:437:G:H22 | 1:AS:620:A:H61 | 1.22 | 0.84 |
| 79:DT:75:SER:HA | 79:DT:116:ILE:HD13 | 1.58 | 0.84 |
| 52:H:95:ASN:OD1 | 52:H:107:LYS:NZ | 2.10 | 0.84 |
| 16:BI:42:PRO:HD3 | 16:BI:61:ILE:HG13 | 1.59 | 0.84 |
| 48:D:180:THR:HG22 | 48:D:183:GLN:CD | 2.02 | 0.84 |
| 55:K:2:GLY:O | 55:K:24:LYS:NZ | 2.11 | 0.84 |
| 82:l1:76:ARG:NH1 | 82:l1:140:HIS:O | 2.10 | 0.83 |
| 46:B:1236:U:O2' | 46:B:1237:C:O2 | 1.96 | 0.83 |
| 1:1:3235:A:N7 | 8:n:45:ARG:NH1 | 2.26 | 0.83 |
| 30:AC:8:THR:HG22 | 30:AC:10:HIS:H | 1.43 | 0.83 |
| 46:CM:880:G:H1 | 46:CM:902:U:H3 | 1.26 | 0.83 |
| 46:CM:1236:U:O2' | 46:CM:1237:C:O2 | 1.95 | 0.82 |
| 1:AS:2334:A:N3 | 18:BK:131:ARG:NH2 | 2.27 | 0.82 |
| 46:CM:538:G:N2 | 77:DR:25:GLU:OE2 | 2.12 | 0.82 |
| 1:1:1519:U:H5' | 26:8:113:LEU:HD13 | 1.62 | 0.82 |
| 1:1:1241:A:H3' | 1:1:1242:G:H5" | 1.60 | 0.82 |
| 1:1:572:U:H2' | 1:1:573:G:H8 | 1.42 | 0.82 |
| 78:DS:127:TYR:CD1 | 78:DS:128:THR:HG23 | 2.15 | 0.82 |
| 46:B:480:U:H2' | 46:B:481:A:C8 | 2.14 | 0.82 |
| 69:DJ:11:LEU:HD11 | 69:DJ:37:PHE:HE2 | 1.45 | 0.82 |
| 18:BK:50:GLN:OE1 | 18:BK:56:ARG:NH2 | 2.12 | 0.82 |
| 84:AS:3401:3K5:H11 | 84:AS:3401:3K5:H7 | 1.62 | 0.82 |
| 1:AS:449:U:H2' | 1:AS:450:G:C8 | 2.15 | 0.81 |
| 1:1:2070:A:O2' | 20:z:114:LYS:NZ | 2.13 | 0.81 |
| 57:M:17:GLN:H | 57:M:88:PRO:HB3 | 1.46 | 0.81 |
| 28:BU:3:LYS:NZ | 28:BU:30:ASP:OD1 | 2.12 | 0.81 |
| 80:p0:33:VAL:HG22 | 80:p0:37:GLN:HB3 | 1.59 | 0.81 |
| 1:1:1233:G:N2 | 1:1:1247:A:N1 | 2.26 | 0.81 |
| 46:CM:1275:U:H2' | 46:CM:1276:G:C8 | 2.16 | 0.81 |
| 51:CR:45:VAL:HG23 | 51:CR:61:VAL:HG11 | 1.62 | 0.81 |
| 46:B:871:U:OP1 | 48:D:214:LYS:NZ | 2.13 | 0.80 |
| 1:1:800:C:OP1 | 6:l:99:ARG:NH2 | 2.14 | 0.80 |
| 1:AS:2461:G:H22 | 1:AS:2464:A:H5" | 1.46 | 0.80 |
| 46:CM:853:G:H1 | 46:CM:945:U:H3 | 1.30 | 0.80 |
| 82:l1:73:ASP:O | 82:l1:75:ASP:N | 2.15 | 0.80 |
| 54:J:48:ASN:OD1 | 54:J:167:GLN:NE2 | 2.15 | 0.80 |
| 46:CM:952:A:OP2 | 60:DA:124:ARG:NH2 | 2.15 | 0.80 |
| 1:1:617:A:H5' | 1:1:619:A:H1' | 1.63 | 0.79 |
| 1:1:2836:A:H5" | 12:r:114:GLY:HA2 | 1.63 | 0.79 |
| 1:AS:2467:C:H3' | 1:AS:2468:C:H2' | 1.65 | 0.79 |
| 59:O:107:ASP:HB3 | 59:O:113:ARG:HG3 | 1.64 | 0.79 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 1:AS:1561:U:O2' | 1:AS:1562:G:OP1 | 2.00 | 0.79 |
| 46:B:1334:G:N3 | 46:B:1365:C:N4 | 2.30 | 0.79 |
| 1:1:1248:A:H2' | 1:1:1249:U:H5' | 1.63 | 0.79 |
| 46:CM:95:G:OP1 | 51:CR:6:LYS:NZ | 2.15 | 0.79 |
| 70:DK:107:PHE:HD2 | 70:DK:114:LYS:HD3 | 1.46 | 0.79 |
| 1:AS:2445:G:N2 | 1:AS:2467:C:O2 | 2.16 | 0.79 |
| 3:4:89:A:OP1 | 36:AI:1:MET:N | 2.16 | 0.79 |
| 1:1:2086:C:H1' | 1:1:3309:A:C8 | 2.18 | 0.79 |
| 1:AS:1542:A:N7 | 16:BI:71:ARG:NH1 | 2.31 | 0.79 |
| 30:BW:8:THR:HG22 | 30:BW:10:HIS:H | 1.48 | 0.79 |
| 1:1:3157:A:OP1 | 11:q:23:ARG:NH1 | 2.16 | 0.79 |
| 82:l1:21:THR:HA | 82:l1:25:LYS:HE3 | 1.65 | 0.79 |
| 64:T:71:PHE:CZ | 64:T:74:GLN:HG2 | 2.19 | 0.78 |
| 1:1:1631:G:N2 | 1:1:1634:A:OP2 | 2.17 | 0.78 |
| 46:B:480:U:H2' | 46:B:481:A:H8 | 1.46 | 0.78 |
| 46:B:509:A:OP2 | 56:L:176:ASN:ND2 | 2.13 | 0.78 |
| 54:CU:94:ILE:HD13 | 54:CU:114:LEU:HD12 | 1.64 | 0.78 |
| 1:1:1253:C:H42 | 1:1:1257:G:N2 | 1.81 | 0.78 |
| 1:1:1279:C:H2' | 1:1:1280:C:H6 | 1.48 | 0.78 |
| 20:z:165:ARG:NE | 46:B:835:A:OP1 | 2.16 | 0.78 |
| 1:AS:2139:G:H5" | 4:AW:227:ARG:HH12 | 1.49 | 0.78 |
| 52:H:36:ALA:C | 52:H:38:ARG:H | 1.91 | 0.78 |
| 1:AS:1657:G:H2' | 1:AS:1658:G:C8 | 2.19 | 0.78 |
| 1:1:1657:G:H2' | 1:1:1658:G:C8 | 2.19 | 0.78 |
| 1:AS:1631:G:N2 | 1:AS:1634:A:OP2 | 2.17 | 0.78 |
| 65:DF:134:ARG:HB2 | 65:DF:136:GLN:HE22 | 1.48 | 0.77 |
| 1:1:653:C:H2' | 1:1:654:A:H8 | 1.49 | 0.77 |
| 1:1:1251:C:H2' | 1:1:1252:G:C8 | 2.19 | 0.77 |
| 63:S:23:ALA:HA | 63:S:62:ILE:HA | 1.64 | 0.77 |
| 23:5:19:VAL:HG23 | 23:5:20:ALA:H | 1.49 | 0.77 |
| 1:1:2420:G:H1 | 1:1:2483:U:H3 | 1.31 | 0.77 |
| 5:AX:10:ARG:NH2 | 5:AX:263:THR:O | 2.17 | 0.77 |
| 23:BP:19:VAL:HG23 | 23:BP:20:ALA:H | 1.49 | 0.77 |
| 58:CY:46:LYS:NZ | 58:CY:50:GLU:OE1 | 2.17 | 0.77 |
| 20:z:165:ARG:HD3 | 46:B:835:A:H5' | 1.64 | 0.77 |
| 46:B:869:A:H62 | 46:B:913:U:H3 | 1.30 | 0.76 |
| 46:CM:1067:C:H4' | 68:DI:58:TYR:HE1 | 1.50 | 0.76 |
| 47:CN:200:ASP:HB2 | 64:DE:85:VAL:HG23 | 1.65 | 0.76 |
| 63:S:19:ALA:HB2 | 63:S:83:ALA:HB1 | 1.67 | 0.76 |
| 46:CM:216:A:N6 | 46:CM:829:A:O2' | 2.18 | 0.76 |
| 59:CZ:36:LEU:HD11 | 59:CZ:43:ARG:HH21 | 1.50 | 0.76 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 46:B:653:G:N1 | 46:B:677:G:O6 | 2.19 | 0.76 |
| 75:DP:12:VAL:HG22 | 75:DP:52:ASP:H | 1.51 | 0.76 |
| 1:1:2334:A:N3 | 18:x:131:ARG:NH2 | 2.34 | 0.76 |
| 46:B:1579:A:H2' | 46:B:1580:A:H8 | 1.51 | 0.76 |
| 53:I:159:ARG:NH1 | 53:I:170:THR:OG1 | 2.18 | 0.76 |
| 13:BF:7:ASN:OD1 | 13:BF:10:ARG:HG3 | 1.85 | 0.76 |
| 46:CM:1431:G:N2 | 78:DS:129:THR:O | 2.18 | 0.76 |
| 50:F:65:ARG:HD2 | 57:M:91:ARG:HH11 | 1.50 | 0.76 |
| 1:AS:2492:U:OP2 | 1:AS:2558:G:N2 | 2.19 | 0.76 |
| 45:CL:67:LYS:HG2 | 65:DF:129:TRP:HZ2 | 1.51 | 0.76 |
| 17:BJ:63:THR:HG21 | 17:BJ:69:LYS:HB2 | 1.67 | 0.76 |
| 69:DJ:75:ILE:HD11 | 69:DJ:93:LEU:HD11 | 1.67 | 0.76 |
| 80:P0:45:LEU:HD21 | 80:P0:99:ILE:HB | 1.68 | 0.76 |
| 46:B:653:G:N2 | 46:B:676:G:N7 | 2.33 | 0.75 |
| 79:AR:42:LEU:HB2 | 79:AR:62:PHE:HB2 | 1.68 | 0.75 |
| 18:BK:122:ALA:HB3 | 18:BK:143:PRO:HB2 | 1.68 | 0.75 |
| 46:CM:1529:G:N2 | 46:CM:1556:A:OP2 | 2.18 | 0.75 |
| 54:J:25:GLU:HG3 | 54:J:35:ARG:HH12 | 1.51 | 0.75 |
| 24:BQ:30:GLY:HA3 | 24:BQ:66:LYS:HE2 | 1.66 | 0.75 |
| 1:1:1251:C:H2' | 1:1:1252:G:H8 | 1.52 | 0.75 |
| 45:i:103:LEU:HB3 | 45:i:109:GLN:HG3 | 1.69 | 0.75 |
| 43:AP:36:PHE:O | 43:AP:41:ARG:NH1 | 2.19 | 0.75 |
| 46:B:217:A:N6 | 46:B:828:U:O2 | 2.19 | 0.75 |
| 11:BD:92:PHE:HB2 | 11:BD:142:ASP:HB3 | 1.69 | 0.75 |
| 55:CV:139:ALA:HB3 | 55:CV:141:ARG:NH1 | 2.01 | 0.75 |
| 1:1:2200:A:H2' | 1:1:2201:A:C8 | 2.21 | 0.75 |
| 12:BE:30:LYS:HG3 | 12:BE:63:GLU:HG3 | 1.69 | 0.75 |
| 46:CM:697:U:H3 | 46:CM:724:G:H1 | 1.34 | 0.75 |
| 82:l1:26:ARG:H | 82:l1:26:ARG:HD3 | 1.50 | 0.75 |
| 1:AS:1091:U:H4' | 1:AS:1092:U:H5' | 1.67 | 0.75 |
| 3:AU:122:U:H3 | 3:AU:131:G:H1 | 1.34 | 0.75 |
| 46:CM:78:A:H8 | 53:CT:154:ARG:HG3 | 1.51 | 0.75 |
| 50:F:138:VAL:HG22 | 50:F:152:LYS:HG2 | 1.68 | 0.75 |
| 63:S:34:PRO:HB2 | 63:S:36:THR:HG22 | 1.67 | 0.75 |
| 1:AS:564:G:H2' | 1:AS:565:A:C8 | 2.22 | 0.75 |
| 1:AS:1034:U:H1' | 7:AZ:3:MET:HE3 | 1.69 | 0.75 |
| 1:1:3021:A:N1 | 24:6:86:ARG:NH2 | 2.34 | 0.74 |
| 1:1:3254:G:H2' | 1:1:3255:G:H8 | 1.52 | 0.74 |
| 46:B:553:A:N3 | 46:B:588:C:O2' | 2.20 | 0.74 |
| 1:AS:628:A:H2' | 1:AS:629:A:H8 | 1.52 | 0.74 |
| 59:CZ:80:ASN:O | 59:CZ:82:PRO:HD3 | 1.87 | 0.74 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 1:1:1172:C:H4' | 17:w:90:PRO:HD3 | 1.69 | 0.74 |
| 1:AS:153:U:OP2 | 36:CC:103:LYS:NZ | 2.19 | 0.74 |
| 84:AS:3401:3K5:H9 | 43:CJ:57:ILE:HG23 | 1.67 | 0.74 |
| 20:BM:160:GLU:OE2 | 20:BM:163:ARG:NH1 | 2.20 | 0.74 |
| 1:1:3194:G:H4' | 15:u:129:VAL:HG11 | 1.70 | 0.74 |
| 1:AS:412:G:H21 | 18:BK:118:GLN:HE22 | 1.35 | 0.74 |
| 1:AS:831:G:O2' | 1:AS:853:G:N2 | 2.18 | 0.74 |
| 1:1:581:A:H5" | 34:AG:106:ASN:HD21 | 1.53 | 0.74 |
| 46:B:1242:U:O2' | 57:M:8:ARG:NH2 | 2.20 | 0.74 |
| 46:CM:139:U:OP1 | 53:CT:149:LYS:NZ | 2.20 | 0.74 |
| 48:CO:97:LEU:HD22 | 48:CO:232:HIS:CD2 | 2.23 | 0.74 |
| 80:P0:71:PRO:O | 80:P0:73:PHE:N | 2.19 | 0.74 |
| 1:AS:2428:G:H22 | 1:AS:2475:U:H3 | 1.31 | 0.74 |
| 46:B:747:A:OP1 | 56:L:79:ARG:NH2 | 2.21 | 0.74 |
| 1:AS:2455:G:O2' | 1:AS:2456:C:O5' | 2.06 | 0.74 |
| 1:1:1091:U:H4' | 1:1:1092:U:H5' | 1.69 | 0.74 |
| 65:DF:69:ILE:HG22 | 65:DF:73:MET:HE2 | 1.68 | 0.74 |
| 46:B:211:A:H62 | 46:B:250:U:H3 | 1.36 | 0.74 |
| 46:B:1665:C:OP1 | 55:K:59:ARG:NH2 | 2.21 | 0.74 |
| 46:CM:1042:U:H3' | 46:CM:1043:U:H2' | 1.70 | 0.74 |
| 1:1:564:G:H2' | 1:1:565:A:C8 | 2.23 | 0.74 |
| 1:1:831:G:O2' | 1:1:853:G:N2 | 2.19 | 0.74 |
| 46:B:721:C:O2' | 46:B:722:A:H5' | 1.88 | 0.74 |
| 1:AS:1384:U:OP1 | 33:BZ:105:LYS:NZ | 2.21 | 0.74 |
| 1:AS:1562:G:N2 | 1:AS:1564:U:O4 | 2.21 | 0.74 |
| 45:CL:156:ALA:HB1 | 57:CX:17:GLN:HG2 | 1.70 | 0.73 |
| 18:x:50:GLN:OE1 | 18:x:56:ARG:NH2 | 2.21 | 0.73 |
| 26:8:75:LYS:HB3 | 26:8:81:THR:HG23 | 1.70 | 0.73 |
| 17:BJ:62:ALA:HA | 17:BJ:71:PRO:HD2 | 1.70 | 0.73 |
| 66:DG:130:ARG:NH1 | 66:DG:131:ASP:OD1 | 2.21 | 0.73 |
| 1:1:3194:G:H5' | 15:u:129:VAL:HG21 | 1.70 | 0.73 |
| 46:B:1511:A:H2' | 46:B:1512:A:C8 | 2.23 | 0.73 |
| 32:AE:45:THR:HG21 | 32:AE:89:PHE:HA | 1.71 | 0.73 |
| 1:1:1436:G:OP1 | 6:l:84:HIS:NE2 | 2.22 | 0.73 |
| 75:e:8:THR:HG21 | 75:e:59:SER:HB2 | 1.69 | 0.73 |
| 1:AS:628:A:H2' | 1:AS:629:A:C8 | 2.22 | 0.73 |
| 1:AS:653:C:H2' | 1:AS:654:A:H8 | 1.52 | 0.73 |
| 22:BO:49:GLN:HA | 22:BO:52:MET:HE3 | 1.70 | 0.73 |
| 46:CM:151:G:O6 | 71:DL:128:ARG:NH2 | 2.21 | 0.73 |
| 70:Z:107:PHE:CE2 | 70:Z:114:LYS:HD3 | 2.24 | 0.73 |
| 1:AS:833:A:OP2 | 44:CK:4:ARG:NH1 | 2.20 | 0.73 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 79:DT:102:GLN:NE2 | 79:DT:138:ILE:O | 2.18 | 0.73 |
| 79:DT:158:SER:HA | 79:DT:201:LEU:HD12 | 1.70 | 0.73 |
| 46:B:697:U:HO2' | 46:B:698:C:H6 | 1.37 | 0.73 |
| 1:AS:316:U:O2' | 37:CD:29:LYS:NZ | 2.20 | 0.73 |
| 80:P0:8:LYS:HG2 | 80:P0:58:MET:HE1 | 1.70 | 0.73 |
| 82:l1:53:LEU:HB3 | 82:l1:189:PHE:CZ | 2.24 | 0.73 |
| 1:1:2191:A:H2' | 1:1:2192:A:C8 | 2.23 | 0.73 |
| 46:B:766:U:H4' | 46:B:767:G:H5" | 1.71 | 0.73 |
| 50:F:54:SER:O | 50:F:95:ARG:NH1 | 2.21 | 0.73 |
| 1:AS:3313:G:H1 | 1:AS:3322:U:H3 | 1.34 | 0.73 |
| 5:AX:211:GLN:NE2 | 5:AX:283:TYR:O | 2.22 | 0.73 |
| 7:AZ:197:LYS:HG2 | 7:AZ:202:GLY:HA3 | 1.70 | 0.73 |
| 46:CM:515:U:H2' | 46:CM:516:A:H8 | 1.54 | 0.73 |
| 46:B:635:C:O2 | 54:J:110:ARG:NH2 | 2.22 | 0.72 |
| 1:AS:429:U:H2' | 1:AS:430:G:H8 | 1.52 | 0.72 |
| 59:CZ:129:ASP:HA | 59:CZ:133:ARG:HD3 | 1.71 | 0.72 |
| 82:l1:17:LEU:HA | 82:l1:20:SER:HB2 | 1.69 | 0.72 |
| 1:1:2470:C:H1' | 82:l1:207:LYS:HE3 | 1.71 | 0.72 |
| 24:BQ:80:ARG:NH1 | 24:BQ:97:ASP:OD1 | 2.22 | 0.72 |
| 46:CM:1353:G:H5" | 66:DG:69:LYS:HE3 | 1.71 | 0.72 |
| 53:CT:159:ARG:NH1 | 53:CT:170:THR:OG1 | 2.22 | 0.72 |
| 1:1:2428:G:H22 | 1:1:2475:U:H3 | 1.36 | 0.72 |
| 46:CM:814:A:O2' | 46:CM:815:U:OP2 | 2.05 | 0.72 |
| 67:DH:52:LYS:HB3 | 67:DH:91:ASP:HB2 | 1.70 | 0.72 |
| 20:z:165:ARG:HD2 | 46:B:835:A:H5' | 1.69 | 0.72 |
| 46:CM:1511:A:H2' | 46:CM:1512:A:C8 | 2.24 | 0.72 |
| 46:CM:1698:U:H2' | 46:CM:1699:G:H4' | 1.71 | 0.72 |
| 78:DS:127:TYR:HD1 | 78:DS:128:THR:HG23 | 1.54 | 0.72 |
| 1:1:2530:C:N4 | 31:AD:59:GLU:OE2 | 2.23 | 0.72 |
| 46:B:945:U:H5' | 60:P:55:ARG:HD3 | 1.71 | 0.72 |
| 51:G:11:ARG:HH12 | 51:G:24:SER:HB3 | 1.52 | 0.72 |
| 23:BP:68:VAL:HG12 | 23:BP:69:SER:H | 1.53 | 0.72 |
| 7:m:289:LYS:HA | 7:m:292:GLU:HG2 | 1.72 | 0.72 |
| 18:x:122:ALA:HB3 | 18:x:143:PRO:HB2 | 1.71 | 0.72 |
| 19:y:96:PHE:O | 19:y:117:ASN:ND2 | 2.22 | 0.72 |
| 1:AS:1479:G:O6 | 35:CB:4:ARG:NH2 | 2.23 | 0.72 |
| 2:AT:39:U:H5' | 45:CL:33:ASN:HD22 | 1.54 | 0.72 |
| 20:BM:30:THR:O | 20:BM:34:ASN:ND2 | 2.21 | 0.72 |
| 46:CM:476:A:OP1 | 77:DR:37:ARG:NH1 | 2.21 | 0.72 |
| 1:1:496:A:H4' | 8:n:27:GLN:HG3 | 1.72 | 0.72 |
| 11:q:92:PHE:HB2 | 11:q:142:ASP:HB3 | 1.70 | 0.72 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 68:X:38:LYS:HD2 | 68:X:49:GLU:HG3 | 1.71 | 0.72 |
| 46:CM:553:A:N3 | 46:CM:588:C:O2' | 2.22 | 0.72 |
| 46:CM:1579:A:H2' | 46:CM:1580:A:H8 | 1.55 | 0.72 |
| 1:1:2899:C:H2' | 1:1:2900:C:C6 | 2.25 | 0.72 |
| 15:u:17:ARG:NH2 | 15:u:58:THR:O | 2.22 | 0.72 |
| 46:B:853:G:H1 | 46:B:945:U:H3 | 1.34 | 0.72 |
| 4:AW:36:GLU:OE1 | 4:AW:163:ARG:NH1 | 2.23 | 0.72 |
| 46:CM:847:A:O2' | 46:CM:948:A:N1 | 2.23 | 0.72 |
| 46:CM:1410:A:H2' | 49:CP:87:ALA:CB | 2.20 | 0.72 |
| 51:G:45:VAL:HG23 | 51:G:61:VAL:HG11 | 1.71 | 0.72 |
| 1:AS:449:U:H3 | 1:AS:480:G:H1 | 1.38 | 0.72 |
| 46:CM:1276:G:H1 | 46:CM:1309:G:H22 | 1.36 | 0.72 |
| 55:K:136:VAL:O | 55:K:141:ARG:NH2 | 2.22 | 0.71 |
| 64:T:71:PHE:HD1 | 64:T:72:LYS:H | 1.35 | 0.71 |
| 1:AS:437:G:N2 | 1:AS:620:A:H61 | 1.87 | 0.71 |
| 46:B:960:C:H5" | 60:P:109:LYS:HD3 | 1.72 | 0.71 |
| 48:CO:30:PHE:CE1 | 48:CO:46:THR:HB | 2.25 | 0.71 |
| 54:CU:48:ASN:OD1 | 54:CU:167:GLN:NE2 | 2.23 | 0.71 |
| 46:B:1218:G:H1 | 46:B:1237:C:H5 | 1.37 | 0.71 |
| 46:B:1753:A:N1 | 73:c:80:HIS:ND1 | 2.35 | 0.71 |
| 52:H:109:LYS:O | 52:H:113:ILE:HD12 | 1.89 | 0.71 |
| 45:CL:124:ASP:OD2 | 50:CQ:118:ARG:NH1 | 2.23 | 0.71 |
| 46:CM:1282:G:N2 | 46:CM:1285:A:OP2 | 2.17 | 0.71 |
| 46:B:1181:A:OP2 | 46:B:1450:G:N2 | 2.21 | 0.71 |
| 46:B:1431:G:N2 | 78:h:129:THR:O | 2.24 | 0.71 |
| 63:S:12:LYS:HG3 | 63:S:13:LYS:H | 1.56 | 0.71 |
| 57:CX:15:LEU:O | 57:CX:19:GLY:HA2 | 1.89 | 0.71 |
| 82:l1:93:LEU:HD21 | 82:l1:100:ILE:HG23 | 1.70 | 0.71 |
| 5:k:284:ARG:NH2 | 5:k:295:ALA:O | 2.24 | 0.71 |
| 16:v:183:THR:HG22 | 16:v:187:ARG:HB2 | 1.72 | 0.71 |
| 31:BX:57:GLU:HB2 | 35:CB:94:LEU:HD11 | 1.72 | 0.71 |
| 46:B:1026:G:H2' | 46:B:1027:G:C8 | 2.26 | 0.71 |
| 1:AS:627:U:H2' | 1:AS:628:A:C8 | 2.26 | 0.71 |
| 46:CM:1598:A:OP1 | 52:CS:107:LYS:NZ | 2.23 | 0.71 |
| 1:1:1230:G:H2' | 1:1:1231:U:C6 | 2.26 | 0.71 |
| 47:C:124:THR:HG22 | 47:C:174:TRP:HE1 | 1.55 | 0.71 |
| 66:V:62:ALA:HB2 | 66:V:108:LEU:HD21 | 1.71 | 0.71 |
| 1:AS:1279:C:OP1 | 80:p0:60:ARG:NH1 | 2.24 | 0.71 |
| 82:l1:36:VAL:HA | 82:l1:204:LEU:HA | 1.73 | 0.71 |
| 1:1:1152:C:OP2 | 9:o:92:LYS:NZ | 2.22 | 0.71 |
| 1:1:429:U:H2' | 1:1:430:G:H8 | 1.54 | 0.71 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 25:BR:80:ARG:HH12 | 53:CT:10:ASN:C | 1.98 | 0.71 |
| 45:CL:64:LEU:O | 45:CL:66:ASN:N | 2.23 | 0.71 |
| 46:CM:869:A:H62 | 46:CM:913:U:H3 | 1.39 | 0.70 |
| 49:CP:211:ALA:O | 49:CP:215:ASN:ND2 | 2.23 | 0.70 |
| 14:t:115:ARG:NH2 | 14:t:147:PHE:O | 2.24 | 0.70 |
| 47:C:84:ARG:NH1 | 47:C:203:PHE:O | 2.24 | 0.70 |
| 46:CM:921:G:OP1 | 46:CM:1059:G:N2 | 2.23 | 0.70 |
| 69:DJ:88:ARG:O | 69:DJ:92:ASN:ND2 | 2.23 | 0.70 |
| 46:B:1741:A:H2' | 46:B:1742:A:C8 | 2.27 | 0.70 |
| 57:M:77:ARG:HD2 | 57:M:84:GLU:HA | 1.73 | 0.70 |
| 15:BH:17:ARG:NH2 | 15:BH:58:THR:O | 2.25 | 0.70 |
| 46:CM:122:U:H2' | 46:CM:123:G:H5" | 1.73 | 0.70 |
| 46:CM:345:G:H5" | 58:CY:85:ILE:HD11 | 1.74 | 0.70 |
| 46:B:700:G:O2' | 46:B:701:G:O4' | 2.09 | 0.70 |
| 1:AS:1020:G:N2 | 1:AS:1023:A:OP2 | 2.25 | 0.70 |
| 19:BL:96:PHE:O | 19:BL:117:ASN:ND2 | 2.25 | 0.70 |
| 46:CM:784:U:H2' | 46:CM:785:G:H8 | 1.54 | 0.70 |
| 54:CU:5:ILE:HG21 | 54:CU:10:PRO:HB3 | 1.71 | 0.70 |
| 79:DT:19:TRP:HB2 | 79:DT:38:ARG:HD2 | 1.73 | 0.70 |
| 1:1:1479:G:O6 | 35:AH:4:ARG:NH2 | 2.24 | 0.70 |
| 1:1:3254:G:H2' | 1:1:3255:G:C8 | 2.26 | 0.70 |
| 46:B:903:U:H2' | 46:B:904:A:C8 | 2.27 | 0.70 |
| 64:T:75:GLU:HA | 64:T:78:ARG:HB2 | 1.73 | 0.70 |
| 7:AZ:41:LYS:NZ | 22:BO:32:LYS:O | 2.23 | 0.70 |
| 82:l1:49:PHE:HB2 | 82:l1:193:LEU:HD22 | 1.73 | 0.70 |
| 3:4:63:G:H1 | 3:4:97:A:H61 | 1.39 | 0.70 |
| 12:r:30:LYS:HG3 | 12:r:63:GLU:HG3 | 1.73 | 0.70 |
| 16:v:159:ARG:HB2 | 16:v:164:LEU:HB2 | 1.73 | 0.70 |
| 46:CM:821:U:H2' | 46:CM:822:G:C8 | 2.26 | 0.70 |
| 46:B:1395:G:N2 | 46:B:1398:G:OP2 | 2.25 | 0.70 |
| 46:CM:79:C:OP1 | 53:CT:159:ARG:NH2 | 2.23 | 0.70 |
| 46:CM:336:C:H5" | 55:CV:10:LYS:HD2 | 1.73 | 0.70 |
| 60:DA:54:LEU:HB3 | 60:DA:60:VAL:HB | 1.73 | 0.70 |
| 46:B:593:G:H5' | 56:L:40:ARG:HH22 | 1.57 | 0.70 |
| 1:AS:3195:G:H5" | 15:BH:125:LYS:HE2 | 1.73 | 0.70 |
| 5:AX:21:ARG:HE | 5:AX:269:GLN:HG3 | 1.57 | 0.70 |
| 12:BE:43:VAL:HG21 | 12:BE:197:VAL:HG13 | 1.74 | 0.70 |
| 31:AD:46:ILE:HG21 | 31:AD:55:LYS:HG3 | 1.74 | 0.69 |
| 46:B:856:G:H2' | 46:B:857:G:C8 | 2.27 | 0.69 |
| 46:B:1673:U:H2' | 46:B:1674:U:O4' | 1.91 | 0.69 |
| 1:AS:1089:A:OP2 | 22:BO:120:LYS:NZ | 2.25 | 0.69 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 81:12:149:HIS:H | 81:12:152:ILE:HD12 | 1.56 | 0.69 |
| 1:1:628:A:H2' | 1:1:629:A:C8 | 2.26 | 0.69 |
| 1:1:628:A:H2' | 1:1:629:A:H8 | 1.57 | 0.69 |
| 1:1:1903:C:O2 | 5:k:240:ARG:NH2 | 2.26 | 0.69 |
| 6:AY:290:LEU:HD22 | 19:BL:129:LEU:HD11 | 1.74 | 0.69 |
| 46:CM:771:G:H4' | 51:CR:256:ARG:HH22 | 1.57 | 0.69 |
| 46:CM:1156:A:H2' | 46:CM:1157:G:C8 | 2.26 | 0.69 |
| 57:CX:54:TYR:HD1 | 57:CX:72:GLY:HA2 | 1.57 | 0.69 |
| 1:1:1253:C:H42 | 1:1:1257:G:H22 | 1.39 | 0.69 |
| 1:AS:1735:U:HO2' | 35:CB:56:THR:HG1 | 1.38 | 0.69 |
| 6:l:42:ARG:HD2 | 6:l:114:VAL:HG22 | 1.75 | 0.69 |
| 17:w:76:ALA:HB3 | 17:w:79:ARG:HG2 | 1.75 | 0.69 |
| 46:B:1131:G:H2' | 46:B:1132:A:C8 | 2.28 | 0.69 |
| 1:AS:976:A:H2' | 1:AS:977:U:H5' | 1.74 | 0.69 |
| 8:BA:34:VAL:HB | 8:BA:89:LYS:HE3 | 1.73 | 0.69 |
| 82:l1:76:ARG:HG2 | 82:l1:144:LEU:HD21 | 1.74 | 0.69 |
| 1:1:1273:C:H2' | 1:1:1274:A:H8 | 1.58 | 0.69 |
| 46:B:139:U:OP1 | 53:I:149:LYS:NZ | 2.21 | 0.69 |
| 1:AS:538:G:N2 | 1:AS:547:U:O2 | 2.24 | 0.69 |
| 1:1:2191:A:H2' | 1:1:2192:A:H8 | 1.58 | 0.69 |
| 11:q:80:THR:HA | 11:q:83:THR:HG22 | 1.74 | 0.69 |
| 46:B:1354:U:N3 | 46:B:1355:A:N7 | 2.40 | 0.69 |
| 52:H:156:ARG:HH12 | 75:e:67:ARG:HG3 | 1.58 | 0.69 |
| 5:AX:284:ARG:NH2 | 5:AX:295:ALA:O | 2.26 | 0.69 |
| 28:BU:115:LYS:NZ | 28:BU:119:GLU:OE2 | 2.25 | 0.69 |
| 46:CM:766:U:H4' | 46:CM:767:G:H5" | 1.74 | 0.69 |
| 46:CM:1670:U:H3 | 46:CM:1705:G:H1 | 1.41 | 0.69 |
| 48:CO:190:PRO:HG2 | 48:CO:192:VAL:HG23 | 1.74 | 0.69 |
| 1:1:653:C:H2' | 1:1:654:A:C8 | 2.27 | 0.69 |
| 46:B:1698:U:H2' | 46:B:1699:G:O4' | 1.93 | 0.69 |
| 52:H:36:ALA:C | 52:H:38:ARG:N | 2.50 | 0.69 |
| 1:AS:2191:A:H2' | 1:AS:2192:A:C8 | 2.27 | 0.69 |
| 1:AS:2444:G:N2 | 1:AS:2467:C:O2' | 2.23 | 0.69 |
| 25:BR:97:LYS:HG3 | 25:BR:98:PRO:HD3 | 1.74 | 0.69 |
| 46:CM:1276:G:H22 | 46:CM:1309:G:N2 | 1.90 | 0.69 |
| 67:DH:21:ILE:HG12 | 67:DH:117:ILE:HG12 | 1.75 | 0.69 |
| 46:B:352:C:H5" | 55:K:16:ALA:HB2 | 1.73 | 0.69 |
| 46:B:952:A:OP2 | 60:P:124:ARG:NH2 | 2.26 | 0.69 |
| 46:B:1422:A:OP2 | 50:F:28:ARG:NH2 | 2.26 | 0.69 |
| 48:D:180:THR:N | 48:D:183:GLN:OE1 | 2.25 | 0.69 |
| 54:J:5:ILE:HG21 | 54:J:10:PRO:HB3 | 1.75 | 0.69 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 59:CZ:59:LEU:HD11 | 59:CZ:89:ILE:HD11 | 1.73 | 0.69 |
| 1:1:572:U:H2' | 1:1:573:G:C8 | 2.25 | 0.69 |
| 4:AW:54:ARG:HH21 | 4:AW:58:LEU:HD11 | 1.55 | 0.69 |
| 46:CM:487:C:O2 | 46:CM:496:G:N2 | 2.25 | 0.69 |
| 46:CM:690:C:H2' | 46:CM:691:U:C6 | 2.28 | 0.68 |
| 1:1:660:U:H2' | 1:1:661:C:C6 | 2.29 | 0.68 |
| 46:B:1578:C:H2' | 46:B:1579:A:H8 | 1.57 | 0.68 |
| 5:AX:218:ILE:HB | 5:AX:337:THR:HB | 1.75 | 0.68 |
| 82:l1:33:GLU:HA | 82:l1:168:ALA:HB3 | 1.75 | 0.68 |
| 1:1:2334:A:H61 | 1:1:2955:C:H5 | 1.37 | 0.68 |
| 32:AE:45:THR:HG22 | 32:AE:47:ASP:H | 1.58 | 0.68 |
| 64:T:103:ASP:OD1 | 64:T:104:ALA:N | 2.26 | 0.68 |
| 1:AS:740:A:OP1 | 19:BL:66:ARG:NH2 | 2.26 | 0.68 |
| 46:CM:578:A:H5" | 50:CQ:144:ARG:HH21 | 1.58 | 0.68 |
| 46:B:671:G:H5" | 46:B:672:U:H6 | 1.58 | 0.68 |
| 15:BH:23:ASN:ND2 | 15:BH:23:ASN:O | 2.25 | 0.68 |
| 46:CM:2:A:OP1 | 49:CP:171:LYS:NZ | 2.19 | 0.68 |
| 82:l1:12:ASN:HB3 | 82:l1:206:ILE:HG21 | 1.74 | 0.68 |
| 64:DE:78:ARG:HH11 | 64:DE:81:LYS:HD3 | 1.59 | 0.68 |
| 72:DM:78:VAL:HG12 | 72:DM:81:ARG:HH21 | 1.59 | 0.68 |
| 46:B:987:G:N2 | 46:B:1747:G:O3' | 2.26 | 0.68 |
| 65:U:29:MET:HB2 | 65:U:54:LEU:HD22 | 1.74 | 0.68 |
| 1:AS:1662:G:H2' | 1:AS:1663:A:H8 | 1.58 | 0.68 |
| 1:1:756:G:O2' | 1:1:766:G:N2 | 2.26 | 0.68 |
| 1:1:1199:A:H2' | 1:1:1200:A:C8 | 2.29 | 0.68 |
| 48:D:128:LYS:HG2 | 48:D:134:VAL:HG22 | 1.76 | 0.68 |
| 1:1:2932:C:H2' | 1:1:2933:G:H8 | 1.58 | 0.68 |
| 46:B:1719:A:H2' | 46:B:1720:C:C6 | 2.29 | 0.68 |
| 1:AS:1218:G:H4' | 1:AS:1219:A:H5" | 1.75 | 0.68 |
| 1:AS:3262:U:O4 | 5:AX:124:LYS:NZ | 2.27 | 0.68 |
| 46:CM:1592:G:OP2 | 63:DD:126:LYS:NZ | 2.21 | 0.68 |
| 52:CS:157:ARG:HG3 | 52:CS:224:ASN:OD1 | 1.93 | 0.68 |
| 1:1:1663:A:H2' | 1:1:1664:G:C8 | 2.28 | 0.68 |
| 46:B:515:U:H2' | 46:B:516:A:H8 | 1.59 | 0.68 |
| 1:AS:662:U:H2' | 1:AS:663:A:C8 | 2.29 | 0.68 |
| 1:AS:2988:A:H2' | 1:AS:2989:A:H8 | 1.59 | 0.68 |
| 46:B:122:U:H2' | 46:B:123:G:H5" | 1.76 | 0.68 |
| 57:M:88:PRO:HD2 | 57:M:91:ARG:HB2 | 1.75 | 0.68 |
| 63:S:26:GLY:HA2 | 63:S:62:ILE:O | 1.94 | 0.68 |
| 1:AS:654:A:H2' | 1:AS:655:A:C8 | 2.28 | 0.68 |
| 46:CM:856:G:H2' | 46:CM:857:G:C8 | 2.29 | 0.68 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 56:CW:38:ASN:HA | 77:DR:36:MET:HE3 | 1.76 | 0.68 |
| 70:DK:107:PHE:CD2 | 70:DK:114:LYS:HD3 | 2.28 | 0.68 |
| 82:L1:28:PHE:HD1 | 82:L1:29:LEU:H | 1.41 | 0.68 |
| 82:L1:30:GLU:H | 82:L1:172:VAL:HB | 1.59 | 0.68 |
| 1:1:2932:C:H2' | 1:1:2933:G:C8 | 2.29 | 0.67 |
| 46:B:1156:A:H2' | 46:B:1157:G:C8 | 2.30 | 0.67 |
| 46:B:1282:G:N2 | 46:B:1285:A:OP2 | 2.24 | 0.67 |
| 79:AR:16:HIS:CE1 | 79:AR:37:SER:HB2 | 2.29 | 0.67 |
| 14:BG:126:PHE:O | 14:BG:130:THR:OG1 | 2.11 | 0.67 |
| 45:CL:42:ALA:O | 45:CL:44:ALA:N | 2.27 | 0.67 |
| 46:CM:12:U:H2' | 46:CM:13:C:C6 | 2.28 | 0.67 |
| 46:CM:855:C:O2 | 74:DO:51:GLN:NE2 | 2.27 | 0.67 |
| 54:CU:5:ILE:HG22 | 54:CU:7:SER:H | 1.60 | 0.67 |
| 1:1:627:U:H2' | 1:1:628:A:C8 | 2.29 | 0.67 |
| 46:B:1579:A:H2' | 46:B:1580:A:C8 | 2.30 | 0.67 |
| 59:O:129:ASP:O | 59:O:131:ASP:N | 2.27 | 0.67 |
| 13:BF:85:LYS:HE3 | 62:DC:11:THR:HA | 1.76 | 0.67 |
| 46:CM:636:C:OP2 | 69:DJ:32:LYS:NZ | 2.25 | 0.67 |
| 46:CM:700:G:O2' | 46:CM:701:G:O5' | 2.11 | 0.67 |
| 64:DE:27:ASP:OD2 | 79:DT:38:ARG:NH2 | 2.22 | 0.67 |
| 67:DH:41:ILE:HD11 | 67:DH:54:PRO:HD3 | 1.77 | 0.67 |
| 1:1:269:G:H5" | 16:v:14:LYS:HE2 | 1.76 | 0.67 |
| 1:1:3014:U:OP2 | 1:1:3064:C:N4 | 2.28 | 0.67 |
| 1:1:3287:A:H2' | 1:1:3288:A:C8 | 2.29 | 0.67 |
| 77:g:50:THR:HB | 77:g:53:LYS:HB2 | 1.76 | 0.67 |
| 1:AS:581:A:H5" | 34:CA:106:ASN:HD21 | 1.60 | 0.67 |
| 1:AS:1663:A:H2' | 1:AS:1664:G:C8 | 2.29 | 0.67 |
| 1:AS:2669:A:H2' | 1:AS:2670:G:C8 | 2.29 | 0.67 |
| 46:B:518:A:H2' | 46:B:519:A:C8 | 2.30 | 0.67 |
| 46:B:1239:U:OP2 | 59:O:46:ARG:NH1 | 2.27 | 0.67 |
| 1:AS:480:G:H2' | 1:AS:480:G:N3 | 2.08 | 0.67 |
| 1:AS:2196:G:H2' | 1:AS:2197:A:H8 | 1.59 | 0.67 |
| 46:CM:63:G:O2' | 46:CM:168:U:OP1 | 2.12 | 0.67 |
| 53:CT:57:ASP:HA | 53:CT:106:LEU:HA | 1.74 | 0.67 |
| 73:DN:74:CYS:SG | 73:DN:75:VAL:N | 2.67 | 0.67 |
| 79:DT:158:SER:HA | 79:DT:201:LEU:CD1 | 2.25 | 0.67 |
| 1:1:1782:G:H2' | 1:1:1783:A:C8 | 2.30 | 0.67 |
| 1:1:2941:A:N7 | 4:j:215:ASN:ND2 | 2.43 | 0.67 |
| 13:s:46:VAL:HG12 | 45:i:33:ASN:HB3 | 1.75 | 0.67 |
| 25:7:80:ARG:HH21 | 53:I:131:LYS:HG2 | 1.60 | 0.67 |
| 46:B:540:A:N6 | 77:g:25:GLU:OE2 | 2.28 | 0.67 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 46:CM:647:C:O2' | 46:CM:648:U:O5' | 2.10 | 0.67 |
| 46:CM:1300:U:OP1 | 46:CM:1313:G:N2 | 2.27 | 0.67 |
| 51:CR:11:ARG:HH12 | 51:CR:24:SER:HB2 | 1.59 | 0.67 |
| 1:1:269:G:N2 | 1:1:295:A:OP2 | 2.24 | 0.67 |
| 1:1:833:A:OP2 | 44:AQ:4:ARG:NH1 | 2.28 | 0.67 |
| 1:1:3199:G:H1 | 1:1:3218:U:H3 | 1.43 | 0.67 |
| 5:k:35:ASP:OD2 | 5:k:191:LYS:NZ | 2.24 | 0.67 |
| 1:AS:3318:G:H5" | 1:AS:3319:U:H4' | 1.76 | 0.67 |
| 8:BA:54:LEU:HD21 | 8:BA:145:LEU:HD11 | 1.76 | 0.67 |
| 46:CM:721:C:H42 | 46:CM:722:A:H62 | 1.40 | 0.67 |
| 1:1:307:A:H2' | 1:1:308:A:C8 | 2.29 | 0.67 |
| 13:s:109:HIS:HD2 | 13:s:123:TYR:H | 1.42 | 0.67 |
| 17:w:2:SER:N | 21:0:161:LYS:HZ3 | 1.93 | 0.67 |
| 65:U:110:ARG:NH2 | 65:U:111:ASP:OD1 | 2.28 | 0.67 |
| 75:e:12:VAL:HG12 | 75:e:30:VAL:HG12 | 1.76 | 0.67 |
| 1:AS:2888:U:H5 | 1:AS:2907:U:HO2' | 1.43 | 0.67 |
| 41:CH:22:LYS:HG3 | 41:CH:42:THR:HG21 | 1.75 | 0.67 |
| 46:CM:78:A:C8 | 53:CT:154:ARG:HG3 | 2.30 | 0.67 |
| 59:CZ:80:ASN:C | 59:CZ:82:PRO:HD3 | 2.20 | 0.67 |
| 1:1:2395:U:H5" | 4:j:221:LYS:HE3 | 1.77 | 0.67 |
| 1:1:2974:C:OP1 | 5:k:26:ARG:NH1 | 2.27 | 0.67 |
| 46:B:944:U:O2 | 60:P:61:SER:OG | 2.11 | 0.67 |
| 57:M:77:ARG:NH1 | 57:M:83:PRO:O | 2.28 | 0.67 |
| 63:S:124:GLU:HG2 | 63:S:133:ALA:HB1 | 1.76 | 0.67 |
| 63:S:128:PHE:O | 63:S:136:ARG:NH1 | 2.24 | 0.67 |
| 1:AS:627:U:H2' | 1:AS:628:A:H8 | 1.59 | 0.67 |
| 1:AS:1436:G:OP1 | 6:AY:84:HIS:NE2 | 2.28 | 0.67 |
| 1:AS:2557:G:O6 | 10:BC:48:SER:OG | 2.13 | 0.67 |
| 11:BD:47:LYS:HE3 | 11:BD:49:ASN:O | 1.94 | 0.67 |
| 46:CM:586:U:OP2 | 77:DR:26:LYS:NZ | 2.27 | 0.67 |
| 46:CM:1463:G:H2' | 46:CM:1464:G:H8 | 1.59 | 0.67 |
| 1:1:1279:C:H2' | 1:1:1280:C:C6 | 2.30 | 0.67 |
| 21:0:73:LYS:NZ | 21:0:97:VAL:O | 2.28 | 0.67 |
| 35:AH:81:CYS:SG | 35:AH:82:ALA:N | 2.68 | 0.67 |
| 46:B:1463:G:H2' | 46:B:1464:G:H8 | 1.60 | 0.67 |
| 50:F:214:ASP:OD1 | 50:F:215:GLU:N | 2.19 | 0.67 |
| 78:h:124:LYS:NZ | 78:h:125:LYS:O | 2.27 | 0.67 |
| 79:AR:52:ASP:O | 79:AR:53:ASN:ND2 | 2.27 | 0.67 |
| 46:B:702:G:H1' | 46:B:703:U:H1' | 1.77 | 0.66 |
| 1:AS:2645:A:O2' | 13:BF:126:ASP:OD1 | 2.10 | 0.66 |
| 16:v:143:ARG:O | 16:v:149:ASN:ND2 | 2.28 | 0.66 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 46:B:57:G:OP1 | 71:a:112:LYS:NZ | 2.29 | 0.66 |
| 1:AS:92:C:OP2 | 1:AS:2736:C:O2' | 2.10 | 0.66 |
| 46:CM:994:U:OP2 | 61:DB:124:LYS:NZ | 2.24 | 0.66 |
| 1:1:739:C:H5" | 19:y:69:ARG:HH22 | 1.60 | 0.66 |
| 57:M:80:LEU:HB3 | 57:M:82:ILE:HG23 | 1.77 | 0.66 |
| 7:AZ:91:GLY:O | 7:AZ:94:ASN:ND2 | 2.28 | 0.66 |
| 28:BU:78:ASN:OD1 | 31:BX:37:ARG:NH2 | 2.24 | 0.66 |
| 32:BY:45:THR:HG21 | 32:BY:89:PHE:HA | 1.76 | 0.66 |
| 46:CM:1145:A:H2' | 46:CM:1146:C:H6 | 1.61 | 0.66 |
| 46:CM:1668:A:H8 | 53:CT:65:GLN:HG3 | 1.59 | 0.66 |
| 63:DD:12:LYS:HG3 | 63:DD:13:LYS:H | 1.60 | 0.66 |
| 46:B:813:U:H2' | 46:B:814:A:C8 | 2.31 | 0.66 |
| 46:B:1470:G:H21 | 46:B:1593:C:H1' | 1.58 | 0.66 |
| 50:F:224:VAL:HG23 | 79:AR:188:ASP:HB2 | 1.76 | 0.66 |
| 55:K:11:ARG:O | 58:N:133:LYS:NZ | 2.29 | 0.66 |
| 1:AS:307:A:H2' | 1:AS:308:A:C8 | 2.30 | 0.66 |
| 1:AS:339:C:OP1 | 1:AS:1376:G:O2' | 2.12 | 0.66 |
| 46:CM:653:G:O2' | 46:CM:655:U:O4 | 2.12 | 0.66 |
| 46:CM:1543:A:OP1 | 62:DC:115:TYR:OH | 2.14 | 0.66 |
| 64:DE:20:PHE:O | 64:DE:24:LEU:HD12 | 1.94 | 0.66 |
| 31:AD:57:GLU:HB2 | 35:AH:94:LEU:HD11 | 1.77 | 0.66 |
| 46:B:681:C:H3' | 46:B:682:A:C8 | 2.31 | 0.66 |
| 46:B:1600:U:OP1 | 52:H:169:ASN:HB2 | 1.96 | 0.66 |
| 1:AS:834:G:O6 | 44:CK:4:ARG:NH2 | 2.29 | 0.66 |
| 31:BX:42:LYS:NZ | 31:BX:95:LEU:O | 2.27 | 0.66 |
| 46:CM:739:A:H5" | 46:CM:740:A:H5' | 1.78 | 0.66 |
| 1:1:3318:G:OP1 | 55:K:170:ARG:NH2 | 2.28 | 0.66 |
| 23:BP:16:VAL:HG12 | 23:BP:65:VAL:HG22 | 1.78 | 0.66 |
| 37:CD:91:GLN:HG3 | 82:L1:3:LYS:HE3 | 1.77 | 0.66 |
| 46:CM:482:C:H2' | 46:CM:483:A:H8 | 1.60 | 0.66 |
| 46:CM:972:G:N2 | 46:CM:998:A:OP1 | 2.27 | 0.66 |
| 46:CM:1026:G:H2' | 46:CM:1027:G:C8 | 2.30 | 0.66 |
| 1:1:581:A:H5" | 34:AG:106:ASN:ND2 | 2.10 | 0.66 |
| 1:1:627:U:H2' | 1:1:628:A:H8 | 1.61 | 0.66 |
| 46:B:345:G:H5" | 58:N:85:ILE:HD11 | 1.78 | 0.66 |
| 1:AS:1761:U:C5 | 20:BM:43:LYS:HE3 | 2.29 | 0.66 |
| 46:CM:672:U:H1' | 46:CM:673:A:C5 | 2.30 | 0.66 |
| 46:CM:1578:C:H2' | 46:CM:1579:A:H8 | 1.61 | 0.66 |
| 79:DT:92:LEU:O | 79:DT:101:THR:N | 2.28 | 0.66 |
| 1:1:662:U:H2' | 1:1:663:A:C8 | 2.30 | 0.66 |
| 1:1:2171:U:H5' | 1:1:2172:G:H5' | 1.78 | 0.66 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 46:B:30:G:OP1 | 70:Z:126:LYS:NZ | 2.27 | 0.66 |
| 46:B:1230:G:H1 | 46:B:1235:U:H3 | 1.43 | 0.66 |
| 1:AS:2171:U:H5' | 1:AS:2172:G:H5' | 1.77 | 0.66 |
| 3:AU:36:G:C5 | 36:CC:86:ARG:HD3 | 2.31 | 0.66 |
| 63:DD:86:LYS:HG2 | 63:DD:116:LEU:HD13 | 1.77 | 0.66 |
| 64:DE:75:GLU:HG3 | 64:DE:76:GLU:OE1 | 1.96 | 0.66 |
| 4:j:101:ILE:HG12 | 4:j:165:VAL:HG22 | 1.77 | 0.66 |
| 46:CM:747:A:OP1 | 56:CW:79:ARG:NH2 | 2.28 | 0.66 |
| 46:CM:1400:U:H5" | 64:DE:3:ARG:HE | 1.60 | 0.66 |
| 1:1:231:A:O2' | 1:AS:246:U:OP1 | 2.11 | 0.66 |
| 1:1:1611:U:H2' | 1:1:1612:U:C6 | 2.31 | 0.66 |
| 1:1:2138:G:H2' | 1:1:2139:G:H8 | 1.61 | 0.66 |
| 23:5:59:GLU:HG2 | 23:5:62:ASN:H | 1.60 | 0.66 |
| 79:AR:90:LEU:HB2 | 79:AR:104:PHE:HB2 | 1.78 | 0.66 |
| 11:BD:110:ASP:HB3 | 11:BD:128:ILE:HD12 | 1.77 | 0.66 |
| 46:CM:452:A:H4' | 51:CR:62:LYS:HE3 | 1.77 | 0.66 |
| 46:CM:1265:C:H2' | 46:CM:1266:G:H8 | 1.61 | 0.66 |
| 80:P0:55:LYS:HD3 | 80:P0:58:MET:HG3 | 1.78 | 0.66 |
| 1:1:2915:G:OP2 | 5:k:2:SER:OG | 2.14 | 0.65 |
| 2:3:64:A:H61 | 12:r:200:LEU:HD21 | 1.60 | 0.65 |
| 46:B:1240:G:N7 | 59:O:46:ARG:NH2 | 2.42 | 0.65 |
| 46:CM:1198:G:OP1 | 78:DS:129:THR:HG21 | 1.96 | 0.65 |
| 82:L1:44:GLN:O | 82:L1:46:ASP:N | 2.29 | 0.65 |
| 1:1:2867:G:O2' | 41:AN:24:TYR:O | 2.13 | 0.65 |
| 8:n:3:GLN:NE2 | 33:AF:76:LEU:O | 2.29 | 0.65 |
| 18:x:32:THR:HG21 | 18:x:87:SER:HB3 | 1.78 | 0.65 |
| 46:B:671:G:H5" | 46:B:672:U:C6 | 2.31 | 0.65 |
| 46:B:1452:G:O2' | 46:B:1589:C:OP1 | 2.14 | 0.65 |
| 1:AS:896:G:H1' | 1:AS:1585:A:N6 | 2.11 | 0.65 |
| 1:AS:2740:U:H2' | 1:AS:2741:A:H8 | 1.61 | 0.65 |
| 50:CQ:124:LEU:HD11 | 50:CQ:153:TYR:HB3 | 1.76 | 0.65 |
| 75:DP:40:ILE:HG23 | 75:DP:62:GLU:HG3 | 1.77 | 0.65 |
| 1:1:115:A:OP2 | 16:v:2:GLY:N | 2.29 | 0.65 |
| 1:1:3207:G:OP1 | 17:w:160:LYS:NZ | 2.17 | 0.65 |
| 51:G:100:ARG:NH2 | 51:G:121:TYR:O | 2.28 | 0.65 |
| 64:T:27:ASP:O | 64:T:31:ASN:ND2 | 2.28 | 0.65 |
| 1:AS:654:A:H2' | 1:AS:655:A:H8 | 1.61 | 0.65 |
| 1:AS:1903:C:O2 | 5:AX:240:ARG:NH2 | 2.29 | 0.65 |
| 16:BI:143:ARG:O | 16:BI:149:ASN:ND2 | 2.28 | 0.65 |
| 46:CM:784:U:H2' | 46:CM:785:G:C8 | 2.31 | 0.65 |
| 52:CS:72:HIS:CD2 | 52:CS:107:LYS:HD3 | 2.30 | 0.65 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 1:1:3318:G:P | 55:K:77:ARG:HH22 | 2.19 | 0.65 |
| 12:r:189:GLU:HG2 | 12:r:200:LEU:HB3 | 1.78 | 0.65 |
| 13:s:92:ARG:HD3 | 13:s:174:LYS:HE3 | 1.78 | 0.65 |
| 46:B:1130:U:O2' | 49:E:84:GLN:O | 2.15 | 0.65 |
| 1:AS:496:A:OP1 | 8:BA:81:ARG:NH1 | 2.27 | 0.65 |
| 1:AS:1662:G:H2' | 1:AS:1663:A:C8 | 2.32 | 0.65 |
| 1:AS:1760:U:OP1 | 20:BM:43:LYS:HE2 | 1.97 | 0.65 |
| 1:AS:2655:U:H2' | 1:AS:2656:C:C6 | 2.31 | 0.65 |
| 23:BP:59:GLU:HG2 | 23:BP:60:SER:H | 1.62 | 0.65 |
| 46:CM:778:U:O2' | 46:CM:779:U:O2 | 2.14 | 0.65 |
| 46:CM:1138:G:OP1 | 73:DN:85:ARG:NH1 | 2.30 | 0.65 |
| 46:CM:1239:U:OP2 | 59:CZ:46:ARG:NH2 | 2.29 | 0.65 |
| 1:1:716:G:OP1 | 29:AB:117:ARG:NH2 | 2.30 | 0.65 |
| 1:1:2442:U:O2' | 1:1:2443:G:N7 | 2.30 | 0.65 |
| 1:AS:2932:C:H2' | 1:AS:2933:G:H8 | 1.61 | 0.65 |
| 46:CM:504:A:H62 | 77:DR:27:PRO:HB3 | 1.61 | 0.65 |
| 46:CM:1520:C:OP2 | 72:DM:77:ARG:NH1 | 2.27 | 0.65 |
| 48:D:190:PRO:HG2 | 48:D:192:VAL:HG23 | 1.78 | 0.65 |
| 70:Z:73:ARG:NH1 | 70:Z:84:THR:OG1 | 2.30 | 0.65 |
| 46:CM:1131:G:H2' | 46:CM:1132:A:C8 | 2.31 | 0.65 |
| 66:DG:117:SER:HB2 | 66:DG:123:ARG:HB2 | 1.77 | 0.65 |
| 1:1:740:A:OP1 | 19:y:66:ARG:NH2 | 2.29 | 0.65 |
| 1:1:2458:G:H4' | 82:l1:102:LYS:HZ1 | 1.60 | 0.65 |
| 54:J:25:GLU:HB2 | 54:J:31:LYS:HG3 | 1.78 | 0.65 |
| 1:AS:1564:U:N3 | 1:AS:1568:U:O4 | 2.29 | 0.65 |
| 20:BM:162:ARG:NH1 | 46:CM:835:A:OP1 | 2.28 | 0.65 |
| 46:CM:200:A:H2' | 46:CM:201:U:C6 | 2.32 | 0.65 |
| 46:CM:211:A:H62 | 46:CM:250:U:H3 | 1.44 | 0.65 |
| 46:CM:1669:U:O4 | 46:CM:1707:G:N2 | 2.30 | 0.65 |
| 75:DP:19:THR:HG23 | 75:DP:25:VAL:HG13 | 1.79 | 0.65 |
| 82:l1:34:LEU:HD11 | 82:l1:183:ILE:HG21 | 1.78 | 0.65 |
| 1:1:1489:G:OP2 | 1:1:1489:G:N2 | 2.26 | 0.65 |
| 11:q:22:ALA:O | 11:q:39:LYS:NZ | 2.27 | 0.65 |
| 42:AO:7:LYS:NZ | 46:B:1761:G:OP1 | 2.30 | 0.65 |
| 1:AS:2634:G:H2' | 1:AS:2635:A:H8 | 1.62 | 0.65 |
| 1:AS:2932:C:H2' | 1:AS:2933:G:C8 | 2.32 | 0.65 |
| 15:BH:20:LEU:HD23 | 15:BH:21:VAL:N | 2.12 | 0.65 |
| 80:P0:25:ILE:HD11 | 80:P0:88:PHE:HA | 1.77 | 0.65 |
| 82:l1:194:LEU:HD13 | 82:l1:200:ASN:HB2 | 1.78 | 0.65 |
| 1:1:1240:A:O2' | 1:1:1244:C:N4 | 2.29 | 0.65 |
| 1:1:1735:U:HO2' | 35:AH:56:THR:HG1 | 1.41 | 0.65 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 1:1:2634:G:H2' | 1:1:2635:A:C8 | 2.32 | 0.65 |
| 46:B:477:C:OP1 | 56:L:121:SER:OG | 2.11 | 0.65 |
| 46:B:1592:G:OP2 | 63:S:126:LYS:NZ | 2.23 | 0.65 |
| 1:AS:394:G:N1 | 1:AS:397:A:OP2 | 2.30 | 0.65 |
| 1:AS:2687:A:O2' | 43:CJ:8:ARG:NH2 | 2.30 | 0.65 |
| 46:CM:1156:A:H2' | 46:CM:1157:G:H8 | 1.61 | 0.65 |
| 55:CV:4:SER:OG | 55:CV:6:ASP:OD1 | 2.14 | 0.65 |
| 1:AS:3160:C:H3' | 1:AS:3161:U:H5" | 1.78 | 0.65 |
| 1:AS:3287:A:H2' | 1:AS:3288:A:C8 | 2.31 | 0.65 |
| 46:CM:502:U:H2' | 46:CM:503:A:H8 | 1.61 | 0.65 |
| 46:CM:1487:C:OP1 | 66:DG:122:ARG:NH2 | 2.28 | 0.65 |
| 62:DC:52:LYS:HB3 | 62:DC:80:LEU:HD13 | 1.78 | 0.65 |
| 69:DJ:81:VAL:O | 69:DJ:122:SER:OG | 2.14 | 0.65 |
| 82:L1:10:ARG:HG2 | 82:L1:180:VAL:HG21 | 1.79 | 0.65 |
| 82:L1:160:LYS:H | 82:L1:162:VAL:HG12 | 1.62 | 0.65 |
| 1:1:896:G:H1' | 1:1:1585:A:N6 | 2.12 | 0.64 |
| 84:1:3402:3K5:H27 | 43:AP:43:TYR:CD2 | 2.32 | 0.64 |
| 46:B:784:U:H2' | 46:B:785:G:H8 | 1.62 | 0.64 |
| 1:AS:476:C:H2' | 1:AS:477:U:C6 | 2.33 | 0.64 |
| 1:AS:2199:G:N2 | 1:AS:2202:A:OP2 | 2.22 | 0.64 |
| 46:B:317:U:H4' | 46:B:321:A:C8 | 2.32 | 0.64 |
| 46:B:1326:A:H1' | 79:AR:66:SER:HB2 | 1.80 | 0.64 |
| 65:U:92:GLN:OE1 | 65:U:115:ARG:NH2 | 2.30 | 0.64 |
| 1:AS:600:U:C2 | 1:AS:602:A:H1' | 2.33 | 0.64 |
| 1:AS:653:C:H2' | 1:AS:654:A:C8 | 2.30 | 0.64 |
| 1:AS:1774:G:O2' | 1:AS:1776:G:OP2 | 2.14 | 0.64 |
| 1:AS:2456:C:O2 | 1:AS:2466:A:N6 | 2.30 | 0.64 |
| 3:AU:63:G:H22 | 3:AU:97:A:H2 | 1.44 | 0.64 |
| 46:CM:1219:A:HO2' | 78:DS:182:TYR:HH | 1.42 | 0.64 |
| 79:DT:132:VAL:HB | 79:DT:145:LEU:HD22 | 1.77 | 0.64 |
| 80:P0:52:LEU:HB3 | 80:P0:86:PHE:HB2 | 1.78 | 0.64 |
| 1:1:654:A:H2' | 1:1:655:A:C8 | 2.32 | 0.64 |
| 1:1:2634:G:H2' | 1:1:2635:A:H8 | 1.60 | 0.64 |
| 20:z:73:GLY:HA2 | 20:z:76:MET:HE2 | 1.79 | 0.64 |
| 46:B:881:U:H5' | 48:D:23:PRO:HG2 | 1.79 | 0.64 |
| 46:B:1144:C:N4 | 46:B:1270:U:OP1 | 2.30 | 0.64 |
| 50:F:124:LEU:HD11 | 50:F:153:TYR:HB3 | 1.79 | 0.64 |
| 55:K:191:GLU:HB3 | 58:N:23:PRO:HG3 | 1.79 | 0.64 |
| 59:O:132:GLU:HG3 | 59:O:133:ARG:H | 1.61 | 0.64 |
| 69:Y:28:ARG:HD3 | 69:Y:60:LYS:HE2 | 1.78 | 0.64 |
| 1:AS:358:G:N2 | 1:AS:361:A:OP2 | 2.29 | 0.64 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 1:AS:1489:G:N2 | 1:AS:1489:G:OP2 | 2.28 | 0.64 |
| 46:CM:870:G:H2' | 46:CM:871:U:C6 | 2.32 | 0.64 |
| 62:R:72:ARG:HH21 | 62:R:93:VAL:HG11 | 1.61 | 0.64 |
| 1:AS:2669:A:H2' | 1:AS:2670:G:H8 | 1.61 | 0.64 |
| 3:AU:94:C:OP1 | 38:CE:75:LYS:NZ | 2.25 | 0.64 |
| 46:CM:1043:U:O2' | 46:CM:1045:U:OP2 | 2.16 | 0.64 |
| 50:CQ:128:MET:HE2 | 50:CQ:135:VAL:HG12 | 1.79 | 0.64 |
| 46:B:778:U:O2' | 46:B:779:U:O2 | 2.15 | 0.64 |
| 46:B:1219:A:O2' | 78:h:187:HIS:ND1 | 2.30 | 0.64 |
| 47:C:147:THR:HG21 | 47:C:159:ALA:HB1 | 1.79 | 0.64 |
| 46:CM:518:A:H2' | 46:CM:519:A:C8 | 2.31 | 0.64 |
| 46:CM:605:G:H5' | 46:CM:611:G:N2 | 2.12 | 0.64 |
| 48:CO:28:ASP:HB3 | 48:CO:50:ARG:CD | 2.28 | 0.64 |
| 69:DJ:2:THR:HG22 | 69:DJ:3:ARG:H | 1.63 | 0.64 |
| 1:1:417:A:H2' | 1:1:418:A:C8 | 2.33 | 0.64 |
| 46:B:219:A:H5" | 46:B:818:U:H1' | 1.77 | 0.64 |
| 69:Y:15:ASN:ND2 | 69:Y:72:CYS:O | 2.25 | 0.64 |
| 1:AS:2634:G:H2' | 1:AS:2635:A:C8 | 2.33 | 0.64 |
| 46:CM:127:G:N7 | 53:CT:202:ARG:NH2 | 2.45 | 0.64 |
| 46:CM:1597:G:N7 | 63:DD:13:LYS:NZ | 2.46 | 0.64 |
| 69:DJ:7:LEU:HD11 | 69:DJ:37:PHE:HD2 | 1.63 | 0.64 |
| 82:l1:14:HIS:O | 82:l1:18:GLU:N | 2.29 | 0.64 |
| 1:1:531:G:HO2' | 1:1:552:G:H1 | 1.45 | 0.64 |
| 43:AP:15:LYS:HD3 | 43:AP:18:ARG:HH21 | 1.60 | 0.64 |
| 1:AS:1283:A:OP2 | 1:AS:1283:A:H8 | 1.81 | 0.64 |
| 1:AS:2391:A:H2' | 1:AS:2392:G:H8 | 1.62 | 0.64 |
| 20:BM:53:LYS:HG2 | 20:BM:54:PRO:HD2 | 1.79 | 0.64 |
| 46:CM:327:G:H5" | 55:CV:98:LYS:HB3 | 1.79 | 0.64 |
| 53:CT:1:MET:HE2 | 53:CT:106:LEU:HB2 | 1.79 | 0.64 |
| 82:L1:116:LEU:HA | 82:L1:119:GLN:HB2 | 1.77 | 0.64 |
| 1:1:482:U:H2' | 1:1:483:U:C6 | 2.33 | 0.64 |
| 1:1:3260:A:H2' | 1:1:3261:A:C8 | 2.33 | 0.64 |
| 15:u:14:GLU:HG2 | 15:u:17:ARG:HG2 | 1.80 | 0.64 |
| 46:B:442:C:OP1 | 71:a:102:LYS:NZ | 2.27 | 0.64 |
| 1:AS:2638:C:O2' | 45:CL:40:ASP:OD2 | 2.15 | 0.64 |
| 1:AS:3014:U:OP2 | 1:AS:3064:C:N4 | 2.29 | 0.64 |
| 46:CM:1600:U:OP1 | 52:CS:169:ASN:HB2 | 1.98 | 0.64 |
| 46:CM:1701:A:H2' | 46:CM:1702:A:C8 | 2.33 | 0.64 |
| 65:DF:134:ARG:HB2 | 65:DF:136:GLN:NE2 | 2.13 | 0.64 |
| 1:1:2079:C:HO2' | 1:1:2080:U:H6 | 1.46 | 0.64 |
| 46:B:985:C:H5 | 46:B:988:A:H5" | 1.61 | 0.64 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 46:B:1410:A:H2' | 49:E:87:ALA:HB3 | 1.79 | 0.64 |
| 70:Z:107:PHE:HE2 | 70:Z:114:LYS:HD3 | 1.63 | 0.64 |
| 1:AS:660:U:H2' | 1:AS:661:C:C6 | 2.33 | 0.64 |
| 8:BA:39:LEU:HD11 | 8:BA:53:TYR:HB2 | 1.80 | 0.64 |
| 18:BK:118:GLN:OE1 | 18:BK:120:ASN:ND2 | 2.29 | 0.64 |
| 46:CM:482:C:H2' | 46:CM:483:A:C8 | 2.32 | 0.64 |
| 46:CM:947:C:H2' | 46:CM:948:A:C8 | 2.33 | 0.64 |
| 46:CM:1211:A:O2' | 46:CM:1241:A:N1 | 2.30 | 0.64 |
| 79:DT:145:LEU:HD21 | 79:DT:178:TRP:CE2 | 2.32 | 0.64 |
| 1:1:2244:U:H2' | 1:1:2245:C:C6 | 2.32 | 0.64 |
| 16:v:27:CYS:HB2 | 16:v:122:ASN:ND2 | 2.13 | 0.64 |
| 54:J:72:ARG:HG2 | 54:J:75:ARG:HH21 | 1.63 | 0.64 |
| 55:K:120:THR:HG21 | 55:K:133:ALA:HA | 1.80 | 0.64 |
| 58:N:7:VAL:HG23 | 58:N:8:GLN:HG2 | 1.78 | 0.64 |
| 60:P:54:LEU:HB3 | 60:P:60:VAL:HB | 1.79 | 0.64 |
| 1:AS:1140:U:OP1 | 1:AS:1363:G:O2' | 2.16 | 0.64 |
| 8:BA:39:LEU:HD13 | 8:BA:83:VAL:HG11 | 1.80 | 0.64 |
| 62:DC:18:LYS:NZ | 65:DF:90:LYS:O | 2.23 | 0.64 |
| 73:DN:12:LYS:HA | 73:DN:15:ARG:HH12 | 1.62 | 0.64 |
| 82:l1:93:LEU:HD22 | 82:l1:99:LEU:HD13 | 1.80 | 0.64 |
| 80:p0:45:LEU:HD22 | 80:p0:99:ILE:HG22 | 1.80 | 0.64 |
| 1:AS:1939:C:O2' | 55:CV:92:ARG:NH1 | 2.31 | 0.63 |
| 46:CM:142:G:O2' | 46:CM:143:A:O5' | 2.17 | 0.63 |
| 46:CM:696:U:H6 | 46:CM:696:U:OP1 | 1.80 | 0.63 |
| 79:DT:235:ALA:HB3 | 79:DT:253:THR:HB | 1.81 | 0.63 |
| 46:B:218:A:OP2 | 46:B:817:U:H5' | 1.98 | 0.63 |
| 46:B:853:G:OP1 | 60:P:121:ARG:NH1 | 2.31 | 0.63 |
| 59:O:104:CYS:SG | 59:O:115:VAL:HA | 2.39 | 0.63 |
| 1:AS:827:G:O2' | 1:AS:1860:A:N3 | 2.28 | 0.63 |
| 1:AS:1259:A:H4' | 1:AS:1260:G:H5" | 1.79 | 0.63 |
| 46:CM:484:G:H1 | 46:CM:499:U:H3 | 0.78 | 0.63 |
| 46:CM:1776:G:OP2 | 61:DB:127:ARG:NH2 | 2.25 | 0.63 |
| 1:1:362:U:O4 | 38:AK:24:ARG:NH2 | 2.31 | 0.63 |
| 46:B:150:U:O2 | 53:I:4:ASN:ND2 | 2.28 | 0.63 |
| 59:O:76:GLU:HB3 | 78:h:153:GLU:OE1 | 1.99 | 0.63 |
| 82:l1:59:PRO:HA | 82:l1:170:GLY:HA2 | 1.80 | 0.63 |
| 10:p:222:ASN:HA | 10:p:226:LYS:HE2 | 1.80 | 0.63 |
| 40:AM:9:THR:HG23 | 40:AM:51:ILE:HG21 | 1.80 | 0.63 |
| 46:B:515:U:H2' | 46:B:516:A:C8 | 2.32 | 0.63 |
| 46:B:1715:U:H2' | 46:B:1716:C:C6 | 2.33 | 0.63 |
| 1:AS:437:G:H22 | 1:AS:620:A:N6 | 1.92 | 0.63 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 1:AS:1400:G:N2 | 1:AS:1403:A:OP2 | 2.28 | 0.63 |
| 1:AS:3156:A:O2' | 11:BD:23:ARG:NH1 | 2.31 | 0.63 |
| 46:CM:1452:G:O2' | 46:CM:1589:C:OP1 | 2.16 | 0.63 |
| 46:CM:1460:G:H2' | 46:CM:1461:A:H8 | 1.64 | 0.63 |
| 1:1:2196:G:H2' | 1:1:2197:A:H8 | 1.63 | 0.63 |
| 4:j:204:MET:SD | 4:j:209:HIS:HB2 | 2.39 | 0.63 |
| 36:AI:1:MET:HB3 | 36:AI:45:HIS:HE1 | 1.63 | 0.63 |
| 66:V:27:LYS:HG2 | 66:V:111:ILE:HD12 | 1.80 | 0.63 |
| 32:BY:45:THR:HG22 | 32:BY:47:ASP:H | 1.62 | 0.63 |
| 46:CM:326:A:OP2 | 58:CY:56:LYS:NZ | 2.26 | 0.63 |
| 46:CM:826:U:H2' | 46:CM:827:C:H5' | 1.79 | 0.63 |
| 46:CM:1659:G:H2' | 46:CM:1660:G:C8 | 2.33 | 0.63 |
| 70:DK:69:ARG:HG3 | 70:DK:117:ILE:HG12 | 1.79 | 0.63 |
| 79:DT:155:VAL:O | 79:DT:156:ARG:NH1 | 2.29 | 0.63 |
| 53:I:163:THR:HA | 53:I:168:THR:HG22 | 1.80 | 0.63 |
| 73:c:7:SER:OG | 73:c:10:ARG:O | 2.17 | 0.63 |
| 1:AS:3294:U:H5" | 5:AX:308:MET:HE2 | 1.81 | 0.63 |
| 29:BV:75:LEU:HD22 | 29:BV:118:LEU:HD11 | 1.80 | 0.63 |
| 33:BZ:106:ARG:NH2 | 33:BZ:122:ASN:O | 2.31 | 0.63 |
| 78:DS:175:ALA:N | 78:DS:182:TYR:O | 2.31 | 0.63 |
| 1:1:1199:A:H2' | 1:1:1200:A:H8 | 1.63 | 0.63 |
| 1:1:2669:A:H2' | 1:1:2670:G:C8 | 2.33 | 0.63 |
| 1:1:2740:U:H2' | 1:1:2741:A:H8 | 1.64 | 0.63 |
| 46:B:305:G:OP2 | 58:N:105:LYS:NZ | 2.32 | 0.63 |
| 47:C:184:LEU:HB3 | 68:X:45:ALA:HB2 | 1.80 | 0.63 |
| 1:AS:1255:A:H61 | 80:p0:33:VAL:HG12 | 1.64 | 0.63 |
| 1:AS:1801:C:H2' | 1:AS:1802:A:H8 | 1.64 | 0.63 |
| 23:BP:28:PHE:CE1 | 23:BP:33:TYR:HB2 | 2.34 | 0.63 |
| 46:B:1301:G:OP1 | 64:T:7:LYS:N | 2.32 | 0.63 |
| 46:B:1350:C:H5" | 63:S:27:LEU:HD22 | 1.81 | 0.63 |
| 1:AS:411:U:H2' | 1:AS:412:G:H8 | 1.63 | 0.63 |
| 1:AS:2862:A:O2' | 1:AS:2905:A:N3 | 2.28 | 0.63 |
| 5:AX:284:ARG:HH11 | 5:AX:356:LEU:HD12 | 1.64 | 0.63 |
| 46:CM:1579:A:H2' | 46:CM:1580:A:C8 | 2.33 | 0.63 |
| 79:DT:90:LEU:HD11 | 79:DT:125:SER:HB3 | 1.79 | 0.63 |
| 1:1:2789:A:H4' | 1:1:2790:U:OP2 | 1.99 | 0.63 |
| 46:B:12:U:H2' | 46:B:13:C:C6 | 2.34 | 0.63 |
| 46:B:697:U:H3 | 46:B:724:G:H1 | 1.47 | 0.63 |
| 46:B:703:U:H2' | 46:B:704:A:C5 | 2.33 | 0.63 |
| 20:BM:165:ARG:NE | 46:CM:835:A:OP1 | 2.32 | 0.63 |
| 46:CM:903:U:H2' | 46:CM:904:A:C8 | 2.33 | 0.63 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 52:CS:159:ALA:O | 75:DP:61:ARG:NH2 | 2.27 | 0.63 |
| 82:L1:191:VAL:HG11 | 82:L1:198:TRP:CD1 | 2.34 | 0.63 |
| 1:1:1662:G:H2' | 1:1:1663:A:H8 | 1.64 | 0.62 |
| 1:AS:93:G:H2' | 1:AS:94:A:C8 | 2.34 | 0.62 |
| 1:AS:185:U:H3 | 1:AS:229:C:N4 | 1.90 | 0.62 |
| 1:AS:448:U:O2' | 1:AS:483:U:OP1 | 2.17 | 0.62 |
| 11:BD:57:VAL:HG23 | 11:BD:68:LEU:HD13 | 1.81 | 0.62 |
| 16:BI:113:LEU:HB2 | 16:BI:134:LEU:HD23 | 1.79 | 0.62 |
| 46:CM:148:C:H42 | 46:CM:162:A:H61 | 1.46 | 0.62 |
| 46:CM:405:A:H2' | 46:CM:406:C:C6 | 2.34 | 0.62 |
| 46:CM:829:A:H2' | 46:CM:830:G:C8 | 2.34 | 0.62 |
| 50:CQ:48:GLU:HG2 | 50:CQ:88:TYR:HE2 | 1.63 | 0.62 |
| 82:L1:194:LEU:HD13 | 82:L1:200:ASN:HD22 | 1.64 | 0.62 |
| 1:1:1202:G:OP1 | 12:r:157:TYR:OH | 2.14 | 0.62 |
| 1:1:1400:G:N2 | 1:1:1403:A:OP2 | 2.24 | 0.62 |
| 8:n:65:SER:HB2 | 8:n:75:LEU:HD23 | 1.80 | 0.62 |
| 46:B:1783:C:OP2 | 73:c:5:ARG:NH2 | 2.32 | 0.62 |
| 62:R:14:GLN:HE22 | 62:R:23:LYS:HB2 | 1.64 | 0.62 |
| 63:S:19:ALA:HA | 63:S:66:VAL:HG12 | 1.80 | 0.62 |
| 63:S:86:LYS:HG2 | 63:S:116:LEU:HD13 | 1.80 | 0.62 |
| 68:X:55:LEU:HD11 | 68:X:69:LEU:HD21 | 1.81 | 0.62 |
| 1:AS:1199:A:H2' | 1:AS:1200:A:C8 | 2.34 | 0.62 |
| 1:AS:2530:C:OP1 | 35:CB:102:LYS:NZ | 2.24 | 0.62 |
| 2:AT:23:A:H2' | 2:AT:24:A:C8 | 2.34 | 0.62 |
| 58:CY:102:LYS:O | 70:DK:13:ARG:NH1 | 2.21 | 0.62 |
| 1:1:2155:G:OP2 | 4:j:128:ARG:NH1 | 2.30 | 0.62 |
| 31:AD:19:THR:HG23 | 31:AD:97:ALA:HA | 1.81 | 0.62 |
| 21:BN:8:GLN:HB2 | 21:BN:64:ILE:HD11 | 1.81 | 0.62 |
| 69:DJ:37:PHE:HE1 | 69:DJ:103:ILE:HG13 | 1.62 | 0.62 |
| 1:1:654:A:H2' | 1:1:655:A:H8 | 1.64 | 0.62 |
| 1:1:976:A:H2' | 1:1:977:U:H5' | 1.80 | 0.62 |
| 1:1:1115:C:H2' | 1:1:1116:A:H8 | 1.65 | 0.62 |
| 1:1:2347:G:H2' | 1:1:2348:G:C8 | 2.35 | 0.62 |
| 1:1:2655:U:H2' | 1:1:2656:C:C6 | 2.34 | 0.62 |
| 45:i:77:GLN:OE1 | 46:B:1446:A:N6 | 2.33 | 0.62 |
| 1:AS:1258:G:O6 | 1:AS:1260:G:N2 | 2.32 | 0.62 |
| 1:AS:2444:G:N2 | 1:AS:2468:C:OP1 | 2.33 | 0.62 |
| 1:AS:3261:A:H2' | 1:AS:3262:U:H6 | 1.64 | 0.62 |
| 46:CM:390:G:OP1 | 55:CV:24:LYS:NZ | 2.23 | 0.62 |
| 46:CM:484:G:N2 | 46:CM:499:U:O2 | 2.26 | 0.62 |
| 50:CQ:107:LYS:HB2 | 50:CQ:176:VAL:HG22 | 1.81 | 0.62 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 51:CR:104:ASP:HB3 | 51:CR:110:ALA:HB2 | 1.82 | 0.62 |
| 79:DT:65:HIS:CG | 79:DT:85:SER:HG | 2.18 | 0.62 |
| 7:m:155:THR:HG22 | 7:m:179:ARG:HD3 | 1.80 | 0.62 |
| 45:i:93:ARG:H | 46:B:1259:C:H5 | 1.47 | 0.62 |
| 1:AS:362:U:O4 | 38:CE:24:ARG:NH2 | 2.31 | 0.62 |
| 46:CM:218:A:H3' | 46:CM:219:A:C5' | 2.28 | 0.62 |
| 1:1:1713:U:H2' | 1:1:1714:G:C8 | 2.34 | 0.62 |
| 1:1:1936:G:H21 | 1:1:3327:A:H8 | 1.45 | 0.62 |
| 47:C:200:ASP:HB2 | 64:T:85:VAL:HG23 | 1.82 | 0.62 |
| 48:D:145:ARG:NH2 | 48:D:151:LYS:O | 2.33 | 0.62 |
| 79:AR:102:GLN:NE2 | 79:AR:103:ARG:O | 2.33 | 0.62 |
| 21:BN:52:LYS:HG2 | 21:BN:55:SER:HB3 | 1.81 | 0.62 |
| 46:CM:1152:G:H21 | 63:DD:138:GLN:HE22 | 1.47 | 0.62 |
| 47:CN:205:ARG:NH2 | 64:DE:82:ASP:OD1 | 2.31 | 0.62 |
| 49:CP:36:LEU:HD21 | 49:CP:51:ILE:HD12 | 1.81 | 0.62 |
| 79:DT:14:GLU:OE2 | 79:DT:53:ASN:ND2 | 2.32 | 0.62 |
| 6:l:113:LYS:HE3 | 16:v:202:TYR:HB3 | 1.81 | 0.62 |
| 52:H:72:HIS:CD2 | 52:H:107:LYS:HD3 | 2.35 | 0.62 |
| 63:S:98:GLU:HG3 | 63:S:101:LYS:HE3 | 1.81 | 0.62 |
| 1:AS:1713:U:H2' | 1:AS:1714:G:C8 | 2.33 | 0.62 |
| 1:AS:3259:A:OP1 | 5:AX:128:LYS:NZ | 2.28 | 0.62 |
| 3:AU:21:C:OP1 | 6:AY:194:LYS:NZ | 2.30 | 0.62 |
| 15:BH:14:GLU:HG2 | 15:BH:17:ARG:HG2 | 1.80 | 0.62 |
| 25:BR:98:PRO:HA | 25:BR:101:ARG:HD2 | 1.81 | 0.62 |
| 46:CM:16:G:H2' | 46:CM:17:C:C6 | 2.34 | 0.62 |
| 46:CM:515:U:H2' | 46:CM:516:A:C8 | 2.33 | 0.62 |
| 46:CM:869:A:OP1 | 48:CO:136:ARG:NH2 | 2.33 | 0.62 |
| 46:CM:1719:A:H2' | 46:CM:1720:C:C6 | 2.35 | 0.62 |
| 49:CP:136:ARG:HB3 | 49:CP:146:PRO:HB2 | 1.81 | 0.62 |
| 59:CZ:82:PRO:HG3 | 59:CZ:85:LYS:HA | 1.81 | 0.62 |
| 80:p0:76:LEU:HD22 | 80:p0:79:PHE:HZ | 1.64 | 0.62 |
| 1:1:1575:A:H5" | 1:1:1576:A:H2 | 1.65 | 0.62 |
| 1:1:2244:U:H2' | 1:1:2245:C:H6 | 1.65 | 0.62 |
| 5:k:372:THR:HG22 | 5:k:374:ALA:H | 1.64 | 0.62 |
| 46:B:854:A:H61 | 46:B:943:U:H5 | 1.45 | 0.62 |
| 46:B:1198:G:H1 | 46:B:1436:U:H3 | 1.46 | 0.62 |
| 46:CM:352:C:H5" | 55:CV:16:ALA:HB2 | 1.80 | 0.62 |
| 46:CM:970:G:H2' | 46:CM:971:G:C8 | 2.34 | 0.62 |
| 46:CM:1245:U:H2' | 46:CM:1246:G:H8 | 1.65 | 0.62 |
| 79:DT:211:ALA:HB2 | 79:DT:217:ILE:HG12 | 1.80 | 0.62 |
| 1:1:483:U:H2' | 1:1:484:U:C6 | 2.35 | 0.62 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 1:1:1692:A:H2' | 1:1:1693:A:C8 | 2.35 | 0.62 |
| 17:w:122:PRO:HA | 17:w:125:LEU:HD12 | 1.81 | 0.62 |
| 46:B:1460:G:H2' | 46:B:1461:A:H8 | 1.63 | 0.62 |
| 52:H:108:LEU:HD21 | 63:S:43:LEU:HD11 | 1.80 | 0.62 |
| 72:b:67:ASP:O | 72:b:70:LYS:NZ | 2.33 | 0.62 |
| 1:AS:2694:U:O2' | 22:BO:88:ARG:O | 2.17 | 0.62 |
| 1:AS:3060:G:OP1 | 5:AX:313:ARG:NH1 | 2.33 | 0.62 |
| 24:BQ:17:LEU:HD13 | 24:BQ:23:MET:HE2 | 1.82 | 0.62 |
| 46:CM:255:A:N3 | 55:CV:64:ASN:ND2 | 2.47 | 0.62 |
| 46:CM:1324:C:O2' | 46:CM:1326:A:N7 | 2.30 | 0.62 |
| 1:1:394:G:N1 | 1:1:397:A:OP2 | 2.33 | 0.62 |
| 1:1:1921:U:O4 | 1:1:2297:U:O2' | 2.17 | 0.62 |
| 1:1:2370:C:H1' | 5:k:266:ARG:HH21 | 1.65 | 0.62 |
| 6:l:359:GLU:OE2 | 21:0:8:GLN:NE2 | 2.33 | 0.62 |
| 1:AS:2936:G:N2 | 1:AS:2939:A:OP2 | 2.26 | 0.62 |
| 6:l:114:VAL:HB | 6:l:119:LYS:HE3 | 1.81 | 0.61 |
| 46:B:739:A:H5" | 46:B:740:A:H5' | 1.81 | 0.61 |
| 46:CM:52:U:H2' | 46:CM:53:G:C8 | 2.35 | 0.61 |
| 65:DF:126:ARG:HB2 | 65:DF:133:VAL:HG12 | 1.82 | 0.61 |
| 82:L1:67:ILE:HG22 | 82:L1:68:PHE:H | 1.64 | 0.61 |
| 1:1:1249:U:H5" | 1:1:1259:A:H2 | 1.65 | 0.61 |
| 1:1:1592:C:H2' | 1:1:1593:C:C6 | 2.35 | 0.61 |
| 13:s:47:GLN:HB2 | 45:i:34:THR:HG22 | 1.80 | 0.61 |
| 46:B:327:G:H5" | 55:K:98:LYS:HB3 | 1.81 | 0.61 |
| 46:B:965:G:H4' | 46:B:1763:A:H4' | 1.82 | 0.61 |
| 46:B:1127:A:H5" | 73:c:2:PRO:HB3 | 1.82 | 0.61 |
| 3:AU:29:U:H5" | 14:BG:27:ASP:HB3 | 1.82 | 0.61 |
| 5:AX:372:THR:HG22 | 5:AX:374:ALA:H | 1.65 | 0.61 |
| 27:BT:39:LEU:HD22 | 27:BT:43:TYR:HE2 | 1.64 | 0.61 |
| 46:CM:673:A:H2' | 46:CM:674:C:C6 | 2.34 | 0.61 |
| 5:k:218:ILE:HB | 5:k:337:THR:HB | 1.82 | 0.61 |
| 46:B:64:U:O2' | 46:B:166:A:N3 | 2.29 | 0.61 |
| 46:B:1275:U:H2' | 46:B:1276:G:C8 | 2.35 | 0.61 |
| 46:B:1578:C:H2' | 46:B:1579:A:C8 | 2.35 | 0.61 |
| 53:I:161:GLU:HB3 | 53:I:170:THR:HG22 | 1.82 | 0.61 |
| 1:AS:880:A:HO2' | 38:CE:2:GLY:N | 1.98 | 0.61 |
| 1:AS:2244:U:H2' | 1:AS:2245:C:C6 | 2.36 | 0.61 |
| 1:AS:3256:G:H2' | 1:AS:3257:A:C8 | 2.35 | 0.61 |
| 46:CM:849:U:OP1 | 69:DJ:28:ARG:NH1 | 2.33 | 0.61 |
| 1:1:2694:U:O2' | 22:2:88:ARG:O | 2.14 | 0.61 |
| 5:k:284:ARG:HH11 | 5:k:356:LEU:HD12 | 1.64 | 0.61 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 32:AE:43:MET:HE3 | 32:AE:76:ARG:HB2 | 1.83 | 0.61 |
| 46:B:511:U:H2' | 46:B:512:G:C8 | 2.35 | 0.61 |
| 46:B:814:A:O2' | 46:B:815:U:OP2 | 2.15 | 0.61 |
| 1:AS:2331:G:H5" | 18:BK:86:LYS:HB2 | 1.82 | 0.61 |
| 1:AS:3179:U:H2' | 15:BH:114:MET:HE1 | 1.82 | 0.61 |
| 1:AS:3233:A:OP1 | 8:BA:45:ARG:NH2 | 2.29 | 0.61 |
| 41:CH:23:CYS:HB2 | 41:CH:38:LYS:HD2 | 1.83 | 0.61 |
| 46:CM:405:A:H2' | 46:CM:406:C:H6 | 1.66 | 0.61 |
| 46:CM:1474:G:H3' | 46:CM:1502:A:H61 | 1.65 | 0.61 |
| 52:CS:116:HIS:HD2 | 72:DM:98:GLN:HB3 | 1.65 | 0.61 |
| 69:DJ:37:PHE:CE1 | 69:DJ:103:ILE:HG13 | 2.34 | 0.61 |
| 75:DP:42:ARG:NH1 | 75:DP:58:GLU:O | 2.34 | 0.61 |
| 79:DT:252:ALA:HB2 | 79:DT:289:LEU:HD11 | 1.82 | 0.61 |
| 1:1:2820:G:OP1 | 41:AN:24:TYR:OH | 2.15 | 0.61 |
| 46:B:1156:A:H2' | 46:B:1157:G:H8 | 1.63 | 0.61 |
| 51:G:104:ASP:HB3 | 51:G:110:ALA:HB2 | 1.82 | 0.61 |
| 1:AS:214:G:OP1 | 27:BT:12:ARG:NH1 | 2.32 | 0.61 |
| 1:AS:2086:C:H1' | 1:AS:3309:A:C8 | 2.35 | 0.61 |
| 46:CM:680:C:HO2' | 46:CM:681:C:H6 | 1.48 | 0.61 |
| 46:CM:1239:U:OP1 | 59:CZ:50:LYS:NZ | 2.33 | 0.61 |
| 48:CO:26:ARG:O | 48:CO:50:ARG:N | 2.34 | 0.61 |
| 48:CO:48:ILE:HG21 | 48:CO:61:LEU:HD11 | 1.81 | 0.61 |
| 82:L1:104:ALA:HB2 | 82:L1:128:LEU:HD12 | 1.81 | 0.61 |
| 1:1:563:U:H2' | 1:1:564:G:C8 | 2.35 | 0.61 |
| 1:1:1774:G:O2' | 1:1:1776:G:OP2 | 2.18 | 0.61 |
| 1:1:2899:C:H2' | 1:1:2900:C:H6 | 1.65 | 0.61 |
| 1:1:2959:A:H2' | 1:1:2960:C:H6 | 1.64 | 0.61 |
| 10:p:144:ILE:HG23 | 10:p:176:VAL:HG21 | 1.83 | 0.61 |
| 46:B:829:A:H2' | 46:B:830:G:H8 | 1.65 | 0.61 |
| 48:D:62:LYS:NZ | 48:D:90:GLU:HA | 2.16 | 0.61 |
| 46:CM:511:U:H2' | 46:CM:512:G:C8 | 2.36 | 0.61 |
| 1:1:582:G:H2' | 1:1:583:A:H8 | 1.66 | 0.61 |
| 1:1:925:A:O2' | 38:AK:49:TRP:O | 2.18 | 0.61 |
| 3:4:150:G:OP1 | 26:8:27:ARG:NH2 | 2.33 | 0.61 |
| 52:H:200:ASN:HB3 | 52:H:208:SER:HB3 | 1.82 | 0.61 |
| 1:AS:1695:A:O2' | 39:CF:3:ARG:NH1 | 2.34 | 0.61 |
| 16:BI:177:GLY:H | 16:BI:184:LYS:NZ | 1.99 | 0.61 |
| 56:CW:101:PRO:O | 56:CW:105:LEU:HD12 | 2.00 | 0.61 |
| 1:1:1080:A:H2' | 1:1:1081:A:C8 | 2.35 | 0.61 |
| 11:q:8:GLN:HB3 | 11:q:72:LYS:HD2 | 1.83 | 0.61 |
| 46:B:1227:A:OP1 | 62:R:59:LYS:NZ | 2.24 | 0.61 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 49:E:78:ILE:HD11 | 49:E:120:ILE:HD11 | 1.83 | 0.61 |
| 51:G:148:ARG:NH2 | 53:I:201:GLN:OE1 | 2.34 | 0.61 |
| 1:AS:2530:C:N4 | 31:BX:59:GLU:OE2 | 2.34 | 0.61 |
| 57:CX:50:THR:HG21 | 57:CX:57:THR:HG22 | 1.83 | 0.61 |
| 29:AB:59:ARG:HH22 | 43:AP:38:GLN:HG2 | 1.64 | 0.61 |
| 1:AS:589:G:N2 | 1:AS:610:U:OP1 | 2.33 | 0.61 |
| 1:AS:2516:U:O2' | 1:AS:2519:A:N1 | 2.31 | 0.61 |
| 46:CM:518:A:H2' | 46:CM:519:A:H8 | 1.66 | 0.61 |
| 1:1:997:G:O2' | 1:1:1037:U:OP2 | 2.19 | 0.61 |
| 1:1:3159:A:H2' | 1:1:3160:C:C6 | 2.35 | 0.61 |
| 46:B:29:U:H2' | 46:B:30:G:H8 | 1.65 | 0.61 |
| 46:B:504:A:H5" | 46:B:505:U:O5' | 2.00 | 0.61 |
| 54:J:92:ARG:NH1 | 54:J:120:LYS:HB3 | 2.15 | 0.61 |
| 1:AS:1217:A:N7 | 80:p0:12:PHE:HB3 | 2.15 | 0.61 |
| 1:AS:1344:U:OP1 | 19:BL:39:ARG:NH2 | 2.34 | 0.61 |
| 1:AS:2345:A:H2' | 1:AS:2346:A:C8 | 2.35 | 0.61 |
| 46:CM:184:C:OP1 | 55:CV:152:ARG:NH2 | 2.31 | 0.61 |
| 46:CM:1230:G:H1 | 46:CM:1235:U:H3 | 1.49 | 0.61 |
| 64:DE:25:THR:HG23 | 64:DE:27:ASP:H | 1.64 | 0.61 |
| 25:7:81:ALA:HB3 | 53:I:130:PRO:HB3 | 1.83 | 0.60 |
| 46:B:1276:G:H1 | 46:B:1309:G:H22 | 1.48 | 0.60 |
| 46:B:1459:U:OP1 | 52:H:183:SER:OG | 2.19 | 0.60 |
| 75:e:19:THR:HG23 | 75:e:25:VAL:HG13 | 1.82 | 0.60 |
| 1:AS:591:C:O2 | 9:BB:24:ARG:NH1 | 2.34 | 0.60 |
| 1:AS:1115:C:H2' | 1:AS:1116:A:H8 | 1.64 | 0.60 |
| 48:CO:28:ASP:HB3 | 48:CO:50:ARG:HD2 | 1.82 | 0.60 |
| 59:CZ:132:GLU:O | 59:CZ:136:LEU:HB2 | 2.01 | 0.60 |
| 79:DT:14:GLU:CD | 79:DT:53:ASN:HD21 | 2.09 | 0.60 |
| 1:1:93:G:H2' | 1:1:94:A:C8 | 2.36 | 0.60 |
| 46:B:52:U:H2' | 46:B:53:G:C8 | 2.36 | 0.60 |
| 53:I:57:ASP:HA | 53:I:106:LEU:HA | 1.84 | 0.60 |
| 1:AS:2812:C:N4 | 1:AS:2817:A:O2' | 2.34 | 0.60 |
| 46:CM:726:C:O2 | 54:CU:103:ARG:NH2 | 2.28 | 0.60 |
| 46:CM:829:A:H2' | 46:CM:830:G:H8 | 1.66 | 0.60 |
| 46:CM:1334:G:N3 | 46:CM:1365:C:N4 | 2.49 | 0.60 |
| 67:DH:26:THR:HG22 | 67:DH:87:LYS:HG3 | 1.82 | 0.60 |
| 1:1:504:G:OP1 | 87:1:4001:HOH:O | 2.16 | 0.60 |
| 1:1:1255:A:N3 | 1:1:1276:C:O2' | 2.31 | 0.60 |
| 1:1:2196:G:H2' | 1:1:2197:A:C8 | 2.36 | 0.60 |
| 1:1:2888:U:H5 | 1:1:2907:U:HO2' | 1.49 | 0.60 |
| 35:AH:16:ARG:HG2 | 35:AH:37:LYS:HD3 | 1.83 | 0.60 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 46:B:1417:C:O2' | 46:B:1423:U:O4 | 2.16 | 0.60 |
| 54:J:5:ILE:HG22 | 54:J:7:SER:H | 1.66 | 0.60 |
| 1:AS:487:C:O2' | 1:AS:488:G:OP1 | 2.19 | 0.60 |
| 1:AS:662:U:H2' | 1:AS:663:A:H8 | 1.65 | 0.60 |
| 1:AS:2196:G:H2' | 1:AS:2197:A:C8 | 2.37 | 0.60 |
| 1:AS:3309:A:H2 | 1:AS:3326:G:H21 | 1.48 | 0.60 |
| 28:BU:15:ARG:HD2 | 28:BU:79:HIS:CD2 | 2.36 | 0.60 |
| 46:CM:39:A:OP1 | 56:CW:3:ARG:NH2 | 2.34 | 0.60 |
| 62:DC:41:VAL:HG13 | 62:DC:84:ILE:HD13 | 1.83 | 0.60 |
| 1:1:1237:U:O2' | 1:1:1239:G:N7 | 2.29 | 0.60 |
| 1:1:1253:C:N4 | 1:1:1257:G:H22 | 1.98 | 0.60 |
| 1:1:2527:G:N2 | 1:1:2527:G:OP2 | 2.34 | 0.60 |
| 1:1:2651:A:H1' | 45:i:50:LYS:HE2 | 1.83 | 0.60 |
| 79:AR:200:THR:HG21 | 79:AR:241:ALA:HA | 1.84 | 0.60 |
| 1:AS:1782:G:H2' | 1:AS:1783:A:C8 | 2.36 | 0.60 |
| 1:AS:2139:G:H5" | 4:AW:227:ARG:NH1 | 2.17 | 0.60 |
| 1:AS:3260:A:H2' | 1:AS:3261:A:C8 | 2.36 | 0.60 |
| 46:CM:1463:G:H2' | 46:CM:1464:G:C8 | 2.36 | 0.60 |
| 51:CR:48:LEU:HD11 | 51:CR:70:VAL:HG21 | 1.84 | 0.60 |
| 52:CS:159:ALA:HB3 | 52:CS:225:ARG:HB3 | 1.84 | 0.60 |
| 1:1:252:U:H5' | 1:1:253:A:C8 | 2.36 | 0.60 |
| 1:1:2206:A:H2' | 1:1:2207:A:C8 | 2.36 | 0.60 |
| 32:AE:30:LYS:NZ | 32:AE:34:GLU:OE2 | 2.34 | 0.60 |
| 46:B:501:G:H2' | 46:B:502:U:H6 | 1.66 | 0.60 |
| 46:B:1486:G:OP2 | 66:V:73:VAL:HG12 | 2.02 | 0.60 |
| 1:AS:1018:U:H2' | 1:AS:1019:U:H5" | 1.83 | 0.60 |
| 1:AS:1795:A:H2' | 1:AS:1796:A:C8 | 2.37 | 0.60 |
| 9:BB:185:GLU:HG2 | 9:BB:196:VAL:HG21 | 1.83 | 0.60 |
| 46:CM:65:A:O2' | 46:CM:67:A:OP2 | 2.16 | 0.60 |
| 46:CM:787:A:O2' | 54:CU:100:ARG:NE | 2.34 | 0.60 |
| 49:CP:53:LEU:HA | 68:DI:12:TYR:HE1 | 1.67 | 0.60 |
| 57:CX:70:ASP:OD1 | 57:CX:71:GLU:N | 2.34 | 0.60 |
| 57:CX:78:THR:O | 57:CX:81:ASN:ND2 | 2.34 | 0.60 |
| 67:DH:32:GLN:HB3 | 67:DH:108:GLU:HG2 | 1.84 | 0.60 |
| 1:1:948:A:H4' | 1:1:964:G:N2 | 2.16 | 0.60 |
| 18:x:120:ASN:HB2 | 18:x:145:HIS:HB2 | 1.84 | 0.60 |
| 62:R:94:VAL:HG21 | 62:R:116:LEU:HD11 | 1.83 | 0.60 |
| 1:AS:118:U:O2' | 10:BC:134:LYS:NZ | 2.34 | 0.60 |
| 1:AS:2709:C:O2' | 30:BW:36:ASP:OD1 | 2.19 | 0.60 |
| 46:CM:558:U:H2' | 46:CM:559:G:H8 | 1.66 | 0.60 |
| 82:L1:117:ILE:HD11 | 82:L1:137:PRO:HB3 | 1.83 | 0.60 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 1:1:631:U:H2' | 1:1:632:C:C6 | 2.36 | 0.60 |
| 1:1:2345:A:H2' | 1:1:2346:A:C8 | 2.37 | 0.60 |
| 20:z:23:TRP:HB3 | 20:z:51:VAL:HG12 | 1.84 | 0.60 |
| 46:B:874:U:H2' | 46:B:875:C:H6 | 1.66 | 0.60 |
| 49:E:53:LEU:HA | 68:X:12:TYR:HE1 | 1.65 | 0.60 |
| 60:P:46:THR:O | 60:P:50:ILE:HD12 | 2.01 | 0.60 |
| 1:AS:498:C:H5" | 8:BA:25:ARG:NH2 | 2.17 | 0.60 |
| 1:AS:1303:G:OP1 | 17:BJ:60:ARG:NH2 | 2.34 | 0.60 |
| 1:AS:2449:U:O4 | 1:AS:2452:G:N2 | 2.28 | 0.60 |
| 10:BC:249:LYS:HE3 | 10:BC:253:ALA:HB2 | 1.84 | 0.60 |
| 48:CO:145:ARG:NH2 | 48:CO:151:LYS:O | 2.34 | 0.60 |
| 48:CO:151:LYS:NZ | 48:CO:153:THR:O | 2.33 | 0.60 |
| 1:1:3192:A:O3' | 15:u:126:LYS:NZ | 2.32 | 0.60 |
| 16:v:96:LYS:NZ | 16:v:104:GLU:OE2 | 2.34 | 0.60 |
| 33:AF:80:VAL:HG12 | 33:AF:112:LYS:HD2 | 1.83 | 0.60 |
| 46:B:1335:U:H2' | 46:B:1336:G:C8 | 2.37 | 0.60 |
| 1:AS:619:A:H2' | 1:AS:620:A:C8 | 2.36 | 0.60 |
| 16:BI:159:ARG:HB2 | 16:BI:164:LEU:HB2 | 1.82 | 0.60 |
| 23:BP:19:VAL:O | 23:BP:21:ALA:N | 2.35 | 0.60 |
| 1:1:591:C:O2 | 9:o:24:ARG:NH1 | 2.34 | 0.60 |
| 46:B:703:U:H2' | 46:B:704:A:N7 | 2.16 | 0.60 |
| 46:B:1265:C:H2' | 46:B:1266:G:H8 | 1.67 | 0.60 |
| 46:B:1575:G:H1 | 46:B:1595:U:H3 | 1.48 | 0.60 |
| 49:E:165:ILE:HB | 49:E:192:TYR:HB2 | 1.84 | 0.60 |
| 1:AS:294:U:OP2 | 16:BI:15:GLN:NE2 | 2.32 | 0.60 |
| 1:AS:1302:G:C5 | 17:BJ:63:THR:HA | 2.37 | 0.60 |
| 1:AS:2138:G:H2' | 1:AS:2139:G:H8 | 1.67 | 0.60 |
| 1:AS:2925:U:H2' | 1:AS:2926:U:H2' | 1.84 | 0.60 |
| 1:AS:2937:U:O2' | 4:AW:221:LYS:HD3 | 2.02 | 0.60 |
| 7:AZ:85:ARG:NH2 | 7:AZ:250:ASP:OD2 | 2.35 | 0.60 |
| 23:BP:28:PHE:HE1 | 23:BP:33:TYR:HB2 | 1.67 | 0.60 |
| 35:CB:57:LEU:HB2 | 35:CB:62:TYR:CE1 | 2.37 | 0.60 |
| 46:CM:870:G:OP1 | 48:CO:216:LYS:NZ | 2.26 | 0.60 |
| 46:CM:1678:G:H1 | 46:CM:1698:U:H3 | 1.49 | 0.60 |
| 46:CM:1715:U:H2' | 46:CM:1716:C:C6 | 2.36 | 0.60 |
| 79:DT:218:ILE:HG23 | 79:DT:230:THR:HG22 | 1.84 | 0.60 |
| 1:1:934:C:H2' | 1:1:935:U:H5" | 1.83 | 0.60 |
| 1:1:2384:C:H2' | 1:1:2385:C:C6 | 2.37 | 0.60 |
| 3:4:63:G:N2 | 3:4:97:A:N1 | 2.50 | 0.60 |
| 46:B:220:A:H2' | 46:B:221:U:C2 | 2.37 | 0.60 |
| 46:B:1635:A:H2' | 46:B:1636:C:C6 | 2.37 | 0.60 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 66:V:28:LEU:HA | 66:V:111:ILE:HD11 | 1.84 | 0.60 |
| 1:AS:2941:A:N7 | 4:AW:215:ASN:ND2 | 2.50 | 0.60 |
| 3:AU:52:A:H62 | 40:CG:27:ILE:HD13 | 1.67 | 0.60 |
| 23:BP:34:VAL:HG21 | 23:BP:58:ALA:HB2 | 1.83 | 0.60 |
| 46:CM:738:A:OP1 | 51:CR:187:ARG:N | 2.35 | 0.60 |
| 46:CM:924:A:H2' | 46:CM:925:A:C8 | 2.36 | 0.60 |
| 46:CM:1265:C:H2' | 46:CM:1266:G:C8 | 2.36 | 0.60 |
| 48:CO:82:ARG:NH1 | 48:CO:191:GLU:OE2 | 2.34 | 0.60 |
| 1:1:712:G:HO2' | 1:1:749:C:HO2' | 1.49 | 0.59 |
| 1:1:1830:U:OP2 | 40:AM:10:LYS:NZ | 2.33 | 0.59 |
| 1:1:2709:C:O2' | 30:AC:36:ASP:OD1 | 2.17 | 0.59 |
| 9:o:13:LYS:HE3 | 9:o:17:GLN:NE2 | 2.17 | 0.59 |
| 46:B:1410:A:H2' | 49:E:87:ALA:CB | 2.31 | 0.59 |
| 46:B:1776:G:OP2 | 61:Q:127:ARG:NH2 | 2.33 | 0.59 |
| 1:AS:1217:A:H4' | 1:AS:1218:G:OP2 | 2.02 | 0.59 |
| 1:AS:2191:A:H2' | 1:AS:2192:A:H8 | 1.66 | 0.59 |
| 1:AS:2384:C:H2' | 1:AS:2385:C:C6 | 2.36 | 0.59 |
| 1:AS:2873:G:O2' | 1:AS:2996:A:N1 | 2.34 | 0.59 |
| 1:AS:3310:G:OP1 | 55:CV:92:ARG:HG2 | 2.02 | 0.59 |
| 2:AT:3:U:H2' | 2:AT:4:U:C6 | 2.37 | 0.59 |
| 31:BX:29:TYR:OH | 31:BX:57:GLU:OE2 | 2.20 | 0.59 |
| 46:CM:521:G:H5' | 71:DL:60:PHE:O | 2.02 | 0.59 |
| 51:CR:21:ASP:OD2 | 51:CR:24:SER:OG | 2.20 | 0.59 |
| 82:l1:49:PHE:CG | 82:l1:193:LEU:HB3 | 2.37 | 0.59 |
| 1:1:1265:U:H5' | 1:1:1266:A:OP2 | 2.01 | 0.59 |
| 1:1:2669:A:H2' | 1:1:2670:G:H8 | 1.67 | 0.59 |
| 46:B:1026:G:H2' | 46:B:1027:G:H8 | 1.67 | 0.59 |
| 1:AS:3136:C:H2' | 1:AS:3137:A:C8 | 2.36 | 0.59 |
| 46:CM:214:U:H4' | 46:CM:215:A:OP2 | 2.02 | 0.59 |
| 66:DG:42:GLY:HA2 | 66:DG:84:LYS:HG3 | 1.85 | 0.59 |
| 1:1:730:A:H4' | 1:1:730:A:OP1 | 2.03 | 0.59 |
| 46:B:216:A:H4' | 46:B:217:A:OP1 | 2.01 | 0.59 |
| 46:B:673:A:H2' | 46:B:674:C:O4' | 2.02 | 0.59 |
| 50:F:65:ARG:HD2 | 57:M:91:ARG:NH1 | 2.17 | 0.59 |
| 62:R:97:TYR:HE1 | 62:R:102:PHE:CZ | 2.19 | 0.59 |
| 1:AS:1830:U:OP2 | 40:CG:10:LYS:NZ | 2.34 | 0.59 |
| 3:AU:8:C:H2' | 3:AU:9:A:H8 | 1.67 | 0.59 |
| 3:AU:9:A:H2' | 3:AU:10:A:C8 | 2.38 | 0.59 |
| 80:p0:45:LEU:HD12 | 80:p0:49:ALA:HB3 | 1.83 | 0.59 |
| 1:1:1231:U:OP2 | 81:12:119:LYS:NZ | 2.36 | 0.59 |
| 1:1:1302:G:O6 | 1:1:2344:C:O2' | 2.18 | 0.59 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 1:1:2482:U:H2' | 1:1:2483:U:H5' | 1.85 | 0.59 |
| 1:1:2679:U:O2' | 45:i:37:LYS:O | 2.19 | 0.59 |
| 23:5:92:ILE:HD12 | 23:5:96:ILE:HD12 | 1.84 | 0.59 |
| 46:B:1551:U:H2' | 46:B:1552:C:H6 | 1.67 | 0.59 |
| 1:AS:431:A:H2' | 1:AS:432:G:C8 | 2.37 | 0.59 |
| 1:AS:1744:G:OP1 | 39:CF:44:LYS:NZ | 2.33 | 0.59 |
| 1:AS:2448:C:N3 | 1:AS:2467:C:H4' | 2.18 | 0.59 |
| 51:CR:126:VAL:HG13 | 51:CR:139:VAL:HG13 | 1.84 | 0.59 |
| 65:DF:63:GLN:O | 65:DF:67:GLU:HG3 | 2.03 | 0.59 |
| 6:l:290:LEU:HD22 | 19:y:129:LEU:HD11 | 1.85 | 0.59 |
| 46:B:1193:A:H4' | 46:B:1255:G:P | 2.42 | 0.59 |
| 64:T:72:LYS:NZ | 64:T:76:GLU:OE2 | 2.34 | 0.59 |
| 1:AS:289:A:H2' | 1:AS:290:G:H8 | 1.68 | 0.59 |
| 1:AS:2958:U:H2' | 1:AS:2959:A:H8 | 1.67 | 0.59 |
| 69:DJ:11:LEU:HD11 | 69:DJ:37:PHE:CE2 | 2.34 | 0.59 |
| 1:1:1662:G:H2' | 1:1:1663:A:C8 | 2.37 | 0.59 |
| 1:1:1758:U:O2' | 1:1:1759:U:C2 | 2.55 | 0.59 |
| 1:1:2628:A:OP2 | 43:AP:97:LYS:HD3 | 2.03 | 0.59 |
| 38:AK:21:ARG:HD2 | 38:AK:37:CYS:SG | 2.42 | 0.59 |
| 1:AS:292:U:OP2 | 16:BI:68:ARG:NH2 | 2.34 | 0.59 |
| 3:AU:140:G:O3' | 16:BI:109:ARG:NH1 | 2.35 | 0.59 |
| 16:BI:46:ASP:OD2 | 16:BI:50:ARG:NH2 | 2.34 | 0.59 |
| 46:CM:349:C:OP1 | 46:CM:628:A:O2' | 2.19 | 0.59 |
| 46:CM:472:A:H5" | 56:CW:144:PRO:HD2 | 1.83 | 0.59 |
| 46:CM:786:G:H21 | 69:DJ:107:SER:HB3 | 1.67 | 0.59 |
| 46:CM:834:C:H2' | 46:CM:835:A:C8 | 2.38 | 0.59 |
| 63:DD:98:GLU:HG3 | 63:DD:101:LYS:HE3 | 1.85 | 0.59 |
| 79:DT:259:ILE:HD12 | 79:DT:268:LEU:HD23 | 1.83 | 0.59 |
| 2:3:13:A:H2 | 7:m:21:ARG:HB2 | 1.67 | 0.59 |
| 13:s:101:ASN:HD22 | 13:s:130:VAL:HA | 1.67 | 0.59 |
| 46:B:219:A:H2' | 46:B:220:A:C8 | 2.38 | 0.59 |
| 46:B:1138:G:OP1 | 73:c:85:ARG:NH1 | 2.35 | 0.59 |
| 46:B:1160:U:H2' | 46:B:1161:G:H8 | 1.67 | 0.59 |
| 50:F:210:ALA:O | 64:T:19:ARG:NH1 | 2.36 | 0.59 |
| 59:O:105:GLN:HG3 | 59:O:113:ARG:HD3 | 1.85 | 0.59 |
| 75:e:12:VAL:HG22 | 75:e:52:ASP:H | 1.67 | 0.59 |
| 1:AS:1148:G:N2 | 1:AS:1148:G:OP2 | 2.36 | 0.59 |
| 46:CM:1036:U:O2 | 46:CM:1052:G:N2 | 2.30 | 0.59 |
| 50:CQ:212:ALA:HB2 | 64:DE:19:ARG:HG3 | 1.84 | 0.59 |
| 55:CV:76:THR:HG21 | 55:CV:104:ILE:HD12 | 1.85 | 0.59 |
| 64:DE:61:ILE:HD11 | 64:DE:69:ILE:HD11 | 1.83 | 0.59 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 6:l:301:ARG:NH2 | 19:y:38:ARG:O | 2.36 | 0.59 |
| 30:AC:17:HIS:CD2 | 30:AC:21:ILE:HG13 | 2.37 | 0.59 |
| 46:B:653:G:O2' | 46:B:672:U:N3 | 2.34 | 0.59 |
| 46:B:1276:G:H22 | 46:B:1309:G:N2 | 2.01 | 0.59 |
| 1:AS:1592:C:H2' | 1:AS:1593:C:C6 | 2.38 | 0.59 |
| 37:CD:57:ILE:HG23 | 37:CD:93:ILE:HD11 | 1.83 | 0.59 |
| 46:CM:824:U:OP2 | 58:CY:28:ASN:HB2 | 2.03 | 0.59 |
| 46:CM:1216:U:H3 | 46:CM:1239:U:H3 | 1.51 | 0.59 |
| 54:CU:52:LYS:O | 54:CU:84:ARG:HA | 2.02 | 0.59 |
| 1:1:481:G:H2' | 1:1:482:U:C6 | 2.37 | 0.59 |
| 1:1:1801:C:H2' | 1:1:1802:A:H8 | 1.67 | 0.59 |
| 1:1:3039:C:H3' | 20:z:62:ARG:HH22 | 1.67 | 0.59 |
| 3:4:75:G:OP2 | 27:9:74:TYR:OH | 2.17 | 0.59 |
| 13:s:93:SER:N | 13:s:172:LEU:O | 2.35 | 0.59 |
| 18:x:126:ARG:HG3 | 18:x:140:GLN:HG2 | 1.82 | 0.59 |
| 23:5:22:PRO:HB2 | 23:5:28:PHE:HB2 | 1.85 | 0.59 |
| 46:B:479:A:H2' | 46:B:480:U:C6 | 2.37 | 0.59 |
| 46:B:578:A:O2' | 46:B:580:U:OP1 | 2.21 | 0.59 |
| 59:O:26:ASP:HA | 59:O:29:LYS:HG2 | 1.85 | 0.59 |
| 79:AR:127:SER:OG | 79:AR:129:ASP:OD1 | 2.18 | 0.59 |
| 1:AS:1208:A:O3' | 21:BN:92:LYS:NZ | 2.35 | 0.59 |
| 46:CM:85:A:N3 | 46:CM:146:A:O2' | 2.36 | 0.59 |
| 1:1:297:G:OP2 | 1:1:297:G:N2 | 2.25 | 0.59 |
| 1:1:754:C:OP1 | 43:AP:15:LYS:NZ | 2.36 | 0.59 |
| 5:k:66:LYS:HZ1 | 24:6:9:ASN:H | 1.51 | 0.59 |
| 27:9:51:ARG:HG2 | 27:9:52:GLN:H | 1.68 | 0.59 |
| 70:Z:109:ARG:HB3 | 70:Z:112:LYS:HG3 | 1.84 | 0.59 |
| 2:AT:112:G:H2' | 2:AT:113:C:C6 | 2.38 | 0.59 |
| 20:BM:134:HIS:HE1 | 20:BM:136:ARG:HE | 1.49 | 0.59 |
| 46:CM:509:A:OP2 | 56:CW:176:ASN:ND2 | 2.36 | 0.59 |
| 51:CR:100:ARG:HG2 | 51:CR:102:VAL:HG13 | 1.85 | 0.59 |
| 1:1:268:A:C4 | 16:v:12:ARG:HG2 | 2.37 | 0.58 |
| 1:1:907:C:N4 | 4:j:3:ARG:HD3 | 2.17 | 0.58 |
| 1:1:3133:G:H2' | 1:1:3134:C:C6 | 2.37 | 0.58 |
| 46:B:217:A:H2' | 46:B:218:A:O4' | 2.02 | 0.58 |
| 46:B:1238:U:H5" | 78:h:172:ILE:HD12 | 1.84 | 0.58 |
| 62:R:26:VAL:HG23 | 62:R:27:GLU:HG3 | 1.85 | 0.58 |
| 46:CM:985:C:H5 | 46:CM:988:A:H5" | 1.66 | 0.58 |
| 50:CQ:65:ARG:HD2 | 57:CX:91:ARG:HE | 1.67 | 0.58 |
| 59:CZ:82:PRO:HB2 | 59:CZ:84:GLU:H | 1.66 | 0.58 |
| 82:l1:41:TYR:HB3 | 82:l1:163:LEU:HD11 | 1.83 | 0.58 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 82:l1:138:VAL:HG13 | 82:l1:147:LYS:HZ1 | 1.67 | 0.58 |
| 1:1:2498:A:H2' | 1:1:2499:U:C6 | 2.37 | 0.58 |
| 53:I:21:GLU:OE2 | 53:I:28:TYR:OH | 2.19 | 0.58 |
| 59:O:63:CYS:HB3 | 59:O:97:LEU:HD11 | 1.84 | 0.58 |
| 79:AR:90:LEU:HD11 | 79:AR:125:SER:HB3 | 1.85 | 0.58 |
| 1:AS:172:C:O2' | 1:AS:173:C:OP1 | 2.21 | 0.58 |
| 1:AS:941:C:H2' | 1:AS:942:U:C6 | 2.38 | 0.58 |
| 1:AS:2322:U:H2' | 1:AS:2323:A:C8 | 2.38 | 0.58 |
| 2:AT:3:U:H2' | 2:AT:4:U:H6 | 1.68 | 0.58 |
| 11:BD:80:THR:HA | 11:BD:83:THR:HG22 | 1.85 | 0.58 |
| 33:BZ:97:ILE:HG21 | 33:BZ:106:ARG:HG3 | 1.85 | 0.58 |
| 45:CL:96:LYS:HE2 | 46:CM:575:G:H2' | 1.85 | 0.58 |
| 46:CM:52:U:H2' | 46:CM:53:G:H8 | 1.67 | 0.58 |
| 46:CM:504:A:N6 | 77:DR:27:PRO:HB3 | 2.17 | 0.58 |
| 46:CM:723:G:H2' | 46:CM:724:G:O4' | 2.02 | 0.58 |
| 1:1:1225:G:H2' | 1:1:1226:G:C8 | 2.39 | 0.58 |
| 2:3:81:U:H2' | 2:3:82:G:H8 | 1.67 | 0.58 |
| 3:4:103:G:OP2 | 3:4:105:A:O2' | 2.22 | 0.58 |
| 11:q:110:ASP:HB3 | 11:q:128:ILE:HD12 | 1.85 | 0.58 |
| 46:B:108:A:H2' | 46:B:109:G:C8 | 2.38 | 0.58 |
| 64:T:17:ILE:HB | 64:T:69:ILE:HD12 | 1.86 | 0.58 |
| 65:U:16:ARG:NH1 | 65:U:21:ASN:OD1 | 2.37 | 0.58 |
| 1:AS:449:U:H2' | 1:AS:450:G:H8 | 1.68 | 0.58 |
| 1:AS:2347:G:H2' | 1:AS:2348:G:C8 | 2.38 | 0.58 |
| 1:AS:2469:A:O5' | 82:L1:212:PRO:HA | 2.04 | 0.58 |
| 1:AS:2988:A:H2' | 1:AS:2989:A:C8 | 2.38 | 0.58 |
| 1:AS:3256:G:H2' | 1:AS:3257:A:H8 | 1.66 | 0.58 |
| 46:CM:68:A:OP1 | 53:CT:160:ARG:NH2 | 2.34 | 0.58 |
| 46:CM:533:A:OP1 | 56:CW:168:ARG:NH2 | 2.34 | 0.58 |
| 46:CM:970:G:H2' | 46:CM:971:G:H8 | 1.68 | 0.58 |
| 52:CS:122:HIS:HB2 | 52:CS:129:PRO:HG3 | 1.85 | 0.58 |
| 81:12:155:ILE:HG13 | 81:12:159:GLU:HB3 | 1.86 | 0.58 |
| 82:L1:36:VAL:HG13 | 82:L1:204:LEU:HG | 1.86 | 0.58 |
| 23:5:30:GLN:HE22 | 23:5:59:GLU:HB2 | 1.68 | 0.58 |
| 29:AB:36:GLY:HA3 | 29:AB:40:HIS:CE1 | 2.38 | 0.58 |
| 45:i:129:LEU:HD21 | 50:F:129:GLY:HA3 | 1.85 | 0.58 |
| 46:B:501:G:H2' | 46:B:502:U:C6 | 2.38 | 0.58 |
| 46:B:1463:G:H2' | 46:B:1464:G:C8 | 2.38 | 0.58 |
| 1:AS:2335:A:H2' | 1:AS:2336:A:H8 | 1.67 | 0.58 |
| 1:AS:2472:A:H1' | 82:L1:163:LEU:HB2 | 1.86 | 0.58 |
| 2:AT:39:U:H5' | 45:CL:33:ASN:ND2 | 2.17 | 0.58 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 10:BC:42:GLN:OE1 | 10:BC:45:ARG:NH2 | 2.30 | 0.58 |
| 46:CM:496:G:H2' | 46:CM:497:U:O4' | 2.04 | 0.58 |
| 46:CM:1637:U:H2' | 46:CM:1638:A:C8 | 2.39 | 0.58 |
| 60:DA:55:ARG:NH2 | 74:DO:51:GLN:OE1 | 2.35 | 0.58 |
| 7:m:197:LYS:HG2 | 7:m:202:GLY:HA3 | 1.85 | 0.58 |
| 28:AA:41:ALA:HB2 | 28:AA:77:TYR:HE1 | 1.69 | 0.58 |
| 46:B:518:A:H2' | 46:B:519:A:H8 | 1.67 | 0.58 |
| 53:I:159:ARG:HB2 | 53:I:170:THR:HB | 1.84 | 0.58 |
| 71:a:6:THR:HB | 71:a:28:LEU:HB2 | 1.85 | 0.58 |
| 46:CM:1399:U:O2' | 46:CM:1402:G:OP1 | 2.20 | 0.58 |
| 1:1:2408:A:H2' | 1:1:2409:C:C6 | 2.39 | 0.58 |
| 3:4:63:G:O2' | 36:AI:49:LYS:NZ | 2.36 | 0.58 |
| 4:j:29:LEU:HD22 | 4:j:101:ILE:HD13 | 1.86 | 0.58 |
| 46:B:671:G:H3' | 46:B:672:U:C5' | 2.24 | 0.58 |
| 1:AS:1635:C:OP2 | 35:CB:74:ARG:NH1 | 2.33 | 0.58 |
| 1:AS:2435:G:H1 | 1:AS:2439:A:H61 | 1.52 | 0.58 |
| 6:AY:301:ARG:NH2 | 19:BL:38:ARG:O | 2.36 | 0.58 |
| 46:CM:768:C:H2' | 46:CM:769:U:O4' | 2.04 | 0.58 |
| 1:1:1779:U:H2' | 1:1:1780:A:C8 | 2.38 | 0.58 |
| 1:1:2322:U:H2' | 1:1:2323:A:C8 | 2.39 | 0.58 |
| 46:B:1129:U:H2' | 46:B:1130:U:C6 | 2.38 | 0.58 |
| 46:B:1445:C:H2' | 65:U:138:THR:OG1 | 2.04 | 0.58 |
| 47:C:63:ILE:HG12 | 68:X:36:ILE:HG12 | 1.86 | 0.58 |
| 51:G:126:VAL:HG13 | 51:G:139:VAL:HG13 | 1.83 | 0.58 |
| 1:AS:112:C:OP1 | 16:BI:147:ARG:NH2 | 2.37 | 0.58 |
| 1:AS:1794:A:H2' | 1:AS:1795:A:C8 | 2.39 | 0.58 |
| 1:AS:1841:G:H5" | 1:AS:1842:C:H5' | 1.85 | 0.58 |
| 1:AS:2545:C:O2' | 1:AS:2547:G:N3 | 2.37 | 0.58 |
| 24:BQ:24:ASN:ND2 | 24:BQ:97:ASP:OD2 | 2.34 | 0.58 |
| 46:CM:189:G:N7 | 55:CV:143:ARG:NH2 | 2.50 | 0.58 |
| 46:CM:965:G:H4' | 46:CM:1763:A:H4' | 1.86 | 0.58 |
| 46:CM:1147:C:H4' | 75:DP:22:ARG:HD3 | 1.86 | 0.58 |
| 46:CM:1548:U:H4' | 46:CM:1586:C:H4' | 1.86 | 0.58 |
| 65:DF:27:LYS:HA | 65:DF:57:ARG:HA | 1.86 | 0.58 |
| 81:12:124:ASN:O | 81:12:126:ALA:N | 2.33 | 0.58 |
| 82:L1:50:SER:HA | 82:L1:158:GLN:HA | 1.86 | 0.58 |
| 82:l1:206:ILE:HG12 | 82:l1:216:ILE:HG13 | 1.85 | 0.58 |
| 1:1:2832:U:O2 | 1:1:2910:G:H4' | 2.03 | 0.58 |
| 1:1:2958:U:H2' | 1:1:2959:A:H8 | 1.67 | 0.58 |
| 43:AP:38:GLN:OE1 | 43:AP:41:ARG:NH2 | 2.37 | 0.58 |
| 46:B:626:G:N1 | 46:B:955:A:OP2 | 2.28 | 0.58 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 46:B:1131:G:H2' | 46:B:1132:A:H8 | 1.69 | 0.58 |
| 46:B:1265:C:O2' | 67:W:69:THR:HG22 | 2.03 | 0.58 |
| 1:AS:236:A:OP1 | 3:AU:95:G:N2 | 2.28 | 0.58 |
| 1:AS:563:U:H2' | 1:AS:564:G:C8 | 2.39 | 0.58 |
| 1:AS:1692:A:H2' | 1:AS:1693:A:C8 | 2.37 | 0.58 |
| 1:AS:1936:G:H21 | 1:AS:3327:A:H8 | 1.51 | 0.58 |
| 1:AS:2580:G:OP1 | 4:AW:2:GLY:N | 2.37 | 0.58 |
| 2:AT:4:U:H2' | 2:AT:5:G:H8 | 1.68 | 0.58 |
| 46:CM:669:G:H2' | 46:CM:671:G:C8 | 2.39 | 0.58 |
| 1:1:1140:U:OP1 | 1:1:1363:G:O2' | 2.21 | 0.58 |
| 1:1:2138:G:H2' | 1:1:2139:G:C8 | 2.39 | 0.58 |
| 1:1:2391:A:H2' | 1:1:2392:G:H8 | 1.68 | 0.58 |
| 1:1:3133:G:H2' | 1:1:3134:C:H6 | 1.69 | 0.58 |
| 8:n:20:THR:HG22 | 8:n:22:LYS:H | 1.69 | 0.58 |
| 19:y:67:ILE:HG12 | 19:y:81:ILE:HG21 | 1.86 | 0.58 |
| 46:B:4:C:O2' | 56:L:17:ARG:NH2 | 2.36 | 0.58 |
| 46:B:924:A:H2' | 46:B:925:A:C8 | 2.39 | 0.58 |
| 46:B:940:A:H4' | 46:B:1058:G:O2' | 2.04 | 0.58 |
| 46:B:1399:U:O2' | 46:B:1400:U:OP1 | 2.21 | 0.58 |
| 46:B:1478:A:O2' | 46:B:1479:A:O4' | 2.21 | 0.58 |
| 46:B:1719:A:H2' | 46:B:1720:C:H6 | 1.66 | 0.58 |
| 59:O:29:LYS:HE2 | 59:O:100:TRP:CE3 | 2.39 | 0.58 |
| 1:AS:1663:A:H2' | 1:AS:1664:G:H8 | 1.67 | 0.58 |
| 1:AS:2158:A:H2' | 1:AS:2159:C:C6 | 2.39 | 0.58 |
| 1:AS:2244:U:H2' | 1:AS:2245:C:H6 | 1.68 | 0.58 |
| 46:CM:78:A:H2 | 53:CT:174:LYS:HG3 | 1.69 | 0.58 |
| 48:CO:174:ARG:NH2 | 48:CO:196:GLU:OE2 | 2.37 | 0.58 |
| 51:CR:100:ARG:NH1 | 51:CR:118:GLU:OE2 | 2.37 | 0.58 |
| 55:CV:120:THR:HG21 | 55:CV:133:ALA:HA | 1.86 | 0.58 |
| 1:1:431:A:H2' | 1:1:432:G:C8 | 2.39 | 0.58 |
| 1:1:2385:C:H2' | 1:1:2386:U:H6 | 1.69 | 0.58 |
| 1:1:3151:C:OP2 | 17:w:172:LYS:NZ | 2.34 | 0.58 |
| 1:1:3287:A:H2' | 1:1:3288:A:H8 | 1.68 | 0.58 |
| 15:u:19:VAL:HG12 | 15:u:57:LEU:HA | 1.85 | 0.58 |
| 16:v:31:ARG:NH1 | 16:v:124:ASP:OD2 | 2.35 | 0.58 |
| 62:R:121:ILE:HD11 | 65:U:125:ILE:HD13 | 1.86 | 0.58 |
| 1:AS:48:A:N7 | 16:BI:187:ARG:HD2 | 2.18 | 0.58 |
| 45:CL:159:GLU:OE2 | 45:CL:163:GLN:NE2 | 2.34 | 0.58 |
| 46:CM:103:A:O3' | 46:CM:306:C:N4 | 2.36 | 0.58 |
| 46:CM:1578:C:H2' | 46:CM:1579:A:C8 | 2.39 | 0.58 |
| 47:CN:59:LEU:HD22 | 68:DI:79:LEU:HD11 | 1.86 | 0.58 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 50:CQ:214:ASP:CG | 50:CQ:215:GLU:H | 2.11 | 0.58 |
| 62:DC:121:ILE:HD11 | 65:DF:125:ILE:HD13 | 1.86 | 0.58 |
| 65:DF:87:ASN:HB2 | 65:DF:99:HIS:CE1 | 2.39 | 0.58 |
| 79:DT:9:LEU:HB2 | 79:DT:310:TRP:CZ3 | 2.39 | 0.58 |
| 82:L1:87:VAL:HA | 82:L1:90:LEU:HD12 | 1.86 | 0.58 |
| 1:1:1691:U:O2' | 1:1:1745:A:N1 | 2.36 | 0.57 |
| 3:4:8:C:H2' | 3:4:9:A:H8 | 1.68 | 0.57 |
| 5:k:260:VAL:HG11 | 5:k:266:ARG:HH11 | 1.69 | 0.57 |
| 7:m:164:LYS:NZ | 7:m:168:ASP:OD1 | 2.34 | 0.57 |
| 48:D:82:ARG:NH2 | 48:D:191:GLU:OE2 | 2.37 | 0.57 |
| 52:H:98:MET:O | 52:H:99:MET:HE2 | 2.03 | 0.57 |
| 54:J:137:ARG:NH2 | 69:Y:49:GLU:OE1 | 2.37 | 0.57 |
| 79:AR:152:VAL:HG12 | 79:AR:170:SER:HB2 | 1.85 | 0.57 |
| 1:AS:782:A:H4' | 1:AS:783:G:H5' | 1.84 | 0.57 |
| 1:AS:2456:C:H3' | 1:AS:2457:C:H5" | 1.84 | 0.57 |
| 1:AS:3165:U:H2' | 1:AS:3166:A:H4' | 1.85 | 0.57 |
| 46:CM:1200:C:OP1 | 78:DS:134:LYS:NZ | 2.33 | 0.57 |
| 51:CR:123:LEU:HD13 | 51:CR:237:VAL:HG13 | 1.86 | 0.57 |
| 59:CZ:75:VAL:HA | 59:CZ:78:LEU:HG | 1.84 | 0.57 |
| 82:L1:66:CYS:HB2 | 82:L1:83:ASP:HB2 | 1.85 | 0.57 |
| 1:1:1255:A:N7 | 80:P0:53:MET:HB3 | 2.19 | 0.57 |
| 1:1:1841:G:H5" | 1:1:1842:C:H5' | 1.85 | 0.57 |
| 1:1:3256:G:H2' | 1:1:3257:A:H8 | 1.68 | 0.57 |
| 46:B:738:A:OP1 | 51:G:187:ARG:N | 2.37 | 0.57 |
| 46:B:784:U:H2' | 46:B:785:G:C8 | 2.39 | 0.57 |
| 46:B:1245:U:H2' | 46:B:1246:G:H8 | 1.69 | 0.57 |
| 46:B:1649:G:H2' | 46:B:1650:G:H8 | 1.69 | 0.57 |
| 49:E:168:PRO:HG3 | 56:L:57:ARG:HD3 | 1.86 | 0.57 |
| 57:M:14:TYR:HD2 | 57:M:21:VAL:HG22 | 1.69 | 0.57 |
| 64:T:96:THR:HG23 | 64:T:98:GLY:H | 1.69 | 0.57 |
| 1:AS:1530:A:H2' | 1:AS:1531:A:C8 | 2.39 | 0.57 |
| 1:AS:1779:U:H2' | 1:AS:1780:A:C8 | 2.38 | 0.57 |
| 1:AS:1795:A:H2' | 1:AS:1796:A:H8 | 1.68 | 0.57 |
| 1:AS:2587:G:H2' | 1:AS:2588:C:H6 | 1.67 | 0.57 |
| 25:BR:82:ILE:HG21 | 53:CT:158:VAL:HG11 | 1.87 | 0.57 |
| 29:BV:36:GLY:HA3 | 29:BV:40:HIS:CE1 | 2.39 | 0.57 |
| 46:CM:610:U:OP2 | 70:DK:5:LYS:NZ | 2.34 | 0.57 |
| 46:CM:1026:G:H2' | 46:CM:1027:G:H8 | 1.69 | 0.57 |
| 46:CM:1192:C:N3 | 46:CM:1442:C:H5 | 2.02 | 0.57 |
| 46:CM:1719:A:H2' | 46:CM:1720:C:H6 | 1.68 | 0.57 |
| 81:12:159:GLU:HG3 | 81:12:160:ILE:HG12 | 1.86 | 0.57 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 5:k:106:TRP:HB2 | 5:k:133:TYR:CE2 | 2.40 | 0.57 |
| 46:B:1400:U:H5" | 64:T:3:ARG:HE | 1.69 | 0.57 |
| 46:B:1469:A:N3 | 46:B:1594:G:O2' | 2.28 | 0.57 |
| 1:AS:115:A:OP2 | 16:BI:2:GLY:N | 2.38 | 0.57 |
| 1:AS:353:G:O6 | 38:CE:55:ARG:NH2 | 2.36 | 0.57 |
| 1:AS:800:C:OP1 | 6:AY:99:ARG:NH2 | 2.37 | 0.57 |
| 1:AS:3287:A:H2' | 1:AS:3288:A:H8 | 1.67 | 0.57 |
| 26:BS:58:ASP:OD2 | 36:CC:25:LYS:NZ | 2.35 | 0.57 |
| 46:CM:119:A:H1' | 46:CM:395:A:C5 | 2.39 | 0.57 |
| 46:CM:560:G:H2' | 46:CM:561:U:O2 | 2.04 | 0.57 |
| 55:CV:113:TYR:OH | 55:CV:156:ALA:O | 2.21 | 0.57 |
| 58:CY:7:VAL:HG23 | 58:CY:8:GLN:HG2 | 1.85 | 0.57 |
| 59:CZ:102:GLY:C | 59:CZ:104:CYS:H | 2.12 | 0.57 |
| 81:12:132:ILE:HA | 81:12:135:THR:HG22 | 1.85 | 0.57 |
| 82:l1:29:LEU:HD13 | 82:l1:173:ASP:HB2 | 1.86 | 0.57 |
| 1:1:294:U:P | 16:v:15:GLN:HE22 | 2.28 | 0.57 |
| 1:1:2492:U:OP2 | 1:1:2558:G:N2 | 2.37 | 0.57 |
| 45:i:107:TRP:HA | 50:F:116:ILE:HD11 | 1.85 | 0.57 |
| 46:B:1216:U:H3 | 46:B:1239:U:H3 | 1.52 | 0.57 |
| 50:F:141:GLY:HA3 | 50:F:183:LEU:HD23 | 1.85 | 0.57 |
| 51:G:199:GLU:OE2 | 51:G:201:HIS:NE2 | 2.35 | 0.57 |
| 59:O:52:LEU:HD21 | 59:O:60:CYS:SG | 2.45 | 0.57 |
| 1:AS:2334:A:H61 | 1:AS:2955:C:H5 | 1.52 | 0.57 |
| 39:CF:32:ASN:C | 39:CF:34:ASN:H | 2.10 | 0.57 |
| 62:DC:13:LYS:H | 62:DC:13:LYS:HD2 | 1.69 | 0.57 |
| 78:DS:168:CYS:SG | 78:DS:186:CYS:HB3 | 2.44 | 0.57 |
| 82:L1:60:ARG:HB2 | 82:L1:63:MET:HE3 | 1.86 | 0.57 |
| 82:l1:208:SER:C | 82:l1:210:MET:H | 2.13 | 0.57 |
| 1:1:662:U:H2' | 1:1:663:A:H8 | 1.67 | 0.57 |
| 1:1:1241:A:H3' | 1:1:1242:G:C5' | 2.31 | 0.57 |
| 1:1:1518:U:O2' | 26:8:113:LEU:HD11 | 2.05 | 0.57 |
| 1:1:2196:G:OP1 | 37:AJ:67:ARG:NH2 | 2.38 | 0.57 |
| 2:3:81:U:H2' | 2:3:82:G:C8 | 2.39 | 0.57 |
| 3:4:9:A:H2' | 3:4:10:A:C8 | 2.40 | 0.57 |
| 46:B:801:A:O4' | 54:J:106:GLN:NE2 | 2.37 | 0.57 |
| 46:B:938:G:H2' | 46:B:939:G:C8 | 2.40 | 0.57 |
| 46:B:1551:U:H2' | 46:B:1552:C:C6 | 2.39 | 0.57 |
| 1:AS:408:A:N3 | 1:AS:653:C:O2' | 2.35 | 0.57 |
| 1:AS:1256:A:O2' | 1:AS:1275:C:O2 | 2.22 | 0.57 |
| 45:CL:67:LYS:HG2 | 65:DF:129:TRP:CZ2 | 2.35 | 0.57 |
| 46:CM:1635:A:H2' | 46:CM:1636:C:C6 | 2.40 | 0.57 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 50:CQ:60:LEU:HD11 | 50:CQ:89:ALA:HB3 | 1.87 | 0.57 |
| 61:DB:124:LYS:HG3 | 61:DB:125:GLY:N | 2.19 | 0.57 |
| 1:1:72:A:N7 | 14:t:66:ASN:HB3 | 2.19 | 0.57 |
| 1:1:99:A:H3' | 1:1:100:G:H21 | 1.69 | 0.57 |
| 1:1:680:U:H5" | 1:1:681:U:H5 | 1.68 | 0.57 |
| 1:1:2126:U:H2' | 1:1:2127:A:C8 | 2.40 | 0.57 |
| 1:1:2959:A:H2' | 1:1:2960:C:C6 | 2.39 | 0.57 |
| 8:n:39:LEU:HB3 | 8:n:83:VAL:HG13 | 1.86 | 0.57 |
| 16:v:46:ASP:OD2 | 16:v:50:ARG:NH2 | 2.36 | 0.57 |
| 20:z:158:GLU:OE2 | 20:z:162:ARG:NH2 | 2.37 | 0.57 |
| 46:B:483:A:H2' | 46:B:484:G:C8 | 2.40 | 0.57 |
| 63:S:27:LEU:HB3 | 63:S:63:ASP:HB2 | 1.85 | 0.57 |
| 1:AS:148:U:H4' | 16:BI:56:LYS:HG2 | 1.86 | 0.57 |
| 1:AS:527:G:H2' | 1:AS:528:A:C8 | 2.39 | 0.57 |
| 4:AW:27:ALA:O | 4:AW:128:ARG:NH2 | 2.37 | 0.57 |
| 23:BP:99:VAL:HG12 | 23:BP:107:LYS:O | 2.05 | 0.57 |
| 45:CL:155:LEU:HD13 | 57:CX:92:LEU:HD13 | 1.87 | 0.57 |
| 46:CM:267:G:H2' | 46:CM:268:C:C6 | 2.40 | 0.57 |
| 46:CM:1302:C:O2' | 46:CM:1386:A:N3 | 2.32 | 0.57 |
| 47:CN:50:ILE:HA | 47:CN:53:THR:HB | 1.87 | 0.57 |
| 80:P0:43:LYS:HD3 | 81:12:121:PHE:HB3 | 1.86 | 0.57 |
| 82:l1:205:VAL:HG13 | 82:l1:213:SER:HB3 | 1.87 | 0.57 |
| 1:1:428:U:H2' | 1:1:429:U:C6 | 2.39 | 0.57 |
| 1:1:679:U:O2' | 1:1:695:G:O6 | 2.15 | 0.57 |
| 1:1:783:G:H2' | 1:1:784:C:C6 | 2.39 | 0.57 |
| 2:3:19:C:H2' | 2:3:20:A:H8 | 1.68 | 0.57 |
| 1:AS:638:U:H2' | 1:AS:639:C:C6 | 2.39 | 0.57 |
| 1:AS:1242:G:O2' | 1:AS:1260:G:OP2 | 2.20 | 0.57 |
| 1:AS:2107:U:H2' | 1:AS:2108:G:C8 | 2.40 | 0.57 |
| 9:BB:143:ARG:HG3 | 9:BB:183:ILE:HD13 | 1.85 | 0.57 |
| 21:BN:73:LYS:NZ | 21:BN:97:VAL:O | 2.37 | 0.57 |
| 46:CM:671:G:H3' | 46:CM:672:U:H5' | 1.87 | 0.57 |
| 46:CM:1395:G:N2 | 46:CM:1398:G:OP2 | 2.36 | 0.57 |
| 46:CM:1486:G:OP2 | 66:DG:73:VAL:HG12 | 2.04 | 0.57 |
| 1:1:1249:U:OP1 | 81:12:137:GLN:NE2 | 2.38 | 0.57 |
| 1:1:2625:C:OP1 | 43:AP:89:LYS:HB2 | 2.05 | 0.57 |
| 16:v:11:GLN:O | 16:v:14:LYS:NZ | 2.36 | 0.57 |
| 21:0:8:GLN:HB2 | 21:0:64:ILE:HD11 | 1.87 | 0.57 |
| 32:AE:7:VAL:HG13 | 32:AE:43:MET:HE1 | 1.87 | 0.57 |
| 46:B:125:U:OP1 | 53:I:201:GLN:NE2 | 2.32 | 0.57 |
| 46:B:874:U:H2' | 46:B:875:C:C6 | 2.40 | 0.57 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 46:B:1300:U:HO2' | 46:B:1301:G:H8 | 1.52 | 0.57 |
| 46:B:1315:G:H21 | 64:T:8:THR:HG21 | 1.68 | 0.57 |
| 55:K:76:THR:HG21 | 55:K:104:ILE:HD12 | 1.85 | 0.57 |
| 1:AS:547:U:H2' | 1:AS:548:G:H8 | 1.70 | 0.57 |
| 46:CM:1145:A:H2' | 46:CM:1146:C:C6 | 2.40 | 0.57 |
| 46:CM:1302:C:H2' | 46:CM:1303:G:O4' | 2.05 | 0.57 |
| 80:p0:66:PHE:HA | 80:p0:69:GLU:HB3 | 1.86 | 0.57 |
| 1:1:1473:A:OP1 | 1:1:3047:G:O2' | 2.16 | 0.57 |
| 1:1:2107:U:H2' | 1:1:2108:G:C8 | 2.40 | 0.57 |
| 4:j:27:ALA:O | 4:j:128:ARG:NH2 | 2.36 | 0.57 |
| 8:n:170:ARG:HB3 | 8:n:172:HIS:CE1 | 2.39 | 0.57 |
| 21:0:92:LYS:HE2 | 21:0:109:ASP:OD1 | 2.05 | 0.57 |
| 46:B:282:G:N7 | 53:I:188:ARG:NH2 | 2.49 | 0.57 |
| 46:B:335:G:O2' | 55:K:10:LYS:NZ | 2.36 | 0.57 |
| 46:B:932:U:H2' | 46:B:933:A:H8 | 1.70 | 0.57 |
| 46:B:1024:A:O2' | 46:B:1025:G:O5' | 2.23 | 0.57 |
| 4:AW:51:ASP:OD2 | 4:AW:54:ARG:NH2 | 2.37 | 0.57 |
| 19:BL:67:ILE:HG12 | 19:BL:81:ILE:HG21 | 1.87 | 0.57 |
| 45:CL:67:LYS:HD2 | 62:DC:125:PRO:HG3 | 1.87 | 0.57 |
| 46:CM:317:U:H4' | 46:CM:321:A:C8 | 2.40 | 0.57 |
| 46:CM:723:G:C4 | 46:CM:724:G:H1' | 2.40 | 0.57 |
| 46:CM:815:U:O2' | 46:CM:816:U:O5' | 2.23 | 0.57 |
| 46:CM:881:U:H5' | 48:CO:23:PRO:HG2 | 1.87 | 0.57 |
| 48:CO:30:PHE:CD1 | 48:CO:96:LEU:HD21 | 2.39 | 0.57 |
| 1:1:292:U:OP2 | 16:v:68:ARG:NH2 | 2.30 | 0.57 |
| 1:1:374:A:N3 | 1:1:376:G:H5" | 2.20 | 0.57 |
| 1:1:1060:A:H4' | 1:1:1061:A:O5' | 2.05 | 0.57 |
| 1:1:1719:A:OP1 | 20:z:128:LYS:NZ | 2.35 | 0.57 |
| 2:3:3:U:H2' | 2:3:4:U:C6 | 2.40 | 0.57 |
| 3:4:36:G:C5 | 36:AI:86:ARG:HD3 | 2.39 | 0.57 |
| 7:m:119:TYR:OH | 7:m:139:PRO:O | 2.21 | 0.57 |
| 59:O:41:LEU:H | 59:O:124:LYS:HG2 | 1.70 | 0.57 |
| 1:AS:649:G:O2' | 1:AS:1431:A:OP1 | 2.22 | 0.57 |
| 1:AS:1275:C:H2' | 1:AS:1276:C:C6 | 2.39 | 0.57 |
| 1:AS:3298:G:N7 | 25:BR:35:LYS:NZ | 2.53 | 0.57 |
| 5:AX:280:HIS:HD1 | 5:AX:328:ILE:HG22 | 1.70 | 0.57 |
| 6:AY:109:ARG:HG2 | 16:BI:203:ARG:HG3 | 1.87 | 0.57 |
| 46:CM:530:U:OP1 | 71:DL:64:PHE:HA | 2.04 | 0.57 |
| 46:CM:1469:A:H2' | 46:CM:1470:G:C8 | 2.40 | 0.57 |
| 48:CO:26:ARG:NH1 | 48:CO:49:ASN:OD1 | 2.38 | 0.57 |
| 57:CX:77:ARG:HD2 | 57:CX:84:GLU:HA | 1.86 | 0.57 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 79:DT:107:HIS:HE2 | 79:DT:125:SER:HG | 1.52 | 0.57 |
| 82:L1:54:LYS:HD2 | 82:L1:150:ASP:HB3 | 1.86 | 0.57 |
| 1:1:1273:C:H2' | 1:1:1274:A:C8 | 2.39 | 0.56 |
| 2:3:4:U:H2' | 2:3:5:G:H8 | 1.70 | 0.56 |
| 46:B:85:A:N3 | 46:B:146:A:O2' | 2.37 | 0.56 |
| 46:B:418:A:OP1 | 53:I:96:SER:OG | 2.18 | 0.56 |
| 46:B:1183:G:OP1 | 46:B:1184:G:O2' | 2.20 | 0.56 |
| 66:V:107:ALA:O | 66:V:111:ILE:HG12 | 2.05 | 0.56 |
| 46:CM:722:A:HO2' | 46:CM:723:G:H8 | 1.51 | 0.56 |
| 66:DG:16:ASN:OD1 | 66:DG:56:LYS:NZ | 2.37 | 0.56 |
| 1:1:268:A:N1 | 1:1:295:A:H5' | 2.19 | 0.56 |
| 1:1:1837:A:H1' | 40:AM:45:ARG:HH22 | 1.70 | 0.56 |
| 1:1:2978:A:H2' | 1:1:2979:U:O4' | 2.05 | 0.56 |
| 46:B:405:A:H2' | 46:B:406:C:H6 | 1.70 | 0.56 |
| 1:AS:2126:U:H2' | 1:AS:2127:A:C8 | 2.40 | 0.56 |
| 1:AS:3260:A:H2' | 1:AS:3261:A:H8 | 1.70 | 0.56 |
| 3:AU:126:A:O2' | 3:AU:129:C:N4 | 2.38 | 0.56 |
| 46:CM:1067:C:H4' | 68:DI:58:TYR:CE1 | 2.36 | 0.56 |
| 68:DI:36:ILE:HD12 | 68:DI:78:LEU:HD13 | 1.87 | 0.56 |
| 1:1:1255:A:C8 | 80:P0:53:MET:HB3 | 2.40 | 0.56 |
| 1:1:1795:A:H2' | 1:1:1796:A:H8 | 1.70 | 0.56 |
| 1:1:2174:C:H2' | 1:1:2220:A:H61 | 1.70 | 0.56 |
| 1:1:2183:U:O4 | 1:1:2216:G:N1 | 2.38 | 0.56 |
| 23:5:19:VAL:O | 23:5:21:ALA:N | 2.38 | 0.56 |
| 46:B:871:U:H2' | 46:B:872:A:H8 | 1.70 | 0.56 |
| 50:F:193:PRO:HG3 | 50:F:203:LEU:HD12 | 1.88 | 0.56 |
| 51:G:175:PHE:HE2 | 51:G:198:ARG:HD2 | 1.70 | 0.56 |
| 57:M:55:VAL:HG12 | 57:M:68:LEU:HA | 1.86 | 0.56 |
| 1:AS:1642:G:O2' | 1:AS:1804:G:N2 | 2.34 | 0.56 |
| 1:AS:2206:A:H2' | 1:AS:2207:A:C8 | 2.40 | 0.56 |
| 1:AS:2651:A:O2' | 13:BF:52:TYR:OH | 2.21 | 0.56 |
| 1:AS:2672:G:H5" | 22:BO:17:ARG:HG2 | 1.86 | 0.56 |
| 8:BA:170:ARG:HB3 | 8:BA:172:HIS:CE1 | 2.40 | 0.56 |
| 12:BE:193:ASP:OD2 | 12:BE:198:LYS:HE3 | 2.05 | 0.56 |
| 26:BS:67:ILE:HD12 | 26:BS:121:LYS:HG3 | 1.87 | 0.56 |
| 39:CF:46:ARG:HD2 | 39:CF:47:GLY:O | 2.05 | 0.56 |
| 46:CM:477:C:OP1 | 56:CW:121:SER:OG | 2.15 | 0.56 |
| 46:CM:589:A:H2' | 46:CM:590:A:C8 | 2.41 | 0.56 |
| 46:CM:652:C:H5' | 46:CM:653:G:OP2 | 2.04 | 0.56 |
| 46:CM:1024:A:O2' | 46:CM:1025:G:O5' | 2.23 | 0.56 |
| 46:CM:1129:U:H2' | 46:CM:1130:U:C6 | 2.39 | 0.56 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 46:CM:1198:G:H1 | 46:CM:1436:U:H3 | 1.53 | 0.56 |
| 46:CM:1593:C:H2' | 46:CM:1594:G:C8 | 2.40 | 0.56 |
| 47:CN:48:ILE:HG12 | 47:CN:149:MET:HE3 | 1.87 | 0.56 |
| 1:1:447:U:H3 | 1:1:483:U:H3 | 1.54 | 0.56 |
| 1:1:496:A:H2' | 1:1:497:U:C6 | 2.40 | 0.56 |
| 46:B:589:A:H2' | 46:B:590:A:C8 | 2.41 | 0.56 |
| 64:T:25:THR:HG23 | 64:T:27:ASP:H | 1.70 | 0.56 |
| 66:V:57:ARG:NH2 | 66:V:101:ASN:OD1 | 2.35 | 0.56 |
| 73:c:5:ARG:HD3 | 73:c:9:GLY:N | 2.21 | 0.56 |
| 1:AS:477:U:H2' | 1:AS:478:G:H8 | 1.70 | 0.56 |
| 1:AS:783:G:H2' | 1:AS:784:C:C6 | 2.40 | 0.56 |
| 1:AS:796:G:H22 | 6:AY:102:ALA:HA | 1.71 | 0.56 |
| 1:AS:1011:C:H4' | 1:AS:1012:U:H6 | 1.71 | 0.56 |
| 1:AS:2933:G:H2' | 1:AS:2934:U:C6 | 2.40 | 0.56 |
| 1:AS:3193:C:H4' | 1:AS:3194:G:O5' | 2.05 | 0.56 |
| 12:BE:101:LYS:HE2 | 12:BE:101:LYS:HA | 1.86 | 0.56 |
| 45:CL:61:GLU:OE1 | 45:CL:61:GLU:N | 2.37 | 0.56 |
| 46:CM:1245:U:H2' | 46:CM:1246:G:C8 | 2.40 | 0.56 |
| 46:CM:1679:A:H2 | 46:CM:1696:U:H3 | 1.51 | 0.56 |
| 47:CN:57:ILE:HG23 | 47:CN:177:LEU:HD23 | 1.87 | 0.56 |
| 60:DA:136:PRO:HG2 | 60:DA:139:TRP:HB2 | 1.87 | 0.56 |
| 1:1:1561:U:H2' | 1:1:1562:G:C8 | 2.40 | 0.56 |
| 1:1:2718:A:H5' | 7:m:178:ASN:OD1 | 2.05 | 0.56 |
| 6:l:155:ASN:OD1 | 6:l:254:GLY:N | 2.30 | 0.56 |
| 20:z:176:ARG:NH1 | 46:B:837:C:OP1 | 2.38 | 0.56 |
| 20:z:176:ARG:NH2 | 46:B:838:G:OP2 | 2.37 | 0.56 |
| 48:D:82:ARG:NH2 | 48:D:188:LEU:O | 2.37 | 0.56 |
| 57:M:86:ILE:HG13 | 57:M:87:LEU:HG | 1.86 | 0.56 |
| 1:AS:429:U:H2' | 1:AS:430:G:C8 | 2.38 | 0.56 |
| 1:AS:2330:A:H5" | 18:BK:83:TRP:O | 2.06 | 0.56 |
| 7:AZ:75:PHE:O | 7:AZ:112:LYS:NZ | 2.36 | 0.56 |
| 16:BI:177:GLY:H | 16:BI:184:LYS:HZ2 | 1.53 | 0.56 |
| 21:BN:99:ARG:NH1 | 21:BN:126:VAL:O | 2.32 | 0.56 |
| 46:CM:834:C:H2' | 46:CM:835:A:H8 | 1.71 | 0.56 |
| 68:DI:64:GLU:OE2 | 74:DO:2:VAL:N | 2.39 | 0.56 |
| 82:l1:113:SER:OG | 82:l1:114:GLU:N | 2.34 | 0.56 |
| 80:p0:45:LEU:HB3 | 80:p0:49:ALA:O | 2.04 | 0.56 |
| 1:1:1079:G:H2' | 1:1:1080:A:H8 | 1.71 | 0.56 |
| 1:1:1199:A:N3 | 1:1:2827:U:O2' | 2.36 | 0.56 |
| 1:1:1493:C:O2' | 1:1:1598:A:N3 | 2.35 | 0.56 |
| 14:t:201:LYS:HE2 | 82:l1:51:GLY:HA2 | 1.88 | 0.56 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 46:B:1087:G:OP2 | 70:Z:7:ARG:NH1 | 2.36 | 0.56 |
| 46:B:1670:U:O2' | 46:B:1671:G:O5' | 2.22 | 0.56 |
| 1:AS:252:U:H5' | 1:AS:253:A:H8 | 1.69 | 0.56 |
| 1:AS:496:A:H4' | 8:BA:27:GLN:HG3 | 1.87 | 0.56 |
| 1:AS:2434:A:H61 | 1:AS:2439:A:H62 | 1.51 | 0.56 |
| 1:AS:3153:A:H2 | 1:AS:3158:G:H4' | 1.70 | 0.56 |
| 10:BC:134:LYS:HD2 | 10:BC:139:HIS:HE1 | 1.69 | 0.56 |
| 17:BJ:11:ASP:HB2 | 17:BJ:118:ARG:HB3 | 1.87 | 0.56 |
| 27:BT:51:ARG:HG2 | 27:BT:52:GLN:H | 1.69 | 0.56 |
| 37:CD:95:GLU:O | 37:CD:98:ARG:NH1 | 2.37 | 0.56 |
| 46:CM:701:G:H5' | 53:CT:230:ARG:NH1 | 2.15 | 0.56 |
| 46:CM:816:U:H2' | 46:CM:817:U:C6 | 2.41 | 0.56 |
| 46:CM:1155:G:C2 | 46:CM:1156:A:C8 | 2.94 | 0.56 |
| 46:CM:1387:A:OP1 | 64:DE:56:HIS:NE2 | 2.26 | 0.56 |
| 46:CM:1566:U:H2' | 46:CM:1567:C:C6 | 2.41 | 0.56 |
| 47:CN:180:GLU:OE2 | 47:CN:191:ARG:NH2 | 2.39 | 0.56 |
| 50:CQ:49:VAL:HB | 50:CQ:87:ILE:HD13 | 1.87 | 0.56 |
| 81:12:116:MET:HB3 | 81:12:119:LYS:HG2 | 1.87 | 0.56 |
| 80:p0:101:VAL:C | 80:p0:102:SER:HG | 2.13 | 0.56 |
| 1:1:2428:G:N2 | 1:1:2475:U:H3 | 2.03 | 0.56 |
| 1:1:3316:U:H3 | 55:K:110:ARG:NH1 | 2.03 | 0.56 |
| 3:4:8:C:H2' | 3:4:9:A:C8 | 2.41 | 0.56 |
| 59:O:26:ASP:HA | 59:O:29:LYS:CG | 2.36 | 0.56 |
| 1:AS:99:A:H3' | 1:AS:100:G:H21 | 1.70 | 0.56 |
| 1:AS:498:C:H2' | 1:AS:499:G:H8 | 1.69 | 0.56 |
| 1:AS:856:G:O2' | 1:AS:891:A:H4' | 2.06 | 0.56 |
| 1:AS:1030:U:H2' | 1:AS:1031:A:C8 | 2.41 | 0.56 |
| 1:AS:2281:A:OP1 | 42:CI:23:ARG:NE | 2.26 | 0.56 |
| 16:BI:38:ARG:HD2 | 16:BI:62:TYR:HE1 | 1.70 | 0.56 |
| 46:CM:723:G:H2' | 46:CM:724:G:C4' | 2.36 | 0.56 |
| 51:CR:129:VAL:HG22 | 51:CR:139:VAL:HG22 | 1.88 | 0.56 |
| 74:DO:49:HIS:HA | 74:DO:70:LYS:HA | 1.88 | 0.56 |
| 1:1:1789:C:H2' | 4:j:184:ARG:HH22 | 1.70 | 0.56 |
| 1:1:2988:A:H2' | 1:1:2989:A:H8 | 1.69 | 0.56 |
| 14:t:158:LEU:HB3 | 29:AB:98:ALA:HB1 | 1.88 | 0.56 |
| 28:AA:12:ILE:HB | 28:AA:81:MET:HB3 | 1.87 | 0.56 |
| 34:AG:42:LYS:HA | 34:AG:45:LEU:HG | 1.88 | 0.56 |
| 41:AN:22:LYS:HG3 | 41:AN:39:CYS:HB2 | 1.88 | 0.56 |
| 46:B:1566:U:H2' | 46:B:1567:C:C6 | 2.40 | 0.56 |
| 50:F:91:ARG:HD2 | 50:F:95:ARG:NH2 | 2.21 | 0.56 |
| 1:AS:438:A:N1 | 1:AS:489:G:O2' | 2.34 | 0.56 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 46:CM:1536:C:OP1 | 62:DC:42:ARG:NH1 | 2.37 | 0.56 |
| 61:DB:76:ILE:HD13 | 61:DB:97:LEU:HD11 | 1.87 | 0.56 |
| 62:DC:130:ARG:HD3 | 62:DC:130:ARG:H | 1.70 | 0.56 |
| 81:12:137:GLN:HB2 | 81:12:148:PRO:HB2 | 1.87 | 0.56 |
| 1:1:527:G:H2' | 1:1:528:A:C8 | 2.41 | 0.56 |
| 1:1:1089:A:OP2 | 22:2:120:LYS:NZ | 2.33 | 0.56 |
| 4:j:77:ILE:HD13 | 4:j:128:ARG:HB3 | 1.87 | 0.56 |
| 46:B:1192:C:N3 | 46:B:1442:C:H5 | 2.03 | 0.56 |
| 46:B:1468:C:H5" | 46:B:1508:G:H22 | 1.70 | 0.56 |
| 46:B:1487:C:P | 66:V:122:ARG:HH22 | 2.28 | 0.56 |
| 72:b:61:SER:H | 72:b:64:VAL:HB | 1.71 | 0.56 |
| 1:AS:1060:A:H4' | 1:AS:1061:A:O5' | 2.05 | 0.56 |
| 1:AS:2740:U:H2' | 1:AS:2741:A:C8 | 2.41 | 0.56 |
| 6:AY:140:GLY:O | 6:AY:142:ARG:NH1 | 2.39 | 0.56 |
| 11:BD:23:ARG:NH2 | 11:BD:39:LYS:O | 2.39 | 0.56 |
| 14:BG:158:LEU:HB3 | 29:BV:98:ALA:HB1 | 1.87 | 0.56 |
| 21:BN:66:GLU:HB2 | 21:BN:98:THR:HG23 | 1.87 | 0.56 |
| 26:BS:75:LYS:HB3 | 26:BS:81:THR:HB | 1.88 | 0.56 |
| 45:CL:96:LYS:HG3 | 46:CM:575:G:C8 | 2.40 | 0.56 |
| 46:CM:165:U:H2' | 46:CM:166:A:H5" | 1.88 | 0.56 |
| 48:CO:86:LEU:HB3 | 48:CO:98:THR:HB | 1.88 | 0.56 |
| 1:1:1795:A:H2' | 1:1:1796:A:C8 | 2.41 | 0.56 |
| 1:1:1804:G:OP2 | 28:AA:133:LYS:NZ | 2.36 | 0.56 |
| 2:3:19:C:H2' | 2:3:20:A:C8 | 2.40 | 0.56 |
| 46:B:681:C:H3' | 46:B:682:A:H8 | 1.71 | 0.56 |
| 46:B:829:A:H2' | 46:B:830:G:C8 | 2.41 | 0.56 |
| 46:B:1637:U:H2' | 46:B:1638:A:C8 | 2.41 | 0.56 |
| 62:R:77:LYS:HB3 | 62:R:102:PHE:CE1 | 2.41 | 0.56 |
| 1:AS:417:A:H2' | 1:AS:418:A:C8 | 2.41 | 0.56 |
| 1:AS:1655:U:H2' | 1:AS:1656:C:C6 | 2.41 | 0.56 |
| 46:CM:1335:U:H2' | 46:CM:1336:G:C8 | 2.41 | 0.56 |
| 50:CQ:215:GLU:HG3 | 50:CQ:216:ASP:N | 2.16 | 0.56 |
| 59:CZ:42:ALA:HB1 | 59:CZ:47:GLU:HB3 | 1.88 | 0.56 |
| 75:DP:58:GLU:OE2 | 75:DP:61:ARG:NE | 2.35 | 0.56 |
| 82:L1:175:GLU:HG3 | 82:L1:177:ASP:H | 1.71 | 0.56 |
| 1:1:429:U:H5" | 34:AG:87:LYS:HE3 | 1.86 | 0.55 |
| 1:1:2270:U:HO2' | 46:B:1643:U:HO2' | 1.52 | 0.55 |
| 12:r:54:SER:OG | 12:r:130:SER:O | 2.24 | 0.55 |
| 23:5:55:SER:HB2 | 23:5:67:VAL:HB | 1.87 | 0.55 |
| 43:AP:61:LYS:NZ | 43:AP:63:LYS:O | 2.38 | 0.55 |
| 46:B:255:A:H1' | 55:K:73:SER:HB2 | 1.88 | 0.55 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 46:B:728:U:OP1 | 54:J:104:LYS:N | 2.36 | 0.55 |
| 46:B:944:U:OP2 | 74:d:20:LYS:NZ | 2.39 | 0.55 |
| 46:B:1436:U:H2' | 46:B:1437:C:H6 | 1.70 | 0.55 |
| 46:B:1659:G:H2' | 46:B:1660:G:C8 | 2.40 | 0.55 |
| 1:AS:252:U:H5' | 1:AS:253:A:C8 | 2.41 | 0.55 |
| 1:AS:1199:A:H2' | 1:AS:1200:A:H8 | 1.70 | 0.55 |
| 1:AS:1632:C:H5" | 28:BU:73:LYS:HZ1 | 1.71 | 0.55 |
| 3:AU:150:G:OP1 | 26:BS:27:ARG:NH2 | 2.38 | 0.55 |
| 4:AW:80:GLU:HG3 | 44:CK:66:GLY:HA2 | 1.88 | 0.55 |
| 46:CM:1160:U:H2' | 46:CM:1161:G:H8 | 1.70 | 0.55 |
| 46:CM:1220:C:H5 | 78:DS:180:ARG:HE | 1.53 | 0.55 |
| 47:CN:11:PRO:O | 47:CN:15:LYS:HG3 | 2.05 | 0.55 |
| 65:DF:22:ILE:HD11 | 65:DF:35:ILE:HG13 | 1.87 | 0.55 |
| 66:DG:7:ARG:NH2 | 66:DG:67:LEU:O | 2.39 | 0.55 |
| 76:DQ:19:ARG:HD2 | 76:DQ:32:ARG:HD3 | 1.88 | 0.55 |
| 82:L1:67:ILE:HB | 82:L1:84:ALA:HA | 1.89 | 0.55 |
| 1:1:629:A:H2' | 1:1:630:G:C8 | 2.41 | 0.55 |
| 1:1:1232:G:N2 | 1:1:1241:A:N7 | 2.53 | 0.55 |
| 1:1:1600:A:H4' | 1:1:1831:A:H4' | 1.89 | 0.55 |
| 1:1:2331:G:H5" | 18:x:86:LYS:HB2 | 1.86 | 0.55 |
| 33:AF:106:ARG:NH2 | 33:AF:122:ASN:O | 2.39 | 0.55 |
| 47:C:48:ILE:HD12 | 47:C:149:MET:HE3 | 1.88 | 0.55 |
| 1:AS:411:U:H2' | 1:AS:412:G:C8 | 2.41 | 0.55 |
| 1:AS:479:C:H2' | 1:AS:480:G:C8 | 2.42 | 0.55 |
| 1:AS:1216:U:H5" | 1:AS:1218:G:C4 | 2.41 | 0.55 |
| 1:AS:2408:A:H2' | 1:AS:2409:C:C6 | 2.41 | 0.55 |
| 1:AS:2876:U:H2' | 1:AS:2877:U:C6 | 2.42 | 0.55 |
| 17:BJ:122:PRO:HA | 17:BJ:125:LEU:HD12 | 1.88 | 0.55 |
| 46:CM:1772:U:H2' | 46:CM:1773:G:H8 | 1.71 | 0.55 |
| 53:CT:159:ARG:HB2 | 53:CT:170:THR:HB | 1.88 | 0.55 |
| 61:DB:59:ALA:HB1 | 61:DB:100:LEU:HG | 1.88 | 0.55 |
| 1:1:172:C:O2' | 1:1:173:C:OP1 | 2.23 | 0.55 |
| 1:1:289:A:H2' | 1:1:290:G:H8 | 1.72 | 0.55 |
| 1:1:795:G:O2' | 14:t:18:TRP:NE1 | 2.35 | 0.55 |
| 1:1:908:G:N7 | 4:j:9:ARG:NH2 | 2.55 | 0.55 |
| 1:1:1115:C:H2' | 1:1:1116:A:C8 | 2.41 | 0.55 |
| 36:AI:1:MET:HG2 | 36:AI:53:ARG:HH22 | 1.70 | 0.55 |
| 45:i:41:ALA:HB1 | 45:i:44:ALA:HB2 | 1.89 | 0.55 |
| 46:B:876:A:H2' | 46:B:877:G:H8 | 1.72 | 0.55 |
| 46:B:878:U:H5' | 46:B:879:U:OP2 | 2.06 | 0.55 |
| 46:B:988:A:H2' | 46:B:990:A:N7 | 2.21 | 0.55 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 47:C:124:THR:O | 47:C:164:ASN:ND2 | 2.39 | 0.55 |
| 1:AS:932:A:OP2 | 29:BV:27:LYS:HE2 | 2.06 | 0.55 |
| 5:AX:292:ALA:HB1 | 5:AX:295:ALA:HB3 | 1.88 | 0.55 |
| 46:CM:1472:G:N2 | 46:CM:1509:U:O4 | 2.39 | 0.55 |
| 80:p0:16:ARG:HD3 | 80:p0:66:PHE:CE1 | 2.42 | 0.55 |
| 1:1:1187:U:OP2 | 17:w:50:ARG:HD2 | 2.06 | 0.55 |
| 1:1:2199:G:N2 | 1:1:2202:A:OP2 | 2.39 | 0.55 |
| 1:1:2925:U:H2' | 1:1:2926:U:H2' | 1.88 | 0.55 |
| 19:y:123:THR:OG1 | 19:y:125:ASP:OD1 | 2.20 | 0.55 |
| 46:B:123:G:OP1 | 51:G:77:ARG:NH2 | 2.29 | 0.55 |
| 46:B:219:A:H3' | 46:B:818:U:O2 | 2.06 | 0.55 |
| 46:B:563:C:O3' | 70:Z:66:SER:OG | 2.24 | 0.55 |
| 46:B:1205:C:H2' | 46:B:1206:A:C8 | 2.42 | 0.55 |
| 54:J:146:GLN:HB2 | 54:J:177:VAL:HG23 | 1.88 | 0.55 |
| 68:X:64:GLU:OE2 | 74:d:2:VAL:N | 2.39 | 0.55 |
| 79:AR:96:GLU:HG2 | 79:AR:97:THR:HG23 | 1.88 | 0.55 |
| 1:AS:2587:G:H2' | 1:AS:2588:C:C6 | 2.42 | 0.55 |
| 3:AU:8:C:H2' | 3:AU:9:A:C8 | 2.40 | 0.55 |
| 28:BU:87:LEU:HD11 | 28:BU:121:LYS:HD2 | 1.88 | 0.55 |
| 46:CM:79:C:H1' | 53:CT:174:LYS:HB2 | 1.89 | 0.55 |
| 46:CM:1399:U:O2' | 46:CM:1400:U:OP1 | 2.24 | 0.55 |
| 46:CM:1495:U:H2' | 46:CM:1496:C:C6 | 2.41 | 0.55 |
| 46:CM:1609:G:H2' | 46:CM:1610:C:C6 | 2.42 | 0.55 |
| 46:CM:1659:G:H2' | 46:CM:1660:G:H8 | 1.70 | 0.55 |
| 48:CO:62:LYS:HA | 48:CO:88:VAL:HG13 | 1.88 | 0.55 |
| 79:DT:20:VAL:HG11 | 79:DT:307:ILE:HG12 | 1.88 | 0.55 |
| 82:l1:44:GLN:HB3 | 82:l1:45:ARG:HE | 1.71 | 0.55 |
| 1:1:85:G:O2' | 1:1:97:G:O6 | 2.22 | 0.55 |
| 1:1:1239:G:N2 | 1:1:1266:A:O2' | 2.27 | 0.55 |
| 1:1:1493:C:H2' | 1:1:1494:A:H8 | 1.71 | 0.55 |
| 1:1:1571:G:H2' | 1:1:1572:G:C8 | 2.42 | 0.55 |
| 1:1:3261:A:H2' | 1:1:3262:U:H6 | 1.72 | 0.55 |
| 3:4:49:G:OP1 | 36:AI:45:HIS:HB2 | 2.06 | 0.55 |
| 46:B:1020:G:OP1 | 60:P:2:GLY:N | 2.39 | 0.55 |
| 46:B:1324:C:O2' | 46:B:1326:A:N7 | 2.35 | 0.55 |
| 47:C:14:ALA:O | 47:C:18:LEU:HD12 | 2.06 | 0.55 |
| 48:D:83:LYS:NZ | 48:D:105:PHE:O | 2.39 | 0.55 |
| 48:D:180:THR:CG2 | 48:D:183:GLN:OE1 | 2.45 | 0.55 |
| 49:E:231:ALA:O | 68:X:33:GLN:NE2 | 2.38 | 0.55 |
| 50:F:171:ILE:HG12 | 50:F:188:LYS:HG3 | 1.89 | 0.55 |
| 62:R:1:MET:HB3 | 65:U:17:LEU:HA | 1.88 | 0.55 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 1:AS:623:A:H2' | 1:AS:624:U:C6 | 2.41 | 0.55 |
| 1:AS:948:A:H4' | 1:AS:964:G:N2 | 2.21 | 0.55 |
| 1:AS:1611:U:H2' | 1:AS:1612:U:C6 | 2.41 | 0.55 |
| 1:AS:1632:C:OP1 | 28:BU:36:HIS:NE2 | 2.39 | 0.55 |
| 1:AS:2466:A:OP2 | 1:AS:2467:C:N4 | 2.39 | 0.55 |
| 12:BE:82:ARG:NH1 | 12:BE:83:ASP:OD1 | 2.39 | 0.55 |
| 32:BY:78:ARG:HA | 32:BY:88:LEU:HD23 | 1.89 | 0.55 |
| 46:CM:1551:U:H2' | 46:CM:1552:C:C6 | 2.40 | 0.55 |
| 46:CM:1615:U:H2' | 46:CM:1616:G:C8 | 2.42 | 0.55 |
| 46:CM:1668:A:O3' | 53:CT:31:ARG:NH2 | 2.40 | 0.55 |
| 47:CN:200:ASP:O | 47:CN:203:PHE:HB2 | 2.07 | 0.55 |
| 65:DF:67:GLU:HA | 65:DF:70:VAL:HG22 | 1.89 | 0.55 |
| 82:l1:41:TYR:HE1 | 82:l1:195:LYS:H | 1.52 | 0.55 |
| 82:l1:87:VAL:HG23 | 82:l1:88:ASP:H | 1.72 | 0.55 |
| 1:1:208:A:H4' | 1:1:210:A:N7 | 2.22 | 0.55 |
| 1:1:1228:C:H2' | 1:1:1229:G:C8 | 2.42 | 0.55 |
| 1:1:2405:U:H2' | 1:1:2406:U:C6 | 2.41 | 0.55 |
| 46:B:309:U:OP2 | 70:Z:20:ARG:HD3 | 2.06 | 0.55 |
| 46:B:826:U:H2' | 46:B:827:C:O4' | 2.06 | 0.55 |
| 46:B:1669:U:O4 | 46:B:1707:G:N2 | 2.39 | 0.55 |
| 64:T:99:GLN:OE1 | 64:T:99:GLN:N | 2.39 | 0.55 |
| 66:V:53:TRP:HH2 | 66:V:100:ILE:HD12 | 1.71 | 0.55 |
| 79:AR:302:TYR:CE2 | 79:AR:308:ARG:HD2 | 2.41 | 0.55 |
| 1:AS:1099:A:H62 | 1:AS:1359:A:H1' | 1.70 | 0.55 |
| 1:AS:1617:A:H2' | 1:AS:1618:U:C6 | 2.42 | 0.55 |
| 11:BD:107:ASP:O | 11:BD:109:GLN:NE2 | 2.38 | 0.55 |
| 25:BR:80:ARG:HH22 | 53:CT:11:GLY:N | 2.05 | 0.55 |
| 46:CM:1193:A:H4' | 46:CM:1255:G:P | 2.47 | 0.55 |
| 54:CU:169:TYR:HE2 | 54:CU:175:LYS:HB2 | 1.71 | 0.55 |
| 1:1:2407:G:H2' | 1:1:2408:A:H8 | 1.72 | 0.55 |
| 36:AI:1:MET:HB3 | 36:AI:45:HIS:CE1 | 2.41 | 0.55 |
| 46:B:338:U:H2' | 46:B:339:A:H8 | 1.71 | 0.55 |
| 46:B:558:U:H2' | 46:B:559:G:H8 | 1.72 | 0.55 |
| 59:O:38:HIS:C | 59:O:40:GLY:H | 2.12 | 0.55 |
| 62:R:60:LEU:HD21 | 62:R:94:VAL:HG12 | 1.88 | 0.55 |
| 67:W:33:LEU:HG | 67:W:88:ARG:HH21 | 1.72 | 0.55 |
| 1:AS:448:U:H2' | 1:AS:481:G:N1 | 2.21 | 0.55 |
| 1:AS:1943:G:O2' | 1:AS:1944:G:OP1 | 2.20 | 0.55 |
| 1:AS:2869:A:H2' | 1:AS:2871:C:H5" | 1.88 | 0.55 |
| 8:BA:39:LEU:HB3 | 8:BA:83:VAL:HG13 | 1.89 | 0.55 |
| 46:CM:711:U:OP1 | 46:CM:713:U:N3 | 2.40 | 0.55 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 46:CM:1663:U:H5” | 55:CV:58:LEU:HD21 | 1.89 | 0.55 |
| 51:CR:36:HIS:CG | 51:CR:85:GLY:HA3 | 2.42 | 0.55 |
| 59:CZ:63:CYS:HB2 | 59:CZ:97:LEU:HD11 | 1.89 | 0.55 |
| 1:1:252:U:H5’ | 1:1:253:A:H8 | 1.71 | 0.55 |
| 1:1:619:A:H2’ | 1:1:620:A:C8 | 2.41 | 0.55 |
| 1:1:624:U:H2’ | 1:1:625:C:C6 | 2.42 | 0.55 |
| 1:1:782:A:H4’ | 1:1:783:G:H5’ | 1.89 | 0.55 |
| 1:1:1493:C:H2’ | 1:1:1494:A:C8 | 2.42 | 0.55 |
| 1:1:2411:U:H1’ | 16:v:125:SER:HB3 | 1.88 | 0.55 |
| 1:1:2766:G:C4 | 84:1:3402:3K5:H1 | 2.41 | 0.55 |
| 46:B:52:U:H2’ | 46:B:53:G:H8 | 1.72 | 0.55 |
| 46:B:1187:A:H1’ | 46:B:1192:C:N4 | 2.22 | 0.55 |
| 1:AS:1600:A:H4’ | 1:AS:1831:A:H4’ | 1.89 | 0.55 |
| 1:AS:1755:U:H2’ | 1:AS:1756:A:H5” | 1.88 | 0.55 |
| 4:AW:227:ARG:HB2 | 4:AW:239:ALA:HB2 | 1.87 | 0.55 |
| 5:AX:4:ARG:HD3 | 5:AX:7:GLU:HG2 | 1.89 | 0.55 |
| 5:AX:92:TYR:HB2 | 5:AX:157:VAL:HB | 1.88 | 0.55 |
| 5:AX:152:LYS:HG2 | 5:AX:189:SER:HA | 1.89 | 0.55 |
| 25:BR:82:ILE:HD13 | 53:CT:131:LYS:HG3 | 1.89 | 0.55 |
| 36:CC:85:THR:O | 36:CC:89:ARG:HG3 | 2.07 | 0.55 |
| 46:CM:238:U:H3’ | 46:CM:239:U:O4’ | 2.07 | 0.55 |
| 46:CM:1262:G:O3’ | 50:CQ:184:GLY:HA3 | 2.07 | 0.55 |
| 46:CM:1470:G:H5’ | 63:DD:14:THR:HG21 | 1.89 | 0.55 |
| 50:CQ:128:MET:HE1 | 50:CQ:134:GLY:HA2 | 1.89 | 0.55 |
| 59:CZ:97:LEU:HD13 | 59:CZ:119:SER:HA | 1.89 | 0.55 |
| 61:DB:76:ILE:HD12 | 61:DB:110:ILE:HG13 | 1.89 | 0.55 |
| 62:DC:68:GLU:OE1 | 62:DC:68:GLU:N | 2.40 | 0.55 |
| 82:L1:180:VAL:O | 82:L1:184:MET:HG2 | 2.07 | 0.55 |
| 1:1:538:G:H2’ | 1:1:539:G:C8 | 2.41 | 0.55 |
| 1:1:705:U:OP2 | 19:y:168:LYS:NZ | 2.33 | 0.55 |
| 1:1:2808:C:H5 | 1:1:2824:C:H42 | 1.53 | 0.55 |
| 1:1:2933:G:H2’ | 1:1:2934:U:C6 | 2.41 | 0.55 |
| 24:6:32:ARG:HH21 | 24:6:64:LYS:HD3 | 1.72 | 0.55 |
| 39:AL:24:ILE:HD13 | 39:AL:76:THR:HB | 1.88 | 0.55 |
| 46:B:583:A:OP1 | 77:g:15:LYS:NZ | 2.39 | 0.55 |
| 46:B:1413:A:O2’ | 46:B:1414:G:OP1 | 2.25 | 0.55 |
| 46:B:1460:G:H2’ | 46:B:1461:A:C8 | 2.42 | 0.55 |
| 47:C:47:ILE:HD12 | 64:T:106:THR:HG22 | 1.88 | 0.55 |
| 56:L:31:ALA:HB2 | 56:L:42:ILE:HD11 | 1.88 | 0.55 |
| 56:L:38:ASN:HA | 77:g:36:MET:HE3 | 1.89 | 0.55 |
| 57:M:70:ASP:OD1 | 57:M:71:GLU:N | 2.40 | 0.55 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 1:AS:647:A:H2' | 1:AS:648:C:C6 | 2.42 | 0.55 |
| 1:AS:1106:U:H2' | 1:AS:1107:U:C6 | 2.42 | 0.55 |
| 1:AS:2174:C:H2' | 1:AS:2220:A:H61 | 1.70 | 0.55 |
| 1:AS:2385:C:H2' | 1:AS:2386:U:H6 | 1.72 | 0.55 |
| 1:AS:2876:U:H2' | 1:AS:2877:U:H6 | 1.72 | 0.55 |
| 7:AZ:83:LEU:HD13 | 7:AZ:88:ILE:HD12 | 1.89 | 0.55 |
| 21:BN:60:SER:OG | 21:BN:62:ASN:OD1 | 2.25 | 0.55 |
| 46:CM:1315:G:H2' | 46:CM:1316:A:H8 | 1.71 | 0.55 |
| 51:CR:148:ARG:NH2 | 53:CT:201:GLN:OE1 | 2.40 | 0.55 |
| 57:CX:81:ASN:HB3 | 59:CZ:37:VAL:HG13 | 1.89 | 0.55 |
| 82:L1:15:LYS:HB2 | 82:L1:214:PHE:CZ | 2.42 | 0.55 |
| 82:l1:12:ASN:ND2 | 82:l1:216:ILE:HD12 | 2.22 | 0.55 |
| 1:1:638:U:H2' | 1:1:639:C:C6 | 2.41 | 0.55 |
| 1:1:1663:A:H2' | 1:1:1664:G:H8 | 1.70 | 0.55 |
| 1:1:2197:A:H2' | 1:1:2198:A:C8 | 2.42 | 0.55 |
| 1:1:2680:C:H2' | 1:1:2681:C:H6 | 1.72 | 0.55 |
| 6:l:38:SER:OG | 6:l:42:ARG:NH2 | 2.33 | 0.55 |
| 46:B:1265:C:H2' | 46:B:1266:G:C8 | 2.42 | 0.55 |
| 54:J:13:LEU:HD21 | 54:J:54:LEU:HD11 | 1.89 | 0.55 |
| 1:AS:1632:C:H5" | 28:BU:73:LYS:NZ | 2.21 | 0.55 |
| 46:CM:702:G:H4' | 46:CM:703:U:OP1 | 2.05 | 0.55 |
| 46:CM:878:U:H5' | 46:CM:879:U:OP2 | 2.07 | 0.55 |
| 71:DL:57:VAL:HB | 71:DL:60:PHE:HE1 | 1.72 | 0.55 |
| 78:DS:178:LYS:O | 78:DS:180:ARG:HG2 | 2.07 | 0.55 |
| 1:1:1174:G:N3 | 1:1:1324:U:O2' | 2.40 | 0.54 |
| 5:k:117:ARG:HD2 | 5:k:176:ALA:O | 2.06 | 0.54 |
| 19:y:94:LEU:HD22 | 29:AB:119:PRO:HG3 | 1.88 | 0.54 |
| 46:B:671:G:C5' | 46:B:672:U:H2' | 2.36 | 0.54 |
| 46:B:1470:G:H5' | 63:S:14:THR:HG21 | 1.89 | 0.54 |
| 1:AS:477:U:H2' | 1:AS:478:G:C8 | 2.43 | 0.54 |
| 1:AS:730:A:H4' | 1:AS:730:A:OP1 | 2.07 | 0.54 |
| 1:AS:1456:A:H2' | 1:AS:1457:A:C8 | 2.42 | 0.54 |
| 1:AS:2423:A:H5' | 37:CD:62:ASN:OD1 | 2.07 | 0.54 |
| 1:AS:3261:A:H2' | 1:AS:3262:U:C6 | 2.41 | 0.54 |
| 5:AX:35:ASP:OD2 | 5:AX:191:LYS:NZ | 2.25 | 0.54 |
| 14:BG:100:ARG:O | 14:BG:102:GLN:NE2 | 2.39 | 0.54 |
| 28:BU:70:PRO:O | 28:BU:111:LYS:HE3 | 2.08 | 0.54 |
| 46:CM:233:G:H2' | 46:CM:234:G:C8 | 2.42 | 0.54 |
| 64:DE:7:LYS:O | 64:DE:11:ARG:HG2 | 2.07 | 0.54 |
| 80:p0:101:VAL:O | 80:p0:103:ASN:N | 2.40 | 0.54 |
| 14:t:63:VAL:HA | 14:t:66:ASN:ND2 | 2.22 | 0.54 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 16:v:73:ARG:HG2 | 16:v:75:VAL:HG13 | 1.89 | 0.54 |
| 28:AA:54:THR:HG22 | 28:AA:57:MET:HE3 | 1.89 | 0.54 |
| 42:AO:1:MET:HB3 | 46:B:1629:G:H5' | 1.88 | 0.54 |
| 46:B:15:U:H2' | 46:B:16:G:O4' | 2.07 | 0.54 |
| 46:B:1672:G:O2' | 46:B:1673:U:H5' | 2.06 | 0.54 |
| 57:M:4:PRO:HG2 | 57:M:7:ASP:HB2 | 1.90 | 0.54 |
| 1:AS:2958:U:H2' | 1:AS:2959:A:C8 | 2.42 | 0.54 |
| 3:AU:47:C:H1' | 3:AU:61:A:H2' | 1.88 | 0.54 |
| 38:CE:21:ARG:HD2 | 38:CE:37:CYS:SG | 2.47 | 0.54 |
| 46:CM:1341:U:H2' | 46:CM:1342:A:C8 | 2.42 | 0.54 |
| 46:CM:1478:A:O2' | 46:CM:1479:A:O4' | 2.21 | 0.54 |
| 53:CT:180:THR:HG23 | 53:CT:183:THR:H | 1.72 | 0.54 |
| 53:CT:218:GLU:HG2 | 53:CT:219:ARG:NH2 | 2.22 | 0.54 |
| 80:P0:16:ARG:NH2 | 80:P0:62:ALA:O | 2.33 | 0.54 |
| 82:l1:189:PHE:O | 82:l1:193:LEU:HG | 2.07 | 0.54 |
| 1:1:359:U:OP1 | 38:AK:11:ARG:NH1 | 2.40 | 0.54 |
| 1:1:403:C:O2' | 1:1:404:G:OP1 | 2.21 | 0.54 |
| 1:1:1079:G:H2' | 1:1:1080:A:C8 | 2.43 | 0.54 |
| 1:1:1182:G:OP2 | 15:u:36:LYS:NZ | 2.28 | 0.54 |
| 1:1:2429:G:H2' | 1:1:2430:G:C8 | 2.42 | 0.54 |
| 1:1:2958:U:H2' | 1:1:2959:A:C8 | 2.41 | 0.54 |
| 2:3:3:U:H2' | 2:3:4:U:H6 | 1.70 | 0.54 |
| 24:6:15:LEU:HD13 | 24:6:51:ALA:HB3 | 1.90 | 0.54 |
| 38:AK:39:TYR:CD1 | 38:AK:40:PRO:HA | 2.43 | 0.54 |
| 52:H:61:TYR:OH | 75:e:52:ASP:OD1 | 2.22 | 0.54 |
| 1:AS:582:G:H2' | 1:AS:583:A:H8 | 1.72 | 0.54 |
| 1:AS:2079:C:HO2' | 1:AS:2080:U:H6 | 1.53 | 0.54 |
| 1:AS:2391:A:H2' | 1:AS:2392:G:C8 | 2.41 | 0.54 |
| 1:AS:2443:G:H1 | 1:AS:2468:C:H5 | 1.54 | 0.54 |
| 2:AT:4:U:H2' | 2:AT:5:G:C8 | 2.42 | 0.54 |
| 6:AY:204:ARG:NH2 | 6:AY:227:GLU:OE2 | 2.35 | 0.54 |
| 17:BJ:76:ALA:HB3 | 17:BJ:79:ARG:HG2 | 1.90 | 0.54 |
| 23:BP:33:TYR:O | 23:BP:37:LEU:HD23 | 2.06 | 0.54 |
| 28:BU:103:GLU:HB2 | 28:BU:106:GLN:HB2 | 1.89 | 0.54 |
| 39:CF:24:ILE:HB | 39:CF:44:LYS:HB2 | 1.89 | 0.54 |
| 46:CM:583:A:H2' | 46:CM:584:G:C8 | 2.43 | 0.54 |
| 46:CM:668:U:H3' | 46:CM:669:G:H8 | 1.72 | 0.54 |
| 46:CM:1072:A:H2' | 46:CM:1073:A:C8 | 2.42 | 0.54 |
| 46:CM:1199:U:HO2' | 76:DQ:3:HIS:HD1 | 1.55 | 0.54 |
| 46:CM:1266:G:O3' | 67:DH:75:SER:OG | 2.22 | 0.54 |
| 49:CP:134:ILE:HD13 | 49:CP:186:ALA:HB1 | 1.88 | 0.54 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 61:DB:107:ILE:HG13 | 73:DN:53:LEU:HD12 | 1.90 | 0.54 |
| 1:1:158:A:H2' | 1:1:159:A:C8 | 2.42 | 0.54 |
| 1:1:411:U:H2' | 1:1:412:G:H8 | 1.73 | 0.54 |
| 1:1:612:U:H2' | 1:1:613:U:C6 | 2.43 | 0.54 |
| 1:1:1233:G:H1 | 1:1:1247:A:H61 | 0.70 | 0.54 |
| 11:q:12:ILE:HD11 | 11:q:53:ILE:HG13 | 1.88 | 0.54 |
| 46:B:1479:A:H4' | 46:B:1480:G:O5' | 2.08 | 0.54 |
| 49:E:217:TYR:OH | 68:X:11:LEU:O | 2.24 | 0.54 |
| 63:S:98:GLU:N | 79:AR:59:LYS:O | 2.31 | 0.54 |
| 69:Y:111:MET:SD | 69:Y:115:GLU:HG2 | 2.48 | 0.54 |
| 78:h:175:ALA:O | 78:h:177:MET:HG3 | 2.06 | 0.54 |
| 79:AR:218:ILE:HG23 | 79:AR:230:THR:HG22 | 1.88 | 0.54 |
| 1:AS:208:A:H4' | 1:AS:210:A:N7 | 2.23 | 0.54 |
| 1:AS:2171:U:O4 | 1:AS:2221:A:N6 | 2.41 | 0.54 |
| 1:AS:2520:A:H1' | 1:AS:2521:C:C5 | 2.42 | 0.54 |
| 1:AS:2718:A:H5' | 7:AZ:178:ASN:OD1 | 2.07 | 0.54 |
| 11:BD:86:TYR:CE2 | 11:BD:151:LEU:HB2 | 2.42 | 0.54 |
| 46:CM:133:U:H4' | 46:CM:134:A:OP2 | 2.08 | 0.54 |
| 82:L1:10:ARG:O | 82:L1:14:HIS:ND1 | 2.40 | 0.54 |
| 1:1:94:A:H5" | 29:AB:34:LYS:HB2 | 1.87 | 0.54 |
| 25:7:83:VAL:HG11 | 46:B:68:A:C2 | 2.43 | 0.54 |
| 39:AL:34:ASN:ND2 | 39:AL:34:ASN:O | 2.41 | 0.54 |
| 46:B:1160:U:H2' | 46:B:1161:G:C8 | 2.43 | 0.54 |
| 54:J:29:ASP:OD1 | 54:J:30:LEU:HD23 | 2.07 | 0.54 |
| 72:b:50:ILE:HG12 | 72:b:69:LEU:HD13 | 1.89 | 0.54 |
| 1:AS:511:C:H5" | 6:AY:344:LYS:HD2 | 1.90 | 0.54 |
| 1:AS:2384:C:H2' | 1:AS:2385:C:H6 | 1.73 | 0.54 |
| 5:AX:58:ARG:HD2 | 5:AX:354:VAL:HG13 | 1.90 | 0.54 |
| 13:BF:117:ASP:HB3 | 13:BF:120:ILE:HD12 | 1.88 | 0.54 |
| 25:BR:1:MET:HE2 | 25:BR:15:PRO:HG2 | 1.88 | 0.54 |
| 31:BX:43:LEU:HD23 | 31:BX:94:ILE:HD12 | 1.89 | 0.54 |
| 31:BX:53:LEU:HD13 | 35:CB:91:ARG:HD3 | 1.89 | 0.54 |
| 45:CL:48:PRO:O | 45:CL:50:LYS:N | 2.40 | 0.54 |
| 46:CM:1:U:OP2 | 56:CW:57:ARG:NH2 | 2.41 | 0.54 |
| 46:CM:585:C:H5' | 77:DR:24:GLN:NE2 | 2.22 | 0.54 |
| 54:CU:137:ARG:NH2 | 69:DJ:49:GLU:OE2 | 2.38 | 0.54 |
| 55:CV:57:ALA:HB2 | 55:CV:183:GLY:HA2 | 1.88 | 0.54 |
| 82:L1:60:ARG:HE | 82:L1:63:MET:HE3 | 1.72 | 0.54 |
| 1:1:48:A:N7 | 16:v:187:ARG:HD2 | 2.23 | 0.54 |
| 1:1:1239:G:O2' | 1:1:1240:A:H5' | 2.07 | 0.54 |
| 1:1:1278:G:OP1 | 80:P0:55:LYS:HE3 | 2.07 | 0.54 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 1:1:2093:G:H22 | 1:1:2098:A:H1' | 1.73 | 0.54 |
| 1:1:2385:C:H2' | 1:1:2386:U:C6 | 2.43 | 0.54 |
| 1:1:2583:U:H2' | 1:1:2584:U:C6 | 2.43 | 0.54 |
| 1:1:2807:U:O2' | 1:1:2808:C:OP1 | 2.26 | 0.54 |
| 9:o:39:ARG:HA | 9:o:42:ILE:HG12 | 1.88 | 0.54 |
| 12:r:140:THR:HG21 | 12:r:148:VAL:HG21 | 1.89 | 0.54 |
| 15:u:14:GLU:HB3 | 21:0:149:LYS:HG2 | 1.90 | 0.54 |
| 21:0:96:ASP:OD1 | 21:0:97:VAL:N | 2.41 | 0.54 |
| 46:B:484:G:H1 | 46:B:499:U:H3 | 1.54 | 0.54 |
| 46:B:605:G:H5' | 46:B:611:G:N2 | 2.23 | 0.54 |
| 46:B:693:U:H4' | 54:J:96:PRO:HG3 | 1.88 | 0.54 |
| 67:W:26:THR:OG1 | 67:W:112:ASP:OD1 | 2.25 | 0.54 |
| 72:b:42:LEU:HD21 | 72:b:47:TYR:HD1 | 1.72 | 0.54 |
| 79:AR:257:ILE:HB | 79:AR:271:LEU:HB2 | 1.90 | 0.54 |
| 1:AS:581:A:H5" | 34:CA:106:ASN:ND2 | 2.22 | 0.54 |
| 1:AS:1007:A:H2' | 1:AS:1008:A:C8 | 2.43 | 0.54 |
| 1:AS:1034:U:H5" | 7:AZ:5:LYS:HG2 | 1.90 | 0.54 |
| 3:AU:26:U:H2' | 3:AU:27:U:C6 | 2.42 | 0.54 |
| 5:AX:293:ASN:HB2 | 5:AX:304:THR:HA | 1.90 | 0.54 |
| 43:CJ:61:LYS:NZ | 43:CJ:63:LYS:O | 2.40 | 0.54 |
| 49:CP:171:LYS:HE2 | 56:CW:57:ARG:NH1 | 2.21 | 0.54 |
| 50:CQ:179:ARG:H | 50:CQ:179:ARG:HD2 | 1.72 | 0.54 |
| 79:DT:42:LEU:HD11 | 79:DT:83:SER:HB3 | 1.88 | 0.54 |
| 82:l1:68:PHE:H | 82:l1:111:ILE:HG12 | 1.72 | 0.54 |
| 1:1:623:A:H2' | 1:1:624:U:C6 | 2.43 | 0.54 |
| 1:1:1249:U:H3' | 1:1:1250:C:H5' | 1.90 | 0.54 |
| 1:1:1556:G:N7 | 26:8:36:LYS:HE2 | 2.22 | 0.54 |
| 1:1:1794:A:H2' | 1:1:1795:A:C8 | 2.43 | 0.54 |
| 1:1:2740:U:H2' | 1:1:2741:A:C8 | 2.43 | 0.54 |
| 1:1:2936:G:N2 | 1:1:2939:A:OP2 | 2.34 | 0.54 |
| 46:B:405:A:H2' | 46:B:406:C:C6 | 2.43 | 0.54 |
| 50:F:68:HIS:CE1 | 57:M:94:ASN:HB3 | 2.43 | 0.54 |
| 1:AS:538:G:O6 | 1:AS:547:U:O4 | 2.25 | 0.54 |
| 1:AS:1580:U:H2' | 1:AS:1581:C:H6 | 1.72 | 0.54 |
| 23:BP:16:VAL:HG21 | 23:BP:105:GLN:HE21 | 1.72 | 0.54 |
| 46:CM:739:A:H5" | 46:CM:740:A:C5' | 2.38 | 0.54 |
| 46:CM:1083:U:OP1 | 49:CP:154:THR:OG1 | 2.24 | 0.54 |
| 46:CM:1628:C:N4 | 86:CM:1902:HYG:O20 | 2.35 | 0.54 |
| 61:DB:79:ARG:HB3 | 61:DB:113:VAL:HG23 | 1.89 | 0.54 |
| 62:DC:24:ASP:O | 62:DC:28:MET:HG3 | 2.08 | 0.54 |
| 1:1:25:A:H2' | 1:1:26:C:H6 | 1.73 | 0.54 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 1:1:314:U:H2' | 1:1:315:C:C6 | 2.43 | 0.54 |
| 1:1:1620:G:O2' | 1:1:1639:A:N1 | 2.40 | 0.54 |
| 1:1:2826:U:P | 12:r:3:ARG:HH22 | 2.30 | 0.54 |
| 36:AI:64:GLU:HA | 36:AI:67:ARG:HB2 | 1.89 | 0.54 |
| 43:AP:8:ARG:HG2 | 43:AP:10:THR:HG23 | 1.89 | 0.54 |
| 46:B:17:C:H2' | 46:B:18:C:C6 | 2.42 | 0.54 |
| 48:D:62:LYS:HZ1 | 48:D:90:GLU:HA | 1.72 | 0.54 |
| 59:O:38:HIS:C | 59:O:40:GLY:N | 2.63 | 0.54 |
| 63:S:131:ARG:HG3 | 63:S:137:PHE:HE1 | 1.72 | 0.54 |
| 1:AS:117:U:O2 | 1:AS:120:A:H5" | 2.07 | 0.54 |
| 1:AS:314:U:H2' | 1:AS:315:C:C6 | 2.43 | 0.54 |
| 1:AS:437:G:O2' | 1:AS:438:A:OP1 | 2.23 | 0.54 |
| 1:AS:1035:U:H2' | 1:AS:1036:A:C8 | 2.43 | 0.54 |
| 4:AW:20:THR:HA | 4:AW:23:ARG:HG3 | 1.89 | 0.54 |
| 5:AX:331:VAL:H | 5:AX:334:ARG:HG3 | 1.73 | 0.54 |
| 15:BH:14:GLU:HB3 | 21:BN:149:LYS:HG2 | 1.89 | 0.54 |
| 46:CM:29:U:H2' | 46:CM:30:G:H8 | 1.73 | 0.54 |
| 46:CM:68:A:N6 | 53:CT:132:ARG:HG3 | 2.22 | 0.54 |
| 46:CM:290:U:H2' | 46:CM:291:U:C6 | 2.42 | 0.54 |
| 46:CM:1064:U:H2' | 46:CM:1065:U:C6 | 2.43 | 0.54 |
| 65:DF:91:ASP:OD1 | 65:DF:92:GLN:N | 2.40 | 0.54 |
| 78:DS:125:LYS:O | 78:DS:126:VAL:HG23 | 2.08 | 0.54 |
| 82:L1:207:LYS:HD2 | 82:L1:208:SER:O | 2.08 | 0.54 |
| 1:1:976:A:N6 | 1:1:1100:G:O2' | 2.38 | 0.54 |
| 1:1:1593:C:P | 35:AH:8:ARG:HH22 | 2.31 | 0.54 |
| 7:m:40:HIS:CE1 | 7:m:42:ALA:HB3 | 2.43 | 0.54 |
| 21:0:12:ARG:HB3 | 21:0:24:LEU:HD23 | 1.89 | 0.54 |
| 46:B:142:G:O2' | 46:B:143:A:O5' | 2.21 | 0.54 |
| 52:H:51:VAL:HA | 52:H:131:GLN:OE1 | 2.07 | 0.54 |
| 1:AS:498:C:H2' | 1:AS:499:G:C8 | 2.43 | 0.54 |
| 1:AS:2194:G:H22 | 1:AS:2207:A:H2 | 1.56 | 0.54 |
| 1:AS:2742:G:H5" | 43:CJ:79:THR:HG23 | 1.88 | 0.54 |
| 4:AW:242:ARG:NH2 | 4:AW:243:THR:O | 2.41 | 0.54 |
| 6:AY:4:ARG:HH22 | 6:AY:25:ALA:HA | 1.73 | 0.54 |
| 27:BT:11:SER:HB3 | 27:BT:14:LYS:HB2 | 1.88 | 0.54 |
| 46:CM:391:C:H2' | 46:CM:392:C:C6 | 2.43 | 0.54 |
| 46:CM:470:U:H5" | 56:CW:11:THR:HG23 | 1.90 | 0.54 |
| 46:CM:904:A:H2' | 46:CM:905:C:C6 | 2.42 | 0.54 |
| 51:CR:15:PRO:HG3 | 51:CR:39:ARG:HD3 | 1.90 | 0.54 |
| 52:CS:25:LEU:HD12 | 63:DD:26:GLY:HA3 | 1.90 | 0.54 |
| 56:CW:53:ARG:O | 56:CW:57:ARG:HG3 | 2.07 | 0.54 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 63:DD:28:ILE:HG22 | 63:DD:64:ILE:HB | 1.89 | 0.54 |
| 71:DL:74:LEU:HD13 | 71:DL:76:TYR:CE1 | 2.43 | 0.54 |
| 79:DT:189:PHE:HD2 | 79:DT:220:TRP:CE3 | 2.26 | 0.54 |
| 82:L1:23:THR:HG22 | 82:L1:24:LYS:H | 1.73 | 0.54 |
| 82:l1:26:ARG:HD3 | 82:l1:26:ARG:N | 2.20 | 0.54 |
| 1:1:715:C:OP1 | 1:1:747:A:O2' | 2.22 | 0.54 |
| 1:1:815:U:H2' | 1:1:816:A:H8 | 1.73 | 0.54 |
| 1:1:1655:U:H3 | 1:1:1786:G:H1 | 1.56 | 0.54 |
| 46:B:330:U:P | 55:K:56:ARG:HH22 | 2.30 | 0.54 |
| 46:B:948:A:N7 | 60:P:70:LYS:NZ | 2.55 | 0.54 |
| 46:B:1237:C:O2' | 78:h:184:GLY:N | 2.38 | 0.54 |
| 46:B:1668:A:H8 | 53:I:65:GLN:HG3 | 1.73 | 0.54 |
| 47:C:41:ARG:HD3 | 47:C:47:ILE:HD11 | 1.90 | 0.54 |
| 64:T:89:SER:C | 64:T:91:LEU:H | 2.16 | 0.54 |
| 1:AS:1104:U:H2' | 1:AS:1105:U:C6 | 2.42 | 0.54 |
| 1:AS:1233:G:H1 | 1:AS:1247:A:H61 | 1.55 | 0.54 |
| 1:AS:2404:U:H3 | 1:AS:2575:G:H1 | 1.56 | 0.54 |
| 1:AS:3240:U:OP2 | 34:CA:66:VAL:HG21 | 2.07 | 0.54 |
| 46:CM:4:C:H5 | 46:CM:20:G:H1 | 1.56 | 0.54 |
| 46:CM:17:C:H2' | 46:CM:18:C:C6 | 2.43 | 0.54 |
| 46:CM:151:G:H2' | 46:CM:152:G:C8 | 2.43 | 0.54 |
| 48:CO:123:ALA:HB2 | 48:CO:165:ARG:HG3 | 1.90 | 0.54 |
| 79:DT:107:HIS:NE2 | 79:DT:125:SER:OG | 2.41 | 0.54 |
| 82:l1:40:ASN:O | 82:l1:200:ASN:ND2 | 2.41 | 0.54 |
| 1:1:1172:C:H2' | 1:1:1173:G:N2 | 2.22 | 0.53 |
| 1:1:1617:A:H2' | 1:1:1618:U:C6 | 2.43 | 0.53 |
| 1:1:2183:U:O2' | 1:1:2184:G:OP1 | 2.26 | 0.53 |
| 1:1:2370:C:H1' | 5:k:266:ARG:NH2 | 2.23 | 0.53 |
| 1:1:2407:G:H2' | 1:1:2408:A:C8 | 2.42 | 0.53 |
| 46:B:151:G:H2' | 46:B:152:G:H8 | 1.72 | 0.53 |
| 46:B:768:C:H2' | 46:B:769:U:O4' | 2.08 | 0.53 |
| 46:B:1742:A:C6 | 77:g:3:LYS:HE3 | 2.43 | 0.53 |
| 59:O:36:LEU:C | 59:O:38:HIS:H | 2.15 | 0.53 |
| 63:S:98:GLU:OE1 | 79:AR:61:SER:N | 2.41 | 0.53 |
| 1:AS:269:G:H5" | 16:BI:14:LYS:HE2 | 1.91 | 0.53 |
| 1:AS:689:A:N1 | 3:AU:28:C:O2' | 2.38 | 0.53 |
| 1:AS:1080:A:H2' | 1:AS:1081:A:C8 | 2.43 | 0.53 |
| 1:AS:1302:G:O6 | 1:AS:2344:C:O2' | 2.25 | 0.53 |
| 1:AS:2183:U:O2' | 1:AS:2184:G:OP1 | 2.24 | 0.53 |
| 25:BR:108:LYS:HA | 25:BR:111:LYS:HD2 | 1.90 | 0.53 |
| 46:CM:17:C:O2' | 46:CM:1122:A:N1 | 2.36 | 0.53 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 46:CM:519:A:N3 | 71:DL:34:ASN:ND2 | 2.53 | 0.53 |
| 46:CM:874:U:H2' | 46:CM:875:C:H6 | 1.72 | 0.53 |
| 46:CM:1160:U:H2' | 46:CM:1161:G:C8 | 2.43 | 0.53 |
| 46:CM:1197:G:OP1 | 78:DS:128:THR:HG21 | 2.07 | 0.53 |
| 46:CM:1218:G:N1 | 46:CM:1238:U:O2 | 2.41 | 0.53 |
| 59:CZ:50:LYS:HG3 | 78:DS:171:GLY:HA3 | 1.88 | 0.53 |
| 79:DT:40:LYS:HD3 | 79:DT:66:SER:C | 2.33 | 0.53 |
| 1:1:1456:A:H2' | 1:1:1457:A:C8 | 2.44 | 0.53 |
| 1:1:2528:U:O4' | 10:p:39:GLN:NE2 | 2.40 | 0.53 |
| 46:B:213:A:C2' | 46:B:214:U:H5' | 2.38 | 0.53 |
| 46:B:1469:A:H2' | 46:B:1470:G:C8 | 2.44 | 0.53 |
| 1:AS:1256:A:H1' | 1:AS:1276:C:H1' | 1.89 | 0.53 |
| 1:AS:1301:U:C2 | 5:AX:257:PRO:HG3 | 2.42 | 0.53 |
| 1:AS:1895:G:O2' | 1:AS:2312:U:O4 | 2.16 | 0.53 |
| 1:AS:2097:A:H2 | 20:BM:82:LYS:HZ1 | 1.56 | 0.53 |
| 5:AX:106:TRP:HB2 | 5:AX:133:TYR:CE1 | 2.43 | 0.53 |
| 13:BF:82:ARG:HH22 | 13:BF:114:ILE:HD11 | 1.74 | 0.53 |
| 19:BL:181:SER:OG | 19:BL:182:ARG:NH1 | 2.41 | 0.53 |
| 44:CK:79:VAL:HA | 44:CK:82:THR:HG1 | 1.73 | 0.53 |
| 46:CM:1445:C:OP1 | 65:DF:126:ARG:NH1 | 2.40 | 0.53 |
| 47:CN:198:MET:HB3 | 64:DE:85:VAL:HG21 | 1.91 | 0.53 |
| 67:DH:32:GLN:OE1 | 67:DH:32:GLN:N | 2.41 | 0.53 |
| 70:DK:100:ASP:OD2 | 70:DK:142:LYS:NZ | 2.31 | 0.53 |
| 71:DL:87:PRO:HD2 | 71:DL:90:ARG:HD2 | 1.89 | 0.53 |
| 1:1:941:C:H2' | 1:1:942:U:C6 | 2.43 | 0.53 |
| 1:1:1188:C:N4 | 1:1:1297:A:O2' | 2.41 | 0.53 |
| 5:k:339:ARG:NH2 | 5:k:342:LEU:HD11 | 2.23 | 0.53 |
| 46:B:671:G:H5" | 46:B:672:U:H2' | 1.89 | 0.53 |
| 46:B:788:A:C8 | 69:Y:107:SER:HA | 2.43 | 0.53 |
| 46:B:839:U:O4 | 46:B:840:A:N6 | 2.42 | 0.53 |
| 46:B:1218:G:N1 | 46:B:1237:C:H5 | 2.06 | 0.53 |
| 51:G:139:VAL:HG23 | 51:G:150:PRO:HG3 | 1.90 | 0.53 |
| 65:U:91:ASP:OD1 | 65:U:92:GLN:N | 2.40 | 0.53 |
| 71:a:57:VAL:HB | 71:a:60:PHE:HE2 | 1.74 | 0.53 |
| 79:AR:126:ALA:HB1 | 79:AR:152:VAL:HG23 | 1.90 | 0.53 |
| 1:AS:547:U:H2' | 1:AS:548:G:C8 | 2.43 | 0.53 |
| 1:AS:1046:U:OP2 | 22:BO:13:TYR:OH | 2.19 | 0.53 |
| 1:AS:2197:A:H2' | 1:AS:2198:A:C8 | 2.43 | 0.53 |
| 1:AS:2434:A:O2' | 1:AS:2435:G:OP1 | 2.24 | 0.53 |
| 20:BM:162:ARG:HD3 | 20:BM:165:ARG:HD3 | 1.89 | 0.53 |
| 46:CM:1200:C:P | 78:DS:134:LYS:HZ1 | 2.30 | 0.53 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 46:CM:1306:A:H4' | 46:CM:1307:A:O5' | 2.09 | 0.53 |
| 46:CM:1551:U:H2' | 46:CM:1552:C:H6 | 1.74 | 0.53 |
| 46:CM:1596:U:O2' | 52:CS:105:GLY:O | 2.18 | 0.53 |
| 82:l1:13:VAL:O | 82:l1:17:LEU:HB3 | 2.08 | 0.53 |
| 1:1:158:A:H2' | 1:1:159:A:H8 | 1.73 | 0.53 |
| 1:1:438:A:N1 | 1:1:489:G:O2' | 2.36 | 0.53 |
| 1:1:1250:C:H2' | 1:1:1251:C:C6 | 2.43 | 0.53 |
| 1:1:1530:A:H2' | 1:1:1531:A:C8 | 2.43 | 0.53 |
| 1:1:2869:A:H2' | 1:1:2871:C:H5" | 1.90 | 0.53 |
| 45:i:48:PRO:C | 45:i:50:LYS:H | 2.15 | 0.53 |
| 46:B:79:C:OP1 | 53:I:159:ARG:NH2 | 2.41 | 0.53 |
| 46:B:151:G:H2' | 46:B:152:G:C8 | 2.44 | 0.53 |
| 46:B:736:G:H2' | 46:B:737:A:H8 | 1.73 | 0.53 |
| 70:Z:59:ILE:HG23 | 77:g:4:VAL:HG22 | 1.90 | 0.53 |
| 79:AR:38:ARG:HB3 | 79:AR:68:ILE:HG12 | 1.89 | 0.53 |
| 1:AS:62:A:H5" | 16:BI:174:ILE:HG21 | 1.91 | 0.53 |
| 1:AS:401:U:H1' | 1:AS:403:C:C4 | 2.43 | 0.53 |
| 1:AS:716:G:OP1 | 29:BV:117:ARG:NH2 | 2.41 | 0.53 |
| 1:AS:1434:U:H4' | 6:AY:89:ALA:HB3 | 1.89 | 0.53 |
| 1:AS:1493:C:H2' | 1:AS:1494:A:H8 | 1.73 | 0.53 |
| 1:AS:2435:G:H1 | 1:AS:2439:A:N6 | 2.06 | 0.53 |
| 1:AS:2603:U:OP2 | 22:BO:4:SER:OG | 2.23 | 0.53 |
| 19:BL:94:LEU:HD22 | 29:BV:119:PRO:HG3 | 1.91 | 0.53 |
| 20:BM:134:HIS:CE1 | 20:BM:136:ARG:HB3 | 2.42 | 0.53 |
| 32:BY:71:ARG:HH11 | 32:BY:103:LEU:HD13 | 1.74 | 0.53 |
| 46:CM:238:U:O2' | 46:CM:239:U:OP1 | 2.23 | 0.53 |
| 46:CM:480:U:H2' | 46:CM:481:A:H8 | 1.74 | 0.53 |
| 46:CM:733:U:O2' | 69:DJ:122:SER:O | 2.24 | 0.53 |
| 46:CM:940:A:H4' | 46:CM:1058:G:O2' | 2.08 | 0.53 |
| 46:CM:1341:U:H2' | 46:CM:1342:A:H8 | 1.73 | 0.53 |
| 46:CM:1472:G:N2 | 46:CM:1580:A:OP1 | 2.32 | 0.53 |
| 73:DN:51:ARG:NH2 | 75:DP:60:GLU:HG3 | 2.23 | 0.53 |
| 1:1:437:G:O2' | 1:1:438:A:OP1 | 2.26 | 0.53 |
| 1:1:1330:U:H2' | 1:1:1331:U:C6 | 2.44 | 0.53 |
| 1:1:1485:A:OP1 | 35:AH:10:ARG:HD2 | 2.09 | 0.53 |
| 1:1:2233:A:N1 | 46:B:1631:C:O2' | 2.40 | 0.53 |
| 1:1:2717:G:N2 | 1:1:2720:A:OP2 | 2.38 | 0.53 |
| 14:t:201:LYS:NZ | 82:l1:50:SER:OG | 2.37 | 0.53 |
| 16:v:65:ARG:HG2 | 16:v:127:TYR:CD1 | 2.43 | 0.53 |
| 46:B:538:G:N2 | 77:g:25:GLU:OE2 | 2.42 | 0.53 |
| 48:D:103:LEU:HD13 | 48:D:188:LEU:HD13 | 1.89 | 0.53 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 57:M:11:ILE:HD11 | 57:M:37:THR:HG21 | 1.89 | 0.53 |
| 1:AS:290:G:H1' | 16:BI:93:LYS:HD2 | 1.91 | 0.53 |
| 1:AS:1115:C:H2' | 1:AS:1116:A:C8 | 2.43 | 0.53 |
| 1:AS:1241:A:H3' | 1:AS:1242:G:C5' | 2.38 | 0.53 |
| 1:AS:1743:G:H21 | 39:CF:2:ALA:HB3 | 1.73 | 0.53 |
| 1:AS:2232:U:H2' | 1:AS:2239:G:N2 | 2.23 | 0.53 |
| 1:AS:2520:A:H1' | 1:AS:2521:C:H5 | 1.72 | 0.53 |
| 23:BP:96:ILE:HG21 | 23:BP:108:LEU:HD13 | 1.91 | 0.53 |
| 45:CL:40:ASP:O | 45:CL:42:ALA:N | 2.37 | 0.53 |
| 46:CM:971:G:H2' | 46:CM:972:G:O4' | 2.07 | 0.53 |
| 46:CM:1183:G:OP1 | 46:CM:1184:G:O2' | 2.20 | 0.53 |
| 57:CX:81:ASN:CB | 59:CZ:37:VAL:HG13 | 2.38 | 0.53 |
| 59:CZ:103:LEU:HD13 | 59:CZ:116:VAL:O | 2.08 | 0.53 |
| 77:DR:55:LYS:HB2 | 77:DR:58:PRO:HG3 | 1.90 | 0.53 |
| 82:l1:21:THR:CA | 82:l1:25:LYS:HE3 | 2.37 | 0.53 |
| 82:l1:75:ASP:HA | 82:l1:78:LYS:HD2 | 1.90 | 0.53 |
| 1:1:173:C:H2' | 1:1:174:C:C6 | 2.43 | 0.53 |
| 1:1:411:U:H2' | 1:1:412:G:C8 | 2.43 | 0.53 |
| 1:1:636:C:N4 | 1:1:637:G:O6 | 2.41 | 0.53 |
| 1:1:1229:G:N2 | 81:12:131:GLU:OE2 | 2.29 | 0.53 |
| 1:1:2737:C:O3' | 43:AP:39:GLY:HA3 | 2.09 | 0.53 |
| 1:1:3046:G:H4' | 32:AE:61:ARG:HD2 | 1.89 | 0.53 |
| 1:1:3150:A:C4 | 17:w:115:LYS:HA | 2.44 | 0.53 |
| 1:1:3196:U:H2' | 1:1:3197:G:H8 | 1.72 | 0.53 |
| 1:1:3260:A:H2' | 1:1:3261:A:H8 | 1.71 | 0.53 |
| 13:s:109:HIS:ND1 | 13:s:114:ILE:HD11 | 2.24 | 0.53 |
| 46:B:333:U:O2' | 58:N:130:PRO:O | 2.20 | 0.53 |
| 46:B:1431:G:O2' | 78:h:127:TYR:OH | 2.17 | 0.53 |
| 46:B:1672:G:N2 | 46:B:1704:C:C2 | 2.77 | 0.53 |
| 47:C:52:LYS:HD3 | 68:X:82:VAL:HG23 | 1.91 | 0.53 |
| 57:M:54:TYR:HD1 | 57:M:72:GLY:HA2 | 1.73 | 0.53 |
| 63:S:14:THR:HB | 63:S:71:GLY:HA2 | 1.91 | 0.53 |
| 1:AS:2441:G:H4' | 1:AS:2442:U:C6 | 2.44 | 0.53 |
| 9:BB:8:GLU:HG3 | 9:BB:9:THR:H | 1.73 | 0.53 |
| 45:CL:90:ARG:HG3 | 46:CM:1624:C:C2 | 2.43 | 0.53 |
| 45:CL:154:TYR:HB2 | 57:CX:86:ILE:HG22 | 1.90 | 0.53 |
| 82:L1:17:LEU:O | 82:L1:21:THR:HG22 | 2.09 | 0.53 |
| 1:1:842:A:N6 | 46:B:956:A:N1 | 2.56 | 0.53 |
| 1:1:3269:C:O2 | 5:k:25:GLN:NE2 | 2.42 | 0.53 |
| 46:B:17:C:H4' | 46:B:1094:G:C8 | 2.43 | 0.53 |
| 46:B:560:G:H2' | 46:B:561:U:O2 | 2.08 | 0.53 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 46:B:1012:A:OP1 | 46:B:1776:G:O2' | 2.15 | 0.53 |
| 46:B:1436:U:H2' | 46:B:1437:C:C6 | 2.44 | 0.53 |
| 50:F:77:ARG:HB2 | 57:M:22:VAL:HG11 | 1.91 | 0.53 |
| 78:h:150:VAL:HG22 | 78:h:153:GLU:H | 1.74 | 0.53 |
| 1:AS:46:C:OP2 | 1:AS:47:A:O2' | 2.19 | 0.53 |
| 1:AS:1593:C:H2' | 1:AS:1594:G:C8 | 2.43 | 0.53 |
| 1:AS:2130:A:H2' | 1:AS:2131:U:H6 | 1.73 | 0.53 |
| 4:AW:180:LEU:HD23 | 44:CK:18:TYR:CD2 | 2.44 | 0.53 |
| 46:CM:1265:C:O2' | 67:DH:69:THR:HG22 | 2.09 | 0.53 |
| 46:CM:1479:A:H4' | 46:CM:1480:G:O5' | 2.07 | 0.53 |
| 50:CQ:65:ARG:HD2 | 57:CX:91:ARG:NE | 2.23 | 0.53 |
| 54:CU:29:ASP:OD1 | 54:CU:30:LEU:HD23 | 2.09 | 0.53 |
| 65:DF:4:VAL:N | 72:DM:82:GLN:OE1 | 2.42 | 0.53 |
| 82:l1:92:LYS:HG3 | 82:l1:93:LEU:H | 1.74 | 0.53 |
| 1:1:783:G:H2' | 1:1:784:C:H6 | 1.74 | 0.53 |
| 1:1:2335:A:H2' | 1:1:2336:A:H8 | 1.72 | 0.53 |
| 1:1:3256:G:H2' | 1:1:3257:A:C8 | 2.43 | 0.53 |
| 2:3:112:G:H2' | 2:3:113:C:C6 | 2.43 | 0.53 |
| 17:w:28:ILE:HD11 | 17:w:89:ILE:HD11 | 1.89 | 0.53 |
| 46:B:746:G:O2' | 56:L:72:GLU:OE2 | 2.24 | 0.53 |
| 46:B:1279:G:O2' | 46:B:1306:A:N1 | 2.41 | 0.53 |
| 1:AS:2421:A:H5' | 1:AS:2422:C:OP2 | 2.09 | 0.53 |
| 1:AS:3093:U:H1' | 1:AS:3094:A:H5" | 1.90 | 0.53 |
| 16:BI:73:ARG:HG2 | 16:BI:75:VAL:HG13 | 1.91 | 0.53 |
| 46:CM:110:U:OP1 | 46:CM:738:A:O2' | 2.26 | 0.53 |
| 46:CM:151:G:N2 | 53:CT:56:ASN:OD1 | 2.38 | 0.53 |
| 46:CM:676:G:OP1 | 46:CM:676:G:H4' | 2.08 | 0.53 |
| 48:CO:23:PRO:HB3 | 48:CO:26:ARG:HH21 | 1.73 | 0.53 |
| 76:DQ:17:GLY:HA2 | 76:DQ:27:HIS:ND1 | 2.24 | 0.53 |
| 82:l1:64:THR:HB | 82:l1:108:ASN:HB2 | 1.91 | 0.53 |
| 1:1:2130:A:H2' | 1:1:2131:U:H6 | 1.74 | 0.53 |
| 3:4:75:G:H2' | 3:4:76:C:C6 | 2.42 | 0.53 |
| 8:n:39:LEU:HD11 | 8:n:53:TYR:HB2 | 1.90 | 0.53 |
| 8:n:71:ASN:ND2 | 8:n:159:LEU:O | 2.36 | 0.53 |
| 46:B:983:A:N6 | 46:B:989:U:OP2 | 2.42 | 0.53 |
| 46:B:1220:C:H3' | 46:B:1221:A:H8 | 1.72 | 0.53 |
| 46:B:1344:C:O2 | 66:V:3:GLY:HA3 | 2.08 | 0.53 |
| 59:O:43:ARG:NH2 | 59:O:103:LEU:HD23 | 2.24 | 0.53 |
| 1:AS:371:G:N1 | 1:AS:374:A:OP2 | 2.37 | 0.53 |
| 1:AS:907:C:OP1 | 4:AW:14:SER:OG | 2.27 | 0.53 |
| 1:AS:1456:A:H2' | 1:AS:1457:A:H8 | 1.74 | 0.53 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 1:AS:2978:A:H2' | 1:AS:2979:U:O4' | 2.09 | 0.53 |
| 1:AS:3244:A:O2' | 1:AS:3245:A:H5' | 2.09 | 0.53 |
| 3:AU:57:C:H4' | 3:AU:63:G:N7 | 2.24 | 0.53 |
| 8:BA:20:THR:HG22 | 8:BA:22:LYS:H | 1.73 | 0.53 |
| 46:CM:1132:A:H2' | 46:CM:1133:C:C6 | 2.44 | 0.53 |
| 46:CM:1367:U:O4 | 46:CM:1368:A:N6 | 2.42 | 0.53 |
| 1:1:2469:A:N3 | 82:l1:209:THR:HA | 2.23 | 0.53 |
| 1:1:3126:U:H2' | 1:1:3128:G:H1' | 1.91 | 0.53 |
| 5:k:92:TYR:HB2 | 5:k:157:VAL:HB | 1.90 | 0.53 |
| 8:n:70:VAL:HG13 | 8:n:160:ALA:HB2 | 1.91 | 0.53 |
| 13:s:62:ASN:HB2 | 43:AP:103:ALA:HA | 1.91 | 0.53 |
| 40:AM:23:LEU:HD12 | 40:AM:24:PRO:HD2 | 1.90 | 0.53 |
| 46:B:700:G:H5" | 46:B:717:G:H22 | 1.74 | 0.53 |
| 46:B:1398:G:H4' | 46:B:1399:U:O5' | 2.08 | 0.53 |
| 46:B:1546:G:C5 | 65:U:134:ARG:HD3 | 2.44 | 0.53 |
| 48:D:56:ASN:OD1 | 48:D:57:ALA:N | 2.42 | 0.53 |
| 1:AS:297:G:OP2 | 1:AS:297:G:N2 | 2.33 | 0.53 |
| 3:AU:75:G:H2' | 3:AU:76:C:C6 | 2.44 | 0.53 |
| 46:CM:1533:G:OP1 | 65:DF:123:ARG:NH1 | 2.41 | 0.53 |
| 59:CZ:31:VAL:O | 59:CZ:35:SER:HB3 | 2.09 | 0.53 |
| 60:DA:83:GLU:OE1 | 60:DA:83:GLU:N | 2.42 | 0.53 |
| 64:DE:79:GLU:O | 64:DE:83:GLN:NE2 | 2.28 | 0.53 |
| 65:DF:36:ARG:NH1 | 65:DF:105:LEU:HD22 | 2.24 | 0.53 |
| 1:1:634:C:O2 | 1:1:2355:G:O2' | 2.22 | 0.52 |
| 1:1:683:G:OP2 | 14:t:35:ARG:NH1 | 2.42 | 0.52 |
| 1:1:2981:G:OP1 | 17:w:67:LYS:HD2 | 2.09 | 0.52 |
| 6:l:157:PHE:CD1 | 6:l:169:VAL:HG11 | 2.44 | 0.52 |
| 27:9:39:LEU:HD22 | 27:9:43:TYR:HE2 | 1.73 | 0.52 |
| 42:AO:10:VAL:HG11 | 46:B:1100:U:H5" | 1.91 | 0.52 |
| 46:B:739:A:H5" | 46:B:740:A:C5' | 2.40 | 0.52 |
| 46:B:932:U:H2' | 46:B:933:A:C8 | 2.44 | 0.52 |
| 46:B:1127:A:H2' | 46:B:1128:A:C8 | 2.45 | 0.52 |
| 46:B:1716:C:H2' | 46:B:1717:A:O4' | 2.09 | 0.52 |
| 53:I:180:THR:HG23 | 53:I:183:THR:H | 1.74 | 0.52 |
| 57:M:87:LEU:HD22 | 57:M:91:ARG:O | 2.10 | 0.52 |
| 68:X:70:ASN:HB3 | 68:X:83:TRP:HB2 | 1.90 | 0.52 |
| 1:AS:431:A:H2' | 1:AS:432:G:H8 | 1.74 | 0.52 |
| 1:AS:1493:C:H2' | 1:AS:1494:A:C8 | 2.45 | 0.52 |
| 1:AS:1810:A:H4' | 1:AS:1811:U:O4' | 2.09 | 0.52 |
| 46:CM:701:G:N2 | 46:CM:721:C:C2 | 2.77 | 0.52 |
| 46:CM:1649:G:H2' | 46:CM:1650:G:H8 | 1.73 | 0.52 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 46:CM:1696:U:H2' | 46:CM:1697:C:C5 | 2.44 | 0.52 |
| 52:CS:98:MET:HB2 | 52:CS:103:ASN:O | 2.10 | 0.52 |
| 53:CT:135:PRO:HB2 | 53:CT:141:ILE:HG12 | 1.91 | 0.52 |
| 59:CZ:74:LEU:HD23 | 78:DS:150:VAL:HG13 | 1.91 | 0.52 |
| 80:p0:59:VAL:HA | 80:p0:62:ALA:HB3 | 1.91 | 0.52 |
| 1:1:208:A:H4' | 1:1:210:A:C8 | 2.44 | 0.52 |
| 1:1:1106:U:H2' | 1:1:1107:U:C6 | 2.44 | 0.52 |
| 1:1:1656:C:H2' | 1:1:1657:G:H8 | 1.74 | 0.52 |
| 1:1:2342:G:H22 | 1:1:2374:G:H1' | 1.74 | 0.52 |
| 7:m:235:ASP:O | 7:m:239:ILE:HG13 | 2.09 | 0.52 |
| 31:AD:26:THR:HG23 | 31:AD:95:LEU:HD11 | 1.90 | 0.52 |
| 46:B:302:U:H2' | 46:B:303:C:C6 | 2.44 | 0.52 |
| 46:B:1245:U:H2' | 46:B:1246:G:C8 | 2.44 | 0.52 |
| 46:B:1435:U:H2' | 46:B:1436:U:H6 | 1.74 | 0.52 |
| 52:H:158:GLN:HG2 | 75:e:66:LEU:HD11 | 1.92 | 0.52 |
| 65:U:4:VAL:HG22 | 72:b:82:GLN:OE1 | 2.10 | 0.52 |
| 1:AS:951:U:H2' | 1:AS:952:U:C6 | 2.44 | 0.52 |
| 1:AS:1199:A:N3 | 1:AS:2827:U:O2' | 2.37 | 0.52 |
| 1:AS:1303:G:H5' | 17:BJ:61:LYS:HE3 | 1.90 | 0.52 |
| 1:AS:2335:A:H2' | 1:AS:2336:A:C8 | 2.44 | 0.52 |
| 1:AS:2440:A:O5' | 1:AS:2441:G:N2 | 2.42 | 0.52 |
| 1:AS:2441:G:H4' | 1:AS:2442:U:C5 | 2.44 | 0.52 |
| 13:BF:92:ARG:HB3 | 13:BF:95:ASN:OD1 | 2.10 | 0.52 |
| 15:BH:20:LEU:CD2 | 15:BH:23:ASN:HA | 2.39 | 0.52 |
| 31:BX:36:LEU:HD13 | 31:BX:61:TYR:HB3 | 1.91 | 0.52 |
| 46:CM:874:U:H2' | 46:CM:875:C:C6 | 2.44 | 0.52 |
| 46:CM:1417:C:O2' | 46:CM:1423:U:O4 | 2.13 | 0.52 |
| 56:CW:68:LYS:HE3 | 56:CW:72:GLU:HG3 | 1.91 | 0.52 |
| 79:DT:198:CYS:O | 79:DT:199:ILE:HG12 | 2.09 | 0.52 |
| 80:P0:53:MET:HE3 | 80:P0:54:GLY:H | 1.74 | 0.52 |
| 1:1:290:G:H1' | 16:v:93:LYS:HD2 | 1.91 | 0.52 |
| 1:1:903:G:H2' | 1:1:922:A:H62 | 1.74 | 0.52 |
| 1:1:1611:U:H2' | 1:1:1612:U:H6 | 1.75 | 0.52 |
| 2:3:23:A:H2' | 2:3:24:A:C8 | 2.43 | 0.52 |
| 4:j:3:ARG:HB2 | 4:j:207:VAL:HG22 | 1.90 | 0.52 |
| 4:j:112:ILE:HG13 | 44:AQ:79:VAL:HG22 | 1.91 | 0.52 |
| 18:x:54:HIS:O | 18:x:72:GLN:NE2 | 2.38 | 0.52 |
| 46:B:92:A:OP1 | 51:G:7:LYS:NZ | 2.43 | 0.52 |
| 54:J:8:GLU:H | 54:J:8:GLU:CD | 2.16 | 0.52 |
| 55:K:56:ARG:NH1 | 55:K:180:GLY:O | 2.41 | 0.52 |
| 59:O:96:LEU:HD12 | 59:O:100:TRP:HZ3 | 1.74 | 0.52 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 62:R:77:LYS:HD2 | 62:R:102:PHE:CZ | 2.44 | 0.52 |
| 1:AS:72:A:C4 | 37:CD:14:ARG:HD2 | 2.44 | 0.52 |
| 1:AS:1481:G:N2 | 35:CB:4:ARG:HD2 | 2.24 | 0.52 |
| 1:AS:1561:U:H6 | 1:AS:1561:U:H5" | 1.75 | 0.52 |
| 1:AS:3285:A:H2' | 1:AS:3286:C:C6 | 2.44 | 0.52 |
| 1:AS:3344:U:H4' | 5:AX:315:GLY:HA2 | 1.91 | 0.52 |
| 45:CL:62:ALA:C | 45:CL:64:LEU:H | 2.15 | 0.52 |
| 46:CM:157:U:O2' | 53:CT:87:ARG:NE | 2.42 | 0.52 |
| 46:CM:226:G:C6 | 46:CM:819:G:C4 | 2.97 | 0.52 |
| 46:CM:876:A:H2' | 46:CM:877:G:H8 | 1.74 | 0.52 |
| 46:CM:1237:C:H2' | 46:CM:1238:U:O4' | 2.10 | 0.52 |
| 46:CM:1369:G:O2' | 46:CM:1370:A:H8 | 1.92 | 0.52 |
| 47:CN:88:LYS:HD2 | 47:CN:201:LEU:HD11 | 1.91 | 0.52 |
| 64:DE:89:SER:C | 64:DE:91:LEU:H | 2.17 | 0.52 |
| 80:p0:19:LEU:HD21 | 80:p0:63:ILE:HD12 | 1.91 | 0.52 |
| 80:p0:19:LEU:HB3 | 80:p0:66:PHE:CE2 | 2.44 | 0.52 |
| 1:1:780:A:C2 | 19:y:69:ARG:HD3 | 2.45 | 0.52 |
| 7:m:60:ILE:HB | 7:m:80:ALA:HB2 | 1.91 | 0.52 |
| 46:B:234:G:H2' | 46:B:235:C:C6 | 2.44 | 0.52 |
| 1:AS:648:C:H2' | 1:AS:649:G:C8 | 2.45 | 0.52 |
| 1:AS:1172:C:H4' | 17:BJ:90:PRO:HD3 | 1.90 | 0.52 |
| 1:AS:2464:A:O2' | 1:AS:2465:U:H5' | 2.10 | 0.52 |
| 1:AS:3088:G:H4' | 11:BD:69:ARG:NH1 | 2.24 | 0.52 |
| 15:BH:20:LEU:HD21 | 15:BH:23:ASN:CA | 2.38 | 0.52 |
| 18:BK:40:LYS:HD2 | 18:BK:113:VAL:HG22 | 1.92 | 0.52 |
| 20:BM:70:LYS:HB3 | 20:BM:76:MET:HE2 | 1.91 | 0.52 |
| 46:CM:635:C:O2 | 54:CU:110:ARG:NH2 | 2.38 | 0.52 |
| 46:CM:1301:G:OP1 | 64:DE:7:LYS:N | 2.31 | 0.52 |
| 61:DB:52:PRO:HB3 | 61:DB:95:SER:OG | 2.09 | 0.52 |
| 80:P0:4:ALA:HB3 | 80:P0:5:ARG:NH1 | 2.24 | 0.52 |
| 82:L1:174:MET:HE3 | 82:L1:178:VAL:HG21 | 1.92 | 0.52 |
| 82:l1:14:HIS:O | 82:l1:15:LYS:C | 2.52 | 0.52 |
| 1:1:299:G:C8 | 37:AJ:30:GLY:HA3 | 2.44 | 0.52 |
| 1:1:1225:G:H2' | 1:1:1226:G:H8 | 1.73 | 0.52 |
| 1:1:1810:A:H4' | 1:1:1811:U:O4' | 2.10 | 0.52 |
| 1:1:2850:G:H5" | 5:k:5:LYS:HE2 | 1.92 | 0.52 |
| 14:t:57:VAL:HG22 | 14:t:69:VAL:HG22 | 1.92 | 0.52 |
| 28:AA:101:LEU:HB3 | 28:AA:107:ARG:HH21 | 1.75 | 0.52 |
| 46:B:674:C:H2' | 46:B:675:U:O4' | 2.09 | 0.52 |
| 46:B:1609:G:H2' | 46:B:1610:C:C6 | 2.44 | 0.52 |
| 56:L:110:GLN:NE2 | 56:L:126:ARG:HB2 | 2.25 | 0.52 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 64:T:14:LYS:HB2 | 64:T:69:ILE:HD11 | 1.91 | 0.52 |
| 1:AS:430:G:H2' | 1:AS:431:A:C8 | 2.45 | 0.52 |
| 1:AS:1023:A:C6 | 1:AS:1025:G:H1' | 2.45 | 0.52 |
| 1:AS:1949:G:O2' | 1:AS:2066:G:N2 | 2.43 | 0.52 |
| 3:AU:137:C:H5" | 26:BS:42:ARG:HH12 | 1.74 | 0.52 |
| 21:BN:42:TRP:O | 21:BN:46:GLN:HG3 | 2.10 | 0.52 |
| 28:BU:34:LYS:C | 28:BU:36:HIS:H | 2.17 | 0.52 |
| 46:CM:695:C:O2' | 46:CM:696:U:OP1 | 2.26 | 0.52 |
| 48:CO:180:THR:HG23 | 48:CO:183:GLN:H | 1.75 | 0.52 |
| 50:CQ:28:ARG:HB3 | 57:CX:58:GLN:HE21 | 1.73 | 0.52 |
| 51:CR:112:HIS:NE2 | 51:CR:238:SER:O | 2.41 | 0.52 |
| 71:DL:29:HIS:HB2 | 71:DL:32:ARG:HB3 | 1.90 | 0.52 |
| 71:DL:122:GLN:HG2 | 71:DL:126:GLN:HE22 | 1.74 | 0.52 |
| 79:DT:67:HIS:CG | 79:DT:68:ILE:H | 2.28 | 0.52 |
| 1:1:788:G:H2' | 1:1:789:C:C6 | 2.44 | 0.52 |
| 1:1:1301:U:C2 | 5:k:257:PRO:HG3 | 2.44 | 0.52 |
| 1:1:1374:U:H2' | 1:1:1375:G:H8 | 1.73 | 0.52 |
| 1:1:1568:U:C4 | 1:1:1569:C:H1' | 2.45 | 0.52 |
| 1:1:1580:U:H2' | 1:1:1581:C:H6 | 1.75 | 0.52 |
| 1:1:2232:U:H2' | 1:1:2239:G:N2 | 2.24 | 0.52 |
| 1:1:2587:G:H2' | 1:1:2588:C:H6 | 1.73 | 0.52 |
| 16:v:113:LEU:HB2 | 16:v:134:LEU:HD23 | 1.91 | 0.52 |
| 46:B:1086:G:H4' | 69:Y:76:GLN:HG3 | 1.91 | 0.52 |
| 46:B:1486:G:OP1 | 66:V:122:ARG:NH1 | 2.42 | 0.52 |
| 54:J:134:LYS:HG3 | 60:P:18:TYR:OH | 2.09 | 0.52 |
| 62:R:10:ARG:HG2 | 62:R:13:LYS:HE2 | 1.92 | 0.52 |
| 1:AS:169:G:C6 | 1:AS:249:G:H1' | 2.44 | 0.52 |
| 1:AS:224:C:OP1 | 27:BT:47:SER:OG | 2.25 | 0.52 |
| 1:AS:430:G:H2' | 1:AS:431:A:H8 | 1.74 | 0.52 |
| 1:AS:2734:A:H2' | 1:AS:2735:U:H6 | 1.75 | 0.52 |
| 1:AS:3035:C:H2' | 1:AS:3036:U:H6 | 1.75 | 0.52 |
| 7:AZ:6:GLU:OE1 | 7:AZ:7:PHE:N | 2.42 | 0.52 |
| 11:BD:47:LYS:NZ | 15:BH:3:SER:HA | 2.24 | 0.52 |
| 36:CC:78:LYS:HA | 36:CC:81:ARG:HD2 | 1.90 | 0.52 |
| 49:CP:177:PRO:HD3 | 56:CW:17:ARG:HH22 | 1.75 | 0.52 |
| 57:CX:76:LEU:O | 57:CX:80:LEU:HB2 | 2.10 | 0.52 |
| 74:DO:75:GLU:OE1 | 74:DO:75:GLU:N | 2.31 | 0.52 |
| 79:DT:94:ASP:OD1 | 79:DT:101:THR:OG1 | 2.28 | 0.52 |
| 82:l1:179:LEU:O | 82:l1:181:ASN:N | 2.43 | 0.52 |
| 1:1:277:G:H2' | 1:1:278:U:C6 | 2.44 | 0.52 |
| 1:1:430:G:H2' | 1:1:431:A:H8 | 1.75 | 0.52 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 1:1:1014:G:H1 | 1:1:1030:U:H3 | 1.56 | 0.52 |
| 1:1:1035:U:H2' | 1:1:1036:A:C8 | 2.45 | 0.52 |
| 1:1:1042:A:H2' | 1:1:1045:C:C5 | 2.45 | 0.52 |
| 1:1:1762:G:O2' | 1:1:1763:C:OP1 | 2.26 | 0.52 |
| 1:1:2090:U:H4' | 1:1:2091:A:O5' | 2.09 | 0.52 |
| 1:1:2158:A:H2' | 1:1:2159:C:C6 | 2.44 | 0.52 |
| 1:1:2681:C:H2' | 1:1:2682:C:C6 | 2.44 | 0.52 |
| 1:1:2802:G:H1 | 1:1:2830:U:H3 | 1.58 | 0.52 |
| 1:1:3164:U:H4' | 1:1:3165:U:C2 | 2.45 | 0.52 |
| 31:AD:18:LEU:HB3 | 31:AD:100:SER:HB2 | 1.91 | 0.52 |
| 32:AE:71:ARG:HH11 | 32:AE:103:LEU:HD13 | 1.74 | 0.52 |
| 46:B:338:U:H2' | 46:B:339:A:C8 | 2.44 | 0.52 |
| 50:F:223:THR:HG21 | 79:AR:225:ASN:HB3 | 1.91 | 0.52 |
| 52:H:91:GLU:HA | 52:H:94:THR:HG22 | 1.92 | 0.52 |
| 62:R:25:LEU:HG | 62:R:87:PRO:HB3 | 1.92 | 0.52 |
| 79:AR:76:ALA:HB3 | 79:AR:120:LEU:HD11 | 1.92 | 0.52 |
| 1:AS:699:G:H2' | 1:AS:700:C:C6 | 2.45 | 0.52 |
| 1:AS:1241:A:H3' | 1:AS:1242:G:H5" | 1.92 | 0.52 |
| 1:AS:2480:A:H4' | 1:AS:2481:G:C8 | 2.44 | 0.52 |
| 1:AS:3142:A:H1' | 17:BJ:102:ARG:HH21 | 1.74 | 0.52 |
| 23:BP:19:VAL:C | 23:BP:21:ALA:H | 2.16 | 0.52 |
| 46:CM:1398:G:H4' | 46:CM:1399:U:O5' | 2.09 | 0.52 |
| 82:l1:49:PHE:CZ | 82:l1:159:LEU:HB2 | 2.44 | 0.52 |
| 1:1:248:U:H2' | 1:1:249:G:H4' | 1.92 | 0.52 |
| 1:1:1265:U:N3 | 1:1:1268:C:OP2 | 2.30 | 0.52 |
| 1:1:2484:U:H2' | 1:1:2485:U:C6 | 2.44 | 0.52 |
| 1:1:2876:U:H2' | 1:1:2877:U:C6 | 2.44 | 0.52 |
| 5:k:66:LYS:NZ | 24:6:9:ASN:H | 2.07 | 0.52 |
| 64:T:45:ARG:HA | 64:T:48:ASN:HD21 | 1.73 | 0.52 |
| 79:AR:155:VAL:O | 79:AR:156:ARG:NH1 | 2.37 | 0.52 |
| 1:AS:2370:C:H1' | 5:AX:266:ARG:NH2 | 2.25 | 0.52 |
| 1:AS:2370:C:H1' | 5:AX:266:ARG:HH21 | 1.75 | 0.52 |
| 1:AS:2583:U:H2' | 1:AS:2584:U:C6 | 2.45 | 0.52 |
| 1:AS:3308:G:O2' | 1:AS:3327:A:N6 | 2.42 | 0.52 |
| 84:AS:3401:3K5:H16 | 84:AS:3401:3K5:H39 | 1.92 | 0.52 |
| 15:BH:23:ASN:HD22 | 15:BH:23:ASN:C | 2.18 | 0.52 |
| 21:BN:96:ASP:OD1 | 21:BN:97:VAL:N | 2.42 | 0.52 |
| 30:BW:16:ALA:HB1 | 30:BW:21:ILE:HD11 | 1.91 | 0.52 |
| 45:CL:69:PHE:CE1 | 62:DC:127:ARG:HD3 | 2.45 | 0.52 |
| 46:CM:43:A:O2' | 46:CM:99:C:OP1 | 2.22 | 0.52 |
| 46:CM:220:A:C8 | 46:CM:221:U:H5 | 2.27 | 0.52 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 46:CM:234:G:H2' | 46:CM:235:C:C6 | 2.45 | 0.52 |
| 54:CU:69:VAL:HG12 | 54:CU:72:ARG:HH21 | 1.74 | 0.52 |
| 78:DS:184:GLY:O | 78:DS:186:CYS:N | 2.43 | 0.52 |
| 1:1:365:A:OP1 | 6:l:85:ARG:NH1 | 2.42 | 0.52 |
| 1:1:480:G:H2' | 1:1:481:G:H8 | 1.74 | 0.52 |
| 1:1:1456:A:H2' | 1:1:1457:A:H8 | 1.74 | 0.52 |
| 1:1:2345:A:H2' | 1:1:2346:A:H8 | 1.74 | 0.52 |
| 3:4:20:U:OP1 | 87:4:301:HOH:O | 2.19 | 0.52 |
| 31:AD:77:ASN:ND2 | 44:AQ:43:GLY:O | 2.39 | 0.52 |
| 46:B:415:A:H5' | 46:B:416:G:C5 | 2.45 | 0.52 |
| 46:B:717:G:H4' | 46:B:719:A:N1 | 2.24 | 0.52 |
| 46:B:786:G:H21 | 69:Y:107:SER:HB3 | 1.74 | 0.52 |
| 46:B:1149:G:H2' | 46:B:1150:G:C8 | 2.45 | 0.52 |
| 79:AR:68:ILE:O | 79:AR:86:TRP:N | 2.34 | 0.52 |
| 1:AS:307:A:H2' | 1:AS:308:A:H8 | 1.75 | 0.52 |
| 1:AS:428:U:H2' | 1:AS:429:U:C6 | 2.44 | 0.52 |
| 1:AS:1616:U:H2' | 1:AS:1617:A:C8 | 2.45 | 0.52 |
| 1:AS:2210:A:H2' | 1:AS:2211:A:C8 | 2.45 | 0.52 |
| 1:AS:2345:A:H2' | 1:AS:2346:A:H8 | 1.75 | 0.52 |
| 10:BC:158:VAL:HG21 | 10:BC:164:VAL:HG21 | 1.90 | 0.52 |
| 45:CL:99:SER:OG | 46:CM:573:C:OP1 | 2.26 | 0.52 |
| 46:CM:852:G:H1 | 46:CM:946:U:H3 | 1.58 | 0.52 |
| 46:CM:1393:U:H2' | 46:CM:1394:G:C8 | 2.44 | 0.52 |
| 60:DA:33:VAL:HG21 | 60:DA:66:VAL:HG11 | 1.91 | 0.52 |
| 78:DS:127:TYR:HD1 | 78:DS:128:THR:CG2 | 2.22 | 0.52 |
| 82:l1:112:ALA:O | 82:l1:116:LEU:HB2 | 2.09 | 0.52 |
| 1:1:281:G:N7 | 16:v:182:LYS:HE2 | 2.25 | 0.52 |
| 1:1:624:U:H2' | 1:1:625:C:H6 | 1.75 | 0.52 |
| 1:1:689:A:N1 | 3:4:28:C:O2' | 2.40 | 0.52 |
| 1:1:856:G:O2' | 1:1:891:A:H4' | 2.10 | 0.52 |
| 1:1:1190:G:H2' | 1:1:1191:A:C8 | 2.44 | 0.52 |
| 1:1:1396:U:H2' | 1:1:1397:G:O4' | 2.09 | 0.52 |
| 1:1:2739:U:H2' | 1:1:2740:U:C6 | 2.45 | 0.52 |
| 34:AG:51:TYR:HD2 | 34:AG:67:ILE:HD12 | 1.75 | 0.52 |
| 46:B:503:A:H2' | 46:B:505:U:C6 | 2.45 | 0.52 |
| 46:B:1602:C:N4 | 52:H:80:LYS:O | 2.43 | 0.52 |
| 46:B:1642:A:N6 | 46:B:1732:G:O2' | 2.42 | 0.52 |
| 52:H:151:SER:OG | 52:H:156:ARG:NH2 | 2.41 | 0.52 |
| 61:Q:20:ASP:OD1 | 61:Q:21:THR:N | 2.41 | 0.52 |
| 62:R:41:VAL:HG13 | 62:R:84:ILE:HD13 | 1.91 | 0.52 |
| 70:Z:37:ALA:HA | 70:Z:41:SER:HB3 | 1.92 | 0.52 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 1:AS:671:U:H2' | 1:AS:672:G:C8 | 2.45 | 0.52 |
| 1:AS:989:G:N3 | 1:AS:2609:A:H2' | 2.25 | 0.52 |
| 1:AS:3136:C:H2' | 1:AS:3137:A:H8 | 1.74 | 0.52 |
| 1:AS:3259:A:H2' | 1:AS:3260:A:O4' | 2.10 | 0.52 |
| 14:BG:126:PHE:HB3 | 14:BG:130:THR:OG1 | 2.10 | 0.52 |
| 21:BN:92:LYS:HE2 | 21:BN:109:ASP:OD2 | 2.09 | 0.52 |
| 31:BX:42:LYS:HB3 | 31:BX:103:LEU:HD21 | 1.91 | 0.52 |
| 46:CM:903:U:H4' | 61:DB:13:ARG:HD3 | 1.92 | 0.52 |
| 46:CM:1436:U:H2' | 46:CM:1437:C:C6 | 2.45 | 0.52 |
| 46:CM:1636:C:H2' | 46:CM:1637:U:C6 | 2.45 | 0.52 |
| 57:CX:54:TYR:CE1 | 57:CX:75:PHE:HB2 | 2.45 | 0.52 |
| 1:1:294:U:OP2 | 16:v:15:GLN:NE2 | 2.30 | 0.51 |
| 1:1:407:A:C2 | 3:4:17:A:H1' | 2.45 | 0.51 |
| 1:1:1434:U:H4' | 6:l:89:ALA:HB3 | 1.91 | 0.51 |
| 1:1:2680:C:H2' | 1:1:2681:C:C6 | 2.46 | 0.51 |
| 1:1:3162:U:H2' | 1:1:3163:U:H4' | 1.92 | 0.51 |
| 1:1:3216:U:H2' | 1:1:3217:G:C8 | 2.45 | 0.51 |
| 3:4:126:A:O2' | 3:4:129:C:N4 | 2.43 | 0.51 |
| 6:l:300:VAL:HB | 19:y:39:ARG:HG2 | 1.91 | 0.51 |
| 46:B:458:A:O2' | 51:G:27:TYR:OH | 2.13 | 0.51 |
| 46:B:915:A:H2' | 48:D:114:VAL:HG11 | 1.92 | 0.51 |
| 46:B:1354:U:C2 | 46:B:1355:A:N7 | 2.78 | 0.51 |
| 57:M:70:ASP:O | 57:M:73:VAL:HG22 | 2.10 | 0.51 |
| 59:O:36:LEU:C | 59:O:38:HIS:N | 2.68 | 0.51 |
| 66:V:10:PRO:HB2 | 66:V:13:ASP:OD1 | 2.09 | 0.51 |
| 1:AS:481:G:P | 1:AS:481:G:O4' | 2.69 | 0.51 |
| 1:AS:565:A:H2' | 1:AS:566:C:O4' | 2.11 | 0.51 |
| 1:AS:631:U:H2' | 1:AS:632:C:C6 | 2.44 | 0.51 |
| 1:AS:1265:U:H5' | 1:AS:1266:A:OP2 | 2.10 | 0.51 |
| 1:AS:1755:U:H3 | 1:AS:1762:G:H1 | 1.58 | 0.51 |
| 1:AS:1799:C:H4' | 35:CB:62:TYR:HB3 | 1.92 | 0.51 |
| 1:AS:1837:A:H1' | 40:CG:45:ARG:HH22 | 1.75 | 0.51 |
| 1:AS:2469:A:H2' | 1:AS:2470:C:C6 | 2.45 | 0.51 |
| 1:AS:2854:U:H2' | 1:AS:2855:U:C6 | 2.45 | 0.51 |
| 1:AS:3171:C:H5" | 1:AS:3172:U:O5' | 2.10 | 0.51 |
| 18:BK:32:THR:HG21 | 18:BK:87:SER:HB3 | 1.92 | 0.51 |
| 21:BN:109:ASP:OD1 | 21:BN:113:ARG:NH1 | 2.39 | 0.51 |
| 22:BO:136:ARG:HD3 | 22:BO:139:ARG:NH2 | 2.26 | 0.51 |
| 36:CC:22:VAL:O | 36:CC:26:GLN:HG3 | 2.10 | 0.51 |
| 45:CL:103:LEU:HB3 | 45:CL:109:GLN:HG3 | 1.90 | 0.51 |
| 46:CM:638:U:H2' | 46:CM:639:G:O4' | 2.09 | 0.51 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 46:CM:654:G:H8 | 46:CM:654:G:O5' | 1.93 | 0.51 |
| 46:CM:1254:U:H5' | 46:CM:1418:U:OP2 | 2.08 | 0.51 |
| 50:CQ:68:HIS:CE1 | 57:CX:93:LYS:HG2 | 2.46 | 0.51 |
| 54:CU:69:VAL:HG12 | 54:CU:72:ARG:NH2 | 2.25 | 0.51 |
| 79:DT:239:ALA:HB3 | 79:DT:289:LEU:HD12 | 1.91 | 0.51 |
| 82:l1:14:HIS:HE2 | 82:l1:176:GLU:HG2 | 1.74 | 0.51 |
| 1:1:1130:G:O2' | 1:1:2614:A:N3 | 2.41 | 0.51 |
| 1:1:1268:C:H3' | 1:1:1269:A:H8 | 1.74 | 0.51 |
| 1:1:1278:G:OP1 | 80:P0:55:LYS:HB2 | 2.09 | 0.51 |
| 1:1:1593:C:H2' | 1:1:1594:G:C8 | 2.45 | 0.51 |
| 84:1:3402:3K5:H13 | 43:AP:57:ILE:HG23 | 1.91 | 0.51 |
| 19:y:67:ILE:HG23 | 19:y:81:ILE:HG13 | 1.91 | 0.51 |
| 21:0:99:ARG:NH1 | 21:0:126:VAL:O | 2.43 | 0.51 |
| 46:B:669:G:H2' | 46:B:671:G:C8 | 2.45 | 0.51 |
| 46:B:1216:U:OP1 | 78:h:136:LYS:NZ | 2.33 | 0.51 |
| 51:G:11:ARG:HA | 51:G:28:ALA:HB2 | 1.92 | 0.51 |
| 52:H:57:SER:HB2 | 75:e:53:ILE:O | 2.10 | 0.51 |
| 54:J:156:THR:HA | 54:J:159:ASP:OD2 | 2.10 | 0.51 |
| 1:AS:647:A:OP2 | 1:AS:2840:U:O2' | 2.25 | 0.51 |
| 1:AS:903:G:H2' | 1:AS:922:A:H62 | 1.75 | 0.51 |
| 1:AS:1059:G:N7 | 1:AS:1093:G:O2' | 2.37 | 0.51 |
| 1:AS:1152:C:OP2 | 9:BB:92:LYS:NZ | 2.39 | 0.51 |
| 1:AS:2197:A:H2' | 1:AS:2198:A:H8 | 1.75 | 0.51 |
| 1:AS:2435:G:H3' | 1:AS:2436:A:C5' | 2.40 | 0.51 |
| 1:AS:2659:G:H4' | 7:AZ:7:PHE:HE2 | 1.73 | 0.51 |
| 1:AS:2995:U:H2' | 1:AS:2996:A:H8 | 1.76 | 0.51 |
| 1:AS:3302:G:H2' | 1:AS:3303:C:C6 | 2.45 | 0.51 |
| 10:BC:79:PHE:HA | 10:BC:180:ILE:HD13 | 1.92 | 0.51 |
| 46:CM:1670:U:O2' | 46:CM:1671:G:O5' | 2.29 | 0.51 |
| 50:CQ:214:ASP:OD1 | 50:CQ:215:GLU:N | 2.29 | 0.51 |
| 67:DH:25:LEU:HD23 | 67:DH:88:ARG:O | 2.10 | 0.51 |
| 1:1:249:G:N2 | 1:1:251:G:N7 | 2.59 | 0.51 |
| 1:1:1443:G:N7 | 18:x:25:SER:OG | 2.40 | 0.51 |
| 1:1:2812:C:N4 | 1:1:2817:A:O2' | 2.43 | 0.51 |
| 1:1:3171:C:H5" | 1:1:3172:U:O5' | 2.10 | 0.51 |
| 46:B:638:U:H2' | 46:B:639:G:O4' | 2.10 | 0.51 |
| 46:B:1582:U:H5' | 46:B:1583:C:OP2 | 2.10 | 0.51 |
| 53:I:68:MET:O | 53:I:69:HIS:ND1 | 2.43 | 0.51 |
| 57:M:15:LEU:O | 57:M:19:GLY:HA2 | 2.11 | 0.51 |
| 59:O:74:LEU:O | 59:O:78:LEU:HD13 | 2.09 | 0.51 |
| 62:R:81:ARG:HB2 | 62:R:117:GLY:HA3 | 1.93 | 0.51 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 63:S:67:LYS:O | 63:S:67:LYS:HG2 | 2.11 | 0.51 |
| 64:T:89:SER:HB3 | 64:T:92:ASP:HB2 | 1.91 | 0.51 |
| 1:AS:496:A:H2' | 1:AS:497:U:C6 | 2.45 | 0.51 |
| 21:BN:8:GLN:HG3 | 21:BN:26:ARG:HD2 | 1.92 | 0.51 |
| 50:CQ:30:LEU:HD22 | 50:CQ:59:VAL:HG22 | 1.92 | 0.51 |
| 54:CU:33:GLU:HG3 | 54:CU:69:VAL:HG11 | 1.92 | 0.51 |
| 1:1:788:G:H2' | 1:1:789:C:H6 | 1.76 | 0.51 |
| 1:1:2164:U:OP2 | 4:j:200:ARG:HD2 | 2.10 | 0.51 |
| 1:1:3166:A:H2' | 1:1:3167:G:H8 | 1.75 | 0.51 |
| 16:v:68:ARG:HG2 | 16:v:128:LYS:HG3 | 1.91 | 0.51 |
| 19:y:90:ASP:O | 19:y:113:ARG:NH1 | 2.44 | 0.51 |
| 46:B:685:C:H5" | 69:Y:119:LYS:HG2 | 1.92 | 0.51 |
| 46:B:1235:U:O2' | 78:h:177:MET:HE2 | 2.10 | 0.51 |
| 51:G:192:VAL:HG23 | 51:G:244:GLY:HA3 | 1.91 | 0.51 |
| 52:H:98:MET:HB2 | 52:H:103:ASN:O | 2.11 | 0.51 |
| 54:J:4:LYS:NZ | 54:J:34:LEU:O | 2.42 | 0.51 |
| 67:W:24:THR:HB | 67:W:114:GLU:HG3 | 1.93 | 0.51 |
| 1:AS:21:G:H5" | 38:CE:43:LYS:HG2 | 1.93 | 0.51 |
| 1:AS:448:U:H2' | 1:AS:481:G:H1 | 1.75 | 0.51 |
| 26:BS:133:LEU:O | 26:BS:137:ASN:ND2 | 2.42 | 0.51 |
| 28:BU:12:ILE:HB | 28:BU:81:MET:HB3 | 1.91 | 0.51 |
| 45:CL:82:LYS:HD2 | 45:CL:83:HIS:N | 2.19 | 0.51 |
| 46:CM:327:G:H5' | 55:CV:99:SER:HB3 | 1.93 | 0.51 |
| 46:CM:583:A:H2' | 46:CM:584:G:H8 | 1.75 | 0.51 |
| 46:CM:1315:G:H2' | 46:CM:1316:A:O4' | 2.10 | 0.51 |
| 46:CM:1373:G:OP1 | 64:DE:32:LYS:NZ | 2.37 | 0.51 |
| 46:CM:1437:C:OP1 | 76:DQ:12:ARG:NH1 | 2.39 | 0.51 |
| 46:CM:1485:G:H5" | 66:DG:72:GLY:HA3 | 1.92 | 0.51 |
| 46:CM:1664:C:H42 | 46:CM:1711:C:H42 | 1.58 | 0.51 |
| 46:CM:1716:C:H2' | 46:CM:1717:A:O4' | 2.10 | 0.51 |
| 66:DG:42:GLY:HA3 | 66:DG:94:VAL:HG21 | 1.92 | 0.51 |
| 1:1:541:U:N3 | 1:1:543:C:O2' | 2.44 | 0.51 |
| 1:1:1141:G:OP1 | 33:AF:45:ARG:HD2 | 2.11 | 0.51 |
| 1:1:1656:C:H2' | 1:1:1657:G:C8 | 2.45 | 0.51 |
| 1:1:1949:G:H22 | 20:z:114:LYS:HE3 | 1.75 | 0.51 |
| 1:1:2239:G:O2' | 1:1:2241:C:N4 | 2.44 | 0.51 |
| 15:u:21:VAL:HG22 | 15:u:55:ILE:HG22 | 1.92 | 0.51 |
| 46:B:79:C:H1' | 53:I:174:LYS:HB2 | 1.93 | 0.51 |
| 46:B:1517:C:O5' | 72:b:96:SER:OG | 2.27 | 0.51 |
| 46:B:1634:U:H2' | 46:B:1635:A:C8 | 2.46 | 0.51 |
| 46:B:1636:C:H2' | 46:B:1637:U:C6 | 2.46 | 0.51 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 47:C:10:THR:HG23 | 47:C:13:ASP:H | 1.76 | 0.51 |
| 49:E:96:VAL:HG22 | 49:E:110:ILE:HG12 | 1.93 | 0.51 |
| 51:G:123:LEU:HD23 | 51:G:159:THR:HG21 | 1.91 | 0.51 |
| 52:H:80:LYS:HB2 | 52:H:83:ARG:HH11 | 1.76 | 0.51 |
| 63:S:21:VAL:HG22 | 63:S:64:ILE:HG12 | 1.92 | 0.51 |
| 1:AS:945:C:O2' | 1:AS:967:G:OP1 | 2.22 | 0.51 |
| 1:AS:1251:C:H2' | 1:AS:1252:G:C8 | 2.46 | 0.51 |
| 1:AS:1539:G:OP1 | 16:BI:35:VAL:N | 2.42 | 0.51 |
| 1:AS:2498:A:H2' | 1:AS:2499:U:C6 | 2.45 | 0.51 |
| 1:AS:2919:G:N3 | 5:AX:250:ALA:HB1 | 2.25 | 0.51 |
| 1:AS:3023:U:C2 | 1:AS:3024:G:C8 | 2.98 | 0.51 |
| 9:BB:108:GLN:HG2 | 9:BB:109:ILE:N | 2.25 | 0.51 |
| 12:BE:194:GLY:C | 12:BE:196:TYR:H | 2.18 | 0.51 |
| 14:BG:127:ASP:OD1 | 14:BG:128:LYS:N | 2.38 | 0.51 |
| 45:CL:129:LEU:HA | 45:CL:132:GLU:OE1 | 2.11 | 0.51 |
| 46:CM:1298:A:N3 | 46:CM:1300:U:H5' | 2.25 | 0.51 |
| 46:CM:1410:A:C2' | 49:CP:87:ALA:HB3 | 2.35 | 0.51 |
| 46:CM:1460:G:H2' | 46:CM:1461:A:C8 | 2.45 | 0.51 |
| 46:CM:1512:A:H2' | 46:CM:1513:A:C8 | 2.44 | 0.51 |
| 50:CQ:172:ALA:HB1 | 50:CQ:174:ARG:NH1 | 2.25 | 0.51 |
| 59:CZ:63:CYS:HA | 59:CZ:91:VAL:O | 2.10 | 0.51 |
| 67:DH:43:ASN:HD21 | 67:DH:105:ILE:HG21 | 1.76 | 0.51 |
| 1:1:2477:U:H2' | 1:1:2478:A:H8 | 1.75 | 0.51 |
| 1:1:2482:U:C2' | 1:1:2483:U:H5' | 2.41 | 0.51 |
| 1:1:2719:A:H2' | 1:1:2720:A:C8 | 2.46 | 0.51 |
| 1:1:2729:U:H4' | 22:2:7:TYR:HB3 | 1.92 | 0.51 |
| 2:3:4:U:H2' | 2:3:5:G:C8 | 2.45 | 0.51 |
| 3:4:36:G:OP1 | 38:AK:66:TYR:OH | 2.19 | 0.51 |
| 4:j:117:GLU:OE2 | 4:j:163:ARG:NE | 2.43 | 0.51 |
| 21:0:42:TRP:O | 21:0:46:GLN:HG3 | 2.10 | 0.51 |
| 45:i:52:LYS:C | 45:i:54:LYS:H | 2.17 | 0.51 |
| 46:B:1187:A:N6 | 46:B:1443:C:O5' | 2.44 | 0.51 |
| 49:E:97:VAL:HG11 | 49:E:124:ILE:HG12 | 1.92 | 0.51 |
| 67:W:32:GLN:OE1 | 67:W:32:GLN:N | 2.44 | 0.51 |
| 1:AS:629:A:H2' | 1:AS:630:G:C8 | 2.46 | 0.51 |
| 1:AS:820:C:H5" | 4:AW:21:ARG:HD3 | 1.91 | 0.51 |
| 14:BG:115:ARG:NH2 | 14:BG:147:PHE:O | 2.40 | 0.51 |
| 36:CC:105:ARG:HG3 | 36:CC:108:ARG:HH21 | 1.75 | 0.51 |
| 44:CK:28:LYS:O | 44:CK:32:GLN:HG3 | 2.10 | 0.51 |
| 45:CL:101:LYS:HD3 | 46:CM:573:C:H4' | 1.92 | 0.51 |
| 46:CM:449:G:H2' | 46:CM:451:C:C5 | 2.46 | 0.51 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 50:CQ:114:LEU:HD23 | 50:CQ:118:ARG:HD3 | 1.91 | 0.51 |
| 66:DG:57:ARG:NH2 | 66:DG:101:ASN:OD1 | 2.40 | 0.51 |
| 72:DM:64:VAL:HG13 | 72:DM:68:ARG:HH21 | 1.75 | 0.51 |
| 81:12:111:GLU:O | 81:12:115:LYS:N | 2.40 | 0.51 |
| 82:l1:93:LEU:HG | 82:l1:94:ASN:H | 1.76 | 0.51 |
| 1:1:541:U:H3 | 1:1:543:C:HO2' | 1.59 | 0.51 |
| 1:1:1383:G:O6 | 6:l:187:LYS:HD3 | 2.11 | 0.51 |
| 1:1:3060:G:OP1 | 5:k:313:ARG:NH1 | 2.44 | 0.51 |
| 5:k:77:THR:HG21 | 5:k:328:ILE:HG12 | 1.93 | 0.51 |
| 13:s:148:ILE:HG23 | 13:s:152:HIS:HB3 | 1.92 | 0.51 |
| 46:B:82:U:H2' | 46:B:83:G:O4' | 2.11 | 0.51 |
| 46:B:87:C:O2' | 46:B:167:A:N1 | 2.41 | 0.51 |
| 46:B:441:C:OP2 | 71:a:105:ARG:HB2 | 2.10 | 0.51 |
| 46:B:1515:U:H2' | 46:B:1516:C:C6 | 2.45 | 0.51 |
| 53:I:116:GLN:NE2 | 53:I:125:THR:HB | 2.26 | 0.51 |
| 61:Q:13:ARG:N | 61:Q:24:HIS:O | 2.41 | 0.51 |
| 1:AS:2342:G:H22 | 1:AS:2374:G:H1' | 1.75 | 0.51 |
| 1:AS:3039:C:OP2 | 20:BM:62:ARG:NH2 | 2.44 | 0.51 |
| 28:BU:34:LYS:O | 28:BU:35:SER:OG | 2.20 | 0.51 |
| 46:CM:255:A:H1' | 55:CV:73:SER:HB2 | 1.91 | 0.51 |
| 48:CO:27:LYS:HD2 | 48:CO:47:LEU:HD13 | 1.91 | 0.51 |
| 48:CO:168:MET:O | 48:CO:172:MET:HG3 | 2.11 | 0.51 |
| 49:CP:96:VAL:HG22 | 49:CP:110:ILE:HG12 | 1.91 | 0.51 |
| 80:p0:92:ASP:HB3 | 80:p0:94:LYS:HG2 | 1.91 | 0.51 |
| 1:1:216:U:H4' | 27:9:100:HIS:CD2 | 2.45 | 0.51 |
| 1:1:1104:U:H2' | 1:1:1105:U:C6 | 2.45 | 0.51 |
| 1:1:2330:A:H5" | 18:x:83:TRP:O | 2.11 | 0.51 |
| 3:4:142:C:H2' | 3:4:143:U:C6 | 2.45 | 0.51 |
| 5:k:260:VAL:HG11 | 5:k:266:ARG:NH1 | 2.25 | 0.51 |
| 29:AB:75:LEU:HD22 | 29:AB:118:LEU:HD11 | 1.92 | 0.51 |
| 46:B:473:A:OP1 | 56:L:126:ARG:HD3 | 2.10 | 0.51 |
| 63:S:30:ILE:HG12 | 63:S:35:ILE:HG22 | 1.92 | 0.51 |
| 1:AS:164:U:H2' | 1:AS:165:C:C6 | 2.45 | 0.51 |
| 1:AS:422:A:C2 | 1:AS:2341:A:H4' | 2.46 | 0.51 |
| 1:AS:437:G:O2' | 1:AS:438:A:H5" | 2.11 | 0.51 |
| 1:AS:1023:A:N6 | 1:AS:1025:G:N3 | 2.59 | 0.51 |
| 1:AS:1057:A:O2' | 22:BO:102:ARG:NH2 | 2.44 | 0.51 |
| 1:AS:1058:A:O2' | 22:BO:108:ARG:NH2 | 2.43 | 0.51 |
| 1:AS:1245:G:H2' | 1:AS:1246:G:H8 | 1.74 | 0.51 |
| 1:AS:1762:G:O2' | 1:AS:1763:C:OP1 | 2.27 | 0.51 |
| 1:AS:2084:A:H2' | 1:AS:2085:A:H8 | 1.76 | 0.51 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 1:AS:2090:U:H4' | 1:AS:2091:A:O5' | 2.10 | 0.51 |
| 1:AS:2961:U:O2' | 5:AX:232:ARG:NH1 | 2.43 | 0.51 |
| 9:BB:8:GLU:HG3 | 9:BB:9:THR:N | 2.26 | 0.51 |
| 13:BF:86:VAL:HG21 | 13:BF:112:LEU:HD22 | 1.91 | 0.51 |
| 46:CM:1127:A:H5" | 73:DN:2:PRO:HB3 | 1.93 | 0.51 |
| 46:CM:1281:A:OP1 | 47:CN:138:TYR:OH | 2.29 | 0.51 |
| 46:CM:1595:U:O3' | 63:DD:72:GLY:HA3 | 2.11 | 0.51 |
| 72:DM:65:LEU:HD13 | 72:DM:69:LEU:HD12 | 1.93 | 0.51 |
| 79:DT:214:ASP:N | 79:DT:214:ASP:OD1 | 2.43 | 0.51 |
| 82:L1:73:ASP:CG | 82:L1:113:SER:HB2 | 2.36 | 0.51 |
| 1:1:694:C:OP2 | 6:l:120:ARG:NH2 | 2.41 | 0.51 |
| 1:1:1931:G:O2' | 46:B:1654:A:O2' | 2.29 | 0.51 |
| 1:1:2408:A:H2' | 1:1:2409:C:H6 | 1.74 | 0.51 |
| 2:3:65:G:O3' | 12:r:204:GLY:HA2 | 2.11 | 0.51 |
| 10:p:145:GLU:OE1 | 37:AJ:35:ARG:NH1 | 2.44 | 0.51 |
| 46:B:30:G:H2' | 46:B:31:C:C6 | 2.46 | 0.51 |
| 49:E:138:TYR:OH | 49:E:144:GLY:O | 2.26 | 0.51 |
| 79:AR:214:ASP:OD1 | 79:AR:214:ASP:N | 2.43 | 0.51 |
| 1:AS:714:A:OP1 | 29:BV:137:LYS:NZ | 2.42 | 0.51 |
| 1:AS:1275:C:H2' | 1:AS:1276:C:H6 | 1.75 | 0.51 |
| 1:AS:1691:U:O2' | 1:AS:1745:A:N1 | 2.35 | 0.51 |
| 1:AS:2385:C:H2' | 1:AS:2386:U:C6 | 2.46 | 0.51 |
| 32:BY:54:LEU:HA | 32:BY:94:PRO:HG3 | 1.93 | 0.51 |
| 46:CM:15:U:H2' | 46:CM:16:G:O4' | 2.11 | 0.51 |
| 46:CM:335:G:H3' | 58:CY:133:LYS:HB2 | 1.92 | 0.51 |
| 46:CM:398:A:H5" | 55:CV:25:ARG:HA | 1.92 | 0.51 |
| 46:CM:1092:G:O2' | 46:CM:1093:G:H5' | 2.11 | 0.51 |
| 46:CM:1149:G:O2' | 46:CM:1599:U:O2 | 2.22 | 0.51 |
| 47:CN:205:ARG:NH2 | 64:DE:84:TYR:HB3 | 2.26 | 0.51 |
| 72:DM:46:LYS:NZ | 72:DM:69:LEU:O | 2.36 | 0.51 |
| 1:1:33:A:N3 | 1:1:806:A:O2' | 2.42 | 0.51 |
| 1:1:164:U:H2' | 1:1:165:C:C6 | 2.46 | 0.51 |
| 1:1:273:A:H2' | 1:1:274:G:H8 | 1.76 | 0.51 |
| 1:1:834:G:O6 | 44:AQ:4:ARG:NH2 | 2.44 | 0.51 |
| 1:1:868:U:H2' | 1:1:869:C:C6 | 2.45 | 0.51 |
| 1:1:1116:A:H2' | 1:1:1117:U:H6 | 1.75 | 0.51 |
| 1:1:2084:A:H2' | 1:1:2085:A:C8 | 2.46 | 0.51 |
| 25:7:13:ILE:HD12 | 25:7:30:ARG:HB3 | 1.93 | 0.51 |
| 25:7:85:ALA:HB1 | 25:7:89:LEU:HD22 | 1.93 | 0.51 |
| 26:8:75:LYS:HB3 | 26:8:81:THR:CG2 | 2.41 | 0.51 |
| 46:B:452:A:O4' | 51:G:66:MET:HG3 | 2.11 | 0.51 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 46:B:870:G:H2' | 46:B:871:U:C6 | 2.46 | 0.51 |
| 77:g:43:ARG:HG2 | 77:g:54:ARG:NH2 | 2.26 | 0.51 |
| 1:AS:2116:A:C4 | 38:CE:3:LYS:HB3 | 2.46 | 0.51 |
| 1:AS:2525:A:H2' | 1:AS:2526:C:O4' | 2.11 | 0.51 |
| 1:AS:3208:A:OP1 | 17:BJ:160:LYS:NZ | 2.31 | 0.51 |
| 15:BH:20:LEU:HD21 | 15:BH:23:ASN:C | 2.35 | 0.51 |
| 27:BT:32:SER:HA | 27:BT:49:PRO:HA | 1.93 | 0.51 |
| 46:CM:78:A:H2' | 46:CM:79:C:H6 | 1.75 | 0.51 |
| 46:CM:338:U:H2' | 46:CM:339:A:H8 | 1.76 | 0.51 |
| 46:CM:674:C:H3' | 46:CM:675:U:C6 | 2.46 | 0.51 |
| 46:CM:1668:A:H2' | 46:CM:1669:U:H5' | 1.93 | 0.51 |
| 46:CM:1678:G:H3' | 46:CM:1679:A:H8 | 1.76 | 0.51 |
| 53:CT:104:GLN:OE1 | 53:CT:104:GLN:N | 2.44 | 0.51 |
| 55:CV:158:ILE:HA | 58:CY:24:LYS:HD3 | 1.92 | 0.51 |
| 68:DI:11:LEU:HD23 | 68:DI:11:LEU:H | 1.75 | 0.51 |
| 70:DK:59:ILE:HD12 | 70:DK:71:CYS:SG | 2.51 | 0.51 |
| 79:DT:159:PRO:HD3 | 79:DT:201:LEU:HD11 | 1.93 | 0.51 |
| 81:12:133:LEU:HB3 | 81:12:152:ILE:HG12 | 1.93 | 0.51 |
| 1:1:15:A:OP1 | 26:8:42:ARG:HG2 | 2.11 | 0.50 |
| 1:1:381:U:H2' | 1:1:382:U:C6 | 2.46 | 0.50 |
| 1:1:1249:U:OP2 | 1:1:1249:U:H2' | 2.12 | 0.50 |
| 1:1:1660:G:H2' | 1:1:1661:U:C6 | 2.46 | 0.50 |
| 25:7:107:SER:O | 25:7:111:LYS:HG2 | 2.11 | 0.50 |
| 46:B:115:G:H5' | 58:N:129:ARG:HD3 | 1.93 | 0.50 |
| 46:B:217:A:N7 | 46:B:218:A:C8 | 2.79 | 0.50 |
| 46:B:871:U:C2 | 46:B:872:A:C8 | 2.98 | 0.50 |
| 46:B:1214:G:N2 | 46:B:1240:G:O2' | 2.44 | 0.50 |
| 52:H:55:ASP:OD1 | 52:H:57:SER:OG | 2.27 | 0.50 |
| 59:O:96:LEU:HD12 | 59:O:100:TRP:CZ3 | 2.46 | 0.50 |
| 79:AR:240:LEU:HD22 | 79:AR:249:LEU:HD11 | 1.92 | 0.50 |
| 1:AS:675:A:N6 | 1:AS:782:A:O4' | 2.44 | 0.50 |
| 1:AS:1116:A:H2' | 1:AS:1117:U:H6 | 1.76 | 0.50 |
| 1:AS:1245:G:O2' | 1:AS:1246:G:OP1 | 2.25 | 0.50 |
| 1:AS:1708:G:N2 | 1:AS:1729:G:O6 | 2.44 | 0.50 |
| 1:AS:2992:U:H2' | 1:AS:3005:A:N6 | 2.26 | 0.50 |
| 6:AY:260:ASP:OD1 | 6:AY:265:SER:HB3 | 2.09 | 0.50 |
| 46:CM:561:U:H4' | 77:DR:17:GLN:OE1 | 2.11 | 0.50 |
| 50:CQ:95:ARG:O | 50:CQ:102:GLN:NE2 | 2.40 | 0.50 |
| 52:CS:109:LYS:HG2 | 52:CS:112:ARG:NH2 | 2.26 | 0.50 |
| 59:CZ:137:LEU:HA | 59:CZ:140:PHE:CZ | 2.45 | 0.50 |
| 63:DD:11:LYS:HG2 | 63:DD:16:THR:HG22 | 1.92 | 0.50 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 73:DN:12:LYS:HA | 73:DN:15:ARG:NH1 | 2.26 | 0.50 |
| 73:DN:35:ALA:O | 73:DN:37:LYS:HD3 | 2.11 | 0.50 |
| 82:L1:76:ARG:HH22 | 82:L1:142:ASP:HB2 | 1.76 | 0.50 |
| 82:l1:35:GLN:HB2 | 82:l1:205:VAL:HB | 1.93 | 0.50 |
| 1:1:907:C:OP1 | 4:j:14:SER:OG | 2.28 | 0.50 |
| 1:1:1258:G:O6 | 1:1:1260:G:N2 | 2.44 | 0.50 |
| 1:1:2197:A:H2' | 1:1:2198:A:H8 | 1.76 | 0.50 |
| 1:1:2206:A:H2' | 1:1:2207:A:H8 | 1.72 | 0.50 |
| 1:1:2632:G:O3' | 1:1:2721:G:N2 | 2.45 | 0.50 |
| 7:m:95:TRP:HD1 | 7:m:158:ARG:HA | 1.76 | 0.50 |
| 46:B:1074:U:O2' | 46:B:1078:A:N1 | 2.44 | 0.50 |
| 46:B:1149:G:H2' | 46:B:1150:G:H8 | 1.75 | 0.50 |
| 46:B:1317:C:O2' | 50:F:163:GLN:HB3 | 2.11 | 0.50 |
| 46:B:1659:G:H2' | 46:B:1660:G:H8 | 1.75 | 0.50 |
| 65:U:69:ILE:HG22 | 65:U:73:MET:HE2 | 1.93 | 0.50 |
| 1:AS:783:G:H2' | 1:AS:784:C:H6 | 1.76 | 0.50 |
| 1:AS:981:U:H2' | 1:AS:982:U:H6 | 1.77 | 0.50 |
| 1:AS:1007:A:H2' | 1:AS:1008:A:H8 | 1.76 | 0.50 |
| 1:AS:1302:G:C6 | 17:BJ:63:THR:HA | 2.46 | 0.50 |
| 1:AS:2447:G:H1' | 1:AS:2466:A:H2 | 1.76 | 0.50 |
| 20:BM:134:HIS:HE1 | 20:BM:136:ARG:NE | 2.09 | 0.50 |
| 27:BT:58:VAL:HA | 27:BT:104:VAL:HG12 | 1.93 | 0.50 |
| 46:CM:149:G:O6 | 71:DL:124:ARG:NH2 | 2.44 | 0.50 |
| 52:CS:112:ARG:HH11 | 72:DM:95:HIS:CE1 | 2.29 | 0.50 |
| 63:DD:21:VAL:HG22 | 63:DD:64:ILE:HG12 | 1.93 | 0.50 |
| 64:DE:69:ILE:O | 64:DE:69:ILE:HG13 | 2.10 | 0.50 |
| 1:1:1758:U:O2' | 1:1:1759:U:O2 | 2.20 | 0.50 |
| 1:1:2872:A:H5' | 41:AN:51:LEU:HD21 | 1.94 | 0.50 |
| 1:1:3091:U:H4' | 41:AN:28:PRO:HG2 | 1.92 | 0.50 |
| 4:j:140:ASN:ND2 | 4:j:143:GLU:OE1 | 2.44 | 0.50 |
| 6:l:326:LEU:O | 9:o:39:ARG:NH2 | 2.40 | 0.50 |
| 17:w:11:ASP:HB2 | 17:w:118:ARG:HB3 | 1.92 | 0.50 |
| 22:2:45:ASN:OD1 | 22:2:47:SER:OG | 2.21 | 0.50 |
| 23:5:19:VAL:C | 23:5:21:ALA:H | 2.20 | 0.50 |
| 34:AG:68:TRP:O | 34:AG:86:LYS:HG2 | 2.11 | 0.50 |
| 46:B:518:A:O2' | 46:B:519:A:OP1 | 2.26 | 0.50 |
| 46:B:718:A:H4' | 46:B:719:A:C6 | 2.46 | 0.50 |
| 46:B:1064:U:H2' | 46:B:1065:U:C6 | 2.45 | 0.50 |
| 46:B:1219:A:O2' | 78:h:182:TYR:OH | 2.25 | 0.50 |
| 46:B:1455:A:H2' | 46:B:1456:C:C6 | 2.46 | 0.50 |
| 62:R:14:GLN:OE1 | 62:R:22:LEU:N | 2.43 | 0.50 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 1:AS:814:C:H2' | 1:AS:815:U:O4' | 2.11 | 0.50 |
| 1:AS:2655:U:H2' | 1:AS:2656:C:H6 | 1.71 | 0.50 |
| 3:AU:9:A:H2' | 3:AU:10:A:H8 | 1.75 | 0.50 |
| 6:AY:6:GLN:HB2 | 6:AY:20:GLN:OE1 | 2.11 | 0.50 |
| 33:BZ:33:TRP:CH2 | 33:BZ:53:GLN:HG2 | 2.46 | 0.50 |
| 57:CX:12:HIS:HB3 | 57:CX:80:LEU:HD21 | 1.93 | 0.50 |
| 82:L1:43:PRO:HB3 | 82:L1:161:LYS:HA | 1.93 | 0.50 |
| 1:1:583:A:H2' | 1:1:584:C:C6 | 2.47 | 0.50 |
| 1:1:3344:U:H4' | 5:k:315:GLY:HA2 | 1.92 | 0.50 |
| 12:r:179:ASP:OD1 | 12:r:180:GLU:N | 2.44 | 0.50 |
| 29:AB:76:ASP:OD1 | 29:AB:76:ASP:N | 2.44 | 0.50 |
| 29:AB:104:THR:OG1 | 29:AB:126:LYS:O | 2.26 | 0.50 |
| 46:B:296:C:H5" | 51:G:38:LEU:HB2 | 1.94 | 0.50 |
| 46:B:671:G:H5' | 46:B:672:U:OP2 | 2.11 | 0.50 |
| 46:B:904:A:H2' | 46:B:905:C:C6 | 2.46 | 0.50 |
| 46:B:1469:A:OP2 | 46:B:1508:G:N2 | 2.40 | 0.50 |
| 59:O:32:LEU:O | 59:O:36:LEU:N | 2.39 | 0.50 |
| 1:AS:46:C:H5" | 14:BG:16:LYS:HG2 | 1.93 | 0.50 |
| 1:AS:179:C:H2' | 1:AS:180:U:H6 | 1.75 | 0.50 |
| 1:AS:1911:A:H2' | 1:AS:1912:U:C6 | 2.46 | 0.50 |
| 1:AS:1949:G:H1 | 1:AS:2070:A:H2' | 1.77 | 0.50 |
| 1:AS:2220:A:H5" | 4:AW:244:GLY:HA3 | 1.92 | 0.50 |
| 1:AS:2659:G:H4' | 7:AZ:7:PHE:CE2 | 2.46 | 0.50 |
| 3:AU:10:A:H2' | 3:AU:11:C:C6 | 2.46 | 0.50 |
| 46:CM:577:A:H2' | 50:CQ:144:ARG:HH22 | 1.75 | 0.50 |
| 46:CM:871:U:C2 | 46:CM:872:A:C8 | 2.99 | 0.50 |
| 46:CM:1231:C:O3' | 78:DS:134:LYS:NZ | 2.41 | 0.50 |
| 46:CM:1582:U:H5' | 46:CM:1583:C:OP2 | 2.11 | 0.50 |
| 55:CV:172:TYR:HB3 | 55:CV:190:LEU:HD12 | 1.92 | 0.50 |
| 79:DT:90:LEU:HB2 | 79:DT:104:PHE:HB2 | 1.93 | 0.50 |
| 82:l1:128:LEU:O | 82:l1:130:LYS:N | 2.44 | 0.50 |
| 1:1:1058:A:O2' | 22:2:108:ARG:NH2 | 2.44 | 0.50 |
| 1:1:1325:U:O3' | 34:AG:19:SER:OG | 2.29 | 0.50 |
| 1:1:2628:A:P | 43:AP:97:LYS:HD3 | 2.52 | 0.50 |
| 1:1:2766:G:N3 | 84:1:3402:3K5:H1 | 2.27 | 0.50 |
| 1:1:3285:A:H2' | 1:1:3286:C:C6 | 2.46 | 0.50 |
| 3:4:21:C:H5" | 6:l:195:LEU:HD21 | 1.94 | 0.50 |
| 3:4:37:A:H5" | 3:4:39:G:O4' | 2.12 | 0.50 |
| 11:q:10:LEU:HD21 | 11:q:79:ILE:CD1 | 2.41 | 0.50 |
| 45:i:42:ALA:HB3 | 45:i:43:PRO:HD3 | 1.94 | 0.50 |
| 46:B:1132:A:H2' | 46:B:1133:C:C6 | 2.47 | 0.50 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 46:B:1656:U:H2' | 46:B:1657:G:O4' | 2.10 | 0.50 |
| 49:E:53:LEU:O | 68:X:15:ARG:NE | 2.45 | 0.50 |
| 1:AS:1662:G:H1 | 1:AS:1779:U:H3 | 1.59 | 0.50 |
| 4:AW:96:LEU:O | 44:CK:87:ARG:HD3 | 2.12 | 0.50 |
| 40:CG:24:PRO:HG2 | 40:CG:27:ILE:HD12 | 1.93 | 0.50 |
| 46:CM:12:U:H2' | 46:CM:13:C:H6 | 1.73 | 0.50 |
| 46:CM:932:U:H2' | 46:CM:933:A:H8 | 1.77 | 0.50 |
| 46:CM:1573:A:H2' | 46:CM:1574:A:O4' | 2.11 | 0.50 |
| 1:1:169:G:N2 | 1:1:248:U:O2 | 2.44 | 0.50 |
| 1:1:849:G:OP2 | 44:AQ:2:THR:HG21 | 2.10 | 0.50 |
| 1:1:1807:G:H2' | 1:1:1808:G:O4' | 2.11 | 0.50 |
| 1:1:2130:A:HO2' | 1:1:2221:A:HO2' | 1.49 | 0.50 |
| 8:n:39:LEU:HD13 | 8:n:83:VAL:HG11 | 1.93 | 0.50 |
| 8:n:59:ASP:HB2 | 8:n:102:VAL:HG22 | 1.94 | 0.50 |
| 26:8:105:VAL:HG23 | 26:8:130:TYR:CG | 2.47 | 0.50 |
| 46:B:265:U:H2' | 46:B:266:C:H6 | 1.76 | 0.50 |
| 46:B:684:C:H2' | 46:B:685:C:C6 | 2.47 | 0.50 |
| 46:B:1145:A:H2' | 46:B:1146:C:C6 | 2.47 | 0.50 |
| 52:H:113:ILE:HG23 | 52:H:191:ALA:HA | 1.93 | 0.50 |
| 57:M:77:ARG:NE | 57:M:86:ILE:HG22 | 2.27 | 0.50 |
| 79:AR:152:VAL:HA | 79:AR:170:SER:HA | 1.94 | 0.50 |
| 1:AS:559:C:H2' | 1:AS:560:C:H6 | 1.76 | 0.50 |
| 1:AS:1225:G:H2' | 1:AS:1226:G:C8 | 2.46 | 0.50 |
| 1:AS:1330:U:H2' | 1:AS:1331:U:C6 | 2.47 | 0.50 |
| 1:AS:1556:G:O2' | 1:AS:1557:U:H5' | 2.11 | 0.50 |
| 1:AS:2251:G:H22 | 1:AS:2290:A:P | 2.34 | 0.50 |
| 1:AS:2426:G:O6 | 1:AS:2477:U:O2 | 2.29 | 0.50 |
| 1:AS:3309:A:N6 | 1:AS:3326:G:O2' | 2.40 | 0.50 |
| 14:BG:141:VAL:HG21 | 36:CC:118:ILE:HB | 1.94 | 0.50 |
| 19:BL:125:ASP:OD1 | 19:BL:126:GLN:N | 2.45 | 0.50 |
| 46:CM:477:C:H5' | 56:CW:124:HIS:HD1 | 1.77 | 0.50 |
| 46:CM:1279:G:O2' | 46:CM:1306:A:N1 | 2.42 | 0.50 |
| 46:CM:1335:U:O2' | 46:CM:1336:G:OP1 | 2.28 | 0.50 |
| 57:CX:80:LEU:HB3 | 57:CX:82:ILE:HG23 | 1.94 | 0.50 |
| 82:L1:48:ARG:NH1 | 82:L1:161:LYS:H | 2.10 | 0.50 |
| 1:1:1469:G:H5" | 20:z:23:TRP:CD1 | 2.47 | 0.50 |
| 1:1:1632:C:OP1 | 28:AA:36:HIS:NE2 | 2.44 | 0.50 |
| 1:1:2391:A:H2' | 1:1:2392:G:C8 | 2.47 | 0.50 |
| 1:1:3244:A:O2' | 1:1:3245:A:H5' | 2.12 | 0.50 |
| 6:l:181:LYS:O | 6:l:185:SER:HB3 | 2.12 | 0.50 |
| 28:AA:23:VAL:HG12 | 28:AA:45:GLY:HA3 | 1.94 | 0.50 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 46:B:1277:G:H21 | 47:C:111:ILE:HD11 | 1.77 | 0.50 |
| 46:B:1487:C:OP1 | 66:V:122:ARG:NH2 | 2.41 | 0.50 |
| 46:B:1584:A:C8 | 76:f:14:PHE:HD1 | 2.30 | 0.50 |
| 46:B:1750:A:H5" | 46:B:1758:U:H5" | 1.93 | 0.50 |
| 52:H:32:ASP:OD1 | 52:H:33:VAL:N | 2.45 | 0.50 |
| 64:T:77:GLU:O | 64:T:81:LYS:HB2 | 2.11 | 0.50 |
| 1:AS:1561:U:H5" | 1:AS:1561:U:C6 | 2.47 | 0.50 |
| 1:AS:1923:G:N7 | 44:CK:16:VAL:HG13 | 2.27 | 0.50 |
| 1:AS:1937:C:H2' | 1:AS:1938:U:C6 | 2.46 | 0.50 |
| 1:AS:3138:U:H2' | 1:AS:3139:U:C6 | 2.47 | 0.50 |
| 5:AX:117:ARG:HD2 | 5:AX:176:ALA:O | 2.11 | 0.50 |
| 6:AY:300:VAL:HB | 19:BL:39:ARG:HG2 | 1.92 | 0.50 |
| 46:CM:643:U:H2' | 46:CM:644:U:O4' | 2.11 | 0.50 |
| 46:CM:673:A:C5 | 46:CM:674:C:C4 | 3.00 | 0.50 |
| 49:CP:171:LYS:HE2 | 56:CW:57:ARG:CZ | 2.42 | 0.50 |
| 55:CV:38:ILE:HG12 | 55:CV:96:LEU:HD11 | 1.94 | 0.50 |
| 59:CZ:82:PRO:HG3 | 59:CZ:85:LYS:CA | 2.42 | 0.50 |
| 79:DT:41:THR:HG22 | 79:DT:42:LEU:N | 2.26 | 0.50 |
| 81:12:104:ILE:HD12 | 81:12:109:ILE:HD13 | 1.93 | 0.50 |
| 1:1:671:U:H2' | 1:1:672:G:C8 | 2.47 | 0.50 |
| 1:1:2285:G:O2' | 1:1:2288:U:OP2 | 2.30 | 0.50 |
| 3:4:9:A:H2' | 3:4:10:A:H8 | 1.73 | 0.50 |
| 3:4:83:U:O2 | 27:9:51:ARG:NH2 | 2.45 | 0.50 |
| 18:x:29:THR:HA | 18:x:32:THR:HG22 | 1.93 | 0.50 |
| 23:5:16:VAL:HG12 | 23:5:65:VAL:HG22 | 1.93 | 0.50 |
| 24:6:36:VAL:HG22 | 24:6:58:VAL:HG11 | 1.94 | 0.50 |
| 46:B:261:C:H4' | 46:B:290:U:H5' | 1.94 | 0.50 |
| 46:B:336:C:H5" | 55:K:10:LYS:HD2 | 1.93 | 0.50 |
| 46:B:701:G:C2' | 46:B:702:G:H2' | 2.35 | 0.50 |
| 46:B:822:G:H3' | 46:B:823:G:C5' | 2.42 | 0.50 |
| 46:B:1219:A:OP2 | 46:B:1230:G:O2' | 2.25 | 0.50 |
| 67:W:68:LYS:HE2 | 67:W:79:ASP:OD1 | 2.12 | 0.50 |
| 79:AR:69:VAL:HA | 79:AR:85:SER:HA | 1.92 | 0.50 |
| 1:AS:605:U:OP2 | 8:BA:21:ARG:HG2 | 2.11 | 0.50 |
| 2:AT:92:A:O2' | 12:BE:57:LEU:O | 2.29 | 0.50 |
| 17:BJ:126:ARG:HG2 | 17:BJ:130:LEU:HD12 | 1.92 | 0.50 |
| 46:CM:873:U:H2' | 46:CM:874:U:C6 | 2.47 | 0.50 |
| 46:CM:1698:U:C2' | 46:CM:1699:G:H4' | 2.41 | 0.50 |
| 70:DK:70:LYS:HB3 | 70:DK:93:LEU:HD22 | 1.94 | 0.50 |
| 79:DT:200:THR:HG21 | 79:DT:242:PHE:H | 1.77 | 0.50 |
| 82:l1:8:GLY:O | 82:l1:12:ASN:ND2 | 2.45 | 0.50 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 82:l1:175:GLU:HB3 | 82:l1:178:VAL:HG23 | 1.94 | 0.50 |
| 1:1:1059:G:N7 | 1:1:1093:G:O2' | 2.30 | 0.50 |
| 1:1:2852:U:H5" | 5:k:236:LYS:HG2 | 1.94 | 0.50 |
| 24:6:135:VAL:HG11 | 25:7:26:SER:HB3 | 1.93 | 0.50 |
| 45:i:93:ARG:HG2 | 46:B:1259:C:C5 | 2.47 | 0.50 |
| 46:B:345:G:H5" | 58:N:80:MET:HE2 | 1.93 | 0.50 |
| 46:B:1349:G:H21 | 66:V:3:GLY:H | 1.60 | 0.50 |
| 46:B:1573:A:H2' | 46:B:1574:A:O4' | 2.12 | 0.50 |
| 64:T:71:PHE:HZ | 64:T:74:GLN:HE21 | 1.60 | 0.50 |
| 68:X:73:ALA:HB1 | 68:X:78:LEU:HB2 | 1.94 | 0.50 |
| 79:AR:16:HIS:CD2 | 79:AR:43:ILE:HD12 | 2.45 | 0.50 |
| 1:AS:493:A:O2' | 1:AS:3238:A:N1 | 2.39 | 0.50 |
| 1:AS:619:A:H2' | 1:AS:620:A:N7 | 2.27 | 0.50 |
| 1:AS:976:A:C2' | 1:AS:977:U:H5' | 2.42 | 0.50 |
| 1:AS:3290:G:O3' | 32:BY:102:GLY:HA2 | 2.11 | 0.50 |
| 46:CM:656:C:H2' | 46:CM:657:C:C6 | 2.47 | 0.50 |
| 46:CM:1325:U:O4 | 63:DD:8:THR:HA | 2.12 | 0.50 |
| 46:CM:1677:G:H3' | 46:CM:1679:A:N6 | 2.26 | 0.50 |
| 59:CZ:53:SER:HB2 | 78:DS:158:ARG:HH21 | 1.77 | 0.50 |
| 82:l1:26:ARG:HH21 | 82:l1:29:LEU:C | 2.19 | 0.50 |
| 1:1:393:U:H2' | 1:1:394:G:O4' | 2.11 | 0.49 |
| 1:1:547:U:H2' | 1:1:548:G:H8 | 1.75 | 0.49 |
| 1:1:590:A:H5' | 8:n:16:ALA:O | 2.11 | 0.49 |
| 1:1:1921:U:O2' | 1:1:1923:G:N7 | 2.45 | 0.49 |
| 1:1:2854:U:H2' | 1:1:2855:U:C6 | 2.47 | 0.49 |
| 5:k:212:ASP:OD2 | 5:k:354:VAL:N | 2.21 | 0.49 |
| 19:y:76:ALA:HA | 19:y:79:LYS:HG3 | 1.93 | 0.49 |
| 31:AD:26:THR:HB | 31:AD:31:SER:HB3 | 1.94 | 0.49 |
| 46:B:4:C:H4' | 49:E:176:SER:HB3 | 1.94 | 0.49 |
| 46:B:17:C:O2' | 46:B:1122:A:N1 | 2.42 | 0.49 |
| 46:B:180:A:H2' | 46:B:181:U:C6 | 2.47 | 0.49 |
| 46:B:385:A:OP1 | 55:K:23:LYS:HE3 | 2.12 | 0.49 |
| 52:H:80:LYS:HB2 | 52:H:83:ARG:NH1 | 2.27 | 0.49 |
| 1:AS:606:A:C5 | 8:BA:21:ARG:HD3 | 2.47 | 0.49 |
| 1:AS:1246:G:H2' | 1:AS:1247:A:C8 | 2.47 | 0.49 |
| 1:AS:1580:U:H2' | 1:AS:1581:C:C6 | 2.47 | 0.49 |
| 1:AS:2434:A:N6 | 1:AS:2439:A:H62 | 2.09 | 0.49 |
| 1:AS:2871:C:O2' | 1:AS:2873:G:OP2 | 2.22 | 0.49 |
| 1:AS:3019:U:O2' | 1:AS:3020:A:H5' | 2.11 | 0.49 |
| 1:AS:3079:U:H2' | 1:AS:3080:G:C8 | 2.47 | 0.49 |
| 39:CF:30:LYS:HB3 | 39:CF:38:PHE:CE2 | 2.47 | 0.49 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 46:CM:822:G:H8 | 46:CM:822:G:O5' | 1.95 | 0.49 |
| 46:CM:872:A:H1' | 61:DB:117:PRO:HB3 | 1.94 | 0.49 |
| 46:CM:1204:A:N3 | 57:CX:51:SER:OG | 2.42 | 0.49 |
| 46:CM:1455:A:H2' | 46:CM:1456:C:C6 | 2.47 | 0.49 |
| 50:CQ:24:GLU:OE1 | 76:DQ:23:HIS:HE1 | 1.95 | 0.49 |
| 63:DD:89:VAL:HG13 | 63:DD:101:LYS:HG2 | 1.94 | 0.49 |
| 81:12:103:ASN:HB2 | 81:12:142:ARG:O | 2.13 | 0.49 |
| 1:1:1007:A:H2' | 1:1:1008:A:C8 | 2.48 | 0.49 |
| 2:3:13:A:C2 | 7:m:21:ARG:HB2 | 2.47 | 0.49 |
| 3:4:29:U:H5" | 14:t:27:ASP:HB3 | 1.94 | 0.49 |
| 4:j:80:GLU:HG3 | 44:AQ:66:GLY:HA2 | 1.93 | 0.49 |
| 7:m:160:PHE:O | 7:m:163:LEU:HB3 | 2.11 | 0.49 |
| 9:o:135:GLY:HA3 | 9:o:233:ILE:HB | 1.94 | 0.49 |
| 18:x:40:LYS:HD2 | 18:x:113:VAL:HG22 | 1.94 | 0.49 |
| 28:AA:15:ARG:HD2 | 28:AA:79:HIS:CD2 | 2.47 | 0.49 |
| 46:B:1241:A:H5' | 46:B:1242:U:C5 | 2.48 | 0.49 |
| 46:B:1337:C:H2' | 46:B:1338:U:O4' | 2.12 | 0.49 |
| 47:C:49:ASN:ND2 | 47:C:52:LYS:HG3 | 2.27 | 0.49 |
| 53:I:84:TYR:HE1 | 53:I:93:LYS:HE3 | 1.77 | 0.49 |
| 1:AS:152:U:H4' | 1:AS:157:G:H4' | 1.93 | 0.49 |
| 1:AS:1079:G:H2' | 1:AS:1080:A:H8 | 1.77 | 0.49 |
| 1:AS:1236:A:H3' | 1:AS:1237:U:C5 | 2.47 | 0.49 |
| 20:BM:39:SER:HA | 20:BM:42:ARG:HH11 | 1.78 | 0.49 |
| 20:BM:162:ARG:HA | 20:BM:165:ARG:HD3 | 1.93 | 0.49 |
| 25:BR:13:ILE:HG12 | 25:BR:32:GLN:HB2 | 1.94 | 0.49 |
| 45:CL:155:LEU:HA | 57:CX:92:LEU:HD21 | 1.94 | 0.49 |
| 46:CM:788:A:C8 | 69:DJ:107:SER:HA | 2.48 | 0.49 |
| 46:CM:1218:G:H22 | 46:CM:1238:U:H1' | 1.76 | 0.49 |
| 46:CM:1344:C:O2 | 66:DG:3:GLY:HA3 | 2.12 | 0.49 |
| 52:CS:116:HIS:CD2 | 72:DM:98:GLN:HB3 | 2.47 | 0.49 |
| 1:1:352:A:N1 | 1:1:365:A:H5" | 2.27 | 0.49 |
| 1:1:792:U:H2' | 1:1:793:U:C6 | 2.47 | 0.49 |
| 1:1:952:U:H2' | 1:1:953:C:C6 | 2.47 | 0.49 |
| 1:1:1017:G:H2' | 1:1:1018:U:C6 | 2.48 | 0.49 |
| 1:1:1230:G:H5" | 81:12:119:LYS:HE2 | 1.93 | 0.49 |
| 1:1:1377:A:H2' | 1:1:1378:G:H8 | 1.77 | 0.49 |
| 1:1:2668:A:H2' | 1:1:2669:A:C8 | 2.48 | 0.49 |
| 1:1:2852:U:H1' | 5:k:250:ALA:HB3 | 1.93 | 0.49 |
| 1:1:3313:G:H1 | 1:1:3322:U:H3 | 1.60 | 0.49 |
| 3:4:23:U:OP1 | 27:9:16:ARG:NH1 | 2.45 | 0.49 |
| 7:m:95:TRP:CD1 | 7:m:158:ARG:HA | 2.47 | 0.49 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 11:q:86:TYR:CE2 | 11:q:151:LEU:HB2 | 2.46 | 0.49 |
| 46:B:29:U:H2' | 46:B:30:G:C8 | 2.44 | 0.49 |
| 46:B:470:U:H5" | 56:L:11:THR:HG23 | 1.94 | 0.49 |
| 46:B:1546:G:N7 | 65:U:134:ARG:HD3 | 2.27 | 0.49 |
| 67:W:34:GLU:OE2 | 67:W:88:ARG:NH2 | 2.45 | 0.49 |
| 70:Z:107:PHE:CD2 | 70:Z:114:LYS:HD3 | 2.47 | 0.49 |
| 79:AR:263:GLN:O | 79:AR:264:GLU:HG2 | 2.13 | 0.49 |
| 1:AS:1345:G:N2 | 6:AY:292:ASN:O | 2.45 | 0.49 |
| 1:AS:1593:C:H2' | 1:AS:1594:G:H8 | 1.76 | 0.49 |
| 1:AS:2404:U:H2' | 1:AS:2405:U:C6 | 2.47 | 0.49 |
| 1:AS:3035:C:H2' | 1:AS:3036:U:C6 | 2.47 | 0.49 |
| 4:AW:112:ILE:HG13 | 44:CK:79:VAL:HG22 | 1.93 | 0.49 |
| 7:AZ:95:TRP:CD1 | 7:AZ:158:ARG:HA | 2.48 | 0.49 |
| 11:BD:48:ILE:HG22 | 11:BD:49:ASN:HD22 | 1.77 | 0.49 |
| 46:CM:623:C:H2' | 46:CM:624:U:C6 | 2.46 | 0.49 |
| 46:CM:815:U:O2' | 46:CM:816:U:H6 | 1.96 | 0.49 |
| 46:CM:1315:G:H2' | 46:CM:1316:A:C8 | 2.47 | 0.49 |
| 46:CM:1629:G:O6 | 86:CM:1902:HYG:N9 | 2.46 | 0.49 |
| 62:DC:44:ARG:NH2 | 62:DC:82:ASN:OD1 | 2.44 | 0.49 |
| 80:P0:19:LEU:HD21 | 80:P0:73:PHE:HZ | 1.76 | 0.49 |
| 81:12:142:ARG:NH1 | 81:12:145:GLY:O | 2.45 | 0.49 |
| 1:1:75:G:H3' | 14:t:73:ARG:HD2 | 1.94 | 0.49 |
| 1:1:2236:U:C2 | 1:1:2237:A:C8 | 3.00 | 0.49 |
| 1:1:2397:A:H2' | 1:1:2398:C:C6 | 2.47 | 0.49 |
| 1:1:2992:U:H2' | 1:1:3005:A:N6 | 2.28 | 0.49 |
| 2:3:26:C:H2' | 2:3:27:A:O4' | 2.12 | 0.49 |
| 7:m:19:PRO:HG2 | 7:m:24:GLN:HB2 | 1.95 | 0.49 |
| 46:B:415:A:H4' | 46:B:416:G:O5' | 2.12 | 0.49 |
| 46:B:704:A:H2 | 46:B:719:A:C4 | 2.30 | 0.49 |
| 46:B:1148:A:H2' | 46:B:1149:G:O4' | 2.12 | 0.49 |
| 46:B:1485:G:H2' | 46:B:1486:G:H8 | 1.78 | 0.49 |
| 76:f:19:ARG:HD2 | 76:f:32:ARG:HD3 | 1.93 | 0.49 |
| 1:AS:169:G:H5" | 36:CC:109:ILE:HD13 | 1.94 | 0.49 |
| 1:AS:1245:G:H2' | 1:AS:1246:G:C8 | 2.48 | 0.49 |
| 1:AS:1651:G:OP1 | 35:CB:40:SER:OG | 2.24 | 0.49 |
| 1:AS:2853:C:H2' | 1:AS:2854:U:C6 | 2.47 | 0.49 |
| 4:AW:54:ARG:NH2 | 4:AW:58:LEU:HD11 | 2.26 | 0.49 |
| 6:AY:11:SER:OG | 6:AY:15:GLU:OE1 | 2.30 | 0.49 |
| 24:BQ:23:MET:HE1 | 24:BQ:78:VAL:HG22 | 1.94 | 0.49 |
| 46:CM:122:U:C2' | 46:CM:123:G:H5" | 2.41 | 0.49 |
| 46:CM:333:U:O2' | 58:CY:130:PRO:O | 2.21 | 0.49 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 46:CM:799:G:H8 | 46:CM:799:G:OP1 | 1.96 | 0.49 |
| 46:CM:1016:U:H4' | 46:CM:1017:G:OP2 | 2.12 | 0.49 |
| 46:CM:1068:G:O2' | 46:CM:1079:G:O2' | 2.22 | 0.49 |
| 46:CM:1218:G:H1 | 46:CM:1237:C:H5 | 1.58 | 0.49 |
| 46:CM:1610:C:H2' | 46:CM:1611:C:H6 | 1.77 | 0.49 |
| 46:CM:1652:U:H3 | 46:CM:1723:G:H1 | 1.59 | 0.49 |
| 52:CS:225:ARG:HD2 | 75:DP:58:GLU:CD | 2.37 | 0.49 |
| 57:CX:28:ASN:HD21 | 76:DQ:7:TRP:HE1 | 1.60 | 0.49 |
| 64:DE:36:SER:OG | 64:DE:47:ARG:NH1 | 2.41 | 0.49 |
| 65:DF:82:PRO:HG2 | 66:DG:36:ILE:HG21 | 1.94 | 0.49 |
| 80:P0:52:LEU:HD22 | 80:P0:88:PHE:CE2 | 2.47 | 0.49 |
| 1:1:6:C:H2' | 1:1:7:C:C6 | 2.48 | 0.49 |
| 1:1:708:A:H2' | 1:1:709:A:C8 | 2.48 | 0.49 |
| 1:1:945:C:O2' | 1:1:967:G:OP1 | 2.27 | 0.49 |
| 1:1:951:U:H2' | 1:1:952:U:C6 | 2.47 | 0.49 |
| 1:1:1149:A:HO2' | 1:1:1150:A:H5' | 1.77 | 0.49 |
| 1:1:1184:U:OP1 | 1:1:1206:U:O2' | 2.15 | 0.49 |
| 1:1:1651:G:H5" | 35:AH:58:ARG:NH1 | 2.28 | 0.49 |
| 1:1:2086:C:H1' | 1:1:3309:A:H8 | 1.76 | 0.49 |
| 1:1:2551:G:OP2 | 1:1:2552:A:O2' | 2.24 | 0.49 |
| 1:1:3019:U:O2' | 1:1:3020:A:H5' | 2.13 | 0.49 |
| 1:1:3024:G:H2' | 1:1:3025:G:H8 | 1.77 | 0.49 |
| 8:n:30:ARG:NE | 34:AG:107:ILE:O | 2.44 | 0.49 |
| 27:9:11:SER:HB3 | 27:9:14:LYS:HB2 | 1.93 | 0.49 |
| 45:i:101:LYS:HD3 | 46:B:573:C:H4' | 1.95 | 0.49 |
| 46:B:161:G:O2' | 53:I:110:ALA:HB1 | 2.12 | 0.49 |
| 46:B:1615:U:H2' | 46:B:1616:G:C8 | 2.46 | 0.49 |
| 50:F:143:LEU:C | 50:F:145:ALA:H | 2.18 | 0.49 |
| 51:G:19:MET:HE2 | 51:G:108:LYS:HG2 | 1.94 | 0.49 |
| 62:R:97:TYR:HE1 | 62:R:102:PHE:CE1 | 2.31 | 0.49 |
| 73:c:3:LYS:NZ | 73:c:6:ALA:HA | 2.27 | 0.49 |
| 76:f:12:ARG:HB2 | 76:f:12:ARG:HH11 | 1.76 | 0.49 |
| 79:AR:200:THR:OG1 | 79:AR:240:LEU:O | 2.30 | 0.49 |
| 1:AS:1655:U:H2' | 1:AS:1656:C:H6 | 1.78 | 0.49 |
| 1:AS:2086:C:H1' | 1:AS:3309:A:H8 | 1.74 | 0.49 |
| 1:AS:2423:A:H4' | 37:CD:61:ARG:HB3 | 1.94 | 0.49 |
| 16:BI:11:GLN:O | 16:BI:14:LYS:NZ | 2.41 | 0.49 |
| 46:CM:557:C:OP1 | 77:DR:59:SER:OG | 2.25 | 0.49 |
| 46:CM:671:G:H5' | 46:CM:672:U:OP2 | 2.11 | 0.49 |
| 46:CM:718:A:H2' | 46:CM:720:C:H5 | 1.77 | 0.49 |
| 46:CM:1183:G:O3' | 76:DQ:40:ARG:NH2 | 2.45 | 0.49 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 46:CM:1475:U:OP1 | 50:CQ:10:LYS:NZ | 2.31 | 0.49 |
| 46:CM:1549:G:OP1 | 66:DG:89:ARG:NH2 | 2.44 | 0.49 |
| 57:CX:8:ARG:O | 57:CX:12:HIS:ND1 | 2.46 | 0.49 |
| 59:CZ:78:LEU:O | 59:CZ:81:GLU:HG3 | 2.12 | 0.49 |
| 65:DF:72:ILE:HD13 | 65:DF:79:TYR:CG | 2.47 | 0.49 |
| 71:DL:63:GLN:CD | 71:DL:68:LYS:HD3 | 2.37 | 0.49 |
| 80:P0:16:ARG:HE | 80:P0:63:ILE:HD13 | 1.78 | 0.49 |
| 82:L1:124:LEU:HD22 | 82:L1:128:LEU:HD13 | 1.93 | 0.49 |
| 82:l1:70:ASP:OD1 | 82:l1:87:VAL:N | 2.46 | 0.49 |
| 82:l1:120:ILE:HB | 82:l1:121:PRO:HD3 | 1.94 | 0.49 |
| 1:1:2601:U:H3 | 1:1:2621:G:H1 | 1.61 | 0.49 |
| 1:1:3166:A:N6 | 1:1:3167:G:O6 | 2.46 | 0.49 |
| 1:1:3179:U:OP2 | 15:u:121:ARG:NH2 | 2.45 | 0.49 |
| 2:3:64:A:N6 | 12:r:200:LEU:HD21 | 2.27 | 0.49 |
| 4:j:107:CYS:HB2 | 4:j:136:ILE:HD12 | 1.94 | 0.49 |
| 28:AA:71:PHE:HA | 28:AA:111:LYS:HE2 | 1.95 | 0.49 |
| 31:AD:55:LYS:O | 31:AD:59:GLU:HG2 | 2.13 | 0.49 |
| 43:AP:34:SER:O | 43:AP:40:LYS:HD3 | 2.13 | 0.49 |
| 46:B:17:C:H2' | 46:B:18:C:H6 | 1.78 | 0.49 |
| 46:B:413:C:O2' | 46:B:416:G:O6 | 2.30 | 0.49 |
| 46:B:653:G:O2' | 46:B:672:U:C2 | 2.63 | 0.49 |
| 79:AR:175:VAL:HB | 79:AR:189:PHE:HB2 | 1.94 | 0.49 |
| 1:AS:25:A:H2' | 1:AS:26:C:H6 | 1.77 | 0.49 |
| 1:AS:243:G:H2' | 1:AS:244:G:H8 | 1.76 | 0.49 |
| 1:AS:602:A:H2' | 1:AS:603:C:C6 | 2.48 | 0.49 |
| 1:AS:2155:G:OP2 | 4:AW:128:ARG:NH1 | 2.45 | 0.49 |
| 1:AS:2432:G:H5' | 1:AS:2433:U:OP2 | 2.11 | 0.49 |
| 1:AS:3153:A:H2' | 1:AS:3154:A:C8 | 2.47 | 0.49 |
| 46:CM:953:U:H2' | 46:CM:954:C:O4' | 2.12 | 0.49 |
| 46:CM:1457:A:H5' | 52:CS:185:ARG:HG2 | 1.94 | 0.49 |
| 62:DC:50:ASP:C | 62:DC:52:LYS:H | 2.20 | 0.49 |
| 80:p0:63:ILE:HB | 80:p0:77:LEU:HD11 | 1.95 | 0.49 |
| 80:p0:76:LEU:HD22 | 80:p0:79:PHE:CZ | 2.45 | 0.49 |
| 1:1:348:A:N3 | 1:1:352:A:O2' | 2.46 | 0.49 |
| 1:1:1248:A:C2' | 1:1:1249:U:H5' | 2.37 | 0.49 |
| 1:1:2084:A:H2' | 1:1:2085:A:H8 | 1.77 | 0.49 |
| 1:1:2335:A:H2' | 1:1:2336:A:C8 | 2.48 | 0.49 |
| 1:1:3225:G:OP2 | 15:u:121:ARG:NH1 | 2.46 | 0.49 |
| 13:s:141:ARG:O | 13:s:145:ARG:HG2 | 2.12 | 0.49 |
| 15:u:116:LEU:HD22 | 17:w:191:ALA:HA | 1.93 | 0.49 |
| 23:5:35:LYS:HZ3 | 23:5:39:GLU:CD | 2.21 | 0.49 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 46:B:974:U:H2' | 46:B:975:C:C6 | 2.48 | 0.49 |
| 46:B:1634:U:H2' | 46:B:1635:A:H8 | 1.76 | 0.49 |
| 1:AS:277:G:H2' | 1:AS:278:U:C6 | 2.46 | 0.49 |
| 1:AS:412:G:H5' | 18:BK:26:PHE:HZ | 1.77 | 0.49 |
| 1:AS:1245:G:HO2' | 1:AS:1246:G:P | 2.35 | 0.49 |
| 1:AS:1494:A:H2' | 1:AS:1495:U:C6 | 2.48 | 0.49 |
| 1:AS:1713:U:H2' | 1:AS:1714:G:H8 | 1.76 | 0.49 |
| 1:AS:2186:A:O2' | 1:AS:2187:U:H5' | 2.13 | 0.49 |
| 1:AS:2405:U:H2' | 1:AS:2406:U:C6 | 2.48 | 0.49 |
| 9:BB:208:PRO:HB3 | 9:BB:239:GLN:HB3 | 1.95 | 0.49 |
| 46:CM:477:C:H4' | 56:CW:120:ARG:HG3 | 1.93 | 0.49 |
| 46:CM:820:U:H2' | 46:CM:821:U:C6 | 2.47 | 0.49 |
| 46:CM:915:A:H2' | 48:CO:114:VAL:HG11 | 1.93 | 0.49 |
| 46:CM:1243:U:C6 | 46:CM:1244:U:H5 | 2.31 | 0.49 |
| 67:DH:68:LYS:HE2 | 67:DH:79:ASP:OD1 | 2.13 | 0.49 |
| 77:DR:13:LYS:O | 77:DR:17:GLN:HG2 | 2.12 | 0.49 |
| 78:DS:160:ARG:NH1 | 78:DS:176:ASN:H | 2.11 | 0.49 |
| 80:P0:8:LYS:NZ | 80:P0:58:MET:SD | 2.86 | 0.49 |
| 82:l1:156:LYS:HG2 | 82:l1:157:PHE:H | 1.78 | 0.49 |
| 1:1:493:A:O2' | 1:1:3238:A:N1 | 2.42 | 0.49 |
| 1:1:510:G:O2' | 6:l:342:SER:HB3 | 2.12 | 0.49 |
| 1:1:648:C:H2' | 1:1:649:G:C8 | 2.48 | 0.49 |
| 1:1:662:U:H5' | 6:l:108:ARG:HA | 1.95 | 0.49 |
| 1:1:1182:G:N3 | 21:0:112:ALA:HB1 | 2.27 | 0.49 |
| 1:1:1239:G:OP2 | 1:1:1239:G:H8 | 1.95 | 0.49 |
| 1:1:1250:C:H2' | 1:1:1251:C:H6 | 1.78 | 0.49 |
| 1:1:1255:A:H8 | 1:1:1255:A:OP1 | 1.94 | 0.49 |
| 1:1:2876:U:H2' | 1:1:2877:U:H6 | 1.77 | 0.49 |
| 1:1:3042:A:OP1 | 20:z:62:ARG:NH1 | 2.44 | 0.49 |
| 14:t:83:VAL:HG23 | 14:t:85:ILE:HG13 | 1.95 | 0.49 |
| 17:w:2:SER:HB2 | 34:AG:34:GLY:HA2 | 1.93 | 0.49 |
| 32:AE:95:VAL:HG12 | 32:AE:97:VAL:HG13 | 1.93 | 0.49 |
| 46:B:233:G:H2' | 46:B:234:G:C8 | 2.47 | 0.49 |
| 46:B:744:U:C2 | 46:B:745:A:C8 | 3.00 | 0.49 |
| 46:B:1593:C:H2' | 46:B:1594:G:C8 | 2.47 | 0.49 |
| 47:C:6:SER:O | 47:C:191:ARG:NH1 | 2.46 | 0.49 |
| 1:AS:249:G:H2' | 1:AS:251:G:OP2 | 2.12 | 0.49 |
| 1:AS:623:A:H2' | 1:AS:624:U:H6 | 1.76 | 0.49 |
| 1:AS:729:C:H3' | 1:AS:730:A:H5" | 1.94 | 0.49 |
| 1:AS:1227:A:H8 | 1:AS:1227:A:O5' | 1.95 | 0.49 |
| 1:AS:1863:A:H2' | 1:AS:1864:G:C8 | 2.48 | 0.49 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 1:AS:3236:G:O2' | 8:BA:107:ARG:NH1 | 2.46 | 0.49 |
| 9:BB:119:LYS:HB2 | 22:BO:133:ALA:HB3 | 1.94 | 0.49 |
| 19:BL:96:PHE:CD1 | 19:BL:97:PRO:HD2 | 2.47 | 0.49 |
| 46:CM:821:U:H2' | 46:CM:822:G:H8 | 1.75 | 0.49 |
| 46:CM:1230:G:N2 | 46:CM:1235:U:O4 | 2.41 | 0.49 |
| 46:CM:1610:C:H2' | 46:CM:1611:C:C6 | 2.48 | 0.49 |
| 46:CM:1677:G:H2' | 46:CM:1678:G:N7 | 2.27 | 0.49 |
| 48:CO:97:LEU:HD22 | 48:CO:232:HIS:CG | 2.47 | 0.49 |
| 62:DC:53:PRO:HB3 | 62:DC:83:MET:SD | 2.53 | 0.49 |
| 82:L1:63:MET:HG2 | 82:L1:65:ILE:HG12 | 1.95 | 0.49 |
| 1:1:582:G:H2' | 1:1:583:A:C8 | 2.47 | 0.49 |
| 1:1:1176:A:C4 | 1:1:1178:G:C8 | 3.01 | 0.49 |
| 1:1:1825:A:H5" | 1:1:1826:G:H5' | 1.94 | 0.49 |
| 1:1:2205:C:OP1 | 43:AP:32:LYS:NZ | 2.46 | 0.49 |
| 1:1:2636:C:O2' | 1:1:2637:U:H5' | 2.13 | 0.49 |
| 13:s:101:ASN:ND2 | 13:s:130:VAL:HG13 | 2.28 | 0.49 |
| 18:x:122:ALA:HA | 18:x:145:HIS:CE1 | 2.47 | 0.49 |
| 46:B:1238:U:H2' | 46:B:1239:U:H6 | 1.78 | 0.49 |
| 46:B:1435:U:H2' | 46:B:1436:U:C6 | 2.47 | 0.49 |
| 53:I:136:LYS:HG3 | 53:I:173:PRO:HB2 | 1.95 | 0.49 |
| 79:AR:44:LYS:NZ | 79:AR:95:LEU:O | 2.37 | 0.49 |
| 79:AR:71:ASP:HB3 | 79:AR:113:SER:HA | 1.95 | 0.49 |
| 1:AS:35:C:H4' | 1:AS:804:A:C2 | 2.47 | 0.49 |
| 1:AS:348:A:N3 | 1:AS:352:A:O2' | 2.45 | 0.49 |
| 1:AS:560:C:O3' | 21:BN:71:LYS:NZ | 2.38 | 0.49 |
| 1:AS:907:C:N4 | 4:AW:3:ARG:HD3 | 2.27 | 0.49 |
| 1:AS:1747:G:H5' | 39:CF:26:LYS:HE2 | 1.95 | 0.49 |
| 1:AS:1777:C:H2' | 1:AS:1778:U:C6 | 2.46 | 0.49 |
| 1:AS:2115:U:OP2 | 1:AS:2120:A:N6 | 2.39 | 0.49 |
| 1:AS:3336:G:H2' | 1:AS:3337:A:H8 | 1.77 | 0.49 |
| 4:AW:117:GLU:OE2 | 4:AW:163:ARG:NH2 | 2.45 | 0.49 |
| 8:BA:65:SER:HB3 | 8:BA:75:LEU:HD23 | 1.95 | 0.49 |
| 46:CM:494:G:H3' | 46:CM:495:G:H5" | 1.95 | 0.49 |
| 46:CM:1143:C:O2' | 46:CM:1568:C:OP2 | 2.28 | 0.49 |
| 69:DJ:28:ARG:HD2 | 69:DJ:60:LYS:HE2 | 1.95 | 0.49 |
| 1:1:1277:G:OP1 | 80:P0:55:LYS:HD2 | 2.13 | 0.49 |
| 1:1:2384:C:H2' | 1:1:2385:C:H6 | 1.76 | 0.49 |
| 1:1:2895:U:H2' | 1:1:2896:U:C6 | 2.48 | 0.49 |
| 1:1:3057:G:OP1 | 25:7:34:SER:OG | 2.27 | 0.49 |
| 15:u:57:LEU:HG | 21:0:172:TYR:OH | 2.13 | 0.49 |
| 16:v:62:TYR:HD2 | 16:v:106:VAL:HG13 | 1.78 | 0.49 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 30:AC:11:ASN:O | 30:AC:11:ASN:ND2 | 2.46 | 0.49 |
| 46:B:1336:G:H2' | 46:B:1337:C:O4' | 2.13 | 0.49 |
| 50:F:62:GLU:HB3 | 50:F:65:ARG:NH2 | 2.28 | 0.49 |
| 51:G:71:GLN:NE2 | 51:G:93:GLU:OE2 | 2.46 | 0.49 |
| 52:H:148:ARG:HB3 | 52:H:157:ARG:HH11 | 1.78 | 0.49 |
| 54:J:6:LEU:HG | 54:J:38:GLN:HB3 | 1.95 | 0.49 |
| 70:Z:57:ILE:HG23 | 70:Z:58:GLY:H | 1.78 | 0.49 |
| 1:AS:200:A:H2' | 1:AS:201:G:H8 | 1.78 | 0.49 |
| 1:AS:634:C:O2 | 1:AS:2355:G:O2' | 2.23 | 0.49 |
| 1:AS:2435:G:H5' | 1:AS:2460:U:O4' | 2.12 | 0.49 |
| 1:AS:2899:C:H2' | 1:AS:2900:C:C6 | 2.47 | 0.49 |
| 2:AT:7:G:OP1 | 7:AZ:33:ARG:NH1 | 2.46 | 0.49 |
| 3:AU:37:A:OP2 | 36:CC:86:ARG:HD2 | 2.13 | 0.49 |
| 7:AZ:187:ALA:O | 7:AZ:189:GLU:N | 2.44 | 0.49 |
| 10:BC:160:PRO:HB2 | 10:BC:162:GLU:OE1 | 2.13 | 0.49 |
| 20:BM:44:LEU:HB3 | 20:BM:49:THR:HB | 1.95 | 0.49 |
| 46:CM:1:U:H1' | 49:CP:174:VAL:HG13 | 1.95 | 0.49 |
| 46:CM:86:A:H5' | 71:DL:119:PHE:CE1 | 2.47 | 0.49 |
| 46:CM:1485:G:H2' | 46:CM:1486:G:H8 | 1.77 | 0.49 |
| 47:CN:52:LYS:HD3 | 68:DI:82:VAL:HG23 | 1.95 | 0.49 |
| 48:CO:59:ASP:OD1 | 48:CO:60:GLY:N | 2.45 | 0.49 |
| 58:CY:22:ASN:HB3 | 58:CY:25:ALA:HB3 | 1.93 | 0.49 |
| 59:CZ:78:LEU:HA | 59:CZ:81:GLU:HG2 | 1.94 | 0.49 |
| 67:DH:27:SER:OG | 67:DH:111:VAL:HA | 2.13 | 0.49 |
| 79:DT:41:THR:HG22 | 79:DT:42:LEU:H | 1.77 | 0.49 |
| 1:1:1268:C:H2' | 1:1:1269:A:O4' | 2.13 | 0.48 |
| 1:1:3039:C:H3' | 20:z:62:ARG:NH2 | 2.27 | 0.48 |
| 1:1:3261:A:H2' | 1:1:3262:U:C6 | 2.48 | 0.48 |
| 3:4:63:G:H1 | 3:4:97:A:N6 | 2.07 | 0.48 |
| 6:l:38:SER:HG | 6:l:42:ARG:HH21 | 1.55 | 0.48 |
| 46:B:103:A:O3' | 46:B:306:C:N4 | 2.45 | 0.48 |
| 46:B:671:G:C3' | 46:B:672:U:H5' | 2.25 | 0.48 |
| 46:B:701:G:H2' | 46:B:702:G:C2' | 2.34 | 0.48 |
| 46:B:1772:U:H2' | 46:B:1773:G:H8 | 1.78 | 0.48 |
| 49:E:133:PRO:HB2 | 49:E:217:TYR:HE2 | 1.77 | 0.48 |
| 53:I:48:TYR:CD2 | 53:I:117:GLY:HA3 | 2.48 | 0.48 |
| 62:R:60:LEU:HD22 | 62:R:92:SER:OG | 2.12 | 0.48 |
| 70:Z:59:ILE:HD11 | 70:Z:84:THR:HG21 | 1.95 | 0.48 |
| 77:g:43:ARG:HG2 | 77:g:54:ARG:HH22 | 1.78 | 0.48 |
| 1:AS:588:G:OP1 | 33:BZ:63:LYS:NZ | 2.31 | 0.48 |
| 1:AS:997:G:O2' | 1:AS:1037:U:OP2 | 2.30 | 0.48 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 1:AS:1250:C:H41 | 1:AS:1259:A:P | 2.36 | 0.48 |
| 1:AS:2135:G:N2 | 1:AS:2155:G:O2' | 2.46 | 0.48 |
| 1:AS:3323:U:H2' | 1:AS:3324:A:H8 | 1.76 | 0.48 |
| 45:CL:92:SER:HB2 | 46:CM:1413:A:H62 | 1.78 | 0.48 |
| 46:CM:302:U:H2' | 46:CM:303:C:C6 | 2.48 | 0.48 |
| 46:CM:510:A:O2' | 56:CW:133:HIS:NE2 | 2.40 | 0.48 |
| 46:CM:520:U:O3' | 71:DL:60:PHE:HB2 | 2.13 | 0.48 |
| 46:CM:529:C:HO2' | 46:CM:530:U:P | 2.36 | 0.48 |
| 49:CP:165:ILE:HB | 49:CP:192:TYR:HB2 | 1.94 | 0.48 |
| 1:1:684:G:C2 | 1:1:693:C:C2 | 3.01 | 0.48 |
| 1:1:1486:A:O2' | 38:AK:12:HIS:O | 2.25 | 0.48 |
| 1:1:1591:U:O2' | 1:1:1602:U:O2 | 2.30 | 0.48 |
| 3:4:21:C:OP1 | 6:l:194:LYS:NZ | 2.37 | 0.48 |
| 3:4:70:G:P | 27:9:121:ARG:HH22 | 2.35 | 0.48 |
| 3:4:81:A:H2' | 3:4:82:U:C6 | 2.48 | 0.48 |
| 46:B:1516:C:H2' | 46:B:1517:C:C6 | 2.48 | 0.48 |
| 46:B:1635:A:H2' | 46:B:1636:C:H6 | 1.75 | 0.48 |
| 47:C:10:THR:OG1 | 47:C:12:GLU:OE1 | 2.30 | 0.48 |
| 1:AS:29:G:H5" | 16:BI:188:ARG:HH12 | 1.78 | 0.48 |
| 1:AS:94:A:H5" | 29:BV:34:LYS:HB2 | 1.95 | 0.48 |
| 1:AS:797:A:OP1 | 29:BV:27:LYS:HE3 | 2.13 | 0.48 |
| 1:AS:2475:U:H2' | 1:AS:2476:C:C5 | 2.48 | 0.48 |
| 1:AS:2557:G:C6 | 26:BS:24:LEU:HD21 | 2.48 | 0.48 |
| 4:AW:54:ARG:HG2 | 4:AW:56:ALA:H | 1.78 | 0.48 |
| 7:AZ:119:TYR:OH | 7:AZ:139:PRO:O | 2.29 | 0.48 |
| 46:CM:310:A:C2 | 46:CM:312:C:H2' | 2.48 | 0.48 |
| 46:CM:1258:G:N7 | 46:CM:1416:U:H3' | 2.28 | 0.48 |
| 46:CM:1277:G:H2' | 46:CM:1278:U:C6 | 2.48 | 0.48 |
| 46:CM:1413:A:O2' | 46:CM:1414:G:OP1 | 2.23 | 0.48 |
| 46:CM:1494:G:H2' | 46:CM:1495:U:C6 | 2.48 | 0.48 |
| 1:1:630:G:H2' | 1:1:631:U:C6 | 2.49 | 0.48 |
| 1:1:910:A:C2 | 4:j:204:MET:HE2 | 2.47 | 0.48 |
| 1:1:935:U:OP2 | 29:AB:26:ARG:NH2 | 2.47 | 0.48 |
| 1:1:1593:C:H2' | 1:1:1594:G:H8 | 1.79 | 0.48 |
| 6:l:296:VAL:O | 6:l:300:VAL:HG13 | 2.12 | 0.48 |
| 7:m:150:LEU:HD12 | 13:s:143:ARG:HG3 | 1.95 | 0.48 |
| 13:s:32:ARG:NH1 | 13:s:123:TYR:OH | 2.46 | 0.48 |
| 46:B:78:A:H2' | 46:B:79:C:H6 | 1.79 | 0.48 |
| 46:B:526:U:H2' | 46:B:527:A:O4' | 2.13 | 0.48 |
| 46:B:1423:U:O2' | 50:F:182:VAL:HG23 | 2.13 | 0.48 |
| 50:F:12:LEU:HD12 | 67:W:85:ILE:HG12 | 1.95 | 0.48 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 50:F:143:LEU:O | 50:F:145:ALA:N | 2.38 | 0.48 |
| 54:J:29:ASP:OD1 | 54:J:30:LEU:N | 2.46 | 0.48 |
| 61:Q:98:ARG:HD2 | 73:c:49:ALA:HB2 | 1.95 | 0.48 |
| 75:e:18:ARG:HD2 | 75:e:26:THR:HG22 | 1.94 | 0.48 |
| 79:AR:22:SER:OG | 79:AR:72:VAL:N | 2.46 | 0.48 |
| 79:AR:50:GLY:H | 79:AR:55:TYR:HA | 1.78 | 0.48 |
| 1:AS:294:U:P | 16:BI:15:GLN:HE22 | 2.36 | 0.48 |
| 1:AS:1779:U:H2' | 1:AS:1780:A:H8 | 1.77 | 0.48 |
| 1:AS:2628:A:H4' | 43:CJ:98:LYS:HE3 | 1.96 | 0.48 |
| 6:AY:284:ASN:HB3 | 6:AY:290:LEU:HD11 | 1.95 | 0.48 |
| 39:CF:16:ARG:HG3 | 39:CF:70:PRO:HG3 | 1.94 | 0.48 |
| 46:CM:108:A:H2' | 46:CM:109:G:C8 | 2.48 | 0.48 |
| 46:CM:518:A:O2' | 46:CM:519:A:OP1 | 2.26 | 0.48 |
| 46:CM:849:U:O2 | 74:DO:21:LEU:HB3 | 2.13 | 0.48 |
| 46:CM:1187:A:H1' | 46:CM:1192:C:N4 | 2.28 | 0.48 |
| 46:CM:1503:A:OP2 | 67:DH:60:LYS:NZ | 2.31 | 0.48 |
| 46:CM:1774:C:H2' | 46:CM:1775:G:C8 | 2.48 | 0.48 |
| 48:CO:46:THR:HG23 | 61:DB:27:ASP:HB2 | 1.96 | 0.48 |
| 48:CO:70:LEU:HD23 | 48:CO:79:HIS:HB3 | 1.94 | 0.48 |
| 49:CP:171:LYS:HE3 | 49:CP:192:TYR:OH | 2.13 | 0.48 |
| 52:CS:58:LEU:HD12 | 52:CS:138:VAL:HG12 | 1.95 | 0.48 |
| 63:DD:27:LEU:HB3 | 63:DD:63:ASP:HB2 | 1.95 | 0.48 |
| 82:L1:174:MET:HB3 | 82:L1:178:VAL:HB | 1.94 | 0.48 |
| 80:p0:19:LEU:HD23 | 80:p0:66:PHE:CD2 | 2.47 | 0.48 |
| 1:1:647:A:OP2 | 1:1:2840:U:O2' | 2.30 | 0.48 |
| 1:1:947:A:H5" | 1:1:1139:A:N1 | 2.29 | 0.48 |
| 1:1:2853:C:H2' | 1:1:2854:U:C6 | 2.48 | 0.48 |
| 1:1:2937:U:O2 | 4:j:221:LYS:NZ | 2.41 | 0.48 |
| 6:l:142:ARG:HB3 | 6:l:177:LYS:HE2 | 1.95 | 0.48 |
| 16:v:38:ARG:HA | 16:v:62:TYR:CD1 | 2.49 | 0.48 |
| 46:B:643:U:H2' | 46:B:644:U:O4' | 2.13 | 0.48 |
| 46:B:857:G:N2 | 46:B:1032:G:H4' | 2.28 | 0.48 |
| 46:B:1648:U:H2' | 46:B:1649:G:H8 | 1.79 | 0.48 |
| 51:G:99:PHE:HE1 | 51:G:113:ARG:HG2 | 1.78 | 0.48 |
| 62:R:18:LYS:N | 65:U:92:GLN:O | 2.38 | 0.48 |
| 1:AS:158:A:H2' | 1:AS:159:A:H8 | 1.78 | 0.48 |
| 1:AS:278:U:H3 | 1:AS:287:G:H1 | 1.61 | 0.48 |
| 1:AS:620:A:OP1 | 34:CA:59:ILE:HD11 | 2.13 | 0.48 |
| 1:AS:679:U:O2' | 1:AS:695:G:O6 | 2.29 | 0.48 |
| 1:AS:964:G:H2' | 1:AS:965:C:C6 | 2.49 | 0.48 |
| 1:AS:1804:G:OP2 | 28:BU:133:LYS:NZ | 2.46 | 0.48 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 1:AS:2183:U:O4 | 1:AS:2216:G:N1 | 2.47 | 0.48 |
| 1:AS:2943:A:H2' | 1:AS:2943:A:N3 | 2.29 | 0.48 |
| 1:AS:2972:A:H2' | 1:AS:2973:U:C6 | 2.49 | 0.48 |
| 35:CB:8:ARG:HD2 | 35:CB:32:ALA:O | 2.13 | 0.48 |
| 46:CM:215:A:H4' | 46:CM:216:A:OP2 | 2.12 | 0.48 |
| 46:CM:338:U:H2' | 46:CM:339:A:C8 | 2.48 | 0.48 |
| 46:CM:480:U:H2' | 46:CM:481:A:C8 | 2.49 | 0.48 |
| 46:CM:484:G:H2' | 46:CM:485:G:C8 | 2.49 | 0.48 |
| 46:CM:593:G:H2' | 46:CM:594:C:C6 | 2.49 | 0.48 |
| 46:CM:1118:A:N3 | 46:CM:1637:U:O2' | 2.45 | 0.48 |
| 49:CP:177:PRO:HG3 | 56:CW:17:ARG:HH12 | 1.79 | 0.48 |
| 51:CR:152:PRO:HG3 | 53:CT:212:LEU:HD23 | 1.95 | 0.48 |
| 77:DR:20:LYS:NZ | 77:DR:21:VAL:O | 2.45 | 0.48 |
| 80:P0:55:LYS:HD3 | 80:P0:58:MET:CG | 2.43 | 0.48 |
| 82:l1:25:LYS:HE2 | 82:l1:27:ASN:O | 2.13 | 0.48 |
| 1:1:71:C:O2' | 14:t:66:ASN:OD1 | 2.16 | 0.48 |
| 1:1:779:A:H5" | 1:1:780:A:H5" | 1.94 | 0.48 |
| 1:1:1611:U:H5" | 35:AH:64:GLN:OE1 | 2.12 | 0.48 |
| 1:1:2201:A:H2' | 1:1:2202:A:C8 | 2.48 | 0.48 |
| 1:1:2957:C:H2' | 1:1:2958:U:H6 | 1.77 | 0.48 |
| 1:1:3302:G:H2' | 1:1:3303:C:C6 | 2.49 | 0.48 |
| 3:4:69:U:H3 | 3:4:89:A:H61 | 1.61 | 0.48 |
| 6:l:3:SER:OG | 6:l:4:ARG:N | 2.36 | 0.48 |
| 46:B:227:C:H2' | 46:B:228:C:O4' | 2.13 | 0.48 |
| 46:B:650:G:H3' | 46:B:678:A:H61 | 1.78 | 0.48 |
| 46:B:1205:C:O3' | 57:M:52:LYS:NZ | 2.37 | 0.48 |
| 46:B:1369:G:O2' | 46:B:1370:A:H8 | 1.97 | 0.48 |
| 63:S:21:VAL:HG21 | 63:S:87:GLY:HA3 | 1.94 | 0.48 |
| 1:AS:636:C:N4 | 1:AS:637:G:O6 | 2.46 | 0.48 |
| 1:AS:779:A:H5" | 1:AS:780:A:H5" | 1.96 | 0.48 |
| 1:AS:964:G:H2' | 1:AS:965:C:H6 | 1.78 | 0.48 |
| 1:AS:983:U:H2' | 1:AS:984:U:C6 | 2.48 | 0.48 |
| 1:AS:1678:U:O2 | 23:BP:85:LYS:HG2 | 2.13 | 0.48 |
| 1:AS:1945:A:OP2 | 20:BM:135:LYS:NZ | 2.31 | 0.48 |
| 1:AS:2814:U:H2' | 1:AS:2814:U:O2 | 2.13 | 0.48 |
| 5:AX:95:THR:OG1 | 5:AX:98:GLY:O | 2.24 | 0.48 |
| 15:BH:20:LEU:HD22 | 15:BH:23:ASN:H | 1.78 | 0.48 |
| 46:CM:116:U:H2' | 46:CM:117:U:C6 | 2.49 | 0.48 |
| 46:CM:1488:C:OP2 | 66:DG:102:ARG:NE | 2.47 | 0.48 |
| 53:CT:149:LYS:HB3 | 53:CT:149:LYS:HE2 | 1.69 | 0.48 |
| 62:DC:29:PRO:HG2 | 62:DC:32:GLU:HG2 | 1.96 | 0.48 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 64:DE:66:VAL:HG13 | 64:DE:69:ILE:HG12 | 1.94 | 0.48 |
| 1:1:79:G:H2' | 1:1:80:C:H6 | 1.79 | 0.48 |
| 1:1:169:G:C6 | 1:1:249:G:H1' | 2.49 | 0.48 |
| 19:y:96:PHE:CD1 | 19:y:97:PRO:HD2 | 2.49 | 0.48 |
| 45:i:48:PRO:O | 45:i:50:LYS:N | 2.43 | 0.48 |
| 45:i:155:LEU:HD12 | 45:i:158:LEU:HG | 1.96 | 0.48 |
| 46:B:1323:C:H1' | 46:B:1396:A:C5 | 2.48 | 0.48 |
| 46:B:1399:U:OP2 | 64:T:3:ARG:NH2 | 2.47 | 0.48 |
| 50:F:106:LEU:HD21 | 50:F:139:ILE:HD11 | 1.96 | 0.48 |
| 67:W:32:GLN:HB3 | 67:W:108:GLU:HG2 | 1.94 | 0.48 |
| 77:g:55:LYS:HB2 | 77:g:58:PRO:HG3 | 1.95 | 0.48 |
| 1:AS:258:U:H2' | 1:AS:259:C:C6 | 2.48 | 0.48 |
| 1:AS:268:A:C4 | 16:BI:12:ARG:HG2 | 2.48 | 0.48 |
| 1:AS:710:G:OP1 | 14:BG:176:ARG:NH1 | 2.46 | 0.48 |
| 1:AS:966:A:OP1 | 30:BW:18:ARG:HD2 | 2.13 | 0.48 |
| 1:AS:2832:U:O2 | 1:AS:2910:G:H4' | 2.13 | 0.48 |
| 2:AT:27:A:H2' | 2:AT:28:C:C6 | 2.48 | 0.48 |
| 24:BQ:15:LEU:HD13 | 24:BQ:51:ALA:HB3 | 1.95 | 0.48 |
| 46:CM:165:U:C2' | 46:CM:166:A:H5" | 2.43 | 0.48 |
| 46:CM:638:U:O2 | 54:CU:175:LYS:HE3 | 2.13 | 0.48 |
| 46:CM:1529:G:H5" | 66:DG:87:GLY:C | 2.39 | 0.48 |
| 60:DA:89:TYR:CE2 | 60:DA:150:VAL:HG12 | 2.49 | 0.48 |
| 68:DI:79:LEU:HD13 | 68:DI:82:VAL:HG11 | 1.95 | 0.48 |
| 82:L1:205:VAL:HG11 | 82:L1:213:SER:HB2 | 1.96 | 0.48 |
| 1:1:200:A:H2' | 1:1:201:G:H8 | 1.77 | 0.48 |
| 1:1:386:A:C5 | 1:1:387:A:H1' | 2.48 | 0.48 |
| 1:1:1642:G:H1' | 1:1:1805:A:N6 | 2.28 | 0.48 |
| 1:1:2210:A:H2' | 1:1:2211:A:C8 | 2.49 | 0.48 |
| 1:1:2469:A:H2' | 82:l1:207:LYS:HE2 | 1.96 | 0.48 |
| 1:1:3235:A:N6 | 18:x:178:SER:OG | 2.44 | 0.48 |
| 1:1:3318:G:OP1 | 55:K:77:ARG:NH2 | 2.46 | 0.48 |
| 46:B:722:A:O2' | 46:B:723:G:H8 | 1.97 | 0.48 |
| 46:B:810:U:H2' | 46:B:811:U:O4' | 2.13 | 0.48 |
| 46:B:817:U:HO2' | 46:B:818:U:H6 | 1.61 | 0.48 |
| 46:B:824:U:OP2 | 58:N:27:ALA:HA | 2.12 | 0.48 |
| 46:B:1396:A:O2' | 46:B:1397:A:OP1 | 2.29 | 0.48 |
| 46:B:1425:C:H2' | 46:B:1426:C:H6 | 1.79 | 0.48 |
| 46:B:1668:A:H1' | 53:I:66:GLY:HA2 | 1.94 | 0.48 |
| 59:O:40:GLY:O | 59:O:41:LEU:HB3 | 2.13 | 0.48 |
| 1:AS:148:U:O2' | 16:BI:56:LYS:NZ | 2.46 | 0.48 |
| 1:AS:629:A:H2' | 1:AS:630:G:H8 | 1.77 | 0.48 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 1:AS:659:G:H4' | 1:AS:660:U:C6 | 2.49 | 0.48 |
| 1:AS:1176:A:C4 | 1:AS:1178:G:C8 | 3.02 | 0.48 |
| 1:AS:1233:G:H2' | 1:AS:1234:C:H6 | 1.78 | 0.48 |
| 1:AS:1261:U:N3 | 1:AS:1273:C:O2 | 2.47 | 0.48 |
| 1:AS:1434:U:H4' | 6:AY:89:ALA:CB | 2.43 | 0.48 |
| 1:AS:2915:G:H2' | 1:AS:2916:U:O4' | 2.13 | 0.48 |
| 1:AS:3066:A:H2' | 1:AS:3067:U:C6 | 2.47 | 0.48 |
| 1:AS:3216:U:H2' | 1:AS:3217:G:C8 | 2.48 | 0.48 |
| 1:AS:3300:A:H2' | 1:AS:3301:A:C8 | 2.49 | 0.48 |
| 46:CM:147:C:C2 | 46:CM:148:C:C5 | 3.02 | 0.48 |
| 46:CM:339:A:H2' | 46:CM:340:C:C6 | 2.49 | 0.48 |
| 46:CM:1549:G:OP1 | 66:DG:89:ARG:NH1 | 2.46 | 0.48 |
| 54:CU:14:GLU:HG2 | 54:CU:42:ILE:HG13 | 1.95 | 0.48 |
| 82:l1:73:ASP:OD1 | 82:l1:113:SER:HB2 | 2.12 | 0.48 |
| 82:l1:126:PRO:HA | 82:l1:130:LYS:HE2 | 1.96 | 0.48 |
| 1:1:291:C:H2' | 1:1:292:U:C6 | 2.49 | 0.48 |
| 1:1:1385:G:H5" | 33:AF:102:SER:HB3 | 1.95 | 0.48 |
| 1:1:1661:U:H2' | 1:1:1662:G:H8 | 1.79 | 0.48 |
| 1:1:2370:C:O2' | 5:k:266:ARG:NH2 | 2.47 | 0.48 |
| 1:1:2985:U:H2' | 1:1:2986:U:C6 | 2.48 | 0.48 |
| 1:1:3104:C:H2' | 1:1:3105:C:C6 | 2.49 | 0.48 |
| 1:1:3138:U:H2' | 1:1:3139:U:C6 | 2.49 | 0.48 |
| 7:m:132:THR:HG21 | 7:m:170:GLY:O | 2.13 | 0.48 |
| 46:B:180:A:H2' | 46:B:181:U:H6 | 1.78 | 0.48 |
| 46:B:673:A:H8 | 46:B:673:A:O5' | 1.96 | 0.48 |
| 46:B:1140:G:H2' | 46:B:1141:C:C6 | 2.48 | 0.48 |
| 46:B:1306:A:H4' | 46:B:1307:A:O5' | 2.13 | 0.48 |
| 47:C:98:ILE:HG12 | 47:C:116:LYS:NZ | 2.28 | 0.48 |
| 62:R:1:MET:CB | 65:U:18:LEU:H | 2.27 | 0.48 |
| 70:Z:70:LYS:HB3 | 70:Z:93:LEU:HD22 | 1.95 | 0.48 |
| 79:AR:202:SER:OG | 79:AR:204:ASP:OD1 | 2.23 | 0.48 |
| 1:AS:139:U:H2' | 1:AS:140:C:C6 | 2.49 | 0.48 |
| 1:AS:1020:G:H4' | 1:AS:1020:G:OP1 | 2.13 | 0.48 |
| 1:AS:2138:G:H2' | 1:AS:2139:G:C8 | 2.47 | 0.48 |
| 1:AS:2417:A:H2' | 1:AS:2418:A:C8 | 2.49 | 0.48 |
| 1:AS:3082:C:H2' | 1:AS:3083:U:C6 | 2.48 | 0.48 |
| 11:BD:8:GLN:HB3 | 11:BD:72:LYS:HD2 | 1.94 | 0.48 |
| 46:CM:78:A:H2' | 46:CM:79:C:C6 | 2.48 | 0.48 |
| 46:CM:473:A:OP1 | 56:CW:126:ARG:HD3 | 2.13 | 0.48 |
| 46:CM:698:C:H2' | 46:CM:699:U:C6 | 2.49 | 0.48 |
| 46:CM:721:C:N4 | 46:CM:722:A:H62 | 2.09 | 0.48 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 46:CM:1131:G:H2' | 46:CM:1132:A:H8 | 1.77 | 0.48 |
| 47:CN:21:ASN:HB3 | 47:CN:24:LEU:HD12 | 1.96 | 0.48 |
| 51:CR:141:THR:OG1 | 51:CR:143:ASP:OD1 | 2.23 | 0.48 |
| 54:CU:122:LEU:HD11 | 54:CU:169:TYR:CD1 | 2.49 | 0.48 |
| 64:DE:93:LEU:HD23 | 64:DE:93:LEU:H | 1.79 | 0.48 |
| 79:DT:202:SER:HB3 | 79:DT:207:LEU:HB2 | 1.95 | 0.48 |
| 1:1:307:A:H2' | 1:1:308:A:H8 | 1.74 | 0.48 |
| 1:1:538:G:O2' | 1:1:539:G:OP1 | 2.29 | 0.48 |
| 1:1:1760:U:OP2 | 1:1:1760:U:C2 | 2.67 | 0.48 |
| 1:1:1945:A:H2' | 1:1:1946:U:C6 | 2.49 | 0.48 |
| 1:1:2915:G:H2' | 1:1:2916:U:O4' | 2.14 | 0.48 |
| 84:1:3402:3K5:H7 | 84:1:3402:3K5:O16 | 2.14 | 0.48 |
| 27:9:71:ASN:ND2 | 27:9:83:ASP:HA | 2.29 | 0.48 |
| 35:AH:58:ARG:CD | 35:AH:59:PRO:HD2 | 2.36 | 0.48 |
| 46:B:872:A:H2' | 46:B:873:U:H6 | 1.78 | 0.48 |
| 46:B:1029:U:H2' | 46:B:1030:C:C6 | 2.48 | 0.48 |
| 50:F:66:ARG:HA | 50:F:69:GLU:HG2 | 1.96 | 0.48 |
| 59:O:76:GLU:CB | 78:h:153:GLU:OE1 | 2.62 | 0.48 |
| 1:AS:385:A:H2' | 1:AS:386:A:C8 | 2.48 | 0.48 |
| 2:AT:19:C:H2' | 2:AT:20:A:C8 | 2.49 | 0.48 |
| 6:AY:40:PHE:CD2 | 6:AY:243:ALA:HB2 | 2.49 | 0.48 |
| 15:BH:20:LEU:CD2 | 15:BH:23:ASN:CA | 2.92 | 0.48 |
| 34:CA:20:LYS:HB2 | 34:CA:20:LYS:HE2 | 1.68 | 0.48 |
| 46:CM:379:C:H5" | 51:CR:10:LYS:HD3 | 1.96 | 0.48 |
| 46:CM:443:A:H1' | 46:CM:523:A:H5' | 1.96 | 0.48 |
| 46:CM:458:A:O2' | 51:CR:27:TYR:OH | 2.17 | 0.48 |
| 46:CM:1226:G:C8 | 62:DC:79:HIS:CE1 | 3.01 | 0.48 |
| 46:CM:1423:U:O2' | 50:CQ:182:VAL:HG23 | 2.14 | 0.48 |
| 53:CT:85:ARG:NH2 | 53:CT:87:ARG:HH12 | 2.11 | 0.48 |
| 54:CU:54:LEU:HD13 | 54:CU:84:ARG:HB3 | 1.96 | 0.48 |
| 56:CW:148:VAL:HG11 | 56:CW:156:ILE:HD11 | 1.96 | 0.48 |
| 82:L1:116:LEU:HD23 | 82:L1:119:GLN:HB2 | 1.94 | 0.48 |
| 1:1:1233:G:H2' | 1:1:1234:C:H6 | 1.79 | 0.48 |
| 1:1:1344:U:OP1 | 19:y:39:ARG:NH2 | 2.47 | 0.48 |
| 1:1:1937:C:H42 | 1:1:2085:A:H61 | 1.61 | 0.48 |
| 1:1:1949:G:H1 | 1:1:2070:A:H2' | 1.79 | 0.48 |
| 1:1:2354:G:H2' | 1:1:2355:G:C8 | 2.48 | 0.48 |
| 44:AQ:72:SER:OG | 44:AQ:80:ARG:NH2 | 2.47 | 0.48 |
| 46:B:479:A:H2' | 46:B:480:U:H6 | 1.78 | 0.48 |
| 46:B:1453:C:O2' | 66:V:88:PHE:O | 2.26 | 0.48 |
| 46:B:1457:A:H2 | 46:B:1460:G:N3 | 2.12 | 0.48 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 46:B:1543:A:H1' | 46:B:1547:U:OP2 | 2.13 | 0.48 |
| 49:E:233:SER:HB3 | 49:E:236:GLU:HG3 | 1.95 | 0.48 |
| 51:G:64:ILE:HA | 51:G:67:GLN:HE21 | 1.79 | 0.48 |
| 58:N:73:GLY:HA3 | 58:N:86:ILE:HD12 | 1.96 | 0.48 |
| 61:Q:101:ALA:HB2 | 73:c:53:LEU:CD2 | 2.44 | 0.48 |
| 65:U:63:GLN:O | 65:U:67:GLU:HG3 | 2.14 | 0.48 |
| 1:AS:164:U:H2' | 1:AS:165:C:H6 | 1.78 | 0.48 |
| 1:AS:612:U:H2' | 1:AS:613:U:C6 | 2.48 | 0.48 |
| 2:AT:19:C:H2' | 2:AT:20:A:H8 | 1.79 | 0.48 |
| 7:AZ:83:LEU:HB3 | 7:AZ:88:ILE:HB | 1.96 | 0.48 |
| 46:CM:222:C:H2' | 46:CM:223:A:C8 | 2.49 | 0.48 |
| 46:CM:573:C:N4 | 70:DK:65:ASN:OD1 | 2.37 | 0.48 |
| 46:CM:1227:A:O2' | 46:CM:1229:A:OP1 | 2.27 | 0.48 |
| 46:CM:1739:U:H2' | 46:CM:1740:A:H8 | 1.78 | 0.48 |
| 46:CM:1785:U:C4 | 73:DN:98:PRO:HG2 | 2.49 | 0.48 |
| 49:CP:93:MET:HG3 | 49:CP:116:VAL:HG23 | 1.96 | 0.48 |
| 82:l1:129:SER:HA | 82:l1:133:LYS:HB2 | 1.96 | 0.48 |
| 1:1:1358:C:H2' | 1:1:1359:A:C8 | 2.48 | 0.47 |
| 1:1:1746:A:OP1 | 39:AL:44:LYS:NZ | 2.30 | 0.47 |
| 1:1:3023:U:C2 | 1:1:3024:G:C8 | 3.02 | 0.47 |
| 1:1:3064:C:O2' | 1:1:3066:A:OP2 | 2.25 | 0.47 |
| 5:k:133:TYR:O | 5:k:136:LYS:HB2 | 2.14 | 0.47 |
| 18:x:14:SER:HA | 18:x:150:LEU:O | 2.14 | 0.47 |
| 27:9:51:ARG:HG2 | 27:9:52:GLN:N | 2.28 | 0.47 |
| 45:i:63:ALA:C | 45:i:65:LYS:H | 2.22 | 0.47 |
| 46:B:740:A:HO2' | 46:B:741:A:P | 2.35 | 0.47 |
| 46:B:786:G:H2' | 46:B:787:A:C8 | 2.49 | 0.47 |
| 46:B:809:G:H2' | 46:B:810:U:C6 | 2.49 | 0.47 |
| 46:B:1141:C:H2' | 46:B:1142:A:C8 | 2.49 | 0.47 |
| 46:B:1498:G:H2' | 46:B:1499:G:H8 | 1.79 | 0.47 |
| 46:B:1575:G:O6 | 46:B:1595:U:O4 | 2.32 | 0.47 |
| 1:AS:2174:C:O2' | 1:AS:2248:A:N3 | 2.40 | 0.47 |
| 84:AS:3401:3K5:H9 | 43:CJ:57:ILE:CG2 | 2.40 | 0.47 |
| 24:BQ:42:THR:HG21 | 24:BQ:50:PRO:HG3 | 1.96 | 0.47 |
| 34:CA:42:LYS:HA | 34:CA:45:LEU:HG | 1.96 | 0.47 |
| 45:CL:53:LYS:C | 45:CL:55:LYS:H | 2.21 | 0.47 |
| 46:CM:724:G:C4 | 46:CM:725:A:C8 | 3.02 | 0.47 |
| 62:DC:10:ARG:NH1 | 62:DC:13:LYS:HE3 | 2.29 | 0.47 |
| 62:DC:68:GLU:N | 62:DC:69:PRO:HD3 | 2.29 | 0.47 |
| 78:DS:142:LEU:HB3 | 78:DS:145:LEU:HG | 1.95 | 0.47 |
| 1:1:859:C:H2' | 1:1:860:G:O4' | 2.13 | 0.47 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 1:1:892:A:H5' | 4:j:183:GLY:HA2 | 1.96 | 0.47 |
| 1:1:1580:U:H2' | 1:1:1581:C:C6 | 2.49 | 0.47 |
| 1:1:1612:U:H2' | 1:1:1613:G:H8 | 1.78 | 0.47 |
| 1:1:1911:A:H2' | 1:1:1912:U:C6 | 2.48 | 0.47 |
| 1:1:2957:C:H2' | 1:1:2958:U:C6 | 2.49 | 0.47 |
| 1:1:2995:U:H2' | 1:1:2996:A:H8 | 1.79 | 0.47 |
| 3:4:10:A:H2' | 3:4:11:C:C6 | 2.49 | 0.47 |
| 36:AI:100:GLU:OE1 | 36:AI:108:ARG:NE | 2.47 | 0.47 |
| 46:B:68:A:N6 | 53:I:132:ARG:HG2 | 2.30 | 0.47 |
| 46:B:486:G:H2' | 46:B:487:C:O4' | 2.14 | 0.47 |
| 46:B:1302:C:H2' | 46:B:1303:G:O4' | 2.14 | 0.47 |
| 46:B:1475:U:H5' | 46:B:1481:C:H1' | 1.96 | 0.47 |
| 56:L:106:GLU:HA | 56:L:111:THR:HG21 | 1.96 | 0.47 |
| 62:R:52:LYS:HB2 | 62:R:53:PRO:HD3 | 1.97 | 0.47 |
| 64:T:77:GLU:O | 64:T:80:ARG:NH1 | 2.47 | 0.47 |
| 73:c:32:LYS:O | 73:c:37:LYS:NZ | 2.45 | 0.47 |
| 1:AS:142:G:H4' | 3:AU:145:U:OP1 | 2.13 | 0.47 |
| 1:AS:516:U:OP1 | 6:AY:352:PRO:HD2 | 2.14 | 0.47 |
| 1:AS:795:G:O2' | 14:BG:18:TRP:NE1 | 2.35 | 0.47 |
| 7:AZ:55:PHE:H | 7:AZ:151:GLN:HE22 | 1.60 | 0.47 |
| 10:BC:147:LYS:HG3 | 10:BC:174:MET:HE3 | 1.96 | 0.47 |
| 33:BZ:10:ILE:HA | 33:BZ:64:THR:HG21 | 1.96 | 0.47 |
| 46:CM:29:U:H2' | 46:CM:30:G:C8 | 2.49 | 0.47 |
| 46:CM:138:C:O4' | 53:CT:179:VAL:HG11 | 2.15 | 0.47 |
| 46:CM:444:A:H5" | 51:CR:57:ASN:HD22 | 1.79 | 0.47 |
| 46:CM:670:C:H3' | 46:CM:671:G:O4' | 2.14 | 0.47 |
| 46:CM:694:C:C3' | 46:CM:695:C:H5" | 2.34 | 0.47 |
| 46:CM:721:C:H42 | 46:CM:722:A:N6 | 2.11 | 0.47 |
| 46:CM:987:G:N2 | 46:CM:1747:G:O3' | 2.43 | 0.47 |
| 46:CM:1668:A:H1' | 53:CT:66:GLY:HA2 | 1.95 | 0.47 |
| 52:CS:108:LEU:HD21 | 63:DD:43:LEU:HD11 | 1.95 | 0.47 |
| 59:CZ:45:LEU:HA | 59:CZ:120:CYS:SG | 2.53 | 0.47 |
| 81:12:143:VAL:HG11 | 81:12:148:PRO:HG3 | 1.96 | 0.47 |
| 1:1:125:U:OP1 | 16:v:144:ARG:NH1 | 2.44 | 0.47 |
| 1:1:962:U:OP1 | 29:AB:44:ASN:ND2 | 2.47 | 0.47 |
| 1:1:1222:G:H5' | 1:1:3089:C:H1' | 1.97 | 0.47 |
| 1:1:2108:G:O4' | 1:1:2122:A:H4' | 2.13 | 0.47 |
| 1:1:2400:C:O5' | 43:AP:52:GLY:HA2 | 2.13 | 0.47 |
| 1:1:2418:A:H2' | 1:1:2419:A:C8 | 2.49 | 0.47 |
| 1:1:2443:G:H5" | 1:1:2443:G:H8 | 1.78 | 0.47 |
| 1:1:2649:G:H2' | 1:1:2649:G:N3 | 2.28 | 0.47 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 1:1:3044:C:H2' | 1:1:3045:A:O4' | 2.14 | 0.47 |
| 21:0:171:PHE:O | 21:0:172:TYR:HB2 | 2.14 | 0.47 |
| 23:5:53:ASP:HA | 23:5:69:SER:HB3 | 1.96 | 0.47 |
| 46:B:1099:G:O2' | 46:B:1115:G:O6 | 2.30 | 0.47 |
| 46:B:1298:A:N3 | 46:B:1300:U:H5' | 2.29 | 0.47 |
| 46:B:1742:A:N1 | 77:g:3:LYS:HE3 | 2.29 | 0.47 |
| 53:I:135:PRO:HB2 | 53:I:141:ILE:HG12 | 1.96 | 0.47 |
| 1:AS:712:G:O2' | 1:AS:749:C:O2' | 2.30 | 0.47 |
| 1:AS:1218:G:OP1 | 80:p0:58:MET:HA | 2.14 | 0.47 |
| 1:AS:1937:C:H42 | 1:AS:2085:A:H61 | 1.62 | 0.47 |
| 1:AS:2418:A:H2' | 1:AS:2419:A:C8 | 2.49 | 0.47 |
| 5:AX:159:ARG:HG2 | 5:AX:182:GLN:HA | 1.96 | 0.47 |
| 13:BF:87:LYS:HG2 | 13:BF:91:LEU:HD23 | 1.95 | 0.47 |
| 14:BG:57:VAL:HG23 | 14:BG:149:VAL:HG13 | 1.96 | 0.47 |
| 15:BH:19:VAL:HG11 | 15:BH:55:ILE:HD12 | 1.96 | 0.47 |
| 18:BK:18:ARG:NH1 | 18:BK:147:GLU:OE1 | 2.45 | 0.47 |
| 42:CI:1:MET:HB3 | 46:CM:1629:G:H5' | 1.95 | 0.47 |
| 46:CM:3:U:O2 | 56:CW:17:ARG:NH2 | 2.47 | 0.47 |
| 46:CM:184:C:H2' | 46:CM:185:G:O4' | 2.14 | 0.47 |
| 46:CM:502:U:H2' | 46:CM:503:A:C8 | 2.47 | 0.47 |
| 46:CM:1325:U:O4' | 46:CM:1364:U:H5" | 2.14 | 0.47 |
| 46:CM:1332:U:C5 | 67:DH:57:MET:HE1 | 2.49 | 0.47 |
| 46:CM:1422:A:OP2 | 50:CQ:28:ARG:NH2 | 2.47 | 0.47 |
| 55:CV:37:LYS:NZ | 55:CV:93:THR:HB | 2.29 | 0.47 |
| 59:CZ:106:LEU:HB3 | 59:CZ:110:GLY:HA2 | 1.96 | 0.47 |
| 59:CZ:131:ASP:O | 59:CZ:135:ILE:HB | 2.14 | 0.47 |
| 79:DT:260:PHE:CE2 | 79:DT:267:LEU:HD13 | 2.50 | 0.47 |
| 82:L1:31:THR:O | 82:L1:209:THR:N | 2.46 | 0.47 |
| 1:1:430:G:H2' | 1:1:431:A:C8 | 2.49 | 0.47 |
| 1:1:431:A:H2' | 1:1:432:G:H8 | 1.76 | 0.47 |
| 1:1:1153:G:H2' | 1:1:1154:A:O4' | 2.15 | 0.47 |
| 1:1:1612:U:H2' | 1:1:1613:G:C8 | 2.49 | 0.47 |
| 1:1:2351:A:N3 | 1:1:2796:G:O2' | 2.44 | 0.47 |
| 2:3:16:U:H2' | 2:3:17:A:C8 | 2.49 | 0.47 |
| 2:3:84:A:H2' | 2:3:85:G:C8 | 2.49 | 0.47 |
| 19:y:147:ARG:HB3 | 19:y:150:VAL:HG23 | 1.96 | 0.47 |
| 46:B:128:U:H1' | 46:B:129:A:N7 | 2.29 | 0.47 |
| 46:B:444:A:N6 | 46:B:459:G:H21 | 2.12 | 0.47 |
| 46:B:1072:A:H2' | 46:B:1073:A:C8 | 2.49 | 0.47 |
| 47:C:167:LYS:NZ | 47:C:204:TYR:O | 2.48 | 0.47 |
| 70:Z:63:GLN:OE1 | 70:Z:64:PRO:HA | 2.15 | 0.47 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 75:e:14:LYS:HB3 | 75:e:29:ARG:HB3 | 1.96 | 0.47 |
| 1:AS:95:G:H5' | 14:BG:15:ARG:CZ | 2.44 | 0.47 |
| 1:AS:421:G:O6 | 1:AS:2361:C:O2' | 2.24 | 0.47 |
| 1:AS:867:U:H2' | 1:AS:868:U:C6 | 2.49 | 0.47 |
| 1:AS:1139:A:H5' | 1:AS:1364:U:H1' | 1.96 | 0.47 |
| 1:AS:1153:G:H2' | 1:AS:1154:A:O4' | 2.15 | 0.47 |
| 1:AS:1231:U:O3' | 1:AS:1232:G:H3' | 2.14 | 0.47 |
| 1:AS:1443:G:OP1 | 18:BK:65:SER:HB2 | 2.14 | 0.47 |
| 1:AS:2785:A:H2' | 1:AS:2786:G:O4' | 2.15 | 0.47 |
| 1:AS:3153:A:H2' | 1:AS:3154:A:H8 | 1.79 | 0.47 |
| 3:AU:75:G:OP2 | 27:BT:74:TYR:OH | 2.28 | 0.47 |
| 7:AZ:155:THR:HB | 7:AZ:179:ARG:HH11 | 1.79 | 0.47 |
| 46:CM:1540:G:O6 | 62:DC:43:ARG:NE | 2.30 | 0.47 |
| 46:CM:1635:A:H2' | 46:CM:1636:C:H6 | 1.77 | 0.47 |
| 46:CM:1743:A:H4' | 46:CM:1744:G:OP2 | 2.13 | 0.47 |
| 48:CO:32:ILE:HG22 | 48:CO:96:LEU:HD11 | 1.95 | 0.47 |
| 48:CO:111:ARG:HB3 | 73:DN:68:TYR:HB2 | 1.95 | 0.47 |
| 51:CR:100:ARG:NH2 | 51:CR:121:TYR:O | 2.48 | 0.47 |
| 57:CX:15:LEU:HD23 | 57:CX:76:LEU:HD11 | 1.94 | 0.47 |
| 62:DC:18:LYS:HB2 | 62:DC:36:LEU:HD12 | 1.96 | 0.47 |
| 70:DK:50:LYS:HD3 | 70:DK:101:GLU:OE2 | 2.14 | 0.47 |
| 82:l1:57:GLN:O | 82:l1:59:PRO:HD3 | 2.13 | 0.47 |
| 1:1:164:U:H2' | 1:1:165:C:H6 | 1.78 | 0.47 |
| 1:1:246:U:H2' | 1:1:247:C:C6 | 2.49 | 0.47 |
| 1:1:2992:U:H2' | 1:1:3005:A:H61 | 1.79 | 0.47 |
| 1:1:3132:U:H2' | 1:1:3133:G:C8 | 2.50 | 0.47 |
| 1:1:3259:A:H2' | 1:1:3260:A:O4' | 2.15 | 0.47 |
| 3:4:6:U:H2' | 3:4:7:U:H6 | 1.80 | 0.47 |
| 8:n:165:LEU:HD11 | 34:AG:102:LEU:HD11 | 1.96 | 0.47 |
| 21:0:27:MET:HE2 | 21:0:27:MET:HB3 | 1.74 | 0.47 |
| 46:B:12:U:H2' | 46:B:13:C:H6 | 1.77 | 0.47 |
| 46:B:137:A:O4' | 46:B:139:U:H5' | 2.15 | 0.47 |
| 46:B:1515:U:OP1 | 52:H:109:LYS:HB2 | 2.15 | 0.47 |
| 51:G:63:ALA:O | 51:G:67:GLN:HG2 | 2.14 | 0.47 |
| 56:L:110:GLN:HE21 | 56:L:126:ARG:HB2 | 1.80 | 0.47 |
| 70:Z:69:ARG:HG3 | 70:Z:117:ILE:HG12 | 1.96 | 0.47 |
| 79:AR:216:VAL:HA | 79:AR:232:GLU:HA | 1.96 | 0.47 |
| 1:AS:299:G:C8 | 37:CD:30:GLY:HA3 | 2.50 | 0.47 |
| 1:AS:787:A:H2' | 1:AS:788:G:H8 | 1.79 | 0.47 |
| 1:AS:2063:C:H3' | 1:AS:2064:A:C8 | 2.49 | 0.47 |
| 19:BL:123:THR:OG1 | 19:BL:125:ASP:OD1 | 2.30 | 0.47 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 22:BO:119:ALA:HB1 | 22:BO:124:GLU:O | 2.14 | 0.47 |
| 46:CM:107:C:H2' | 46:CM:108:A:H8 | 1.79 | 0.47 |
| 46:CM:813:U:O2' | 46:CM:814:A:H5' | 2.14 | 0.47 |
| 46:CM:1132:A:O2' | 46:CM:1623:C:OP2 | 2.31 | 0.47 |
| 46:CM:1183:G:O4' | 67:DH:72:GLY:HA3 | 2.13 | 0.47 |
| 46:CM:1648:U:H2' | 46:CM:1649:G:C8 | 2.49 | 0.47 |
| 48:CO:97:LEU:HD11 | 48:CO:228:LEU:HD21 | 1.96 | 0.47 |
| 53:CT:64:LYS:HB2 | 53:CT:97:VAL:HG21 | 1.97 | 0.47 |
| 56:CW:63:ASP:OD1 | 56:CW:64:GLU:N | 2.48 | 0.47 |
| 82:l1:6:SER:O | 82:l1:10:ARG:HG3 | 2.13 | 0.47 |
| 82:l1:66:CYS:HB2 | 82:l1:107:TYR:CG | 2.49 | 0.47 |
| 1:1:629:A:H2' | 1:1:630:G:H8 | 1.79 | 0.47 |
| 1:1:2437:A:H3' | 1:1:2438:U:H5" | 1.96 | 0.47 |
| 1:1:2584:U:H2' | 1:1:2585:U:O4' | 2.15 | 0.47 |
| 13:s:110:ILE:HG21 | 13:s:116:TYR:HD2 | 1.79 | 0.47 |
| 46:B:65:A:H2 | 46:B:84:A:H62 | 1.62 | 0.47 |
| 46:B:114:C:O2' | 58:N:65:SER:OG | 2.22 | 0.47 |
| 46:B:809:G:H2' | 46:B:810:U:H6 | 1.79 | 0.47 |
| 46:B:1155:G:C2 | 46:B:1156:A:C8 | 3.03 | 0.47 |
| 46:B:1303:G:H5" | 64:T:67:ARG:NH1 | 2.30 | 0.47 |
| 49:E:71:LEU:HB3 | 49:E:99:ILE:HD11 | 1.97 | 0.47 |
| 50:F:56:THR:O | 50:F:60:LEU:HG | 2.14 | 0.47 |
| 51:G:64:ILE:O | 51:G:67:GLN:HG3 | 2.14 | 0.47 |
| 57:M:59:PHE:CZ | 57:M:62:GLN:HA | 2.49 | 0.47 |
| 1:AS:595:G:OP2 | 9:BB:32:LYS:NZ | 2.44 | 0.47 |
| 1:AS:1358:C:H2' | 1:AS:1359:A:C8 | 2.50 | 0.47 |
| 1:AS:1656:C:H2' | 1:AS:1657:G:H8 | 1.80 | 0.47 |
| 1:AS:1718:U:OP1 | 20:BM:100:ARG:NE | 2.47 | 0.47 |
| 1:AS:2270:U:HO2' | 46:CM:1643:U:HO2' | 1.63 | 0.47 |
| 5:AX:217:VAL:HG11 | 5:AX:328:ILE:HB | 1.96 | 0.47 |
| 45:CL:70:ASN:OD1 | 45:CL:70:ASN:N | 2.48 | 0.47 |
| 46:CM:415:A:H4' | 46:CM:416:G:O5' | 2.13 | 0.47 |
| 46:CM:815:U:HO2' | 46:CM:816:U:H6 | 1.62 | 0.47 |
| 46:CM:886:G:H2' | 46:CM:887:G:C8 | 2.50 | 0.47 |
| 46:CM:1043:U:O2 | 46:CM:1045:U:N3 | 2.46 | 0.47 |
| 46:CM:1062:C:H2' | 46:CM:1063:C:H6 | 1.78 | 0.47 |
| 46:CM:1609:G:H2' | 46:CM:1610:C:H6 | 1.79 | 0.47 |
| 49:CP:74:ASP:OD2 | 49:CP:181:ARG:NE | 2.47 | 0.47 |
| 60:DA:4:MET:HE1 | 60:DA:121:ARG:HG3 | 1.96 | 0.47 |
| 67:DH:101:ARG:O | 67:DH:105:ILE:HG12 | 2.13 | 0.47 |
| 82:L1:3:LYS:HD3 | 82:L1:3:LYS:HA | 1.66 | 0.47 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 1:1:108:A:N1 | 1:1:322:U:O2' | 2.47 | 0.47 |
| 1:1:486:C:H2' | 1:1:487:C:C6 | 2.49 | 0.47 |
| 1:1:567:G:OP2 | 6:l:349:LYS:HE2 | 2.15 | 0.47 |
| 1:1:892:A:H4' | 4:j:186:PHE:CD2 | 2.50 | 0.47 |
| 1:1:964:G:H2' | 1:1:965:C:C6 | 2.50 | 0.47 |
| 1:1:1029:U:H2' | 1:1:1030:U:C6 | 2.49 | 0.47 |
| 1:1:1217:A:H1' | 80:P0:8:LYS:HZ1 | 1.80 | 0.47 |
| 1:1:1616:U:H2' | 1:1:1617:A:C8 | 2.49 | 0.47 |
| 1:1:1642:G:O2' | 1:1:1804:G:N2 | 2.43 | 0.47 |
| 1:1:1937:C:H2' | 1:1:1938:U:C6 | 2.50 | 0.47 |
| 1:1:1940:U:H2' | 1:1:1941:A:C8 | 2.49 | 0.47 |
| 1:1:2546:U:H5' | 1:1:2547:G:O4' | 2.14 | 0.47 |
| 1:1:2557:G:C6 | 26:8:24:LEU:HD21 | 2.50 | 0.47 |
| 1:1:3193:C:H4' | 1:1:3194:G:O5' | 2.13 | 0.47 |
| 2:3:6:C:H5" | 7:m:54:ARG:NH2 | 2.30 | 0.47 |
| 2:3:107:A:H2' | 2:3:108:U:C6 | 2.49 | 0.47 |
| 3:4:75:G:H2' | 3:4:76:C:H6 | 1.80 | 0.47 |
| 5:k:25:GLN:HE21 | 5:k:334:ARG:HD3 | 1.80 | 0.47 |
| 5:k:123:TYR:CZ | 5:k:124:LYS:HG3 | 2.48 | 0.47 |
| 7:m:50:ARG:NH2 | 7:m:72:ASP:OD2 | 2.45 | 0.47 |
| 7:m:85:ARG:NH2 | 7:m:250:ASP:OD2 | 2.48 | 0.47 |
| 11:q:173:ARG:HH11 | 41:AN:50:LYS:C | 2.23 | 0.47 |
| 12:r:49:CYS:HB3 | 12:r:168:SER:HB3 | 1.95 | 0.47 |
| 12:r:190:VAL:HG22 | 12:r:199:PHE:HD1 | 1.78 | 0.47 |
| 14:t:8:PRO:HD3 | 19:y:164:ARG:HB3 | 1.97 | 0.47 |
| 14:t:143:VAL:HG13 | 14:t:147:PHE:HD2 | 1.80 | 0.47 |
| 19:y:89:ASP:OD1 | 19:y:90:ASP:N | 2.46 | 0.47 |
| 21:0:161:LYS:NZ | 21:0:161:LYS:HB3 | 2.29 | 0.47 |
| 46:B:507:G:H2' | 46:B:508:G:C8 | 2.49 | 0.47 |
| 46:B:886:G:H2' | 46:B:887:G:C8 | 2.50 | 0.47 |
| 46:B:989:U:H3' | 46:B:990:A:H5" | 1.96 | 0.47 |
| 46:B:1016:U:H4' | 46:B:1017:G:OP2 | 2.13 | 0.47 |
| 46:B:1156:A:O2' | 46:B:1557:A:N3 | 2.41 | 0.47 |
| 46:B:1242:U:O2 | 46:B:1242:U:H2' | 2.13 | 0.47 |
| 46:B:1375:C:O2' | 64:T:52:GLY:HA3 | 2.15 | 0.47 |
| 46:B:1495:U:H2' | 46:B:1496:C:C6 | 2.49 | 0.47 |
| 59:O:47:GLU:HG2 | 59:O:50:LYS:HE2 | 1.97 | 0.47 |
| 62:R:68:GLU:N | 62:R:69:PRO:HD3 | 2.30 | 0.47 |
| 68:X:79:LEU:HD13 | 68:X:82:VAL:HG11 | 1.97 | 0.47 |
| 69:Y:41:MET:HG2 | 69:Y:129:VAL:HG21 | 1.97 | 0.47 |
| 70:Z:62:LYS:H | 70:Z:116:ASP:HB2 | 1.78 | 0.47 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 72:b:54:VAL:HA | 72:b:57:TYR:CD2 | 2.49 | 0.47 |
| 1:AS:37:U:H2' | 1:AS:38:A:O4' | 2.14 | 0.47 |
| 1:AS:158:A:H2' | 1:AS:159:A:C8 | 2.49 | 0.47 |
| 1:AS:180:U:H4' | 38:CE:75:LYS:CG | 2.45 | 0.47 |
| 1:AS:242:C:O2' | 1:AS:243:G:H8 | 1.98 | 0.47 |
| 1:AS:1050:A:H5" | 1:AS:2609:A:H61 | 1.78 | 0.47 |
| 1:AS:1190:G:H2' | 1:AS:1191:A:C8 | 2.50 | 0.47 |
| 1:AS:2236:U:C2 | 1:AS:2237:A:C8 | 3.03 | 0.47 |
| 1:AS:2503:G:OP2 | 4:AW:37:ARG:NH2 | 2.48 | 0.47 |
| 1:AS:3135:A:H2' | 1:AS:3136:C:C6 | 2.50 | 0.47 |
| 84:AS:3401:3K5:H21 | 43:CJ:43:TYR:CE2 | 2.50 | 0.47 |
| 2:AT:39:U:O2' | 13:BF:43:GLN:HB3 | 2.15 | 0.47 |
| 3:AU:142:C:H2' | 3:AU:143:U:C6 | 2.49 | 0.47 |
| 3:AU:153:U:OP1 | 10:BC:64:LYS:NZ | 2.36 | 0.47 |
| 8:BA:59:ASP:HB2 | 8:BA:102:VAL:HG22 | 1.96 | 0.47 |
| 16:BI:183:THR:HG22 | 16:BI:187:ARG:HB2 | 1.96 | 0.47 |
| 17:BJ:131:LYS:HB3 | 17:BJ:134:ARG:HG2 | 1.97 | 0.47 |
| 45:CL:64:LEU:HB2 | 62:DC:103:ASN:HD21 | 1.79 | 0.47 |
| 46:CM:25:C:H4' | 46:CM:26:A:O5' | 2.15 | 0.47 |
| 46:CM:151:G:H2' | 46:CM:152:G:H8 | 1.78 | 0.47 |
| 46:CM:1218:G:N2 | 46:CM:1238:U:H1' | 2.30 | 0.47 |
| 46:CM:1301:G:HO2' | 46:CM:1387:A:HO2' | 1.63 | 0.47 |
| 46:CM:1323:C:H1' | 46:CM:1396:A:C5 | 2.49 | 0.47 |
| 46:CM:1436:U:H2' | 46:CM:1437:C:H6 | 1.79 | 0.47 |
| 46:CM:1500:G:H1' | 46:CM:1505:C:O2 | 2.15 | 0.47 |
| 46:CM:1520:C:OP2 | 72:DM:77:ARG:NH2 | 2.47 | 0.47 |
| 46:CM:1571:G:O2' | 46:CM:1597:G:O6 | 2.27 | 0.47 |
| 47:CN:53:THR:OG1 | 47:CN:161:PRO:HG2 | 2.15 | 0.47 |
| 48:CO:85:LYS:HB2 | 48:CO:101:HIS:HB3 | 1.96 | 0.47 |
| 50:CQ:208:LYS:HB3 | 64:DE:40:VAL:HB | 1.95 | 0.47 |
| 55:CV:65:PHE:CZ | 55:CV:78:ILE:HD11 | 2.50 | 0.47 |
| 64:DE:93:LEU:HD12 | 64:DE:98:GLY:O | 2.14 | 0.47 |
| 71:DL:57:VAL:HB | 71:DL:60:PHE:CE1 | 2.50 | 0.47 |
| 75:DP:60:GLU:H | 75:DP:60:GLU:CD | 2.22 | 0.47 |
| 78:DS:177:MET:SD | 78:DS:180:ARG:NH2 | 2.87 | 0.47 |
| 79:DT:41:THR:CG2 | 79:DT:61:SER:HB2 | 2.44 | 0.47 |
| 1:1:1075:A:H4' | 7:m:140:ARG:O | 2.15 | 0.47 |
| 1:1:1635:C:OP2 | 35:AH:74:ARG:NH1 | 2.42 | 0.47 |
| 1:1:1852:C:H2' | 1:1:1853:C:H6 | 1.80 | 0.47 |
| 1:1:2902:A:H2' | 1:1:2903:C:C6 | 2.49 | 0.47 |
| 2:3:27:A:H2' | 2:3:28:C:C6 | 2.49 | 0.47 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 11:q:10:LEU:HD23 | 11:q:11:ASP:N | 2.29 | 0.47 |
| 36:AI:118:ILE:HG22 | 36:AI:119:LYS:N | 2.29 | 0.47 |
| 46:B:55:A:OP1 | 71:a:112:LYS:NZ | 2.39 | 0.47 |
| 46:B:700:G:H2' | 46:B:701:G:H8 | 1.79 | 0.47 |
| 46:B:1241:A:H5' | 46:B:1242:U:C6 | 2.49 | 0.47 |
| 46:B:1343:G:H4' | 66:V:130:ARG:HA | 1.96 | 0.47 |
| 46:B:1502:A:O2' | 46:B:1505:C:N4 | 2.48 | 0.47 |
| 46:B:1648:U:H2' | 46:B:1649:G:C8 | 2.49 | 0.47 |
| 48:D:26:ARG:HA | 48:D:50:ARG:HH12 | 1.79 | 0.47 |
| 1:AS:859:C:H2' | 1:AS:860:G:O4' | 2.14 | 0.47 |
| 1:AS:1396:U:H2' | 1:AS:1397:G:O4' | 2.14 | 0.47 |
| 1:AS:2417:A:H2' | 1:AS:2418:A:H8 | 1.80 | 0.47 |
| 11:BD:147:SER:HB2 | 11:BD:187:ILE:HD11 | 1.96 | 0.47 |
| 26:BS:96:LYS:HG3 | 26:BS:107:ALA:HB3 | 1.97 | 0.47 |
| 28:BU:101:LEU:HB3 | 28:BU:107:ARG:NH2 | 2.29 | 0.47 |
| 45:CL:120:GLU:HG2 | 50:CQ:118:ARG:HE | 1.80 | 0.47 |
| 46:CM:30:G:H4' | 70:DK:131:SER:HB2 | 1.97 | 0.47 |
| 46:CM:93:A:O2' | 51:CR:4:GLY:HA3 | 2.15 | 0.47 |
| 46:CM:309:U:OP2 | 70:DK:20:ARG:HD3 | 2.14 | 0.47 |
| 46:CM:810:U:H2' | 46:CM:811:U:O4' | 2.15 | 0.47 |
| 46:CM:946:U:H5" | 60:DA:71:ILE:HD12 | 1.97 | 0.47 |
| 46:CM:1214:G:N2 | 46:CM:1240:G:O2' | 2.47 | 0.47 |
| 46:CM:1276:G:H22 | 46:CM:1309:G:H22 | 1.61 | 0.47 |
| 1:1:130:U:H2' | 1:1:131:C:H6 | 1.80 | 0.47 |
| 1:1:178:U:H2' | 1:1:179:C:H6 | 1.80 | 0.47 |
| 1:1:528:A:O2' | 1:1:529:A:H5' | 2.15 | 0.47 |
| 1:1:787:A:H2' | 1:1:788:G:H8 | 1.79 | 0.47 |
| 1:1:2404:U:H2' | 1:1:2405:U:C6 | 2.50 | 0.47 |
| 1:1:2472:A:H3' | 1:1:2473:C:H5" | 1.96 | 0.47 |
| 1:1:2734:A:H2' | 1:1:2735:U:H6 | 1.79 | 0.47 |
| 6:l:318:PRO:HG2 | 9:o:147:TYR:HB3 | 1.96 | 0.47 |
| 20:z:165:ARG:HD2 | 46:B:835:A:C5' | 2.43 | 0.47 |
| 28:AA:27:LYS:HE3 | 28:AA:97:THR:HG22 | 1.97 | 0.47 |
| 45:i:96:LYS:HA | 46:B:575:G:C6 | 2.50 | 0.47 |
| 46:B:1258:G:N7 | 46:B:1416:U:H3' | 2.30 | 0.47 |
| 46:B:1610:C:H2' | 46:B:1611:C:H6 | 1.78 | 0.47 |
| 46:B:1626:C:H2' | 46:B:1627:C:O4' | 2.15 | 0.47 |
| 46:B:1706:A:H2' | 46:B:1707:G:O4' | 2.15 | 0.47 |
| 47:C:84:ARG:NE | 64:T:82:ASP:OD1 | 2.46 | 0.47 |
| 52:H:108:LEU:HD21 | 63:S:43:LEU:CD1 | 2.44 | 0.47 |
| 53:I:169:TYR:HE2 | 53:I:171:LYS:HE3 | 1.79 | 0.47 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 59:O:59:LEU:HD22 | 59:O:123:VAL:CG2 | 2.45 | 0.47 |
| 63:S:22:LYS:HB3 | 63:S:63:ASP:OD1 | 2.15 | 0.47 |
| 72:b:78:VAL:HG12 | 72:b:81:ARG:HH21 | 1.80 | 0.47 |
| 1:AS:289:A:H2' | 1:AS:290:G:C8 | 2.47 | 0.47 |
| 1:AS:359:U:OP1 | 38:CE:11:ARG:NH1 | 2.48 | 0.47 |
| 1:AS:1079:G:H2' | 1:AS:1080:A:C8 | 2.50 | 0.47 |
| 1:AS:1642:G:H1' | 1:AS:1805:A:N6 | 2.30 | 0.47 |
| 1:AS:2628:A:C8 | 1:AS:2630:G:C8 | 3.03 | 0.47 |
| 2:AT:107:A:H2' | 2:AT:108:U:C6 | 2.49 | 0.47 |
| 3:AU:122:U:O2 | 3:AU:131:G:N2 | 2.38 | 0.47 |
| 4:AW:5:ILE:HG12 | 4:AW:8:GLN:HG3 | 1.97 | 0.47 |
| 8:BA:145:LEU:HD23 | 8:BA:145:LEU:HA | 1.80 | 0.47 |
| 11:BD:76:ALA:O | 11:BD:79:ILE:HG22 | 2.15 | 0.47 |
| 12:BE:142:ASP:CG | 12:BE:178:ARG:HH22 | 2.23 | 0.47 |
| 27:BT:51:ARG:HG2 | 27:BT:52:GLN:N | 2.30 | 0.47 |
| 28:BU:46:ILE:HG23 | 28:BU:68:VAL:HG13 | 1.96 | 0.47 |
| 36:CC:31:LEU:HD22 | 36:CC:41:LEU:HD21 | 1.97 | 0.47 |
| 45:CL:112:LYS:HG3 | 45:CL:113:ARG:H | 1.79 | 0.47 |
| 46:CM:157:U:O3' | 53:CT:87:ARG:NH2 | 2.47 | 0.47 |
| 46:CM:1375:C:O2' | 64:DE:52:GLY:HA3 | 2.15 | 0.47 |
| 46:CM:1772:U:OP1 | 61:DB:131:ARG:NH2 | 2.40 | 0.47 |
| 1:1:1298:A:N7 | 1:1:2829:C:O2' | 2.47 | 0.47 |
| 1:1:1895:G:O2' | 1:1:2312:U:O4 | 2.20 | 0.47 |
| 1:1:2557:G:H2' | 1:1:2557:G:N3 | 2.30 | 0.47 |
| 1:1:2687:A:HO2' | 43:AP:8:ARG:HH22 | 1.58 | 0.47 |
| 1:1:2912:A:OP2 | 5:k:2:SER:N | 2.48 | 0.47 |
| 1:1:3320:U:H5" | 1:1:3321:G:OP1 | 2.14 | 0.47 |
| 2:3:77:G:H3' | 21:0:46:GLN:O | 2.15 | 0.47 |
| 3:4:87:G:OP2 | 36:AI:5:LYS:HD2 | 2.14 | 0.47 |
| 7:m:94:ASN:HB2 | 7:m:97:ALA:H | 1.80 | 0.47 |
| 8:n:146:LEU:O | 8:n:150:LYS:HG2 | 2.15 | 0.47 |
| 46:B:485:G:C2 | 46:B:486:G:C8 | 3.03 | 0.47 |
| 46:B:1043:U:O2' | 46:B:1045:U:OP2 | 2.32 | 0.47 |
| 46:B:1067:C:H4' | 68:X:58:TYR:CE2 | 2.50 | 0.47 |
| 46:B:1644:U:O5' | 46:B:1645:G:H5" | 2.15 | 0.47 |
| 46:B:1672:G:H2' | 46:B:1673:U:C6 | 2.49 | 0.47 |
| 46:B:1749:A:H1' | 46:B:1770:C:H5' | 1.96 | 0.47 |
| 50:F:52:LYS:NZ | 50:F:90:GLU:OE1 | 2.44 | 0.47 |
| 60:P:26:PHE:CE1 | 60:P:28:LEU:HB2 | 2.49 | 0.47 |
| 60:P:69:ASN:HB3 | 60:P:73:ARG:HD2 | 1.96 | 0.47 |
| 1:AS:583:A:H2' | 1:AS:584:C:C6 | 2.50 | 0.47 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 1:AS:786:U:H5” | 6:AY:113:LYS:HD3 | 1.96 | 0.47 |
| 1:AS:1180:A:H2’ | 1:AS:1181:C:C6 | 2.50 | 0.47 |
| 1:AS:1251:C:H2’ | 1:AS:1252:G:H8 | 1.79 | 0.47 |
| 1:AS:1563:A:H2 | 1:AS:1569:C:C4 | 2.33 | 0.47 |
| 1:AS:1714:G:H2’ | 1:AS:1715:G:H8 | 1.80 | 0.47 |
| 1:AS:2739:U:H2’ | 1:AS:2740:U:C6 | 2.49 | 0.47 |
| 1:AS:3023:U:H2’ | 1:AS:3024:G:H8 | 1.80 | 0.47 |
| 1:AS:3194:G:H4’ | 15:BH:129:VAL:HG11 | 1.96 | 0.47 |
| 5:AX:260:VAL:HG11 | 5:AX:266:ARG:NH1 | 2.30 | 0.47 |
| 46:CM:17:C:H2’ | 46:CM:18:C:H6 | 1.80 | 0.47 |
| 46:CM:1029:U:H2’ | 46:CM:1030:C:C6 | 2.50 | 0.47 |
| 46:CM:1074:U:O2’ | 46:CM:1078:A:N1 | 2.41 | 0.47 |
| 46:CM:1783:C:OP1 | 73:DN:87:ARG:NE | 2.48 | 0.47 |
| 51:CR:103:TYR:HE2 | 51:CR:184:THR:HG23 | 1.80 | 0.47 |
| 62:DC:49:LEU:HB3 | 62:DC:50:ASP:H | 1.45 | 0.47 |
| 79:DT:244:PRO:HD3 | 79:DT:291:TRP:HB3 | 1.97 | 0.47 |
| 1:1:2116:A:C4 | 38:AK:3:LYS:HB3 | 2.50 | 0.46 |
| 1:1:2855:U:H2’ | 1:1:2856:C:C6 | 2.50 | 0.46 |
| 2:3:7:G:OP1 | 7:m:33:ARG:NH1 | 2.47 | 0.46 |
| 45:i:77:GLN:NE2 | 46:B:1165:C:H5’ | 2.31 | 0.46 |
| 46:B:216:A:N6 | 46:B:829:A:O2’ | 2.47 | 0.46 |
| 46:B:397:A:H4’ | 51:G:3:ARG:HG2 | 1.96 | 0.46 |
| 46:B:827:C:H5” | 46:B:828:U:OP2 | 2.14 | 0.46 |
| 46:B:880:G:H4’ | 61:Q:32:GLU:OE1 | 2.15 | 0.46 |
| 46:B:953:U:H5” | 46:B:1018:C:O2’ | 2.15 | 0.46 |
| 46:B:1227:A:O2’ | 46:B:1229:A:OP1 | 2.28 | 0.46 |
| 50:F:71:THR:HB | 50:F:87:ILE:HD12 | 1.96 | 0.46 |
| 54:J:169:TYR:OH | 54:J:175:LYS:HE3 | 2.15 | 0.46 |
| 1:AS:239:A:OP1 | 36:CC:94:LYS:NZ | 2.31 | 0.46 |
| 1:AS:870:U:H5” | 1:AS:2922:G:OP1 | 2.15 | 0.46 |
| 1:AS:1568:U:C4 | 1:AS:1569:C:H1’ | 2.50 | 0.46 |
| 1:AS:2084:A:H2’ | 1:AS:2085:A:C8 | 2.49 | 0.46 |
| 1:AS:2354:G:H2’ | 1:AS:2355:G:C8 | 2.50 | 0.46 |
| 1:AS:3019:U:H5’ | 5:AX:329:PRO:HA | 1.96 | 0.46 |
| 33:BZ:14:TYR:CE2 | 33:BZ:16:LYS:HB2 | 2.50 | 0.46 |
| 46:CM:7:G:H4’ | 46:CM:571:C:H4’ | 1.97 | 0.46 |
| 46:CM:565:A:H5” | 70:DK:70:LYS:NZ | 2.31 | 0.46 |
| 46:CM:938:G:H2’ | 46:CM:939:G:C8 | 2.50 | 0.46 |
| 46:CM:938:G:H2’ | 46:CM:939:G:H8 | 1.80 | 0.46 |
| 46:CM:1678:G:H3’ | 46:CM:1679:A:C8 | 2.50 | 0.46 |
| 46:CM:1679:A:H2’ | 46:CM:1680:A:C8 | 2.50 | 0.46 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 50:CQ:183:LEU:HD23 | 50:CQ:183:LEU:H | 1.79 | 0.46 |
| 51:CR:45:VAL:HA | 51:CR:61:VAL:HG21 | 1.96 | 0.46 |
| 79:DT:240:LEU:HD22 | 79:DT:249:LEU:HD11 | 1.97 | 0.46 |
| 79:DT:259:ILE:HG13 | 79:DT:268:LEU:HB3 | 1.96 | 0.46 |
| 79:DT:302:TYR:CE2 | 79:DT:308:ARG:HD2 | 2.50 | 0.46 |
| 1:1:95:G:H5' | 14:t:15:ARG:CZ | 2.45 | 0.46 |
| 1:1:169:G:N1 | 1:1:249:G:H1' | 2.30 | 0.46 |
| 1:1:669:U:H2' | 1:1:670:A:C8 | 2.50 | 0.46 |
| 1:1:729:C:H3' | 1:1:730:A:H5" | 1.97 | 0.46 |
| 1:1:907:C:H42 | 4:j:3:ARG:HD3 | 1.79 | 0.46 |
| 1:1:1920:U:O2' | 1:1:1923:G:O6 | 2.30 | 0.46 |
| 1:1:1949:G:N1 | 1:1:2070:A:H2' | 2.30 | 0.46 |
| 1:1:2946:U:H2' | 1:1:2947:U:C6 | 2.50 | 0.46 |
| 1:1:3124:U:O2' | 1:1:3126:U:H1' | 2.14 | 0.46 |
| 1:1:3153:A:H2' | 1:1:3154:A:C8 | 2.50 | 0.46 |
| 15:u:62:LEU:HD21 | 15:u:77:LYS:HB3 | 1.97 | 0.46 |
| 16:v:90:ASN:O | 43:AP:50:TYR:OH | 2.30 | 0.46 |
| 17:w:83:LYS:HE2 | 17:w:83:LYS:HB3 | 1.65 | 0.46 |
| 33:AF:77:VAL:HG13 | 33:AF:82:ASP:HB2 | 1.97 | 0.46 |
| 46:B:1:U:H1' | 49:E:174:VAL:HG13 | 1.97 | 0.46 |
| 46:B:432:G:N1 | 46:B:435:A:OP2 | 2.48 | 0.46 |
| 46:B:583:A:H2' | 46:B:584:G:H8 | 1.79 | 0.46 |
| 46:B:653:G:N2 | 46:B:654:G:O6 | 2.48 | 0.46 |
| 46:B:1219:A:H3' | 46:B:1230:G:C8 | 2.51 | 0.46 |
| 46:B:1544:U:OP2 | 46:B:1546:G:O2' | 2.25 | 0.46 |
| 48:D:66:PHE:CE1 | 61:Q:29:SER:HB3 | 2.50 | 0.46 |
| 57:M:11:ILE:HA | 57:M:35:ILE:HD13 | 1.98 | 0.46 |
| 69:Y:40:VAL:HG11 | 69:Y:103:ILE:HD12 | 1.97 | 0.46 |
| 79:AR:67:HIS:CG | 79:AR:68:ILE:H | 2.33 | 0.46 |
| 1:AS:477:U:O5' | 1:AS:477:U:H6 | 1.99 | 0.46 |
| 1:AS:629:A:C2 | 34:CA:91:PRO:HG2 | 2.50 | 0.46 |
| 1:AS:755:U:H2' | 1:AS:756:G:O4' | 2.16 | 0.46 |
| 1:AS:883:G:H2' | 1:AS:884:A:C8 | 2.50 | 0.46 |
| 1:AS:1444:U:H2' | 1:AS:1445:A:C8 | 2.51 | 0.46 |
| 1:AS:1617:A:H2' | 1:AS:1618:U:H6 | 1.79 | 0.46 |
| 21:BN:164:GLN:HG2 | 21:BN:166:THR:H | 1.80 | 0.46 |
| 24:BQ:38:ALA:HB3 | 24:BQ:59:MET:HB2 | 1.97 | 0.46 |
| 26:BS:105:VAL:HG23 | 26:BS:130:TYR:CG | 2.50 | 0.46 |
| 36:CC:118:ILE:HG22 | 36:CC:119:LYS:N | 2.30 | 0.46 |
| 46:CM:483:A:H2' | 46:CM:484:G:H8 | 1.80 | 0.46 |
| 46:CM:840:A:O2' | 46:CM:841:A:H3' | 2.15 | 0.46 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 46:CM:1637:U:H2' | 46:CM:1638:A:H8 | 1.78 | 0.46 |
| 46:CM:1714:G:H21 | 55:CV:32:GLN:HE21 | 1.63 | 0.46 |
| 51:CR:139:VAL:HG23 | 51:CR:150:PRO:HG3 | 1.97 | 0.46 |
| 52:CS:116:HIS:O | 52:CS:120:ILE:HG13 | 2.15 | 0.46 |
| 82:l1:33:GLU:H | 82:l1:208:SER:HA | 1.80 | 0.46 |
| 1:1:511:C:H5" | 6:l:344:LYS:HD2 | 1.98 | 0.46 |
| 1:1:716:G:O2' | 1:1:717:A:OP1 | 2.26 | 0.46 |
| 1:1:1020:G:H22 | 1:1:1023:A:H5" | 1.81 | 0.46 |
| 1:1:2873:G:O2' | 1:1:2996:A:N1 | 2.47 | 0.46 |
| 1:1:2919:G:N3 | 5:k:250:ALA:HB1 | 2.30 | 0.46 |
| 1:1:3038:U:H2' | 1:1:3039:C:C6 | 2.49 | 0.46 |
| 1:1:3125:U:H4' | 1:1:3126:U:O5' | 2.14 | 0.46 |
| 11:q:12:ILE:HB | 11:q:51:ARG:HA | 1.97 | 0.46 |
| 19:y:165:ILE:HD11 | 19:y:172:PHE:HB3 | 1.96 | 0.46 |
| 33:AF:97:ILE:HG21 | 33:AF:106:ARG:HG3 | 1.97 | 0.46 |
| 35:AH:109:GLN:OE1 | 35:AH:113:LYS:NZ | 2.49 | 0.46 |
| 39:AL:46:ARG:HD3 | 39:AL:47:GLY:O | 2.15 | 0.46 |
| 46:B:70:C:OP2 | 53:I:164:LYS:NZ | 2.48 | 0.46 |
| 46:B:119:A:H1' | 46:B:395:A:C5 | 2.50 | 0.46 |
| 46:B:335:G:H3' | 58:N:133:LYS:HB2 | 1.98 | 0.46 |
| 46:B:1485:G:H5" | 66:V:72:GLY:HA3 | 1.97 | 0.46 |
| 46:B:1668:A:H2' | 46:B:1669:U:H5' | 1.96 | 0.46 |
| 51:G:45:VAL:HA | 51:G:61:VAL:HG21 | 1.98 | 0.46 |
| 59:O:36:LEU:HG | 59:O:102:GLY:HA3 | 1.97 | 0.46 |
| 1:AS:762:U:H4' | 1:AS:763:U:O4' | 2.14 | 0.46 |
| 1:AS:777:G:OP1 | 19:BL:151:ARG:HD2 | 2.15 | 0.46 |
| 1:AS:1863:A:H2' | 1:AS:1864:G:H8 | 1.79 | 0.46 |
| 1:AS:3021:A:C5 | 5:AX:75:ALA:HB2 | 2.50 | 0.46 |
| 1:AS:3285:A:H2' | 1:AS:3286:C:H6 | 1.80 | 0.46 |
| 46:CM:696:U:OP1 | 46:CM:696:U:C6 | 2.65 | 0.46 |
| 46:CM:740:A:H2' | 46:CM:741:A:H8 | 1.81 | 0.46 |
| 55:CV:78:ILE:HD13 | 55:CV:104:ILE:HG22 | 1.97 | 0.46 |
| 61:DB:107:ILE:HG21 | 73:DN:53:LEU:HD11 | 1.97 | 0.46 |
| 65:DF:24:GLY:HA2 | 65:DF:58:ALA:HB3 | 1.96 | 0.46 |
| 72:DM:43:ASP:CG | 72:DM:44:GLN:H | 2.23 | 0.46 |
| 82:l1:144:LEU:HD23 | 82:l1:144:LEU:HA | 1.66 | 0.46 |
| 1:1:185:U:H3 | 1:1:229:C:H42 | 1.63 | 0.46 |
| 1:1:1020:G:H21 | 1:1:1023:A:H8 | 1.62 | 0.46 |
| 1:1:1466:U:H2' | 1:1:1467:U:C6 | 2.49 | 0.46 |
| 1:1:1713:U:H2' | 1:1:1714:G:H8 | 1.80 | 0.46 |
| 1:1:2871:C:N3 | 11:q:173:ARG:NH2 | 2.62 | 0.46 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 1:1:3016:A:H2' | 1:1:3017:G:C8 | 2.50 | 0.46 |
| 3:4:6:U:H2' | 3:4:7:U:C6 | 2.49 | 0.46 |
| 5:k:122:TRP:CE2 | 5:k:127:LYS:HE3 | 2.51 | 0.46 |
| 15:u:34:ASP:OD2 | 15:u:37:ARG:NH2 | 2.48 | 0.46 |
| 46:B:484:G:H2' | 46:B:485:G:C8 | 2.50 | 0.46 |
| 46:B:736:G:H2' | 46:B:737:A:C8 | 2.51 | 0.46 |
| 46:B:1675:U:O2' | 46:B:1700:G:N7 | 2.44 | 0.46 |
| 62:R:81:ARG:NH2 | 62:R:117:GLY:O | 2.48 | 0.46 |
| 65:U:24:GLY:HA2 | 65:U:58:ALA:HB3 | 1.96 | 0.46 |
| 66:V:74:GLY:HA2 | 66:V:77:ASN:HD22 | 1.79 | 0.46 |
| 67:W:81:TYR:HB3 | 76:f:52:PHE:HB3 | 1.97 | 0.46 |
| 74:d:36:LYS:HZ1 | 74:d:43:ILE:HD13 | 1.79 | 0.46 |
| 1:AS:546:C:H2' | 1:AS:547:U:O4' | 2.14 | 0.46 |
| 1:AS:3064:C:O2' | 1:AS:3066:A:OP2 | 2.33 | 0.46 |
| 7:AZ:235:ASP:OD1 | 7:AZ:235:ASP:N | 2.48 | 0.46 |
| 9:BB:135:GLY:N | 9:BB:233:ILE:HD12 | 2.30 | 0.46 |
| 17:BJ:160:LYS:O | 17:BJ:163:VAL:HG12 | 2.14 | 0.46 |
| 19:BL:158:HIS:NE2 | 19:BL:186:VAL:HG12 | 2.31 | 0.46 |
| 29:BV:95:SER:OG | 29:BV:96:ALA:N | 2.48 | 0.46 |
| 43:CJ:8:ARG:HG2 | 43:CJ:10:THR:HG23 | 1.96 | 0.46 |
| 46:CM:558:U:H2' | 46:CM:559:G:C8 | 2.49 | 0.46 |
| 46:CM:559:G:H2' | 46:CM:560:G:H8 | 1.80 | 0.46 |
| 46:CM:976:G:P | 61:DB:124:LYS:HD2 | 2.54 | 0.46 |
| 79:DT:70:GLN:OE1 | 79:DT:86:TRP:NE1 | 2.41 | 0.46 |
| 1:1:179:C:H2' | 1:1:180:U:H6 | 1.80 | 0.46 |
| 1:1:234:A:H2' | 1:1:235:G:O4' | 2.16 | 0.46 |
| 1:1:1569:C:H2' | 1:1:1570:A:C8 | 2.51 | 0.46 |
| 1:1:1684:U:H2' | 1:1:1685:U:C6 | 2.51 | 0.46 |
| 1:1:2367:C:O2' | 1:1:3272:A:N1 | 2.42 | 0.46 |
| 1:1:2431:U:C6 | 1:1:2439:A:H5" | 2.51 | 0.46 |
| 12:r:77:THR:HG22 | 12:r:82:ARG:HA | 1.98 | 0.46 |
| 46:B:261:C:O2' | 46:B:262:G:H5' | 2.16 | 0.46 |
| 46:B:444:A:H5" | 51:G:57:ASN:HD22 | 1.79 | 0.46 |
| 46:B:1145:A:H2' | 46:B:1146:C:H6 | 1.79 | 0.46 |
| 46:B:1757:U:H2' | 46:B:1758:U:C6 | 2.51 | 0.46 |
| 52:H:43:PHE:O | 52:H:44:ASN:C | 2.59 | 0.46 |
| 54:J:81:PHE:HB3 | 54:J:84:ARG:HG3 | 1.97 | 0.46 |
| 71:a:63:GLN:CD | 71:a:68:LYS:HD3 | 2.41 | 0.46 |
| 79:AR:261:LYS:HZ2 | 79:AR:268:LEU:HD13 | 1.80 | 0.46 |
| 1:AS:66:A:O2' | 1:AS:315:C:O2 | 2.31 | 0.46 |
| 1:AS:212:A:OP1 | 27:BT:2:ALA:N | 2.49 | 0.46 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 1:AS:364:G:OP1 | 6:AY:61:THR:HG23 | 2.15 | 0.46 |
| 1:AS:1329:C:OP1 | 19:BL:2:GLY:N | 2.48 | 0.46 |
| 1:AS:1632:C:H1' | 28:BU:76:ASN:HB2 | 1.98 | 0.46 |
| 1:AS:1949:G:N1 | 1:AS:2070:A:H2' | 2.31 | 0.46 |
| 1:AS:2130:A:H2' | 1:AS:2131:U:C6 | 2.51 | 0.46 |
| 1:AS:2967:A:H2' | 1:AS:2968:U:O4' | 2.16 | 0.46 |
| 1:AS:3067:U:H2' | 1:AS:3068:C:H6 | 1.79 | 0.46 |
| 3:AU:49:G:OP1 | 36:CC:45:HIS:HB2 | 2.15 | 0.46 |
| 10:BC:158:VAL:HG21 | 10:BC:164:VAL:CG2 | 2.46 | 0.46 |
| 39:CF:73:LEU:HD12 | 39:CF:75:ILE:HG23 | 1.96 | 0.46 |
| 45:CL:156:ALA:N | 57:CX:92:LEU:HD11 | 2.30 | 0.46 |
| 46:CM:769:U:O2' | 46:CM:770:C:OP2 | 2.33 | 0.46 |
| 46:CM:1187:A:N6 | 46:CM:1443:C:O5' | 2.48 | 0.46 |
| 46:CM:1477:U:H4' | 46:CM:1478:A:H5' | 1.98 | 0.46 |
| 46:CM:1672:G:H2' | 46:CM:1673:U:C6 | 2.51 | 0.46 |
| 51:CR:59:ARG:HH22 | 71:DL:87:PRO:HG3 | 1.80 | 0.46 |
| 51:CR:173:ILE:HD11 | 51:CR:236:TRP:CE2 | 2.50 | 0.46 |
| 82:L1:76:ARG:NH2 | 82:L1:139:SER:O | 2.49 | 0.46 |
| 82:l1:27:ASN:HB3 | 82:l1:28:PHE:HD1 | 1.80 | 0.46 |
| 1:1:1239:G:C2' | 1:1:1240:A:H5' | 2.45 | 0.46 |
| 3:4:7:U:H2' | 3:4:8:C:C6 | 2.51 | 0.46 |
| 4:j:147:ARG:HG2 | 4:j:157:ILE:HG12 | 1.97 | 0.46 |
| 7:m:119:TYR:OH | 7:m:135:VAL:HG22 | 2.16 | 0.46 |
| 22:2:44:ALA:HB2 | 22:2:53:PRO:HG2 | 1.97 | 0.46 |
| 46:B:391:C:H2' | 46:B:392:C:C6 | 2.50 | 0.46 |
| 46:B:485:G:N2 | 46:B:499:U:C2 | 2.84 | 0.46 |
| 46:B:521:G:OP2 | 71:a:37:LYS:NZ | 2.36 | 0.46 |
| 46:B:1409:U:OP1 | 50:F:152:LYS:NZ | 2.48 | 0.46 |
| 46:B:1701:A:H2' | 46:B:1702:A:H4' | 1.97 | 0.46 |
| 46:B:1783:C:H5 | 73:c:6:ALA:HB3 | 1.79 | 0.46 |
| 1:AS:538:G:H2' | 1:AS:539:G:C8 | 2.51 | 0.46 |
| 1:AS:638:U:OP1 | 29:BV:21:ARG:NH1 | 2.48 | 0.46 |
| 1:AS:1239:G:O2' | 1:AS:1240:A:H5' | 2.15 | 0.46 |
| 1:AS:2465:U:H4' | 1:AS:2466:A:OP2 | 2.13 | 0.46 |
| 3:AU:34:U:H4' | 36:CC:85:THR:HG21 | 1.97 | 0.46 |
| 15:BH:65:LEU:HD12 | 15:BH:77:LYS:HD2 | 1.97 | 0.46 |
| 42:CI:9:ARG:HH12 | 46:CM:1630:U:P | 2.39 | 0.46 |
| 46:CM:30:G:H2' | 46:CM:31:C:C6 | 2.51 | 0.46 |
| 46:CM:59:C:H5" | 46:CM:449:G:N2 | 2.31 | 0.46 |
| 46:CM:107:C:H2' | 46:CM:108:A:C8 | 2.51 | 0.46 |
| 46:CM:491:U:H3' | 46:CM:492:U:C6 | 2.51 | 0.46 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 46:CM:715:G:N2 | 46:CM:715:G:OP2 | 2.48 | 0.46 |
| 46:CM:1648:U:H2' | 46:CM:1649:G:H8 | 1.80 | 0.46 |
| 47:CN:13:ASP:CG | 47:CN:179:ARG:HH22 | 2.23 | 0.46 |
| 59:CZ:80:ASN:O | 59:CZ:82:PRO:CD | 2.58 | 0.46 |
| 59:CZ:103:LEU:O | 59:CZ:115:VAL:HG13 | 2.16 | 0.46 |
| 62:DC:34:THR:HG21 | 62:DC:45:PHE:CD2 | 2.51 | 0.46 |
| 64:DE:75:GLU:O | 64:DE:79:GLU:HB2 | 2.15 | 0.46 |
| 64:DE:81:LYS:N | 64:DE:83:GLN:OE1 | 2.49 | 0.46 |
| 78:DS:127:TYR:CD1 | 78:DS:128:THR:CG2 | 2.94 | 0.46 |
| 1:1:27:C:C2 | 1:1:56:A:C6 | 3.04 | 0.46 |
| 1:1:117:U:O2 | 1:1:120:A:H5" | 2.16 | 0.46 |
| 1:1:249:G:H2' | 1:1:251:G:OP2 | 2.15 | 0.46 |
| 1:1:533:G:H2' | 1:1:534:G:O4' | 2.16 | 0.46 |
| 1:1:1231:U:H1' | 1:1:1233:G:OP2 | 2.16 | 0.46 |
| 1:1:1309:G:O2' | 1:1:1314:A:N1 | 2.44 | 0.46 |
| 1:1:1695:A:C6 | 1:1:1743:G:C6 | 3.03 | 0.46 |
| 1:1:2988:A:H2' | 1:1:2989:A:C8 | 2.48 | 0.46 |
| 7:m:290:ILE:HG13 | 12:r:206:LEU:HD21 | 1.97 | 0.46 |
| 13:s:88:GLU:HB3 | 62:R:10:ARG:NH1 | 2.31 | 0.46 |
| 46:B:1612:C:H2' | 46:B:1613:U:H6 | 1.81 | 0.46 |
| 50:F:209:ILE:HD12 | 64:T:16:LEU:HD21 | 1.96 | 0.46 |
| 60:P:46:THR:OG1 | 60:P:49:GLN:HG3 | 2.16 | 0.46 |
| 66:V:108:LEU:HD12 | 66:V:108:LEU:HA | 1.82 | 0.46 |
| 1:AS:875:U:O2' | 18:BK:131:ARG:HD2 | 2.15 | 0.46 |
| 1:AS:1825:A:H5" | 1:AS:1826:G:H5' | 1.96 | 0.46 |
| 1:AS:2407:G:H2' | 1:AS:2408:A:C8 | 2.51 | 0.46 |
| 1:AS:2956:C:H2' | 1:AS:2957:C:H6 | 1.80 | 0.46 |
| 14:BG:143:VAL:HG13 | 14:BG:147:PHE:HD2 | 1.80 | 0.46 |
| 16:BI:94:TYR:OH | 16:BI:96:LYS:HE2 | 2.16 | 0.46 |
| 46:CM:839:U:O4 | 46:CM:840:A:N6 | 2.48 | 0.46 |
| 57:CX:77:ARG:NH1 | 57:CX:86:ILE:O | 2.47 | 0.46 |
| 59:CZ:135:ILE:HA | 59:CZ:138:GLU:OE2 | 2.15 | 0.46 |
| 62:DC:55:GLY:O | 62:DC:58:LYS:HG2 | 2.15 | 0.46 |
| 68:DI:53:TYR:OH | 68:DI:76:ASP:OD2 | 2.23 | 0.46 |
| 71:DL:10:ARG:NH1 | 71:DL:26:ASP:OD2 | 2.44 | 0.46 |
| 72:DM:61:SER:H | 72:DM:64:VAL:HB | 1.80 | 0.46 |
| 79:DT:40:LYS:HG2 | 79:DT:67:HIS:O | 2.16 | 0.46 |
| 79:DT:104:PHE:CD2 | 79:DT:139:GLY:HA2 | 2.51 | 0.46 |
| 79:DT:159:PRO:HD3 | 79:DT:201:LEU:CD1 | 2.45 | 0.46 |
| 1:1:337:G:O4' | 6:l:49:GLN:NE2 | 2.49 | 0.46 |
| 1:1:408:A:N3 | 1:1:653:C:O2' | 2.48 | 0.46 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 1:1:1076:A:H5' | 7:m:139:PRO:HB3 | 1.98 | 0.46 |
| 1:1:1142:C:H4' | 1:1:1327:U:C4 | 2.50 | 0.46 |
| 1:1:1163:U:H2' | 1:1:1164:U:O4' | 2.16 | 0.46 |
| 1:1:1377:A:C2 | 1:1:1422:C:C2 | 3.04 | 0.46 |
| 1:1:1482:G:N2 | 35:AH:6:THR:HG22 | 2.31 | 0.46 |
| 1:1:1746:A:H1' | 1:1:1748:A:N7 | 2.31 | 0.46 |
| 1:1:1834:C:H4' | 1:1:1835:A:O4' | 2.15 | 0.46 |
| 1:1:2221:A:H3' | 4:j:244:GLY:HA2 | 1.98 | 0.46 |
| 1:1:3082:C:H2' | 1:1:3083:U:C6 | 2.50 | 0.46 |
| 46:B:67:A:O2' | 46:B:69:G:OP1 | 2.33 | 0.46 |
| 46:B:366:U:H2' | 46:B:367:A:O4' | 2.16 | 0.46 |
| 46:B:553:A:H2' | 46:B:554:A:C8 | 2.51 | 0.46 |
| 46:B:1628:C:H2' | 46:B:1629:G:C8 | 2.50 | 0.46 |
| 55:K:67:TRP:NE1 | 55:K:191:GLU:OE2 | 2.45 | 0.46 |
| 79:AR:12:THR:O | 79:AR:53:ASN:HA | 2.16 | 0.46 |
| 79:AR:42:LEU:HD11 | 79:AR:83:SER:HB3 | 1.96 | 0.46 |
| 1:AS:515:A:N7 | 6:AY:361:LEU:HD11 | 2.31 | 0.46 |
| 1:AS:531:G:HO2' | 1:AS:552:G:H1 | 1.62 | 0.46 |
| 1:AS:787:A:H2' | 1:AS:788:G:C8 | 2.51 | 0.46 |
| 1:AS:1277:G:OP1 | 80:p0:55:LYS:HG2 | 2.16 | 0.46 |
| 1:AS:2339:A:H2' | 1:AS:2340:C:H6 | 1.81 | 0.46 |
| 6:AY:65:SER:HA | 6:AY:76:PRO:HA | 1.98 | 0.46 |
| 18:BK:29:THR:HA | 18:BK:32:THR:HG22 | 1.98 | 0.46 |
| 46:CM:703:U:H2' | 46:CM:704:A:N7 | 2.31 | 0.46 |
| 46:CM:904:A:H2' | 46:CM:905:C:H6 | 1.81 | 0.46 |
| 46:CM:1482:C:O2' | 46:CM:1506:U:O2 | 2.30 | 0.46 |
| 46:CM:1676:A:H1' | 46:CM:1700:G:C6 | 2.51 | 0.46 |
| 47:CN:79:ARG:O | 47:CN:83:GLN:HG3 | 2.15 | 0.46 |
| 50:CQ:109:LYS:HE3 | 50:CQ:114:LEU:HD22 | 1.98 | 0.46 |
| 55:CV:56:ARG:NH1 | 55:CV:180:GLY:O | 2.48 | 0.46 |
| 56:CW:31:ALA:HB2 | 56:CW:42:ILE:HD11 | 1.97 | 0.46 |
| 59:CZ:62:LEU:HG | 59:CZ:63:CYS:N | 2.31 | 0.46 |
| 81:12:151:ILE:H | 81:12:151:ILE:HD12 | 1.81 | 0.46 |
| 1:1:130:U:H2' | 1:1:131:C:C6 | 2.50 | 0.46 |
| 1:1:385:A:H2' | 1:1:386:A:C8 | 2.51 | 0.46 |
| 1:1:412:G:H2' | 1:1:413:U:C6 | 2.51 | 0.46 |
| 1:1:514:G:H2' | 1:1:516:U:H5' | 1.98 | 0.46 |
| 1:1:547:U:H2' | 1:1:548:G:C8 | 2.51 | 0.46 |
| 1:1:972:U:H2' | 1:1:973:C:O4' | 2.16 | 0.46 |
| 1:1:988:A:O2' | 1:1:989:G:H5' | 2.16 | 0.46 |
| 1:1:1255:A:N6 | 80:P0:53:MET:HE2 | 2.30 | 0.46 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 1:1:1916:U:O2' | 1:1:1928:A:N7 | 2.43 | 0.46 |
| 1:1:2601:U:O2 | 1:1:2621:G:N2 | 2.41 | 0.46 |
| 1:1:3300:A:H2' | 1:1:3301:A:C8 | 2.51 | 0.46 |
| 46:B:167:A:OP1 | 53:I:137:ARG:NE | 2.48 | 0.46 |
| 46:B:1552:C:H2' | 46:B:1553:U:H6 | 1.81 | 0.46 |
| 46:B:1669:U:O2' | 46:B:1670:U:H6 | 1.98 | 0.46 |
| 72:b:36:ALA:HB1 | 72:b:38:HIS:CE1 | 2.51 | 0.46 |
| 1:AS:270:U:H2' | 1:AS:271:C:H6 | 1.81 | 0.46 |
| 1:AS:2485:U:H2' | 1:AS:2486:U:C6 | 2.51 | 0.46 |
| 3:AU:156:U:O2' | 3:AU:157:U:P | 2.74 | 0.46 |
| 12:BE:77:THR:HG22 | 12:BE:82:ARG:HA | 1.97 | 0.46 |
| 13:BF:148:ILE:HG22 | 13:BF:152:HIS:HB3 | 1.97 | 0.46 |
| 25:BR:80:ARG:HH21 | 46:CM:163:G:H4' | 1.80 | 0.46 |
| 46:CM:801:A:O4' | 54:CU:106:GLN:NE2 | 2.49 | 0.46 |
| 46:CM:885:A:H2' | 46:CM:886:G:H8 | 1.81 | 0.46 |
| 46:CM:1012:A:OP1 | 46:CM:1776:G:O2' | 2.27 | 0.46 |
| 46:CM:1548:U:H2' | 46:CM:1549:G:H8 | 1.81 | 0.46 |
| 48:CO:115:ARG:HA | 48:CO:115:ARG:HD3 | 1.79 | 0.46 |
| 57:CX:92:LEU:HD23 | 57:CX:92:LEU:HA | 1.77 | 0.46 |
| 1:1:95:G:H2' | 1:1:96:U:O4' | 2.16 | 0.46 |
| 1:1:498:C:H2' | 1:1:499:G:C8 | 2.50 | 0.46 |
| 1:1:638:U:OP1 | 29:AB:21:ARG:NH1 | 2.47 | 0.46 |
| 1:1:663:A:OP1 | 16:v:203:ARG:HD2 | 2.16 | 0.46 |
| 1:1:712:G:N2 | 29:AB:72:GLU:OE1 | 2.49 | 0.46 |
| 1:1:798:C:H2' | 1:1:799:C:H6 | 1.80 | 0.46 |
| 1:1:1240:A:H5" | 1:1:1241:A:N7 | 2.31 | 0.46 |
| 1:1:1621:A:H4' | 1:1:1639:A:C5 | 2.51 | 0.46 |
| 1:1:2130:A:H2' | 1:1:2131:U:C6 | 2.50 | 0.46 |
| 16:v:27:CYS:HB2 | 16:v:122:ASN:HD21 | 1.78 | 0.46 |
| 21:0:44:PHE:O | 21:0:48:LEU:HD12 | 2.16 | 0.46 |
| 22:2:80:VAL:O | 22:2:83:ARG:NH1 | 2.49 | 0.46 |
| 32:AE:45:THR:HG22 | 32:AE:47:ASP:N | 2.28 | 0.46 |
| 45:i:77:GLN:HE22 | 46:B:1165:C:H5' | 1.80 | 0.46 |
| 46:B:339:A:H2' | 46:B:340:C:C6 | 2.50 | 0.46 |
| 46:B:583:A:H2' | 46:B:584:G:C8 | 2.50 | 0.46 |
| 46:B:870:G:P | 48:D:136:ARG:HH11 | 2.39 | 0.46 |
| 46:B:1102:U:H2' | 46:B:1103:G:C8 | 2.51 | 0.46 |
| 46:B:1254:U:H5' | 46:B:1418:U:OP2 | 2.16 | 0.46 |
| 46:B:1548:U:H2' | 46:B:1549:G:H8 | 1.81 | 0.46 |
| 46:B:1597:G:H5" | 52:H:107:LYS:HD2 | 1.98 | 0.46 |
| 53:I:161:GLU:HA | 53:I:170:THR:HA | 1.97 | 0.46 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 67:W:68:LYS:O | 76:f:44:ARG:NH1 | 2.48 | 0.46 |
| 79:AR:145:LEU:HD13 | 79:AR:178:TRP:CD2 | 2.51 | 0.46 |
| 1:AS:67:C:N4 | 1:AS:314:U:O2' | 2.49 | 0.46 |
| 1:AS:126:G:H2' | 1:AS:127:G:H8 | 1.81 | 0.46 |
| 1:AS:1761:U:H5 | 20:BM:43:LYS:HE3 | 1.80 | 0.46 |
| 1:AS:2434:A:H2' | 1:AS:2435:G:C8 | 2.51 | 0.46 |
| 1:AS:2645:A:H5" | 13:BF:95:ASN:HD22 | 1.81 | 0.46 |
| 4:AW:54:ARG:HD2 | 4:AW:56:ALA:HB3 | 1.97 | 0.46 |
| 11:BD:113:GLU:CD | 11:BD:115:ARG:HE | 2.24 | 0.46 |
| 13:BF:106:ILE:HD11 | 13:BF:125:MET:HB3 | 1.97 | 0.46 |
| 21:BN:12:ARG:HB3 | 21:BN:24:LEU:HD23 | 1.97 | 0.46 |
| 27:BT:31:LEU:HB3 | 27:BT:101:PRO:HG2 | 1.98 | 0.46 |
| 33:BZ:98:ALA:HB3 | 33:BZ:101:VAL:HG23 | 1.97 | 0.46 |
| 45:CL:112:LYS:C | 45:CL:114:GLU:H | 2.23 | 0.46 |
| 46:CM:195:A:N6 | 55:CV:144:LYS:HD3 | 2.31 | 0.46 |
| 46:CM:341:C:H2' | 46:CM:342:A:H8 | 1.80 | 0.46 |
| 46:CM:511:U:H5' | 56:CW:133:HIS:CE1 | 2.51 | 0.46 |
| 46:CM:770:C:OP1 | 46:CM:770:C:H6 | 1.99 | 0.46 |
| 46:CM:872:A:H2' | 46:CM:873:U:H6 | 1.79 | 0.46 |
| 46:CM:1071:A:H2' | 46:CM:1072:A:C8 | 2.50 | 0.46 |
| 46:CM:1133:C:O2' | 46:CM:1752:A:N1 | 2.47 | 0.46 |
| 51:CR:151:ASP:HB3 | 51:CR:154:ILE:HG13 | 1.97 | 0.46 |
| 51:CR:158:ASP:OD1 | 51:CR:175:PHE:N | 2.45 | 0.46 |
| 75:DP:12:VAL:CG2 | 75:DP:52:ASP:H | 2.26 | 0.46 |
| 1:1:157:G:H2' | 1:1:158:A:H8 | 1.81 | 0.45 |
| 1:1:243:G:H2' | 1:1:244:G:H8 | 1.81 | 0.45 |
| 1:1:1099:A:N6 | 1:1:1359:A:H1' | 2.31 | 0.45 |
| 1:1:1208:A:O3' | 21:0:92:LYS:NZ | 2.48 | 0.45 |
| 1:1:1552:C:O2' | 10:p:55:GLU:OE2 | 2.34 | 0.45 |
| 1:1:3047:G:H5" | 32:AE:61:ARG:O | 2.16 | 0.45 |
| 1:1:3153:A:H2 | 1:1:3158:G:H4' | 1.80 | 0.45 |
| 4:j:247:ARG:HB3 | 46:B:997:U:H4' | 1.98 | 0.45 |
| 40:AM:9:THR:O | 40:AM:13:LEU:HG | 2.17 | 0.45 |
| 46:B:702:G:H1' | 46:B:703:U:C1' | 2.44 | 0.45 |
| 46:B:1597:G:N7 | 63:S:13:LYS:NZ | 2.63 | 0.45 |
| 46:B:1649:G:H2' | 46:B:1650:G:C8 | 2.49 | 0.45 |
| 46:B:1739:U:H2' | 46:B:1740:A:H8 | 1.81 | 0.45 |
| 62:R:80:LEU:HD12 | 62:R:80:LEU:O | 2.15 | 0.45 |
| 1:AS:868:U:H2' | 1:AS:869:C:C6 | 2.51 | 0.45 |
| 1:AS:2435:G:N1 | 1:AS:2439:A:N6 | 2.63 | 0.45 |
| 3:AU:155:G:C5 | 3:AU:156:U:C4 | 3.04 | 0.45 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 7:AZ:41:LYS:HD3 | 7:AZ:41:LYS:HA | 1.80 | 0.45 |
| 21:BN:171:PHE:O | 21:BN:172:TYR:HB2 | 2.16 | 0.45 |
| 35:CB:58:ARG:CD | 35:CB:59:PRO:HD2 | 2.37 | 0.45 |
| 46:CM:415:A:H5' | 46:CM:416:G:C5 | 2.50 | 0.45 |
| 46:CM:497:U:O2' | 46:CM:498:C:H5' | 2.16 | 0.45 |
| 46:CM:1191:U:OP2 | 46:CM:1192:C:O2' | 2.22 | 0.45 |
| 46:CM:1308:C:H2' | 46:CM:1309:G:O4' | 2.16 | 0.45 |
| 46:CM:1396:A:HO2' | 46:CM:1397:A:P | 2.39 | 0.45 |
| 70:DK:107:PHE:HE1 | 70:DK:120:VAL:HG12 | 1.80 | 0.45 |
| 82:l1:37:GLY:N | 82:l1:203:SER:O | 2.49 | 0.45 |
| 1:1:72:A:C4 | 37:AJ:14:ARG:HD2 | 2.51 | 0.45 |
| 1:1:713:A:HO2' | 1:1:748:C:HO2' | 1.64 | 0.45 |
| 1:1:883:G:H2' | 1:1:884:A:C8 | 2.51 | 0.45 |
| 1:1:1617:A:H2' | 1:1:1618:U:H6 | 1.81 | 0.45 |
| 1:1:1852:C:H2' | 1:1:1853:C:C6 | 2.51 | 0.45 |
| 1:1:2079:C:O2' | 1:1:2080:U:H6 | 1.99 | 0.45 |
| 1:1:3190:C:C2 | 1:1:3191:A:C8 | 3.04 | 0.45 |
| 1:1:3218:U:H2' | 1:1:3219:G:C8 | 2.52 | 0.45 |
| 2:3:113:C:H2' | 2:3:114:U:O4' | 2.15 | 0.45 |
| 3:4:142:C:H2' | 3:4:143:U:H6 | 1.81 | 0.45 |
| 20:z:165:ARG:CD | 46:B:835:A:C5' | 2.86 | 0.45 |
| 33:AF:67:LEU:HD23 | 33:AF:73:LYS:HG3 | 1.98 | 0.45 |
| 38:AK:28:HIS:HB3 | 38:AK:31:LYS:HB2 | 1.97 | 0.45 |
| 46:B:608:G:H21 | 70:Z:19:ARG:HH22 | 1.63 | 0.45 |
| 46:B:1318:C:H2' | 46:B:1319:U:C6 | 2.51 | 0.45 |
| 46:B:1609:G:H2' | 46:B:1610:C:H6 | 1.81 | 0.45 |
| 46:B:1704:C:C2 | 46:B:1705:G:C8 | 3.04 | 0.45 |
| 47:C:118:PRO:HG2 | 47:C:141:ILE:HD13 | 1.98 | 0.45 |
| 51:G:59:ARG:NH1 | 71:a:87:PRO:HG3 | 2.30 | 0.45 |
| 65:U:49:LYS:HD3 | 65:U:49:LYS:HA | 1.72 | 0.45 |
| 79:AR:40:LYS:HD2 | 79:AR:65:HIS:O | 2.16 | 0.45 |
| 79:AR:156:ARG:HD3 | 79:AR:156:ARG:HA | 1.84 | 0.45 |
| 1:AS:178:U:H2' | 1:AS:179:C:H6 | 1.81 | 0.45 |
| 1:AS:3044:C:H2' | 1:AS:3045:A:O4' | 2.16 | 0.45 |
| 7:AZ:40:HIS:CE1 | 7:AZ:42:ALA:HB3 | 2.51 | 0.45 |
| 10:BC:90:GLN:O | 10:BC:93:LYS:HG2 | 2.15 | 0.45 |
| 15:BH:57:LEU:HG | 21:BN:172:TYR:OH | 2.16 | 0.45 |
| 40:CG:23:LEU:HD12 | 40:CG:24:PRO:HD2 | 1.98 | 0.45 |
| 46:CM:244:G:N2 | 58:CY:38:VAL:O | 2.44 | 0.45 |
| 46:CM:814:A:H2' | 46:CM:814:A:OP2 | 2.16 | 0.45 |
| 46:CM:1205:C:H2' | 46:CM:1206:A:C8 | 2.50 | 0.45 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 46:CM:1220:C:H5 | 78:DS:180:ARG:NE | 2.13 | 0.45 |
| 46:CM:1396:A:O2' | 46:CM:1397:A:OP1 | 2.29 | 0.45 |
| 46:CM:1519:U:P | 72:DM:77:ARG:HH11 | 2.39 | 0.45 |
| 46:CM:1656:U:H2' | 46:CM:1657:G:O4' | 2.17 | 0.45 |
| 57:CX:55:VAL:HG12 | 57:CX:68:LEU:HA | 1.98 | 0.45 |
| 79:DT:65:HIS:CE1 | 79:DT:83:SER:HG | 2.33 | 0.45 |
| 79:DT:88:ARG:HA | 79:DT:111:VAL:HG23 | 1.98 | 0.45 |
| 80:P0:30:VAL:HB | 80:P0:33:VAL:HG21 | 1.96 | 0.45 |
| 80:P0:96:ILE:O | 80:P0:99:ILE:HG13 | 2.16 | 0.45 |
| 1:1:269:G:H5' | 16:v:120:TRP:CE3 | 2.52 | 0.45 |
| 1:1:781:G:N2 | 1:1:782:A:H62 | 2.14 | 0.45 |
| 1:1:1329:C:C2 | 1:1:1330:U:C5 | 3.04 | 0.45 |
| 1:1:1872:U:OP1 | 20:z:19:LYS:NZ | 2.47 | 0.45 |
| 1:1:3228:G:H2' | 1:1:3229:G:H8 | 1.80 | 0.45 |
| 15:u:19:VAL:HG11 | 15:u:55:ILE:HD12 | 1.98 | 0.45 |
| 45:i:108:GLY:HA3 | 50:F:117:ARG:HG3 | 1.99 | 0.45 |
| 46:B:154:A:H2' | 46:B:155:A:O4' | 2.16 | 0.45 |
| 46:B:349:C:OP1 | 46:B:628:A:O2' | 2.31 | 0.45 |
| 46:B:673:A:C5 | 46:B:674:C:C2 | 3.04 | 0.45 |
| 46:B:857:G:H2' | 46:B:858:U:O4' | 2.16 | 0.45 |
| 46:B:872:A:H2' | 46:B:873:U:C6 | 2.52 | 0.45 |
| 46:B:1102:U:H2' | 46:B:1103:G:H8 | 1.81 | 0.45 |
| 46:B:1238:U:C2 | 46:B:1239:U:C5 | 3.04 | 0.45 |
| 46:B:1277:G:H2' | 46:B:1278:U:C6 | 2.52 | 0.45 |
| 46:B:1347:U:H1' | 46:B:1348:U:O2 | 2.17 | 0.45 |
| 46:B:1596:U:OP1 | 63:S:75:SER:N | 2.40 | 0.45 |
| 46:B:1636:C:H2' | 46:B:1637:U:H6 | 1.81 | 0.45 |
| 46:B:1714:G:N2 | 55:K:32:GLN:OE1 | 2.41 | 0.45 |
| 47:C:117:GLU:HB2 | 49:E:35:LYS:HE2 | 1.98 | 0.45 |
| 50:F:159:ILE:HG23 | 50:F:165:THR:HG22 | 1.98 | 0.45 |
| 57:M:47:GLN:O | 57:M:51:SER:HB3 | 2.15 | 0.45 |
| 57:M:77:ARG:NH2 | 57:M:86:ILE:HA | 2.31 | 0.45 |
| 64:T:6:THR:HG23 | 64:T:8:THR:HG22 | 1.98 | 0.45 |
| 78:h:180:ARG:HA | 78:h:190:LEU:O | 2.17 | 0.45 |
| 1:AS:154:G:H5" | 1:AS:155:A:H2' | 1.97 | 0.45 |
| 1:AS:835:C:H4' | 1:AS:1720:U:H2' | 1.97 | 0.45 |
| 1:AS:925:A:H2' | 1:AS:926:U:C6 | 2.52 | 0.45 |
| 1:AS:2065:C:H5' | 1:AS:2066:G:OP2 | 2.16 | 0.45 |
| 1:AS:2584:U:H2' | 1:AS:2585:U:O4' | 2.17 | 0.45 |
| 1:AS:2719:A:H2' | 1:AS:2720:A:C8 | 2.50 | 0.45 |
| 1:AS:3005:A:H2' | 1:AS:3006:C:H6 | 1.82 | 0.45 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 1:AS:3013:U:H2' | 1:AS:3014:U:C6 | 2.51 | 0.45 |
| 1:AS:3110:U:OP1 | 5:AX:274:HIS:ND1 | 2.44 | 0.45 |
| 3:AU:69:U:H3 | 3:AU:89:A:H61 | 1.65 | 0.45 |
| 4:AW:79:ASN:ND2 | 4:AW:165:VAL:HG12 | 2.32 | 0.45 |
| 27:BT:27:ARG:NH1 | 27:BT:76:LEU:HA | 2.32 | 0.45 |
| 27:BT:85:LEU:HD23 | 27:BT:85:LEU:HA | 1.81 | 0.45 |
| 39:CF:16:ARG:HG3 | 39:CF:70:PRO:CG | 2.46 | 0.45 |
| 46:CM:65:A:H8 | 46:CM:65:A:H5" | 1.81 | 0.45 |
| 46:CM:368:A:H2' | 46:CM:369:G:C8 | 2.51 | 0.45 |
| 46:CM:740:A:O2' | 46:CM:741:A:OP1 | 2.33 | 0.45 |
| 46:CM:974:U:H2' | 46:CM:975:C:C6 | 2.51 | 0.45 |
| 46:CM:983:A:N6 | 46:CM:989:U:OP2 | 2.50 | 0.45 |
| 46:CM:1181:A:OP2 | 46:CM:1450:G:N2 | 2.40 | 0.45 |
| 46:CM:1305:U:O2 | 46:CM:1307:A:H5' | 2.17 | 0.45 |
| 48:CO:53:GLY:O | 48:CO:55:LYS:N | 2.41 | 0.45 |
| 50:CQ:59:VAL:HG12 | 50:CQ:60:LEU:HD12 | 1.98 | 0.45 |
| 54:CU:14:GLU:HA | 54:CU:42:ILE:HD12 | 1.97 | 0.45 |
| 58:CY:101:GLU:OE1 | 70:DK:16:ARG:NH2 | 2.50 | 0.45 |
| 59:CZ:132:GLU:OE1 | 59:CZ:132:GLU:N | 2.46 | 0.45 |
| 65:DF:29:MET:HB2 | 65:DF:54:LEU:HD23 | 1.98 | 0.45 |
| 65:DF:132:LYS:NZ | 65:DF:141:THR:OG1 | 2.50 | 0.45 |
| 67:DH:81:TYR:HB3 | 76:DQ:52:PHE:HB3 | 1.97 | 0.45 |
| 79:DT:26:THR:CG2 | 79:DT:74:ILE:HG21 | 2.46 | 0.45 |
| 80:P0:52:LEU:HD22 | 80:P0:88:PHE:HE2 | 1.78 | 0.45 |
| 82:l1:201:VAL:HB | 82:l1:217:TYR:HE2 | 1.80 | 0.45 |
| 1:1:62:A:H5" | 16:v:174:ILE:HG21 | 1.99 | 0.45 |
| 1:1:712:G:H1 | 29:AB:72:GLU:CD | 2.23 | 0.45 |
| 1:1:942:U:H2' | 1:1:943:G:H8 | 1.81 | 0.45 |
| 1:1:1434:U:H2' | 1:1:1435:U:C6 | 2.51 | 0.45 |
| 1:1:1478:A:H4' | 1:1:1479:G:OP2 | 2.16 | 0.45 |
| 4:j:211:HIS:CD2 | 4:j:219:ILE:HG23 | 2.52 | 0.45 |
| 8:n:164:SER:OG | 8:n:166:LYS:NZ | 2.49 | 0.45 |
| 31:AD:101:ASP:OD1 | 31:AD:101:ASP:N | 2.49 | 0.45 |
| 46:B:415:A:H5' | 46:B:416:G:C4 | 2.52 | 0.45 |
| 46:B:789:U:O4 | 54:J:100:ARG:NH2 | 2.47 | 0.45 |
| 46:B:913:U:OP1 | 73:c:19:LYS:HE3 | 2.17 | 0.45 |
| 46:B:1610:C:H2' | 46:B:1611:C:C6 | 2.51 | 0.45 |
| 59:O:55:ARG:HH22 | 59:O:81:GLU:CD | 2.24 | 0.45 |
| 64:T:100:LEU:HB3 | 64:T:102:ILE:HG23 | 1.99 | 0.45 |
| 1:AS:173:C:H2' | 1:AS:174:C:C6 | 2.52 | 0.45 |
| 1:AS:248:U:H2' | 1:AS:249:G:H4' | 1.97 | 0.45 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 1:AS:413:U:H2' | 1:AS:414:U:H6 | 1.81 | 0.45 |
| 1:AS:699:G:H2' | 1:AS:700:C:H6 | 1.80 | 0.45 |
| 1:AS:941:C:H2' | 1:AS:942:U:H6 | 1.80 | 0.45 |
| 1:AS:1029:U:H2' | 1:AS:1030:U:C6 | 2.52 | 0.45 |
| 1:AS:1116:A:H2' | 1:AS:1117:U:C6 | 2.51 | 0.45 |
| 1:AS:3199:G:H1 | 1:AS:3218:U:H3 | 1.63 | 0.45 |
| 1:AS:3218:U:H2' | 1:AS:3219:G:C8 | 2.51 | 0.45 |
| 6:AY:262:VAL:HA | 6:AY:271:ILE:HG12 | 1.99 | 0.45 |
| 17:BJ:86:ARG:HG3 | 17:BJ:100:LEU:HD11 | 1.97 | 0.45 |
| 46:CM:432:G:OP1 | 70:DK:78:LYS:HA | 2.16 | 0.45 |
| 46:CM:695:C:H1' | 46:CM:696:U:P | 2.57 | 0.45 |
| 46:CM:823:G:H4' | 46:CM:824:U:OP2 | 2.16 | 0.45 |
| 46:CM:852:G:H5" | 60:DA:4:MET:HE2 | 1.98 | 0.45 |
| 46:CM:1611:C:H2' | 46:CM:1612:C:H6 | 1.81 | 0.45 |
| 55:CV:37:LYS:HA | 55:CV:37:LYS:HD2 | 1.87 | 0.45 |
| 70:DK:107:PHE:CE1 | 70:DK:120:VAL:HG12 | 2.52 | 0.45 |
| 82:L1:55:LEU:HD13 | 82:L1:182:GLN:HE21 | 1.82 | 0.45 |
| 82:L1:70:ASP:HB3 | 82:L1:87:VAL:HG21 | 1.98 | 0.45 |
| 82:l1:19:TYR:CD2 | 82:l1:210:MET:HB3 | 2.51 | 0.45 |
| 80:p0:48:ASP:N | 80:p0:48:ASP:OD1 | 2.39 | 0.45 |
| 1:1:126:G:H2' | 1:1:127:G:H8 | 1.81 | 0.45 |
| 1:1:531:G:O2' | 1:1:552:G:N1 | 2.44 | 0.45 |
| 1:1:814:C:H2' | 1:1:815:U:O4' | 2.16 | 0.45 |
| 1:1:1559:C:O2' | 1:1:1560:U:OP1 | 2.25 | 0.45 |
| 1:1:1714:G:H2' | 1:1:1715:G:H8 | 1.82 | 0.45 |
| 1:1:1800:A:H2' | 1:1:1801:C:H6 | 1.81 | 0.45 |
| 1:1:2655:U:H2' | 1:1:2656:C:H6 | 1.80 | 0.45 |
| 1:1:2978:A:C2 | 1:1:3113:A:C4 | 3.04 | 0.45 |
| 5:k:214:MET:HE2 | 5:k:350:ALA:HA | 1.98 | 0.45 |
| 5:k:283:TYR:CZ | 5:k:325:LYS:HB2 | 2.52 | 0.45 |
| 17:w:160:LYS:O | 17:w:164:GLN:HG3 | 2.16 | 0.45 |
| 28:AA:85:TYR:OH | 35:AH:97:GLU:OE2 | 2.24 | 0.45 |
| 46:B:231:C:H4' | 46:B:232:G:C2 | 2.52 | 0.45 |
| 46:B:302:U:H2' | 46:B:303:C:H6 | 1.80 | 0.45 |
| 46:B:411:U:H2' | 46:B:412:C:C6 | 2.52 | 0.45 |
| 46:B:446:C:OP1 | 51:G:29:PRO:HD3 | 2.17 | 0.45 |
| 46:B:840:A:O2' | 46:B:841:A:H3' | 2.17 | 0.45 |
| 47:C:41:ARG:HG2 | 47:C:42:PRO:HD2 | 1.98 | 0.45 |
| 60:P:25:TRP:CE3 | 74:d:82:LYS:HE3 | 2.51 | 0.45 |
| 1:AS:716:G:O2' | 1:AS:717:A:OP1 | 2.30 | 0.45 |
| 1:AS:972:U:H2' | 1:AS:973:C:O4' | 2.16 | 0.45 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 1:AS:1186:A:H4' | 41:CH:37:ARG:NH2 | 2.32 | 0.45 |
| 1:AS:1206:U:H5" | 11:BD:62:ARG:HD3 | 1.97 | 0.45 |
| 1:AS:2257:A:C8 | 1:AS:2266:G:C8 | 3.05 | 0.45 |
| 1:AS:2407:G:H2' | 1:AS:2408:A:H8 | 1.82 | 0.45 |
| 1:AS:2420:G:H1 | 1:AS:2483:U:H3 | 1.62 | 0.45 |
| 1:AS:2460:U:H2' | 1:AS:2461:G:C8 | 2.51 | 0.45 |
| 1:AS:2814:U:OP1 | 1:AS:2816:C:N4 | 2.49 | 0.45 |
| 6:AY:186:LYS:HE3 | 6:AY:200:PHE:HB3 | 1.97 | 0.45 |
| 13:BF:32:ARG:HD2 | 13:BF:120:ILE:HA | 1.98 | 0.45 |
| 46:CM:58:U:O2' | 46:CM:449:G:N3 | 2.50 | 0.45 |
| 46:CM:191:U:H4' | 46:CM:192:U:H5' | 1.99 | 0.45 |
| 46:CM:260:U:O2' | 46:CM:261:C:H5' | 2.17 | 0.45 |
| 46:CM:826:U:C2' | 46:CM:827:C:H5' | 2.45 | 0.45 |
| 46:CM:977:A:O2' | 46:CM:1772:U:O2 | 2.34 | 0.45 |
| 46:CM:1725:U:H2' | 46:CM:1726:C:C6 | 2.51 | 0.45 |
| 47:CN:157:ASP:O | 68:DI:66:ASP:HA | 2.17 | 0.45 |
| 51:CR:123:LEU:HD23 | 51:CR:159:THR:HG21 | 1.98 | 0.45 |
| 82:L1:55:LEU:HB2 | 82:L1:153:SER:HB2 | 1.98 | 0.45 |
| 82:l1:196:LYS:HD2 | 82:l1:200:ASN:HD21 | 1.81 | 0.45 |
| 1:1:14:C:H5" | 26:8:42:ARG:HG3 | 1.99 | 0.45 |
| 1:1:273:A:H2' | 1:1:274:G:C8 | 2.51 | 0.45 |
| 1:1:908:G:H2' | 1:1:910:A:N7 | 2.31 | 0.45 |
| 1:1:922:A:H2' | 1:1:923:C:C6 | 2.52 | 0.45 |
| 1:1:964:G:H2' | 1:1:965:C:H6 | 1.82 | 0.45 |
| 1:1:981:U:H2' | 1:1:982:U:H6 | 1.80 | 0.45 |
| 1:1:1011:C:O5' | 1:1:1011:C:H6 | 2.00 | 0.45 |
| 1:1:1233:G:N2 | 81:12:138:SER:HB2 | 2.32 | 0.45 |
| 1:1:1494:A:H2' | 1:1:1495:U:C6 | 2.52 | 0.45 |
| 1:1:1777:C:H2' | 1:1:1778:U:C6 | 2.51 | 0.45 |
| 1:1:2469:A:H5' | 1:1:2470:C:OP2 | 2.17 | 0.45 |
| 1:1:2646:A:C2 | 13:s:124:GLY:HA3 | 2.51 | 0.45 |
| 6:l:4:ARG:HH12 | 6:l:25:ALA:HA | 1.82 | 0.45 |
| 16:v:48:ALA:HA | 16:v:133:ILE:HD11 | 1.99 | 0.45 |
| 34:AG:35:VAL:HG12 | 34:AG:79:GLY:HA3 | 1.99 | 0.45 |
| 36:AI:3:GLY:HA3 | 36:AI:50:ASN:OD1 | 2.17 | 0.45 |
| 46:B:404:U:H2' | 46:B:405:A:H8 | 1.82 | 0.45 |
| 46:B:521:G:H5' | 71:a:60:PHE:O | 2.17 | 0.45 |
| 46:B:611:G:OP2 | 46:B:1084:U:O2' | 2.30 | 0.45 |
| 46:B:1235:U:O2' | 78:h:177:MET:HB3 | 2.16 | 0.45 |
| 46:B:1419:G:O2' | 76:f:24:CYS:SG | 2.68 | 0.45 |
| 51:G:194:VAL:HG11 | 51:G:232:ALA:HB2 | 1.97 | 0.45 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 52:H:122:HIS:HB2 | 52:H:129:PRO:HG3 | 1.97 | 0.45 |
| 63:S:39:GLN:OE1 | 63:S:39:GLN:N | 2.42 | 0.45 |
| 78:h:182:TYR:CE1 | 78:h:187:HIS:HA | 2.51 | 0.45 |
| 1:AS:1182:G:N3 | 21:BN:112:ALA:HB1 | 2.32 | 0.45 |
| 1:AS:1374:U:H2' | 1:AS:1375:G:H8 | 1.80 | 0.45 |
| 1:AS:2639:A:N6 | 1:AS:2659:G:O2' | 2.50 | 0.45 |
| 2:AT:7:G:O3' | 7:AZ:33:ARG:NH2 | 2.49 | 0.45 |
| 3:AU:2:A:C4 | 3:AU:3:A:C8 | 3.05 | 0.45 |
| 16:BI:36:ILE:HG12 | 16:BI:64:ILE:HG13 | 1.99 | 0.45 |
| 23:BP:12:VAL:HB | 23:BP:68:VAL:O | 2.16 | 0.45 |
| 23:BP:60:SER:OG | 23:BP:61:ASP:OD1 | 2.21 | 0.45 |
| 46:CM:78:A:H5' | 53:CT:154:ARG:O | 2.17 | 0.45 |
| 46:CM:457:G:OP2 | 71:DL:105:ARG:NH2 | 2.42 | 0.45 |
| 46:CM:526:U:H2' | 46:CM:527:A:O4' | 2.17 | 0.45 |
| 46:CM:985:C:H6 | 46:CM:988:A:H8 | 1.64 | 0.45 |
| 46:CM:992:C:OP1 | 61:DB:130:ARG:HA | 2.16 | 0.45 |
| 46:CM:1425:C:H2' | 46:CM:1426:C:H6 | 1.81 | 0.45 |
| 52:CS:143:ARG:HG2 | 75:DP:55:CYS:SG | 2.57 | 0.45 |
| 53:CT:88:ARG:HG3 | 53:CT:91:GLU:HB2 | 1.98 | 0.45 |
| 64:DE:90:ALA:HA | 64:DE:95:HIS:CD2 | 2.51 | 0.45 |
| 82:L1:37:GLY:O | 82:L1:202:GLY:HA3 | 2.16 | 0.45 |
| 82:L1:59:PRO:HD3 | 82:L1:153:SER:HA | 1.98 | 0.45 |
| 1:1:206:U:H2' | 1:1:207:C:H6 | 1.81 | 0.45 |
| 1:1:762:U:H4' | 1:1:763:U:O4' | 2.16 | 0.45 |
| 1:1:1519:U:OP1 | 1:1:1603:U:N3 | 2.41 | 0.45 |
| 1:1:1800:A:H2' | 1:1:1801:C:C6 | 2.52 | 0.45 |
| 1:1:2590:G:OP2 | 30:AC:3:LYS:HE3 | 2.16 | 0.45 |
| 1:1:2828:G:H2' | 1:1:2829:C:C6 | 2.52 | 0.45 |
| 1:1:2902:A:H2' | 1:1:2903:C:H6 | 1.82 | 0.45 |
| 1:1:3293:G:OP1 | 5:k:385:LYS:HE3 | 2.17 | 0.45 |
| 6:l:182:VAL:HG11 | 6:l:225:GLY:HA3 | 1.99 | 0.45 |
| 8:n:135:VAL:O | 8:n:139:LYS:HD3 | 2.17 | 0.45 |
| 13:s:52:TYR:HA | 13:s:61:ARG:HG3 | 1.98 | 0.45 |
| 20:z:159:ALA:HB1 | 20:z:163:ARG:HH22 | 1.81 | 0.45 |
| 46:B:569:G:H5" | 70:Z:114:LYS:CE | 2.46 | 0.45 |
| 46:B:598:U:P | 70:Z:108:GLY:HA2 | 2.57 | 0.45 |
| 46:B:672:U:OP2 | 46:B:672:U:H3' | 2.17 | 0.45 |
| 46:B:1150:G:H2' | 46:B:1151:A:C8 | 2.52 | 0.45 |
| 50:F:24:GLU:OE1 | 76:f:23:HIS:HE1 | 2.00 | 0.45 |
| 56:L:37:LYS:HA | 77:g:33:ARG:HA | 1.99 | 0.45 |
| 75:e:35:ASP:O | 75:e:37:SER:N | 2.48 | 0.45 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 1:AS:1921:U:O4 | 1:AS:2297:U:O2' | 2.33 | 0.45 |
| 1:AS:2290:A:OP1 | 1:AS:2292:U:H5 | 2.00 | 0.45 |
| 1:AS:2796:G:H2' | 1:AS:2797:C:H6 | 1.81 | 0.45 |
| 1:AS:2852:U:OP1 | 24:BQ:47:ASN:ND2 | 2.47 | 0.45 |
| 3:AU:5:U:H2' | 3:AU:6:U:C6 | 2.52 | 0.45 |
| 11:BD:180:TYR:CD1 | 41:CH:13:TYR:HD2 | 2.33 | 0.45 |
| 28:BU:41:ALA:HB2 | 28:BU:77:TYR:HE1 | 1.82 | 0.45 |
| 46:CM:243:U:O2' | 46:CM:245:A:N7 | 2.48 | 0.45 |
| 46:CM:283:G:H2' | 46:CM:284:C:C6 | 2.51 | 0.45 |
| 46:CM:852:G:H21 | 60:DA:87:ASP:CG | 2.24 | 0.45 |
| 46:CM:1739:U:H2' | 46:CM:1740:A:C8 | 2.52 | 0.45 |
| 50:CQ:105:ALA:O | 50:CQ:109:LYS:HG2 | 2.16 | 0.45 |
| 50:CQ:128:MET:HE3 | 50:CQ:155:ASP:HB3 | 1.99 | 0.45 |
| 50:CQ:140:SER:O | 50:CQ:184:GLY:N | 2.48 | 0.45 |
| 51:CR:91:THR:HG23 | 51:CR:98:HIS:CE1 | 2.51 | 0.45 |
| 54:CU:169:TYR:CE2 | 54:CU:175:LYS:HB2 | 2.51 | 0.45 |
| 82:l1:70:ASP:HA | 82:l1:74:VAL:HG12 | 1.98 | 0.45 |
| 1:1:37:U:H2' | 1:1:38:A:O4' | 2.16 | 0.45 |
| 1:1:150:A:C5 | 1:1:151:U:C5 | 3.05 | 0.45 |
| 1:1:1829:G:H5" | 40:AM:10:LYS:HD2 | 1.97 | 0.45 |
| 1:1:2339:A:H2' | 1:1:2340:C:H6 | 1.82 | 0.45 |
| 1:1:3313:G:H2' | 1:1:3314:C:C6 | 2.52 | 0.45 |
| 28:AA:40:HIS:CE1 | 28:AA:74:LEU:HD11 | 2.51 | 0.45 |
| 46:B:634:A:H5" | 69:Y:31:SER:HB3 | 1.98 | 0.45 |
| 46:B:1318:C:H2' | 46:B:1319:U:H6 | 1.81 | 0.45 |
| 46:B:1458:C:OP1 | 52:H:102:ARG:NH2 | 2.46 | 0.45 |
| 47:C:77:SER:HB2 | 47:C:124:THR:HG21 | 1.99 | 0.45 |
| 63:S:19:ALA:CB | 63:S:83:ALA:HB1 | 2.43 | 0.45 |
| 66:V:38:LYS:NZ | 66:V:41:ALA:HA | 2.31 | 0.45 |
| 1:AS:673:C:O2' | 1:AS:677:U:OP1 | 2.28 | 0.45 |
| 1:AS:1124:U:H2' | 1:AS:1125:A:O4' | 2.16 | 0.45 |
| 1:AS:1357:U:H2' | 1:AS:1358:C:C6 | 2.51 | 0.45 |
| 1:AS:1714:G:H2' | 1:AS:1715:G:C8 | 2.52 | 0.45 |
| 1:AS:2646:A:C2 | 13:BF:124:GLY:HA3 | 2.52 | 0.45 |
| 1:AS:2668:A:H2' | 1:AS:2669:A:C8 | 2.52 | 0.45 |
| 1:AS:2957:C:H2' | 1:AS:2958:U:H6 | 1.81 | 0.45 |
| 1:AS:3208:A:H4' | 5:AX:95:THR:HG22 | 1.99 | 0.45 |
| 20:BM:162:ARG:HD3 | 20:BM:162:ARG:HA | 1.83 | 0.45 |
| 21:BN:81:TYR:CE1 | 21:BN:90:MET:HE3 | 2.51 | 0.45 |
| 22:BO:52:MET:HA | 22:BO:95:HIS:CE1 | 2.51 | 0.45 |
| 32:BY:61:ARG:HB2 | 32:BY:65:GLY:HA3 | 1.99 | 0.45 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 46:CM:214:U:H5' | 46:CM:815:U:H4' | 1.98 | 0.45 |
| 46:CM:226:G:H2' | 46:CM:227:C:O4' | 2.16 | 0.45 |
| 46:CM:744:U:C2 | 46:CM:745:A:C8 | 3.04 | 0.45 |
| 46:CM:753:C:C2 | 56:CW:143:ILE:HG21 | 2.51 | 0.45 |
| 46:CM:845:U:O4' | 54:CU:110:ARG:HG3 | 2.17 | 0.45 |
| 46:CM:1128:A:OP2 | 73:DN:2:PRO:HG3 | 2.17 | 0.45 |
| 46:CM:1539:U:O2' | 46:CM:1584:A:N3 | 2.42 | 0.45 |
| 54:CU:52:LYS:O | 54:CU:85:HIS:N | 2.39 | 0.45 |
| 59:CZ:51:ALA:HB3 | 59:CZ:122:VAL:HG11 | 1.98 | 0.45 |
| 66:DG:103:LYS:HD3 | 66:DG:103:LYS:HA | 1.83 | 0.45 |
| 82:l1:67:ILE:HG23 | 82:l1:111:ILE:HD13 | 1.99 | 0.45 |
| 82:l1:87:VAL:HG12 | 82:l1:90:LEU:HD12 | 1.98 | 0.45 |
| 80:p0:77:LEU:O | 80:p0:80:ILE:HD12 | 2.17 | 0.45 |
| 1:1:798:C:C2 | 1:1:799:C:C5 | 3.05 | 0.45 |
| 1:1:815:U:H2' | 1:1:816:A:C8 | 2.52 | 0.45 |
| 1:1:1023:A:H2' | 1:1:1025:G:C8 | 2.52 | 0.45 |
| 1:1:1163:U:P | 34:AG:73:ARG:HH12 | 2.40 | 0.45 |
| 1:1:1197:C:N4 | 1:1:2829:C:OP1 | 2.48 | 0.45 |
| 1:1:1230:G:H2' | 1:1:1231:U:C5 | 2.50 | 0.45 |
| 1:1:1299:A:O4' | 1:1:2857:C:O2' | 2.35 | 0.45 |
| 1:1:1468:U:H5' | 20:z:4:LEU:HB2 | 1.98 | 0.45 |
| 1:1:2334:A:N6 | 1:1:2955:C:H5 | 2.11 | 0.45 |
| 1:1:2525:A:H2' | 1:1:2526:C:O4' | 2.17 | 0.45 |
| 1:1:2587:G:H2' | 1:1:2588:C:C6 | 2.51 | 0.45 |
| 1:1:3013:U:H2' | 1:1:3014:U:C6 | 2.52 | 0.45 |
| 1:1:3184:G:H4' | 1:1:3185:G:H5' | 1.99 | 0.45 |
| 5:k:160:VAL:HB | 5:k:183:ILE:HD11 | 1.99 | 0.45 |
| 6:l:272:LYS:HB2 | 6:l:275:TYR:HB3 | 1.99 | 0.45 |
| 16:v:116:LEU:HB2 | 16:v:135:VAL:HG23 | 1.99 | 0.45 |
| 19:y:78:GLU:OE1 | 19:y:78:GLU:N | 2.50 | 0.45 |
| 24:6:38:ALA:O | 24:6:58:VAL:HG13 | 2.16 | 0.45 |
| 33:AF:5:VAL:N | 33:AF:91:LYS:O | 2.48 | 0.45 |
| 40:AM:41:ARG:HA | 40:AM:41:ARG:HD2 | 1.73 | 0.45 |
| 46:B:379:C:H2' | 46:B:380:C:H6 | 1.81 | 0.45 |
| 46:B:1206:A:H2' | 46:B:1207:C:O4' | 2.17 | 0.45 |
| 46:B:1276:G:H22 | 46:B:1309:G:H22 | 1.64 | 0.45 |
| 46:B:1611:C:H2' | 46:B:1612:C:H6 | 1.82 | 0.45 |
| 49:E:173:ILE:HG21 | 49:E:180:LYS:HA | 1.98 | 0.45 |
| 71:a:42:GLU:HG3 | 71:a:52:LYS:HE3 | 1.98 | 0.45 |
| 78:h:178:LYS:HB3 | 78:h:179:ASP:H | 1.49 | 0.45 |
| 1:AS:108:A:O2' | 1:AS:323:A:N6 | 2.50 | 0.45 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 1:AS:713:A:H8 | 29:BV:115:LYS:HG3 | 1.82 | 0.45 |
| 1:AS:912:G:N1 | 4:AW:207:VAL:HG11 | 2.32 | 0.45 |
| 1:AS:1029:U:O2' | 1:AS:1030:U:OP1 | 2.28 | 0.45 |
| 1:AS:1225:G:H2' | 1:AS:1226:G:H8 | 1.82 | 0.45 |
| 1:AS:1575:A:H5" | 1:AS:1576:A:H2 | 1.81 | 0.45 |
| 1:AS:2557:G:N3 | 1:AS:2557:G:H2' | 2.32 | 0.45 |
| 45:CL:77:GLN:HG3 | 46:CM:1446:A:H62 | 1.82 | 0.45 |
| 46:CM:82:U:H2' | 46:CM:83:G:O4' | 2.17 | 0.45 |
| 46:CM:188:U:H2' | 46:CM:189:G:C8 | 2.52 | 0.45 |
| 46:CM:582:C:C4 | 46:CM:583:A:N7 | 2.85 | 0.45 |
| 46:CM:600:U:H2' | 46:CM:601:U:C6 | 2.52 | 0.45 |
| 46:CM:1140:G:H2' | 46:CM:1141:C:C6 | 2.51 | 0.45 |
| 46:CM:1458:C:OP1 | 52:CS:102:ARG:NH2 | 2.42 | 0.45 |
| 54:CU:40:LYS:HG3 | 54:CU:59:PRO:HD3 | 1.99 | 0.45 |
| 75:DP:10:ALA:HB1 | 75:DP:30:VAL:HB | 1.98 | 0.45 |
| 79:DT:179:ASP:HB2 | 79:DT:186:ASN:HD21 | 1.81 | 0.45 |
| 82:L1:126:PRO:HA | 82:L1:129:SER:HB2 | 1.99 | 0.45 |
| 82:l1:44:GLN:O | 82:l1:46:ASP:N | 2.46 | 0.45 |
| 82:l1:204:LEU:HB3 | 82:l1:217:TYR:HB3 | 1.99 | 0.45 |
| 1:1:275:U:H2' | 1:1:276:U:C6 | 2.52 | 0.45 |
| 1:1:480:G:H2' | 1:1:481:G:C8 | 2.52 | 0.45 |
| 1:1:623:A:H2' | 1:1:624:U:H6 | 1.79 | 0.45 |
| 1:1:641:U:O2' | 1:1:1149:A:N1 | 2.37 | 0.45 |
| 1:1:716:G:H3' | 1:1:717:A:H5" | 1.98 | 0.45 |
| 1:1:892:A:H5' | 4:j:183:GLY:CA | 2.47 | 0.45 |
| 1:1:1424:A:OP2 | 29:AB:2:PRO:HA | 2.17 | 0.45 |
| 1:1:2186:A:O2' | 1:1:2187:U:H5' | 2.17 | 0.45 |
| 1:1:2869:A:OP2 | 41:AN:48:LYS:NZ | 2.43 | 0.45 |
| 1:1:2956:C:H2' | 1:1:2957:C:H6 | 1.81 | 0.45 |
| 1:1:3025:G:H2' | 1:1:3026:U:H6 | 1.82 | 0.45 |
| 6:l:16:GLN:NE2 | 6:l:147:LYS:HD2 | 2.32 | 0.45 |
| 8:n:45:ARG:HH12 | 18:x:178:SER:CB | 2.30 | 0.45 |
| 13:s:4:LYS:HG3 | 13:s:6:GLN:H | 1.81 | 0.45 |
| 26:8:141:TYR:HB3 | 36:AI:33:VAL:HG13 | 1.98 | 0.45 |
| 28:AA:103:GLU:HB2 | 28:AA:106:GLN:HB2 | 1.98 | 0.45 |
| 46:B:232:G:C2 | 46:B:233:G:H1' | 2.51 | 0.45 |
| 48:D:59:ASP:OD1 | 48:D:60:GLY:N | 2.49 | 0.45 |
| 49:E:223:ASN:HD21 | 68:X:1:MET:HE3 | 1.82 | 0.45 |
| 51:G:67:GLN:NE2 | 71:a:17:LEU:O | 2.42 | 0.45 |
| 56:L:108:ARG:NH1 | 56:L:110:GLN:OE1 | 2.50 | 0.45 |
| 59:O:38:HIS:HE1 | 59:O:43:ARG:HD2 | 1.82 | 0.45 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 62:R:26:VAL:HA | 62:R:87:PRO:HB2 | 1.98 | 0.45 |
| 69:Y:77:PRO:HD3 | 70:Z:7:ARG:O | 2.17 | 0.45 |
| 78:h:182:TYR:OH | 78:h:187:HIS:ND1 | 2.42 | 0.45 |
| 1:AS:19:A:H2' | 1:AS:20:G:C8 | 2.52 | 0.45 |
| 1:AS:21:G:H1' | 3:AU:104:A:N3 | 2.32 | 0.45 |
| 1:AS:179:C:H2' | 1:AS:180:U:C6 | 2.51 | 0.45 |
| 1:AS:206:U:H2' | 1:AS:207:C:H6 | 1.82 | 0.45 |
| 1:AS:785:A:H2' | 1:AS:786:U:C6 | 2.51 | 0.45 |
| 1:AS:1247:A:H3' | 1:AS:1248:A:H5" | 1.99 | 0.45 |
| 1:AS:1870:A:OP2 | 20:BM:20:ARG:NH1 | 2.49 | 0.45 |
| 1:AS:2108:G:O4' | 1:AS:2122:A:H4' | 2.16 | 0.45 |
| 1:AS:2435:G:H2' | 1:AS:2437:A:N7 | 2.32 | 0.45 |
| 10:BC:113:GLU:HA | 10:BC:126:VAL:HG11 | 1.99 | 0.45 |
| 15:BH:26:LEU:HD11 | 15:BH:87:TRP:CG | 2.51 | 0.45 |
| 23:BP:27:VAL:HG12 | 23:BP:92:ILE:HD13 | 1.98 | 0.45 |
| 35:CB:25:THR:OG1 | 35:CB:29:LYS:HG2 | 2.17 | 0.45 |
| 45:CL:107:TRP:HA | 50:CQ:116:ILE:HD11 | 1.98 | 0.45 |
| 46:CM:98:U:H2' | 46:CM:99:C:C6 | 2.52 | 0.45 |
| 46:CM:236:U:O2' | 46:CM:237:C:H5" | 2.17 | 0.45 |
| 46:CM:261:C:H4' | 46:CM:290:U:H5' | 1.98 | 0.45 |
| 46:CM:462:A:C2 | 46:CM:463:G:C8 | 3.05 | 0.45 |
| 46:CM:627:U:C2 | 46:CM:628:A:C8 | 3.04 | 0.45 |
| 46:CM:871:U:H2' | 46:CM:872:A:H8 | 1.82 | 0.45 |
| 46:CM:1255:G:OP2 | 78:DS:122:ARG:NH2 | 2.49 | 0.45 |
| 46:CM:1468:C:H5" | 46:CM:1508:G:H22 | 1.82 | 0.45 |
| 46:CM:1720:C:H2' | 46:CM:1721:U:C6 | 2.52 | 0.45 |
| 47:CN:92:HIS:ND1 | 47:CN:202:TYR:OH | 2.33 | 0.45 |
| 48:CO:28:ASP:O | 48:CO:29:TRP:HB2 | 2.17 | 0.45 |
| 49:CP:122:ALA:O | 49:CP:126:ILE:HG13 | 2.17 | 0.45 |
| 70:DK:48:HIS:HB3 | 70:DK:103:LEU:HD11 | 1.99 | 0.45 |
| 79:DT:33:LEU:O | 79:DT:45:TRP:HD1 | 2.00 | 0.45 |
| 82:l1:98:LYS:O | 82:l1:100:ILE:N | 2.50 | 0.45 |
| 1:1:559:C:H2' | 1:1:560:C:C6 | 2.52 | 0.44 |
| 1:1:867:U:H2' | 1:1:868:U:C6 | 2.53 | 0.44 |
| 1:1:1571:G:H2' | 1:1:1572:G:H8 | 1.82 | 0.44 |
| 1:1:1829:G:P | 26:8:114:ILE:HD12 | 2.57 | 0.44 |
| 1:1:1852:C:C2 | 1:1:1853:C:C5 | 3.05 | 0.44 |
| 1:1:1863:A:H2' | 1:1:1864:G:C8 | 2.52 | 0.44 |
| 1:1:2478:A:N3 | 1:1:2478:A:H2' | 2.32 | 0.44 |
| 1:1:3005:A:H2' | 1:1:3006:C:H6 | 1.82 | 0.44 |
| 9:o:86:ARG:O | 9:o:110:ASN:N | 2.44 | 0.44 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 22:2:28:SER:O | 22:2:32:LYS:HG3 | 2.16 | 0.44 |
| 31:AD:20:ILE:HG23 | 31:AD:25:TYR:CZ | 2.52 | 0.44 |
| 42:AO:13:LEU:HD11 | 46:B:1737:A:O5' | 2.17 | 0.44 |
| 46:B:573:C:H41 | 70:Z:65:ASN:ND2 | 2.16 | 0.44 |
| 46:B:733:U:O2' | 69:Y:122:SER:O | 2.28 | 0.44 |
| 46:B:982:G:C6 | 46:B:993:G:C6 | 3.04 | 0.44 |
| 46:B:1469:A:C2 | 46:B:1594:G:H1' | 2.52 | 0.44 |
| 46:B:1654:A:H2' | 46:B:1655:G:C8 | 2.52 | 0.44 |
| 47:C:88:LYS:HD3 | 47:C:88:LYS:HA | 1.80 | 0.44 |
| 52:H:29:ILE:HB | 52:H:34:GLN:HE21 | 1.82 | 0.44 |
| 59:O:34:THR:HA | 59:O:37:VAL:HG23 | 1.99 | 0.44 |
| 59:O:132:GLU:C | 59:O:134:ASN:H | 2.24 | 0.44 |
| 62:R:1:MET:HB2 | 65:U:18:LEU:H | 1.82 | 0.44 |
| 68:X:4:ASP:OD1 | 68:X:5:LYS:N | 2.50 | 0.44 |
| 76:f:12:ARG:HB2 | 76:f:12:ARG:NH1 | 2.32 | 0.44 |
| 1:AS:406:G:H1' | 3:AU:16:G:N2 | 2.32 | 0.44 |
| 1:AS:640:U:OP1 | 29:BV:22:ILE:HG23 | 2.17 | 0.44 |
| 1:AS:740:A:H1' | 19:BL:141:ARG:HE | 1.82 | 0.44 |
| 1:AS:1908:U:O2' | 1:AS:2099:G:N7 | 2.44 | 0.44 |
| 1:AS:2134:U:OP1 | 4:AW:241:ARG:NH2 | 2.50 | 0.44 |
| 1:AS:2902:A:H2' | 1:AS:2903:C:C6 | 2.52 | 0.44 |
| 1:AS:2912:A:OP2 | 5:AX:2:SER:N | 2.50 | 0.44 |
| 1:AS:3314:C:H2' | 1:AS:3315:C:C6 | 2.53 | 0.44 |
| 5:AX:80:ASP:OD1 | 5:AX:82:PRO:HD3 | 2.17 | 0.44 |
| 33:BZ:33:TRP:HH2 | 33:BZ:53:GLN:HG2 | 1.82 | 0.44 |
| 46:CM:222:C:C2 | 46:CM:823:G:N2 | 2.85 | 0.44 |
| 46:CM:366:U:H2' | 46:CM:367:A:O4' | 2.17 | 0.44 |
| 46:CM:498:C:O2' | 46:CM:499:U:H5' | 2.16 | 0.44 |
| 46:CM:690:C:H4' | 46:CM:691:U:OP1 | 2.17 | 0.44 |
| 46:CM:1248:G:H2' | 46:CM:1249:G:O4' | 2.17 | 0.44 |
| 46:CM:1332:U:C4 | 67:DH:57:MET:HE1 | 2.52 | 0.44 |
| 46:CM:1636:C:H2' | 46:CM:1637:U:H6 | 1.81 | 0.44 |
| 53:CT:232:GLU:OE2 | 53:CT:236:ASN:ND2 | 2.50 | 0.44 |
| 57:CX:32:HIS:HB2 | 57:CX:39:ASN:HA | 1.98 | 0.44 |
| 59:CZ:54:LYS:HA | 78:DS:170:ALA:HB3 | 1.99 | 0.44 |
| 65:DF:30:TYR:O | 65:DF:33:THR:OG1 | 2.33 | 0.44 |
| 81:12:153:ASP:HA | 81:12:156:ASN:HB2 | 2.00 | 0.44 |
| 1:1:38:A:H61 | 1:1:41:C:H3' | 1.82 | 0.44 |
| 1:1:149:A:C4 | 1:1:150:A:C8 | 3.05 | 0.44 |
| 1:1:755:U:H2' | 1:1:756:G:O4' | 2.17 | 0.44 |
| 1:1:1189:A:H4' | 1:1:1294:C:OP1 | 2.17 | 0.44 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 1:1:1456:A:H5' | 32:AE:50:LEU:O | 2.17 | 0.44 |
| 1:1:2492:U:H5' | 10:p:69:ARG:HG3 | 1.99 | 0.44 |
| 1:1:2679:U:H2' | 1:1:2680:C:C6 | 2.52 | 0.44 |
| 1:1:3035:C:H2' | 1:1:3036:U:H6 | 1.82 | 0.44 |
| 1:1:3153:A:H2' | 1:1:3154:A:H8 | 1.82 | 0.44 |
| 1:1:3336:G:H2' | 1:1:3337:A:H8 | 1.82 | 0.44 |
| 3:4:19:C:H2' | 3:4:20:U:C6 | 2.52 | 0.44 |
| 6:l:155:ASN:O | 6:l:158:GLU:HB2 | 2.17 | 0.44 |
| 7:m:179:ARG:HD3 | 7:m:179:ARG:HA | 1.80 | 0.44 |
| 17:w:9:VAL:HG12 | 17:w:118:ARG:HG3 | 1.99 | 0.44 |
| 28:AA:119:GLU:O | 28:AA:123:GLN:HG2 | 2.16 | 0.44 |
| 29:AB:112:VAL:HB | 29:AB:130:VAL:HG12 | 1.99 | 0.44 |
| 46:B:16:G:H2' | 46:B:17:C:C6 | 2.52 | 0.44 |
| 46:B:94:U:H2' | 46:B:95:G:O4' | 2.16 | 0.44 |
| 46:B:721:C:C2' | 46:B:722:A:H5' | 2.47 | 0.44 |
| 46:B:1062:C:H2' | 46:B:1063:C:H6 | 1.82 | 0.44 |
| 46:B:1220:C:N4 | 78:h:177:MET:HE1 | 2.32 | 0.44 |
| 46:B:1594:G:N7 | 63:S:123:MET:HE1 | 2.32 | 0.44 |
| 46:B:1700:G:N3 | 46:B:1700:G:H2' | 2.32 | 0.44 |
| 46:B:1727:A:H2' | 46:B:1728:U:C6 | 2.52 | 0.44 |
| 51:G:100:ARG:HG2 | 51:G:102:VAL:HG13 | 1.99 | 0.44 |
| 52:H:42:LEU:HB3 | 52:H:46:TRP:HB2 | 1.99 | 0.44 |
| 59:O:38:HIS:HE1 | 59:O:43:ARG:HH11 | 1.64 | 0.44 |
| 78:h:147:TYR:HD2 | 78:h:173:PHE:CD2 | 2.34 | 0.44 |
| 1:AS:48:A:OP1 | 16:BI:191:TRP:NE1 | 2.48 | 0.44 |
| 1:AS:843:A:H2' | 1:AS:844:A:C8 | 2.52 | 0.44 |
| 1:AS:922:A:H2' | 1:AS:923:C:C6 | 2.52 | 0.44 |
| 1:AS:1484:G:C2 | 1:AS:1485:A:C8 | 3.06 | 0.44 |
| 1:AS:1486:A:O2' | 38:CE:12:HIS:O | 2.27 | 0.44 |
| 1:AS:2329:U:H2' | 1:AS:2330:A:H8 | 1.82 | 0.44 |
| 1:AS:2415:G:C6 | 1:AS:2489:A:C5 | 3.05 | 0.44 |
| 1:AS:2457:C:C4 | 1:AS:2458:G:C6 | 3.04 | 0.44 |
| 1:AS:2627:U:H4' | 1:AS:2628:A:O4' | 2.17 | 0.44 |
| 1:AS:2656:C:H2' | 1:AS:2657:C:C6 | 2.52 | 0.44 |
| 5:AX:122:TRP:CE2 | 5:AX:127:LYS:HE3 | 2.53 | 0.44 |
| 45:CL:102:LYS:HB3 | 50:CQ:144:ARG:O | 2.17 | 0.44 |
| 46:CM:426:A:N3 | 46:CM:438:U:O2' | 2.33 | 0.44 |
| 46:CM:483:A:H2' | 46:CM:484:G:C8 | 2.53 | 0.44 |
| 46:CM:705:G:H21 | 46:CM:716:C:H2' | 1.82 | 0.44 |
| 46:CM:1574:A:O2' | 52:CS:104:ASN:OD1 | 2.31 | 0.44 |
| 46:CM:1700:G:H5' | 46:CM:1701:A:OP2 | 2.18 | 0.44 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 51:CR:32:SER:HG | 51:CR:81:THR:HG23 | 1.82 | 0.44 |
| 81:12:119:LYS:HD2 | 81:12:119:LYS:N | 2.33 | 0.44 |
| 1:1:487:C:H2' | 1:1:488:G:O4' | 2.17 | 0.44 |
| 1:1:649:G:O2' | 1:1:1431:A:OP1 | 2.35 | 0.44 |
| 1:1:816:A:H2' | 1:1:817:U:C6 | 2.52 | 0.44 |
| 1:1:1116:A:H2' | 1:1:1117:U:C6 | 2.50 | 0.44 |
| 1:1:1338:G:H2' | 1:1:1339:A:O4' | 2.17 | 0.44 |
| 1:1:1434:U:H4' | 6:l:89:ALA:CB | 2.47 | 0.44 |
| 1:1:1632:C:H4' | 28:AA:74:LEU:O | 2.17 | 0.44 |
| 1:1:2401:U:H2' | 1:1:2402:A:C8 | 2.52 | 0.44 |
| 1:1:2802:G:H1' | 1:1:2833:U:C2 | 2.52 | 0.44 |
| 1:1:2855:U:H2' | 1:1:2856:C:H6 | 1.83 | 0.44 |
| 1:1:2933:G:H2' | 1:1:2934:U:H6 | 1.80 | 0.44 |
| 3:4:141:C:O3' | 16:v:62:TYR:OH | 2.35 | 0.44 |
| 5:k:292:ALA:HB1 | 5:k:295:ALA:HB3 | 2.00 | 0.44 |
| 12:r:86:HIS:HB3 | 12:r:139:ARG:CG | 2.46 | 0.44 |
| 38:AK:36:SER:OG | 38:AK:57:ARG:NH2 | 2.48 | 0.44 |
| 44:AQ:84:ARG:O | 44:AQ:88:GLU:HG2 | 2.17 | 0.44 |
| 46:B:558:U:H2' | 46:B:559:G:C8 | 2.53 | 0.44 |
| 46:B:1092:G:O2' | 46:B:1093:G:H5' | 2.17 | 0.44 |
| 49:E:36:LEU:HD21 | 49:E:51:ILE:HD12 | 1.99 | 0.44 |
| 49:E:138:TYR:CD1 | 49:E:142:ASN:HA | 2.52 | 0.44 |
| 57:M:77:ARG:CZ | 57:M:86:ILE:HG22 | 2.47 | 0.44 |
| 61:Q:15:PHE:HB3 | 61:Q:22:PHE:HB2 | 1.98 | 0.44 |
| 78:h:174:MET:HB3 | 78:h:181:GLN:HB3 | 2.00 | 0.44 |
| 1:AS:377:A:H1' | 1:AS:392:G:N2 | 2.32 | 0.44 |
| 1:AS:1203:G:OP1 | 41:CH:43:ASN:ND2 | 2.45 | 0.44 |
| 1:AS:1286:A:H2' | 1:AS:1287:A:C8 | 2.51 | 0.44 |
| 1:AS:2628:A:C4 | 1:AS:2630:G:N7 | 2.86 | 0.44 |
| 9:BB:149:ARG:HD2 | 9:BB:205:LEU:HD23 | 1.98 | 0.44 |
| 14:BG:57:VAL:HG22 | 14:BG:69:VAL:HG22 | 1.98 | 0.44 |
| 19:BL:44:PHE:CD2 | 19:BL:134:GLY:HA3 | 2.53 | 0.44 |
| 23:BP:18:ASP:HA | 23:BP:63:LYS:HG2 | 1.98 | 0.44 |
| 29:BV:28:HIS:CD2 | 29:BV:32:ARG:HG2 | 2.52 | 0.44 |
| 46:CM:66:U:H5" | 53:CT:172:ALA:C | 2.42 | 0.44 |
| 46:CM:584:G:H2' | 46:CM:585:C:C6 | 2.52 | 0.44 |
| 46:CM:647:C:O2' | 46:CM:648:U:H6 | 2.00 | 0.44 |
| 46:CM:721:C:H2' | 46:CM:722:A:H5' | 1.99 | 0.44 |
| 46:CM:932:U:H2' | 46:CM:933:A:C8 | 2.51 | 0.44 |
| 46:CM:1275:U:H2' | 46:CM:1276:G:H8 | 1.77 | 0.44 |
| 46:CM:1345:A:N1 | 46:CM:1349:G:C6 | 2.85 | 0.44 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 46:CM:1712:U:H2' | 46:CM:1713:G:C8 | 2.53 | 0.44 |
| 60:DA:5:HIS:HB2 | 60:DA:121:ARG:HH21 | 1.83 | 0.44 |
| 65:DF:36:ARG:HH12 | 65:DF:105:LEU:HD22 | 1.82 | 0.44 |
| 79:DT:34:LEU:HB3 | 79:DT:74:ILE:HD11 | 1.99 | 0.44 |
| 79:DT:46:LYS:HD2 | 79:DT:59:LYS:HE3 | 1.98 | 0.44 |
| 82:L1:181:ASN:O | 82:L1:185:MET:HG3 | 2.18 | 0.44 |
| 1:1:4:G:C6 | 3:4:155:G:O6 | 2.71 | 0.44 |
| 1:1:502:U:H2' | 1:1:503:U:C6 | 2.52 | 0.44 |
| 1:1:798:C:H2' | 1:1:799:C:C6 | 2.52 | 0.44 |
| 1:1:1908:U:H2' | 1:1:1909:A:O4' | 2.18 | 0.44 |
| 1:1:2771:A:O2' | 29:AB:42:ARG:NH2 | 2.51 | 0.44 |
| 1:1:3038:U:H2' | 1:1:3039:C:H6 | 1.82 | 0.44 |
| 84:1:3402:3K5:H47 | 84:1:3402:3K5:H15 | 2.00 | 0.44 |
| 17:w:116:LYS:O | 17:w:118:ARG:NH1 | 2.51 | 0.44 |
| 36:AI:31:LEU:HD22 | 36:AI:41:LEU:HD21 | 2.00 | 0.44 |
| 52:H:103:ASN:HA | 52:H:106:LYS:HD2 | 1.99 | 0.44 |
| 63:S:25:LYS:H | 63:S:25:LYS:HG2 | 1.66 | 0.44 |
| 1:AS:171:G:H1 | 1:AS:246:U:H3 | 1.66 | 0.44 |
| 1:AS:281:G:N7 | 16:BI:182:LYS:NZ | 2.51 | 0.44 |
| 1:AS:1298:A:N7 | 1:AS:2829:C:O2' | 2.49 | 0.44 |
| 1:AS:1625:U:H3 | 28:BU:111:LYS:HE2 | 1.82 | 0.44 |
| 1:AS:2115:U:C6 | 1:AS:2119:U:C4 | 3.05 | 0.44 |
| 1:AS:2479:U:H5" | 1:AS:2480:A:C2 | 2.52 | 0.44 |
| 1:AS:3067:U:H2' | 1:AS:3068:C:C6 | 2.52 | 0.44 |
| 3:AU:13:A:C6 | 3:AU:14:C:C4 | 3.06 | 0.44 |
| 3:AU:26:U:O2' | 6:AY:52:ALA:O | 2.34 | 0.44 |
| 7:AZ:240:TYR:O | 7:AZ:244:HIS:ND1 | 2.50 | 0.44 |
| 10:BC:215:LEU:HD23 | 10:BC:215:LEU:HA | 1.84 | 0.44 |
| 46:CM:520:U:H2' | 46:CM:521:G:O4' | 2.18 | 0.44 |
| 47:CN:15:LYS:HZ1 | 64:DE:93:LEU:HD13 | 1.81 | 0.44 |
| 51:CR:88:ASP:OD1 | 51:CR:122:LYS:NZ | 2.49 | 0.44 |
| 60:DA:38:ILE:HD11 | 60:DA:78:ASN:ND2 | 2.32 | 0.44 |
| 61:DB:27:ASP:OD1 | 61:DB:30:GLY:N | 2.47 | 0.44 |
| 63:DD:22:LYS:HG2 | 63:DD:63:ASP:OD1 | 2.16 | 0.44 |
| 82:L1:194:LEU:HD13 | 82:L1:200:ASN:HB2 | 1.98 | 0.44 |
| 82:l1:180:VAL:O | 82:l1:184:MET:HG3 | 2.16 | 0.44 |
| 1:1:206:U:H2' | 1:1:207:C:C6 | 2.53 | 0.44 |
| 1:1:3207:G:O6 | 5:k:150:ARG:NH2 | 2.50 | 0.44 |
| 21:0:119:ARG:HE | 21:0:119:ARG:HB2 | 1.56 | 0.44 |
| 46:B:226:G:H2' | 46:B:227:C:C6 | 2.53 | 0.44 |
| 46:B:953:U:H2' | 46:B:954:C:O4' | 2.16 | 0.44 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 46:B:1039:U:H2' | 46:B:1040:U:C6 | 2.53 | 0.44 |
| 46:B:1042:U:C5 | 46:B:1048:U:C4 | 3.06 | 0.44 |
| 46:B:1341:U:H2' | 46:B:1342:A:C8 | 2.52 | 0.44 |
| 53:I:85:ARG:O | 53:I:87:ARG:NH1 | 2.50 | 0.44 |
| 59:O:43:ARG:HH21 | 59:O:103:LEU:HD23 | 1.82 | 0.44 |
| 71:a:27:VAL:O | 71:a:68:LYS:HA | 2.17 | 0.44 |
| 1:AS:120:A:C2 | 10:BC:130:PRO:HB3 | 2.51 | 0.44 |
| 1:AS:284:A:N6 | 1:AS:2757:A:O4' | 2.50 | 0.44 |
| 1:AS:352:A:N1 | 1:AS:365:A:H5" | 2.32 | 0.44 |
| 1:AS:582:G:H2' | 1:AS:583:A:C8 | 2.51 | 0.44 |
| 1:AS:925:A:O2' | 38:CE:49:TRP:O | 2.35 | 0.44 |
| 1:AS:1661:U:H2' | 1:AS:1662:G:H8 | 1.82 | 0.44 |
| 1:AS:2681:C:H2' | 1:AS:2682:C:C6 | 2.52 | 0.44 |
| 1:AS:2957:C:H2' | 1:AS:2958:U:C6 | 2.52 | 0.44 |
| 3:AU:139:U:H2' | 3:AU:140:G:H8 | 1.83 | 0.44 |
| 4:AW:47:GLN:HG2 | 4:AW:49:ILE:HG23 | 1.99 | 0.44 |
| 10:BC:162:GLU:OE2 | 16:BI:26:ARG:NH1 | 2.47 | 0.44 |
| 20:BM:38:ARG:O | 20:BM:42:ARG:HG3 | 2.17 | 0.44 |
| 22:BO:66:ASN:OD1 | 30:BW:35:VAL:HA | 2.16 | 0.44 |
| 46:CM:704:A:O2' | 46:CM:705:G:O5' | 2.35 | 0.44 |
| 46:CM:720:C:O2' | 46:CM:721:C:OP2 | 2.36 | 0.44 |
| 46:CM:908:A:H2' | 46:CM:909:A:C8 | 2.53 | 0.44 |
| 46:CM:1066:A:O2' | 46:CM:1068:G:N7 | 2.43 | 0.44 |
| 53:CT:220:LYS:HD2 | 53:CT:223:ARG:HH21 | 1.82 | 0.44 |
| 54:CU:29:ASP:OD1 | 54:CU:30:LEU:N | 2.49 | 0.44 |
| 60:DA:45:LEU:HD22 | 60:DA:49:GLN:CD | 2.42 | 0.44 |
| 82:L1:16:LEU:HD11 | 82:L1:208:SER:H | 1.82 | 0.44 |
| 1:1:214:G:OP1 | 27:9:12:ARG:NH1 | 2.46 | 0.44 |
| 1:1:657:G:H2' | 1:1:1428:C:H42 | 1.81 | 0.44 |
| 1:1:812:A:H5' | 1:1:902:A:H61 | 1.83 | 0.44 |
| 1:1:1110:U:OP1 | 29:AB:23:GLY:N | 2.37 | 0.44 |
| 1:1:1556:G:O2' | 1:1:1557:U:H5' | 2.17 | 0.44 |
| 1:1:1754:G:H2' | 1:1:1755:U:O4' | 2.17 | 0.44 |
| 1:1:2649:G:O2' | 1:1:2651:A:N1 | 2.33 | 0.44 |
| 1:1:2771:A:H1' | 29:AB:42:ARG:CZ | 2.48 | 0.44 |
| 1:1:3197:G:H2' | 1:1:3198:C:C6 | 2.52 | 0.44 |
| 1:1:3314:C:H2' | 1:1:3315:C:C6 | 2.53 | 0.44 |
| 14:t:2:ALA:HB1 | 29:AB:33:GLY:O | 2.18 | 0.44 |
| 29:AB:94:SER:HB3 | 29:AB:121:VAL:HG13 | 1.99 | 0.44 |
| 32:AE:84:ALA:C | 32:AE:86:GLU:H | 2.25 | 0.44 |
| 46:B:217:A:H5" | 46:B:816:U:O2 | 2.18 | 0.44 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 46:B:294:U:H2' | 46:B:295:U:C6 | 2.53 | 0.44 |
| 46:B:569:G:H5" | 70:Z:114:LYS:HD2 | 1.99 | 0.44 |
| 46:B:1293:G:H2' | 46:B:1294:C:C6 | 2.53 | 0.44 |
| 46:B:1436:U:C2 | 46:B:1437:C:C5 | 3.06 | 0.44 |
| 52:H:99:MET:O | 52:H:103:ASN:HB2 | 2.18 | 0.44 |
| 78:h:168:CYS:HB3 | 78:h:172:ILE:HB | 2.00 | 0.44 |
| 1:AS:314:U:H2' | 1:AS:315:C:H6 | 1.81 | 0.44 |
| 1:AS:1021:A:C6 | 1:AS:1022:A:H1' | 2.52 | 0.44 |
| 1:AS:1042:A:H2' | 1:AS:1045:C:C5 | 2.53 | 0.44 |
| 1:AS:1104:U:H2' | 1:AS:1105:U:H6 | 1.82 | 0.44 |
| 1:AS:1385:G:O6 | 6:AY:187:LYS:NZ | 2.46 | 0.44 |
| 1:AS:1618:U:H2' | 1:AS:1619:G:C8 | 2.52 | 0.44 |
| 1:AS:1725:A:C6 | 44:CK:42:CYS:HA | 2.53 | 0.44 |
| 1:AS:2371:G:O2' | 1:AS:2954:A:N6 | 2.40 | 0.44 |
| 1:AS:2958:U:C2 | 1:AS:2959:A:C8 | 3.05 | 0.44 |
| 7:AZ:19:PRO:HG2 | 7:AZ:24:GLN:HB2 | 1.99 | 0.44 |
| 46:CM:94:U:H2' | 46:CM:95:G:O4' | 2.17 | 0.44 |
| 46:CM:261:C:O2' | 46:CM:262:G:H5' | 2.18 | 0.44 |
| 46:CM:584:G:H2' | 46:CM:585:C:H6 | 1.83 | 0.44 |
| 46:CM:696:U:C2' | 46:CM:697:U:H5' | 2.47 | 0.44 |
| 54:CU:134:LYS:C | 54:CU:135:ARG:HD2 | 2.42 | 0.44 |
| 64:DE:89:SER:HB3 | 64:DE:92:ASP:HB2 | 1.99 | 0.44 |
| 76:DQ:23:HIS:CG | 76:DQ:42:CYS:SG | 3.11 | 0.44 |
| 78:DS:178:LYS:N | 78:DS:178:LYS:HD2 | 2.32 | 0.44 |
| 82:l1:93:LEU:CG | 82:l1:94:ASN:H | 2.30 | 0.44 |
| 82:l1:118:LYS:HB3 | 82:l1:118:LYS:HE3 | 1.84 | 0.44 |
| 1:1:417:A:H2' | 1:1:418:A:H8 | 1.79 | 0.44 |
| 1:1:614:G:H2' | 1:1:615:G:C8 | 2.53 | 0.44 |
| 1:1:669:U:H2' | 1:1:670:A:H8 | 1.81 | 0.44 |
| 1:1:1944:G:H2' | 1:1:1945:A:H8 | 1.82 | 0.44 |
| 1:1:2242:U:H2' | 1:1:2243:C:H6 | 1.82 | 0.44 |
| 1:1:2857:C:O2' | 1:1:2858:U:H5' | 2.17 | 0.44 |
| 1:1:2938:G:H2' | 1:1:2939:A:C8 | 2.52 | 0.44 |
| 1:1:3066:A:H2' | 1:1:3067:U:C6 | 2.52 | 0.44 |
| 5:k:74:GLU:OE2 | 5:k:325:LYS:HE3 | 2.18 | 0.44 |
| 9:o:52:GLU:OE2 | 9:o:184:HIS:NE2 | 2.50 | 0.44 |
| 10:p:202:THR:O | 10:p:203:GLU:HG2 | 2.18 | 0.44 |
| 20:z:98:ARG:HD2 | 20:z:133:LYS:O | 2.18 | 0.44 |
| 22:2:77:ASN:OD1 | 30:AC:24:PRO:HG3 | 2.18 | 0.44 |
| 24:6:121:GLU:OE1 | 24:6:121:GLU:N | 2.49 | 0.44 |
| 25:7:112:ASP:HB3 | 46:B:278:U:O4 | 2.18 | 0.44 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 32:AE:18:ARG:HB3 | 32:AE:34:GLU:HG3 | 2.00 | 0.44 |
| 46:B:846:U:H5' | 46:B:847:A:OP2 | 2.17 | 0.44 |
| 46:B:1345:A:N1 | 46:B:1349:G:C6 | 2.86 | 0.44 |
| 48:D:174:ARG:NH2 | 48:D:196:GLU:OE2 | 2.51 | 0.44 |
| 66:V:30:VAL:HG13 | 66:V:34:VAL:HG11 | 1.99 | 0.44 |
| 78:h:168:CYS:HB3 | 78:h:172:ILE:CB | 2.47 | 0.44 |
| 1:AS:206:U:H2' | 1:AS:207:C:C6 | 2.52 | 0.44 |
| 1:AS:445:A:H2' | 1:AS:446:U:C6 | 2.53 | 0.44 |
| 1:AS:716:G:H3' | 1:AS:717:A:H5" | 1.98 | 0.44 |
| 1:AS:2201:A:H2' | 1:AS:2202:A:C8 | 2.53 | 0.44 |
| 1:AS:2853:C:H2' | 1:AS:2854:U:H6 | 1.82 | 0.44 |
| 10:BC:145:GLU:OE2 | 37:CD:35:ARG:NH1 | 2.50 | 0.44 |
| 46:CM:1555:C:H4' | 46:CM:1556:A:O5' | 2.18 | 0.44 |
| 46:CM:1676:A:H2' | 46:CM:1677:G:H1' | 1.99 | 0.44 |
| 46:CM:1697:C:H2' | 46:CM:1698:U:C2 | 2.52 | 0.44 |
| 54:CU:59:PRO:HG2 | 54:CU:62:SER:HB3 | 1.99 | 0.44 |
| 59:CZ:33:ARG:HD2 | 59:CZ:34:THR:HG23 | 2.00 | 0.44 |
| 69:DJ:75:ILE:HD12 | 69:DJ:125:ILE:CD1 | 2.48 | 0.44 |
| 82:l1:93:LEU:C | 82:l1:95:LYS:H | 2.26 | 0.44 |
| 1:1:1030:U:H2' | 1:1:1031:A:C8 | 2.53 | 0.44 |
| 1:1:1256:A:H2' | 1:1:1257:G:C8 | 2.53 | 0.44 |
| 1:1:1278:G:C5 | 1:1:1279:C:C5 | 3.05 | 0.44 |
| 1:1:1562:G:C2 | 1:1:1563:A:H1' | 2.53 | 0.44 |
| 1:1:1714:G:H2' | 1:1:1715:G:C8 | 2.52 | 0.44 |
| 1:1:2458:G:H2' | 1:1:2458:G:N3 | 2.33 | 0.44 |
| 1:1:3240:U:H5" | 34:AG:68:TRP:HZ2 | 1.83 | 0.44 |
| 1:1:3316:U:H3 | 55:K:110:ARG:HH12 | 1.64 | 0.44 |
| 13:s:47:GLN:OE1 | 13:s:64:LYS:HD3 | 2.18 | 0.44 |
| 22:2:40:VAL:HB | 22:2:96:VAL:HG13 | 2.00 | 0.44 |
| 25:7:96:GLN:NE2 | 25:7:101:ARG:HE | 2.16 | 0.44 |
| 36:AI:22:VAL:O | 36:AI:26:GLN:HG3 | 2.18 | 0.44 |
| 37:AJ:94:ALA:O | 37:AJ:97:ARG:HB2 | 2.18 | 0.44 |
| 46:B:97:C:H2' | 46:B:98:U:C6 | 2.53 | 0.44 |
| 46:B:700:G:C2 | 46:B:701:G:C5 | 3.05 | 0.44 |
| 46:B:701:G:C2 | 46:B:721:C:O2 | 2.71 | 0.44 |
| 46:B:781:G:H4' | 58:N:69:LYS:NZ | 2.32 | 0.44 |
| 46:B:875:C:H2' | 46:B:876:A:H8 | 1.83 | 0.44 |
| 46:B:1040:U:H3 | 46:B:1049:G:H1 | 1.66 | 0.44 |
| 49:E:44:LYS:HA | 49:E:44:LYS:HD3 | 1.78 | 0.44 |
| 49:E:134:ILE:HD13 | 49:E:186:ALA:HB1 | 1.99 | 0.44 |
| 1:AS:268:A:N1 | 1:AS:295:A:H5' | 2.33 | 0.44 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 1:AS:477:U:C2 | 1:AS:478:G:C8 | 3.05 | 0.44 |
| 1:AS:481:G:H2' | 1:AS:481:G:N3 | 2.33 | 0.44 |
| 1:AS:1149:A:O2' | 1:AS:1150:A:H5' | 2.18 | 0.44 |
| 1:AS:1560:U:H2' | 1:AS:1561:U:C6 | 2.53 | 0.44 |
| 1:AS:2502:A:H1' | 1:AS:2503:G:C8 | 2.53 | 0.44 |
| 1:AS:2504:C:H2' | 1:AS:2505:G:H8 | 1.83 | 0.44 |
| 1:AS:2660:U:O4 | 7:AZ:19:PRO:HD3 | 2.18 | 0.44 |
| 5:AX:4:ARG:HD3 | 5:AX:7:GLU:HA | 1.99 | 0.44 |
| 7:AZ:4:GLN:HG3 | 7:AZ:5:LYS:N | 2.31 | 0.44 |
| 7:AZ:95:TRP:CE3 | 7:AZ:198:TYR:HB3 | 2.53 | 0.44 |
| 27:BT:47:SER:O | 27:BT:122:LYS:HE2 | 2.18 | 0.44 |
| 39:CF:69:LEU:HB3 | 39:CF:73:LEU:HD21 | 2.00 | 0.44 |
| 45:CL:112:LYS:HG3 | 45:CL:113:ARG:N | 2.32 | 0.44 |
| 45:CL:120:GLU:HG2 | 50:CQ:118:ARG:NE | 2.33 | 0.44 |
| 46:CM:91:G:H2' | 46:CM:92:A:O4' | 2.18 | 0.44 |
| 46:CM:166:A:H2' | 46:CM:167:A:C8 | 2.52 | 0.44 |
| 46:CM:446:C:OP1 | 51:CR:29:PRO:HD3 | 2.17 | 0.44 |
| 46:CM:1601:A:H5' | 75:DP:47:PRO:HG3 | 2.00 | 0.44 |
| 46:CM:1623:C:O2 | 46:CM:1752:A:N6 | 2.50 | 0.44 |
| 79:DT:24:ALA:HB1 | 79:DT:74:ILE:HG13 | 2.00 | 0.44 |
| 79:DT:44:LYS:NZ | 79:DT:95:LEU:O | 2.34 | 0.44 |
| 7:m:95:TRP:CE3 | 7:m:198:TYR:HB3 | 2.53 | 0.44 |
| 14:t:115:ARG:HH22 | 14:t:148:PRO:C | 2.26 | 0.44 |
| 46:B:25:C:H4' | 46:B:26:A:O5' | 2.17 | 0.44 |
| 46:B:182:C:H2' | 46:B:183:C:H6 | 1.83 | 0.44 |
| 46:B:489:C:N4 | 46:B:490:U:O2 | 2.51 | 0.44 |
| 46:B:787:A:C4 | 54:J:100:ARG:HD2 | 2.53 | 0.44 |
| 46:B:946:U:H5" | 60:P:71:ILE:HD12 | 2.00 | 0.44 |
| 46:B:1432:A:O2' | 46:B:1433:C:H3' | 2.18 | 0.44 |
| 53:I:136:LYS:NZ | 53:I:174:LYS:O | 2.41 | 0.44 |
| 54:J:40:LYS:HG3 | 54:J:59:PRO:HD3 | 2.00 | 0.44 |
| 59:O:105:GLN:H | 59:O:105:GLN:HG2 | 1.60 | 0.44 |
| 65:U:4:VAL:HG12 | 72:b:78:VAL:HG23 | 1.99 | 0.44 |
| 1:AS:88:G:N7 | 19:BL:171:LYS:NZ | 2.66 | 0.44 |
| 1:AS:602:A:H2' | 1:AS:603:C:H6 | 1.83 | 0.44 |
| 1:AS:659:G:H4' | 1:AS:660:U:H6 | 1.83 | 0.44 |
| 1:AS:1502:A:H1' | 1:AS:1844:G:O6 | 2.18 | 0.44 |
| 1:AS:1558:G:H5' | 1:AS:1559:C:OP2 | 2.18 | 0.44 |
| 1:AS:2206:A:H2' | 1:AS:2207:A:H8 | 1.80 | 0.44 |
| 1:AS:2515:G:H1' | 1:AS:2516:U:O4' | 2.18 | 0.44 |
| 3:AU:87:G:OP2 | 36:CC:5:LYS:HD2 | 2.17 | 0.44 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 10:BC:150:LYS:HE3 | 10:BC:203:GLU:HA | 1.99 | 0.44 |
| 14:BG:31:LYS:O | 14:BG:35:ARG:HB2 | 2.17 | 0.44 |
| 14:BG:83:VAL:HG23 | 14:BG:85:ILE:HG13 | 1.99 | 0.44 |
| 16:BI:101:THR:O | 16:BI:105:ARG:HD2 | 2.18 | 0.44 |
| 21:BN:27:MET:HE2 | 21:BN:27:MET:HB3 | 1.80 | 0.44 |
| 21:BN:44:PHE:HE1 | 21:BN:122:HIS:ND1 | 2.16 | 0.44 |
| 44:CK:46:THR:OG1 | 44:CK:57:CYS:SG | 2.75 | 0.44 |
| 46:CM:451:C:O2 | 46:CM:451:C:H2' | 2.17 | 0.44 |
| 46:CM:690:C:H2' | 46:CM:691:U:H6 | 1.82 | 0.44 |
| 46:CM:1212:A:H2 | 59:CZ:43:ARG:HB3 | 1.83 | 0.44 |
| 46:CM:1238:U:H2' | 46:CM:1239:U:H6 | 1.82 | 0.44 |
| 46:CM:1342:A:H3' | 46:CM:1343:G:H8 | 1.83 | 0.44 |
| 46:CM:1378:U:H2' | 46:CM:1379:C:C6 | 2.53 | 0.44 |
| 46:CM:1634:U:H2' | 46:CM:1635:A:C8 | 2.53 | 0.44 |
| 48:CO:53:GLY:C | 48:CO:55:LYS:H | 2.24 | 0.44 |
| 52:CS:200:ASN:CB | 52:CS:208:SER:HB3 | 2.48 | 0.44 |
| 53:CT:136:LYS:HG3 | 53:CT:173:PRO:HB2 | 2.00 | 0.44 |
| 63:DD:46:LYS:HD2 | 63:DD:46:LYS:HA | 1.72 | 0.44 |
| 65:DF:115:ARG:HG2 | 65:DF:118:LYS:HE2 | 2.00 | 0.44 |
| 73:DN:87:ARG:NH2 | 73:DN:91:ASP:O | 2.50 | 0.44 |
| 76:DQ:23:HIS:CE1 | 76:DQ:46:LYS:HE3 | 2.52 | 0.44 |
| 82:l1:3:LYS:HG3 | 82:l1:217:TYR:CE1 | 2.52 | 0.44 |
| 80:p0:16:ARG:HA | 80:p0:16:ARG:HH11 | 1.83 | 0.44 |
| 1:1:1132:A:O4' | 1:1:2608:A:N6 | 2.51 | 0.43 |
| 1:1:1201:A:C6 | 1:1:1296:G:N2 | 2.85 | 0.43 |
| 1:1:1228:C:H2' | 1:1:1229:G:H8 | 1.82 | 0.43 |
| 1:1:1696:G:H5' | 39:AL:3:ARG:NH1 | 2.33 | 0.43 |
| 1:1:1779:U:H2' | 1:1:1780:A:H8 | 1.80 | 0.43 |
| 1:1:1923:G:C8 | 44:AQ:16:VAL:HG12 | 2.53 | 0.43 |
| 1:1:3093:U:H1' | 1:1:3094:A:H5" | 1.99 | 0.43 |
| 3:4:38:U:O2' | 36:AI:83:LYS:NZ | 2.40 | 0.43 |
| 3:4:47:C:H1' | 3:4:61:A:H2' | 2.00 | 0.43 |
| 8:n:7:LYS:H | 8:n:10:GLN:HG3 | 1.82 | 0.43 |
| 18:x:42:GLU:HG2 | 18:x:43:LYS:N | 2.32 | 0.43 |
| 46:B:78:A:H2' | 46:B:79:C:C6 | 2.53 | 0.43 |
| 46:B:962:A:H2' | 46:B:963:A:O4' | 2.17 | 0.43 |
| 46:B:1596:U:O2' | 52:H:105:GLY:O | 2.19 | 0.43 |
| 46:B:1712:U:H2' | 46:B:1713:G:C8 | 2.53 | 0.43 |
| 57:M:35:ILE:O | 57:M:37:THR:N | 2.50 | 0.43 |
| 66:V:114:LEU:HD13 | 66:V:122:ARG:HB3 | 2.00 | 0.43 |
| 72:b:65:LEU:O | 72:b:69:LEU:HB2 | 2.18 | 0.43 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 1:AS:157:G:H2' | 1:AS:158:A:H8 | 1.82 | 0.43 |
| 1:AS:229:C:H2' | 1:AS:230:G:O4' | 2.18 | 0.43 |
| 1:AS:357:A:O4' | 6:AY:82:GLY:HA3 | 2.17 | 0.43 |
| 1:AS:605:U:OP1 | 8:BA:23:THR:HB | 2.17 | 0.43 |
| 1:AS:911:A:H8 | 1:AS:2114:C:O2' | 2.01 | 0.43 |
| 1:AS:1241:A:N7 | 1:AS:1267:A:O2' | 2.48 | 0.43 |
| 1:AS:1853:C:O2 | 35:CB:4:ARG:HB3 | 2.18 | 0.43 |
| 1:AS:2093:G:H22 | 1:AS:2098:A:H1' | 1.83 | 0.43 |
| 1:AS:2468:C:H1' | 1:AS:2469:A:H5" | 2.00 | 0.43 |
| 1:AS:2475:U:H2' | 1:AS:2476:C:H5 | 1.83 | 0.43 |
| 1:AS:3019:U:OP1 | 5:AX:222:LYS:N | 2.45 | 0.43 |
| 16:BI:104:GLU:OE2 | 16:BI:161:ALA:HA | 2.17 | 0.43 |
| 46:CM:1161:G:C6 | 46:CM:1450:G:C6 | 3.06 | 0.43 |
| 46:CM:1238:U:C2 | 46:CM:1239:U:C5 | 3.07 | 0.43 |
| 46:CM:1602:C:H5" | 46:CM:1603:G:O5' | 2.18 | 0.43 |
| 47:CN:33:ASN:HD22 | 47:CN:149:MET:HA | 1.84 | 0.43 |
| 50:CQ:178:MET:HG3 | 50:CQ:183:LEU:CD2 | 2.48 | 0.43 |
| 68:DI:85:TYR:O | 74:DO:6:ASP:N | 2.51 | 0.43 |
| 1:1:291:C:H2' | 1:1:292:U:H6 | 1.82 | 0.43 |
| 1:1:413:U:H2' | 1:1:414:U:H6 | 1.82 | 0.43 |
| 1:1:1209:G:H5' | 21:0:137:ARG:HH21 | 1.83 | 0.43 |
| 1:1:1242:G:H2' | 1:1:1243:U:C6 | 2.52 | 0.43 |
| 1:1:1639:A:H2' | 1:1:1640:C:C2 | 2.53 | 0.43 |
| 1:1:2583:U:H2' | 1:1:2584:U:H6 | 1.80 | 0.43 |
| 1:1:2615:A:OP2 | 22:2:3:LYS:HE2 | 2.17 | 0.43 |
| 2:3:7:G:OP1 | 7:m:33:ARG:HD2 | 2.18 | 0.43 |
| 10:p:48:SER:HA | 10:p:51:VAL:HG23 | 2.00 | 0.43 |
| 10:p:167:LEU:HD23 | 10:p:167:LEU:HA | 1.87 | 0.43 |
| 35:AH:105:LEU:O | 35:AH:109:GLN:NE2 | 2.51 | 0.43 |
| 44:AQ:28:LYS:O | 44:AQ:32:GLN:HG3 | 2.18 | 0.43 |
| 45:i:99:SER:OG | 45:i:102:LYS:HD2 | 2.18 | 0.43 |
| 46:B:99:C:H2' | 46:B:376:A:H4' | 2.00 | 0.43 |
| 46:B:122:U:C2' | 46:B:123:G:H5" | 2.45 | 0.43 |
| 46:B:607:U:O2 | 70:Z:19:ARG:NH1 | 2.50 | 0.43 |
| 46:B:1772:U:P | 61:Q:128:ARG:HH22 | 2.41 | 0.43 |
| 58:N:125:VAL:HG12 | 58:N:139:VAL:HA | 2.00 | 0.43 |
| 1:AS:25:A:H4' | 1:AS:329:U:H2' | 2.00 | 0.43 |
| 1:AS:373:A:N1 | 1:AS:394:G:H4' | 2.33 | 0.43 |
| 1:AS:1075:A:H4' | 7:AZ:140:ARG:O | 2.19 | 0.43 |
| 1:AS:1466:U:H2' | 1:AS:1467:U:C6 | 2.53 | 0.43 |
| 1:AS:1945:A:H2' | 1:AS:1946:U:C6 | 2.54 | 0.43 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 1:AS:2425:G:C2 | 1:AS:2426:G:H1' | 2.53 | 0.43 |
| 1:AS:2933:G:H2' | 1:AS:2934:U:H6 | 1.83 | 0.43 |
| 84:AS:3401:3K5:H16 | 84:AS:3401:3K5:H32 | 1.99 | 0.43 |
| 5:AX:256:HIS:HA | 5:AX:257:PRO:C | 2.43 | 0.43 |
| 9:BB:39:ARG:HA | 9:BB:42:ILE:HG12 | 1.99 | 0.43 |
| 11:BD:12:ILE:HD11 | 11:BD:53:ILE:HG13 | 2.00 | 0.43 |
| 46:CM:59:C:H5" | 46:CM:449:G:H21 | 1.83 | 0.43 |
| 46:CM:392:C:H2' | 46:CM:393:U:C6 | 2.53 | 0.43 |
| 46:CM:672:U:O3' | 46:CM:673:A:C8 | 2.71 | 0.43 |
| 46:CM:857:G:H2' | 46:CM:858:U:O4' | 2.18 | 0.43 |
| 46:CM:876:A:H2' | 46:CM:877:G:C8 | 2.52 | 0.43 |
| 46:CM:1503:A:O2' | 46:CM:1504:U:H5' | 2.18 | 0.43 |
| 47:CN:23:HIS:O | 47:CN:48:ILE:HD12 | 2.18 | 0.43 |
| 50:CQ:52:LYS:HA | 50:CQ:90:GLU:O | 2.19 | 0.43 |
| 51:CR:175:PHE:HE1 | 51:CR:198:ARG:HD2 | 1.84 | 0.43 |
| 59:CZ:93:ASP:OD1 | 59:CZ:93:ASP:N | 2.50 | 0.43 |
| 79:DT:157:ILE:O | 79:DT:201:LEU:HD11 | 2.18 | 0.43 |
| 80:p0:34:SER:OG | 80:p0:35:SER:N | 2.47 | 0.43 |
| 80:p0:45:LEU:CD1 | 80:p0:49:ALA:HB3 | 2.48 | 0.43 |
| 1:1:260:C:H2' | 1:1:261:U:C6 | 2.53 | 0.43 |
| 1:1:498:C:H2' | 1:1:499:G:H8 | 1.82 | 0.43 |
| 1:1:671:U:H2' | 1:1:672:G:H8 | 1.82 | 0.43 |
| 1:1:1124:U:H2' | 1:1:1125:A:O4' | 2.18 | 0.43 |
| 1:1:1562:G:C4 | 1:1:1563:A:H1' | 2.53 | 0.43 |
| 1:1:1863:A:H2' | 1:1:1864:G:H8 | 1.82 | 0.43 |
| 1:1:2251:G:O2' | 1:1:2289:G:O6 | 2.27 | 0.43 |
| 1:1:3343:C:H4' | 5:k:313:ARG:HG3 | 2.01 | 0.43 |
| 11:q:47:LYS:HB2 | 15:u:5:VAL:HB | 2.00 | 0.43 |
| 11:q:134:MET:SD | 11:q:146:VAL:HG22 | 2.58 | 0.43 |
| 16:v:143:ARG:HB3 | 36:AI:96:GLU:OE1 | 2.19 | 0.43 |
| 18:x:94:LEU:HD23 | 18:x:94:LEU:HA | 1.86 | 0.43 |
| 40:AM:18:LYS:HG2 | 40:AM:21:ARG:NH2 | 2.34 | 0.43 |
| 45:i:64:LEU:HA | 45:i:67:LYS:HG2 | 2.00 | 0.43 |
| 46:B:740:A:O2' | 46:B:741:A:OP1 | 2.28 | 0.43 |
| 46:B:818:U:H3' | 46:B:819:G:H5' | 2.00 | 0.43 |
| 46:B:1305:U:O2 | 46:B:1307:A:H5' | 2.18 | 0.43 |
| 59:O:32:LEU:HA | 59:O:32:LEU:HD23 | 1.67 | 0.43 |
| 62:R:50:ASP:N | 62:R:50:ASP:OD1 | 2.51 | 0.43 |
| 75:e:9:LEU:HA | 75:e:55:CYS:HA | 2.00 | 0.43 |
| 79:AR:118:LYS:HD2 | 79:AR:159:PRO:HA | 1.99 | 0.43 |
| 79:AR:235:ALA:HB3 | 79:AR:253:THR:HB | 2.00 | 0.43 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 1:AS:440:U:O4 | 1:AS:489:G:H1' | 2.18 | 0.43 |
| 1:AS:942:U:H2' | 1:AS:943:G:H8 | 1.84 | 0.43 |
| 1:AS:988:A:O2' | 1:AS:989:G:H5' | 2.18 | 0.43 |
| 1:AS:1065:C:H2' | 1:AS:1066:U:H6 | 1.83 | 0.43 |
| 1:AS:1338:G:H2' | 1:AS:1339:A:O4' | 2.18 | 0.43 |
| 1:AS:1443:G:N7 | 18:BK:25:SER:OG | 2.49 | 0.43 |
| 1:AS:1569:C:H2' | 1:AS:1570:A:C8 | 2.53 | 0.43 |
| 1:AS:1596:U:H5" | 20:BM:42:ARG:NH2 | 2.33 | 0.43 |
| 1:AS:1743:G:N2 | 39:CF:2:ALA:HB3 | 2.33 | 0.43 |
| 1:AS:2855:U:H2' | 1:AS:2856:C:C6 | 2.53 | 0.43 |
| 2:AT:26:C:H2' | 2:AT:27:A:O4' | 2.18 | 0.43 |
| 2:AT:84:A:H2' | 2:AT:85:G:C8 | 2.52 | 0.43 |
| 3:AU:49:G:OP2 | 36:CC:48:ARG:NH1 | 2.51 | 0.43 |
| 46:CM:260:U:C2' | 46:CM:261:C:H5' | 2.48 | 0.43 |
| 46:CM:289:G:H2' | 46:CM:290:U:C5 | 2.53 | 0.43 |
| 46:CM:518:A:HO2' | 46:CM:519:A:P | 2.41 | 0.43 |
| 46:CM:588:C:H5" | 77:DR:56:MET:SD | 2.58 | 0.43 |
| 46:CM:857:G:N2 | 46:CM:1032:G:H4' | 2.33 | 0.43 |
| 46:CM:879:U:H1' | 61:DB:31:LYS:NZ | 2.32 | 0.43 |
| 46:CM:943:U:OP2 | 74:DO:20:LYS:NZ | 2.44 | 0.43 |
| 46:CM:1579:A:O2' | 46:CM:1580:A:OP1 | 2.33 | 0.43 |
| 46:CM:1626:C:H2' | 46:CM:1627:C:O4' | 2.17 | 0.43 |
| 46:CM:1720:C:H2' | 46:CM:1721:U:H6 | 1.83 | 0.43 |
| 48:CO:81:TYR:HB2 | 48:CO:109:LYS:HG2 | 1.99 | 0.43 |
| 48:CO:120:LEU:HD13 | 48:CO:142:PHE:CE2 | 2.52 | 0.43 |
| 52:CS:109:LYS:HB3 | 52:CS:109:LYS:HE2 | 1.79 | 0.43 |
| 59:CZ:50:LYS:HE3 | 59:CZ:54:LYS:HE3 | 1.99 | 0.43 |
| 70:DK:79:ASN:OD1 | 70:DK:79:ASN:N | 2.50 | 0.43 |
| 73:DN:41:ILE:HG12 | 73:DN:68:TYR:CD2 | 2.53 | 0.43 |
| 75:DP:14:LYS:HB3 | 75:DP:29:ARG:HB3 | 1.99 | 0.43 |
| 1:1:258:U:H2' | 1:1:259:C:C6 | 2.53 | 0.43 |
| 1:1:546:C:H2' | 1:1:547:U:O4' | 2.18 | 0.43 |
| 1:1:1350:G:N1 | 1:1:1354:C:H5' | 2.34 | 0.43 |
| 1:1:1606:G:H2' | 1:1:1607:G:O4' | 2.18 | 0.43 |
| 1:1:2426:G:H22 | 1:1:2478:A:H1' | 1.84 | 0.43 |
| 6:l:6:GLN:HB3 | 6:l:20:GLN:HB3 | 2.00 | 0.43 |
| 10:p:99:ARG:NH2 | 10:p:189:THR:O | 2.48 | 0.43 |
| 16:v:37:HIS:NE2 | 16:v:63:ARG:HB3 | 2.32 | 0.43 |
| 21:0:26:ARG:HH22 | 21:0:28:ARG:HH11 | 1.65 | 0.43 |
| 37:AJ:57:ILE:HG23 | 37:AJ:93:ILE:HD11 | 1.98 | 0.43 |
| 46:B:593:G:H2' | 46:B:594:C:C6 | 2.53 | 0.43 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 46:B:945:U:H5' | 60:P:55:ARG:CD | 2.44 | 0.43 |
| 46:B:1376:U:C5 | 64:T:3:ARG:HG3 | 2.53 | 0.43 |
| 46:B:1512:A:H2' | 46:B:1513:A:C8 | 2.54 | 0.43 |
| 54:J:63:LEU:HD13 | 54:J:90:ALA:HB2 | 1.98 | 0.43 |
| 57:M:56:LYS:NZ | 57:M:69:THR:HG22 | 2.33 | 0.43 |
| 65:U:33:THR:HA | 65:U:38:VAL:O | 2.19 | 0.43 |
| 68:X:58:TYR:OH | 69:Y:20:THR:HA | 2.18 | 0.43 |
| 69:Y:77:PRO:HD2 | 69:Y:79:PHE:CZ | 2.53 | 0.43 |
| 79:AR:9:LEU:HB2 | 79:AR:310:TRP:CZ3 | 2.52 | 0.43 |
| 1:AS:38:A:H5" | 29:BV:35:ALA:HB2 | 2.00 | 0.43 |
| 1:AS:268:A:H61 | 1:AS:295:A:H3' | 1.83 | 0.43 |
| 1:AS:374:A:N3 | 1:AS:376:G:H5" | 2.34 | 0.43 |
| 1:AS:785:A:H2' | 1:AS:786:U:H6 | 1.83 | 0.43 |
| 1:AS:1790:U:C2 | 4:AW:187:HIS:CD2 | 3.07 | 0.43 |
| 1:AS:2474:C:H5' | 1:AS:2475:U:OP2 | 2.18 | 0.43 |
| 1:AS:2810:A:H4' | 12:BE:74:LYS:HD3 | 1.99 | 0.43 |
| 1:AS:2852:U:O2 | 5:AX:250:ALA:HB3 | 2.19 | 0.43 |
| 84:AS:3401:3K5:H7 | 84:AS:3401:3K5:C33 | 2.32 | 0.43 |
| 3:AU:6:U:H2' | 3:AU:7:U:H6 | 1.83 | 0.43 |
| 5:AX:260:VAL:HG11 | 5:AX:266:ARG:HH11 | 1.83 | 0.43 |
| 8:BA:39:LEU:HB3 | 8:BA:83:VAL:CG1 | 2.49 | 0.43 |
| 22:BO:45:ASN:H | 22:BO:95:HIS:CD2 | 2.36 | 0.43 |
| 24:BQ:108:GLU:HG2 | 24:BQ:128:ARG:HG3 | 2.00 | 0.43 |
| 38:CE:28:HIS:HB3 | 38:CE:31:LYS:HB2 | 1.99 | 0.43 |
| 46:CM:125:U:H5" | 51:CR:148:ARG:CZ | 2.48 | 0.43 |
| 46:CM:137:A:O4' | 46:CM:139:U:H5' | 2.18 | 0.43 |
| 46:CM:176:U:O2' | 46:CM:177:A:OP2 | 2.36 | 0.43 |
| 46:CM:504:A:H5" | 46:CM:505:U:P | 2.57 | 0.43 |
| 46:CM:1039:U:H2' | 46:CM:1040:U:C6 | 2.53 | 0.43 |
| 46:CM:1212:A:C2 | 59:CZ:43:ARG:HB3 | 2.53 | 0.43 |
| 50:CQ:77:ARG:HB2 | 57:CX:22:VAL:HG11 | 2.00 | 0.43 |
| 51:CR:71:GLN:HB3 | 51:CR:91:THR:HB | 1.98 | 0.43 |
| 53:CT:229:LYS:HB3 | 53:CT:229:LYS:HE3 | 1.62 | 0.43 |
| 54:CU:109:PRO:HG2 | 54:CU:112:ARG:HD3 | 2.00 | 0.43 |
| 62:DC:60:LEU:HD22 | 62:DC:92:SER:HB3 | 2.00 | 0.43 |
| 64:DE:74:GLN:O | 64:DE:78:ARG:HB3 | 2.19 | 0.43 |
| 82:L1:14:HIS:CE1 | 82:L1:176:GLU:HB2 | 2.53 | 0.43 |
| 80:p0:61:ARG:HG2 | 80:p0:64:ARG:CG | 2.49 | 0.43 |
| 1:1:304:G:H3' | 1:1:304:G:OP2 | 2.19 | 0.43 |
| 1:1:757:A:H2' | 1:1:758:U:C6 | 2.53 | 0.43 |
| 1:1:925:A:H2' | 1:1:926:U:C6 | 2.53 | 0.43 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 1:1:1014:G:N2 | 1:1:1030:U:O2 | 2.47 | 0.43 |
| 1:1:1099:A:H62 | 1:1:1338:G:H21 | 1.66 | 0.43 |
| 1:1:1262:G:N2 | 1:1:1272:U:H1' | 2.33 | 0.43 |
| 1:1:1721:C:H2' | 1:1:1722:C:C6 | 2.54 | 0.43 |
| 1:1:2651:A:H1' | 45:i:50:LYS:HG3 | 2.00 | 0.43 |
| 1:1:2753:U:H2' | 1:1:2754:U:C6 | 2.53 | 0.43 |
| 1:1:3309:A:H2 | 1:1:3326:G:H21 | 1.65 | 0.43 |
| 12:r:34:TYR:O | 12:r:88:ARG:HA | 2.18 | 0.43 |
| 46:B:404:U:H2' | 46:B:405:A:C8 | 2.54 | 0.43 |
| 46:B:511:U:O4 | 56:L:171:ARG:NH2 | 2.52 | 0.43 |
| 46:B:1416:U:H1' | 67:W:71:ASN:HB3 | 1.99 | 0.43 |
| 46:B:1654:A:H2' | 46:B:1655:G:H8 | 1.84 | 0.43 |
| 57:M:14:TYR:CD2 | 57:M:21:VAL:HG22 | 2.51 | 0.43 |
| 61:Q:11:VAL:HG12 | 61:Q:13:ARG:HG3 | 2.00 | 0.43 |
| 69:Y:24:GLN:HA | 69:Y:63:VAL:O | 2.19 | 0.43 |
| 78:h:161:ARG:HD3 | 78:h:161:ARG:HA | 1.69 | 0.43 |
| 79:AR:38:ARG:HG2 | 79:AR:68:ILE:HG23 | 2.01 | 0.43 |
| 1:AS:246:U:H2' | 1:AS:247:C:C6 | 2.53 | 0.43 |
| 1:AS:624:U:H2' | 1:AS:625:C:C6 | 2.54 | 0.43 |
| 1:AS:2176:A:C2 | 1:AS:2177:G:C8 | 3.07 | 0.43 |
| 1:AS:2480:A:H4' | 1:AS:2481:G:H8 | 1.83 | 0.43 |
| 2:AT:81:U:H2' | 2:AT:82:G:H8 | 1.82 | 0.43 |
| 3:AU:156:U:H2' | 3:AU:157:U:C6 | 2.54 | 0.43 |
| 19:BL:176:ARG:N | 29:BV:51:GLY:HA2 | 2.33 | 0.43 |
| 27:BT:69:LYS:HE2 | 27:BT:69:LYS:HB3 | 1.86 | 0.43 |
| 28:BU:23:VAL:HG12 | 28:BU:45:GLY:HA3 | 2.00 | 0.43 |
| 46:CM:154:A:H2' | 46:CM:155:A:O4' | 2.18 | 0.43 |
| 46:CM:1062:C:OP1 | 73:DN:13:LYS:NZ | 2.51 | 0.43 |
| 46:CM:1220:C:H3' | 46:CM:1221:A:H8 | 1.83 | 0.43 |
| 58:CY:26:LYS:CG | 58:CY:29:LYS:HE2 | 2.48 | 0.43 |
| 61:DB:76:ILE:HD13 | 61:DB:97:LEU:CD1 | 2.48 | 0.43 |
| 80:P0:80:ILE:C | 80:P0:81:LYS:HD2 | 2.43 | 0.43 |
| 81:12:112:ILE:HG22 | 81:12:132:ILE:HD13 | 2.00 | 0.43 |
| 82:L1:212:PRO:HB2 | 82:L1:213:SER:H | 1.54 | 0.43 |
| 82:l1:26:ARG:NH2 | 82:l1:28:PHE:O | 2.52 | 0.43 |
| 80:p0:70:LEU:HD13 | 80:p0:72:GLU:CD | 2.43 | 0.43 |
| 80:p0:96:ILE:O | 80:p0:100:VAL:HG22 | 2.18 | 0.43 |
| 1:1:200:A:H2' | 1:1:201:G:C8 | 2.54 | 0.43 |
| 1:1:1221:A:H2' | 1:1:1222:G:C8 | 2.53 | 0.43 |
| 1:1:1380:U:OP2 | 6:l:203:ARG:HA | 2.18 | 0.43 |
| 1:1:2251:G:H22 | 1:1:2290:A:P | 2.42 | 0.43 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 1:1:2383:C:O2 | 1:1:2791:A:N1 | 2.52 | 0.43 |
| 3:4:40:A:H2' | 3:4:41:A:C8 | 2.53 | 0.43 |
| 3:4:119:C:H2' | 3:4:120:U:C6 | 2.54 | 0.43 |
| 4:j:117:GLU:HB2 | 4:j:162:ALA:HB1 | 2.00 | 0.43 |
| 11:q:137:SER:HB3 | 11:q:143:GLU:HB3 | 2.00 | 0.43 |
| 16:v:23:TYR:O | 16:v:122:ASN:ND2 | 2.52 | 0.43 |
| 26:8:108:LEU:N | 26:8:125:ARG:O | 2.44 | 0.43 |
| 30:AC:17:HIS:NE2 | 30:AC:21:ILE:HG13 | 2.34 | 0.43 |
| 38:AK:18:LEU:HD11 | 40:AM:51:ILE:HD12 | 2.00 | 0.43 |
| 44:AQ:49:ARG:HB2 | 44:AQ:55:TRP:CZ3 | 2.54 | 0.43 |
| 46:B:1:U:C2 | 46:B:3:U:C4 | 3.07 | 0.43 |
| 46:B:283:G:H2' | 46:B:284:C:C6 | 2.54 | 0.43 |
| 46:B:443:A:C2 | 46:B:444:A:C8 | 3.07 | 0.43 |
| 46:B:792:U:H2' | 46:B:793:A:C8 | 2.53 | 0.43 |
| 46:B:795:A:N6 | 54:J:109:PRO:HD3 | 2.33 | 0.43 |
| 46:B:975:C:H2' | 46:B:976:G:O4' | 2.19 | 0.43 |
| 46:B:1300:U:O2' | 46:B:1301:G:H8 | 2.00 | 0.43 |
| 46:B:1503:A:H8 | 67:W:57:MET:HE1 | 1.83 | 0.43 |
| 48:D:115:ARG:HA | 48:D:115:ARG:HD3 | 1.65 | 0.43 |
| 65:U:22:ILE:HD11 | 65:U:35:ILE:HD11 | 1.99 | 0.43 |
| 1:AS:403:C:O2' | 1:AS:404:G:OP1 | 2.25 | 0.43 |
| 1:AS:908:G:N7 | 4:AW:9:ARG:NH2 | 2.66 | 0.43 |
| 1:AS:1232:G:H1' | 1:AS:1241:A:O4' | 2.18 | 0.43 |
| 1:AS:2074:A:H2' | 1:AS:2075:U:C6 | 2.53 | 0.43 |
| 1:AS:2430:G:O2' | 1:AS:2431:U:OP2 | 2.33 | 0.43 |
| 1:AS:2621:G:H4' | 1:AS:2668:A:O4' | 2.18 | 0.43 |
| 1:AS:2852:U:H1' | 5:AX:250:ALA:HB3 | 2.01 | 0.43 |
| 1:AS:2902:A:H2' | 1:AS:2903:C:H6 | 1.83 | 0.43 |
| 1:AS:3172:U:C4 | 21:BN:159:SER:HB2 | 2.54 | 0.43 |
| 2:AT:39:U:H3 | 13:BF:70:THR:HB | 1.83 | 0.43 |
| 3:AU:19:C:H2' | 3:AU:20:U:C6 | 2.53 | 0.43 |
| 6:AY:303:ALA:CA | 19:BL:39:ARG:HH12 | 2.30 | 0.43 |
| 7:AZ:95:TRP:HD1 | 7:AZ:158:ARG:HA | 1.83 | 0.43 |
| 21:BN:79:LEU:HD13 | 21:BN:110:LEU:HD21 | 2.00 | 0.43 |
| 36:CC:6:THR:HG22 | 36:CC:53:ARG:HD3 | 2.01 | 0.43 |
| 45:CL:82:LYS:HE2 | 46:CM:1175:C:N4 | 2.33 | 0.43 |
| 46:CM:871:U:O2' | 61:DB:116:VAL:O | 2.35 | 0.43 |
| 46:CM:1746:C:H2' | 46:CM:1747:G:O4' | 2.19 | 0.43 |
| 50:CQ:176:VAL:HB | 50:CQ:183:LEU:CD2 | 2.49 | 0.43 |
| 59:CZ:82:PRO:HB2 | 59:CZ:84:GLU:N | 2.33 | 0.43 |
| 62:DC:8:LYS:HD3 | 62:DC:8:LYS:HA | 1.73 | 0.43 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 70:DK:103:LEU:HD22 | 70:DK:126:LYS:NZ | 2.34 | 0.43 |
| 1:1:152:U:O2' | 1:1:153:U:H5' | 2.19 | 0.43 |
| 1:1:216:U:H4' | 27:9:100:HIS:CG | 2.53 | 0.43 |
| 1:1:242:C:O2' | 1:1:243:G:H8 | 2.02 | 0.43 |
| 1:1:412:G:H5' | 18:x:26:PHE:HZ | 1.83 | 0.43 |
| 1:1:421:G:O6 | 1:1:2361:C:O2' | 2.31 | 0.43 |
| 1:1:426:G:H2' | 1:1:427:C:C6 | 2.54 | 0.43 |
| 1:1:495:C:H2' | 1:1:496:A:H8 | 1.83 | 0.43 |
| 1:1:1006:G:N2 | 12:r:193:ASP:O | 2.37 | 0.43 |
| 1:1:1165:A:H2' | 1:1:1166:A:C8 | 2.54 | 0.43 |
| 1:1:1217:A:C2 | 80:P0:12:PHE:HE2 | 2.36 | 0.43 |
| 1:1:1678:U:O2 | 23:5:85:LYS:HG2 | 2.19 | 0.43 |
| 1:1:2642:G:H2' | 1:1:2643:A:C8 | 2.53 | 0.43 |
| 5:k:145:GLU:OE2 | 5:k:196:LYS:HE2 | 2.19 | 0.43 |
| 7:m:125:VAL:HG11 | 7:m:199:ILE:HG21 | 1.99 | 0.43 |
| 46:B:139:U:P | 53:I:149:LYS:HZ1 | 2.35 | 0.43 |
| 46:B:165:U:H2' | 46:B:166:A:H5" | 1.99 | 0.43 |
| 46:B:400:C:OP1 | 51:G:3:ARG:NH1 | 2.51 | 0.43 |
| 46:B:451:C:O2 | 46:B:451:C:H2' | 2.19 | 0.43 |
| 46:B:814:A:H2 | 46:B:815:U:H3 | 1.66 | 0.43 |
| 46:B:885:A:H2' | 46:B:886:G:H8 | 1.84 | 0.43 |
| 46:B:1007:C:H4' | 46:B:1110:A:H61 | 1.83 | 0.43 |
| 46:B:1595:U:O3' | 63:S:72:GLY:HA3 | 2.19 | 0.43 |
| 47:C:144:ILE:HG12 | 47:C:158:VAL:HB | 2.01 | 0.43 |
| 48:D:24:PHE:HZ | 61:Q:34:ILE:HA | 1.83 | 0.43 |
| 52:H:63:GLN:HE22 | 52:H:66:ASN:HB2 | 1.84 | 0.43 |
| 57:M:35:ILE:HG22 | 57:M:37:THR:HG22 | 2.00 | 0.43 |
| 57:M:70:ASP:OD1 | 57:M:71:GLU:HG3 | 2.19 | 0.43 |
| 67:W:34:GLU:HG2 | 67:W:88:ARG:HH22 | 1.83 | 0.43 |
| 1:AS:669:U:OP1 | 19:BL:55:SER:OG | 2.35 | 0.43 |
| 1:AS:744:U:H2' | 1:AS:745:C:C6 | 2.54 | 0.43 |
| 1:AS:849:G:OP2 | 44:CK:2:THR:HG21 | 2.19 | 0.43 |
| 1:AS:1214:U:H5" | 80:p0:5:ARG:HD3 | 2.01 | 0.43 |
| 1:AS:1329:C:C2 | 1:AS:1330:U:C5 | 3.06 | 0.43 |
| 1:AS:1618:U:H2' | 1:AS:1619:G:H8 | 1.83 | 0.43 |
| 1:AS:1719:A:OP1 | 20:BM:128:LYS:NZ | 2.45 | 0.43 |
| 1:AS:2157:C:C4 | 4:AW:131:GLY:HA3 | 2.54 | 0.43 |
| 1:AS:2210:A:N3 | 1:AS:2406:U:O2' | 2.46 | 0.43 |
| 1:AS:2485:U:H2' | 1:AS:2486:U:H6 | 1.83 | 0.43 |
| 1:AS:2927:U:H2' | 1:AS:2928:A:O4' | 2.19 | 0.43 |
| 4:AW:66:PRO:HG2 | 4:AW:67:TYR:CE2 | 2.53 | 0.43 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 9:BB:130:PRO:HG2 | 9:BB:131:TYR:CE2 | 2.53 | 0.43 |
| 22:BO:97:LYS:HB3 | 22:BO:97:LYS:HE2 | 1.67 | 0.43 |
| 23:BP:19:VAL:HG12 | 23:BP:108:LEU:HG | 2.00 | 0.43 |
| 45:CL:83:HIS:CD2 | 45:CL:84:SER:H | 2.36 | 0.43 |
| 46:CM:657:C:O2 | 46:CM:669:G:N2 | 2.51 | 0.43 |
| 46:CM:736:G:H2' | 46:CM:737:A:H8 | 1.84 | 0.43 |
| 46:CM:903:U:H2' | 46:CM:904:A:H8 | 1.76 | 0.43 |
| 46:CM:1311:A:H2' | 46:CM:1312:C:H6 | 1.84 | 0.43 |
| 46:CM:1326:A:H1' | 79:DT:66:SER:OG | 2.19 | 0.43 |
| 50:CQ:24:GLU:OE1 | 76:DQ:23:HIS:CE1 | 2.72 | 0.43 |
| 64:DE:99:GLN:OE1 | 64:DE:120:GLN:NE2 | 2.52 | 0.43 |
| 79:DT:113:SER:CB | 79:DT:154:ALA:HA | 2.49 | 0.43 |
| 1:1:58:G:H2' | 3:4:33:A:O2' | 2.18 | 0.43 |
| 1:1:364:G:OP1 | 6:l:61:THR:HG23 | 2.18 | 0.43 |
| 1:1:559:C:H2' | 1:1:560:C:H6 | 1.83 | 0.43 |
| 1:1:1747:G:H5' | 39:AL:26:LYS:HE2 | 2.01 | 0.43 |
| 1:1:1902:G:H1' | 1:1:1904:A:N6 | 2.34 | 0.43 |
| 1:1:2628:A:C8 | 1:1:2630:G:C8 | 3.07 | 0.43 |
| 1:1:3336:G:H2' | 1:1:3337:A:C8 | 2.54 | 0.43 |
| 3:4:27:U:H2' | 3:4:28:C:C6 | 2.54 | 0.43 |
| 4:j:30:ARG:HG2 | 4:j:74:GLU:HG3 | 2.01 | 0.43 |
| 4:j:117:GLU:OE2 | 4:j:163:ARG:HB2 | 2.19 | 0.43 |
| 7:m:204:VAL:O | 7:m:208:MET:HG3 | 2.18 | 0.43 |
| 32:AE:78:ARG:HA | 32:AE:88:LEU:HD23 | 2.01 | 0.43 |
| 46:B:147:C:C2 | 46:B:148:C:C5 | 3.06 | 0.43 |
| 46:B:213:A:H2' | 46:B:214:U:H5' | 2.00 | 0.43 |
| 46:B:384:G:H2' | 46:B:385:A:C8 | 2.54 | 0.43 |
| 46:B:638:U:HO2' | 46:B:639:G:P | 2.41 | 0.43 |
| 46:B:787:A:O2' | 54:J:100:ARG:NE | 2.51 | 0.43 |
| 46:B:1438:U:P | 76:f:10:HIS:HD1 | 2.41 | 0.43 |
| 47:C:79:ARG:O | 47:C:83:GLN:HG3 | 2.18 | 0.43 |
| 50:F:139:ILE:HG12 | 50:F:185:ILE:HG22 | 1.99 | 0.43 |
| 53:I:6:SER:O | 53:I:113:ILE:HG13 | 2.19 | 0.43 |
| 54:J:109:PRO:HG2 | 54:J:112:ARG:HD3 | 2.01 | 0.43 |
| 72:b:78:VAL:HG12 | 72:b:81:ARG:NH2 | 2.33 | 0.43 |
| 77:g:54:ARG:HH12 | 77:g:56:MET:HE2 | 1.83 | 0.43 |
| 79:AR:92:LEU:HB2 | 79:AR:104:PHE:HE1 | 1.83 | 0.43 |
| 1:AS:166:U:H2' | 1:AS:167:U:H6 | 1.84 | 0.43 |
| 1:AS:275:U:H2' | 1:AS:276:U:C6 | 2.54 | 0.43 |
| 1:AS:437:G:H1 | 1:AS:620:A:N6 | 2.16 | 0.43 |
| 1:AS:614:G:H2' | 1:AS:615:G:C8 | 2.54 | 0.43 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 1:AS:1296:G:OP2 | 1:AS:1297:A:O2' | 2.30 | 0.43 |
| 1:AS:1478:A:H4' | 1:AS:1479:G:OP2 | 2.19 | 0.43 |
| 1:AS:1692:A:H2' | 1:AS:1693:A:H8 | 1.83 | 0.43 |
| 1:AS:2919:G:C2 | 5:AX:250:ALA:HB1 | 2.54 | 0.43 |
| 1:AS:3264:C:H2' | 1:AS:3265:U:C6 | 2.53 | 0.43 |
| 2:AT:24:A:H2' | 2:AT:25:G:C8 | 2.54 | 0.43 |
| 7:AZ:119:TYR:OH | 7:AZ:135:VAL:HG22 | 2.19 | 0.43 |
| 20:BM:176:ARG:NH2 | 46:CM:838:G:OP2 | 2.51 | 0.43 |
| 45:CL:67:LYS:HG3 | 45:CL:69:PHE:HD2 | 1.82 | 0.43 |
| 46:CM:382:G:H2' | 46:CM:383:A:C8 | 2.54 | 0.43 |
| 46:CM:1383:U:O2' | 46:CM:1386:A:N6 | 2.37 | 0.43 |
| 52:CS:166:ARG:HB2 | 75:DP:46:GLY:HA3 | 2.01 | 0.43 |
| 53:CT:56:ASN:HB2 | 53:CT:108:VAL:HG12 | 2.00 | 0.43 |
| 57:CX:15:LEU:HD21 | 57:CX:68:LEU:HD13 | 2.01 | 0.43 |
| 78:DS:181:GLN:O | 78:DS:189:THR:HA | 2.19 | 0.43 |
| 82:L1:119:GLN:HA | 82:L1:122:ARG:HB2 | 2.00 | 0.43 |
| 82:l1:5:THR:O | 82:l1:9:VAL:HG23 | 2.19 | 0.43 |
| 82:l1:49:PHE:CD1 | 82:l1:193:LEU:HD13 | 2.53 | 0.43 |
| 82:l1:174:MET:HB3 | 82:l1:178:VAL:HB | 2.00 | 0.43 |
| 1:1:72:A:C5 | 37:AJ:14:ARG:HD2 | 2.54 | 0.43 |
| 1:1:561:U:H2' | 1:1:562:C:C6 | 2.53 | 0.43 |
| 1:1:1252:G:H2' | 1:1:1253:C:C6 | 2.54 | 0.43 |
| 1:1:1258:G:H3' | 1:1:1258:G:OP2 | 2.19 | 0.43 |
| 1:1:1787:U:H2' | 1:1:1788:C:C6 | 2.54 | 0.43 |
| 1:1:1908:U:O2' | 1:1:2099:G:N7 | 2.32 | 0.43 |
| 1:1:1940:U:H2' | 1:1:1941:A:H8 | 1.82 | 0.43 |
| 1:1:2260:U:O2 | 1:1:2288:U:H4' | 2.18 | 0.43 |
| 1:1:2373:G:H5" | 5:k:255:TRP:CD1 | 2.54 | 0.43 |
| 1:1:2406:U:H2' | 1:1:2407:G:H8 | 1.84 | 0.43 |
| 1:1:2828:G:H2' | 1:1:2829:C:H6 | 1.84 | 0.43 |
| 1:1:3136:C:H2' | 1:1:3137:A:C8 | 2.54 | 0.43 |
| 1:1:3234:U:H3 | 8:n:134:ARG:NH1 | 2.17 | 0.43 |
| 4:j:77:ILE:CD1 | 4:j:128:ARG:HB3 | 2.49 | 0.43 |
| 5:k:159:ARG:HG2 | 5:k:182:GLN:HA | 2.00 | 0.43 |
| 9:o:36:LYS:HE2 | 9:o:36:LYS:HB2 | 1.88 | 0.43 |
| 9:o:233:ILE:HD12 | 9:o:233:ILE:HA | 1.92 | 0.43 |
| 13:s:19:LEU:O | 13:s:68:HIS:HA | 2.19 | 0.43 |
| 15:u:14:GLU:CB | 21:0:149:LYS:HG2 | 2.49 | 0.43 |
| 46:B:31:C:O2' | 46:B:545:U:OP1 | 2.37 | 0.43 |
| 46:B:649:G:C5 | 46:B:650:G:H1' | 2.54 | 0.43 |
| 46:B:891:A:H2' | 46:B:892:A:C8 | 2.54 | 0.43 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 46:B:997:U:H2' | 46:B:998:A:H8 | 1.84 | 0.43 |
| 46:B:1230:G:N2 | 46:B:1235:U:O4 | 2.43 | 0.43 |
| 46:B:1248:G:H2' | 46:B:1249:G:O4' | 2.19 | 0.43 |
| 46:B:1335:U:H5' | 63:S:67:LYS:NZ | 2.33 | 0.43 |
| 46:B:1756:U:H1' | 61:Q:131:ARG:HB3 | 2.01 | 0.43 |
| 57:M:17:GLN:O | 57:M:18:GLU:HB2 | 2.19 | 0.43 |
| 61:Q:101:ALA:HB2 | 73:c:53:LEU:HD23 | 2.00 | 0.43 |
| 63:S:46:LYS:HA | 63:S:46:LYS:HD2 | 1.79 | 0.43 |
| 65:U:57:ARG:NH1 | 72:b:40:VAL:HB | 2.34 | 0.43 |
| 70:Z:48:HIS:CD2 | 70:Z:105:ALA:HB2 | 2.53 | 0.43 |
| 79:AR:133:LYS:HD3 | 79:AR:141:CYS:SG | 2.59 | 0.43 |
| 1:AS:243:G:H2' | 1:AS:244:G:C8 | 2.53 | 0.43 |
| 1:AS:447:U:C2' | 1:AS:448:U:H5" | 2.38 | 0.43 |
| 1:AS:1468:U:H5' | 20:BM:4:LEU:HB2 | 2.01 | 0.43 |
| 1:AS:2623:G:H5" | 1:AS:2624:U:O4' | 2.19 | 0.43 |
| 1:AS:2632:G:OP1 | 1:AS:2722:U:O2' | 2.37 | 0.43 |
| 1:AS:2645:A:H5" | 13:BF:95:ASN:ND2 | 2.33 | 0.43 |
| 1:AS:3038:U:H2' | 1:AS:3039:C:H6 | 1.84 | 0.43 |
| 11:BD:16:VAL:HG11 | 11:BD:79:ILE:HG13 | 2.01 | 0.43 |
| 11:BD:47:LYS:HE2 | 15:BH:3:SER:HB3 | 2.01 | 0.43 |
| 15:BH:14:GLU:HG2 | 15:BH:17:ARG:CG | 2.47 | 0.43 |
| 24:BQ:75:PRO:HG2 | 24:BQ:103:VAL:O | 2.19 | 0.43 |
| 29:BV:112:VAL:HB | 29:BV:130:VAL:HG12 | 2.00 | 0.43 |
| 44:CK:5:THR:HB | 44:CK:8:VAL:HG22 | 2.01 | 0.43 |
| 46:CM:246:U:H5' | 58:CY:36:LYS:HG3 | 1.99 | 0.43 |
| 46:CM:654:G:H5" | 46:CM:655:U:OP2 | 2.18 | 0.43 |
| 46:CM:667:A:H2' | 46:CM:668:U:C6 | 2.53 | 0.43 |
| 46:CM:1318:C:H2' | 46:CM:1319:U:C6 | 2.53 | 0.43 |
| 46:CM:1377:A:H2' | 46:CM:1378:U:C6 | 2.54 | 0.43 |
| 46:CM:1490:A:H2' | 46:CM:1491:G:O4' | 2.18 | 0.43 |
| 46:CM:1494:G:H2' | 46:CM:1495:U:H6 | 1.84 | 0.43 |
| 48:CO:61:LEU:HD23 | 48:CO:96:LEU:HD22 | 2.00 | 0.43 |
| 48:CO:136:ARG:HG3 | 48:CO:218:LEU:HD11 | 2.00 | 0.43 |
| 49:CP:78:ILE:HD11 | 49:CP:120:ILE:HD11 | 2.00 | 0.43 |
| 57:CX:25:LYS:HD2 | 57:CX:59:PHE:CZ | 2.54 | 0.43 |
| 80:P0:43:LYS:HD2 | 80:P0:43:LYS:HA | 1.75 | 0.43 |
| 82:l1:49:PHE:CE1 | 82:l1:159:LEU:HB2 | 2.53 | 0.43 |
| 1:1:583:A:H2' | 1:1:584:C:H6 | 1.84 | 0.43 |
| 1:1:602:A:H8 | 1:1:602:A:OP1 | 2.02 | 0.43 |
| 1:1:696:U:H2' | 1:1:697:A:O4' | 2.18 | 0.43 |
| 1:1:705:U:H1' | 1:1:750:G:O2' | 2.18 | 0.43 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 1:1:817:U:H2' | 1:1:818:G:H8 | 1.83 | 0.43 |
| 1:1:1237:U:H2' | 1:1:1239:G:OP2 | 2.18 | 0.43 |
| 1:1:1725:A:N6 | 44:AQ:42:CYS:HA | 2.34 | 0.43 |
| 1:1:1809:A:OP1 | 1:1:1813:G:O2' | 2.33 | 0.43 |
| 1:1:2115:U:C6 | 1:1:2119:U:C4 | 3.06 | 0.43 |
| 1:1:2397:A:H2' | 1:1:2398:C:H6 | 1.83 | 0.43 |
| 1:1:2958:U:C2 | 1:1:2959:A:C8 | 3.06 | 0.43 |
| 4:j:117:GLU:OE1 | 4:j:121:GLY:N | 2.46 | 0.43 |
| 5:k:57:VAL:HG22 | 5:k:73:VAL:HG22 | 2.01 | 0.43 |
| 10:p:69:ARG:HD3 | 10:p:238:ILE:O | 2.19 | 0.43 |
| 21:0:14:LEU:HD23 | 21:0:14:LEU:HA | 1.90 | 0.43 |
| 23:5:19:VAL:HG12 | 23:5:108:LEU:HG | 2.01 | 0.43 |
| 46:B:14:C:H2' | 46:B:15:U:C6 | 2.53 | 0.43 |
| 46:B:672:U:O3' | 46:B:673:A:C8 | 2.72 | 0.43 |
| 46:B:1300:U:OP1 | 46:B:1313:G:N2 | 2.37 | 0.43 |
| 46:B:1612:C:H2' | 46:B:1613:U:C6 | 2.54 | 0.43 |
| 46:B:1637:U:H2' | 46:B:1638:A:H8 | 1.83 | 0.43 |
| 56:L:101:PRO:O | 56:L:105:LEU:HD12 | 2.19 | 0.43 |
| 1:AS:76:A:H5' | 14:BG:100:ARG:CZ | 2.48 | 0.43 |
| 1:AS:347:G:O6 | 38:CE:55:ARG:NH1 | 2.52 | 0.43 |
| 1:AS:437:G:H1 | 1:AS:620:A:H61 | 1.66 | 0.43 |
| 1:AS:807:U:H2' | 1:AS:808:G:C8 | 2.54 | 0.43 |
| 1:AS:1313:A:O2' | 1:AS:1314:A:H3' | 2.19 | 0.43 |
| 1:AS:1452:A:N1 | 1:AS:1472:G:O2' | 2.51 | 0.43 |
| 1:AS:2649:G:H2' | 1:AS:2649:G:N3 | 2.33 | 0.43 |
| 1:AS:2855:U:H2' | 1:AS:2856:C:H6 | 1.84 | 0.43 |
| 1:AS:3199:G:H2' | 1:AS:3200:C:H6 | 1.84 | 0.43 |
| 4:AW:64:ARG:NH2 | 10:BC:39:GLN:O | 2.52 | 0.43 |
| 8:BA:53:TYR:CE1 | 8:BA:62:LEU:HB3 | 2.54 | 0.43 |
| 11:BD:17:THR:OG1 | 11:BD:28:THR:HB | 2.19 | 0.43 |
| 12:BE:140:THR:HG21 | 12:BE:148:VAL:HG21 | 2.00 | 0.43 |
| 27:BT:77:LYS:HE3 | 40:CG:31:THR:HG21 | 2.01 | 0.43 |
| 36:CC:12:LYS:HD3 | 36:CC:16:GLN:HB3 | 2.01 | 0.43 |
| 46:CM:14:C:H2' | 46:CM:15:U:C6 | 2.53 | 0.43 |
| 46:CM:404:U:H2' | 46:CM:405:A:C8 | 2.54 | 0.43 |
| 46:CM:487:C:O2 | 46:CM:496:G:C2 | 2.72 | 0.43 |
| 46:CM:723:G:H2' | 46:CM:724:G:H4' | 2.01 | 0.43 |
| 46:CM:945:U:O2' | 60:DA:48:SER:O | 2.31 | 0.43 |
| 46:CM:953:U:H5" | 46:CM:1018:C:O2' | 2.19 | 0.43 |
| 46:CM:1032:G:H2' | 46:CM:1033:U:H6 | 1.84 | 0.43 |
| 46:CM:1105:U:H2' | 46:CM:1106:C:C6 | 2.53 | 0.43 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 46:CM:1167:U:H2' | 46:CM:1168:A:O3' | 2.18 | 0.43 |
| 46:CM:1318:C:H2' | 46:CM:1319:U:H6 | 1.84 | 0.43 |
| 46:CM:1453:C:O2' | 66:DG:88:PHE:O | 2.22 | 0.43 |
| 46:CM:1672:G:H2' | 46:CM:1673:U:H6 | 1.84 | 0.43 |
| 51:CR:32:SER:OG | 51:CR:81:THR:HG23 | 2.19 | 0.43 |
| 53:CT:2:LYS:O | 53:CT:108:VAL:HA | 2.19 | 0.43 |
| 62:DC:33:PHE:CZ | 62:DC:112:VAL:HG22 | 2.54 | 0.43 |
| 63:DD:94:LYS:O | 79:DT:60:LYS:NZ | 2.39 | 0.43 |
| 65:DF:56:LYS:HE3 | 65:DF:60:GLU:HB2 | 2.00 | 0.43 |
| 82:L1:158:GLN:H | 82:L1:158:GLN:CD | 2.26 | 0.43 |
| 82:l1:163:LEU:HD12 | 82:l1:163:LEU:HA | 1.81 | 0.43 |
| 80:p0:64:ARG:HA | 80:p0:64:ARG:HD2 | 1.84 | 0.43 |
| 1:1:35:C:H4' | 1:1:804:A:N1 | 2.33 | 0.42 |
| 1:1:413:U:H2' | 1:1:414:U:C6 | 2.54 | 0.42 |
| 1:1:538:G:C6 | 1:1:548:G:C6 | 3.07 | 0.42 |
| 1:1:976:A:C2' | 1:1:977:U:H5' | 2.48 | 0.42 |
| 1:1:1128:C:H2' | 1:1:1129:A:H8 | 1.84 | 0.42 |
| 1:1:1235:C:C2 | 1:1:1236:A:C8 | 3.07 | 0.42 |
| 1:1:1499:A:C4 | 1:1:1500:A:C8 | 3.06 | 0.42 |
| 1:1:2814:U:O2 | 1:1:2814:U:H2' | 2.18 | 0.42 |
| 1:1:3090:C:H2' | 1:1:3091:U:O4' | 2.18 | 0.42 |
| 1:1:3319:U:H5" | 1:1:3320:U:H3' | 2.00 | 0.42 |
| 2:3:16:U:H2' | 2:3:17:A:H8 | 1.82 | 0.42 |
| 3:4:45:C:OP1 | 40:AM:12:LYS:HD2 | 2.19 | 0.42 |
| 3:4:126:A:O2' | 3:4:128:U:OP2 | 2.23 | 0.42 |
| 12:r:47:PRO:HB3 | 12:r:171:TRP:CZ2 | 2.54 | 0.42 |
| 17:w:35:VAL:HG22 | 17:w:104:LYS:HB2 | 2.01 | 0.42 |
| 19:y:133:LYS:HB2 | 19:y:135:GLN:NE2 | 2.34 | 0.42 |
| 25:7:86:SER:O | 25:7:90:ILE:HG12 | 2.18 | 0.42 |
| 46:B:30:G:H2' | 46:B:31:C:H6 | 1.82 | 0.42 |
| 46:B:702:G:H4' | 46:B:703:U:H4' | 2.00 | 0.42 |
| 46:B:1071:A:H2' | 46:B:1072:A:C8 | 2.53 | 0.42 |
| 46:B:1238:U:H2' | 46:B:1239:U:C6 | 2.54 | 0.42 |
| 46:B:1242:U:O2 | 57:M:2:LEU:HD23 | 2.18 | 0.42 |
| 62:R:77:LYS:HD2 | 62:R:102:PHE:CE1 | 2.53 | 0.42 |
| 1:AS:96:U:H2' | 1:AS:97:G:C8 | 2.54 | 0.42 |
| 1:AS:414:U:H2' | 1:AS:415:G:H8 | 1.84 | 0.42 |
| 1:AS:523:G:H1 | 1:AS:563:U:H3 | 1.67 | 0.42 |
| 1:AS:559:C:H2' | 1:AS:560:C:C6 | 2.54 | 0.42 |
| 1:AS:662:U:H5' | 6:AY:108:ARG:HA | 2.00 | 0.42 |
| 1:AS:844:A:C5 | 1:AS:845:C:H1' | 2.54 | 0.42 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 1:AS:952:U:H2' | 1:AS:953:C:C6 | 2.54 | 0.42 |
| 1:AS:1189:A:H2' | 1:AS:1190:G:C8 | 2.54 | 0.42 |
| 1:AS:1852:C:H2' | 1:AS:1853:C:H6 | 1.84 | 0.42 |
| 1:AS:2745:C:C2 | 1:AS:2746:C:C5 | 3.06 | 0.42 |
| 1:AS:3038:U:H2' | 1:AS:3039:C:C6 | 2.54 | 0.42 |
| 1:AS:3068:C:H2' | 1:AS:3069:U:C6 | 2.54 | 0.42 |
| 1:AS:3322:U:H2' | 1:AS:3323:U:C6 | 2.54 | 0.42 |
| 13:BF:47:GLN:OE1 | 13:BF:64:LYS:HD3 | 2.18 | 0.42 |
| 17:BJ:13:LYS:HD2 | 17:BJ:38:ARG:NH2 | 2.34 | 0.42 |
| 32:BY:45:THR:HG22 | 32:BY:47:ASP:N | 2.31 | 0.42 |
| 34:CA:53:TYR:CZ | 34:CA:65:ARG:HB2 | 2.54 | 0.42 |
| 45:CL:86:LYS:HD3 | 45:CL:86:LYS:HA | 1.77 | 0.42 |
| 46:CM:507:G:H2' | 46:CM:508:G:C8 | 2.54 | 0.42 |
| 46:CM:1127:A:H2' | 46:CM:1128:A:C8 | 2.54 | 0.42 |
| 46:CM:1148:A:H2' | 46:CM:1149:G:O4' | 2.18 | 0.42 |
| 46:CM:1206:A:H2' | 46:CM:1207:C:O4' | 2.18 | 0.42 |
| 46:CM:1337:C:H2' | 46:CM:1338:U:O4' | 2.18 | 0.42 |
| 46:CM:1369:G:O2' | 46:CM:1370:A:O5' | 2.31 | 0.42 |
| 46:CM:1376:U:H5" | 64:DE:3:ARG:HD2 | 2.01 | 0.42 |
| 46:CM:1518:G:N2 | 66:DG:48:GLN:OE1 | 2.52 | 0.42 |
| 46:CM:1546:G:C5 | 65:DF:134:ARG:HD3 | 2.54 | 0.42 |
| 49:CP:138:TYR:OH | 68:DI:3:ASN:HB3 | 2.19 | 0.42 |
| 53:CT:48:TYR:CD2 | 53:CT:117:GLY:HA3 | 2.53 | 0.42 |
| 54:CU:51:LYS:HB3 | 54:CU:85:HIS:CD2 | 2.54 | 0.42 |
| 54:CU:60:PRO:N | 54:CU:61:PRO:HD2 | 2.34 | 0.42 |
| 1:1:149:A:C5 | 1:1:150:A:C8 | 3.07 | 0.42 |
| 1:1:787:A:H2' | 1:1:788:G:C8 | 2.54 | 0.42 |
| 1:1:1221:A:H2' | 1:1:1222:G:H8 | 1.84 | 0.42 |
| 1:1:1255:A:H62 | 80:P0:53:MET:HE2 | 1.84 | 0.42 |
| 1:1:1856:G:O3' | 20:z:60:ARG:NH1 | 2.52 | 0.42 |
| 1:1:2406:U:H2' | 1:1:2407:G:C8 | 2.54 | 0.42 |
| 1:1:2739:U:H2' | 1:1:2740:U:H6 | 1.84 | 0.42 |
| 1:1:2972:A:H2' | 1:1:2973:U:C6 | 2.54 | 0.42 |
| 1:1:3285:A:H2' | 1:1:3286:C:H6 | 1.83 | 0.42 |
| 4:j:242:ARG:NH2 | 4:j:243:THR:O | 2.52 | 0.42 |
| 5:k:262:TRP:CD1 | 5:k:262:TRP:H | 2.37 | 0.42 |
| 13:s:53:THR:HG23 | 13:s:60:ARG:HA | 2.01 | 0.42 |
| 13:s:108:GLU:OE1 | 65:U:110:ARG:NH1 | 2.51 | 0.42 |
| 17:w:75:ARG:HD2 | 17:w:146:VAL:O | 2.20 | 0.42 |
| 25:7:4:GLU:HB2 | 25:7:13:ILE:HB | 2.01 | 0.42 |
| 29:AB:119:PRO:O | 29:AB:121:VAL:N | 2.51 | 0.42 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 42:AO:7:LYS:HD3 | 42:AO:11:ARG:NH2 | 2.34 | 0.42 |
| 46:B:167:A:H8 | 46:B:167:A:OP2 | 2.02 | 0.42 |
| 46:B:602:A:H2' | 46:B:603:A:O4' | 2.19 | 0.42 |
| 46:B:770:C:H6 | 46:B:770:C:OP1 | 2.02 | 0.42 |
| 46:B:824:U:H2' | 46:B:825:U:C6 | 2.54 | 0.42 |
| 46:B:1181:A:H4' | 46:B:1182:C:H5" | 2.00 | 0.42 |
| 46:B:1739:U:H2' | 46:B:1740:A:C8 | 2.54 | 0.42 |
| 57:M:11:ILE:HD13 | 57:M:35:ILE:HG21 | 2.00 | 0.42 |
| 59:O:81:GLU:HG3 | 78:h:155:ASN:HB2 | 2.01 | 0.42 |
| 61:Q:73:ALA:HB2 | 61:Q:106:ARG:HB2 | 2.02 | 0.42 |
| 1:AS:561:U:H2' | 1:AS:562:C:C6 | 2.54 | 0.42 |
| 1:AS:815:U:H2' | 1:AS:816:A:H8 | 1.84 | 0.42 |
| 1:AS:1202:G:OP1 | 12:BE:157:TYR:OH | 2.20 | 0.42 |
| 1:AS:1725:A:O4' | 31:BX:54:ARG:NH1 | 2.51 | 0.42 |
| 1:AS:2236:U:H2' | 1:AS:2237:A:H8 | 1.84 | 0.42 |
| 1:AS:2239:G:O2' | 1:AS:2241:C:N4 | 2.52 | 0.42 |
| 1:AS:2397:A:H2' | 1:AS:2398:C:C6 | 2.54 | 0.42 |
| 1:AS:2766:G:N3 | 84:AS:3401:3K5:H1 | 2.34 | 0.42 |
| 1:AS:2809:A:H2 | 1:AS:2823:A:N7 | 2.17 | 0.42 |
| 1:AS:3061:C:H2' | 1:AS:3062:U:O4' | 2.18 | 0.42 |
| 1:AS:3135:A:H2' | 1:AS:3136:C:H6 | 1.84 | 0.42 |
| 1:AS:3159:A:O2' | 1:AS:3160:C:OP1 | 2.30 | 0.42 |
| 13:BF:96:PHE:CD2 | 13:BF:102:PHE:HB3 | 2.54 | 0.42 |
| 27:BT:113:LYS:HE2 | 27:BT:113:LYS:HB2 | 1.76 | 0.42 |
| 46:CM:32:U:O2' | 46:CM:592:A:N1 | 2.44 | 0.42 |
| 46:CM:289:G:H2' | 46:CM:290:U:C6 | 2.53 | 0.42 |
| 46:CM:703:U:OP2 | 53:CT:234:LEU:HD13 | 2.19 | 0.42 |
| 46:CM:824:U:N3 | 46:CM:825:U:O4 | 2.52 | 0.42 |
| 46:CM:962:A:H2' | 46:CM:963:A:O4' | 2.19 | 0.42 |
| 46:CM:1239:U:H5' | 78:DS:185:LYS:HG3 | 2.01 | 0.42 |
| 46:CM:1286:U:H5' | 49:CP:83:LYS:HD2 | 2.00 | 0.42 |
| 46:CM:1697:C:H2' | 46:CM:1698:U:C6 | 2.55 | 0.42 |
| 48:CO:23:PRO:O | 48:CO:27:LYS:NZ | 2.52 | 0.42 |
| 48:CO:26:ARG:C | 48:CO:50:ARG:HG2 | 2.43 | 0.42 |
| 50:CQ:23:ASN:O | 50:CQ:27:THR:HG23 | 2.19 | 0.42 |
| 56:CW:66:ASP:OD1 | 56:CW:67:PRO:HD2 | 2.19 | 0.42 |
| 61:DB:53:TYR:CE2 | 61:DB:57:LEU:HD11 | 2.54 | 0.42 |
| 64:DE:89:SER:C | 64:DE:91:LEU:N | 2.77 | 0.42 |
| 65:DF:6:GLN:OE1 | 65:DF:6:GLN:N | 2.52 | 0.42 |
| 73:DN:13:LYS:H | 73:DN:15:ARG:NH2 | 2.16 | 0.42 |
| 73:DN:23:CYS:SG | 73:DN:77:CYS:CB | 3.07 | 0.42 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 79:DT:88:ARG:HG2 | 79:DT:109:GLY:C | 2.44 | 0.42 |
| 81:12:149:HIS:H | 81:12:152:ILE:CD1 | 2.29 | 0.42 |
| 82:l1:140:HIS:O | 82:l1:142:ASP:N | 2.52 | 0.42 |
| 1:1:46:C:OP2 | 1:1:47:A:O2' | 2.30 | 0.42 |
| 1:1:50:A:C4 | 1:1:51:A:C8 | 3.07 | 0.42 |
| 1:1:1147:U:O4 | 1:1:1196:A:N6 | 2.53 | 0.42 |
| 1:1:2296:U:H2' | 1:1:2297:U:O4' | 2.20 | 0.42 |
| 1:1:2656:C:H2' | 1:1:2657:C:C6 | 2.54 | 0.42 |
| 1:1:2785:A:H2' | 1:1:2786:G:O4' | 2.20 | 0.42 |
| 1:1:3035:C:H2' | 1:1:3036:U:C6 | 2.54 | 0.42 |
| 16:v:45:PRO:O | 16:v:49:ARG:HG3 | 2.19 | 0.42 |
| 21:0:41:TYR:O | 21:0:45:LEU:HD23 | 2.19 | 0.42 |
| 22:2:90:ASN:O | 22:2:91:LEU:HD23 | 2.20 | 0.42 |
| 32:AE:61:ARG:HB2 | 32:AE:65:GLY:HA3 | 2.01 | 0.42 |
| 46:B:151:G:C6 | 46:B:160:A:C6 | 3.07 | 0.42 |
| 46:B:627:U:C2 | 46:B:628:A:C8 | 3.08 | 0.42 |
| 46:B:671:G:H5' | 46:B:672:U:H2' | 2.01 | 0.42 |
| 46:B:761:G:N2 | 46:B:769:U:H1' | 2.34 | 0.42 |
| 46:B:1335:U:H2' | 46:B:1336:G:H8 | 1.83 | 0.42 |
| 46:B:1571:G:H22 | 46:B:1598:A:P | 2.41 | 0.42 |
| 47:C:57:ILE:HG23 | 47:C:177:LEU:HD23 | 2.02 | 0.42 |
| 47:C:182:LEU:HB3 | 47:C:187:ILE:HB | 2.00 | 0.42 |
| 48:D:135:LEU:HD23 | 48:D:217:LEU:HA | 2.00 | 0.42 |
| 50:F:46:LYS:HD2 | 50:F:86:ALA:HB2 | 2.01 | 0.42 |
| 52:H:200:ASN:CB | 52:H:208:SER:HB3 | 2.47 | 0.42 |
| 59:O:63:CYS:HB3 | 59:O:97:LEU:CD1 | 2.48 | 0.42 |
| 59:O:105:GLN:NE2 | 59:O:114:LYS:HD2 | 2.35 | 0.42 |
| 78:h:182:TYR:CE2 | 78:h:184:GLY:HA2 | 2.54 | 0.42 |
| 1:AS:1191:A:H2' | 1:AS:1305:U:O2 | 2.19 | 0.42 |
| 1:AS:1233:G:H2' | 1:AS:1234:C:C6 | 2.54 | 0.42 |
| 1:AS:1615:A:H2' | 1:AS:1616:U:O4' | 2.19 | 0.42 |
| 1:AS:1656:C:H2' | 1:AS:1657:G:C8 | 2.54 | 0.42 |
| 1:AS:2276:U:O2' | 1:AS:2277:A:H5' | 2.19 | 0.42 |
| 1:AS:2432:G:N3 | 1:AS:2432:G:H2' | 2.34 | 0.42 |
| 1:AS:2583:U:H2' | 1:AS:2584:U:H6 | 1.84 | 0.42 |
| 1:AS:2985:U:H2' | 1:AS:2986:U:C6 | 2.54 | 0.42 |
| 1:AS:3199:G:H2' | 1:AS:3200:C:C6 | 2.54 | 0.42 |
| 1:AS:3281:A:C6 | 5:AX:124:LYS:HG2 | 2.54 | 0.42 |
| 3:AU:46:G:O2' | 3:AU:61:A:N1 | 2.44 | 0.42 |
| 3:AU:142:C:H2' | 3:AU:143:U:H6 | 1.84 | 0.42 |
| 5:AX:108:GLU:HG2 | 5:AX:109:HIS:CE1 | 2.53 | 0.42 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 15:BH:20:LEU:HD21 | 15:BH:23:ASN:HA | 2.00 | 0.42 |
| 31:BX:12:ILE:H | 31:BX:12:ILE:HD12 | 1.84 | 0.42 |
| 32:BY:95:VAL:HG12 | 32:BY:97:VAL:HG13 | 2.01 | 0.42 |
| 46:CM:673:A:H2' | 46:CM:674:C:H6 | 1.80 | 0.42 |
| 46:CM:825:U:O2' | 46:CM:826:U:H5" | 2.19 | 0.42 |
| 46:CM:861:G:H2' | 46:CM:921:G:N2 | 2.35 | 0.42 |
| 46:CM:1156:A:O2' | 46:CM:1557:A:N3 | 2.40 | 0.42 |
| 46:CM:1205:C:H4' | 57:CX:52:LYS:HG2 | 2.00 | 0.42 |
| 46:CM:1300:U:O2' | 46:CM:1301:G:H8 | 2.01 | 0.42 |
| 46:CM:1308:C:H2' | 46:CM:1309:G:C8 | 2.55 | 0.42 |
| 46:CM:1760:C:H2' | 46:CM:1761:G:C8 | 2.55 | 0.42 |
| 51:CR:87:MET:O | 51:CR:122:LYS:HE3 | 2.19 | 0.42 |
| 53:CT:218:GLU:HG2 | 53:CT:219:ARG:CZ | 2.49 | 0.42 |
| 57:CX:46:LEU:HD23 | 57:CX:66:TYR:CG | 2.54 | 0.42 |
| 69:DJ:106:THR:HG23 | 69:DJ:108:ALA:H | 1.83 | 0.42 |
| 69:DJ:115:GLU:O | 69:DJ:119:LYS:HG2 | 2.19 | 0.42 |
| 82:L1:15:LYS:HB2 | 82:L1:214:PHE:HZ | 1.83 | 0.42 |
| 1:1:19:A:H2' | 1:1:20:G:C8 | 2.55 | 0.42 |
| 1:1:259:C:H2' | 1:1:260:C:H6 | 1.85 | 0.42 |
| 1:1:377:A:H1' | 1:1:392:G:N2 | 2.34 | 0.42 |
| 1:1:640:U:OP1 | 29:AB:22:ILE:HG23 | 2.20 | 0.42 |
| 1:1:843:A:H2' | 1:1:844:A:C8 | 2.53 | 0.42 |
| 1:1:941:C:H2' | 1:1:942:U:H6 | 1.84 | 0.42 |
| 1:1:1556:G:C2 | 1:1:1575:A:C8 | 3.07 | 0.42 |
| 1:1:1905:A:H2' | 1:1:1906:A:C8 | 2.54 | 0.42 |
| 1:1:3085:A:H2' | 1:1:3086:A:O4' | 2.20 | 0.42 |
| 2:3:4:U:H4' | 2:3:26:C:H4' | 2.01 | 0.42 |
| 3:4:18:U:H2' | 3:4:19:C:H6 | 1.83 | 0.42 |
| 3:4:155:G:H5' | 10:p:186:ARG:HD2 | 2.01 | 0.42 |
| 8:n:59:ASP:HB2 | 8:n:102:VAL:CG2 | 2.49 | 0.42 |
| 16:v:146:ALA:HA | 16:v:149:ASN:OD1 | 2.19 | 0.42 |
| 20:z:72:ALA:O | 20:z:74:ARG:NH1 | 2.52 | 0.42 |
| 27:9:58:VAL:HA | 27:9:104:VAL:HG12 | 2.00 | 0.42 |
| 27:9:109:LEU:HD22 | 27:9:115:ARG:NH2 | 2.34 | 0.42 |
| 46:B:191:U:H4' | 46:B:192:U:H5' | 2.01 | 0.42 |
| 46:B:218:A:N1 | 46:B:219:A:C5 | 2.87 | 0.42 |
| 46:B:265:U:H2' | 46:B:266:C:C6 | 2.54 | 0.42 |
| 46:B:496:G:H2' | 46:B:497:U:O4' | 2.19 | 0.42 |
| 46:B:1477:U:H4' | 46:B:1478:A:H5' | 2.00 | 0.42 |
| 48:D:167:LYS:HD3 | 48:D:170:GLU:OE2 | 2.19 | 0.42 |
| 50:F:105:ALA:O | 50:F:109:LYS:HG2 | 2.19 | 0.42 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 79:AR:118:LYS:HD2 | 79:AR:159:PRO:C | 2.44 | 0.42 |
| 1:AS:4:G:C6 | 3:AU:155:G:O6 | 2.73 | 0.42 |
| 1:AS:393:U:H2' | 1:AS:394:G:O4' | 2.20 | 0.42 |
| 1:AS:649:G:C6 | 1:AS:650:G:C6 | 3.07 | 0.42 |
| 1:AS:718:A:H5" | 19:BL:69:ARG:HH12 | 1.84 | 0.42 |
| 1:AS:756:G:H1' | 1:AS:767:A:N6 | 2.34 | 0.42 |
| 1:AS:1637:U:O2' | 1:AS:1638:A:H3' | 2.18 | 0.42 |
| 1:AS:2093:G:O2' | 20:BM:82:LYS:NZ | 2.44 | 0.42 |
| 1:AS:2493:A:H5" | 16:BI:28:TRP:CD1 | 2.54 | 0.42 |
| 1:AS:2744:C:H4' | 1:AS:2745:C:H5' | 2.02 | 0.42 |
| 1:AS:2946:U:H2' | 1:AS:2947:U:C6 | 2.54 | 0.42 |
| 1:AS:3313:G:H2' | 1:AS:3314:C:C6 | 2.54 | 0.42 |
| 4:AW:29:LEU:HA | 4:AW:76:PHE:CE1 | 2.54 | 0.42 |
| 6:AY:17:GLY:O | 6:AY:18:SER:OG | 2.32 | 0.42 |
| 9:BB:146:VAL:HG12 | 9:BB:179:ILE:HD11 | 2.00 | 0.42 |
| 14:BG:2:ALA:HB1 | 29:BV:33:GLY:O | 2.18 | 0.42 |
| 22:BO:51:GLY:HA3 | 22:BO:92:ARG:HG3 | 2.01 | 0.42 |
| 28:BU:42:ILE:HD11 | 28:BU:74:LEU:HD12 | 2.00 | 0.42 |
| 31:BX:11:ASN:O | 31:BX:14:SER:OG | 2.37 | 0.42 |
| 45:CL:101:LYS:NZ | 46:CM:579:U:OP1 | 2.46 | 0.42 |
| 46:CM:404:U:H2' | 46:CM:405:A:H8 | 1.83 | 0.42 |
| 46:CM:961:G:N1 | 46:CM:1008:A:O2' | 2.39 | 0.42 |
| 46:CM:1157:G:H2' | 46:CM:1158:C:C6 | 2.55 | 0.42 |
| 46:CM:1174:A:N3 | 46:CM:1179:A:O2' | 2.52 | 0.42 |
| 46:CM:1634:U:H2' | 46:CM:1635:A:H8 | 1.85 | 0.42 |
| 48:CO:30:PHE:CG | 48:CO:96:LEU:HD21 | 2.55 | 0.42 |
| 50:CQ:19:TYR:HE1 | 50:CQ:38:VAL:HG13 | 1.84 | 0.42 |
| 54:CU:30:LEU:HD12 | 54:CU:34:LEU:HD21 | 2.01 | 0.42 |
| 56:CW:34:TYR:CD2 | 56:CW:105:LEU:HD22 | 2.54 | 0.42 |
| 57:CX:73:VAL:HG21 | 57:CX:91:ARG:NH1 | 2.35 | 0.42 |
| 62:DC:83:MET:HB3 | 62:DC:116:LEU:HD22 | 2.01 | 0.42 |
| 82:L1:6:SER:HA | 82:L1:9:VAL:HB | 2.01 | 0.42 |
| 82:l1:32:VAL:HB | 82:l1:169:VAL:O | 2.18 | 0.42 |
| 1:1:619:A:H8 | 1:1:619:A:OP2 | 2.02 | 0.42 |
| 1:1:1012:U:C4' | 1:1:1013:U:H4' | 2.50 | 0.42 |
| 1:1:1467:U:H2' | 1:1:1468:U:C6 | 2.55 | 0.42 |
| 1:1:1690:U:O2' | 1:1:1691:U:H5' | 2.20 | 0.42 |
| 1:1:1789:C:O2 | 4:j:188:LYS:NZ | 2.46 | 0.42 |
| 1:1:2545:C:O2' | 1:1:2547:G:H1' | 2.20 | 0.42 |
| 1:1:2610:C:H3' | 1:1:2611:G:C8 | 2.53 | 0.42 |
| 1:1:2686:G:H4' | 1:1:2687:A:H5" | 2.02 | 0.42 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 3:4:104:A:OP2 | 3:4:105:A:H2' | 2.20 | 0.42 |
| 4:j:70:LYS:HG3 | 4:j:71:LEU:N | 2.34 | 0.42 |
| 11:q:89:LYS:HB2 | 11:q:183:GLU:HB3 | 2.02 | 0.42 |
| 15:u:78:TRP:CE2 | 15:u:83:ILE:HB | 2.55 | 0.42 |
| 26:8:86:VAL:HG11 | 26:8:95:ILE:HG12 | 2.01 | 0.42 |
| 46:B:68:A:OP1 | 53:I:160:ARG:NH2 | 2.33 | 0.42 |
| 46:B:515:U:C2 | 46:B:516:A:C8 | 3.07 | 0.42 |
| 46:B:873:U:H2' | 46:B:874:U:C6 | 2.54 | 0.42 |
| 49:E:139:TRP:CE2 | 69:Y:97:ARG:HD2 | 2.54 | 0.42 |
| 53:I:84:TYR:CE1 | 53:I:93:LYS:HB2 | 2.55 | 0.42 |
| 54:J:11:THR:HG23 | 54:J:14:GLU:H | 1.84 | 0.42 |
| 55:K:113:TYR:OH | 55:K:156:ALA:O | 2.36 | 0.42 |
| 56:L:63:ASP:OD1 | 56:L:64:GLU:N | 2.52 | 0.42 |
| 57:M:79:GLU:OE1 | 57:M:80:LEU:HD22 | 2.19 | 0.42 |
| 59:O:103:LEU:HD13 | 59:O:116:VAL:HB | 2.01 | 0.42 |
| 73:c:51:ARG:O | 73:c:55:GLU:HG3 | 2.19 | 0.42 |
| 1:AS:413:U:H2' | 1:AS:414:U:C6 | 2.55 | 0.42 |
| 1:AS:1459:U:H2' | 1:AS:1460:G:O4' | 2.20 | 0.42 |
| 1:AS:1706:C:H2' | 1:AS:1707:U:H6 | 1.83 | 0.42 |
| 1:AS:1725:A:N6 | 44:CK:42:CYS:HA | 2.35 | 0.42 |
| 1:AS:2310:A:H2' | 1:AS:2311:C:O4' | 2.19 | 0.42 |
| 1:AS:2653:U:O2 | 13:BF:20:ASN:ND2 | 2.52 | 0.42 |
| 1:AS:2739:U:H2' | 1:AS:2740:U:H6 | 1.84 | 0.42 |
| 2:AT:13:A:H2 | 7:AZ:21:ARG:HB2 | 1.84 | 0.42 |
| 13:BF:6:GLN:OE1 | 13:BF:6:GLN:N | 2.53 | 0.42 |
| 13:BF:62:ASN:O | 43:CJ:103:ALA:HB2 | 2.20 | 0.42 |
| 16:BI:146:ALA:HA | 16:BI:149:ASN:OD1 | 2.19 | 0.42 |
| 25:BR:102:LYS:HA | 25:BR:105:ARG:HB2 | 2.00 | 0.42 |
| 29:BV:27:LYS:HA | 29:BV:27:LYS:HD2 | 1.82 | 0.42 |
| 46:CM:390:G:H5" | 46:CM:1716:C:O2' | 2.18 | 0.42 |
| 51:CR:185:GLY:HA3 | 51:CR:224:ASN:OD1 | 2.19 | 0.42 |
| 53:CT:126:ASP:OD1 | 53:CT:127:THR:N | 2.51 | 0.42 |
| 54:CU:155:SER:O | 54:CU:157:ALA:N | 2.44 | 0.42 |
| 57:CX:58:GLN:HB3 | 57:CX:65:TYR:HB2 | 2.00 | 0.42 |
| 62:DC:81:ARG:HH12 | 62:DC:122:THR:HG22 | 1.85 | 0.42 |
| 80:P0:71:PRO:HB2 | 80:P0:72:GLU:H | 1.68 | 0.42 |
| 81:12:120:SER:HB3 | 81:12:128:VAL:HA | 2.01 | 0.42 |
| 1:1:212:A:OP1 | 27:9:2:ALA:N | 2.53 | 0.42 |
| 1:1:259:C:H2' | 1:1:260:C:C6 | 2.54 | 0.42 |
| 1:1:997:G:H1' | 1:1:1037:U:H5' | 2.00 | 0.42 |
| 1:1:1312:C:H5' | 1:1:1313:A:C2 | 2.55 | 0.42 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 1:1:1379:G:OP1 | 6:l:204:ARG:HD3 | 2.19 | 0.42 |
| 1:1:1767:G:H2' | 1:1:1768:U:O4' | 2.20 | 0.42 |
| 1:1:2690:U:H2' | 1:1:2691:U:O4' | 2.20 | 0.42 |
| 1:1:2853:C:H2' | 1:1:2854:U:H6 | 1.84 | 0.42 |
| 1:1:3006:C:H1' | 11:q:120:GLU:OE1 | 2.19 | 0.42 |
| 1:1:3067:U:H2' | 1:1:3068:C:H6 | 1.84 | 0.42 |
| 2:3:11:A:N1 | 2:3:67:G:O2' | 2.42 | 0.42 |
| 8:n:45:ARG:HD3 | 8:n:46:PHE:CZ | 2.54 | 0.42 |
| 9:o:9:THR:HA | 9:o:12:LYS:HE3 | 2.01 | 0.42 |
| 10:p:178:TYR:CZ | 10:p:223:TYR:HB3 | 2.54 | 0.42 |
| 16:v:53:TYR:HB2 | 16:v:133:ILE:HD13 | 2.00 | 0.42 |
| 22:2:39:ILE:HG12 | 22:2:63:ILE:CD1 | 2.49 | 0.42 |
| 33:AF:33:TRP:CH2 | 33:AF:53:GLN:HG2 | 2.54 | 0.42 |
| 38:AK:26:SER:HB3 | 38:AK:35:SER:OG | 2.20 | 0.42 |
| 39:AL:58:ASP:OD1 | 39:AL:61:LYS:N | 2.40 | 0.42 |
| 45:i:99:SER:HB2 | 46:B:573:C:OP1 | 2.20 | 0.42 |
| 46:B:393:U:H2' | 46:B:394:G:O4' | 2.20 | 0.42 |
| 46:B:1580:A:H2' | 46:B:1581:G:H8 | 1.85 | 0.42 |
| 47:C:88:LYS:HG3 | 47:C:201:LEU:HD11 | 2.02 | 0.42 |
| 49:E:135:ARG:HB3 | 49:E:216:THR:HB | 2.01 | 0.42 |
| 51:G:98:HIS:ND1 | 51:G:116:ALA:HA | 2.34 | 0.42 |
| 66:V:35:ASP:OD1 | 66:V:35:ASP:N | 2.44 | 0.42 |
| 66:V:37:VAL:HG21 | 66:V:100:ILE:HD11 | 2.00 | 0.42 |
| 68:X:30:ALA:O | 68:X:60:ARG:NE | 2.47 | 0.42 |
| 1:AS:87:A:H2' | 1:AS:88:G:O4' | 2.19 | 0.42 |
| 1:AS:122:A:C6 | 1:AS:149:A:C5 | 3.07 | 0.42 |
| 1:AS:624:U:H2' | 1:AS:625:C:H6 | 1.85 | 0.42 |
| 1:AS:2233:A:O2' | 46:CM:1744:G:O2' | 2.16 | 0.42 |
| 1:AS:3129:C:H2' | 1:AS:3130:C:H6 | 1.85 | 0.42 |
| 1:AS:3336:G:H2' | 1:AS:3337:A:C8 | 2.52 | 0.42 |
| 5:AX:66:LYS:NZ | 24:BQ:9:ASN:H | 2.18 | 0.42 |
| 13:BF:25:GLU:OE2 | 13:BF:29:ARG:HD3 | 2.20 | 0.42 |
| 13:BF:37:LEU:HD23 | 13:BF:37:LEU:HA | 1.85 | 0.42 |
| 23:BP:90:ASN:O | 23:BP:92:ILE:HG13 | 2.19 | 0.42 |
| 30:BW:28:LYS:HG2 | 30:BW:29:TYR:CD1 | 2.55 | 0.42 |
| 34:CA:73:ARG:HD3 | 34:CA:82:ARG:HD2 | 2.01 | 0.42 |
| 46:CM:602:A:H2' | 46:CM:603:A:O4' | 2.20 | 0.42 |
| 46:CM:891:A:H2' | 46:CM:892:A:C8 | 2.55 | 0.42 |
| 46:CM:1519:U:OP2 | 72:DM:77:ARG:HD2 | 2.19 | 0.42 |
| 46:CM:1584:A:C8 | 76:DQ:14:PHE:HB2 | 2.54 | 0.42 |
| 49:CP:53:LEU:O | 68:DI:15:ARG:NE | 2.52 | 0.42 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 55:CV:84:HIS:CE1 | 55:CV:86:SER:HB3 | 2.54 | 0.42 |
| 61:DB:127:ARG:HA | 73:DN:29:CYS:SG | 2.59 | 0.42 |
| 75:DP:8:THR:O | 75:DP:56:LEU:N | 2.53 | 0.42 |
| 79:DT:171:TRP:CG | 79:DT:195:TYR:HB2 | 2.55 | 0.42 |
| 81:12:143:VAL:HG21 | 81:12:148:PRO:HG3 | 2.02 | 0.42 |
| 81:12:154:ALA:HB1 | 81:12:159:GLU:HB2 | 2.00 | 0.42 |
| 82:l1:111:ILE:HA | 82:l1:136:THR:HB | 2.02 | 0.42 |
| 1:1:38:A:H5" | 29:AB:35:ALA:HB2 | 2.01 | 0.42 |
| 1:1:224:C:H5' | 27:9:34:PRO:HD3 | 2.01 | 0.42 |
| 1:1:263:C:H2' | 1:1:264:G:O4' | 2.19 | 0.42 |
| 1:1:429:U:H2' | 1:1:430:G:C8 | 2.43 | 0.42 |
| 1:1:652:C:H2' | 1:1:653:C:C6 | 2.54 | 0.42 |
| 1:1:1347:U:O2' | 1:1:1348:U:OP2 | 2.30 | 0.42 |
| 1:1:1444:U:H5" | 18:x:66:SER:O | 2.19 | 0.42 |
| 1:1:2394:U:H2' | 1:1:2395:U:C6 | 2.55 | 0.42 |
| 1:1:2663:A:H2' | 1:1:2664:A:C8 | 2.55 | 0.42 |
| 1:1:3133:G:H2' | 1:1:3134:C:O4' | 2.20 | 0.42 |
| 1:1:3298:G:N2 | 1:1:3334:G:O2' | 2.53 | 0.42 |
| 3:4:60:U:OP1 | 26:8:54:TYR:OH | 2.33 | 0.42 |
| 3:4:85:G:H4' | 3:4:86:U:OP1 | 2.20 | 0.42 |
| 5:k:60:LEU:HD11 | 5:k:62:ARG:NH1 | 2.35 | 0.42 |
| 5:k:95:THR:OG1 | 5:k:98:GLY:O | 2.33 | 0.42 |
| 9:o:86:ARG:NH1 | 9:o:106:LEU:O | 2.39 | 0.42 |
| 21:0:119:ARG:H | 21:0:119:ARG:HG3 | 1.63 | 0.42 |
| 46:B:1282:G:C4 | 46:B:1284:G:OP2 | 2.73 | 0.42 |
| 46:B:1469:A:H2 | 46:B:1594:G:H1' | 1.85 | 0.42 |
| 46:B:1669:U:O2' | 46:B:1670:U:O5' | 2.38 | 0.42 |
| 50:F:72:SER:O | 50:F:76:LYS:HD2 | 2.20 | 0.42 |
| 50:F:158:MET:SD | 50:F:188:LYS:HD2 | 2.60 | 0.42 |
| 73:c:9:GLY:O | 73:c:34:LYS:HG3 | 2.20 | 0.42 |
| 1:AS:67:C:O3' | 16:BI:177:GLY:HA2 | 2.19 | 0.42 |
| 1:AS:259:C:H2' | 1:AS:260:C:C6 | 2.54 | 0.42 |
| 1:AS:663:A:OP1 | 16:BI:203:ARG:HD2 | 2.19 | 0.42 |
| 1:AS:706:G:N2 | 1:AS:709:A:OP2 | 2.47 | 0.42 |
| 1:AS:745:C:H5" | 30:BW:32:LEU:HD12 | 2.02 | 0.42 |
| 1:AS:798:C:C2 | 1:AS:799:C:C5 | 3.08 | 0.42 |
| 1:AS:897:G:OP1 | 38:CE:13:ASN:ND2 | 2.35 | 0.42 |
| 1:AS:1218:G:N2 | 1:AS:1282:A:N7 | 2.68 | 0.42 |
| 1:AS:1620:G:O2' | 1:AS:1639:A:N1 | 2.50 | 0.42 |
| 1:AS:2408:A:H2' | 1:AS:2409:C:H6 | 1.81 | 0.42 |
| 1:AS:2668:A:N7 | 1:AS:2730:A:N6 | 2.68 | 0.42 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 1:AS:2686:G:OP2 | 43:CJ:10:THR:HG22 | 2.20 | 0.42 |
| 3:AU:143:U:H2' | 3:AU:144:G:O4' | 2.18 | 0.42 |
| 8:BA:105:PHE:HA | 8:BA:134:ARG:HH22 | 1.84 | 0.42 |
| 14:BG:69:VAL:O | 14:BG:151:GLN:NE2 | 2.51 | 0.42 |
| 16:BI:4:TYR:CZ | 16:BI:49:ARG:HD2 | 2.55 | 0.42 |
| 16:BI:65:ARG:HG2 | 16:BI:127:TYR:CD1 | 2.55 | 0.42 |
| 25:BR:80:ARG:HH22 | 53:CT:11:GLY:CA | 2.31 | 0.42 |
| 46:CM:1:U:C2 | 46:CM:3:U:C4 | 3.08 | 0.42 |
| 46:CM:144:U:H5 | 46:CM:166:A:N7 | 2.17 | 0.42 |
| 46:CM:608:G:H2' | 46:CM:612:C:C5 | 2.55 | 0.42 |
| 46:CM:1370:A:H2' | 46:CM:1371:G:O4' | 2.20 | 0.42 |
| 47:CN:41:ARG:CD | 47:CN:47:ILE:HD11 | 2.49 | 0.42 |
| 49:CP:217:TYR:O | 68:DI:23:ILE:HG21 | 2.20 | 0.42 |
| 50:CQ:35:TYR:HE1 | 50:CQ:51:VAL:HG23 | 1.85 | 0.42 |
| 50:CQ:69:GLU:O | 57:CX:20:VAL:HG11 | 2.19 | 0.42 |
| 52:CS:27:THR:OG1 | 63:DD:27:LEU:HD12 | 2.19 | 0.42 |
| 79:DT:145:LEU:HD11 | 79:DT:178:TRP:CD2 | 2.54 | 0.42 |
| 79:DT:200:THR:HG21 | 79:DT:241:ALA:HA | 2.02 | 0.42 |
| 82:l1:67:ILE:N | 82:l1:83:ASP:OD2 | 2.49 | 0.42 |
| 1:1:296:A:N3 | 1:1:299:G:O2' | 2.51 | 0.42 |
| 1:1:358:G:N2 | 1:1:361:A:OP2 | 2.48 | 0.42 |
| 1:1:983:U:H2' | 1:1:984:U:C6 | 2.54 | 0.42 |
| 1:1:1560:U:H3 | 1:1:1571:G:H1 | 1.66 | 0.42 |
| 1:1:1801:C:O2' | 35:AH:76:TYR:HA | 2.20 | 0.42 |
| 1:1:2497:A:H2' | 1:1:2498:A:C8 | 2.55 | 0.42 |
| 1:1:2650:A:C8 | 45:i:55:LYS:HG2 | 2.55 | 0.42 |
| 1:1:3025:G:H2' | 1:1:3026:U:C6 | 2.55 | 0.42 |
| 5:k:80:ASP:OD1 | 5:k:319:ASN:HB2 | 2.20 | 0.42 |
| 9:o:15:LYS:HE2 | 9:o:15:LYS:HB3 | 1.94 | 0.42 |
| 11:q:90:MET:HE3 | 11:q:181:VAL:HG23 | 2.02 | 0.42 |
| 17:w:187:ALA:O | 17:w:188:GLU:HG2 | 2.19 | 0.42 |
| 29:AB:73:ILE:HB | 29:AB:109:TYR:CD2 | 2.54 | 0.42 |
| 33:AF:98:ALA:HB3 | 33:AF:101:VAL:HG23 | 2.02 | 0.42 |
| 38:AK:84:LYS:HE3 | 38:AK:84:LYS:HB2 | 1.73 | 0.42 |
| 46:B:472:A:H5" | 56:L:144:PRO:HD2 | 2.01 | 0.42 |
| 46:B:495:G:H2' | 46:B:496:G:C8 | 2.55 | 0.42 |
| 46:B:938:G:H2' | 46:B:939:G:H8 | 1.82 | 0.42 |
| 46:B:1127:A:H2' | 46:B:1128:A:H8 | 1.84 | 0.42 |
| 46:B:1580:A:H2' | 46:B:1581:G:C8 | 2.55 | 0.42 |
| 46:B:1606:C:O3' | 52:H:152:SER:OG | 2.38 | 0.42 |
| 51:G:36:HIS:CG | 51:G:85:GLY:HA3 | 2.55 | 0.42 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 52:H:109:LYS:HB2 | 52:H:109:LYS:HE2 | 1.78 | 0.42 |
| 53:I:182:GLN:HE21 | 53:I:186:ARG:HG3 | 1.84 | 0.42 |
| 59:O:47:GLU:HA | 59:O:50:LYS:HG2 | 2.02 | 0.42 |
| 59:O:63:CYS:HB2 | 59:O:92:SER:HB2 | 2.02 | 0.42 |
| 1:AS:208:A:H4' | 1:AS:210:A:C8 | 2.54 | 0.42 |
| 1:AS:533:G:H2' | 1:AS:534:G:O4' | 2.20 | 0.42 |
| 1:AS:849:G:N7 | 44:CK:2:THR:HG23 | 2.35 | 0.42 |
| 1:AS:1045:C:H2' | 1:AS:1046:U:C6 | 2.55 | 0.42 |
| 1:AS:1204:U:O2 | 1:AS:3087:C:N4 | 2.53 | 0.42 |
| 1:AS:1560:U:H3 | 1:AS:1571:G:H1 | 1.66 | 0.42 |
| 1:AS:1690:U:O2' | 1:AS:1691:U:H5' | 2.20 | 0.42 |
| 1:AS:2696:U:OP1 | 22:BO:78:LYS:NZ | 2.46 | 0.42 |
| 1:AS:3111:A:H2' | 1:AS:3112:G:O4' | 2.19 | 0.42 |
| 3:AU:27:U:H2' | 3:AU:28:C:H6 | 1.85 | 0.42 |
| 3:AU:40:A:H2' | 3:AU:41:A:C8 | 2.54 | 0.42 |
| 3:AU:139:U:H2' | 3:AU:140:G:C8 | 2.54 | 0.42 |
| 31:BX:102:ILE:O | 31:BX:106:ILE:HG23 | 2.20 | 0.42 |
| 44:CK:47:VAL:HA | 44:CK:56:ASN:O | 2.19 | 0.42 |
| 46:CM:598:U:OP2 | 70:DK:108:GLY:HA2 | 2.19 | 0.42 |
| 46:CM:598:U:P | 70:DK:108:GLY:HA2 | 2.59 | 0.42 |
| 46:CM:721:C:N3 | 46:CM:722:A:N7 | 2.67 | 0.42 |
| 46:CM:850:A:OP1 | 69:DJ:28:ARG:NH2 | 2.52 | 0.42 |
| 46:CM:1431:G:C5 | 78:DS:131:LYS:HD3 | 2.54 | 0.42 |
| 46:CM:1696:U:O2 | 46:CM:1697:C:N4 | 2.53 | 0.42 |
| 53:CT:222:GLU:O | 53:CT:226:ILE:HG12 | 2.20 | 0.42 |
| 55:CV:123:LYS:HE3 | 55:CV:123:LYS:HB3 | 1.92 | 0.42 |
| 60:DA:15:ALA:O | 74:DO:28:PRO:HD3 | 2.20 | 0.42 |
| 63:DD:124:GLU:HG3 | 63:DD:125:PRO:HD2 | 2.02 | 0.42 |
| 65:DF:83:ALA:HB1 | 65:DF:97:ASP:OD2 | 2.19 | 0.42 |
| 79:DT:12:THR:O | 79:DT:53:ASN:HA | 2.20 | 0.42 |
| 82:l1:67:ILE:HB | 82:l1:84:ALA:HA | 2.01 | 0.42 |
| 82:l1:208:SER:C | 82:l1:210:MET:N | 2.77 | 0.42 |
| 1:1:39:A:H5" | 29:AB:35:ALA:HB1 | 2.02 | 0.42 |
| 1:1:564:G:H2' | 1:1:565:A:H8 | 1.77 | 0.42 |
| 1:1:742:C:H2' | 1:1:743:A:C8 | 2.54 | 0.42 |
| 1:1:870:U:H5" | 1:1:2922:G:OP1 | 2.20 | 0.42 |
| 1:1:1011:C:HO2' | 1:1:1012:U:P | 2.43 | 0.42 |
| 1:1:1256:A:N6 | 80:P0:38:MET:SD | 2.91 | 0.42 |
| 1:1:1738:U:H2' | 1:1:1739:G:H8 | 1.84 | 0.42 |
| 1:1:2367:C:H2' | 1:1:2368:A:C8 | 2.55 | 0.42 |
| 1:1:2420:G:H2' | 1:1:2421:A:C8 | 2.55 | 0.42 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 1:1:2470:C:O2 | 82:l1:35:GLN:NE2 | 2.53 | 0.42 |
| 1:1:2686:G:OP2 | 43:AP:10:THR:HG22 | 2.20 | 0.42 |
| 1:1:3067:U:H2' | 1:1:3068:C:C6 | 2.55 | 0.42 |
| 1:1:3264:C:H2' | 1:1:3265:U:C6 | 2.55 | 0.42 |
| 6:l:36:VAL:HG21 | 6:l:245:LEU:HD21 | 2.02 | 0.42 |
| 16:v:62:TYR:HE2 | 16:v:110:ALA:HB2 | 1.85 | 0.42 |
| 18:x:18:ARG:NH1 | 18:x:147:GLU:OE1 | 2.52 | 0.42 |
| 46:B:650:G:C4 | 46:B:678:A:C6 | 3.08 | 0.42 |
| 46:B:1184:G:O6 | 67:W:66:THR:HG22 | 2.20 | 0.42 |
| 46:B:1537:A:H2' | 46:B:1538:U:C6 | 2.54 | 0.42 |
| 51:G:129:VAL:HG22 | 51:G:139:VAL:HG22 | 2.02 | 0.42 |
| 53:I:126:ASP:OD1 | 53:I:127:THR:N | 2.52 | 0.42 |
| 54:J:33:GLU:O | 54:J:37:LEU:HG | 2.20 | 0.42 |
| 58:N:56:LYS:HE2 | 58:N:57:LYS:HE3 | 2.02 | 0.42 |
| 60:P:87:ASP:N | 60:P:87:ASP:OD1 | 2.51 | 0.42 |
| 63:S:72:GLY:H | 63:S:75:SER:HB3 | 1.84 | 0.42 |
| 79:AR:118:LYS:HE2 | 79:AR:118:LYS:HB3 | 1.80 | 0.42 |
| 1:AS:40:G:N2 | 1:AS:2775:A:H62 | 2.17 | 0.42 |
| 1:AS:259:C:H2' | 1:AS:260:C:H6 | 1.84 | 0.42 |
| 1:AS:730:A:H2' | 1:AS:731:U:H2' | 2.01 | 0.42 |
| 1:AS:756:G:O2' | 1:AS:766:G:N2 | 2.49 | 0.42 |
| 1:AS:1559:C:O2' | 1:AS:1560:U:OP1 | 2.29 | 0.42 |
| 1:AS:1628:A:OP1 | 28:BU:48:ARG:NH1 | 2.45 | 0.42 |
| 1:AS:2078:A:H3' | 1:AS:2078:A:N3 | 2.35 | 0.42 |
| 1:AS:2367:C:H2' | 1:AS:2368:A:C8 | 2.55 | 0.42 |
| 1:AS:2485:U:C2 | 1:AS:2486:U:C5 | 3.08 | 0.42 |
| 1:AS:2771:A:H5" | 1:AS:2772:G:O5' | 2.19 | 0.42 |
| 1:AS:3091:U:H4' | 41:CH:28:PRO:HG2 | 2.01 | 0.42 |
| 3:AU:156:U:H2' | 3:AU:157:U:C5 | 2.54 | 0.42 |
| 19:BL:147:ARG:HB3 | 19:BL:150:VAL:HG23 | 2.02 | 0.42 |
| 46:CM:205:U:H2' | 46:CM:206:U:C6 | 2.55 | 0.42 |
| 46:CM:265:U:H2' | 46:CM:266:C:H6 | 1.85 | 0.42 |
| 46:CM:452:A:O4' | 51:CR:66:MET:HG3 | 2.19 | 0.42 |
| 46:CM:746:G:O2' | 56:CW:72:GLU:OE2 | 2.38 | 0.42 |
| 46:CM:1149:G:H2' | 46:CM:1150:G:C8 | 2.55 | 0.42 |
| 46:CM:1464:G:O2' | 66:DG:56:LYS:HD2 | 2.20 | 0.42 |
| 48:CO:26:ARG:HG3 | 48:CO:49:ASN:OD1 | 2.19 | 0.42 |
| 52:CS:63:GLN:HE22 | 52:CS:66:ASN:HB2 | 1.85 | 0.42 |
| 59:CZ:62:LEU:HA | 59:CZ:119:SER:O | 2.19 | 0.42 |
| 75:DP:12:VAL:HG12 | 75:DP:30:VAL:HG12 | 2.01 | 0.42 |
| 77:DR:34:ALA:O | 77:DR:37:ARG:HG2 | 2.20 | 0.42 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 79:DT:65:HIS:CE1 | 79:DT:85:SER:HG | 2.31 | 0.42 |
| 82:l1:41:TYR:HE1 | 82:l1:195:LYS:N | 2.18 | 0.42 |
| 1:1:563:U:H2' | 1:1:564:G:H8 | 1.82 | 0.42 |
| 1:1:713:A:O2' | 1:1:748:C:O2' | 2.34 | 0.42 |
| 1:1:1203:G:H4' | 41:AN:41:HIS:O | 2.20 | 0.42 |
| 1:1:1368:C:P | 29:AB:7:LYS:HE2 | 2.60 | 0.42 |
| 1:1:1377:A:H2' | 1:1:1378:G:C8 | 2.53 | 0.42 |
| 1:1:1586:G:C2 | 1:1:1587:G:C8 | 3.08 | 0.42 |
| 1:1:1591:U:C2 | 1:1:1592:C:C5 | 3.08 | 0.42 |
| 1:1:1912:U:H5" | 20:z:85:LYS:HB2 | 2.02 | 0.42 |
| 1:1:2079:C:O2' | 1:1:2080:U:H5" | 2.20 | 0.42 |
| 1:1:2681:C:H2' | 1:1:2682:C:H6 | 1.82 | 0.42 |
| 1:1:3262:U:O4 | 5:k:124:LYS:NZ | 2.53 | 0.42 |
| 1:1:3264:C:C2 | 1:1:3265:U:C5 | 3.07 | 0.42 |
| 2:3:24:A:H2' | 2:3:25:G:O4' | 2.20 | 0.42 |
| 5:k:286:GLY:HA3 | 5:k:321:PHE:CE1 | 2.55 | 0.42 |
| 5:k:313:ARG:O | 5:k:333:LYS:HE3 | 2.19 | 0.42 |
| 9:o:78:GLN:OE1 | 22:2:136:ARG:HG2 | 2.19 | 0.42 |
| 10:p:201:LEU:HD23 | 10:p:203:GLU:H | 1.85 | 0.42 |
| 11:q:95:ALA:O | 41:AN:1:MET:N | 2.51 | 0.42 |
| 28:AA:68:VAL:O | 28:AA:115:LYS:HG3 | 2.19 | 0.42 |
| 45:i:60:ASN:O | 45:i:62:ALA:N | 2.46 | 0.42 |
| 46:B:112:A:C2 | 46:B:301:U:H1' | 2.55 | 0.42 |
| 46:B:426:A:N3 | 46:B:438:U:O2' | 2.36 | 0.42 |
| 46:B:600:U:H2' | 46:B:601:U:C6 | 2.55 | 0.42 |
| 46:B:883:A:N3 | 46:B:884:G:H1' | 2.35 | 0.42 |
| 46:B:1537:A:H2' | 46:B:1538:U:H6 | 1.84 | 0.42 |
| 46:B:1709:A:H5" | 53:I:75:LEU:HD22 | 2.02 | 0.42 |
| 47:C:201:LEU:O | 47:C:202:TYR:HB2 | 2.19 | 0.42 |
| 66:V:124:ILE:HD11 | 66:V:132:LEU:HD12 | 2.02 | 0.42 |
| 78:h:156:VAL:HG22 | 78:h:158:ARG:HG2 | 2.02 | 0.42 |
| 1:AS:58:G:H2' | 3:AU:33:A:O2' | 2.20 | 0.42 |
| 1:AS:169:G:N1 | 1:AS:249:G:H1' | 2.35 | 0.42 |
| 1:AS:671:U:H2' | 1:AS:672:G:H8 | 1.83 | 0.42 |
| 1:AS:881:U:H2' | 1:AS:882:C:H6 | 1.85 | 0.42 |
| 1:AS:1494:A:H2' | 1:AS:1495:U:H6 | 1.83 | 0.42 |
| 1:AS:1576:A:H5" | 1:AS:1577:C:C5 | 2.55 | 0.42 |
| 1:AS:1695:A:C6 | 1:AS:1743:G:C6 | 3.08 | 0.42 |
| 1:AS:1705:C:H2' | 1:AS:1706:C:H6 | 1.83 | 0.42 |
| 1:AS:1756:A:C6 | 1:AS:1762:G:C5 | 3.08 | 0.42 |
| 1:AS:1802:A:H2' | 1:AS:1803:G:C8 | 2.54 | 0.42 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 1:AS:2279:U:H2' | 1:AS:2280:G:H8 | 1.85 | 0.42 |
| 1:AS:2332:C:H2' | 1:AS:2333:G:O4' | 2.20 | 0.42 |
| 1:AS:2718:A:H2' | 1:AS:2719:A:O4' | 2.20 | 0.42 |
| 1:AS:3159:A:H2' | 1:AS:3160:C:C6 | 2.55 | 0.42 |
| 3:AU:85:G:H4' | 3:AU:86:U:OP1 | 2.19 | 0.42 |
| 5:AX:214:MET:HE2 | 5:AX:350:ALA:HA | 2.00 | 0.42 |
| 11:BD:17:THR:HG1 | 11:BD:28:THR:HB | 1.85 | 0.42 |
| 15:BH:17:ARG:HD2 | 15:BH:61:VAL:HG22 | 2.01 | 0.42 |
| 35:CB:67:LYS:O | 35:CB:71:THR:HG22 | 2.20 | 0.42 |
| 39:CF:32:ASN:C | 39:CF:34:ASN:N | 2.77 | 0.42 |
| 42:CI:4:LYS:HB2 | 46:CM:1760:C:P | 2.59 | 0.42 |
| 46:CM:167:A:OP2 | 46:CM:167:A:H8 | 2.03 | 0.42 |
| 46:CM:488:C:N3 | 46:CM:489:C:N4 | 2.67 | 0.42 |
| 46:CM:517:C:H6 | 46:CM:517:C:H2' | 1.68 | 0.42 |
| 46:CM:565:A:H1' | 77:DR:14:VAL:HG23 | 2.01 | 0.42 |
| 46:CM:818:U:H5' | 46:CM:819:G:H5' | 2.01 | 0.42 |
| 46:CM:1181:A:H4' | 46:CM:1182:C:H5" | 2.01 | 0.42 |
| 46:CM:1508:G:O2' | 46:CM:1510:G:OP2 | 2.31 | 0.42 |
| 46:CM:1518:G:H21 | 66:DG:48:GLN:CD | 2.27 | 0.42 |
| 46:CM:1709:A:H2' | 46:CM:1710:G:O4' | 2.19 | 0.42 |
| 46:CM:1774:C:H2' | 46:CM:1775:G:H8 | 1.85 | 0.42 |
| 52:CS:99:MET:O | 52:CS:103:ASN:HB2 | 2.19 | 0.42 |
| 57:CX:44:LYS:HD3 | 57:CX:44:LYS:HA | 1.81 | 0.42 |
| 59:CZ:61:VAL:HB | 59:CZ:91:VAL:HG11 | 2.01 | 0.42 |
| 62:DC:56:LEU:HD21 | 62:DC:78:THR:OG1 | 2.19 | 0.42 |
| 72:DM:54:VAL:N | 72:DM:55:PRO:HD2 | 2.35 | 0.42 |
| 82:L1:5:THR:O | 82:L1:9:VAL:HG23 | 2.20 | 0.42 |
| 82:l1:35:GLN:HA | 82:l1:166:ALA:HB1 | 2.02 | 0.42 |
| 82:l1:70:ASP:OD1 | 82:l1:87:VAL:HG13 | 2.20 | 0.42 |
| 1:1:480:G:C4 | 1:1:481:G:C8 | 3.07 | 0.41 |
| 1:1:1627:C:H5" | 1:1:1628:A:H5" | 2.02 | 0.41 |
| 1:1:2431:U:H5' | 1:1:2439:A:H5' | 2.01 | 0.41 |
| 1:1:2836:A:H5" | 12:r:114:GLY:CA | 2.43 | 0.41 |
| 1:1:2919:G:H2' | 1:1:2920:C:C6 | 2.55 | 0.41 |
| 1:1:3061:C:H2' | 1:1:3062:U:O4' | 2.20 | 0.41 |
| 1:1:3176:C:H2' | 1:1:3177:C:C6 | 2.55 | 0.41 |
| 4:j:10:LYS:HA | 4:j:16:PHE:CD2 | 2.55 | 0.41 |
| 8:n:58:GLU:H | 8:n:58:GLU:CD | 2.27 | 0.41 |
| 26:8:43:SER:O | 26:8:43:SER:OG | 2.22 | 0.41 |
| 46:B:119:A:H1' | 46:B:395:A:C8 | 2.55 | 0.41 |
| 46:B:517:C:H6 | 46:B:517:C:H2' | 1.68 | 0.41 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 46:B:876:A:H2' | 46:B:877:G:C8 | 2.52 | 0.41 |
| 46:B:935:C:H2' | 46:B:936:A:C8 | 2.55 | 0.41 |
| 46:B:1640:C:C2 | 46:B:1735:G:C2 | 3.08 | 0.41 |
| 53:I:64:LYS:HB2 | 53:I:97:VAL:HG21 | 2.02 | 0.41 |
| 56:L:32:GLY:HA3 | 77:g:40:TYR:CG | 2.54 | 0.41 |
| 62:R:81:ARG:NH1 | 62:R:98:ASN:HA | 2.35 | 0.41 |
| 64:T:24:LEU:HD23 | 64:T:34:LEU:HD23 | 2.02 | 0.41 |
| 65:U:6:GLN:OE1 | 65:U:6:GLN:N | 2.52 | 0.41 |
| 79:AR:104:PHE:CE2 | 79:AR:139:GLY:HA2 | 2.54 | 0.41 |
| 1:AS:436:A:H2' | 1:AS:437:G:C8 | 2.55 | 0.41 |
| 1:AS:943:G:H2' | 1:AS:944:C:C6 | 2.55 | 0.41 |
| 1:AS:949:G:O2' | 1:AS:1111:G:H4' | 2.20 | 0.41 |
| 1:AS:1344:U:OP2 | 19:BL:38:ARG:NH2 | 2.44 | 0.41 |
| 1:AS:1444:U:H2' | 1:AS:1445:A:H8 | 1.83 | 0.41 |
| 1:AS:1754:G:H2' | 1:AS:1755:U:O4' | 2.20 | 0.41 |
| 1:AS:1852:C:H2' | 1:AS:1853:C:C6 | 2.55 | 0.41 |
| 1:AS:2269:A:H2' | 1:AS:2270:U:C6 | 2.55 | 0.41 |
| 1:AS:2470:C:H5' | 82:L1:213:SER:HB3 | 2.02 | 0.41 |
| 6:AY:7:VAL:HG11 | 6:AY:256:PHE:CZ | 2.55 | 0.41 |
| 9:BB:19:LYS:HE3 | 9:BB:23:GLU:OE2 | 2.20 | 0.41 |
| 24:BQ:36:VAL:HG22 | 24:BQ:58:VAL:HG11 | 2.01 | 0.41 |
| 26:BS:68:ALA:HB3 | 36:CC:36:LEU:HD13 | 2.02 | 0.41 |
| 30:BW:20:GLY:HA3 | 30:BW:21:ILE:HA | 1.81 | 0.41 |
| 40:CG:16:ALA:HB1 | 40:CG:42:ARG:HE | 1.85 | 0.41 |
| 46:CM:81:G:H2' | 46:CM:82:U:C6 | 2.55 | 0.41 |
| 46:CM:1152:G:N2 | 63:DD:138:GLN:HE22 | 2.17 | 0.41 |
| 46:CM:1357:A:H4' | 46:CM:1358:G:OP1 | 2.20 | 0.41 |
| 53:CT:220:LYS:HD2 | 53:CT:220:LYS:HA | 1.82 | 0.41 |
| 55:CV:48:THR:HG22 | 55:CV:52:ASN:C | 2.45 | 0.41 |
| 57:CX:35:ILE:HG22 | 57:CX:37:THR:HG22 | 2.02 | 0.41 |
| 69:DJ:106:THR:HG22 | 69:DJ:109:GLY:O | 2.20 | 0.41 |
| 77:DR:37:ARG:O | 77:DR:41:THR:HG23 | 2.20 | 0.41 |
| 79:DT:294:ASP:OD1 | 79:DT:294:ASP:N | 2.53 | 0.41 |
| 82:L1:206:ILE:HB | 82:L1:216:ILE:HD12 | 2.02 | 0.41 |
| 1:1:277:G:H2' | 1:1:278:U:H6 | 1.85 | 0.41 |
| 1:1:516:U:C4 | 6:l:350:VAL:HG23 | 2.55 | 0.41 |
| 1:1:677:U:H2' | 1:1:678:G:C8 | 2.55 | 0.41 |
| 1:1:797:A:OP1 | 29:AB:27:LYS:HE3 | 2.20 | 0.41 |
| 1:1:1180:A:H2' | 1:1:1181:C:C6 | 2.56 | 0.41 |
| 1:1:1459:U:H2' | 1:1:1460:G:O4' | 2.20 | 0.41 |
| 1:1:1650:A:O2' | 35:AH:59:PRO:HD3 | 2.21 | 0.41 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 1:1:1802:A:C5 | 1:1:1803:G:C5 | 3.07 | 0.41 |
| 1:1:2493:A:H5" | 16:v:28:TRP:CD1 | 2.54 | 0.41 |
| 1:1:2610:C:H3' | 1:1:2611:G:H8 | 1.85 | 0.41 |
| 1:1:2919:G:OP1 | 1:1:2954:A:N6 | 2.44 | 0.41 |
| 5:k:284:ARG:NH1 | 5:k:356:LEU:HD12 | 2.33 | 0.41 |
| 9:o:174:PHE:HB3 | 9:o:192:ASN:ND2 | 2.35 | 0.41 |
| 12:r:38:ARG:HG2 | 12:r:41:ALA:HB2 | 2.02 | 0.41 |
| 22:2:88:ARG:NH1 | 30:AC:33:LYS:O | 2.53 | 0.41 |
| 35:AH:67:LYS:HA | 35:AH:70:LYS:HE2 | 2.03 | 0.41 |
| 45:i:52:LYS:HG3 | 45:i:53:LYS:N | 2.35 | 0.41 |
| 45:i:69:PHE:HB3 | 45:i:70:ASN:H | 1.76 | 0.41 |
| 45:i:101:LYS:HD2 | 46:B:580:U:C5 | 2.55 | 0.41 |
| 46:B:151:G:O6 | 71:a:128:ARG:NH2 | 2.52 | 0.41 |
| 46:B:209:U:H5" | 58:N:20:PHE:CG | 2.55 | 0.41 |
| 46:B:326:A:H2' | 46:B:327:G:O4' | 2.20 | 0.41 |
| 46:B:536:A:H1' | 46:B:539:A:C8 | 2.55 | 0.41 |
| 46:B:1697:C:H2' | 46:B:1698:U:C2 | 2.56 | 0.41 |
| 47:C:200:ASP:O | 47:C:203:PHE:HB2 | 2.20 | 0.41 |
| 50:F:64:GLY:HA3 | 57:M:96:PRO:HD3 | 2.02 | 0.41 |
| 54:J:60:PRO:N | 54:J:61:PRO:HD2 | 2.34 | 0.41 |
| 59:O:56:GLU:HG2 | 59:O:124:LYS:HE3 | 2.02 | 0.41 |
| 63:S:130:GLY:HA3 | 63:S:136:ARG:HA | 2.00 | 0.41 |
| 64:T:89:SER:C | 64:T:91:LEU:N | 2.76 | 0.41 |
| 1:AS:343:U:H1' | 6:AY:96:ARG:HG3 | 2.01 | 0.41 |
| 1:AS:1209:G:H4' | 21:BN:90:MET:HB2 | 2.03 | 0.41 |
| 1:AS:1410:G:C6 | 1:AS:1411:U:C4 | 3.08 | 0.41 |
| 1:AS:1707:U:C4 | 1:AS:1708:G:C6 | 3.08 | 0.41 |
| 1:AS:1767:G:H2' | 1:AS:1768:U:O4' | 2.19 | 0.41 |
| 1:AS:2117:A:C4 | 38:CE:3:LYS:HE2 | 2.55 | 0.41 |
| 1:AS:2790:U:H6 | 1:AS:2790:U:H5' | 1.85 | 0.41 |
| 1:AS:2854:U:H2' | 1:AS:2855:U:H6 | 1.84 | 0.41 |
| 1:AS:3088:G:H4' | 11:BD:69:ARG:HH12 | 1.83 | 0.41 |
| 1:AS:3157:A:OP1 | 11:BD:23:ARG:HG3 | 2.19 | 0.41 |
| 1:AS:3159:A:C6 | 1:AS:3160:C:N4 | 2.88 | 0.41 |
| 1:AS:3256:G:C2 | 1:AS:3257:A:C5 | 3.08 | 0.41 |
| 3:AU:37:A:H5" | 3:AU:39:G:O4' | 2.20 | 0.41 |
| 3:AU:72:A:C5 | 3:AU:73:U:C5 | 3.08 | 0.41 |
| 6:AY:5:PRO:O | 6:AY:23:LEU:HB2 | 2.20 | 0.41 |
| 7:AZ:40:HIS:CE1 | 22:BO:69:LYS:HA | 2.56 | 0.41 |
| 9:BB:15:LYS:HE3 | 9:BB:15:LYS:HB3 | 1.89 | 0.41 |
| 18:BK:123:PRO:O | 18:BK:143:PRO:HG2 | 2.20 | 0.41 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 19:BL:91:ASN:ND2 | 29:BV:80:THR:HG21 | 2.35 | 0.41 |
| 21:BN:23:LYS:HD3 | 21:BN:23:LYS:HA | 1.87 | 0.41 |
| 27:BT:106:ILE:HG21 | 27:BT:109:LEU:HD23 | 2.03 | 0.41 |
| 30:BW:44:ARG:HE | 30:BW:44:ARG:HB2 | 1.66 | 0.41 |
| 42:CI:4:LYS:HB2 | 46:CM:1760:C:OP2 | 2.20 | 0.41 |
| 46:CM:188:U:H2' | 46:CM:189:G:H8 | 1.85 | 0.41 |
| 46:CM:498:C:C2 | 46:CM:499:U:C6 | 3.08 | 0.41 |
| 46:CM:528:C:O2 | 71:DL:61:ARG:NH1 | 2.29 | 0.41 |
| 46:CM:530:U:OP2 | 56:CW:132:ARG:NH2 | 2.53 | 0.41 |
| 46:CM:975:C:H2' | 46:CM:976:G:O4' | 2.19 | 0.41 |
| 46:CM:1485:G:H2' | 46:CM:1486:G:C8 | 2.55 | 0.41 |
| 48:CO:58:ALA:CB | 48:CO:91:VAL:HG11 | 2.50 | 0.41 |
| 57:CX:50:THR:OG1 | 57:CX:55:VAL:HG23 | 2.20 | 0.41 |
| 1:1:21:G:H1' | 3:4:104:A:N3 | 2.35 | 0.41 |
| 1:1:229:C:H2' | 1:1:230:G:O4' | 2.20 | 0.41 |
| 1:1:780:A:H2' | 1:1:780:A:N3 | 2.33 | 0.41 |
| 1:1:948:A:H4' | 1:1:964:G:H21 | 1.82 | 0.41 |
| 1:1:1559:C:HO2' | 1:1:1560:U:P | 2.43 | 0.41 |
| 1:1:1619:G:H2' | 1:1:1620:G:O4' | 2.19 | 0.41 |
| 1:1:1900:C:H2' | 1:1:1901:G:O4' | 2.20 | 0.41 |
| 1:1:2182:C:H2' | 1:1:2183:U:H6 | 1.84 | 0.41 |
| 1:1:2202:A:H5' | 37:AJ:73:LYS:NZ | 2.35 | 0.41 |
| 1:1:2618:C:H5" | 12:r:119:TRP:CG | 2.55 | 0.41 |
| 1:1:2627:U:H4' | 1:1:2628:A:O4' | 2.20 | 0.41 |
| 1:1:2658:A:H2' | 1:1:2659:G:O4' | 2.19 | 0.41 |
| 2:3:69:A:C6 | 2:3:110:G:C6 | 3.09 | 0.41 |
| 3:4:18:U:H2' | 3:4:19:C:C6 | 2.55 | 0.41 |
| 3:4:27:U:H2' | 3:4:28:C:H6 | 1.85 | 0.41 |
| 3:4:95:G:N7 | 38:AK:83:ALA:HB2 | 2.36 | 0.41 |
| 4:j:68:LYS:HE3 | 4:j:68:LYS:HB2 | 1.95 | 0.41 |
| 7:m:41:LYS:HD3 | 7:m:41:LYS:HA | 1.80 | 0.41 |
| 9:o:108:GLN:HG3 | 9:o:111:ALA:HB2 | 2.02 | 0.41 |
| 13:s:82:ARG:HA | 13:s:85:LYS:HE2 | 2.02 | 0.41 |
| 18:x:153:GLU:HG3 | 18:x:155:GLU:HG3 | 2.02 | 0.41 |
| 32:AE:84:ALA:C | 32:AE:86:GLU:N | 2.78 | 0.41 |
| 34:AG:20:LYS:HE2 | 34:AG:20:LYS:HB2 | 1.64 | 0.41 |
| 46:B:10:G:O2' | 49:E:82:GLN:OE1 | 2.36 | 0.41 |
| 46:B:399:A:O2' | 46:B:400:C:H4' | 2.20 | 0.41 |
| 46:B:1118:A:N3 | 46:B:1637:U:O2' | 2.43 | 0.41 |
| 46:B:1552:C:H5" | 65:U:41:ARG:HG2 | 2.01 | 0.41 |
| 46:B:1553:U:N3 | 46:B:1554:U:C5 | 2.89 | 0.41 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 47:C:35:PRO:HG3 | 68:X:87:ARG:CZ | 2.50 | 0.41 |
| 47:C:147:THR:OG1 | 47:C:151:SER:HB2 | 2.20 | 0.41 |
| 51:G:31:PRO:HD2 | 51:G:38:LEU:HD11 | 2.03 | 0.41 |
| 52:H:116:HIS:O | 52:H:120:ILE:HG13 | 2.20 | 0.41 |
| 59:O:67:THR:C | 59:O:69:GLU:H | 2.28 | 0.41 |
| 62:R:34:THR:HA | 62:R:37:CYS:SG | 2.60 | 0.41 |
| 67:W:98:THR:O | 67:W:102:ILE:HG13 | 2.19 | 0.41 |
| 1:AS:95:G:H2' | 1:AS:96:U:O4' | 2.21 | 0.41 |
| 1:AS:441:U:O2' | 1:AS:442:G:H5" | 2.21 | 0.41 |
| 1:AS:912:G:H5' | 1:AS:913:A:OP1 | 2.20 | 0.41 |
| 1:AS:1011:C:H4' | 1:AS:1012:U:C6 | 2.52 | 0.41 |
| 1:AS:1575:A:OP1 | 1:AS:2500:G:N2 | 2.52 | 0.41 |
| 1:AS:1865:C:H4' | 1:AS:3049:A:O2' | 2.20 | 0.41 |
| 1:AS:1918:A:H2' | 1:AS:1919:C:O4' | 2.20 | 0.41 |
| 1:AS:2603:U:H2' | 1:AS:2604:G:C8 | 2.55 | 0.41 |
| 1:AS:2679:U:H2' | 1:AS:2680:C:C6 | 2.55 | 0.41 |
| 1:AS:3111:A:O4' | 5:AX:18:PRO:HD2 | 2.20 | 0.41 |
| 3:AU:6:U:H2' | 3:AU:7:U:C6 | 2.55 | 0.41 |
| 3:AU:12:A:C6 | 3:AU:13:A:N7 | 2.87 | 0.41 |
| 8:BA:59:ASP:OD2 | 8:BA:77:ARG:NH1 | 2.54 | 0.41 |
| 12:BE:17:TYR:H | 12:BE:95:HIS:CD2 | 2.38 | 0.41 |
| 16:BI:180:PHE:O | 16:BI:184:LYS:HG3 | 2.20 | 0.41 |
| 21:BN:5:ASN:HB2 | 21:BN:7:TYR:CE1 | 2.55 | 0.41 |
| 46:CM:2:A:C2 | 49:CP:165:ILE:HD12 | 2.54 | 0.41 |
| 46:CM:680:C:O2' | 46:CM:681:C:H6 | 2.01 | 0.41 |
| 46:CM:787:A:H8 | 46:CM:787:A:OP2 | 2.04 | 0.41 |
| 46:CM:988:A:H2' | 46:CM:990:A:N7 | 2.35 | 0.41 |
| 47:CN:201:LEU:O | 47:CN:202:TYR:HB2 | 2.20 | 0.41 |
| 52:CS:145:ASP:OD1 | 52:CS:146:SER:N | 2.54 | 0.41 |
| 65:DF:77:THR:HG23 | 65:DF:86:LEU:HD11 | 2.02 | 0.41 |
| 68:DI:58:TYR:OH | 69:DJ:20:THR:HA | 2.19 | 0.41 |
| 79:DT:145:LEU:HD21 | 79:DT:178:TRP:CZ2 | 2.55 | 0.41 |
| 79:DT:174:THR:HG22 | 79:DT:190:ILE:HG22 | 2.01 | 0.41 |
| 81:12:130:LYS:HA | 81:12:133:LEU:HB2 | 2.02 | 0.41 |
| 82:l1:41:TYR:CE1 | 82:l1:195:LYS:HG2 | 2.55 | 0.41 |
| 82:l1:183:ILE:H | 82:l1:183:ILE:HG13 | 1.69 | 0.41 |
| 1:1:35:C:H4' | 1:1:804:A:C2 | 2.55 | 0.41 |
| 1:1:122:A:C6 | 1:1:149:A:C5 | 3.08 | 0.41 |
| 1:1:215:G:C2 | 1:1:224:C:C2 | 3.08 | 0.41 |
| 1:1:745:C:H5" | 30:AC:32:LEU:HD12 | 2.03 | 0.41 |
| 1:1:831:G:H1' | 1:1:854:A:N6 | 2.36 | 0.41 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 1:1:846:U:H2' | 1:1:847:C:H6 | 1.86 | 0.41 |
| 1:1:908:G:C2 | 1:1:910:A:C2 | 3.08 | 0.41 |
| 1:1:1558:G:H5' | 1:1:1559:C:OP2 | 2.20 | 0.41 |
| 1:1:1882:A:O2' | 5:k:226:PHE:O | 2.32 | 0.41 |
| 1:1:2455:G:H2' | 1:1:2456:C:C5 | 2.55 | 0.41 |
| 1:1:3010:U:H5" | 5:k:62:ARG:HG2 | 2.01 | 0.41 |
| 1:1:3197:G:C6 | 1:1:3221:G:C6 | 3.09 | 0.41 |
| 2:3:56:A:H4' | 13:s:152:HIS:HB2 | 2.02 | 0.41 |
| 3:4:119:C:H2' | 3:4:120:U:H6 | 1.84 | 0.41 |
| 6:l:143:VAL:O | 6:l:143:VAL:HG12 | 2.21 | 0.41 |
| 7:m:7:PHE:CD1 | 7:m:7:PHE:C | 2.98 | 0.41 |
| 9:o:212:PHE:HB3 | 9:o:225:ASP:OD2 | 2.21 | 0.41 |
| 20:z:162:ARG:HD2 | 46:B:799:G:O4' | 2.20 | 0.41 |
| 20:z:163:ARG:NH2 | 46:B:799:G:N7 | 2.68 | 0.41 |
| 29:AB:59:ARG:NH2 | 43:AP:38:GLN:HG2 | 2.33 | 0.41 |
| 45:i:55:LYS:HE3 | 45:i:55:LYS:HB3 | 1.86 | 0.41 |
| 46:B:386:G:OP1 | 46:B:400:C:H5 | 2.03 | 0.41 |
| 46:B:1159:C:C4 | 46:B:1160:U:C4 | 3.09 | 0.41 |
| 46:B:1335:U:O2' | 46:B:1336:G:OP1 | 2.34 | 0.41 |
| 46:B:1378:U:H2' | 46:B:1379:C:C6 | 2.55 | 0.41 |
| 46:B:1503:A:O2' | 46:B:1504:U:H5' | 2.20 | 0.41 |
| 46:B:1604:U:H2' | 46:B:1605:C:C6 | 2.56 | 0.41 |
| 48:D:26:ARG:HA | 48:D:50:ARG:NH1 | 2.36 | 0.41 |
| 50:F:27:THR:O | 50:F:31:ALA:HB2 | 2.21 | 0.41 |
| 51:G:185:GLY:HA3 | 51:G:224:ASN:OD1 | 2.21 | 0.41 |
| 59:O:62:LEU:HD11 | 59:O:90:LYS:HD3 | 2.01 | 0.41 |
| 72:b:60:VAL:HG23 | 72:b:101:TYR:HB2 | 2.02 | 0.41 |
| 1:AS:313:A:H2' | 1:AS:314:U:C6 | 2.55 | 0.41 |
| 1:AS:487:C:HO2' | 1:AS:488:G:P | 2.43 | 0.41 |
| 1:AS:502:U:H2' | 1:AS:503:U:C6 | 2.55 | 0.41 |
| 1:AS:528:A:O2' | 1:AS:529:A:H5' | 2.20 | 0.41 |
| 1:AS:861:U:C2 | 1:AS:862:A:C8 | 3.08 | 0.41 |
| 1:AS:939:U:H3' | 29:BV:13:GLY:HA2 | 2.02 | 0.41 |
| 1:AS:1006:G:N2 | 12:BE:193:ASP:O | 2.34 | 0.41 |
| 1:AS:1186:A:N3 | 1:AS:1186:A:H2' | 2.35 | 0.41 |
| 1:AS:1293:C:H2' | 1:AS:1294:C:H6 | 1.85 | 0.41 |
| 1:AS:1900:C:H2' | 1:AS:1901:G:O4' | 2.21 | 0.41 |
| 1:AS:2062:G:H2' | 1:AS:2063:C:H5 | 1.85 | 0.41 |
| 1:AS:2184:G:H5' | 1:AS:2185:A:C2 | 2.55 | 0.41 |
| 1:AS:2461:G:N2 | 1:AS:2464:A:H5" | 2.24 | 0.41 |
| 1:AS:2650:A:OP1 | 45:CL:57:PRO:HD2 | 2.19 | 0.41 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 1:AS:3318:G:C6 | 1:AS:3321:G:C5 | 3.09 | 0.41 |
| 4:AW:68:LYS:HE3 | 4:AW:68:LYS:HB2 | 1.89 | 0.41 |
| 9:BB:45:ARG:NH2 | 9:BB:175:ASN:OD1 | 2.45 | 0.41 |
| 13:BF:160:ILE:HG23 | 13:BF:171:VAL:HG21 | 2.01 | 0.41 |
| 14:BG:69:VAL:HG12 | 14:BG:151:GLN:OE1 | 2.20 | 0.41 |
| 17:BJ:151:GLU:O | 17:BJ:155:GLU:HG2 | 2.20 | 0.41 |
| 18:BK:94:LEU:HD23 | 18:BK:94:LEU:HA | 1.88 | 0.41 |
| 26:BS:46:TYR:CD1 | 36:CC:75:TYR:HB3 | 2.55 | 0.41 |
| 26:BS:69:THR:O | 26:BS:73:MET:HG2 | 2.20 | 0.41 |
| 28:BU:50:PRO:HD3 | 28:BU:68:VAL:HG22 | 2.02 | 0.41 |
| 45:CL:107:TRP:CE2 | 50:CQ:143:LEU:HB2 | 2.56 | 0.41 |
| 46:CM:158:C:H2' | 46:CM:159:U:O4' | 2.21 | 0.41 |
| 46:CM:890:A:H5" | 61:DB:47:ARG:HB2 | 2.02 | 0.41 |
| 46:CM:1277:G:H21 | 47:CN:111:ILE:HD11 | 1.86 | 0.41 |
| 49:CP:233:SER:OG | 49:CP:236:GLU:HG2 | 2.21 | 0.41 |
| 50:CQ:73:LEU:CD2 | 57:CX:20:VAL:HB | 2.50 | 0.41 |
| 60:DA:5:HIS:HD1 | 60:DA:121:ARG:HE | 1.68 | 0.41 |
| 64:DE:5:ARG:O | 64:DE:10:LYS:HE2 | 2.20 | 0.41 |
| 69:DJ:8:ALA:HB2 | 69:DJ:74:VAL:HG21 | 2.03 | 0.41 |
| 78:DS:127:TYR:HD1 | 78:DS:128:THR:N | 2.18 | 0.41 |
| 80:P0:19:LEU:HD21 | 80:P0:73:PHE:CZ | 2.55 | 0.41 |
| 80:p0:14:LYS:O | 80:p0:18:LEU:HG | 2.21 | 0.41 |
| 1:1:180:U:H4' | 38:AK:75:LYS:CG | 2.51 | 0.41 |
| 1:1:422:A:C2 | 1:1:2341:A:H4' | 2.55 | 0.41 |
| 1:1:427:C:OP1 | 33:AF:14:TYR:OH | 2.35 | 0.41 |
| 1:1:626:U:H2' | 1:1:627:U:O4' | 2.21 | 0.41 |
| 1:1:952:U:H2' | 1:1:953:C:H6 | 1.84 | 0.41 |
| 1:1:1004:U:H4' | 12:r:34:TYR:CD1 | 2.55 | 0.41 |
| 1:1:1080:A:H4' | 7:m:44:TYR:CE2 | 2.55 | 0.41 |
| 1:1:1149:A:O2' | 1:1:1150:A:H5' | 2.20 | 0.41 |
| 1:1:1341:U:H2' | 1:1:1342:G:O4' | 2.21 | 0.41 |
| 1:1:2176:A:C2 | 1:1:2177:G:C8 | 3.08 | 0.41 |
| 1:1:3256:G:C2 | 1:1:3257:A:C5 | 3.09 | 0.41 |
| 5:k:35:ASP:HA | 5:k:184:ASN:OD1 | 2.20 | 0.41 |
| 6:l:140:GLY:O | 6:l:142:ARG:NH1 | 2.53 | 0.41 |
| 8:n:28:LYS:HE3 | 8:n:28:LYS:HB3 | 1.81 | 0.41 |
| 26:8:142:ILE:HD12 | 26:8:142:ILE:HA | 1.88 | 0.41 |
| 28:AA:29:HIS:CE1 | 28:AA:42:ILE:HG12 | 2.55 | 0.41 |
| 32:AE:43:MET:CE | 32:AE:76:ARG:HB2 | 2.49 | 0.41 |
| 46:B:260:U:O2' | 46:B:261:C:H5' | 2.20 | 0.41 |
| 46:B:260:U:C2' | 46:B:261:C:H5' | 2.50 | 0.41 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 46:B:392:C:H2' | 46:B:393:U:C6 | 2.56 | 0.41 |
| 46:B:494:G:H2' | 46:B:495:G:O4' | 2.20 | 0.41 |
| 46:B:1008:A:OP1 | 46:B:1111:G:N2 | 2.52 | 0.41 |
| 46:B:1455:A:H4' | 46:B:1528:G:H4' | 2.01 | 0.41 |
| 46:B:1474:G:H3' | 46:B:1502:A:H61 | 1.86 | 0.41 |
| 47:C:148:ASP:N | 47:C:164:ASN:OD1 | 2.54 | 0.41 |
| 50:F:63:GLN:OE1 | 50:F:65:ARG:NH2 | 2.47 | 0.41 |
| 54:J:33:GLU:HG2 | 54:J:34:LEU:HD12 | 2.01 | 0.41 |
| 62:R:41:VAL:HG13 | 62:R:84:ILE:HG21 | 2.02 | 0.41 |
| 64:T:7:LYS:O | 64:T:11:ARG:HG2 | 2.20 | 0.41 |
| 74:d:31:PHE:CD1 | 74:d:81:ARG:HG3 | 2.54 | 0.41 |
| 1:AS:39:A:H5" | 29:BV:35:ALA:HB1 | 2.03 | 0.41 |
| 1:AS:107:A:H2 | 14:BG:73:ARG:HE | 1.68 | 0.41 |
| 1:AS:280:U:O2' | 16:BI:182:LYS:NZ | 2.53 | 0.41 |
| 1:AS:630:G:H2' | 1:AS:631:U:C6 | 2.55 | 0.41 |
| 1:AS:999:A:N1 | 1:AS:1045:C:O2' | 2.51 | 0.41 |
| 1:AS:1227:A:H5" | 1:AS:1228:C:C5' | 2.50 | 0.41 |
| 1:AS:1231:U:H1' | 1:AS:1233:G:OP2 | 2.21 | 0.41 |
| 1:AS:1562:G:OP1 | 1:AS:1562:G:O4' | 2.38 | 0.41 |
| 1:AS:2872:A:C4 | 1:AS:2873:G:C8 | 3.09 | 0.41 |
| 1:AS:3315:C:H4' | 1:AS:3316:U:OP1 | 2.21 | 0.41 |
| 3:AU:104:A:C8 | 3:AU:105:A:C8 | 3.08 | 0.41 |
| 3:AU:152:G:H2' | 3:AU:153:U:O4' | 2.21 | 0.41 |
| 31:BX:11:ASN:HB3 | 31:BX:12:ILE:HD12 | 2.01 | 0.41 |
| 36:CC:70:TYR:HA | 36:CC:73:LYS:HG3 | 2.02 | 0.41 |
| 46:CM:854:A:H61 | 46:CM:943:U:H5 | 1.67 | 0.41 |
| 46:CM:872:A:C4 | 46:CM:873:U:C5 | 3.08 | 0.41 |
| 52:CS:63:GLN:NE2 | 52:CS:66:ASN:H | 2.17 | 0.41 |
| 52:CS:93:LEU:HD12 | 52:CS:172:ILE:HG23 | 2.02 | 0.41 |
| 62:DC:56:LEU:HD13 | 62:DC:80:LEU:HD12 | 2.02 | 0.41 |
| 69:DJ:75:ILE:HD12 | 69:DJ:125:ILE:HD13 | 2.03 | 0.41 |
| 69:DJ:77:PRO:HD3 | 70:DK:7:ARG:O | 2.21 | 0.41 |
| 71:DL:56:SER:HB3 | 71:DL:74:LEU:CD1 | 2.51 | 0.41 |
| 79:DT:145:LEU:HD11 | 79:DT:178:TRP:CG | 2.56 | 0.41 |
| 82:l1:9:VAL:HB | 82:l1:180:VAL:HG13 | 2.01 | 0.41 |
| 82:l1:191:VAL:O | 82:l1:197:ASN:HA | 2.21 | 0.41 |
| 1:1:99:A:H2' | 1:1:100:G:N3 | 2.36 | 0.41 |
| 1:1:179:C:H2' | 1:1:180:U:C6 | 2.55 | 0.41 |
| 1:1:181:U:H2' | 1:1:182:G:H8 | 1.84 | 0.41 |
| 1:1:313:A:H2' | 1:1:314:U:C6 | 2.55 | 0.41 |
| 1:1:339:C:OP1 | 1:1:1376:G:O2' | 2.29 | 0.41 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 1:1:595:G:H21 | 6:l:323:GLN:CD | 2.28 | 0.41 |
| 1:1:1477:A:H1' | 1:1:1854:A:N3 | 2.36 | 0.41 |
| 1:1:1705:C:H2' | 1:1:1706:C:H6 | 1.86 | 0.41 |
| 1:1:2163:G:O2' | 1:1:2292:U:OP2 | 2.38 | 0.41 |
| 1:1:2183:U:HO2' | 1:1:2184:G:P | 2.43 | 0.41 |
| 1:1:2223:C:H4' | 4:j:221:LYS:O | 2.21 | 0.41 |
| 1:1:2404:U:H2' | 1:1:2405:U:H6 | 1.86 | 0.41 |
| 1:1:2458:G:H4' | 82:l1:102:LYS:NZ | 2.33 | 0.41 |
| 1:1:2713:C:O2 | 43:AP:20:HIS:HE1 | 2.04 | 0.41 |
| 1:1:3108:G:C5 | 1:1:3109:C:C5 | 3.08 | 0.41 |
| 1:1:3264:C:H2' | 1:1:3265:U:H6 | 1.85 | 0.41 |
| 2:3:94:C:H2' | 2:3:95:A:H8 | 1.86 | 0.41 |
| 3:4:83:U:H4' | 3:4:85:G:N3 | 2.36 | 0.41 |
| 6:l:61:THR:HG22 | 6:l:63:ALA:N | 2.35 | 0.41 |
| 19:y:150:VAL:HA | 19:y:153:PHE:CD2 | 2.56 | 0.41 |
| 21:0:106:MET:HE3 | 21:0:106:MET:HB3 | 1.96 | 0.41 |
| 31:AD:12:ILE:H | 31:AD:12:ILE:HD12 | 1.85 | 0.41 |
| 34:AG:49:ILE:HG12 | 34:AG:100:ILE:HD13 | 2.03 | 0.41 |
| 46:B:36:C:H2' | 46:B:37:U:H6 | 1.86 | 0.41 |
| 46:B:71:A:H2' | 46:B:72:A:C8 | 2.56 | 0.41 |
| 46:B:94:U:O2' | 51:G:8:HIS:ND1 | 2.47 | 0.41 |
| 46:B:978:A:O3' | 46:B:1765:G:H4' | 2.20 | 0.41 |
| 46:B:1417:C:OP1 | 46:B:1418:U:H2' | 2.21 | 0.41 |
| 46:B:1472:G:N2 | 46:B:1580:A:OP1 | 2.37 | 0.41 |
| 46:B:1720:C:H2' | 46:B:1721:U:C6 | 2.55 | 0.41 |
| 49:E:73:ASP:HB3 | 49:E:99:ILE:HD13 | 2.02 | 0.41 |
| 50:F:7:SER:HB3 | 50:F:10:LYS:HG3 | 2.03 | 0.41 |
| 51:G:123:LEU:HD13 | 51:G:237:VAL:HG13 | 2.02 | 0.41 |
| 69:Y:11:LEU:HD12 | 69:Y:74:VAL:HG13 | 2.02 | 0.41 |
| 1:AS:277:G:H2' | 1:AS:278:U:H6 | 1.84 | 0.41 |
| 1:AS:1268:C:H3' | 1:AS:1269:A:H8 | 1.85 | 0.41 |
| 1:AS:2184:G:H4' | 1:AS:2185:A:C5 | 2.56 | 0.41 |
| 1:AS:2427:A:C6 | 1:AS:2428:G:C4 | 3.08 | 0.41 |
| 1:AS:2650:A:H8 | 45:CL:56:SER:OG | 2.03 | 0.41 |
| 5:AX:123:TYR:CZ | 5:AX:124:LYS:HG3 | 2.55 | 0.41 |
| 11:BD:7:ASP:OD2 | 11:BD:54:LYS:HD3 | 2.19 | 0.41 |
| 12:BE:19:LYS:HB3 | 12:BE:19:LYS:HE2 | 1.77 | 0.41 |
| 12:BE:54:SER:HB2 | 12:BE:135:ILE:HD11 | 2.03 | 0.41 |
| 22:BO:54:HIS:CE1 | 22:BO:55:LYS:HG2 | 2.56 | 0.41 |
| 28:BU:73:LYS:CD | 28:BU:75:VAL:HG22 | 2.50 | 0.41 |
| 28:BU:108:GLU:O | 28:BU:112:LYS:HG2 | 2.20 | 0.41 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 46:CM:384:G:OP2 | 55:CV:25:ARG:NH2 | 2.53 | 0.41 |
| 46:CM:391:C:OP1 | 55:CV:2:GLY:HA3 | 2.20 | 0.41 |
| 46:CM:415:A:H5' | 46:CM:416:G:C4 | 2.56 | 0.41 |
| 46:CM:484:G:O6 | 46:CM:499:U:O4 | 2.38 | 0.41 |
| 46:CM:734:U:H2' | 46:CM:735:U:C6 | 2.55 | 0.41 |
| 46:CM:741:A:H5' | 51:CR:16:SER:HB3 | 2.02 | 0.41 |
| 46:CM:872:A:H2' | 46:CM:873:U:C6 | 2.55 | 0.41 |
| 46:CM:1143:C:H6 | 46:CM:1143:C:H2' | 1.73 | 0.41 |
| 46:CM:1262:G:C5 | 46:CM:1422:A:C2 | 3.09 | 0.41 |
| 46:CM:1330:A:H1' | 67:DH:55:VAL:HG22 | 2.03 | 0.41 |
| 46:CM:1469:A:C2 | 46:CM:1594:G:H1' | 2.55 | 0.41 |
| 46:CM:1484:U:C4 | 46:CM:1498:G:C2 | 3.08 | 0.41 |
| 46:CM:1699:G:C6 | 46:CM:1700:G:C8 | 3.09 | 0.41 |
| 46:CM:1740:A:H2' | 46:CM:1741:A:C8 | 2.56 | 0.41 |
| 46:CM:1757:U:H2' | 46:CM:1758:U:C6 | 2.56 | 0.41 |
| 50:CQ:80:LEU:HD13 | 50:CQ:85:ILE:HB | 2.03 | 0.41 |
| 52:CS:57:SER:HA | 75:DP:53:ILE:HB | 2.03 | 0.41 |
| 52:CS:58:LEU:HD22 | 52:CS:168:VAL:HG23 | 2.03 | 0.41 |
| 56:CW:68:LYS:HE2 | 56:CW:68:LYS:HB3 | 1.80 | 0.41 |
| 61:DB:9:PHE:HA | 61:DB:73:ALA:O | 2.21 | 0.41 |
| 66:DG:108:LEU:HA | 66:DG:111:ILE:HG22 | 2.01 | 0.41 |
| 78:DS:128:THR:OG1 | 78:DS:129:THR:N | 2.53 | 0.41 |
| 82:l1:30:GLU:HB3 | 82:l1:31:THR:H | 1.56 | 0.41 |
| 82:l1:216:ILE:HG22 | 82:l1:217:TYR:H | 1.85 | 0.41 |
| 1:1:2796:G:H2' | 1:1:2797:C:H6 | 1.85 | 0.41 |
| 1:1:2874:A:H2' | 1:1:2875:A:O4' | 2.20 | 0.41 |
| 1:1:2887:U:OP1 | 5:k:9:PRO:HD3 | 2.21 | 0.41 |
| 2:3:31:U:H4' | 7:m:218:LYS:NZ | 2.36 | 0.41 |
| 3:4:141:C:H2' | 3:4:142:C:H6 | 1.85 | 0.41 |
| 5:k:215:ILE:HD12 | 5:k:338:LEU:HB3 | 2.03 | 0.41 |
| 6:l:299:VAL:HG21 | 19:y:133:LYS:HG3 | 2.02 | 0.41 |
| 8:n:44:GLY:O | 8:n:47:ARG:NH1 | 2.46 | 0.41 |
| 15:u:87:TRP:CE2 | 15:u:93:ALA:HB2 | 2.55 | 0.41 |
| 17:w:62:ALA:HA | 17:w:71:PRO:HD2 | 2.01 | 0.41 |
| 25:7:24:GLY:C | 25:7:26:SER:H | 2.28 | 0.41 |
| 45:i:102:LYS:HE3 | 46:B:574:G:OP1 | 2.20 | 0.41 |
| 46:B:217:A:C5 | 46:B:218:A:C8 | 3.08 | 0.41 |
| 46:B:474:U:OP1 | 46:B:475:A:O2' | 2.37 | 0.41 |
| 46:B:804:U:H2' | 46:B:805:U:H5 | 1.84 | 0.41 |
| 46:B:1529:G:H5" | 66:V:87:GLY:C | 2.45 | 0.41 |
| 46:B:1602:C:C5 | 52:H:81:ARG:HA | 2.56 | 0.41 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 1:AS:381:U:H2' | 1:AS:382:U:C6 | 2.55 | 0.41 |
| 1:AS:446:U:H2' | 1:AS:447:U:H1' | 2.03 | 0.41 |
| 1:AS:707:A:H1' | 29:BV:57:GLY:HA2 | 2.02 | 0.41 |
| 1:AS:842:A:N6 | 46:CM:956:A:N1 | 2.69 | 0.41 |
| 1:AS:987:G:C5 | 1:AS:1055:G:C6 | 3.08 | 0.41 |
| 1:AS:1028:C:H2' | 1:AS:1029:U:O4' | 2.21 | 0.41 |
| 1:AS:1151:C:H2' | 1:AS:1152:C:C6 | 2.56 | 0.41 |
| 1:AS:1496:G:H2' | 1:AS:1497:U:O4' | 2.20 | 0.41 |
| 1:AS:1882:A:O2' | 5:AX:226:PHE:O | 2.34 | 0.41 |
| 1:AS:2239:G:H21 | 1:AS:2240:A:N6 | 2.19 | 0.41 |
| 1:AS:2455:G:H2' | 1:AS:2456:C:C6 | 2.56 | 0.41 |
| 1:AS:2540:G:H2' | 1:AS:2541:C:H6 | 1.86 | 0.41 |
| 1:AS:2560:U:OP1 | 10:BC:242:LYS:NZ | 2.49 | 0.41 |
| 1:AS:2959:A:H2' | 1:AS:2960:C:H6 | 1.84 | 0.41 |
| 1:AS:2990:C:C4 | 1:AS:2991:U:C4 | 3.09 | 0.41 |
| 1:AS:3146:G:C6 | 1:AS:3178:A:C2 | 3.09 | 0.41 |
| 1:AS:3264:C:H2' | 1:AS:3265:U:H6 | 1.84 | 0.41 |
| 8:BA:39:LEU:CD1 | 8:BA:53:TYR:HB2 | 2.50 | 0.41 |
| 13:BF:109:HIS:ND1 | 13:BF:122:ILE:HD12 | 2.35 | 0.41 |
| 19:BL:133:LYS:HB2 | 19:BL:135:GLN:NE2 | 2.36 | 0.41 |
| 26:BS:142:ILE:HD12 | 26:BS:142:ILE:HA | 1.90 | 0.41 |
| 28:BU:14:VAL:HB | 35:CB:86:LYS:HG3 | 2.02 | 0.41 |
| 38:CE:14:LYS:NZ | 40:CG:51:ILE:HG22 | 2.36 | 0.41 |
| 46:CM:53:G:H2' | 46:CM:54:C:C6 | 2.55 | 0.41 |
| 46:CM:325:U:H2' | 46:CM:326:A:C8 | 2.55 | 0.41 |
| 46:CM:853:G:C2 | 46:CM:946:U:C2 | 3.08 | 0.41 |
| 46:CM:1102:U:H2' | 46:CM:1103:G:C8 | 2.56 | 0.41 |
| 46:CM:1455:A:H4' | 46:CM:1528:G:H4' | 2.02 | 0.41 |
| 46:CM:1575:G:O2' | 52:CS:106:LYS:NZ | 2.54 | 0.41 |
| 47:CN:48:ILE:CG2 | 47:CN:161:PRO:HB2 | 2.50 | 0.41 |
| 51:CR:103:TYR:CD1 | 51:CR:189:LEU:HD21 | 2.55 | 0.41 |
| 52:CS:109:LYS:HG2 | 52:CS:112:ARG:HH21 | 1.85 | 0.41 |
| 59:CZ:41:LEU:HA | 59:CZ:122:VAL:O | 2.21 | 0.41 |
| 63:DD:124:GLU:HG2 | 63:DD:133:ALA:HB1 | 2.02 | 0.41 |
| 73:DN:37:LYS:HE2 | 73:DN:37:LYS:HB2 | 1.84 | 0.41 |
| 79:DT:29:HIS:CD2 | 79:DT:32:LEU:HD23 | 2.56 | 0.41 |
| 79:DT:113:SER:HB3 | 79:DT:154:ALA:HA | 2.03 | 0.41 |
| 80:P0:94:LYS:HA | 80:P0:97:ARG:HD2 | 2.03 | 0.41 |
| 1:1:426:G:H2' | 1:1:427:C:H6 | 1.86 | 0.41 |
| 1:1:698:C:H2' | 1:1:699:G:H8 | 1.86 | 0.41 |
| 1:1:721:U:O2' | 30:AC:29:TYR:OH | 2.36 | 0.41 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 1:1:742:C:H2' | 1:1:743:A:H8 | 1.86 | 0.41 |
| 1:1:943:G:H2' | 1:1:944:C:C6 | 2.55 | 0.41 |
| 1:1:1286:A:H2' | 1:1:1287:A:C8 | 2.56 | 0.41 |
| 1:1:1474:C:H2' | 1:1:1475:U:C6 | 2.56 | 0.41 |
| 1:1:1506:G:H8 | 1:1:1506:G:O5' | 2.04 | 0.41 |
| 1:1:2111:U:O4 | 1:1:2125:A:H2 | 2.04 | 0.41 |
| 1:1:2202:A:P | 37:AJ:73:LYS:HZ3 | 2.44 | 0.41 |
| 1:1:2520:A:H1' | 1:1:2521:C:C5 | 2.55 | 0.41 |
| 1:1:2733:G:O6 | 1:1:2768:G:H8 | 2.04 | 0.41 |
| 3:4:26:U:H2' | 3:4:27:U:C6 | 2.55 | 0.41 |
| 3:4:155:G:C5 | 3:4:156:U:C4 | 3.09 | 0.41 |
| 6:l:303:ALA:CA | 19:y:39:ARG:HH12 | 2.33 | 0.41 |
| 9:o:13:LYS:HE3 | 9:o:17:GLN:HE22 | 1.82 | 0.41 |
| 12:r:200:LEU:HD12 | 12:r:213:PHE:CG | 2.56 | 0.41 |
| 17:w:151:GLU:O | 17:w:155:GLU:HG2 | 2.20 | 0.41 |
| 46:B:182:C:H2' | 46:B:183:C:C6 | 2.56 | 0.41 |
| 46:B:267:G:H2' | 46:B:268:C:C6 | 2.55 | 0.41 |
| 46:B:673:A:C6 | 46:B:674:C:C2 | 3.08 | 0.41 |
| 46:B:697:U:H2' | 46:B:698:C:H6 | 1.86 | 0.41 |
| 46:B:961:G:N2 | 46:B:1008:A:HO2' | 2.18 | 0.41 |
| 46:B:963:A:H2' | 46:B:964:A:O4' | 2.20 | 0.41 |
| 46:B:1130:U:H2' | 46:B:1131:G:O4' | 2.21 | 0.41 |
| 46:B:1226:G:C4 | 62:R:79:HIS:CE1 | 3.09 | 0.41 |
| 46:B:1237:C:H2' | 46:B:1238:U:H6 | 1.86 | 0.41 |
| 46:B:1350:C:O3' | 63:S:29:LYS:HE2 | 2.21 | 0.41 |
| 46:B:1472:G:N2 | 46:B:1509:U:O4 | 2.54 | 0.41 |
| 46:B:1709:A:H2' | 46:B:1710:G:O4' | 2.21 | 0.41 |
| 47:C:53:THR:OG1 | 47:C:161:PRO:HG2 | 2.21 | 0.41 |
| 48:D:36:THR:HG23 | 48:D:231:LEU:O | 2.21 | 0.41 |
| 55:K:124:LYS:HB3 | 55:K:129:HIS:ND1 | 2.36 | 0.41 |
| 57:M:22:VAL:O | 57:M:32:HIS:NE2 | 2.39 | 0.41 |
| 57:M:54:TYR:CE1 | 57:M:75:PHE:HB2 | 2.55 | 0.41 |
| 66:V:73:VAL:O | 66:V:77:ASN:ND2 | 2.54 | 0.41 |
| 78:h:178:LYS:HD2 | 78:h:178:LYS:HA | 1.94 | 0.41 |
| 1:AS:234:A:H2' | 1:AS:235:G:O4' | 2.21 | 0.41 |
| 1:AS:427:C:OP1 | 33:BZ:14:TYR:OH | 2.37 | 0.41 |
| 1:AS:1021:A:C5 | 1:AS:1022:A:H1' | 2.56 | 0.41 |
| 1:AS:1113:G:OP1 | 30:BW:4:SER:HB2 | 2.21 | 0.41 |
| 1:AS:1164:U:H2' | 1:AS:1165:A:H8 | 1.86 | 0.41 |
| 1:AS:1291:G:H2' | 1:AS:1292:C:C6 | 2.55 | 0.41 |
| 1:AS:1706:C:H2' | 1:AS:1707:U:C6 | 2.56 | 0.41 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 1:AS:1852:C:C2 | 1:AS:1853:C:C5 | 3.08 | 0.41 |
| 1:AS:2435:G:C6 | 1:AS:2439:A:N6 | 2.86 | 0.41 |
| 1:AS:2961:U:H2' | 1:AS:2962:G:O4' | 2.21 | 0.41 |
| 1:AS:3079:U:H2' | 1:AS:3080:G:H8 | 1.85 | 0.41 |
| 1:AS:3240:U:N3 | 1:AS:3242:U:O4' | 2.54 | 0.41 |
| 3:AU:78:G:H2' | 3:AU:79:A:N3 | 2.36 | 0.41 |
| 3:AU:81:A:H2' | 3:AU:82:U:C6 | 2.55 | 0.41 |
| 10:BC:35:PHE:CD1 | 10:BC:43:PRO:HD3 | 2.55 | 0.41 |
| 22:BO:16:GLN:HG2 | 22:BO:17:ARG:O | 2.21 | 0.41 |
| 27:BT:5:SER:HB3 | 27:BT:8:VAL:HG23 | 2.03 | 0.41 |
| 32:BY:109:GLU:O | 32:BY:110:ASP:HB2 | 2.21 | 0.41 |
| 38:CE:82:VAL:HG12 | 38:CE:83:ALA:N | 2.36 | 0.41 |
| 42:CI:2:ARG:HD3 | 42:CI:5:TRP:NE1 | 2.35 | 0.41 |
| 42:CI:11:ARG:NH2 | 46:CM:1762:U:OP1 | 2.50 | 0.41 |
| 44:CK:49:ARG:HB2 | 44:CK:55:TRP:CZ3 | 2.55 | 0.41 |
| 46:CM:291:U:H2' | 46:CM:292:C:C6 | 2.56 | 0.41 |
| 46:CM:302:U:H2' | 46:CM:303:C:H6 | 1.86 | 0.41 |
| 46:CM:335:G:O2' | 55:CV:10:LYS:NZ | 2.54 | 0.41 |
| 46:CM:565:A:N3 | 77:DR:14:VAL:HG21 | 2.35 | 0.41 |
| 46:CM:684:C:H2' | 46:CM:685:C:H6 | 1.85 | 0.41 |
| 46:CM:1226:G:H4' | 62:DC:77:LYS:O | 2.20 | 0.41 |
| 46:CM:1414:G:OP2 | 46:CM:1414:G:H3' | 2.21 | 0.41 |
| 46:CM:1424:G:H2' | 46:CM:1425:C:C6 | 2.56 | 0.41 |
| 48:CO:29:TRP:HA | 48:CO:46:THR:O | 2.21 | 0.41 |
| 51:CR:176:ASP:OD1 | 51:CR:177:THR:N | 2.50 | 0.41 |
| 52:CS:80:LYS:HA | 52:CS:80:LYS:HD2 | 1.90 | 0.41 |
| 54:CU:76:GLU:HG3 | 54:CU:79:LYS:NZ | 2.36 | 0.41 |
| 61:DB:73:ALA:HB2 | 61:DB:106:ARG:HB2 | 2.02 | 0.41 |
| 62:DC:83:MET:HB3 | 62:DC:116:LEU:HD13 | 2.02 | 0.41 |
| 64:DE:103:ASP:OD2 | 64:DE:105:ASP:HB2 | 2.21 | 0.41 |
| 66:DG:135:ILE:O | 66:DG:139:THR:OG1 | 2.35 | 0.41 |
| 79:DT:25:THR:HG21 | 79:DT:291:TRP:O | 2.21 | 0.41 |
| 82:L1:100:ILE:HB | 82:L1:124:LEU:HD23 | 2.03 | 0.41 |
| 82:l1:48:ARG:HA | 82:l1:159:LEU:HD23 | 2.02 | 0.41 |
| 80:p0:45:LEU:HD21 | 80:p0:100:VAL:HA | 2.03 | 0.41 |
| 1:1:96:U:H2' | 1:1:97:G:C8 | 2.56 | 0.41 |
| 1:1:593:G:C8 | 1:1:607:G:C6 | 3.08 | 0.41 |
| 1:1:953:C:H4' | 1:1:2771:A:C5 | 2.56 | 0.41 |
| 1:1:1004:U:H4' | 12:r:34:TYR:HD1 | 1.85 | 0.41 |
| 1:1:1046:U:OP2 | 22:2:13:TYR:OH | 2.24 | 0.41 |
| 1:1:1093:G:N3 | 1:1:1093:G:H2' | 2.36 | 0.41 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 1:1:1454:U:H2' | 1:1:1455:C:C6 | 2.55 | 0.41 |
| 1:1:2070:A:H5" | 1:1:2072:C:H1' | 2.02 | 0.41 |
| 1:1:2195:U:H2' | 1:1:2196:G:H8 | 1.86 | 0.41 |
| 1:1:2199:G:H2' | 1:1:2201:A:OP2 | 2.21 | 0.41 |
| 1:1:2220:A:H5" | 4:j:244:GLY:HA3 | 2.03 | 0.41 |
| 1:1:2242:U:H2' | 1:1:2243:C:C6 | 2.56 | 0.41 |
| 1:1:2325:U:H2' | 1:1:2326:A:O4' | 2.21 | 0.41 |
| 1:1:2413:G:H4' | 16:v:24:ARG:HH12 | 1.86 | 0.41 |
| 1:1:3043:U:C4 | 1:1:3044:C:C4 | 3.09 | 0.41 |
| 1:1:3111:A:H2' | 1:1:3112:G:O4' | 2.21 | 0.41 |
| 1:1:3138:U:C2 | 1:1:3139:U:C5 | 3.09 | 0.41 |
| 2:3:94:C:H2' | 2:3:95:A:C8 | 2.56 | 0.41 |
| 3:4:12:A:C6 | 3:4:13:A:N7 | 2.89 | 0.41 |
| 5:k:67:MET:SD | 5:k:70:ARG:HD2 | 2.61 | 0.41 |
| 5:k:214:MET:CE | 5:k:350:ALA:HA | 2.51 | 0.41 |
| 6:l:61:THR:HG21 | 6:l:78:VAL:HG22 | 2.02 | 0.41 |
| 10:p:83:LEU:HD23 | 10:p:83:LEU:HA | 1.83 | 0.41 |
| 15:u:57:LEU:HG | 21:0:172:TYR:CZ | 2.56 | 0.41 |
| 16:v:68:ARG:CG | 16:v:128:LYS:HG3 | 2.51 | 0.41 |
| 17:w:189:SER:O | 17:w:193:GLN:HG2 | 2.21 | 0.41 |
| 19:y:40:THR:C | 19:y:42:ALA:H | 2.28 | 0.41 |
| 21:0:73:LYS:HD2 | 21:0:75:PHE:CZ | 2.56 | 0.41 |
| 36:AI:1:MET:N | 36:AI:1:MET:SD | 2.77 | 0.41 |
| 41:AN:3:GLU:HG3 | 41:AN:6:LEU:H | 1.86 | 0.41 |
| 45:i:115:LEU:HD12 | 49:E:116:VAL:HG11 | 2.01 | 0.41 |
| 46:B:141:G:H2' | 46:B:142:G:C8 | 2.56 | 0.41 |
| 46:B:530:U:OP1 | 71:a:64:PHE:HA | 2.21 | 0.41 |
| 46:B:695:C:H1' | 46:B:696:U:P | 2.61 | 0.41 |
| 46:B:767:G:HO2' | 46:B:768:C:H6 | 1.69 | 0.41 |
| 46:B:1032:G:H2' | 46:B:1033:U:H6 | 1.86 | 0.41 |
| 46:B:1393:U:H2' | 46:B:1394:G:C8 | 2.56 | 0.41 |
| 46:B:1546:G:H5" | 65:U:135:GLY:HA3 | 2.02 | 0.41 |
| 51:G:103:TYR:CD1 | 51:G:189:LEU:HD21 | 2.56 | 0.41 |
| 51:G:150:PRO:O | 53:I:208:TYR:HE1 | 2.03 | 0.41 |
| 56:L:29:LYS:HA | 77:g:40:TYR:CE1 | 2.56 | 0.41 |
| 59:O:57:ALA:HB1 | 59:O:125:ASN:HB2 | 2.03 | 0.41 |
| 60:P:16:LEU:HG | 60:P:17:PRO:HD2 | 2.03 | 0.41 |
| 62:R:14:GLN:OE1 | 62:R:23:LYS:N | 2.41 | 0.41 |
| 62:R:78:THR:OG1 | 62:R:80:LEU:HG | 2.21 | 0.41 |
| 65:U:132:LYS:HD3 | 65:U:136:GLN:HB2 | 2.03 | 0.41 |
| 65:U:140:THR:HG23 | 65:U:141:THR:HG23 | 2.03 | 0.41 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 74:d:36:LYS:O | 74:d:77:CYS:HA | 2.20 | 0.41 |
| 75:e:16:LEU:HD23 | 75:e:16:LEU:HA | 1.88 | 0.41 |
| 79:AR:121:ARG:HA | 79:AR:137:THR:OG1 | 2.21 | 0.41 |
| 1:AS:447:U:O2 | 1:AS:483:U:N3 | 2.54 | 0.41 |
| 1:AS:495:C:H2' | 1:AS:496:A:H8 | 1.86 | 0.41 |
| 1:AS:1065:C:H2' | 1:AS:1066:U:C6 | 2.55 | 0.41 |
| 1:AS:1261:U:H2' | 1:AS:1262:G:O4' | 2.21 | 0.41 |
| 1:AS:1336:G:H2' | 1:AS:1337:U:H6 | 1.86 | 0.41 |
| 1:AS:1347:U:O2 | 1:AS:1347:U:H2' | 2.20 | 0.41 |
| 1:AS:1467:U:H2' | 1:AS:1468:U:C6 | 2.56 | 0.41 |
| 1:AS:1612:U:H2' | 1:AS:1613:G:C8 | 2.55 | 0.41 |
| 1:AS:1622:U:H2' | 1:AS:1623:U:C6 | 2.55 | 0.41 |
| 1:AS:1807:G:H2' | 1:AS:1808:G:O4' | 2.20 | 0.41 |
| 1:AS:2658:A:H2' | 1:AS:2659:G:O4' | 2.21 | 0.41 |
| 1:AS:2857:C:O2' | 1:AS:2858:U:H5' | 2.21 | 0.41 |
| 1:AS:2995:U:H2' | 1:AS:2996:A:C8 | 2.56 | 0.41 |
| 1:AS:3132:U:H2' | 1:AS:3133:G:C8 | 2.56 | 0.41 |
| 1:AS:3277:U:C4 | 1:AS:3278:U:C5 | 3.09 | 0.41 |
| 2:AT:59:U:H2' | 2:AT:60:G:C8 | 2.56 | 0.41 |
| 2:AT:113:C:H2' | 2:AT:114:U:O4' | 2.20 | 0.41 |
| 2:AT:118:A:H5" | 7:AZ:253:PHE:CZ | 2.55 | 0.41 |
| 7:AZ:134:ALA:HA | 7:AZ:141:PRO:HD3 | 2.03 | 0.41 |
| 10:BC:95:LEU:HD23 | 10:BC:95:LEU:HA | 1.93 | 0.41 |
| 10:BC:162:GLU:OE2 | 16:BI:22:LEU:HD13 | 2.21 | 0.41 |
| 12:BE:47:PRO:HB3 | 12:BE:171:TRP:CZ2 | 2.55 | 0.41 |
| 19:BL:165:ILE:HD11 | 19:BL:172:PHE:HB3 | 2.03 | 0.41 |
| 20:BM:45:TYR:HA | 20:BM:50:ILE:O | 2.21 | 0.41 |
| 25:BR:83:VAL:HG11 | 46:CM:68:A:N1 | 2.35 | 0.41 |
| 33:BZ:83:LEU:HD11 | 33:BZ:109:ILE:HG23 | 2.03 | 0.41 |
| 35:CB:57:LEU:HB2 | 35:CB:62:TYR:HE1 | 1.85 | 0.41 |
| 46:CM:67:A:O2' | 46:CM:69:G:OP1 | 2.39 | 0.41 |
| 46:CM:69:G:H2' | 46:CM:70:C:C6 | 2.56 | 0.41 |
| 46:CM:327:G:H2' | 46:CM:328:G:H8 | 1.86 | 0.41 |
| 46:CM:397:A:P | 55:CV:49:ARG:HH12 | 2.44 | 0.41 |
| 46:CM:497:U:H2' | 46:CM:498:C:C6 | 2.55 | 0.41 |
| 46:CM:578:A:H5" | 50:CQ:144:ARG:NH2 | 2.30 | 0.41 |
| 46:CM:668:U:H3' | 46:CM:669:G:C8 | 2.53 | 0.41 |
| 46:CM:918:A:OP1 | 73:DN:70:LYS:NZ | 2.53 | 0.41 |
| 46:CM:964:A:C4 | 46:CM:965:G:C8 | 3.09 | 0.41 |
| 46:CM:985:C:H6 | 46:CM:988:A:C8 | 2.39 | 0.41 |
| 46:CM:1035:G:C6 | 46:CM:1054:A:C6 | 3.09 | 0.41 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 46:CM:1215:A:H2 | 46:CM:1243:U:O2 | 2.04 | 0.41 |
| 46:CM:1222:G:H2' | 46:CM:1223:A:H8 | 1.85 | 0.41 |
| 46:CM:1378:U:H2' | 46:CM:1379:C:H6 | 1.85 | 0.41 |
| 46:CM:1496:C:H2' | 46:CM:1497:U:C6 | 2.56 | 0.41 |
| 46:CM:1706:A:H2' | 46:CM:1707:G:O4' | 2.21 | 0.41 |
| 48:CO:26:ARG:O | 48:CO:50:ARG:HG2 | 2.21 | 0.41 |
| 50:CQ:107:LYS:HB2 | 50:CQ:176:VAL:CG2 | 2.50 | 0.41 |
| 50:CQ:110:LEU:HA | 50:CQ:110:LEU:HD23 | 1.80 | 0.41 |
| 51:CR:192:VAL:HG23 | 51:CR:244:GLY:HA3 | 2.02 | 0.41 |
| 53:CT:225:GLU:O | 53:CT:228:LYS:HB3 | 2.21 | 0.41 |
| 66:DG:30:VAL:HG13 | 66:DG:34:VAL:HG11 | 2.02 | 0.41 |
| 73:DN:87:ARG:HH21 | 73:DN:92:ARG:C | 2.29 | 0.41 |
| 75:DP:30:VAL:HG22 | 75:DP:40:ILE:O | 2.21 | 0.41 |
| 82:L1:21:THR:HG23 | 82:L1:22:GLU:OE1 | 2.21 | 0.41 |
| 82:l1:17:LEU:O | 82:l1:17:LEU:HG | 2.21 | 0.41 |
| 80:p0:61:ARG:HG2 | 80:p0:64:ARG:HG3 | 2.03 | 0.41 |
| 1:1:342:A:C4 | 1:1:368:G:N7 | 2.89 | 0.41 |
| 1:1:647:A:H2' | 1:1:648:C:C6 | 2.56 | 0.41 |
| 1:1:780:A:O2' | 1:1:781:G:OP2 | 2.36 | 0.41 |
| 1:1:1194:C:OP2 | 1:1:1195:C:O2' | 2.26 | 0.41 |
| 1:1:1312:C:OP2 | 17:w:134:ARG:HG3 | 2.21 | 0.41 |
| 1:1:1666:C:H4' | 1:1:1855:A:O3' | 2.20 | 0.41 |
| 1:1:2182:C:H2' | 1:1:2183:U:C6 | 2.56 | 0.41 |
| 1:1:2737:C:H1' | 84:1:3402:3K5:C19 | 2.51 | 0.41 |
| 1:1:2771:A:H5" | 1:1:2772:G:O5' | 2.21 | 0.41 |
| 1:1:3023:U:H2' | 1:1:3024:G:H8 | 1.86 | 0.41 |
| 1:1:3166:A:C5 | 1:1:3167:G:N7 | 2.89 | 0.41 |
| 1:1:3196:U:H2' | 1:1:3197:G:C8 | 2.53 | 0.41 |
| 2:3:103:A:H2' | 2:3:104:A:O4' | 2.21 | 0.41 |
| 3:4:72:A:P | 27:9:52:GLN:HB2 | 2.61 | 0.41 |
| 12:r:12:CYS:SG | 12:r:59:GLN:HG3 | 2.61 | 0.41 |
| 14:t:99:HIS:CE1 | 14:t:100:ARG:HG3 | 2.56 | 0.41 |
| 21:0:79:LEU:HD13 | 21:0:110:LEU:HD21 | 2.03 | 0.41 |
| 45:i:157:GLU:H | 45:i:157:GLU:CD | 2.27 | 0.41 |
| 46:B:184:C:H2' | 46:B:185:G:O4' | 2.21 | 0.41 |
| 46:B:193:G:N7 | 55:K:147:ARG:NH2 | 2.69 | 0.41 |
| 46:B:519:A:H2' | 46:B:520:U:C6 | 2.56 | 0.41 |
| 46:B:1203:G:H4' | 46:B:1250:G:N2 | 2.35 | 0.41 |
| 46:B:1262:G:O3' | 50:F:184:GLY:HA3 | 2.21 | 0.41 |
| 46:B:1354:U:C2 | 46:B:1355:A:C8 | 3.09 | 0.41 |
| 46:B:1457:A:H5' | 52:H:185:ARG:HG2 | 2.03 | 0.41 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 46:B:1539:U:H2' | 46:B:1540:G:C8 | 2.56 | 0.41 |
| 53:I:69:HIS:HD2 | 53:I:73:VAL:HG11 | 1.86 | 0.41 |
| 58:N:91:LEU:HB3 | 58:N:100:TYR:HB3 | 2.02 | 0.41 |
| 59:O:68:GLU:O | 59:O:69:GLU:HG3 | 2.21 | 0.41 |
| 62:R:90:ILE:HD11 | 62:R:112:VAL:HG21 | 2.03 | 0.41 |
| 64:T:93:LEU:O | 64:T:93:LEU:HD12 | 2.21 | 0.41 |
| 65:U:88:ARG:HH21 | 65:U:92:GLN:HG2 | 1.85 | 0.41 |
| 66:V:84:LYS:HZ2 | 66:V:86:ARG:HG3 | 1.85 | 0.41 |
| 75:e:10:ALA:HB1 | 75:e:30:VAL:HB | 2.02 | 0.41 |
| 79:AR:84:ALA:HA | 79:AR:90:LEU:HD23 | 2.03 | 0.41 |
| 1:AS:97:G:N7 | 14:BG:13:HIS:NE2 | 2.66 | 0.41 |
| 1:AS:615:G:H2' | 1:AS:616:C:C6 | 2.56 | 0.41 |
| 1:AS:935:U:OP2 | 29:BV:26:ARG:NH2 | 2.54 | 0.41 |
| 1:AS:962:U:H2' | 1:AS:963:A:C8 | 2.56 | 0.41 |
| 1:AS:1172:C:H2' | 1:AS:1173:G:N2 | 2.36 | 0.41 |
| 1:AS:1303:G:H4' | 1:AS:1304:A:O5' | 2.21 | 0.41 |
| 1:AS:1521:G:N3 | 1:AS:1521:G:H2' | 2.35 | 0.41 |
| 1:AS:2514:G:C4 | 1:AS:2515:G:N2 | 2.88 | 0.41 |
| 1:AS:2753:U:H2' | 1:AS:2754:U:C6 | 2.55 | 0.41 |
| 1:AS:2972:A:H2' | 1:AS:2973:U:H6 | 1.85 | 0.41 |
| 3:AU:75:G:H2' | 3:AU:76:C:H6 | 1.84 | 0.41 |
| 3:AU:126:A:O2' | 3:AU:128:U:OP2 | 2.30 | 0.41 |
| 9:BB:86:ARG:O | 9:BB:110:ASN:N | 2.45 | 0.41 |
| 22:BO:113:ALA:O | 22:BO:117:ARG:HG3 | 2.21 | 0.41 |
| 33:BZ:43:VAL:HG22 | 33:BZ:50:THR:HB | 2.02 | 0.41 |
| 35:CB:99:LYS:O | 35:CB:103:ARG:HG3 | 2.21 | 0.41 |
| 46:CM:436:A:O2' | 46:CM:463:G:N2 | 2.53 | 0.41 |
| 46:CM:897:U:OP1 | 46:CM:898:G:O2' | 2.33 | 0.41 |
| 46:CM:1220:C:H6 | 46:CM:1220:C:H2' | 1.69 | 0.41 |
| 46:CM:1394:G:H2' | 46:CM:1395:G:O4' | 2.20 | 0.41 |
| 46:CM:1537:A:H2' | 46:CM:1538:U:H6 | 1.85 | 0.41 |
| 46:CM:1742:A:OP1 | 70:DK:63:GLN:HG2 | 2.21 | 0.41 |
| 51:CR:162:ILE:HG22 | 51:CR:164:LEU:H | 1.85 | 0.41 |
| 51:CR:249:ILE:HD12 | 56:CW:71:PHE:CD2 | 2.55 | 0.41 |
| 53:CT:48:TYR:OH | 53:CT:121:ILE:HG12 | 2.21 | 0.41 |
| 59:CZ:69:GLU:HA | 59:CZ:72:ILE:HD12 | 2.03 | 0.41 |
| 79:DT:180:LEU:HD23 | 79:DT:180:LEU:HA | 1.92 | 0.41 |
| 82:l1:144:LEU:HB3 | 82:l1:145:TYR:H | 1.68 | 0.41 |
| 1:1:989:G:N3 | 1:1:2609:A:H2' | 2.35 | 0.40 |
| 1:1:1331:U:H2' | 1:1:1332:C:C6 | 2.56 | 0.40 |
| 1:1:1466:U:H2' | 1:1:1467:U:H6 | 1.86 | 0.40 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 1:1:1644:A:H2' | 1:1:1645:U:O4' | 2.21 | 0.40 |
| 1:1:1725:A:C6 | 44:AQ:42:CYS:HA | 2.55 | 0.40 |
| 1:1:1740:G:H2' | 1:1:1741:C:C6 | 2.56 | 0.40 |
| 1:1:2077:A:O2' | 1:1:2078:A:H5' | 2.21 | 0.40 |
| 1:1:2232:U:H2' | 1:1:2239:G:H22 | 1.86 | 0.40 |
| 1:1:2641:G:H2' | 1:1:2642:G:H8 | 1.86 | 0.40 |
| 1:1:2807:U:O2' | 1:1:2808:C:P | 2.79 | 0.40 |
| 1:1:2871:C:C5 | 11:q:171:ASP:HA | 2.56 | 0.40 |
| 1:1:2919:G:C2 | 5:k:250:ALA:HB1 | 2.55 | 0.40 |
| 1:1:3228:G:H2' | 1:1:3229:G:C8 | 2.56 | 0.40 |
| 3:4:78:G:H2' | 3:4:79:A:N3 | 2.36 | 0.40 |
| 5:k:283:TYR:CE1 | 5:k:354:VAL:HG21 | 2.57 | 0.40 |
| 7:m:78:ALA:HB3 | 7:m:105:VAL:HB | 2.03 | 0.40 |
| 7:m:187:ALA:O | 7:m:189:GLU:N | 2.48 | 0.40 |
| 16:v:7:LEU:HB3 | 16:v:46:ASP:CG | 2.45 | 0.40 |
| 17:w:17:LEU:HD11 | 17:w:81:LEU:HA | 2.02 | 0.40 |
| 46:B:444:A:C6 | 46:B:445:U:C4 | 3.09 | 0.40 |
| 46:B:562:G:O2' | 46:B:575:G:H4' | 2.21 | 0.40 |
| 46:B:1005:A:C6 | 46:B:1006:C:C5 | 3.09 | 0.40 |
| 46:B:1131:G:H1' | 49:E:84:GLN:HG2 | 2.03 | 0.40 |
| 46:B:1257:U:O2' | 46:B:1260:A:OP2 | 2.28 | 0.40 |
| 46:B:1283:U:H2' | 46:B:1284:G:O4' | 2.21 | 0.40 |
| 46:B:1357:A:C8 | 46:B:1359:U:C5 | 3.09 | 0.40 |
| 46:B:1675:U:O2' | 46:B:1700:G:O6 | 2.39 | 0.40 |
| 49:E:111:LYS:HG2 | 49:E:122:ALA:HB3 | 2.03 | 0.40 |
| 51:G:183:VAL:HG21 | 51:G:218:PHE:HE2 | 1.86 | 0.40 |
| 54:J:67:ARG:HD2 | 54:J:127:PHE:CD1 | 2.56 | 0.40 |
| 64:T:99:GLN:HB2 | 64:T:118:PRO:O | 2.22 | 0.40 |
| 66:V:86:ARG:NH2 | 66:V:92:LYS:HD2 | 2.37 | 0.40 |
| 67:W:21:ILE:HD13 | 67:W:99:VAL:HG21 | 2.03 | 0.40 |
| 68:X:37:ALA:HA | 68:X:50:ASN:OD1 | 2.21 | 0.40 |
| 79:AR:224:LYS:HE3 | 79:AR:226:LYS:HE3 | 2.03 | 0.40 |
| 1:AS:380:U:H2' | 1:AS:381:U:H6 | 1.86 | 0.40 |
| 1:AS:830:U:H2' | 1:AS:831:G:O4' | 2.21 | 0.40 |
| 1:AS:1216:U:H1' | 80:p0:61:ARG:CZ | 2.51 | 0.40 |
| 1:AS:1282:A:H2' | 1:AS:1282:A:N3 | 2.36 | 0.40 |
| 1:AS:1720:U:H1' | 1:AS:1721:C:C6 | 2.56 | 0.40 |
| 1:AS:2296:U:H2' | 1:AS:2297:U:O4' | 2.20 | 0.40 |
| 1:AS:2564:G:H4' | 1:AS:2566:C:C2 | 2.56 | 0.40 |
| 1:AS:2713:C:HO2' | 43:CJ:20:HIS:CE1 | 2.30 | 0.40 |
| 2:AT:47:C:H2' | 2:AT:48:C:C6 | 2.57 | 0.40 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 5:AX:57:VAL:HG22 | 5:AX:73:VAL:HG22 | 2.01 | 0.40 |
| 12:BE:96:VAL:HG22 | 12:BE:125:LEU:HD21 | 2.03 | 0.40 |
| 35:CB:104:VAL:O | 35:CB:108:GLN:HG2 | 2.21 | 0.40 |
| 46:CM:298:A:H2' | 46:CM:299:A:C8 | 2.56 | 0.40 |
| 46:CM:368:A:H2' | 46:CM:369:G:H8 | 1.85 | 0.40 |
| 46:CM:498:C:C2 | 46:CM:499:U:C5 | 3.09 | 0.40 |
| 46:CM:1628:C:H2' | 46:CM:1629:G:C8 | 2.56 | 0.40 |
| 46:CM:1784:A:N6 | 73:DN:84:VAL:HB | 2.36 | 0.40 |
| 47:CN:55:GLU:HB3 | 68:DI:79:LEU:HD22 | 2.03 | 0.40 |
| 51:CR:51:ARG:HD3 | 51:CR:51:ARG:HA | 1.78 | 0.40 |
| 54:CU:85:HIS:ND1 | 54:CU:161:LYS:HG2 | 2.36 | 0.40 |
| 54:CU:150:LEU:HB2 | 54:CU:181:ILE:HG12 | 2.02 | 0.40 |
| 59:CZ:62:LEU:HD22 | 59:CZ:75:VAL:HG21 | 2.04 | 0.40 |
| 74:DO:57:ASP:OD1 | 74:DO:58:SER:N | 2.53 | 0.40 |
| 79:DT:156:ARG:HD3 | 79:DT:156:ARG:HA | 1.82 | 0.40 |
| 82:l1:26:ARG:HG2 | 82:l1:27:ASN:N | 2.36 | 0.40 |
| 82:l1:74:VAL:O | 82:l1:77:ALA:N | 2.44 | 0.40 |
| 82:l1:179:LEU:HB3 | 82:l1:180:VAL:H | 1.53 | 0.40 |
| 1:1:276:U:O2 | 16:v:93:LYS:HE2 | 2.22 | 0.40 |
| 1:1:278:U:H2' | 1:1:279:U:C6 | 2.56 | 0.40 |
| 1:1:907:C:OP2 | 4:j:9:ARG:HD2 | 2.22 | 0.40 |
| 1:1:1011:C:O2' | 1:1:1012:U:OP2 | 2.36 | 0.40 |
| 1:1:1791:U:H2' | 4:j:50:HIS:CD2 | 2.56 | 0.40 |
| 1:1:2663:A:HO2' | 1:1:2664:A:P | 2.44 | 0.40 |
| 1:1:3190:C:H2' | 1:1:3191:A:H8 | 1.86 | 0.40 |
| 3:4:97:A:OP1 | 36:AI:63:ARG:NH2 | 2.52 | 0.40 |
| 3:4:152:G:H2' | 3:4:153:U:O4' | 2.21 | 0.40 |
| 6:l:144:GLU:OE1 | 6:l:177:LYS:NZ | 2.47 | 0.40 |
| 6:l:260:ASP:OD1 | 6:l:265:SER:HB3 | 2.21 | 0.40 |
| 8:n:166:LYS:NZ | 34:AG:4:SER:HB3 | 2.37 | 0.40 |
| 11:q:10:LEU:HD21 | 11:q:79:ILE:HD11 | 2.01 | 0.40 |
| 14:t:2:ALA:HB2 | 29:AB:31:GLY:O | 2.21 | 0.40 |
| 21:0:28:ARG:NH2 | 21:0:64:ILE:HG21 | 2.37 | 0.40 |
| 25:7:124:LYS:HB3 | 25:7:124:LYS:HE2 | 1.82 | 0.40 |
| 26:8:34:LEU:HD12 | 26:8:35:PRO:HD2 | 2.02 | 0.40 |
| 27:9:31:LEU:HB3 | 27:9:101:PRO:HG2 | 2.03 | 0.40 |
| 27:9:82:VAL:HG12 | 27:9:83:ASP:H | 1.85 | 0.40 |
| 28:AA:42:ILE:HD11 | 28:AA:74:LEU:HD12 | 2.04 | 0.40 |
| 45:i:80:ALA:HB1 | 46:B:1164:G:O4' | 2.22 | 0.40 |
| 46:B:623:C:H2' | 46:B:624:U:C6 | 2.56 | 0.40 |
| 46:B:627:U:H2' | 46:B:628:A:H8 | 1.86 | 0.40 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 46:B:670:C:H6 | 46:B:670:C:H2' | 1.66 | 0.40 |
| 46:B:704:A:C8 | 46:B:705:G:C2 | 3.09 | 0.40 |
| 46:B:903:U:H2' | 46:B:904:A:H8 | 1.79 | 0.40 |
| 46:B:972:G:N2 | 46:B:998:A:OP1 | 2.52 | 0.40 |
| 46:B:989:U:H3' | 46:B:990:A:C5' | 2.51 | 0.40 |
| 46:B:1216:U:HO2' | 46:B:1243:U:HO2' | 1.67 | 0.40 |
| 46:B:1377:A:H2' | 46:B:1378:U:C6 | 2.56 | 0.40 |
| 46:B:1602:C:C4 | 52:H:81:ARG:HA | 2.56 | 0.40 |
| 52:H:157:ARG:HB3 | 52:H:224:ASN:OD1 | 2.20 | 0.40 |
| 53:I:58:LYS:HG2 | 53:I:105:ASP:O | 2.20 | 0.40 |
| 56:L:140:ILE:HD12 | 71:a:65:GLY:HA3 | 2.04 | 0.40 |
| 61:Q:52:PRO:HB3 | 61:Q:95:SER:OG | 2.21 | 0.40 |
| 62:R:72:ARG:HH21 | 62:R:93:VAL:CG1 | 2.31 | 0.40 |
| 70:Z:130:VAL:HG21 | 70:Z:143:PRO:HD3 | 2.02 | 0.40 |
| 72:b:54:VAL:HG13 | 72:b:60:VAL:HG11 | 2.03 | 0.40 |
| 75:e:34:GLU:OE1 | 75:e:34:GLU:N | 2.42 | 0.40 |
| 1:AS:215:G:H4' | 27:BT:19:TYR:CE2 | 2.56 | 0.40 |
| 1:AS:703:A:C6 | 29:BV:113:LEU:HD13 | 2.56 | 0.40 |
| 1:AS:1163:U:H2' | 1:AS:1164:U:O4' | 2.20 | 0.40 |
| 1:AS:1336:G:H2' | 1:AS:1337:U:C6 | 2.56 | 0.40 |
| 1:AS:1586:G:C2 | 1:AS:1587:G:C8 | 3.09 | 0.40 |
| 1:AS:1814:U:O2' | 1:AS:1815:U:O5' | 2.39 | 0.40 |
| 1:AS:2163:G:C6 | 1:AS:2164:U:C4 | 3.10 | 0.40 |
| 1:AS:2514:G:N7 | 1:AS:2515:G:N1 | 2.69 | 0.40 |
| 1:AS:2656:C:H2' | 1:AS:2657:C:H6 | 1.85 | 0.40 |
| 1:AS:2749:G:H5" | 1:AS:2750:G:OP1 | 2.21 | 0.40 |
| 1:AS:3139:U:N3 | 1:AS:3247:A:C2 | 2.90 | 0.40 |
| 4:AW:101:ILE:HG13 | 4:AW:165:VAL:HG22 | 2.03 | 0.40 |
| 19:BL:173:GLU:HA | 29:BV:51:GLY:C | 2.47 | 0.40 |
| 23:BP:102:LYS:HE3 | 23:BP:102:LYS:HB2 | 1.88 | 0.40 |
| 37:CD:69:LYS:HE3 | 37:CD:69:LYS:HB2 | 1.78 | 0.40 |
| 46:CM:524:A:H2' | 46:CM:525:A:O4' | 2.21 | 0.40 |
| 46:CM:1232:U:H2' | 46:CM:1233:C:C6 | 2.56 | 0.40 |
| 46:CM:1416:U:H1' | 67:DH:71:ASN:HB3 | 2.02 | 0.40 |
| 46:CM:1438:U:H2' | 46:CM:1439:G:C8 | 2.57 | 0.40 |
| 46:CM:1454:U:O2' | 66:DG:87:GLY:O | 2.37 | 0.40 |
| 46:CM:1649:G:H2' | 46:CM:1650:G:C8 | 2.56 | 0.40 |
| 57:CX:25:LYS:HD2 | 57:CX:59:PHE:HZ | 1.85 | 0.40 |
| 59:CZ:139:HIS:O | 59:CZ:139:HIS:CG | 2.74 | 0.40 |
| 61:DB:47:ARG:HG3 | 61:DB:48:ASP:OD1 | 2.21 | 0.40 |
| 82:L1:44:GLN:C | 82:L1:45:ARG:HG2 | 2.47 | 0.40 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 1:1:29:G:C6 | 1:1:54:G:C6 | 3.09 | 0.40 |
| 1:1:163:A:H2' | 1:1:164:U:O4' | 2.22 | 0.40 |
| 1:1:293:C:H2' | 1:1:294:U:O4' | 2.20 | 0.40 |
| 1:1:656:G:N2 | 6:l:94:MET:HB2 | 2.36 | 0.40 |
| 1:1:929:A:C2 | 6:l:99:ARG:NH2 | 2.89 | 0.40 |
| 1:1:1007:A:H2' | 1:1:1008:A:H8 | 1.85 | 0.40 |
| 1:1:1012:U:C3' | 1:1:1013:U:H4' | 2.52 | 0.40 |
| 1:1:1099:A:N3 | 1:1:1099:A:H2' | 2.37 | 0.40 |
| 1:1:1140:U:OP2 | 33:AF:44:ARG:NH1 | 2.51 | 0.40 |
| 1:1:1332:C:H2' | 1:1:1333:A:H8 | 1.87 | 0.40 |
| 1:1:1660:G:H2' | 1:1:1661:U:H6 | 1.87 | 0.40 |
| 1:1:1907:A:H2 | 1:1:2100:G:C8 | 2.39 | 0.40 |
| 1:1:2308:C:H2' | 1:1:2309:C:H6 | 1.86 | 0.40 |
| 1:1:2502:A:H1' | 1:1:2503:G:C8 | 2.57 | 0.40 |
| 1:1:2557:G:C5 | 26:8:24:LEU:HD21 | 2.56 | 0.40 |
| 1:1:3056:C:H2' | 1:1:3057:G:O4' | 2.21 | 0.40 |
| 1:1:3077:U:C2 | 1:1:3078:A:C8 | 3.09 | 0.40 |
| 1:1:3148:A:C2 | 17:w:116:LYS:HD2 | 2.57 | 0.40 |
| 1:1:3207:G:H5' | 1:1:3210:A:N3 | 2.37 | 0.40 |
| 1:1:3344:U:H2' | 1:1:3345:C:C6 | 2.56 | 0.40 |
| 3:4:68:A:H2' | 3:4:69:U:C6 | 2.57 | 0.40 |
| 5:k:293:ASN:HB2 | 5:k:304:THR:HA | 2.03 | 0.40 |
| 6:l:30:PRO:HB3 | 19:y:25:TYR:HE2 | 1.86 | 0.40 |
| 11:q:77:ASN:HA | 11:q:80:THR:HG22 | 2.03 | 0.40 |
| 13:s:112:LEU:HD23 | 13:s:112:LEU:HA | 1.97 | 0.40 |
| 18:x:19:GLY:HA3 | 18:x:22:LEU:HD11 | 2.03 | 0.40 |
| 18:x:51:VAL:HA | 18:x:56:ARG:O | 2.21 | 0.40 |
| 19:y:55:SER:O | 19:y:59:ARG:HG2 | 2.21 | 0.40 |
| 27:9:69:LYS:HE3 | 27:9:69:LYS:HB3 | 1.93 | 0.40 |
| 41:AN:19:ILE:HA | 41:AN:25:ALA:O | 2.22 | 0.40 |
| 46:B:45:U:O2 | 46:B:432:G:H1' | 2.21 | 0.40 |
| 46:B:290:U:H2' | 46:B:291:U:C6 | 2.55 | 0.40 |
| 46:B:303:C:H2' | 46:B:304:U:C6 | 2.56 | 0.40 |
| 46:B:635:C:OP1 | 69:Y:32:LYS:HG3 | 2.20 | 0.40 |
| 46:B:1167:U:H2' | 46:B:1168:A:O3' | 2.20 | 0.40 |
| 46:B:1219:A:H5' | 46:B:1220:C:OP1 | 2.20 | 0.40 |
| 46:B:1239:U:H2' | 46:B:1240:G:C8 | 2.56 | 0.40 |
| 46:B:1414:G:H3' | 46:B:1414:G:OP2 | 2.21 | 0.40 |
| 46:B:1437:C:C2 | 46:B:1438:U:C5 | 3.09 | 0.40 |
| 46:B:1699:G:H2' | 46:B:1700:G:H5" | 2.04 | 0.40 |
| 52:H:124:LEU:HD23 | 72:b:58:LYS:HG2 | 2.03 | 0.40 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 55:K:62:THR:HA | 55:K:77:ARG:HA | 2.04 | 0.40 |
| 56:L:65:LYS:HA | 56:L:70:LEU:HD11 | 2.03 | 0.40 |
| 79:AR:80:TYR:HD2 | 79:AR:92:LEU:HD21 | 1.85 | 0.40 |
| 1:AS:661:C:H2' | 1:AS:662:U:C6 | 2.56 | 0.40 |
| 1:AS:672:G:OP1 | 6:AY:32:ARG:NH1 | 2.44 | 0.40 |
| 1:AS:1025:G:N2 | 1:AS:1026:A:H1' | 2.35 | 0.40 |
| 1:AS:1129:A:H1' | 1:AS:2590:G:O6 | 2.20 | 0.40 |
| 1:AS:1233:G:C4 | 1:AS:1234:C:C5 | 3.10 | 0.40 |
| 1:AS:1612:U:H2' | 1:AS:1613:G:H8 | 1.84 | 0.40 |
| 1:AS:1937:C:OP2 | 20:BM:74:ARG:HB3 | 2.22 | 0.40 |
| 1:AS:2273:A:N3 | 1:AS:2901:C:O2' | 2.41 | 0.40 |
| 1:AS:2325:U:H2' | 1:AS:2326:A:O4' | 2.21 | 0.40 |
| 1:AS:2367:C:H1' | 18:BK:69:ARG:CZ | 2.51 | 0.40 |
| 1:AS:2394:U:H2' | 1:AS:2395:U:C6 | 2.56 | 0.40 |
| 1:AS:2603:U:H2' | 1:AS:2604:G:H8 | 1.86 | 0.40 |
| 1:AS:3176:C:H2' | 1:AS:3177:C:C6 | 2.56 | 0.40 |
| 1:AS:3269:C:O2' | 5:AX:334:ARG:NH1 | 2.54 | 0.40 |
| 4:AW:247:ARG:HB3 | 46:CM:997:U:H4' | 2.03 | 0.40 |
| 16:BI:193:LYS:HE2 | 16:BI:193:LYS:HB3 | 1.77 | 0.40 |
| 23:BP:23:VAL:C | 23:BP:25:ASN:H | 2.29 | 0.40 |
| 25:BR:101:ARG:O | 25:BR:105:ARG:HG3 | 2.22 | 0.40 |
| 29:BV:75:LEU:HD11 | 29:BV:134:ALA:HA | 2.03 | 0.40 |
| 33:BZ:73:LYS:HD2 | 33:BZ:93:TYR:CZ | 2.56 | 0.40 |
| 45:CL:65:LYS:HG2 | 62:DC:119:PHE:O | 2.20 | 0.40 |
| 46:CM:10:G:H1' | 49:CP:84:GLN:HE21 | 1.86 | 0.40 |
| 46:CM:514:G:HO2' | 46:CM:515:U:P | 2.42 | 0.40 |
| 46:CM:597:A:H2' | 46:CM:598:U:C6 | 2.56 | 0.40 |
| 46:CM:652:C:N4 | 46:CM:654:G:C6 | 2.89 | 0.40 |
| 46:CM:722:A:C6 | 46:CM:723:G:C6 | 3.09 | 0.40 |
| 46:CM:1070:G:H2' | 46:CM:1072:A:OP2 | 2.21 | 0.40 |
| 46:CM:1083:U:H1' | 69:DJ:71:LYS:HD2 | 2.02 | 0.40 |
| 46:CM:1239:U:H2' | 46:CM:1240:G:C8 | 2.56 | 0.40 |
| 46:CM:1612:C:H2' | 46:CM:1613:U:H6 | 1.85 | 0.40 |
| 46:CM:1664:C:H2' | 46:CM:1665:C:C6 | 2.57 | 0.40 |
| 50:CQ:28:ARG:HB3 | 57:CX:58:GLN:NE2 | 2.35 | 0.40 |
| 52:CS:128:ASN:OD1 | 52:CS:130:ILE:HG12 | 2.21 | 0.40 |
| 52:CS:163:SER:HB2 | 75:DP:48:VAL:HG22 | 2.04 | 0.40 |
| 63:DD:96:VAL:HG12 | 63:DD:97:ASP:N | 2.36 | 0.40 |
| 65:DF:89:GLN:HA | 65:DF:97:ASP:HA | 2.03 | 0.40 |
| 79:DT:71:ASP:HB3 | 79:DT:113:SER:HA | 2.04 | 0.40 |
| 79:DT:97:THR:OG1 | 79:DT:99:GLU:HG2 | 2.21 | 0.40 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 81:12:109:ILE:HD12 | 81:12:109:ILE:HA | 1.94 | 0.40 |
| 82:L1:60:ARG:HH11 | 82:L1:168:ALA:HB3 | 1.87 | 0.40 |
| 1:1:955:C:O2 | 1:1:2586:G:O2' | 2.33 | 0.40 |
| 1:1:1018:U:O2' | 1:1:1019:U:H5' | 2.22 | 0.40 |
| 1:1:1222:G:H2' | 1:1:1223:C:C6 | 2.57 | 0.40 |
| 1:1:1322:A:O2' | 34:AG:77:ASN:OD1 | 2.33 | 0.40 |
| 1:1:1405:G:H21 | 8:n:1:MET:HG2 | 1.87 | 0.40 |
| 1:1:2128:G:O2' | 1:1:2167:U:OP1 | 2.29 | 0.40 |
| 1:1:2367:C:H1' | 18:x:69:ARG:CZ | 2.52 | 0.40 |
| 1:1:2405:U:H2' | 1:1:2406:U:H6 | 1.87 | 0.40 |
| 1:1:2423:A:O2' | 37:AJ:61:ARG:NH1 | 2.52 | 0.40 |
| 1:1:2628:A:C4 | 1:1:2630:G:N7 | 2.90 | 0.40 |
| 1:1:2650:A:H8 | 45:i:55:LYS:HG2 | 1.86 | 0.40 |
| 1:1:3290:G:O3' | 32:AE:102:GLY:HA2 | 2.22 | 0.40 |
| 3:4:57:C:OP2 | 38:AK:68:LYS:NZ | 2.52 | 0.40 |
| 9:o:208:PRO:HB3 | 9:o:239:GLN:HB3 | 2.03 | 0.40 |
| 15:u:14:GLU:HG2 | 15:u:17:ARG:CG | 2.48 | 0.40 |
| 25:7:83:VAL:HG11 | 46:B:68:A:H2 | 1.83 | 0.40 |
| 45:i:107:TRP:HB2 | 45:i:109:GLN:HG2 | 2.03 | 0.40 |
| 46:B:608:G:H2' | 46:B:612:C:C5 | 2.56 | 0.40 |
| 46:B:886:G:C6 | 46:B:887:G:C6 | 3.09 | 0.40 |
| 46:B:1109:A:H2' | 46:B:1110:A:C8 | 2.57 | 0.40 |
| 46:B:1231:C:H6 | 78:h:132:LYS:HZ3 | 1.69 | 0.40 |
| 46:B:1464:G:C4 | 46:B:1465:A:C8 | 3.09 | 0.40 |
| 46:B:1747:G:H1' | 46:B:1768:A:C2 | 2.56 | 0.40 |
| 47:C:55:GLU:HB3 | 68:X:79:LEU:HD22 | 2.02 | 0.40 |
| 48:D:32:ILE:HA | 48:D:96:LEU:HB2 | 2.03 | 0.40 |
| 48:D:58:ALA:O | 48:D:62:LYS:HG3 | 2.21 | 0.40 |
| 54:J:59:PRO:HG2 | 54:J:62:SER:HB3 | 2.03 | 0.40 |
| 63:S:131:ARG:HG3 | 63:S:137:PHE:CE1 | 2.54 | 0.40 |
| 78:h:124:LYS:HA | 78:h:124:LYS:HD2 | 1.96 | 0.40 |
| 79:AR:40:LYS:HG2 | 79:AR:67:HIS:O | 2.21 | 0.40 |
| 79:AR:90:LEU:HD21 | 79:AR:111:VAL:HG11 | 2.04 | 0.40 |
| 1:AS:79:G:O2' | 1:AS:326:U:H4' | 2.20 | 0.40 |
| 1:AS:291:C:H2' | 1:AS:292:U:C6 | 2.56 | 0.40 |
| 1:AS:487:C:H2' | 1:AS:488:G:O4' | 2.21 | 0.40 |
| 1:AS:607:G:N7 | 6:AY:309:LYS:NZ | 2.65 | 0.40 |
| 1:AS:742:C:H2' | 1:AS:743:A:C8 | 2.56 | 0.40 |
| 1:AS:903:G:C4 | 1:AS:922:A:C8 | 3.09 | 0.40 |
| 1:AS:1217:A:H62 | 80:p0:9:VAL:HA | 1.87 | 0.40 |
| 1:AS:1264:G:H21 | 1:AS:1269:A:H62 | 1.69 | 0.40 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 1:AS:1576:A:H5" | 1:AS:1577:C:H5 | 1.86 | 0.40 |
| 1:AS:2738:U:H2' | 1:AS:2739:U:C6 | 2.56 | 0.40 |
| 3:AU:156:U:O2' | 3:AU:157:U:OP1 | 2.38 | 0.40 |
| 4:AW:10:LYS:HA | 4:AW:16:PHE:CD2 | 2.57 | 0.40 |
| 4:AW:80:GLU:HB2 | 4:AW:170:ALA:HA | 2.03 | 0.40 |
| 9:BB:135:GLY:HA3 | 9:BB:233:ILE:HB | 2.03 | 0.40 |
| 11:BD:48:ILE:HG22 | 11:BD:49:ASN:ND2 | 2.36 | 0.40 |
| 16:BI:56:LYS:HE3 | 16:BI:56:LYS:HB3 | 1.88 | 0.40 |
| 16:BI:123:GLN:OE1 | 16:BI:128:LYS:NZ | 2.55 | 0.40 |
| 18:BK:178:SER:O | 18:BK:182:LEU:HG | 2.21 | 0.40 |
| 46:CM:393:U:H2' | 46:CM:394:G:O4' | 2.20 | 0.40 |
| 46:CM:496:G:C6 | 46:CM:497:U:C2 | 3.09 | 0.40 |
| 46:CM:737:A:H2 | 46:CM:781:G:H22 | 1.68 | 0.40 |
| 46:CM:825:U:O2' | 46:CM:826:U:C6 | 2.72 | 0.40 |
| 47:CN:23:HIS:HD2 | 64:DE:106:THR:HG21 | 1.87 | 0.40 |
| 47:CN:43:ASP:OD1 | 47:CN:44:GLY:N | 2.54 | 0.40 |
| 55:CV:92:ARG:HE | 55:CV:92:ARG:HB2 | 1.78 | 0.40 |
| 63:DD:12:LYS:HD2 | 63:DD:12:LYS:HA | 1.96 | 0.40 |
| 65:DF:70:VAL:HA | 65:DF:73:MET:HE3 | 2.03 | 0.40 |
| 78:DS:161:ARG:HG2 | 78:DS:174:MET:SD | 2.61 | 0.40 |
| 79:DT:189:PHE:CD1 | 79:DT:189:PHE:N | 2.90 | 0.40 |
| 79:DT:247:TYR:HB3 | 79:DT:262:LEU:HD12 | 2.03 | 0.40 |
| 79:DT:271:LEU:HD21 | 79:DT:310:TRP:CD2 | 2.56 | 0.40 |
| 80:P0:64:ARG:HD2 | 80:P0:67:LEU:HD12 | 2.04 | 0.40 |
| 82:l1:3:LYS:HG3 | 82:l1:217:TYR:CD1 | 2.56 | 0.40 |
| 1:1:15:A:H2' | 1:1:16:G:O4' | 2.22 | 0.40 |
| 1:1:25:A:H2' | 1:1:26:C:C6 | 2.55 | 0.40 |
| 1:1:195:G:N2 | 1:1:197:A:H3' | 2.37 | 0.40 |
| 1:1:1560:U:H3 | 1:1:1571:G:H22 | 1.70 | 0.40 |
| 1:1:1738:U:H2' | 1:1:1739:G:C8 | 2.57 | 0.40 |
| 1:1:2638:C:H5' | 45:i:39:SER:HA | 2.02 | 0.40 |
| 3:4:141:C:H2' | 3:4:142:C:C6 | 2.56 | 0.40 |
| 4:j:3:ARG:HG2 | 4:j:4:VAL:N | 2.37 | 0.40 |
| 22:2:112:ASN:HB3 | 22:2:128:LEU:HD13 | 2.04 | 0.40 |
| 27:9:86:GLN:HB3 | 27:9:94:SER:HB3 | 2.04 | 0.40 |
| 28:AA:115:LYS:NZ | 28:AA:119:GLU:OE2 | 2.34 | 0.40 |
| 31:AD:45:ILE:HD12 | 31:AD:92:LEU:HD11 | 2.02 | 0.40 |
| 46:B:23:G:O2' | 46:B:366:U:OP1 | 2.40 | 0.40 |
| 46:B:156:U:O2' | 46:B:157:U:H3' | 2.22 | 0.40 |
| 46:B:215:A:N3 | 46:B:215:A:H2' | 2.36 | 0.40 |
| 46:B:267:G:H2' | 46:B:268:C:H6 | 1.86 | 0.40 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 46:B:286:A:H2' | 46:B:287:U:O4' | 2.22 | 0.40 |
| 46:B:341:C:H2' | 46:B:342:A:H8 | 1.87 | 0.40 |
| 46:B:378:U:C4 | 56:L:5:PRO:HB3 | 2.56 | 0.40 |
| 46:B:1105:U:H2' | 46:B:1106:C:C6 | 2.56 | 0.40 |
| 46:B:1265:C:H5' | 76:f:44:ARG:HH12 | 1.87 | 0.40 |
| 50:F:225:LYS:HG3 | 79:AR:187:ALA:HB2 | 2.03 | 0.40 |
| 52:H:148:ARG:HB3 | 52:H:157:ARG:NH1 | 2.36 | 0.40 |
| 54:J:5:ILE:HD13 | 54:J:10:PRO:CB | 2.52 | 0.40 |
| 62:R:8:LYS:NZ | 62:R:10:ARG:HH21 | 2.19 | 0.40 |
| 63:S:22:LYS:HG2 | 63:S:23:ALA:H | 1.87 | 0.40 |
| 63:S:30:ILE:CG1 | 63:S:35:ILE:HG22 | 2.52 | 0.40 |
| 63:S:34:PRO:HD2 | 63:S:37:LEU:CD1 | 2.51 | 0.40 |
| 63:S:68:VAL:HG11 | 63:S:80:ILE:HD11 | 2.04 | 0.40 |
| 65:U:114:GLU:O | 65:U:118:LYS:N | 2.36 | 0.40 |
| 68:X:86:SER:HB2 | 74:d:9:HIS:O | 2.21 | 0.40 |
| 1:AS:1797:U:H2' | 1:AS:1798:C:C6 | 2.57 | 0.40 |
| 1:AS:2959:A:H2' | 1:AS:2960:C:C6 | 2.56 | 0.40 |
| 1:AS:3024:G:H2' | 1:AS:3025:G:H8 | 1.87 | 0.40 |
| 1:AS:3085:A:H2' | 1:AS:3086:A:O4' | 2.22 | 0.40 |
| 1:AS:3161:U:OP1 | 1:AS:3161:U:H4' | 2.21 | 0.40 |
| 2:AT:16:U:H2' | 2:AT:17:A:C8 | 2.56 | 0.40 |
| 4:AW:4:VAL:HG13 | 4:AW:8:GLN:HB2 | 2.02 | 0.40 |
| 4:AW:77:ILE:HD13 | 4:AW:128:ARG:HB3 | 2.03 | 0.40 |
| 11:BD:47:LYS:HZ1 | 15:BH:3:SER:HA | 1.86 | 0.40 |
| 17:BJ:53:LEU:HD23 | 17:BJ:53:LEU:HA | 1.87 | 0.40 |
| 21:BN:14:LEU:HD23 | 21:BN:14:LEU:HA | 1.93 | 0.40 |
| 21:BN:125:LYS:HG2 | 21:BN:127:VAL:HG23 | 2.02 | 0.40 |
| 31:BX:26:THR:OG1 | 31:BX:93:SER:OG | 2.40 | 0.40 |
| 34:CA:103:TYR:HA | 34:CA:104:PRO:C | 2.46 | 0.40 |
| 37:CD:56:LEU:HD23 | 37:CD:56:LEU:HA | 1.95 | 0.40 |
| 40:CG:20:ASN:OD1 | 40:CG:42:ARG:HG2 | 2.21 | 0.40 |
| 46:CM:233:G:H2' | 46:CM:234:G:H8 | 1.84 | 0.40 |
| 46:CM:479:A:H2' | 46:CM:480:U:C6 | 2.57 | 0.40 |
| 46:CM:801:A:H2' | 46:CM:802:C:H6 | 1.87 | 0.40 |
| 46:CM:1064:U:H2' | 46:CM:1065:U:H6 | 1.87 | 0.40 |
| 46:CM:1233:C:C2 | 46:CM:1234:U:H5 | 2.40 | 0.40 |
| 46:CM:1537:A:H2' | 46:CM:1538:U:C6 | 2.56 | 0.40 |
| 49:CP:213:ILE:HD12 | 49:CP:213:ILE:HA | 1.93 | 0.40 |
| 52:CS:186:ASN:HD21 | 52:CS:188:LYS:HD2 | 1.86 | 0.40 |
| 57:CX:14:TYR:CD2 | 57:CX:35:ILE:HD11 | 2.57 | 0.40 |
| 58:CY:7:VAL:HG12 | 58:CY:53:TYR:HA | 2.03 | 0.40 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 63:DD:14:THR:HB | 63:DD:71:GLY:HA2 | 2.02 | 0.40 |
| 69:DJ:55:ASP:O | 69:DJ:57:ARG:NH1 | 2.53 | 0.40 |
| 73:DN:11:ASN:HB3 | 73:DN:33:ASP:HB2 | 2.02 | 0.40 |
| 75:DP:43:ASN:ND2 | 75:DP:66:LEU:HD13 | 2.36 | 0.40 |
| 81:12:133:LEU:HD13 | 81:12:152:ILE:HG12 | 2.04 | 0.40 |
| 81:12:137:GLN:HA | 81:12:148:PRO:HG2 | 2.04 | 0.40 |
| 82:L1:49:PHE:CE1 | 82:L1:159:LEU:HD22 | 2.57 | 0.40 |
| 82:L1:176:GLU:O | 82:L1:180:VAL:HG23 | 2.22 | 0.40 |
| 82:l1:42:ASP:OD1 | 82:l1:45:ARG:NH2 | 2.55 | 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 X-ray entries followed by that with respect to entries of similar resolution.

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

| Mol | Chain | Analysed | Favoured | Allowed | Outliers | Percentiles | |
|---|---|---|---|---|---|---|---|
| 4 | AW | 247/254 (97%) | 239 (97%) | 8 (3%) | 0 | 100 | 100 |
| 4 | j | 247/254 (97%) | 239 (97%) | 8 (3%) | 0 | 100 | 100 |
| 5 | AX | 384/389 (99%) | 372 (97%) | 12 (3%) | 0 | 100 | 100 |
| 5 | k | 384/389 (99%) | 372 (97%) | 12 (3%) | 0 | 100 | 100 |
| 6 | AY | 359/363 (99%) | 349 (97%) | 10 (3%) | 0 | 100 | 100 |
| 6 | l | 359/363 (99%) | 348 (97%) | 11 (3%) | 0 | 100 | 100 |
| 7 | AZ | 290/298 (97%) | 278 (96%) | 12 (4%) | 0 | 100 | 100 |
| 7 | m | 294/298 (99%) | 281 (96%) | 12 (4%) | 1 (0%) | 36 | 63 |
| 8 | BA | 149/176 (85%) | 147 (99%) | 2 (1%) | 0 | 100 | 100 |
| 8 | n | 153/176 (87%) | 150 (98%) | 3 (2%) | 0 | 100 | 100 |
| 9 | BB | 232/241 (96%) | 226 (97%) | 5 (2%) | 1 (0%) | 30 | 57 |
| 9 | o | 223/241 (92%) | 215 (96%) | 7 (3%) | 1 (0%) | 30 | 57 |
| 10 | BC | 225/262 (86%) | 210 (93%) | 11 (5%) | 4 (2%) | 6 | 24 |

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| Mol | Chain | Analysed | Favoured | Allowed | Outliers | Percentiles |
|---|---|---|---|---|---|---|
| 10 | p | 231/262 (88%) | 223 (96%) | 7 (3%) | 1 (0%) | 30 57 |
| 11 | BD | 188/191 (98%) | 184 (98%) | 4 (2%) | 0 | 100 100 |
| 11 | q | 187/191 (98%) | 182 (97%) | 5 (3%) | 0 | 100 100 |
| 12 | BE | 204/220 (93%) | 199 (98%) | 5 (2%) | 0 | 100 100 |
| 12 | r | 204/220 (93%) | 201 (98%) | 3 (2%) | 0 | 100 100 |
| 13 | BF | 169/174 (97%) | 163 (96%) | 6 (4%) | 0 | 100 100 |
| 13 | s | 169/174 (97%) | 161 (95%) | 8 (5%) | 0 | 100 100 |
| 14 | BG | 198/202 (98%) | 193 (98%) | 5 (2%) | 0 | 100 100 |
| 14 | t | 198/202 (98%) | 196 (99%) | 2 (1%) | 0 | 100 100 |
| 15 | BH | 128/131 (98%) | 124 (97%) | 4 (3%) | 0 | 100 100 |
| 15 | u | 128/131 (98%) | 125 (98%) | 3 (2%) | 0 | 100 100 |
| 16 | BI | 201/204 (98%) | 197 (98%) | 4 (2%) | 0 | 100 100 |
| 16 | v | 201/204 (98%) | 196 (98%) | 5 (2%) | 0 | 100 100 |
| 17 | BJ | 197/200 (98%) | 195 (99%) | 2 (1%) | 0 | 100 100 |
| 17 | w | 197/200 (98%) | 195 (99%) | 2 (1%) | 0 | 100 100 |
| 18 | BK | 172/185 (93%) | 167 (97%) | 5 (3%) | 0 | 100 100 |
| 18 | x | 169/185 (91%) | 166 (98%) | 3 (2%) | 0 | 100 100 |
| 19 | BL | 183/186 (98%) | 179 (98%) | 4 (2%) | 0 | 100 100 |
| 19 | y | 183/186 (98%) | 179 (98%) | 4 (2%) | 0 | 100 100 |
| 20 | BM | 177/190 (93%) | 173 (98%) | 4 (2%) | 0 | 100 100 |
| 20 | z | 177/190 (93%) | 174 (98%) | 3 (2%) | 0 | 100 100 |
| 21 | 0 | 168/172 (98%) | 166 (99%) | 2 (1%) | 0 | 100 100 |
| 21 | BN | 168/172 (98%) | 166 (99%) | 2 (1%) | 0 | 100 100 |
| 22 | 2 | 157/160 (98%) | 154 (98%) | 3 (2%) | 0 | 100 100 |
| 22 | BO | 157/160 (98%) | 154 (98%) | 3 (2%) | 0 | 100 100 |
| 23 | 5 | 100/124 (81%) | 89 (89%) | 10 (10%) | 1 (1%) | 12 37 |
| 23 | BP | 100/124 (81%) | 87 (87%) | 11 (11%) | 2 (2%) | 6 21 |
| 24 | 6 | 129/137 (94%) | 126 (98%) | 3 (2%) | 0 | 100 100 |
| 24 | BQ | 129/137 (94%) | 126 (98%) | 3 (2%) | 0 | 100 100 |
| 25 | 7 | 114/155 (74%) | 103 (90%) | 11 (10%) | 0 | 100 100 |
| 25 | BR | 94/155 (61%) | 90 (96%) | 4 (4%) | 0 | 100 100 |

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| Mol | Chain | Analysed | Favoured | Allowed | Outliers | Percentiles | |
|---|---|---|---|---|---|---|---|
| 26 | 8 | 118/142 (83%) | 116 (98%) | 2 (2%) | 0 | 100 | 100 |
| 26 | BS | 117/142 (82%) | 115 (98%) | 2 (2%) | 0 | 100 | 100 |
| 27 | 9 | 124/127 (98%) | 123 (99%) | 1 (1%) | 0 | 100 | 100 |
| 27 | BT | 124/127 (98%) | 123 (99%) | 1 (1%) | 0 | 100 | 100 |
| 28 | AA | 133/136 (98%) | 132 (99%) | 1 (1%) | 0 | 100 | 100 |
| 28 | BU | 133/136 (98%) | 131 (98%) | 2 (2%) | 0 | 100 | 100 |
| 29 | AB | 146/149 (98%) | 139 (95%) | 7 (5%) | 0 | 100 | 100 |
| 29 | BV | 146/149 (98%) | 139 (95%) | 7 (5%) | 0 | 100 | 100 |
| 30 | AC | 60/63 (95%) | 57 (95%) | 1 (2%) | 2 (3%) | 3 | 13 |
| 30 | BW | 59/63 (94%) | 58 (98%) | 1 (2%) | 0 | 100 | 100 |
| 31 | AD | 94/106 (89%) | 93 (99%) | 1 (1%) | 0 | 100 | 100 |
| 31 | BX | 94/106 (89%) | 92 (98%) | 2 (2%) | 0 | 100 | 100 |
| 32 | AE | 108/112 (96%) | 106 (98%) | 2 (2%) | 0 | 100 | 100 |
| 32 | BY | 108/112 (96%) | 103 (95%) | 5 (5%) | 0 | 100 | 100 |
| 33 | AF | 122/131 (93%) | 122 (100%) | 0 | 0 | 100 | 100 |
| 33 | BZ | 122/131 (93%) | 122 (100%) | 0 | 0 | 100 | 100 |
| 34 | AG | 104/107 (97%) | 102 (98%) | 2 (2%) | 0 | 100 | 100 |
| 34 | CA | 104/107 (97%) | 101 (97%) | 3 (3%) | 0 | 100 | 100 |
| 35 | AH | 110/122 (90%) | 108 (98%) | 2 (2%) | 0 | 100 | 100 |
| 35 | CB | 110/122 (90%) | 107 (97%) | 3 (3%) | 0 | 100 | 100 |
| 36 | AI | 118/120 (98%) | 114 (97%) | 4 (3%) | 0 | 100 | 100 |
| 36 | CC | 116/120 (97%) | 114 (98%) | 2 (2%) | 0 | 100 | 100 |
| 37 | AJ | 95/99 (96%) | 93 (98%) | 2 (2%) | 0 | 100 | 100 |
| 37 | CD | 95/99 (96%) | 94 (99%) | 1 (1%) | 0 | 100 | 100 |
| 38 | AK | 84/90 (93%) | 81 (96%) | 3 (4%) | 0 | 100 | 100 |
| 38 | CE | 84/90 (93%) | 81 (96%) | 3 (4%) | 0 | 100 | 100 |
| 39 | AL | 75/78 (96%) | 72 (96%) | 3 (4%) | 0 | 100 | 100 |
| 39 | CF | 75/78 (96%) | 68 (91%) | 7 (9%) | 0 | 100 | 100 |
| 40 | AM | 48/51 (94%) | 46 (96%) | 1 (2%) | 1 (2%) | 5 | 21 |
| 40 | CG | 48/51 (94%) | 48 (100%) | 0 | 0 | 100 | 100 |
| 41 | AN | 50/52 (96%) | 49 (98%) | 1 (2%) | 0 | 100 | 100 |

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| Mol | Chain | Analysed | Favoured | Allowed | Outliers | Percentiles |
|---|---|---|---|---|---|---|
| 41 | CH | 49/52 (94%) | 46 (94%) | 1 (2%) | 2 (4%) | 2 10 |
| 42 | AO | 23/25 (92%) | 22 (96%) | 1 (4%) | 0 | 100 100 |
| 42 | CI | 22/25 (88%) | 22 (100%) | 0 | 0 | 100 100 |
| 43 | AP | 101/106 (95%) | 100 (99%) | 1 (1%) | 0 | 100 100 |
| 43 | CJ | 101/106 (95%) | 100 (99%) | 1 (1%) | 0 | 100 100 |
| 44 | AQ | 89/92 (97%) | 85 (96%) | 4 (4%) | 0 | 100 100 |
| 44 | CK | 89/92 (97%) | 85 (96%) | 4 (4%) | 0 | 100 100 |
| 45 | CL | 117/267 (44%) | 91 (78%) | 22 (19%) | 4 (3%) | 3 13 |
| 45 | i | 116/267 (43%) | 91 (78%) | 23 (20%) | 2 (2%) | 7 25 |
| 47 | C | 206/261 (79%) | 201 (98%) | 5 (2%) | 0 | 100 100 |
| 47 | CN | 206/261 (79%) | 198 (96%) | 8 (4%) | 0 | 100 100 |
| 48 | CO | 212/256 (83%) | 204 (96%) | 8 (4%) | 0 | 100 100 |
| 48 | D | 212/256 (83%) | 207 (98%) | 5 (2%) | 0 | 100 100 |
| 49 | CP | 215/249 (86%) | 209 (97%) | 6 (3%) | 0 | 100 100 |
| 49 | E | 215/249 (86%) | 210 (98%) | 5 (2%) | 0 | 100 100 |
| 50 | CQ | 221/251 (88%) | 211 (96%) | 10 (4%) | 0 | 100 100 |
| 50 | F | 221/251 (88%) | 213 (96%) | 8 (4%) | 0 | 100 100 |
| 51 | CR | 258/262 (98%) | 254 (98%) | 4 (2%) | 0 | 100 100 |
| 51 | G | 257/262 (98%) | 253 (98%) | 4 (2%) | 0 | 100 100 |
| 52 | CS | 204/225 (91%) | 196 (96%) | 8 (4%) | 0 | 100 100 |
| 52 | H | 204/225 (91%) | 185 (91%) | 17 (8%) | 2 (1%) | 12 37 |
| 53 | CT | 234/236 (99%) | 231 (99%) | 3 (1%) | 0 | 100 100 |
| 53 | I | 224/236 (95%) | 221 (99%) | 3 (1%) | 0 | 100 100 |
| 54 | CU | 181/186 (97%) | 171 (94%) | 9 (5%) | 1 (1%) | 21 48 |
| 54 | J | 182/186 (98%) | 172 (94%) | 10 (6%) | 0 | 100 100 |
| 55 | CV | 201/206 (98%) | 199 (99%) | 2 (1%) | 0 | 100 100 |
| 55 | K | 201/206 (98%) | 200 (100%) | 1 (0%) | 0 | 100 100 |
| 56 | CW | 176/189 (93%) | 175 (99%) | 1 (1%) | 0 | 100 100 |
| 56 | L | 176/189 (93%) | 175 (99%) | 1 (1%) | 0 | 100 100 |
| 57 | CX | 92/118 (78%) | 86 (94%) | 6 (6%) | 0 | 100 100 |
| 57 | M | 96/118 (81%) | 81 (84%) | 13 (14%) | 2 (2%) | 5 21 |

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| Mol | Chain | Analysed | Favoured | Allowed | Outliers | Percentiles |
|---|---|---|---|---|---|---|
| 58 | CY | 139/155 (90%) | 133 (96%) | 4 (3%) | 2 (1%) | 9 29 |
| 58 | N | 142/155 (92%) | 137 (96%) | 5 (4%) | 0 | 100 100 |
| 59 | CZ | 117/143 (82%) | 90 (77%) | 22 (19%) | 5 (4%) | 2 10 |
| 59 | O | 114/143 (80%) | 89 (78%) | 23 (20%) | 2 (2%) | 6 24 |
| 60 | DA | 148/151 (98%) | 146 (99%) | 2 (1%) | 0 | 100 100 |
| 60 | P | 148/151 (98%) | 146 (99%) | 2 (1%) | 0 | 100 100 |
| 61 | DB | 125/132 (95%) | 120 (96%) | 5 (4%) | 0 | 100 100 |
| 61 | Q | 125/132 (95%) | 119 (95%) | 5 (4%) | 1 (1%) | 16 42 |
| 62 | DC | 128/142 (90%) | 111 (87%) | 17 (13%) | 0 | 100 100 |
| 62 | R | 127/142 (89%) | 115 (91%) | 11 (9%) | 1 (1%) | 16 42 |
| 63 | DD | 138/142 (97%) | 134 (97%) | 4 (3%) | 0 | 100 100 |
| 63 | S | 138/142 (97%) | 132 (96%) | 6 (4%) | 0 | 100 100 |
| 64 | DE | 122/137 (89%) | 119 (98%) | 3 (2%) | 0 | 100 100 |
| 64 | T | 122/137 (89%) | 118 (97%) | 4 (3%) | 0 | 100 100 |
| 65 | DF | 139/145 (96%) | 133 (96%) | 5 (4%) | 1 (1%) | 18 45 |
| 65 | U | 142/145 (98%) | 137 (96%) | 5 (4%) | 0 | 100 100 |
| 66 | DG | 139/145 (96%) | 133 (96%) | 5 (4%) | 1 (1%) | 18 45 |
| 66 | V | 139/145 (96%) | 136 (98%) | 3 (2%) | 0 | 100 100 |
| 67 | DH | 95/119 (80%) | 93 (98%) | 2 (2%) | 0 | 100 100 |
| 67 | W | 100/119 (84%) | 97 (97%) | 3 (3%) | 0 | 100 100 |
| 68 | DI | 85/87 (98%) | 83 (98%) | 2 (2%) | 0 | 100 100 |
| 68 | X | 85/87 (98%) | 83 (98%) | 2 (2%) | 0 | 100 100 |
| 69 | DJ | 127/130 (98%) | 126 (99%) | 1 (1%) | 0 | 100 100 |
| 69 | Y | 127/130 (98%) | 125 (98%) | 2 (2%) | 0 | 100 100 |
| 70 | DK | 141/145 (97%) | 139 (99%) | 2 (1%) | 0 | 100 100 |
| 70 | Z | 141/145 (97%) | 138 (98%) | 3 (2%) | 0 | 100 100 |
| 71 | DL | 130/135 (96%) | 130 (100%) | 0 | 0 | 100 100 |
| 71 | a | 132/135 (98%) | 130 (98%) | 2 (2%) | 0 | 100 100 |
| 72 | DM | 69/105 (66%) | 65 (94%) | 4 (6%) | 0 | 100 100 |
| 72 | b | 70/105 (67%) | 69 (99%) | 1 (1%) | 0 | 100 100 |
| 73 | DN | 95/119 (80%) | 93 (98%) | 2 (2%) | 0 | 100 100 |

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| Mol | Chain | Analysed | Favoured | Allowed | Outliers | Percentiles |
|---|---|---|---|---|---|---|
| 73 | c | 96/119 (81%) | 93 (97%) | 3 (3%) | 0 | 100 100 |
| 74 | DO | 79/82 (96%) | 73 (92%) | 6 (8%) | 0 | 100 100 |
| 74 | d | 79/82 (96%) | 75 (95%) | 4 (5%) | 0 | 100 100 |
| 75 | DP | 59/67 (88%) | 53 (90%) | 6 (10%) | 0 | 100 100 |
| 75 | e | 60/67 (90%) | 57 (95%) | 3 (5%) | 0 | 100 100 |
| 76 | DQ | 52/56 (93%) | 50 (96%) | 2 (4%) | 0 | 100 100 |
| 76 | f | 53/56 (95%) | 51 (96%) | 2 (4%) | 0 | 100 100 |
| 77 | DR | 56/63 (89%) | 52 (93%) | 3 (5%) | 1 (2%) | 6 24 |
| 77 | g | 58/63 (92%) | 55 (95%) | 3 (5%) | 0 | 100 100 |
| 78 | DS | 68/193 (35%) | 57 (84%) | 10 (15%) | 1 (2%) | 8 28 |
| 78 | h | 68/193 (35%) | 55 (81%) | 13 (19%) | 0 | 100 100 |
| 79 | AR | 309/317 (98%) | 292 (94%) | 17 (6%) | 0 | 100 100 |
| 79 | DT | 302/317 (95%) | 281 (93%) | 19 (6%) | 2 (1%) | 18 45 |
| 80 | P0 | 105/312 (34%) | 81 (77%) | 21 (20%) | 3 (3%) | 3 16 |
| 80 | p0 | 69/312 (22%) | 46 (67%) | 20 (29%) | 3 (4%) | 2 10 |
| 81 | 12 | 61/165 (37%) | 36 (59%) | 25 (41%) | 0 | 100 100 |
| 82 | L1 | 215/217 (99%) | 166 (77%) | 46 (21%) | 3 (1%) | 9 29 |
| 82 | l1 | 215/217 (99%) | 131 (61%) | 72 (34%) | 12 (6%) | 1 7 |
| All | All | 22741/25499 (89%) | 21725 (96%) | 951 (4%) | 65 (0%) | 36 63 |

All (65) Ramachandran outliers are listed below:

| Mol | Chain | Res | Type |
|---|---|---|---|
| 30 | AC | 21 | ILE |
| 40 | AM | 49 | LEU |
| 45 | i | 55 | LYS |
| 59 | O | 130 | SER |
| 41 | CH | 3 | GLU |
| 45 | CL | 41 | ALA |
| 45 | CL | 43 | PRO |
| 45 | CL | 72 | ASP |
| 59 | CZ | 82 | PRO |
| 59 | CZ | 112 | ALA |
| 78 | DS | 127 | TYR |
| 80 | P0 | 24 | SER |
| 80 | P0 | 71 | PRO |

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| Mol | Chain | Res | Type |
|---|---|---|---|
| 80 | P0 | 72 | GLU |
| 82 | L1 | 45 | ARG |
| 82 | l1 | 71 | ALA |
| 82 | l1 | 74 | VAL |
| 82 | l1 | 87 | VAL |
| 82 | l1 | 129 | SER |
| 82 | l1 | 157 | PHE |
| 82 | l1 | 212 | PRO |
| 80 | p0 | 46 | ARG |
| 80 | p0 | 71 | PRO |
| 80 | p0 | 101 | VAL |
| 10 | p | 205 | ASN |
| 52 | H | 44 | ASN |
| 57 | M | 88 | PRO |
| 10 | BC | 207 | ALA |
| 41 | CH | 4 | PRO |
| 58 | CY | 26 | LYS |
| 59 | CZ | 34 | THR |
| 59 | CZ | 108 | ARG |
| 65 | DF | 57 | ARG |
| 79 | DT | 75 | SER |
| 82 | L1 | 212 | PRO |
| 82 | l1 | 27 | ASN |
| 82 | l1 | 59 | PRO |
| 9 | o | 230 | GLU |
| 62 | R | 2 | VAL |
| 9 | BB | 230 | GLU |
| 45 | CL | 49 | ALA |
| 66 | DG | 119 | LYS |
| 82 | l1 | 14 | HIS |
| 23 | 5 | 20 | ALA |
| 57 | M | 92 | LEU |
| 59 | O | 38 | HIS |
| 10 | BC | 127 | SER |
| 10 | BC | 128 | PRO |
| 23 | BP | 20 | ALA |
| 23 | BP | 24 | GLU |
| 79 | DT | 28 | ALA |
| 7 | m | 44 | TYR |
| 54 | CU | 156 | THR |
| 59 | CZ | 103 | LEU |
| 77 | DR | 7 | SER |

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| Mol | Chain | Res | Type |
|---|---|---|---|
| 30 | AC | 3 | LYS |
| 45 | i | 44 | ALA |
| 61 | Q | 119 | ASP |
| 10 | BC | 126 | VAL |
| 58 | CY | 27 | ALA |
| 52 | H | 53 | VAL |
| 82 | L1 | 59 | PRO |
| 82 | l1 | 216 | ILE |
| 82 | l1 | 82 | VAL |
| 82 | l1 | 180 | VAL |

### 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 X-ray entries followed by that with respect to entries of similar resolution.

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

| Mol | Chain | Analysed | Rotameric | Outliers | Percentiles | |
|---|---|---|---|---|---|---|
| 4 | AW | 190/194 (98%) | 190 (100%) | 0 | 100 | 100 |
| 4 | j | 190/194 (98%) | 190 (100%) | 0 | 100 | 100 |
| 5 | AX | 325/328 (99%) | 325 (100%) | 0 | 100 | 100 |
| 5 | k | 325/328 (99%) | 325 (100%) | 0 | 100 | 100 |
| 6 | AY | 290/292 (99%) | 290 (100%) | 0 | 100 | 100 |
| 6 | l | 290/292 (99%) | 290 (100%) | 0 | 100 | 100 |
| 7 | AZ | 247/252 (98%) | 247 (100%) | 0 | 100 | 100 |
| 7 | m | 250/252 (99%) | 250 (100%) | 0 | 100 | 100 |
| 8 | BA | 132/154 (86%) | 132 (100%) | 0 | 100 | 100 |
| 8 | n | 136/154 (88%) | 136 (100%) | 0 | 100 | 100 |
| 9 | BB | 198/204 (97%) | 198 (100%) | 0 | 100 | 100 |
| 9 | o | 197/204 (97%) | 197 (100%) | 0 | 100 | 100 |
| 10 | BC | 191/216 (88%) | 191 (100%) | 0 | 100 | 100 |
| 10 | p | 193/216 (89%) | 193 (100%) | 0 | 100 | 100 |
| 11 | BD | 169/170 (99%) | 169 (100%) | 0 | 100 | 100 |
| 11 | q | 168/170 (99%) | 168 (100%) | 0 | 100 | 100 |

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| Mol | Chain | Analysed | Rotameric | Outliers | Percentiles | |
|---|---|---|---|---|---|---|
| 12 | BE | 178/186 (96%) | 177 (99%) | 1 (1%) | 78 | 81 |
| 12 | r | 178/186 (96%) | 178 (100%) | 0 | 100 | 100 |
| 13 | BF | 146/149 (98%) | 146 (100%) | 0 | 100 | 100 |
| 13 | s | 146/149 (98%) | 146 (100%) | 0 | 100 | 100 |
| 14 | BG | 166/168 (99%) | 166 (100%) | 0 | 100 | 100 |
| 14 | t | 166/168 (99%) | 166 (100%) | 0 | 100 | 100 |
| 15 | BH | 108/109 (99%) | 108 (100%) | 0 | 100 | 100 |
| 15 | u | 108/109 (99%) | 108 (100%) | 0 | 100 | 100 |
| 16 | BI | 177/178 (99%) | 177 (100%) | 0 | 100 | 100 |
| 16 | v | 177/178 (99%) | 177 (100%) | 0 | 100 | 100 |
| 17 | BJ | 166/167 (99%) | 166 (100%) | 0 | 100 | 100 |
| 17 | w | 166/167 (99%) | 166 (100%) | 0 | 100 | 100 |
| 18 | BK | 145/154 (94%) | 145 (100%) | 0 | 100 | 100 |
| 18 | x | 144/154 (94%) | 144 (100%) | 0 | 100 | 100 |
| 19 | BL | 153/154 (99%) | 153 (100%) | 0 | 100 | 100 |
| 19 | y | 153/154 (99%) | 153 (100%) | 0 | 100 | 100 |
| 20 | BM | 146/153 (95%) | 145 (99%) | 1 (1%) | 76 | 80 |
| 20 | z | 146/153 (95%) | 146 (100%) | 0 | 100 | 100 |
| 21 | 0 | 155/157 (99%) | 155 (100%) | 0 | 100 | 100 |
| 21 | BN | 155/157 (99%) | 155 (100%) | 0 | 100 | 100 |
| 22 | 2 | 133/134 (99%) | 133 (100%) | 0 | 100 | 100 |
| 22 | BO | 133/134 (99%) | 133 (100%) | 0 | 100 | 100 |
| 23 | 5 | 93/112 (83%) | 93 (100%) | 0 | 100 | 100 |
| 23 | BP | 93/112 (83%) | 93 (100%) | 0 | 100 | 100 |
| 24 | 6 | 101/104 (97%) | 101 (100%) | 0 | 100 | 100 |
| 24 | BQ | 101/104 (97%) | 101 (100%) | 0 | 100 | 100 |
| 25 | 7 | 97/127 (76%) | 97 (100%) | 0 | 100 | 100 |
| 25 | BR | 86/127 (68%) | 86 (100%) | 0 | 100 | 100 |
| 26 | 8 | 107/121 (88%) | 107 (100%) | 0 | 100 | 100 |
| 26 | BS | 107/121 (88%) | 107 (100%) | 0 | 100 | 100 |
| 27 | 9 | 111/112 (99%) | 111 (100%) | 0 | 100 | 100 |

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| Mol | Chain | Analysed | Rotameric | Outliers | Percentiles | |
|---|---|---|---|---|---|---|
| 27 | BT | 111/112 (99%) | 111 (100%) | 0 | 100 | 100 |
| 28 | AA | 117/118 (99%) | 117 (100%) | 0 | 100 | 100 |
| 28 | BU | 117/118 (99%) | 117 (100%) | 0 | 100 | 100 |
| 29 | AB | 120/121 (99%) | 120 (100%) | 0 | 100 | 100 |
| 29 | BV | 120/121 (99%) | 120 (100%) | 0 | 100 | 100 |
| 30 | AC | 48/49 (98%) | 48 (100%) | 0 | 100 | 100 |
| 30 | BW | 48/49 (98%) | 48 (100%) | 0 | 100 | 100 |
| 31 | AD | 81/90 (90%) | 81 (100%) | 0 | 100 | 100 |
| 31 | BX | 81/90 (90%) | 81 (100%) | 0 | 100 | 100 |
| 32 | AE | 98/100 (98%) | 98 (100%) | 0 | 100 | 100 |
| 32 | BY | 98/100 (98%) | 98 (100%) | 0 | 100 | 100 |
| 33 | AF | 109/115 (95%) | 109 (100%) | 0 | 100 | 100 |
| 33 | BZ | 110/115 (96%) | 110 (100%) | 0 | 100 | 100 |
| 34 | AG | 91/92 (99%) | 91 (100%) | 0 | 100 | 100 |
| 34 | CA | 91/92 (99%) | 91 (100%) | 0 | 100 | 100 |
| 35 | AH | 95/102 (93%) | 95 (100%) | 0 | 100 | 100 |
| 35 | CB | 95/102 (93%) | 95 (100%) | 0 | 100 | 100 |
| 36 | AI | 106/106 (100%) | 106 (100%) | 0 | 100 | 100 |
| 36 | CC | 105/106 (99%) | 105 (100%) | 0 | 100 | 100 |
| 37 | AJ | 77/79 (98%) | 76 (99%) | 1 (1%) | 61 | 74 |
| 37 | CD | 77/79 (98%) | 77 (100%) | 0 | 100 | 100 |
| 38 | AK | 70/73 (96%) | 70 (100%) | 0 | 100 | 100 |
| 38 | CE | 70/73 (96%) | 70 (100%) | 0 | 100 | 100 |
| 39 | AL | 68/69 (99%) | 68 (100%) | 0 | 100 | 100 |
| 39 | CF | 68/69 (99%) | 68 (100%) | 0 | 100 | 100 |
| 40 | AM | 46/47 (98%) | 46 (100%) | 0 | 100 | 100 |
| 40 | CG | 46/47 (98%) | 46 (100%) | 0 | 100 | 100 |
| 41 | AN | 47/47 (100%) | 47 (100%) | 0 | 100 | 100 |
| 41 | CH | 46/47 (98%) | 46 (100%) | 0 | 100 | 100 |
| 42 | AO | 24/24 (100%) | 24 (100%) | 0 | 100 | 100 |
| 42 | CI | 23/24 (96%) | 23 (100%) | 0 | 100 | 100 |

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| Mol | Chain | Analysed | Rotameric | Outliers | Percentiles | |
|---|---|---|---|---|---|---|
| 43 | AP | 88/91 (97%) | 88 (100%) | 0 | 100 | 100 |
| 43 | CJ | 88/91 (97%) | 88 (100%) | 0 | 100 | 100 |
| 44 | AQ | 72/73 (99%) | 72 (100%) | 0 | 100 | 100 |
| 44 | CK | 72/73 (99%) | 72 (100%) | 0 | 100 | 100 |
| 45 | CL | 100/212 (47%) | 99 (99%) | 1 (1%) | 68 | 77 |
| 45 | i | 99/212 (47%) | 99 (100%) | 0 | 100 | 100 |
| 47 | C | 176/215 (82%) | 176 (100%) | 0 | 100 | 100 |
| 47 | CN | 176/215 (82%) | 176 (100%) | 0 | 100 | 100 |
| 48 | CO | 194/229 (85%) | 194 (100%) | 0 | 100 | 100 |
| 48 | D | 194/229 (85%) | 194 (100%) | 0 | 100 | 100 |
| 49 | CP | 175/198 (88%) | 175 (100%) | 0 | 100 | 100 |
| 49 | E | 175/198 (88%) | 175 (100%) | 0 | 100 | 100 |
| 50 | CQ | 174/196 (89%) | 174 (100%) | 0 | 100 | 100 |
| 50 | F | 174/196 (89%) | 174 (100%) | 0 | 100 | 100 |
| 51 | CR | 218/220 (99%) | 218 (100%) | 0 | 100 | 100 |
| 51 | G | 218/220 (99%) | 218 (100%) | 0 | 100 | 100 |
| 52 | CS | 178/197 (90%) | 178 (100%) | 0 | 100 | 100 |
| 52 | H | 178/197 (90%) | 177 (99%) | 1 (1%) | 78 | 81 |
| 53 | CT | 204/204 (100%) | 204 (100%) | 0 | 100 | 100 |
| 53 | I | 195/204 (96%) | 195 (100%) | 0 | 100 | 100 |
| 54 | CU | 164/167 (98%) | 164 (100%) | 0 | 100 | 100 |
| 54 | J | 165/167 (99%) | 165 (100%) | 0 | 100 | 100 |
| 55 | CV | 157/160 (98%) | 157 (100%) | 0 | 100 | 100 |
| 55 | K | 157/160 (98%) | 157 (100%) | 0 | 100 | 100 |
| 56 | CW | 153/160 (96%) | 153 (100%) | 0 | 100 | 100 |
| 56 | L | 153/160 (96%) | 153 (100%) | 0 | 100 | 100 |
| 57 | CX | 88/104 (85%) | 88 (100%) | 0 | 100 | 100 |
| 57 | M | 90/104 (86%) | 90 (100%) | 0 | 100 | 100 |
| 58 | CY | 122/134 (91%) | 122 (100%) | 0 | 100 | 100 |
| 58 | N | 124/134 (92%) | 124 (100%) | 0 | 100 | 100 |
| 59 | CZ | 101/123 (82%) | 101 (100%) | 0 | 100 | 100 |

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| Mol | Chain | Analysed | Rotameric | Outliers | Percentiles | |
|---|---|---|---|---|---|---|
| 59 | O | 98/123 (80%) | 96 (98%) | 2 (2%) | 48 | 69 |
| 60 | DA | 129/130 (99%) | 129 (100%) | 0 | 100 | 100 |
| 60 | P | 129/130 (99%) | 129 (100%) | 0 | 100 | 100 |
| 61 | DB | 97/102 (95%) | 97 (100%) | 0 | 100 | 100 |
| 61 | Q | 97/102 (95%) | 97 (100%) | 0 | 100 | 100 |
| 62 | DC | 112/121 (93%) | 112 (100%) | 0 | 100 | 100 |
| 62 | R | 111/121 (92%) | 111 (100%) | 0 | 100 | 100 |
| 63 | DD | 114/116 (98%) | 114 (100%) | 0 | 100 | 100 |
| 63 | S | 114/116 (98%) | 114 (100%) | 0 | 100 | 100 |
| 64 | DE | 112/122 (92%) | 112 (100%) | 0 | 100 | 100 |
| 64 | T | 112/122 (92%) | 111 (99%) | 1 (1%) | 70 | 78 |
| 65 | DF | 125/129 (97%) | 125 (100%) | 0 | 100 | 100 |
| 65 | U | 128/129 (99%) | 128 (100%) | 0 | 100 | 100 |
| 66 | DG | 113/117 (97%) | 113 (100%) | 0 | 100 | 100 |
| 66 | V | 113/117 (97%) | 113 (100%) | 0 | 100 | 100 |
| 67 | DH | 87/105 (83%) | 87 (100%) | 0 | 100 | 100 |
| 67 | W | 92/105 (88%) | 92 (100%) | 0 | 100 | 100 |
| 68 | DI | 71/71 (100%) | 71 (100%) | 0 | 100 | 100 |
| 68 | X | 71/71 (100%) | 71 (100%) | 0 | 100 | 100 |
| 69 | DJ | 112/113 (99%) | 112 (100%) | 0 | 100 | 100 |
| 69 | Y | 112/113 (99%) | 112 (100%) | 0 | 100 | 100 |
| 70 | DK | 116/118 (98%) | 116 (100%) | 0 | 100 | 100 |
| 70 | Z | 116/118 (98%) | 116 (100%) | 0 | 100 | 100 |
| 71 | DL | 109/112 (97%) | 109 (100%) | 0 | 100 | 100 |
| 71 | a | 111/112 (99%) | 111 (100%) | 0 | 100 | 100 |
| 72 | DM | 63/85 (74%) | 63 (100%) | 0 | 100 | 100 |
| 72 | b | 64/85 (75%) | 64 (100%) | 0 | 100 | 100 |
| 73 | DN | 83/102 (81%) | 83 (100%) | 0 | 100 | 100 |
| 73 | c | 84/102 (82%) | 84 (100%) | 0 | 100 | 100 |
| 74 | DO | 72/73 (99%) | 72 (100%) | 0 | 100 | 100 |
| 74 | d | 72/73 (99%) | 72 (100%) | 0 | 100 | 100 |

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| Mol | Chain | Analysed | Rotameric | Outliers | Percentiles |
|---|---|---|---|---|---|
| 75 | DP | 53/58 (91%) | 53 (100%) | 0 | 100 100 |
| 75 | e | 54/58 (93%) | 54 (100%) | 0 | 100 100 |
| 76 | DQ | 47/48 (98%) | 47 (100%) | 0 | 100 100 |
| 76 | f | 47/48 (98%) | 47 (100%) | 0 | 100 100 |
| 77 | DR | 50/54 (93%) | 50 (100%) | 0 | 100 100 |
| 77 | g | 51/54 (94%) | 51 (100%) | 0 | 100 100 |
| 78 | DS | 62/175 (35%) | 60 (97%) | 2 (3%) | 34 60 |
| 78 | h | 62/175 (35%) | 59 (95%) | 3 (5%) | 23 50 |
| 79 | AR | 259/263 (98%) | 259 (100%) | 0 | 100 100 |
| 79 | DT | 255/263 (97%) | 255 (100%) | 0 | 100 100 |
| 80 | P0 | 92/247 (37%) | 92 (100%) | 0 | 100 100 |
| 80 | p0 | 71/247 (29%) | 69 (97%) | 2 (3%) | 38 63 |
| 81 | 12 | 53/137 (39%) | 53 (100%) | 0 | 100 100 |
| 82 | L1 | 196/196 (100%) | 196 (100%) | 0 | 100 100 |
| 82 | l1 | 196/196 (100%) | 194 (99%) | 2 (1%) | 68 77 |
| All | All | 19544/21471 (91%) | 19527 (100%) | 17 (0%) | 88 89 |

All (17) residues with a non-rotameric sidechain are listed below:

| Mol | Chain | Res | Type |
|---|---|---|---|
| 37 | AJ | 98 | ARG |
| 52 | H | 21 | GLN |
| 59 | O | 36 | LEU |
| 59 | O | 39 | ASP |
| 64 | T | 48 | ASN |
| 78 | h | 153 | GLU |
| 78 | h | 159 | LEU |
| 78 | h | 160 | ARG |
| 12 | BE | 3 | ARG |
| 20 | BM | 130 | ASN |
| 45 | CL | 82 | LYS |
| 78 | DS | 183 | CYS |
| 78 | DS | 186 | CYS |
| 82 | l1 | 4 | ILE |
| 82 | l1 | 215 | ARG |
| 80 | p0 | 5 | ARG |
| 80 | p0 | 12 | PHE |

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (170) such sidechains are listed below:

| Mol | Chain | Res | Type |
|---|---|---|---|
| 4 | j | 205 | ASN |
| 5 | k | 25 | GLN |
| 5 | k | 182 | GLN |
| 5 | k | 259 | ASN |
| 5 | k | 316 | ASN |
| 6 | l | 16 | GLN |
| 6 | l | 49 | GLN |
| 6 | l | 56 | ASN |
| 6 | l | 321 | ASN |
| 7 | m | 17 | GLN |
| 7 | m | 45 | ASN |
| 7 | m | 151 | GLN |
| 9 | o | 17 | GLN |
| 9 | o | 91 | ASN |
| 9 | o | 192 | ASN |
| 9 | o | 198 | ASN |
| 9 | o | 239 | GLN |
| 10 | p | 192 | HIS |
| 11 | q | 102 | ASN |
| 11 | q | 116 | ASN |
| 12 | r | 100 | ASN |
| 15 | u | 112 | GLN |
| 16 | v | 123 | GLN |
| 17 | w | 51 | ASN |
| 18 | x | 121 | HIS |
| 18 | x | 125 | GLN |
| 18 | x | 133 | HIS |
| 18 | x | 169 | ASN |
| 18 | x | 179 | GLN |
| 19 | y | 58 | ASN |
| 20 | z | 92 | GLN |
| 20 | z | 166 | ASN |
| 21 | 0 | 13 | ASN |
| 22 | 2 | 54 | HIS |
| 23 | 5 | 30 | GLN |
| 23 | 5 | 62 | ASN |
| 27 | 9 | 42 | GLN |
| 27 | 9 | 81 | GLN |
| 28 | AA | 122 | HIS |
| 29 | AB | 40 | HIS |
| 31 | AD | 73 | GLN |

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| Mol | Chain | Res | Type |
|---|---|---|---|
| 34 | AG | 24 | ASN |
| 36 | AI | 45 | HIS |
| 36 | AI | 59 | ASN |
| 36 | AI | 107 | GLN |
| 36 | AI | 113 | GLN |
| 38 | AK | 69 | HIS |
| 39 | AL | 40 | GLN |
| 39 | AL | 51 | GLN |
| 39 | AL | 57 | ASN |
| 39 | AL | 77 | ASN |
| 41 | AN | 41 | HIS |
| 44 | AQ | 32 | GLN |
| 44 | AQ | 56 | ASN |
| 47 | C | 21 | ASN |
| 47 | C | 30 | GLN |
| 47 | C | 33 | ASN |
| 47 | C | 46 | ASN |
| 47 | C | 49 | ASN |
| 49 | E | 54 | HIS |
| 49 | E | 84 | GLN |
| 51 | G | 188 | ASN |
| 52 | H | 34 | GLN |
| 52 | H | 37 | GLN |
| 53 | I | 139 | ASN |
| 54 | J | 19 | GLN |
| 59 | O | 38 | HIS |
| 59 | O | 134 | ASN |
| 60 | P | 123 | HIS |
| 61 | Q | 75 | HIS |
| 63 | S | 93 | GLN |
| 64 | T | 48 | ASN |
| 64 | T | 74 | GLN |
| 65 | U | 19 | ASN |
| 65 | U | 63 | GLN |
| 66 | V | 23 | GLN |
| 67 | W | 35 | ASN |
| 69 | Y | 12 | ASN |
| 69 | Y | 42 | GLN |
| 69 | Y | 70 | ASN |
| 69 | Y | 80 | ASN |
| 70 | Z | 94 | ASN |
| 71 | a | 106 | GLN |

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| Mol | Chain | Res | Type |
|---|---|---|---|
| 72 | b | 37 | GLN |
| 79 | AR | 53 | ASN |
| 79 | AR | 102 | GLN |
| 5 | AX | 25 | GLN |
| 5 | AX | 182 | GLN |
| 5 | AX | 198 | HIS |
| 5 | AX | 259 | ASN |
| 5 | AX | 279 | ASN |
| 5 | AX | 316 | ASN |
| 6 | AY | 6 | GLN |
| 6 | AY | 16 | GLN |
| 6 | AY | 117 | ASN |
| 6 | AY | 202 | GLN |
| 6 | AY | 321 | ASN |
| 7 | AZ | 151 | GLN |
| 8 | BA | 60 | ASN |
| 9 | BB | 50 | GLN |
| 9 | BB | 144 | GLN |
| 10 | BC | 146 | ASN |
| 10 | BC | 192 | HIS |
| 11 | BD | 102 | ASN |
| 12 | BE | 55 | ASN |
| 12 | BE | 100 | ASN |
| 12 | BE | 187 | ASN |
| 13 | BF | 43 | GLN |
| 13 | BF | 161 | GLN |
| 14 | BG | 106 | GLN |
| 16 | BI | 175 | ASN |
| 17 | BJ | 51 | ASN |
| 18 | BK | 125 | GLN |
| 19 | BL | 27 | GLN |
| 20 | BM | 130 | ASN |
| 20 | BM | 134 | HIS |
| 20 | BM | 174 | GLN |
| 20 | BM | 175 | GLN |
| 27 | BT | 81 | GLN |
| 30 | BW | 6 | ASN |
| 30 | BW | 48 | HIS |
| 31 | BX | 73 | GLN |
| 33 | BZ | 36 | GLN |
| 34 | CA | 5 | HIS |
| 34 | CA | 24 | ASN |

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| Mol | Chain | Res | Type |
|---|---|---|---|
| 38 | CE | 69 | HIS |
| 38 | CE | 79 | GLN |
| 39 | CF | 51 | GLN |
| 41 | CH | 33 | ASN |
| 43 | CJ | 22 | GLN |
| 45 | CL | 33 | ASN |
| 47 | CN | 21 | ASN |
| 47 | CN | 33 | ASN |
| 48 | CO | 40 | ASN |
| 48 | CO | 232 | HIS |
| 49 | CP | 54 | HIS |
| 49 | CP | 84 | GLN |
| 51 | CR | 17 | HIS |
| 51 | CR | 98 | HIS |
| 51 | CR | 188 | ASN |
| 51 | CR | 216 | ASN |
| 51 | CR | 260 | GLN |
| 52 | CS | 34 | GLN |
| 53 | CT | 22 | HIS |
| 53 | CT | 81 | HIS |
| 53 | CT | 139 | ASN |
| 54 | CU | 176 | GLN |
| 55 | CV | 32 | GLN |
| 55 | CV | 35 | ASN |
| 55 | CV | 116 | HIS |
| 57 | CX | 17 | GLN |
| 57 | CX | 58 | GLN |
| 58 | CY | 18 | HIS |
| 58 | CY | 92 | HIS |
| 63 | DD | 138 | GLN |
| 64 | DE | 42 | GLN |
| 66 | DG | 12 | GLN |
| 66 | DG | 93 | HIS |
| 68 | DI | 21 | ASN |
| 68 | DI | 33 | GLN |
| 69 | DJ | 44 | HIS |
| 69 | DJ | 64 | GLN |
| 70 | DK | 10 | ASN |
| 72 | DM | 38 | HIS |
| 74 | DO | 9 | HIS |
| 75 | DP | 27 | GLN |
| 79 | DT | 311 | GLN |

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| Mol | Chain | Res | Type |
|---|---|---|---|
| 80 | P0 | 103 | ASN |
| 82 | L1 | 182 | GLN |
| 82 | l1 | 12 | ASN |

### 5.3.3 RNA

| Mol | Chain | Analysed | Backbone Outliers | Pucker Outliers |
|---|---|---|---|---|
| 1 | 1 | 3203/3359 (95%) | 594 (18%) | 44 (1%) |
| 1 | AS | 3223/3359 (95%) | 625 (19%) | 52 (1%) |
| 2 | 3 | 120/121 (99%) | 9 (7%) | 0 |
| 2 | AT | 120/121 (99%) | 9 (7%) | 0 |
| 3 | 4 | 156/158 (98%) | 23 (14%) | 3 (1%) |
| 3 | AU | 156/158 (98%) | 23 (14%) | 3 (1%) |
| 46 | B | 1736/1787 (97%) | 433 (24%) | 42 (2%) |
| 46 | CM | 1762/1787 (98%) | 454 (25%) | 55 (3%) |
| All | All | 10476/10850 (96%) | 2170 (20%) | 199 (1%) |

All (2170) RNA backbone outliers are listed below:

| Mol | Chain | Res | Type |
|---|---|---|---|
| 1 | 1 | 15 | A |
| 1 | 1 | 24 | U |
| 1 | 1 | 25 | A |
| 1 | 1 | 29 | G |
| 1 | 1 | 39 | A |
| 1 | 1 | 42 | A |
| 1 | 1 | 48 | A |
| 1 | 1 | 56 | A |
| 1 | 1 | 58 | G |
| 1 | 1 | 59 | A |
| 1 | 1 | 64 | A |
| 1 | 1 | 65 | A |
| 1 | 1 | 91 | G |
| 1 | 1 | 98 | A |
| 1 | 1 | 104 | C |
| 1 | 1 | 108 | A |
| 1 | 1 | 109 | G |
| 1 | 1 | 110 | C |
| 1 | 1 | 121 | A |
| 1 | 1 | 134 | U |
| 1 | 1 | 135 | G |

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| Mol | Chain | Res | Type |
|---|---|---|---|
| 1 | 1 | 155 | A |
| 1 | 1 | 156 | A |
| 1 | 1 | 164 | U |
| 1 | 1 | 169 | G |
| 1 | 1 | 172 | C |
| 1 | 1 | 173 | C |
| 1 | 1 | 175 | G |
| 1 | 1 | 186 | A |
| 1 | 1 | 189 | U |
| 1 | 1 | 190 | U |
| 1 | 1 | 199 | C |
| 1 | 1 | 205 | G |
| 1 | 1 | 209 | C |
| 1 | 1 | 212 | A |
| 1 | 1 | 217 | G |
| 1 | 1 | 218 | A |
| 1 | 1 | 219 | G |
| 1 | 1 | 230 | G |
| 1 | 1 | 236 | A |
| 1 | 1 | 239 | A |
| 1 | 1 | 240 | C |
| 1 | 1 | 243 | G |
| 1 | 1 | 245 | G |
| 1 | 1 | 249 | G |
| 1 | 1 | 250 | U |
| 1 | 1 | 269 | G |
| 1 | 1 | 286 | U |
| 1 | 1 | 295 | A |
| 1 | 1 | 305 | U |
| 1 | 1 | 311 | C |
| 1 | 1 | 323 | A |
| 1 | 1 | 329 | U |
| 1 | 1 | 337 | G |
| 1 | 1 | 338 | A |
| 1 | 1 | 339 | C |
| 1 | 1 | 349 | A |
| 1 | 1 | 350 | C |
| 1 | 1 | 376 | G |
| 1 | 1 | 377 | A |
| 1 | 1 | 387 | A |
| 1 | 1 | 395 | A |
| 1 | 1 | 398 | A |

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| Mol | Chain | Res | Type |
|---|---|---|---|
| 1 | 1 | 402 | A |
| 1 | 1 | 403 | C |
| 1 | 1 | 404 | G |
| 1 | 1 | 420 | G |
| 1 | 1 | 421 | G |
| 1 | 1 | 422 | A |
| 1 | 1 | 438 | A |
| 1 | 1 | 439 | C |
| 1 | 1 | 448 | U |
| 1 | 1 | 482 | U |
| 1 | 1 | 506 | A |
| 1 | 1 | 517 | A |
| 1 | 1 | 519 | U |
| 1 | 1 | 531 | G |
| 1 | 1 | 532 | U |
| 1 | 1 | 538 | G |
| 1 | 1 | 539 | G |
| 1 | 1 | 540 | C |
| 1 | 1 | 541 | U |
| 1 | 1 | 542 | U |
| 1 | 1 | 543 | C |
| 1 | 1 | 544 | U |
| 1 | 1 | 545 | G |
| 1 | 1 | 546 | C |
| 1 | 1 | 555 | A |
| 1 | 1 | 556 | U |
| 1 | 1 | 557 | A |
| 1 | 1 | 564 | G |
| 1 | 1 | 576 | A |
| 1 | 1 | 577 | G |
| 1 | 1 | 589 | G |
| 1 | 1 | 590 | A |
| 1 | 1 | 598 | U |
| 1 | 1 | 609 | A |
| 1 | 1 | 618 | U |
| 1 | 1 | 619 | A |
| 1 | 1 | 620 | A |
| 1 | 1 | 635 | C |
| 1 | 1 | 647 | A |
| 1 | 1 | 658 | A |
| 1 | 1 | 665 | C |
| 1 | 1 | 675 | A |

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| Mol | Chain | Res | Type |
|---|---|---|---|
| 1 | 1 | 679 | U |
| 1 | 1 | 681 | U |
| 1 | 1 | 688 | A |
| 1 | 1 | 689 | A |
| 1 | 1 | 703 | A |
| 1 | 1 | 710 | G |
| 1 | 1 | 713 | A |
| 1 | 1 | 717 | A |
| 1 | 1 | 723 | G |
| 1 | 1 | 730 | A |
| 1 | 1 | 732 | U |
| 1 | 1 | 760 | U |
| 1 | 1 | 763 | U |
| 1 | 1 | 772 | U |
| 1 | 1 | 773 | U |
| 1 | 1 | 776 | A |
| 1 | 1 | 777 | G |
| 1 | 1 | 780 | A |
| 1 | 1 | 781 | G |
| 1 | 1 | 802 | A |
| 1 | 1 | 813 | A |
| 1 | 1 | 826 | A |
| 1 | 1 | 845 | C |
| 1 | 1 | 857 | C |
| 1 | 1 | 861 | U |
| 1 | 1 | 870 | U |
| 1 | 1 | 875 | U |
| 1 | 1 | 903 | G |
| 1 | 1 | 904 | G |
| 1 | 1 | 910 | A |
| 1 | 1 | 912 | G |
| 1 | 1 | 913 | A |
| 1 | 1 | 917 | A |
| 1 | 1 | 919 | C |
| 1 | 1 | 921 | A |
| 1 | 1 | 933 | G |
| 1 | 1 | 935 | U |
| 1 | 1 | 940 | C |
| 1 | 1 | 949 | G |
| 1 | 1 | 955 | C |
| 1 | 1 | 956 | U |
| 1 | 1 | 958 | A |

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| Mol | Chain | Res | Type |
|---|---|---|---|
| 1 | 1 | 959 | G |
| 1 | 1 | 977 | U |
| 1 | 1 | 990 | G |
| 1 | 1 | 991 | U |
| 1 | 1 | 996 | C |
| 1 | 1 | 997 | G |
| 1 | 1 | 998 | A |
| 1 | 1 | 1006 | G |
| 1 | 1 | 1011 | C |
| 1 | 1 | 1012 | U |
| 1 | 1 | 1013 | U |
| 1 | 1 | 1014 | G |
| 1 | 1 | 1019 | U |
| 1 | 1 | 1020 | G |
| 1 | 1 | 1021 | A |
| 1 | 1 | 1023 | A |
| 1 | 1 | 1024 | U |
| 1 | 1 | 1025 | G |
| 1 | 1 | 1027 | C |
| 1 | 1 | 1030 | U |
| 1 | 1 | 1033 | C |
| 1 | 1 | 1043 | A |
| 1 | 1 | 1045 | C |
| 1 | 1 | 1060 | A |
| 1 | 1 | 1061 | A |
| 1 | 1 | 1068 | G |
| 1 | 1 | 1077 | U |
| 1 | 1 | 1078 | U |
| 1 | 1 | 1089 | A |
| 1 | 1 | 1090 | A |
| 1 | 1 | 1091 | U |
| 1 | 1 | 1092 | U |
| 1 | 1 | 1094 | A |
| 1 | 1 | 1099 | A |
| 1 | 1 | 1100 | G |
| 1 | 1 | 1113 | G |
| 1 | 1 | 1127 | G |
| 1 | 1 | 1140 | U |
| 1 | 1 | 1149 | A |
| 1 | 1 | 1150 | A |
| 1 | 1 | 1151 | C |
| 1 | 1 | 1155 | A |

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| Mol | Chain | Res | Type |
|---|---|---|---|
| 1 | 1 | 1156 | C |
| 1 | 1 | 1164 | U |
| 1 | 1 | 1174 | G |
| 1 | 1 | 1176 | A |
| 1 | 1 | 1177 | U |
| 1 | 1 | 1178 | G |
| 1 | 1 | 1188 | C |
| 1 | 1 | 1189 | A |
| 1 | 1 | 1192 | C |
| 1 | 1 | 1197 | C |
| 1 | 1 | 1204 | U |
| 1 | 1 | 1205 | G |
| 1 | 1 | 1218 | G |
| 1 | 1 | 1223 | C |
| 1 | 1 | 1224 | C |
| 1 | 1 | 1230 | G |
| 1 | 1 | 1231 | U |
| 1 | 1 | 1232 | G |
| 1 | 1 | 1239 | G |
| 1 | 1 | 1240 | A |
| 1 | 1 | 1241 | A |
| 1 | 1 | 1242 | G |
| 1 | 1 | 1244 | C |
| 1 | 1 | 1245 | G |
| 1 | 1 | 1246 | G |
| 1 | 1 | 1247 | A |
| 1 | 1 | 1249 | U |
| 1 | 1 | 1250 | C |
| 1 | 1 | 1252 | G |
| 1 | 1 | 1254 | U |
| 1 | 1 | 1255 | A |
| 1 | 1 | 1257 | G |
| 1 | 1 | 1258 | G |
| 1 | 1 | 1259 | A |
| 1 | 1 | 1261 | U |
| 1 | 1 | 1262 | G |
| 1 | 1 | 1263 | U |
| 1 | 1 | 1264 | G |
| 1 | 1 | 1265 | U |
| 1 | 1 | 1266 | A |
| 1 | 1 | 1267 | A |
| 1 | 1 | 1270 | A |

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| Mol | Chain | Res | Type |
|---|---|---|---|
| 1 | 1 | 1271 | C |
| 1 | 1 | 1273 | C |
| 1 | 1 | 1274 | A |
| 1 | 1 | 1278 | G |
| 1 | 1 | 1280 | C |
| 1 | 1 | 1282 | A |
| 1 | 1 | 1303 | G |
| 1 | 1 | 1304 | A |
| 1 | 1 | 1305 | U |
| 1 | 1 | 1309 | G |
| 1 | 1 | 1312 | C |
| 1 | 1 | 1326 | A |
| 1 | 1 | 1345 | G |
| 1 | 1 | 1346 | U |
| 1 | 1 | 1347 | U |
| 1 | 1 | 1348 | U |
| 1 | 1 | 1349 | U |
| 1 | 1 | 1382 | A |
| 1 | 1 | 1395 | U |
| 1 | 1 | 1415 | A |
| 1 | 1 | 1417 | G |
| 1 | 1 | 1421 | U |
| 1 | 1 | 1427 | G |
| 1 | 1 | 1430 | G |
| 1 | 1 | 1433 | C |
| 1 | 1 | 1442 | A |
| 1 | 1 | 1446 | G |
| 1 | 1 | 1465 | C |
| 1 | 1 | 1471 | A |
| 1 | 1 | 1477 | A |
| 1 | 1 | 1484 | G |
| 1 | 1 | 1498 | C |
| 1 | 1 | 1504 | C |
| 1 | 1 | 1520 | A |
| 1 | 1 | 1523 | C |
| 1 | 1 | 1525 | A |
| 1 | 1 | 1526 | U |
| 1 | 1 | 1532 | G |
| 1 | 1 | 1535 | A |
| 1 | 1 | 1552 | C |
| 1 | 1 | 1556 | G |
| 1 | 1 | 1558 | G |

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| Mol | Chain | Res | Type |
|---|---|---|---|
| 1 | 1 | 1559 | C |
| 1 | 1 | 1560 | U |
| 1 | 1 | 1561 | U |
| 1 | 1 | 1562 | G |
| 1 | 1 | 1563 | A |
| 1 | 1 | 1565 | U |
| 1 | 1 | 1566 | U |
| 1 | 1 | 1567 | U |
| 1 | 1 | 1568 | U |
| 1 | 1 | 1569 | C |
| 1 | 1 | 1571 | G |
| 1 | 1 | 1572 | G |
| 1 | 1 | 1574 | C |
| 1 | 1 | 1576 | A |
| 1 | 1 | 1577 | C |
| 1 | 1 | 1585 | A |
| 1 | 1 | 1589 | A |
| 1 | 1 | 1601 | A |
| 1 | 1 | 1603 | U |
| 1 | 1 | 1624 | C |
| 1 | 1 | 1625 | U |
| 1 | 1 | 1635 | C |
| 1 | 1 | 1638 | A |
| 1 | 1 | 1639 | A |
| 1 | 1 | 1641 | U |
| 1 | 1 | 1648 | G |
| 1 | 1 | 1653 | C |
| 1 | 1 | 1654 | G |
| 1 | 1 | 1679 | A |
| 1 | 1 | 1720 | U |
| 1 | 1 | 1721 | C |
| 1 | 1 | 1732 | G |
| 1 | 1 | 1746 | A |
| 1 | 1 | 1747 | G |
| 1 | 1 | 1755 | U |
| 1 | 1 | 1756 | A |
| 1 | 1 | 1757 | A |
| 1 | 1 | 1758 | U |
| 1 | 1 | 1760 | U |
| 1 | 1 | 1761 | U |
| 1 | 1 | 1762 | G |
| 1 | 1 | 1763 | C |

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| Mol | Chain | Res | Type |
|---|---|---|---|
| 1 | 1 | 1776 | G |
| 1 | 1 | 1793 | A |
| 1 | 1 | 1804 | G |
| 1 | 1 | 1809 | A |
| 1 | 1 | 1810 | A |
| 1 | 1 | 1811 | U |
| 1 | 1 | 1812 | A |
| 1 | 1 | 1814 | U |
| 1 | 1 | 1815 | U |
| 1 | 1 | 1816 | U |
| 1 | 1 | 1817 | U |
| 1 | 1 | 1837 | A |
| 1 | 1 | 1838 | A |
| 1 | 1 | 1842 | C |
| 1 | 1 | 1845 | C |
| 1 | 1 | 1862 | C |
| 1 | 1 | 1874 | G |
| 1 | 1 | 1882 | A |
| 1 | 1 | 1889 | A |
| 1 | 1 | 1902 | G |
| 1 | 1 | 1944 | G |
| 1 | 1 | 1949 | G |
| 1 | 1 | 2068 | U |
| 1 | 1 | 2069 | U |
| 1 | 1 | 2070 | A |
| 1 | 1 | 2071 | A |
| 1 | 1 | 2078 | A |
| 1 | 1 | 2088 | G |
| 1 | 1 | 2089 | G |
| 1 | 1 | 2091 | A |
| 1 | 1 | 2092 | C |
| 1 | 1 | 2099 | G |
| 1 | 1 | 2100 | G |
| 1 | 1 | 2109 | A |
| 1 | 1 | 2118 | U |
| 1 | 1 | 2122 | A |
| 1 | 1 | 2136 | A |
| 1 | 1 | 2147 | G |
| 1 | 1 | 2149 | G |
| 1 | 1 | 2183 | U |
| 1 | 1 | 2184 | G |
| 1 | 1 | 2185 | A |

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| Mol | Chain | Res | Type |
|---|---|---|---|
| 1 | 1 | 2186 | A |
| 1 | 1 | 2187 | U |
| 1 | 1 | 2188 | G |
| 1 | 1 | 2201 | A |
| 1 | 1 | 2222 | A |
| 1 | 1 | 2227 | G |
| 1 | 1 | 2233 | A |
| 1 | 1 | 2234 | A |
| 1 | 1 | 2235 | C |
| 1 | 1 | 2250 | G |
| 1 | 1 | 2251 | G |
| 1 | 1 | 2259 | A |
| 1 | 1 | 2260 | U |
| 1 | 1 | 2276 | U |
| 1 | 1 | 2285 | G |
| 1 | 1 | 2286 | C |
| 1 | 1 | 2288 | U |
| 1 | 1 | 2291 | A |
| 1 | 1 | 2292 | U |
| 1 | 1 | 2293 | G |
| 1 | 1 | 2313 | G |
| 1 | 1 | 2314 | U |
| 1 | 1 | 2341 | A |
| 1 | 1 | 2351 | A |
| 1 | 1 | 2352 | C |
| 1 | 1 | 2353 | G |
| 1 | 1 | 2363 | G |
| 1 | 1 | 2366 | U |
| 1 | 1 | 2371 | G |
| 1 | 1 | 2372 | G |
| 1 | 1 | 2375 | A |
| 1 | 1 | 2380 | A |
| 1 | 1 | 2381 | G |
| 1 | 1 | 2382 | A |
| 1 | 1 | 2389 | U |
| 1 | 1 | 2396 | G |
| 1 | 1 | 2397 | A |
| 1 | 1 | 2413 | G |
| 1 | 1 | 2420 | G |
| 1 | 1 | 2421 | A |
| 1 | 1 | 2422 | C |
| 1 | 1 | 2423 | A |

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| Mol | Chain | Res | Type |
|---|---|---|---|
| 1 | 1 | 2427 | A |
| 1 | 1 | 2430 | G |
| 1 | 1 | 2431 | U |
| 1 | 1 | 2432 | G |
| 1 | 1 | 2433 | U |
| 1 | 1 | 2437 | A |
| 1 | 1 | 2438 | U |
| 1 | 1 | 2439 | A |
| 1 | 1 | 2441 | G |
| 1 | 1 | 2442 | U |
| 1 | 1 | 2443 | G |
| 1 | 1 | 2444 | G |
| 1 | 1 | 2445 | G |
| 1 | 1 | 2446 | A |
| 1 | 1 | 2448 | C |
| 1 | 1 | 2449 | U |
| 1 | 1 | 2451 | C |
| 1 | 1 | 2452 | G |
| 1 | 1 | 2456 | C |
| 1 | 1 | 2457 | C |
| 1 | 1 | 2459 | G |
| 1 | 1 | 2460 | U |
| 1 | 1 | 2464 | A |
| 1 | 1 | 2468 | C |
| 1 | 1 | 2470 | C |
| 1 | 1 | 2471 | U |
| 1 | 1 | 2472 | A |
| 1 | 1 | 2473 | C |
| 1 | 1 | 2475 | U |
| 1 | 1 | 2476 | C |
| 1 | 1 | 2477 | U |
| 1 | 1 | 2480 | A |
| 1 | 1 | 2482 | U |
| 1 | 1 | 2483 | U |
| 1 | 1 | 2489 | A |
| 1 | 1 | 2492 | U |
| 1 | 1 | 2493 | A |
| 1 | 1 | 2511 | G |
| 1 | 1 | 2513 | A |
| 1 | 1 | 2515 | G |
| 1 | 1 | 2516 | U |
| 1 | 1 | 2517 | C |

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| Mol | Chain | Res | Type |
|---|---|---|---|
| 1 | 1 | 2518 | A |
| 1 | 1 | 2519 | A |
| 1 | 1 | 2520 | A |
| 1 | 1 | 2521 | C |
| 1 | 1 | 2529 | U |
| 1 | 1 | 2530 | C |
| 1 | 1 | 2533 | G |
| 1 | 1 | 2536 | U |
| 1 | 1 | 2538 | A |
| 1 | 1 | 2545 | C |
| 1 | 1 | 2546 | U |
| 1 | 1 | 2554 | C |
| 1 | 1 | 2557 | G |
| 1 | 1 | 2565 | A |
| 1 | 1 | 2566 | C |
| 1 | 1 | 2578 | G |
| 1 | 1 | 2579 | G |
| 1 | 1 | 2586 | G |
| 1 | 1 | 2598 | A |
| 1 | 1 | 2623 | G |
| 1 | 1 | 2624 | U |
| 1 | 1 | 2628 | A |
| 1 | 1 | 2638 | C |
| 1 | 1 | 2644 | G |
| 1 | 1 | 2646 | A |
| 1 | 1 | 2649 | G |
| 1 | 1 | 2661 | A |
| 1 | 1 | 2662 | G |
| 1 | 1 | 2663 | A |
| 1 | 1 | 2664 | A |
| 1 | 1 | 2666 | A |
| 1 | 1 | 2676 | A |
| 1 | 1 | 2677 | A |
| 1 | 1 | 2686 | G |
| 1 | 1 | 2691 | U |
| 1 | 1 | 2699 | A |
| 1 | 1 | 2700 | G |
| 1 | 1 | 2701 | U |
| 1 | 1 | 2724 | U |
| 1 | 1 | 2725 | G |
| 1 | 1 | 2734 | A |
| 1 | 1 | 2745 | C |

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| Mol | Chain | Res | Type |
|---|---|---|---|
| 1 | 1 | 2749 | G |
| 1 | 1 | 2750 | G |
| 1 | 1 | 2768 | G |
| 1 | 1 | 2771 | A |
| 1 | 1 | 2772 | G |
| 1 | 1 | 2773 | A |
| 1 | 1 | 2774 | A |
| 1 | 1 | 2782 | C |
| 1 | 1 | 2786 | G |
| 1 | 1 | 2789 | A |
| 1 | 1 | 2790 | U |
| 1 | 1 | 2808 | C |
| 1 | 1 | 2814 | U |
| 1 | 1 | 2815 | U |
| 1 | 1 | 2817 | A |
| 1 | 1 | 2833 | U |
| 1 | 1 | 2839 | C |
| 1 | 1 | 2843 | G |
| 1 | 1 | 2844 | A |
| 1 | 1 | 2847 | U |
| 1 | 1 | 2859 | A |
| 1 | 1 | 2861 | C |
| 1 | 1 | 2866 | C |
| 1 | 1 | 2870 | G |
| 1 | 1 | 2871 | C |
| 1 | 1 | 2886 | G |
| 1 | 1 | 2895 | U |
| 1 | 1 | 2907 | U |
| 1 | 1 | 2908 | A |
| 1 | 1 | 2911 | G |
| 1 | 1 | 2914 | C |
| 1 | 1 | 2919 | G |
| 1 | 1 | 2920 | C |
| 1 | 1 | 2923 | G |
| 1 | 1 | 2926 | U |
| 1 | 1 | 2943 | A |
| 1 | 1 | 2955 | C |
| 1 | 1 | 2962 | G |
| 1 | 1 | 2969 | G |
| 1 | 1 | 2984 | A |
| 1 | 1 | 3021 | A |
| 1 | 1 | 3028 | U |

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| Mol | Chain | Res | Type |
|---|---|---|---|
| 1 | 1 | 3031 | G |
| 1 | 1 | 3050 | A |
| 1 | 1 | 3051 | C |
| 1 | 1 | 3052 | G |
| 1 | 1 | 3058 | A |
| 1 | 1 | 3064 | C |
| 1 | 1 | 3073 | G |
| 1 | 1 | 3094 | A |
| 1 | 1 | 3101 | A |
| 1 | 1 | 3102 | A |
| 1 | 1 | 3103 | U |
| 1 | 1 | 3114 | A |
| 1 | 1 | 3115 | C |
| 1 | 1 | 3126 | U |
| 1 | 1 | 3127 | U |
| 1 | 1 | 3143 | G |
| 1 | 1 | 3144 | A |
| 1 | 1 | 3146 | G |
| 1 | 1 | 3149 | U |
| 1 | 1 | 3151 | C |
| 1 | 1 | 3157 | A |
| 1 | 1 | 3160 | C |
| 1 | 1 | 3161 | U |
| 1 | 1 | 3162 | U |
| 1 | 1 | 3163 | U |
| 1 | 1 | 3164 | U |
| 1 | 1 | 3165 | U |
| 1 | 1 | 3166 | A |
| 1 | 1 | 3167 | G |
| 1 | 1 | 3171 | C |
| 1 | 1 | 3172 | U |
| 1 | 1 | 3182 | C |
| 1 | 1 | 3183 | A |
| 1 | 1 | 3184 | G |
| 1 | 1 | 3194 | G |
| 1 | 1 | 3208 | A |
| 1 | 1 | 3210 | A |
| 1 | 1 | 3212 | G |
| 1 | 1 | 3214 | U |
| 1 | 1 | 3221 | G |
| 1 | 1 | 3224 | U |
| 1 | 1 | 3228 | G |

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| Mol | Chain | Res | Type |
|---|---|---|---|
| 1 | 1 | 3235 | A |
| 1 | 1 | 3241 | G |
| 1 | 1 | 3246 | C |
| 1 | 1 | 3252 | C |
| 1 | 1 | 3259 | A |
| 1 | 1 | 3260 | A |
| 1 | 1 | 3268 | G |
| 1 | 1 | 3269 | C |
| 1 | 1 | 3272 | A |
| 1 | 1 | 3278 | U |
| 1 | 1 | 3281 | A |
| 1 | 1 | 3284 | U |
| 1 | 1 | 3285 | A |
| 1 | 1 | 3306 | U |
| 1 | 1 | 3307 | A |
| 1 | 1 | 3309 | A |
| 1 | 1 | 3310 | G |
| 1 | 1 | 3316 | U |
| 1 | 1 | 3317 | U |
| 1 | 1 | 3318 | G |
| 1 | 1 | 3319 | U |
| 1 | 1 | 3320 | U |
| 1 | 1 | 3321 | G |
| 1 | 1 | 3334 | G |
| 1 | 1 | 3343 | C |
| 1 | 1 | 3351 | G |
| 1 | 1 | 3361 | U |
| 2 | 3 | 7 | G |
| 2 | 3 | 22 | A |
| 2 | 3 | 54 | U |
| 2 | 3 | 55 | A |
| 2 | 3 | 65 | G |
| 2 | 3 | 73 | C |
| 2 | 3 | 76 | A |
| 2 | 3 | 102 | A |
| 2 | 3 | 112 | G |
| 3 | 4 | 23 | U |
| 3 | 4 | 34 | U |
| 3 | 4 | 35 | C |
| 3 | 4 | 59 | A |
| 3 | 4 | 62 | C |
| 3 | 4 | 63 | G |

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| Mol | Chain | Res | Type |
|---|---|---|---|
| 3 | 4 | 81 | A |
| 3 | 4 | 84 | C |
| 3 | 4 | 85 | G |
| 3 | 4 | 86 | U |
| 3 | 4 | 87 | G |
| 3 | 4 | 92 | A |
| 3 | 4 | 95 | G |
| 3 | 4 | 102 | U |
| 3 | 4 | 104 | A |
| 3 | 4 | 106 | C |
| 3 | 4 | 111 | A |
| 3 | 4 | 113 | U |
| 3 | 4 | 125 | U |
| 3 | 4 | 126 | A |
| 3 | 4 | 148 | G |
| 3 | 4 | 152 | G |
| 3 | 4 | 157 | U |
| 46 | B | 17 | C |
| 46 | B | 25 | C |
| 46 | B | 26 | A |
| 46 | B | 27 | U |
| 46 | B | 34 | G |
| 46 | B | 47 | A |
| 46 | B | 57 | G |
| 46 | B | 66 | U |
| 46 | B | 74 | U |
| 46 | B | 75 | U |
| 46 | B | 76 | A |
| 46 | B | 78 | A |
| 46 | B | 79 | C |
| 46 | B | 81 | G |
| 46 | B | 84 | A |
| 46 | B | 93 | A |
| 46 | B | 104 | A |
| 46 | B | 114 | C |
| 46 | B | 115 | G |
| 46 | B | 123 | G |
| 46 | B | 126 | A |
| 46 | B | 127 | G |
| 46 | B | 128 | U |
| 46 | B | 129 | A |
| 46 | B | 130 | C |

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| Mol | Chain | Res | Type |
|---|---|---|---|
| 46 | B | 131 | C |
| 46 | B | 138 | C |
| 46 | B | 139 | U |
| 46 | B | 142 | G |
| 46 | B | 143 | A |
| 46 | B | 150 | U |
| 46 | B | 151 | G |
| 46 | B | 152 | G |
| 46 | B | 154 | A |
| 46 | B | 159 | U |
| 46 | B | 166 | A |
| 46 | B | 168 | U |
| 46 | B | 173 | G |
| 46 | B | 174 | C |
| 46 | B | 176 | U |
| 46 | B | 177 | A |
| 46 | B | 179 | A |
| 46 | B | 190 | U |
| 46 | B | 191 | U |
| 46 | B | 193 | G |
| 46 | B | 199 | G |
| 46 | B | 200 | A |
| 46 | B | 202 | G |
| 46 | B | 206 | U |
| 46 | B | 211 | A |
| 46 | B | 213 | A |
| 46 | B | 214 | U |
| 46 | B | 215 | A |
| 46 | B | 216 | A |
| 46 | B | 217 | A |
| 46 | B | 218 | A |
| 46 | B | 220 | A |
| 46 | B | 221 | U |
| 46 | B | 224 | A |
| 46 | B | 226 | G |
| 46 | B | 229 | U |
| 46 | B | 230 | U |
| 46 | B | 231 | C |
| 46 | B | 233 | G |
| 46 | B | 237 | C |
| 46 | B | 238 | U |
| 46 | B | 247 | U |

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| Mol | Chain | Res | Type |
|---|---|---|---|
| 46 | B | 255 | A |
| 46 | B | 259 | U |
| 46 | B | 260 | U |
| 46 | B | 261 | C |
| 46 | B | 262 | G |
| 46 | B | 266 | C |
| 46 | B | 269 | A |
| 46 | B | 270 | U |
| 46 | B | 274 | C |
| 46 | B | 276 | U |
| 46 | B | 277 | G |
| 46 | B | 278 | U |
| 46 | B | 279 | G |
| 46 | B | 283 | G |
| 46 | B | 285 | G |
| 46 | B | 297 | A |
| 46 | B | 312 | C |
| 46 | B | 314 | A |
| 46 | B | 318 | U |
| 46 | B | 319 | C |
| 46 | B | 320 | G |
| 46 | B | 335 | G |
| 46 | B | 336 | C |
| 46 | B | 350 | A |
| 46 | B | 357 | A |
| 46 | B | 358 | A |
| 46 | B | 359 | C |
| 46 | B | 388 | G |
| 46 | B | 398 | A |
| 46 | B | 400 | C |
| 46 | B | 402 | G |
| 46 | B | 414 | A |
| 46 | B | 416 | G |
| 46 | B | 421 | G |
| 46 | B | 422 | C |
| 46 | B | 423 | A |
| 46 | B | 424 | G |
| 46 | B | 432 | G |
| 46 | B | 437 | U |
| 46 | B | 442 | C |
| 46 | B | 446 | C |
| 46 | B | 452 | A |

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| Mol | Chain | Res | Type |
|---|---|---|---|
| 46 | B | 458 | A |
| 46 | B | 466 | A |
| 46 | B | 475 | A |
| 46 | B | 480 | U |
| 46 | B | 482 | C |
| 46 | B | 483 | A |
| 46 | B | 485 | G |
| 46 | B | 487 | C |
| 46 | B | 489 | C |
| 46 | B | 490 | U |
| 46 | B | 491 | U |
| 46 | B | 499 | U |
| 46 | B | 503 | A |
| 46 | B | 505 | U |
| 46 | B | 506 | U |
| 46 | B | 509 | A |
| 46 | B | 512 | G |
| 46 | B | 513 | A |
| 46 | B | 515 | U |
| 46 | B | 518 | A |
| 46 | B | 519 | A |
| 46 | B | 525 | A |
| 46 | B | 530 | U |
| 46 | B | 534 | C |
| 46 | B | 536 | A |
| 46 | B | 537 | G |
| 46 | B | 539 | A |
| 46 | B | 540 | A |
| 46 | B | 547 | G |
| 46 | B | 553 | A |
| 46 | B | 554 | A |
| 46 | B | 555 | G |
| 46 | B | 556 | U |
| 46 | B | 557 | C |
| 46 | B | 563 | C |
| 46 | B | 566 | G |
| 46 | B | 575 | G |
| 46 | B | 576 | U |
| 46 | B | 580 | U |
| 46 | B | 592 | A |
| 46 | B | 593 | G |
| 46 | B | 604 | A |

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| Mol | Chain | Res | Type |
|---|---|---|---|
| 46 | B | 609 | U |
| 46 | B | 617 | A |
| 46 | B | 618 | A |
| 46 | B | 620 | A |
| 46 | B | 621 | A |
| 46 | B | 633 | A |
| 46 | B | 639 | G |
| 46 | B | 645 | G |
| 46 | B | 647 | C |
| 46 | B | 648 | U |
| 46 | B | 649 | G |
| 46 | B | 650 | G |
| 46 | B | 651 | C |
| 46 | B | 652 | C |
| 46 | B | 653 | G |
| 46 | B | 654 | G |
| 46 | B | 670 | C |
| 46 | B | 671 | G |
| 46 | B | 672 | U |
| 46 | B | 673 | A |
| 46 | B | 674 | C |
| 46 | B | 675 | U |
| 46 | B | 676 | G |
| 46 | B | 677 | G |
| 46 | B | 678 | A |
| 46 | B | 679 | C |
| 46 | B | 680 | C |
| 46 | B | 681 | C |
| 46 | B | 688 | G |
| 46 | B | 695 | C |
| 46 | B | 696 | U |
| 46 | B | 697 | U |
| 46 | B | 698 | C |
| 46 | B | 701 | G |
| 46 | B | 702 | G |
| 46 | B | 703 | U |
| 46 | B | 704 | A |
| 46 | B | 705 | G |
| 46 | B | 706 | C |
| 46 | B | 707 | C |
| 46 | B | 718 | A |
| 46 | B | 719 | A |

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| Mol | Chain | Res | Type |
|---|---|---|---|
| 46 | B | 723 | G |
| 46 | B | 729 | U |
| 46 | B | 739 | A |
| 46 | B | 740 | A |
| 46 | B | 741 | A |
| 46 | B | 750 | G |
| 46 | B | 751 | U |
| 46 | B | 756 | A |
| 46 | B | 759 | A |
| 46 | B | 760 | G |
| 46 | B | 762 | C |
| 46 | B | 764 | U |
| 46 | B | 765 | U |
| 46 | B | 766 | U |
| 46 | B | 767 | G |
| 46 | B | 768 | C |
| 46 | B | 770 | C |
| 46 | B | 771 | G |
| 46 | B | 773 | A |
| 46 | B | 775 | A |
| 46 | B | 778 | U |
| 46 | B | 779 | U |
| 46 | B | 796 | A |
| 46 | B | 798 | A |
| 46 | B | 799 | G |
| 46 | B | 802 | C |
| 46 | B | 803 | G |
| 46 | B | 804 | U |
| 46 | B | 805 | U |
| 46 | B | 807 | U |
| 46 | B | 808 | G |
| 46 | B | 813 | U |
| 46 | B | 815 | U |
| 46 | B | 817 | U |
| 46 | B | 819 | G |
| 46 | B | 820 | U |
| 46 | B | 821 | U |
| 46 | B | 822 | G |
| 46 | B | 823 | G |
| 46 | B | 824 | U |
| 46 | B | 825 | U |
| 46 | B | 826 | U |

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| Mol | Chain | Res | Type |
|---|---|---|---|
| 46 | B | 828 | U |
| 46 | B | 829 | A |
| 46 | B | 831 | G |
| 46 | B | 840 | A |
| 46 | B | 842 | U |
| 46 | B | 847 | A |
| 46 | B | 848 | A |
| 46 | B | 856 | G |
| 46 | B | 857 | G |
| 46 | B | 869 | A |
| 46 | B | 871 | U |
| 46 | B | 875 | C |
| 46 | B | 877 | G |
| 46 | B | 878 | U |
| 46 | B | 879 | U |
| 46 | B | 881 | U |
| 46 | B | 891 | A |
| 46 | B | 909 | A |
| 46 | B | 910 | G |
| 46 | B | 911 | A |
| 46 | B | 918 | A |
| 46 | B | 920 | U |
| 46 | B | 927 | G |
| 46 | B | 945 | U |
| 46 | B | 951 | A |
| 46 | B | 973 | A |
| 46 | B | 975 | C |
| 46 | B | 977 | A |
| 46 | B | 988 | A |
| 46 | B | 989 | U |
| 46 | B | 990 | A |
| 46 | B | 997 | U |
| 46 | B | 998 | A |
| 46 | B | 1004 | A |
| 46 | B | 1005 | A |
| 46 | B | 1011 | A |
| 46 | B | 1013 | C |
| 46 | B | 1017 | G |
| 46 | B | 1024 | A |
| 46 | B | 1025 | G |
| 46 | B | 1039 | U |
| 46 | B | 1042 | U |

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| Mol | Chain | Res | Type |
|---|---|---|---|
| 46 | B | 1043 | U |
| 46 | B | 1044 | U |
| 46 | B | 1047 | U |
| 46 | B | 1055 | A |
| 46 | B | 1056 | U |
| 46 | B | 1057 | C |
| 46 | B | 1058 | G |
| 46 | B | 1059 | G |
| 46 | B | 1060 | C |
| 46 | B | 1061 | A |
| 46 | B | 1067 | C |
| 46 | B | 1077 | A |
| 46 | B | 1081 | C |
| 46 | B | 1085 | G |
| 46 | B | 1123 | A |
| 46 | B | 1135 | G |
| 46 | B | 1143 | C |
| 46 | B | 1145 | A |
| 46 | B | 1152 | G |
| 46 | B | 1168 | A |
| 46 | B | 1169 | A |
| 46 | B | 1170 | U |
| 46 | B | 1179 | A |
| 46 | B | 1181 | A |
| 46 | B | 1184 | G |
| 46 | B | 1185 | G |
| 46 | B | 1187 | A |
| 46 | B | 1193 | A |
| 46 | B | 1202 | A |
| 46 | B | 1203 | G |
| 46 | B | 1206 | A |
| 46 | B | 1207 | C |
| 46 | B | 1212 | A |
| 46 | B | 1215 | A |
| 46 | B | 1219 | A |
| 46 | B | 1220 | C |
| 46 | B | 1221 | A |
| 46 | B | 1229 | A |
| 46 | B | 1230 | G |
| 46 | B | 1231 | C |
| 46 | B | 1236 | U |
| 46 | B | 1243 | U |

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| Mol | Chain | Res | Type |
|---|---|---|---|
| 46 | B | 1250 | G |
| 46 | B | 1270 | U |
| 46 | B | 1299 | U |
| 46 | B | 1300 | U |
| 46 | B | 1301 | G |
| 46 | B | 1306 | A |
| 46 | B | 1325 | U |
| 46 | B | 1330 | A |
| 46 | B | 1336 | G |
| 46 | B | 1339 | G |
| 46 | B | 1342 | A |
| 46 | B | 1343 | G |
| 46 | B | 1345 | A |
| 46 | B | 1346 | U |
| 46 | B | 1348 | U |
| 46 | B | 1349 | G |
| 46 | B | 1352 | G |
| 46 | B | 1355 | A |
| 46 | B | 1356 | U |
| 46 | B | 1357 | A |
| 46 | B | 1359 | U |
| 46 | B | 1360 | C |
| 46 | B | 1364 | U |
| 46 | B | 1369 | G |
| 46 | B | 1370 | A |
| 46 | B | 1376 | U |
| 46 | B | 1380 | G |
| 46 | B | 1381 | A |
| 46 | B | 1382 | U |
| 46 | B | 1384 | U |
| 46 | B | 1385 | C |
| 46 | B | 1392 | A |
| 46 | B | 1397 | A |
| 46 | B | 1398 | G |
| 46 | B | 1399 | U |
| 46 | B | 1400 | U |
| 46 | B | 1401 | U |
| 46 | B | 1410 | A |
| 46 | B | 1413 | A |
| 46 | B | 1414 | G |
| 46 | B | 1415 | G |
| 46 | B | 1422 | A |

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| Mol | Chain | Res | Type |
|---|---|---|---|
| 46 | B | 1431 | G |
| 46 | B | 1433 | C |
| 46 | B | 1445 | C |
| 46 | B | 1446 | A |
| 46 | B | 1455 | A |
| 46 | B | 1457 | A |
| 46 | B | 1458 | C |
| 46 | B | 1461 | A |
| 46 | B | 1462 | C |
| 46 | B | 1463 | G |
| 46 | B | 1468 | C |
| 46 | B | 1476 | A |
| 46 | B | 1477 | U |
| 46 | B | 1480 | G |
| 46 | B | 1483 | U |
| 46 | B | 1485 | G |
| 46 | B | 1491 | G |
| 46 | B | 1502 | A |
| 46 | B | 1503 | A |
| 46 | B | 1508 | G |
| 46 | B | 1510 | G |
| 46 | B | 1511 | A |
| 46 | B | 1523 | G |
| 46 | B | 1524 | C |
| 46 | B | 1529 | G |
| 46 | B | 1530 | A |
| 46 | B | 1541 | U |
| 46 | B | 1544 | U |
| 46 | B | 1546 | G |
| 46 | B | 1560 | A |
| 46 | B | 1561 | G |
| 46 | B | 1571 | G |
| 46 | B | 1574 | A |
| 46 | B | 1575 | G |
| 46 | B | 1577 | G |
| 46 | B | 1580 | A |
| 46 | B | 1582 | U |
| 46 | B | 1584 | A |
| 46 | B | 1588 | G |
| 46 | B | 1621 | C |
| 46 | B | 1644 | U |
| 46 | B | 1645 | G |

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| Mol | Chain | Res | Type |
|---|---|---|---|
| 46 | B | 1665 | C |
| 46 | B | 1667 | G |
| 46 | B | 1670 | U |
| 46 | B | 1671 | G |
| 46 | B | 1672 | G |
| 46 | B | 1673 | U |
| 46 | B | 1696 | U |
| 46 | B | 1697 | C |
| 46 | B | 1699 | G |
| 46 | B | 1700 | G |
| 46 | B | 1701 | A |
| 46 | B | 1702 | A |
| 46 | B | 1703 | C |
| 46 | B | 1704 | C |
| 46 | B | 1737 | A |
| 46 | B | 1742 | A |
| 46 | B | 1743 | A |
| 46 | B | 1744 | G |
| 46 | B | 1747 | G |
| 46 | B | 1749 | A |
| 46 | B | 1753 | A |
| 46 | B | 1756 | U |
| 46 | B | 1767 | G |
| 46 | B | 1769 | A |
| 46 | B | 1770 | C |
| 46 | B | 1779 | G |
| 46 | B | 1780 | G |
| 46 | B | 1781 | A |
| 46 | B | 1782 | U |
| 46 | B | 1783 | C |
| 1 | AS | 24 | U |
| 1 | AS | 25 | A |
| 1 | AS | 29 | G |
| 1 | AS | 39 | A |
| 1 | AS | 42 | A |
| 1 | AS | 48 | A |
| 1 | AS | 56 | A |
| 1 | AS | 58 | G |
| 1 | AS | 59 | A |
| 1 | AS | 64 | A |
| 1 | AS | 65 | A |
| 1 | AS | 91 | G |

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| Mol | Chain | Res | Type |
|---|---|---|---|
| 1 | AS | 98 | A |
| 1 | AS | 104 | C |
| 1 | AS | 108 | A |
| 1 | AS | 109 | G |
| 1 | AS | 110 | C |
| 1 | AS | 121 | A |
| 1 | AS | 134 | U |
| 1 | AS | 135 | G |
| 1 | AS | 155 | A |
| 1 | AS | 156 | A |
| 1 | AS | 164 | U |
| 1 | AS | 169 | G |
| 1 | AS | 172 | C |
| 1 | AS | 173 | C |
| 1 | AS | 175 | G |
| 1 | AS | 186 | A |
| 1 | AS | 189 | U |
| 1 | AS | 190 | U |
| 1 | AS | 199 | C |
| 1 | AS | 205 | G |
| 1 | AS | 209 | C |
| 1 | AS | 212 | A |
| 1 | AS | 217 | G |
| 1 | AS | 218 | A |
| 1 | AS | 219 | G |
| 1 | AS | 230 | G |
| 1 | AS | 236 | A |
| 1 | AS | 239 | A |
| 1 | AS | 240 | C |
| 1 | AS | 243 | G |
| 1 | AS | 245 | G |
| 1 | AS | 249 | G |
| 1 | AS | 250 | U |
| 1 | AS | 251 | G |
| 1 | AS | 269 | G |
| 1 | AS | 286 | U |
| 1 | AS | 295 | A |
| 1 | AS | 305 | U |
| 1 | AS | 311 | C |
| 1 | AS | 323 | A |
| 1 | AS | 329 | U |
| 1 | AS | 337 | G |

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| Mol | Chain | Res | Type |
|---|---|---|---|
| 1 | AS | 338 | A |
| 1 | AS | 339 | C |
| 1 | AS | 343 | U |
| 1 | AS | 349 | A |
| 1 | AS | 350 | C |
| 1 | AS | 376 | G |
| 1 | AS | 377 | A |
| 1 | AS | 395 | A |
| 1 | AS | 398 | A |
| 1 | AS | 402 | A |
| 1 | AS | 403 | C |
| 1 | AS | 404 | G |
| 1 | AS | 420 | G |
| 1 | AS | 421 | G |
| 1 | AS | 422 | A |
| 1 | AS | 438 | A |
| 1 | AS | 439 | C |
| 1 | AS | 442 | G |
| 1 | AS | 445 | A |
| 1 | AS | 447 | U |
| 1 | AS | 448 | U |
| 1 | AS | 449 | U |
| 1 | AS | 450 | G |
| 1 | AS | 451 | C |
| 1 | AS | 453 | U |
| 1 | AS | 454 | G |
| 1 | AS | 474 | C |
| 1 | AS | 479 | C |
| 1 | AS | 480 | G |
| 1 | AS | 481 | G |
| 1 | AS | 482 | U |
| 1 | AS | 483 | U |
| 1 | AS | 484 | U |
| 1 | AS | 486 | C |
| 1 | AS | 487 | C |
| 1 | AS | 488 | G |
| 1 | AS | 506 | A |
| 1 | AS | 517 | A |
| 1 | AS | 519 | U |
| 1 | AS | 531 | G |
| 1 | AS | 532 | U |
| 1 | AS | 538 | G |

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| Mol | Chain | Res | Type |
|---|---|---|---|
| 1 | AS | 539 | G |
| 1 | AS | 541 | U |
| 1 | AS | 542 | U |
| 1 | AS | 543 | C |
| 1 | AS | 544 | U |
| 1 | AS | 545 | G |
| 1 | AS | 546 | C |
| 1 | AS | 555 | A |
| 1 | AS | 556 | U |
| 1 | AS | 557 | A |
| 1 | AS | 564 | G |
| 1 | AS | 577 | G |
| 1 | AS | 589 | G |
| 1 | AS | 590 | A |
| 1 | AS | 598 | U |
| 1 | AS | 600 | U |
| 1 | AS | 601 | U |
| 1 | AS | 602 | A |
| 1 | AS | 609 | A |
| 1 | AS | 618 | U |
| 1 | AS | 619 | A |
| 1 | AS | 620 | A |
| 1 | AS | 635 | C |
| 1 | AS | 647 | A |
| 1 | AS | 658 | A |
| 1 | AS | 675 | A |
| 1 | AS | 679 | U |
| 1 | AS | 688 | A |
| 1 | AS | 689 | A |
| 1 | AS | 703 | A |
| 1 | AS | 710 | G |
| 1 | AS | 713 | A |
| 1 | AS | 717 | A |
| 1 | AS | 723 | G |
| 1 | AS | 730 | A |
| 1 | AS | 732 | U |
| 1 | AS | 760 | U |
| 1 | AS | 763 | U |
| 1 | AS | 772 | U |
| 1 | AS | 773 | U |
| 1 | AS | 776 | A |
| 1 | AS | 777 | G |

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| Mol | Chain | Res | Type |
|---|---|---|---|
| 1 | AS | 780 | A |
| 1 | AS | 781 | G |
| 1 | AS | 802 | A |
| 1 | AS | 813 | A |
| 1 | AS | 826 | A |
| 1 | AS | 845 | C |
| 1 | AS | 857 | C |
| 1 | AS | 861 | U |
| 1 | AS | 870 | U |
| 1 | AS | 875 | U |
| 1 | AS | 892 | A |
| 1 | AS | 893 | U |
| 1 | AS | 903 | G |
| 1 | AS | 904 | G |
| 1 | AS | 910 | A |
| 1 | AS | 912 | G |
| 1 | AS | 913 | A |
| 1 | AS | 917 | A |
| 1 | AS | 919 | C |
| 1 | AS | 921 | A |
| 1 | AS | 933 | G |
| 1 | AS | 940 | C |
| 1 | AS | 949 | G |
| 1 | AS | 955 | C |
| 1 | AS | 956 | U |
| 1 | AS | 959 | G |
| 1 | AS | 970 | G |
| 1 | AS | 976 | A |
| 1 | AS | 977 | U |
| 1 | AS | 990 | G |
| 1 | AS | 991 | U |
| 1 | AS | 996 | C |
| 1 | AS | 997 | G |
| 1 | AS | 998 | A |
| 1 | AS | 1006 | G |
| 1 | AS | 1011 | C |
| 1 | AS | 1012 | U |
| 1 | AS | 1014 | G |
| 1 | AS | 1016 | G |
| 1 | AS | 1017 | G |
| 1 | AS | 1019 | U |
| 1 | AS | 1020 | G |

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| Mol | Chain | Res | Type |
|---|---|---|---|
| 1 | AS | 1022 | A |
| 1 | AS | 1023 | A |
| 1 | AS | 1024 | U |
| 1 | AS | 1025 | G |
| 1 | AS | 1026 | A |
| 1 | AS | 1027 | C |
| 1 | AS | 1030 | U |
| 1 | AS | 1033 | C |
| 1 | AS | 1043 | A |
| 1 | AS | 1045 | C |
| 1 | AS | 1060 | A |
| 1 | AS | 1061 | A |
| 1 | AS | 1068 | G |
| 1 | AS | 1077 | U |
| 1 | AS | 1078 | U |
| 1 | AS | 1089 | A |
| 1 | AS | 1090 | A |
| 1 | AS | 1091 | U |
| 1 | AS | 1092 | U |
| 1 | AS | 1094 | A |
| 1 | AS | 1099 | A |
| 1 | AS | 1100 | G |
| 1 | AS | 1113 | G |
| 1 | AS | 1127 | G |
| 1 | AS | 1140 | U |
| 1 | AS | 1149 | A |
| 1 | AS | 1150 | A |
| 1 | AS | 1151 | C |
| 1 | AS | 1155 | A |
| 1 | AS | 1156 | C |
| 1 | AS | 1164 | U |
| 1 | AS | 1174 | G |
| 1 | AS | 1176 | A |
| 1 | AS | 1177 | U |
| 1 | AS | 1178 | G |
| 1 | AS | 1188 | C |
| 1 | AS | 1189 | A |
| 1 | AS | 1192 | C |
| 1 | AS | 1197 | C |
| 1 | AS | 1204 | U |
| 1 | AS | 1205 | G |
| 1 | AS | 1218 | G |

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| Mol | Chain | Res | Type |
|---|---|---|---|
| 1 | AS | 1219 | A |
| 1 | AS | 1224 | C |
| 1 | AS | 1228 | C |
| 1 | AS | 1231 | U |
| 1 | AS | 1232 | G |
| 1 | AS | 1233 | G |
| 1 | AS | 1237 | U |
| 1 | AS | 1238 | G |
| 1 | AS | 1239 | G |
| 1 | AS | 1241 | A |
| 1 | AS | 1242 | G |
| 1 | AS | 1243 | U |
| 1 | AS | 1244 | C |
| 1 | AS | 1246 | G |
| 1 | AS | 1248 | A |
| 1 | AS | 1249 | U |
| 1 | AS | 1250 | C |
| 1 | AS | 1252 | G |
| 1 | AS | 1254 | U |
| 1 | AS | 1255 | A |
| 1 | AS | 1256 | A |
| 1 | AS | 1258 | G |
| 1 | AS | 1259 | A |
| 1 | AS | 1260 | G |
| 1 | AS | 1261 | U |
| 1 | AS | 1263 | U |
| 1 | AS | 1264 | G |
| 1 | AS | 1265 | U |
| 1 | AS | 1266 | A |
| 1 | AS | 1267 | A |
| 1 | AS | 1270 | A |
| 1 | AS | 1271 | C |
| 1 | AS | 1273 | C |
| 1 | AS | 1278 | G |
| 1 | AS | 1281 | G |
| 1 | AS | 1282 | A |
| 1 | AS | 1283 | A |
| 1 | AS | 1303 | G |
| 1 | AS | 1304 | A |
| 1 | AS | 1305 | U |
| 1 | AS | 1309 | G |
| 1 | AS | 1326 | A |

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| Mol | Chain | Res | Type |
|---|---|---|---|
| 1 | AS | 1345 | G |
| 1 | AS | 1346 | U |
| 1 | AS | 1347 | U |
| 1 | AS | 1348 | U |
| 1 | AS | 1349 | U |
| 1 | AS | 1382 | A |
| 1 | AS | 1395 | U |
| 1 | AS | 1415 | A |
| 1 | AS | 1417 | G |
| 1 | AS | 1421 | U |
| 1 | AS | 1427 | G |
| 1 | AS | 1430 | G |
| 1 | AS | 1433 | C |
| 1 | AS | 1442 | A |
| 1 | AS | 1446 | G |
| 1 | AS | 1465 | C |
| 1 | AS | 1471 | A |
| 1 | AS | 1477 | A |
| 1 | AS | 1484 | G |
| 1 | AS | 1498 | C |
| 1 | AS | 1504 | C |
| 1 | AS | 1520 | A |
| 1 | AS | 1523 | C |
| 1 | AS | 1532 | G |
| 1 | AS | 1535 | A |
| 1 | AS | 1552 | C |
| 1 | AS | 1556 | G |
| 1 | AS | 1558 | G |
| 1 | AS | 1559 | C |
| 1 | AS | 1560 | U |
| 1 | AS | 1561 | U |
| 1 | AS | 1562 | G |
| 1 | AS | 1563 | A |
| 1 | AS | 1564 | U |
| 1 | AS | 1565 | U |
| 1 | AS | 1566 | U |
| 1 | AS | 1567 | U |
| 1 | AS | 1568 | U |
| 1 | AS | 1569 | C |
| 1 | AS | 1571 | G |
| 1 | AS | 1572 | G |
| 1 | AS | 1574 | C |

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| Mol | Chain | Res | Type |
|---|---|---|---|
| 1 | AS | 1576 | A |
| 1 | AS | 1577 | C |
| 1 | AS | 1585 | A |
| 1 | AS | 1589 | A |
| 1 | AS | 1601 | A |
| 1 | AS | 1603 | U |
| 1 | AS | 1624 | C |
| 1 | AS | 1625 | U |
| 1 | AS | 1635 | C |
| 1 | AS | 1638 | A |
| 1 | AS | 1639 | A |
| 1 | AS | 1641 | U |
| 1 | AS | 1648 | G |
| 1 | AS | 1654 | G |
| 1 | AS | 1679 | A |
| 1 | AS | 1720 | U |
| 1 | AS | 1721 | C |
| 1 | AS | 1732 | G |
| 1 | AS | 1746 | A |
| 1 | AS | 1747 | G |
| 1 | AS | 1755 | U |
| 1 | AS | 1756 | A |
| 1 | AS | 1757 | A |
| 1 | AS | 1758 | U |
| 1 | AS | 1759 | U |
| 1 | AS | 1761 | U |
| 1 | AS | 1762 | G |
| 1 | AS | 1763 | C |
| 1 | AS | 1776 | G |
| 1 | AS | 1793 | A |
| 1 | AS | 1804 | G |
| 1 | AS | 1809 | A |
| 1 | AS | 1810 | A |
| 1 | AS | 1811 | U |
| 1 | AS | 1812 | A |
| 1 | AS | 1814 | U |
| 1 | AS | 1815 | U |
| 1 | AS | 1816 | U |
| 1 | AS | 1817 | U |
| 1 | AS | 1835 | A |
| 1 | AS | 1838 | A |
| 1 | AS | 1842 | C |

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| Mol | Chain | Res | Type |
|---|---|---|---|
| 1 | AS | 1845 | C |
| 1 | AS | 1862 | C |
| 1 | AS | 1874 | G |
| 1 | AS | 1882 | A |
| 1 | AS | 1889 | A |
| 1 | AS | 1902 | G |
| 1 | AS | 1944 | G |
| 1 | AS | 1949 | G |
| 1 | AS | 2063 | C |
| 1 | AS | 2064 | A |
| 1 | AS | 2065 | C |
| 1 | AS | 2066 | G |
| 1 | AS | 2067 | U |
| 1 | AS | 2068 | U |
| 1 | AS | 2069 | U |
| 1 | AS | 2070 | A |
| 1 | AS | 2071 | A |
| 1 | AS | 2078 | A |
| 1 | AS | 2088 | G |
| 1 | AS | 2089 | G |
| 1 | AS | 2091 | A |
| 1 | AS | 2092 | C |
| 1 | AS | 2099 | G |
| 1 | AS | 2100 | G |
| 1 | AS | 2109 | A |
| 1 | AS | 2118 | U |
| 1 | AS | 2122 | A |
| 1 | AS | 2136 | A |
| 1 | AS | 2147 | G |
| 1 | AS | 2149 | G |
| 1 | AS | 2183 | U |
| 1 | AS | 2184 | G |
| 1 | AS | 2185 | A |
| 1 | AS | 2186 | A |
| 1 | AS | 2187 | U |
| 1 | AS | 2188 | G |
| 1 | AS | 2201 | A |
| 1 | AS | 2222 | A |
| 1 | AS | 2227 | G |
| 1 | AS | 2233 | A |
| 1 | AS | 2234 | A |
| 1 | AS | 2250 | G |

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| Mol | Chain | Res | Type |
|---|---|---|---|
| 1 | AS | 2251 | G |
| 1 | AS | 2259 | A |
| 1 | AS | 2260 | U |
| 1 | AS | 2276 | U |
| 1 | AS | 2285 | G |
| 1 | AS | 2286 | C |
| 1 | AS | 2288 | U |
| 1 | AS | 2291 | A |
| 1 | AS | 2292 | U |
| 1 | AS | 2293 | G |
| 1 | AS | 2312 | U |
| 1 | AS | 2313 | G |
| 1 | AS | 2314 | U |
| 1 | AS | 2341 | A |
| 1 | AS | 2351 | A |
| 1 | AS | 2352 | C |
| 1 | AS | 2353 | G |
| 1 | AS | 2363 | G |
| 1 | AS | 2366 | U |
| 1 | AS | 2371 | G |
| 1 | AS | 2372 | G |
| 1 | AS | 2375 | A |
| 1 | AS | 2380 | A |
| 1 | AS | 2381 | G |
| 1 | AS | 2382 | A |
| 1 | AS | 2389 | U |
| 1 | AS | 2396 | G |
| 1 | AS | 2397 | A |
| 1 | AS | 2413 | G |
| 1 | AS | 2415 | G |
| 1 | AS | 2420 | G |
| 1 | AS | 2421 | A |
| 1 | AS | 2422 | C |
| 1 | AS | 2425 | G |
| 1 | AS | 2426 | G |
| 1 | AS | 2427 | A |
| 1 | AS | 2428 | G |
| 1 | AS | 2429 | G |
| 1 | AS | 2430 | G |
| 1 | AS | 2431 | U |
| 1 | AS | 2432 | G |
| 1 | AS | 2433 | U |

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| Mol | Chain | Res | Type |
|---|---|---|---|
| 1 | AS | 2434 | A |
| 1 | AS | 2435 | G |
| 1 | AS | 2436 | A |
| 1 | AS | 2437 | A |
| 1 | AS | 2439 | A |
| 1 | AS | 2440 | A |
| 1 | AS | 2441 | G |
| 1 | AS | 2442 | U |
| 1 | AS | 2443 | G |
| 1 | AS | 2444 | G |
| 1 | AS | 2445 | G |
| 1 | AS | 2446 | A |
| 1 | AS | 2447 | G |
| 1 | AS | 2448 | C |
| 1 | AS | 2449 | U |
| 1 | AS | 2450 | U |
| 1 | AS | 2452 | G |
| 1 | AS | 2453 | G |
| 1 | AS | 2455 | G |
| 1 | AS | 2456 | C |
| 1 | AS | 2457 | C |
| 1 | AS | 2458 | G |
| 1 | AS | 2459 | G |
| 1 | AS | 2464 | A |
| 1 | AS | 2465 | U |
| 1 | AS | 2466 | A |
| 1 | AS | 2467 | C |
| 1 | AS | 2468 | C |
| 1 | AS | 2469 | A |
| 1 | AS | 2471 | U |
| 1 | AS | 2472 | A |
| 1 | AS | 2473 | C |
| 1 | AS | 2474 | C |
| 1 | AS | 2475 | U |
| 1 | AS | 2476 | C |
| 1 | AS | 2477 | U |
| 1 | AS | 2478 | A |
| 1 | AS | 2480 | A |
| 1 | AS | 2481 | G |
| 1 | AS | 2482 | U |
| 1 | AS | 2483 | U |
| 1 | AS | 2489 | A |

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| Mol | Chain | Res | Type |
|---|---|---|---|
| 1 | AS | 2492 | U |
| 1 | AS | 2493 | A |
| 1 | AS | 2510 | U |
| 1 | AS | 2511 | G |
| 1 | AS | 2513 | A |
| 1 | AS | 2515 | G |
| 1 | AS | 2516 | U |
| 1 | AS | 2517 | C |
| 1 | AS | 2518 | A |
| 1 | AS | 2519 | A |
| 1 | AS | 2520 | A |
| 1 | AS | 2521 | C |
| 1 | AS | 2529 | U |
| 1 | AS | 2530 | C |
| 1 | AS | 2533 | G |
| 1 | AS | 2536 | U |
| 1 | AS | 2538 | A |
| 1 | AS | 2545 | C |
| 1 | AS | 2546 | U |
| 1 | AS | 2554 | C |
| 1 | AS | 2557 | G |
| 1 | AS | 2565 | A |
| 1 | AS | 2566 | C |
| 1 | AS | 2578 | G |
| 1 | AS | 2579 | G |
| 1 | AS | 2586 | G |
| 1 | AS | 2598 | A |
| 1 | AS | 2623 | G |
| 1 | AS | 2624 | U |
| 1 | AS | 2628 | A |
| 1 | AS | 2646 | A |
| 1 | AS | 2649 | G |
| 1 | AS | 2661 | A |
| 1 | AS | 2662 | G |
| 1 | AS | 2663 | A |
| 1 | AS | 2666 | A |
| 1 | AS | 2676 | A |
| 1 | AS | 2677 | A |
| 1 | AS | 2686 | G |
| 1 | AS | 2699 | A |
| 1 | AS | 2700 | G |
| 1 | AS | 2701 | U |

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| Mol | Chain | Res | Type |
|---|---|---|---|
| 1 | AS | 2724 | U |
| 1 | AS | 2725 | G |
| 1 | AS | 2734 | A |
| 1 | AS | 2745 | C |
| 1 | AS | 2749 | G |
| 1 | AS | 2750 | G |
| 1 | AS | 2768 | G |
| 1 | AS | 2771 | A |
| 1 | AS | 2772 | G |
| 1 | AS | 2773 | A |
| 1 | AS | 2774 | A |
| 1 | AS | 2782 | C |
| 1 | AS | 2786 | G |
| 1 | AS | 2789 | A |
| 1 | AS | 2790 | U |
| 1 | AS | 2814 | U |
| 1 | AS | 2815 | U |
| 1 | AS | 2817 | A |
| 1 | AS | 2833 | U |
| 1 | AS | 2839 | C |
| 1 | AS | 2843 | G |
| 1 | AS | 2844 | A |
| 1 | AS | 2847 | U |
| 1 | AS | 2859 | A |
| 1 | AS | 2861 | C |
| 1 | AS | 2866 | C |
| 1 | AS | 2870 | G |
| 1 | AS | 2871 | C |
| 1 | AS | 2886 | G |
| 1 | AS | 2895 | U |
| 1 | AS | 2907 | U |
| 1 | AS | 2908 | A |
| 1 | AS | 2911 | G |
| 1 | AS | 2914 | C |
| 1 | AS | 2919 | G |
| 1 | AS | 2920 | C |
| 1 | AS | 2923 | G |
| 1 | AS | 2926 | U |
| 1 | AS | 2943 | A |
| 1 | AS | 2955 | C |
| 1 | AS | 2960 | C |
| 1 | AS | 2962 | G |

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| Mol | Chain | Res | Type |
|---|---|---|---|
| 1 | AS | 2969 | G |
| 1 | AS | 2984 | A |
| 1 | AS | 3021 | A |
| 1 | AS | 3028 | U |
| 1 | AS | 3031 | G |
| 1 | AS | 3050 | A |
| 1 | AS | 3051 | C |
| 1 | AS | 3052 | G |
| 1 | AS | 3058 | A |
| 1 | AS | 3064 | C |
| 1 | AS | 3076 | U |
| 1 | AS | 3094 | A |
| 1 | AS | 3101 | A |
| 1 | AS | 3102 | A |
| 1 | AS | 3103 | U |
| 1 | AS | 3114 | A |
| 1 | AS | 3115 | C |
| 1 | AS | 3134 | C |
| 1 | AS | 3143 | G |
| 1 | AS | 3144 | A |
| 1 | AS | 3146 | G |
| 1 | AS | 3149 | U |
| 1 | AS | 3151 | C |
| 1 | AS | 3157 | A |
| 1 | AS | 3160 | C |
| 1 | AS | 3161 | U |
| 1 | AS | 3166 | A |
| 1 | AS | 3167 | G |
| 1 | AS | 3171 | C |
| 1 | AS | 3172 | U |
| 1 | AS | 3182 | C |
| 1 | AS | 3183 | A |
| 1 | AS | 3184 | G |
| 1 | AS | 3194 | G |
| 1 | AS | 3208 | A |
| 1 | AS | 3210 | A |
| 1 | AS | 3212 | G |
| 1 | AS | 3214 | U |
| 1 | AS | 3224 | U |
| 1 | AS | 3228 | G |
| 1 | AS | 3235 | A |
| 1 | AS | 3241 | G |

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| Mol | Chain | Res | Type |
|---|---|---|---|
| 1 | AS | 3246 | C |
| 1 | AS | 3252 | C |
| 1 | AS | 3259 | A |
| 1 | AS | 3260 | A |
| 1 | AS | 3268 | G |
| 1 | AS | 3269 | C |
| 1 | AS | 3272 | A |
| 1 | AS | 3278 | U |
| 1 | AS | 3281 | A |
| 1 | AS | 3284 | U |
| 1 | AS | 3285 | A |
| 1 | AS | 3306 | U |
| 1 | AS | 3307 | A |
| 1 | AS | 3309 | A |
| 1 | AS | 3310 | G |
| 1 | AS | 3316 | U |
| 1 | AS | 3317 | U |
| 1 | AS | 3318 | G |
| 1 | AS | 3319 | U |
| 1 | AS | 3320 | U |
| 1 | AS | 3321 | G |
| 1 | AS | 3334 | G |
| 1 | AS | 3343 | C |
| 1 | AS | 3351 | G |
| 1 | AS | 3361 | U |
| 2 | AT | 7 | G |
| 2 | AT | 22 | A |
| 2 | AT | 54 | U |
| 2 | AT | 55 | A |
| 2 | AT | 65 | G |
| 2 | AT | 73 | C |
| 2 | AT | 76 | A |
| 2 | AT | 102 | A |
| 2 | AT | 112 | G |
| 3 | AU | 23 | U |
| 3 | AU | 34 | U |
| 3 | AU | 35 | C |
| 3 | AU | 59 | A |
| 3 | AU | 62 | C |
| 3 | AU | 63 | G |
| 3 | AU | 81 | A |
| 3 | AU | 84 | C |

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| Mol | Chain | Res | Type |
|---|---|---|---|
| 3 | AU | 85 | G |
| 3 | AU | 86 | U |
| 3 | AU | 87 | G |
| 3 | AU | 92 | A |
| 3 | AU | 95 | G |
| 3 | AU | 102 | U |
| 3 | AU | 104 | A |
| 3 | AU | 105 | A |
| 3 | AU | 106 | C |
| 3 | AU | 111 | A |
| 3 | AU | 113 | U |
| 3 | AU | 125 | U |
| 3 | AU | 126 | A |
| 3 | AU | 152 | G |
| 3 | AU | 157 | U |
| 46 | CM | 17 | C |
| 46 | CM | 25 | C |
| 46 | CM | 26 | A |
| 46 | CM | 27 | U |
| 46 | CM | 34 | G |
| 46 | CM | 47 | A |
| 46 | CM | 57 | G |
| 46 | CM | 66 | U |
| 46 | CM | 74 | U |
| 46 | CM | 75 | U |
| 46 | CM | 76 | A |
| 46 | CM | 78 | A |
| 46 | CM | 79 | C |
| 46 | CM | 81 | G |
| 46 | CM | 84 | A |
| 46 | CM | 104 | A |
| 46 | CM | 114 | C |
| 46 | CM | 115 | G |
| 46 | CM | 123 | G |
| 46 | CM | 126 | A |
| 46 | CM | 127 | G |
| 46 | CM | 128 | U |
| 46 | CM | 129 | A |
| 46 | CM | 130 | C |
| 46 | CM | 131 | C |
| 46 | CM | 132 | U |
| 46 | CM | 133 | U |

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| Mol | Chain | Res | Type |
|---|---|---|---|
| 46 | CM | 134 | A |
| 46 | CM | 135 | C |
| 46 | CM | 138 | C |
| 46 | CM | 139 | U |
| 46 | CM | 142 | G |
| 46 | CM | 143 | A |
| 46 | CM | 150 | U |
| 46 | CM | 151 | G |
| 46 | CM | 152 | G |
| 46 | CM | 154 | A |
| 46 | CM | 159 | U |
| 46 | CM | 166 | A |
| 46 | CM | 168 | U |
| 46 | CM | 173 | G |
| 46 | CM | 176 | U |
| 46 | CM | 177 | A |
| 46 | CM | 190 | U |
| 46 | CM | 193 | G |
| 46 | CM | 199 | G |
| 46 | CM | 200 | A |
| 46 | CM | 201 | U |
| 46 | CM | 202 | G |
| 46 | CM | 206 | U |
| 46 | CM | 211 | A |
| 46 | CM | 213 | A |
| 46 | CM | 214 | U |
| 46 | CM | 215 | A |
| 46 | CM | 216 | A |
| 46 | CM | 217 | A |
| 46 | CM | 218 | A |
| 46 | CM | 219 | A |
| 46 | CM | 220 | A |
| 46 | CM | 221 | U |
| 46 | CM | 222 | C |
| 46 | CM | 223 | A |
| 46 | CM | 226 | G |
| 46 | CM | 229 | U |
| 46 | CM | 230 | U |
| 46 | CM | 231 | C |
| 46 | CM | 232 | G |
| 46 | CM | 236 | U |
| 46 | CM | 237 | C |

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| Mol | Chain | Res | Type |
|---|---|---|---|
| 46 | CM | 238 | U |
| 46 | CM | 239 | U |
| 46 | CM | 240 | U |
| 46 | CM | 247 | U |
| 46 | CM | 255 | A |
| 46 | CM | 259 | U |
| 46 | CM | 260 | U |
| 46 | CM | 261 | C |
| 46 | CM | 262 | G |
| 46 | CM | 266 | C |
| 46 | CM | 269 | A |
| 46 | CM | 270 | U |
| 46 | CM | 274 | C |
| 46 | CM | 276 | U |
| 46 | CM | 277 | G |
| 46 | CM | 278 | U |
| 46 | CM | 279 | G |
| 46 | CM | 283 | G |
| 46 | CM | 285 | G |
| 46 | CM | 297 | A |
| 46 | CM | 312 | C |
| 46 | CM | 314 | A |
| 46 | CM | 318 | U |
| 46 | CM | 319 | C |
| 46 | CM | 320 | G |
| 46 | CM | 335 | G |
| 46 | CM | 336 | C |
| 46 | CM | 350 | A |
| 46 | CM | 357 | A |
| 46 | CM | 358 | A |
| 46 | CM | 359 | C |
| 46 | CM | 388 | G |
| 46 | CM | 398 | A |
| 46 | CM | 400 | C |
| 46 | CM | 402 | G |
| 46 | CM | 414 | A |
| 46 | CM | 416 | G |
| 46 | CM | 421 | G |
| 46 | CM | 422 | C |
| 46 | CM | 423 | A |
| 46 | CM | 424 | G |
| 46 | CM | 432 | G |

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| Mol | Chain | Res | Type |
|---|---|---|---|
| 46 | CM | 437 | U |
| 46 | CM | 442 | C |
| 46 | CM | 446 | C |
| 46 | CM | 452 | A |
| 46 | CM | 458 | A |
| 46 | CM | 462 | A |
| 46 | CM | 466 | A |
| 46 | CM | 475 | A |
| 46 | CM | 480 | U |
| 46 | CM | 482 | C |
| 46 | CM | 489 | C |
| 46 | CM | 490 | U |
| 46 | CM | 491 | U |
| 46 | CM | 495 | G |
| 46 | CM | 498 | C |
| 46 | CM | 499 | U |
| 46 | CM | 503 | A |
| 46 | CM | 504 | A |
| 46 | CM | 505 | U |
| 46 | CM | 506 | U |
| 46 | CM | 509 | A |
| 46 | CM | 512 | G |
| 46 | CM | 513 | A |
| 46 | CM | 515 | U |
| 46 | CM | 518 | A |
| 46 | CM | 519 | A |
| 46 | CM | 525 | A |
| 46 | CM | 530 | U |
| 46 | CM | 534 | C |
| 46 | CM | 536 | A |
| 46 | CM | 537 | G |
| 46 | CM | 539 | A |
| 46 | CM | 540 | A |
| 46 | CM | 547 | G |
| 46 | CM | 553 | A |
| 46 | CM | 554 | A |
| 46 | CM | 555 | G |
| 46 | CM | 556 | U |
| 46 | CM | 557 | C |
| 46 | CM | 563 | C |
| 46 | CM | 566 | G |
| 46 | CM | 575 | G |

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| Mol | Chain | Res | Type |
|---|---|---|---|
| 46 | CM | 576 | U |
| 46 | CM | 592 | A |
| 46 | CM | 593 | G |
| 46 | CM | 604 | A |
| 46 | CM | 609 | U |
| 46 | CM | 617 | A |
| 46 | CM | 618 | A |
| 46 | CM | 620 | A |
| 46 | CM | 621 | A |
| 46 | CM | 633 | A |
| 46 | CM | 639 | G |
| 46 | CM | 645 | G |
| 46 | CM | 648 | U |
| 46 | CM | 649 | G |
| 46 | CM | 650 | G |
| 46 | CM | 652 | C |
| 46 | CM | 653 | G |
| 46 | CM | 654 | G |
| 46 | CM | 659 | U |
| 46 | CM | 668 | U |
| 46 | CM | 670 | C |
| 46 | CM | 671 | G |
| 46 | CM | 672 | U |
| 46 | CM | 673 | A |
| 46 | CM | 674 | C |
| 46 | CM | 675 | U |
| 46 | CM | 676 | G |
| 46 | CM | 678 | A |
| 46 | CM | 679 | C |
| 46 | CM | 680 | C |
| 46 | CM | 681 | C |
| 46 | CM | 682 | A |
| 46 | CM | 688 | G |
| 46 | CM | 691 | U |
| 46 | CM | 694 | C |
| 46 | CM | 695 | C |
| 46 | CM | 696 | U |
| 46 | CM | 697 | U |
| 46 | CM | 700 | G |
| 46 | CM | 701 | G |
| 46 | CM | 702 | G |
| 46 | CM | 703 | U |

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| Mol | Chain | Res | Type |
|---|---|---|---|
| 46 | CM | 704 | A |
| 46 | CM | 705 | G |
| 46 | CM | 706 | C |
| 46 | CM | 707 | C |
| 46 | CM | 709 | U |
| 46 | CM | 711 | U |
| 46 | CM | 712 | A |
| 46 | CM | 714 | G |
| 46 | CM | 716 | C |
| 46 | CM | 717 | G |
| 46 | CM | 719 | A |
| 46 | CM | 720 | C |
| 46 | CM | 722 | A |
| 46 | CM | 723 | G |
| 46 | CM | 724 | G |
| 46 | CM | 729 | U |
| 46 | CM | 739 | A |
| 46 | CM | 740 | A |
| 46 | CM | 741 | A |
| 46 | CM | 750 | G |
| 46 | CM | 751 | U |
| 46 | CM | 756 | A |
| 46 | CM | 759 | A |
| 46 | CM | 760 | G |
| 46 | CM | 762 | C |
| 46 | CM | 764 | U |
| 46 | CM | 765 | U |
| 46 | CM | 766 | U |
| 46 | CM | 767 | G |
| 46 | CM | 768 | C |
| 46 | CM | 770 | C |
| 46 | CM | 771 | G |
| 46 | CM | 773 | A |
| 46 | CM | 775 | A |
| 46 | CM | 778 | U |
| 46 | CM | 779 | U |
| 46 | CM | 796 | A |
| 46 | CM | 798 | A |
| 46 | CM | 799 | G |
| 46 | CM | 802 | C |
| 46 | CM | 803 | G |
| 46 | CM | 804 | U |

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| Mol | Chain | Res | Type |
|---|---|---|---|
| 46 | CM | 805 | U |
| 46 | CM | 807 | U |
| 46 | CM | 808 | G |
| 46 | CM | 812 | C |
| 46 | CM | 814 | A |
| 46 | CM | 815 | U |
| 46 | CM | 816 | U |
| 46 | CM | 818 | U |
| 46 | CM | 819 | G |
| 46 | CM | 820 | U |
| 46 | CM | 821 | U |
| 46 | CM | 823 | G |
| 46 | CM | 824 | U |
| 46 | CM | 825 | U |
| 46 | CM | 826 | U |
| 46 | CM | 827 | C |
| 46 | CM | 828 | U |
| 46 | CM | 829 | A |
| 46 | CM | 840 | A |
| 46 | CM | 842 | U |
| 46 | CM | 848 | A |
| 46 | CM | 856 | G |
| 46 | CM | 857 | G |
| 46 | CM | 869 | A |
| 46 | CM | 871 | U |
| 46 | CM | 875 | C |
| 46 | CM | 877 | G |
| 46 | CM | 878 | U |
| 46 | CM | 879 | U |
| 46 | CM | 881 | U |
| 46 | CM | 891 | A |
| 46 | CM | 909 | A |
| 46 | CM | 910 | G |
| 46 | CM | 911 | A |
| 46 | CM | 918 | A |
| 46 | CM | 920 | U |
| 46 | CM | 927 | G |
| 46 | CM | 945 | U |
| 46 | CM | 951 | A |
| 46 | CM | 973 | A |
| 46 | CM | 975 | C |
| 46 | CM | 977 | A |

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| Mol | Chain | Res | Type |
|---|---|---|---|
| 46 | CM | 988 | A |
| 46 | CM | 989 | U |
| 46 | CM | 990 | A |
| 46 | CM | 997 | U |
| 46 | CM | 998 | A |
| 46 | CM | 1004 | A |
| 46 | CM | 1005 | A |
| 46 | CM | 1011 | A |
| 46 | CM | 1013 | C |
| 46 | CM | 1017 | G |
| 46 | CM | 1024 | A |
| 46 | CM | 1025 | G |
| 46 | CM | 1039 | U |
| 46 | CM | 1042 | U |
| 46 | CM | 1043 | U |
| 46 | CM | 1044 | U |
| 46 | CM | 1047 | U |
| 46 | CM | 1055 | A |
| 46 | CM | 1056 | U |
| 46 | CM | 1057 | C |
| 46 | CM | 1058 | G |
| 46 | CM | 1059 | G |
| 46 | CM | 1060 | C |
| 46 | CM | 1061 | A |
| 46 | CM | 1067 | C |
| 46 | CM | 1074 | U |
| 46 | CM | 1077 | A |
| 46 | CM | 1081 | C |
| 46 | CM | 1085 | G |
| 46 | CM | 1123 | A |
| 46 | CM | 1135 | G |
| 46 | CM | 1143 | C |
| 46 | CM | 1145 | A |
| 46 | CM | 1152 | G |
| 46 | CM | 1168 | A |
| 46 | CM | 1169 | A |
| 46 | CM | 1170 | U |
| 46 | CM | 1179 | A |
| 46 | CM | 1181 | A |
| 46 | CM | 1184 | G |
| 46 | CM | 1185 | G |
| 46 | CM | 1186 | G |

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| Mol | Chain | Res | Type |
|---|---|---|---|
| 46 | CM | 1187 | A |
| 46 | CM | 1193 | A |
| 46 | CM | 1202 | A |
| 46 | CM | 1203 | G |
| 46 | CM | 1206 | A |
| 46 | CM | 1207 | C |
| 46 | CM | 1212 | A |
| 46 | CM | 1215 | A |
| 46 | CM | 1219 | A |
| 46 | CM | 1220 | C |
| 46 | CM | 1221 | A |
| 46 | CM | 1229 | A |
| 46 | CM | 1230 | G |
| 46 | CM | 1231 | C |
| 46 | CM | 1236 | U |
| 46 | CM | 1243 | U |
| 46 | CM | 1250 | G |
| 46 | CM | 1270 | U |
| 46 | CM | 1284 | G |
| 46 | CM | 1299 | U |
| 46 | CM | 1300 | U |
| 46 | CM | 1301 | G |
| 46 | CM | 1306 | A |
| 46 | CM | 1325 | U |
| 46 | CM | 1330 | A |
| 46 | CM | 1336 | G |
| 46 | CM | 1339 | G |
| 46 | CM | 1342 | A |
| 46 | CM | 1343 | G |
| 46 | CM | 1345 | A |
| 46 | CM | 1346 | U |
| 46 | CM | 1348 | U |
| 46 | CM | 1349 | G |
| 46 | CM | 1352 | G |
| 46 | CM | 1355 | A |
| 46 | CM | 1356 | U |
| 46 | CM | 1357 | A |
| 46 | CM | 1358 | G |
| 46 | CM | 1359 | U |
| 46 | CM | 1360 | C |
| 46 | CM | 1364 | U |
| 46 | CM | 1365 | C |

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| Mol | Chain | Res | Type |
|---|---|---|---|
| 46 | CM | 1369 | G |
| 46 | CM | 1370 | A |
| 46 | CM | 1376 | U |
| 46 | CM | 1380 | G |
| 46 | CM | 1381 | A |
| 46 | CM | 1382 | U |
| 46 | CM | 1384 | U |
| 46 | CM | 1385 | C |
| 46 | CM | 1392 | A |
| 46 | CM | 1397 | A |
| 46 | CM | 1398 | G |
| 46 | CM | 1399 | U |
| 46 | CM | 1400 | U |
| 46 | CM | 1401 | U |
| 46 | CM | 1410 | A |
| 46 | CM | 1413 | A |
| 46 | CM | 1414 | G |
| 46 | CM | 1415 | G |
| 46 | CM | 1422 | A |
| 46 | CM | 1431 | G |
| 46 | CM | 1433 | C |
| 46 | CM | 1445 | C |
| 46 | CM | 1446 | A |
| 46 | CM | 1455 | A |
| 46 | CM | 1457 | A |
| 46 | CM | 1458 | C |
| 46 | CM | 1461 | A |
| 46 | CM | 1462 | C |
| 46 | CM | 1463 | G |
| 46 | CM | 1468 | C |
| 46 | CM | 1476 | A |
| 46 | CM | 1477 | U |
| 46 | CM | 1480 | G |
| 46 | CM | 1483 | U |
| 46 | CM | 1491 | G |
| 46 | CM | 1502 | A |
| 46 | CM | 1503 | A |
| 46 | CM | 1508 | G |
| 46 | CM | 1510 | G |
| 46 | CM | 1511 | A |
| 46 | CM | 1523 | G |
| 46 | CM | 1524 | C |

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| Mol | Chain | Res | Type |
|---|---|---|---|
| 46 | CM | 1529 | G |
| 46 | CM | 1530 | A |
| 46 | CM | 1541 | U |
| 46 | CM | 1544 | U |
| 46 | CM | 1546 | G |
| 46 | CM | 1556 | A |
| 46 | CM | 1560 | A |
| 46 | CM | 1561 | G |
| 46 | CM | 1571 | G |
| 46 | CM | 1574 | A |
| 46 | CM | 1575 | G |
| 46 | CM | 1577 | G |
| 46 | CM | 1580 | A |
| 46 | CM | 1582 | U |
| 46 | CM | 1584 | A |
| 46 | CM | 1588 | G |
| 46 | CM | 1621 | C |
| 46 | CM | 1644 | U |
| 46 | CM | 1645 | G |
| 46 | CM | 1665 | C |
| 46 | CM | 1667 | G |
| 46 | CM | 1670 | U |
| 46 | CM | 1671 | G |
| 46 | CM | 1673 | U |
| 46 | CM | 1675 | U |
| 46 | CM | 1677 | G |
| 46 | CM | 1678 | G |
| 46 | CM | 1680 | A |
| 46 | CM | 1697 | C |
| 46 | CM | 1699 | G |
| 46 | CM | 1700 | G |
| 46 | CM | 1701 | A |
| 46 | CM | 1702 | A |
| 46 | CM | 1704 | C |
| 46 | CM | 1737 | A |
| 46 | CM | 1742 | A |
| 46 | CM | 1743 | A |
| 46 | CM | 1744 | G |
| 46 | CM | 1747 | G |
| 46 | CM | 1749 | A |
| 46 | CM | 1753 | A |
| 46 | CM | 1756 | U |

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| Mol | Chain | Res | Type |
|---|---|---|---|
| 46 | CM | 1767 | G |
| 46 | CM | 1770 | C |
| 46 | CM | 1779 | G |
| 46 | CM | 1780 | G |
| 46 | CM | 1781 | A |
| 46 | CM | 1782 | U |
| 46 | CM | 1783 | C |

All (199) RNA pucker outliers are listed below:

| Mol | Chain | Res | Type |
|---|---|---|---|
| 1 | 1 | 172 | C |
| 1 | 1 | 403 | C |
| 1 | 1 | 538 | G |
| 1 | 1 | 563 | U |
| 1 | 1 | 759 | G |
| 1 | 1 | 912 | G |
| 1 | 1 | 1011 | C |
| 1 | 1 | 1012 | U |
| 1 | 1 | 1023 | A |
| 1 | 1 | 1029 | U |
| 1 | 1 | 1060 | A |
| 1 | 1 | 1099 | A |
| 1 | 1 | 1346 | U |
| 1 | 1 | 1347 | U |
| 1 | 1 | 1559 | C |
| 1 | 1 | 1561 | U |
| 1 | 1 | 1576 | A |
| 1 | 1 | 1762 | G |
| 1 | 1 | 1815 | U |
| 1 | 1 | 1943 | G |
| 1 | 1 | 2090 | U |
| 1 | 1 | 2182 | C |
| 1 | 1 | 2183 | U |
| 1 | 1 | 2441 | G |
| 1 | 1 | 2442 | U |
| 1 | 1 | 2447 | G |
| 1 | 1 | 2455 | G |
| 1 | 1 | 2476 | C |
| 1 | 1 | 2515 | G |
| 1 | 1 | 2519 | A |
| 1 | 1 | 2545 | C |

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| Mol | Chain | Res | Type |
|---|---|---|---|
| 1 | 1 | 2663 | A |
| 1 | 1 | 2789 | A |
| 1 | 1 | 2790 | U |
| 1 | 1 | 2807 | U |
| 1 | 1 | 3093 | U |
| 1 | 1 | 3164 | U |
| 1 | 1 | 3165 | U |
| 1 | 1 | 3193 | C |
| 1 | 1 | 3234 | U |
| 1 | 1 | 3240 | U |
| 1 | 1 | 3284 | U |
| 1 | 1 | 3309 | A |
| 1 | 1 | 3317 | U |
| 3 | 4 | 85 | G |
| 3 | 4 | 125 | U |
| 3 | 4 | 156 | U |
| 46 | B | 25 | C |
| 46 | B | 78 | A |
| 46 | B | 137 | A |
| 46 | B | 151 | G |
| 46 | B | 176 | U |
| 46 | B | 215 | A |
| 46 | B | 216 | A |
| 46 | B | 259 | U |
| 46 | B | 265 | U |
| 46 | B | 278 | U |
| 46 | B | 415 | A |
| 46 | B | 451 | C |
| 46 | B | 505 | U |
| 46 | B | 514 | G |
| 46 | B | 518 | A |
| 46 | B | 529 | C |
| 46 | B | 533 | A |
| 46 | B | 553 | A |
| 46 | B | 556 | U |
| 46 | B | 638 | U |
| 46 | B | 695 | C |
| 46 | B | 740 | A |
| 46 | B | 763 | C |
| 46 | B | 769 | U |
| 46 | B | 814 | A |
| 46 | B | 855 | C |

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| Mol | Chain | Res | Type |
|---|---|---|---|
| 46 | B | 874 | U |
| 46 | B | 876 | A |
| 46 | B | 1168 | A |
| 46 | B | 1335 | U |
| 46 | B | 1369 | G |
| 46 | B | 1396 | A |
| 46 | B | 1398 | G |
| 46 | B | 1457 | A |
| 46 | B | 1467 | C |
| 46 | B | 1479 | A |
| 46 | B | 1484 | U |
| 46 | B | 1523 | G |
| 46 | B | 1573 | A |
| 46 | B | 1579 | A |
| 46 | B | 1581 | G |
| 46 | B | 1703 | C |
| 1 | AS | 172 | C |
| 1 | AS | 403 | C |
| 1 | AS | 447 | U |
| 1 | AS | 452 | A |
| 1 | AS | 453 | U |
| 1 | AS | 481 | G |
| 1 | AS | 487 | C |
| 1 | AS | 538 | G |
| 1 | AS | 563 | U |
| 1 | AS | 601 | U |
| 1 | AS | 759 | G |
| 1 | AS | 912 | G |
| 1 | AS | 1029 | U |
| 1 | AS | 1060 | A |
| 1 | AS | 1099 | A |
| 1 | AS | 1217 | A |
| 1 | AS | 1245 | G |
| 1 | AS | 1346 | U |
| 1 | AS | 1347 | U |
| 1 | AS | 1559 | C |
| 1 | AS | 1576 | A |
| 1 | AS | 1762 | G |
| 1 | AS | 1815 | U |
| 1 | AS | 1943 | G |
| 1 | AS | 2090 | U |
| 1 | AS | 2182 | C |

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| Mol | Chain | Res | Type |
|---|---|---|---|
| 1 | AS | 2183 | U |
| 1 | AS | 2430 | G |
| 1 | AS | 2431 | U |
| 1 | AS | 2434 | A |
| 1 | AS | 2447 | G |
| 1 | AS | 2448 | C |
| 1 | AS | 2449 | U |
| 1 | AS | 2452 | G |
| 1 | AS | 2455 | G |
| 1 | AS | 2458 | G |
| 1 | AS | 2465 | U |
| 1 | AS | 2476 | C |
| 1 | AS | 2515 | G |
| 1 | AS | 2519 | A |
| 1 | AS | 2545 | C |
| 1 | AS | 2789 | A |
| 1 | AS | 2790 | U |
| 1 | AS | 3093 | U |
| 1 | AS | 3159 | A |
| 1 | AS | 3193 | C |
| 1 | AS | 3234 | U |
| 1 | AS | 3240 | U |
| 1 | AS | 3284 | U |
| 1 | AS | 3309 | A |
| 1 | AS | 3315 | C |
| 1 | AS | 3317 | U |
| 3 | AU | 85 | G |
| 3 | AU | 125 | U |
| 3 | AU | 156 | U |
| 46 | CM | 25 | C |
| 46 | CM | 65 | A |
| 46 | CM | 78 | A |
| 46 | CM | 133 | U |
| 46 | CM | 137 | A |
| 46 | CM | 151 | G |
| 46 | CM | 176 | U |
| 46 | CM | 214 | U |
| 46 | CM | 216 | A |
| 46 | CM | 237 | C |
| 46 | CM | 238 | U |
| 46 | CM | 259 | U |
| 46 | CM | 265 | U |

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| Mol | Chain | Res | Type |
|---|---|---|---|
| 46 | CM | 278 | U |
| 46 | CM | 415 | A |
| 46 | CM | 451 | C |
| 46 | CM | 505 | U |
| 46 | CM | 514 | G |
| 46 | CM | 518 | A |
| 46 | CM | 529 | C |
| 46 | CM | 533 | A |
| 46 | CM | 553 | A |
| 46 | CM | 556 | U |
| 46 | CM | 638 | U |
| 46 | CM | 680 | C |
| 46 | CM | 681 | C |
| 46 | CM | 690 | C |
| 46 | CM | 695 | C |
| 46 | CM | 700 | G |
| 46 | CM | 702 | G |
| 46 | CM | 711 | U |
| 46 | CM | 740 | A |
| 46 | CM | 763 | C |
| 46 | CM | 769 | U |
| 46 | CM | 814 | A |
| 46 | CM | 817 | U |
| 46 | CM | 823 | G |
| 46 | CM | 855 | C |
| 46 | CM | 874 | U |
| 46 | CM | 876 | A |
| 46 | CM | 1168 | A |
| 46 | CM | 1335 | U |
| 46 | CM | 1359 | U |
| 46 | CM | 1369 | G |
| 46 | CM | 1396 | A |
| 46 | CM | 1398 | G |
| 46 | CM | 1457 | A |
| 46 | CM | 1467 | C |
| 46 | CM | 1479 | A |
| 46 | CM | 1523 | G |
| 46 | CM | 1555 | C |
| 46 | CM | 1573 | A |
| 46 | CM | 1579 | A |
| 46 | CM | 1581 | G |
| 46 | CM | 1743 | A |

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

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

## 5.5 Carbohydrates (i)

There are no oligosaccharides in this entry.

## 5.6 Ligand geometry (i)

Of 1231 ligands modelled in this entry, 1227 are monoatomic - leaving 4 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 | $\#\|Z\| > 2$ |
| 84 | 3K5 | AS | 3401 | - | 63,63,63 | 0.31 | 0 | 84,95,95 | 0.98 | 4 (4%) |
| 86 | HYG | B | 1953 | 83 | 36,39,39 | 0.66 | 1 (2%) | 44,60,60 | 1.10 | 4 (9%) |
| 86 | HYG | CM | 1902 | 83 | 36,39,39 | 0.71 | 1 (2%) | 44,60,60 | 1.23 | 5 (11%) |
| 84 | 3K5 | 1 | 3402 | - | 63,63,63 | 0.35 | 0 | 84,95,95 | 0.93 | 6 (7%) |

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 |
|---|---|---|---|---|---|---|---|
| 84 | 3K5 | AS | 3401 | - | - | 3/29/121/121 | 0/7/7/7 |
| 86 | HYG | B | 1953 | 83 | - | 5/12/87/87 | 0/4/4/4 |
| 86 | HYG | CM | 1902 | 83 | - | 7/12/87/87 | 0/4/4/4 |
| 84 | 3K5 | 1 | 3402 | - | - | 6/29/121/121 | 0/7/7/7 |

All (2) bond length outliers are listed below:

| Mol | Chain | Res | Type | Atoms | Z | Observed(Å) | Ideal(Å) |
|---|---|---|---|---|---|---|---|
| 86 | CM | 1902 | HYG | C4-N9 | 3.19 | 1.50 | 1.47 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(Å) | Ideal(Å) |
|---|---|---|---|---|---|---|---|
| 86 | B | 1953 | HYG | C4-N9 | 3.14 | 1.50 | 1.47 |

All (19) bond angle outliers are listed below:

| Mol | Chain | Res | Type | Atoms | Z | Observed($^o$) | Ideal($^o$) |
|---|---|---|---|---|---|---|---|
| 84 | AS | 3401 | 3K5 | O14-C34-C33 | 4.65 | 118.45 | 107.76 |
| 84 | AS | 3401 | 3K5 | C34-O14-C38 | 3.79 | 123.60 | 117.72 |
| 86 | CM | 1902 | HYG | C16-C17-C12 | -3.74 | 104.56 | 113.50 |
| 86 | B | 1953 | HYG | C16-C17-C12 | -3.41 | 105.34 | 113.50 |
| 86 | CM | 1902 | HYG | O29-C12-C13 | 3.30 | 119.32 | 110.89 |
| 86 | B | 1953 | HYG | O22-C17-C16 | 3.29 | 119.08 | 111.22 |
| 84 | 1 | 3402 | 3K5 | O14-C34-C35 | -3.10 | 100.63 | 107.76 |
| 86 | CM | 1902 | HYG | O22-C17-C16 | 2.85 | 118.03 | 111.22 |
| 84 | 1 | 3402 | 3K5 | C34-O14-C38 | 2.59 | 121.74 | 117.72 |
| 84 | 1 | 3402 | 3K5 | O14-C34-C33 | 2.55 | 113.63 | 107.76 |
| 84 | 1 | 3402 | 3K5 | C15-C17-C22 | -2.37 | 97.57 | 102.89 |
| 84 | AS | 3401 | 3K5 | O14-C34-C35 | 2.34 | 113.15 | 107.76 |
| 84 | 1 | 3402 | 3K5 | C18-C17-C22 | -2.33 | 102.30 | 107.43 |
| 86 | B | 1953 | HYG | O11-C5-C4 | -2.25 | 104.73 | 109.40 |
| 84 | AS | 3401 | 3K5 | O1-C5-C1 | 2.22 | 110.37 | 107.23 |
| 84 | 1 | 3402 | 3K5 | C9-C8-C7 | -2.20 | 122.11 | 126.92 |
| 86 | CM | 1902 | HYG | C26-C25-C24 | -2.17 | 108.08 | 111.18 |
| 86 | B | 1953 | HYG | O29-C12-C13 | 2.16 | 116.41 | 110.89 |
| 86 | CM | 1902 | HYG | O14-C13-C12 | -2.12 | 105.37 | 109.49 |

There are no chirality outliers.

All (21) torsion outliers are listed below:

| Mol | Chain | Res | Type | Atoms |
|---|---|---|---|---|
| 84 | 1 | 3402 | 3K5 | O15-C38-O14-C34 |
| 84 | AS | 3401 | 3K5 | O15-C38-O14-C34 |
| 86 | B | 1953 | HYG | N36-C33-C34-O35 |
| 86 | CM | 1902 | HYG | O28-C27-C33-C34 |
| 84 | 1 | 3402 | 3K5 | C39-C38-O14-C34 |
| 84 | AS | 3401 | 3K5 | C39-C38-O14-C34 |
| 86 | B | 1953 | HYG | O14-C13-O18-C6 |
| 86 | CM | 1902 | HYG | O14-C13-O18-C6 |
| 84 | AS | 3401 | 3K5 | C35-C34-O14-C38 |
| 86 | B | 1953 | HYG | O14-C15-C19-O20 |
| 86 | B | 1953 | HYG | C16-C15-C19-O20 |
| 86 | CM | 1902 | HYG | N36-C33-C34-O35 |
| 86 | B | 1953 | HYG | C27-C33-C34-O35 |

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| Mol | Chain | Res | Type | Atoms |
|---|---|---|---|---|
| 84 | 1 | 3402 | 3K5 | O7-C24-O6-C23 |
| 84 | 1 | 3402 | 3K5 | C25-C24-O6-C23 |
| 86 | CM | 1902 | HYG | C16-C15-C19-O20 |
| 86 | CM | 1902 | HYG | C26-C27-C33-C34 |
| 84 | 1 | 3402 | 3K5 | C1-C5-O1-C6 |
| 86 | CM | 1902 | HYG | O14-C15-C19-O20 |
| 86 | CM | 1902 | HYG | C27-C33-C34-O35 |
| 84 | 1 | 3402 | 3K5 | C21-C20-C23-O6 |

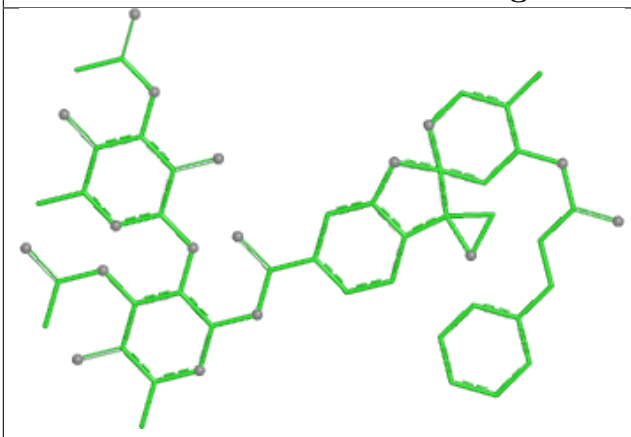
There are no ring outliers.

3 monomers are involved in 17 short contacts:

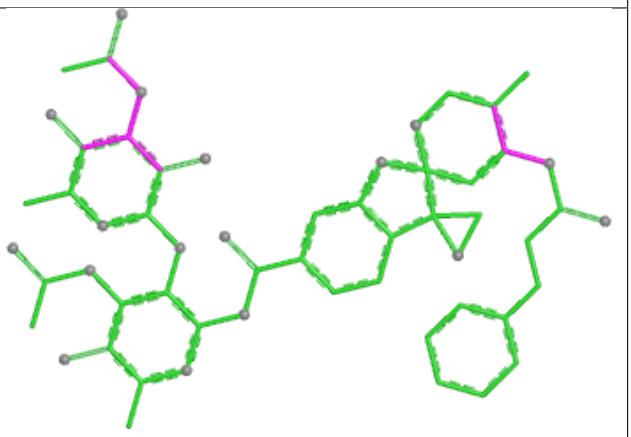
| Mol | Chain | Res | Type | Clashes | Symm-Clashes |
|---|---|---|---|---|---|
| 84 | AS | 3401 | 3K5 | 8 | 0 |
| 86 | CM | 1902 | HYG | 2 | 0 |
| 84 | 1 | 3402 | 3K5 | 7 | 0 |

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

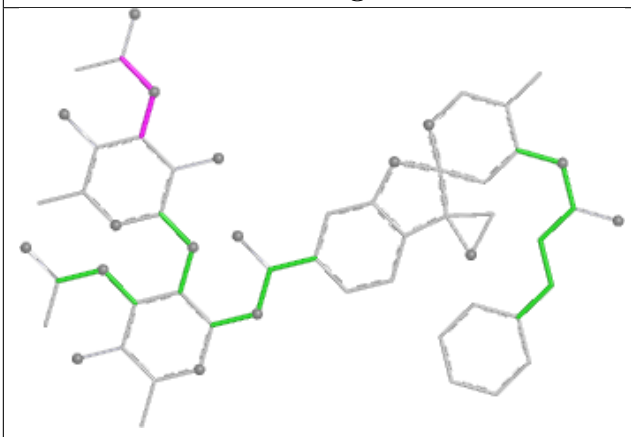
**Ligand 3K5 AS 3401**



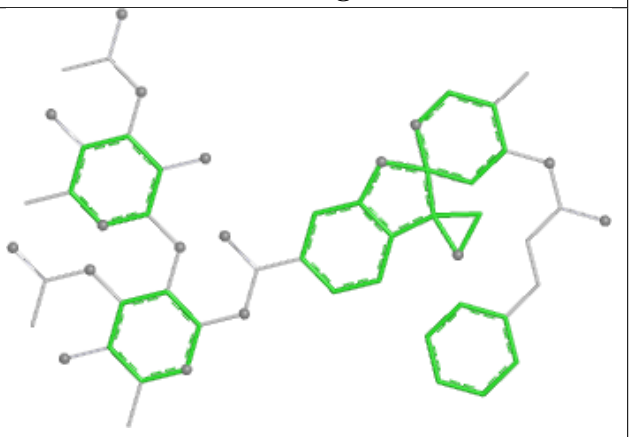
**Bond lengths**



**Bond angles**

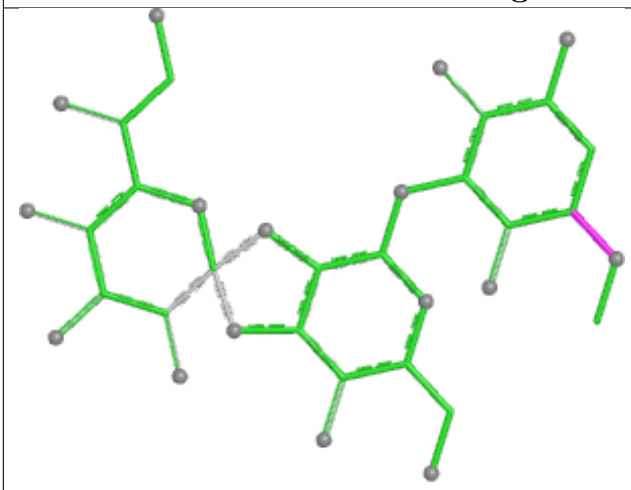


**Torsions**

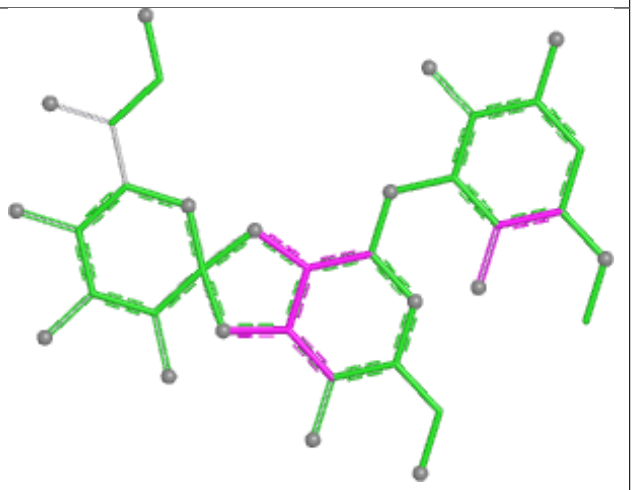


**Rings**

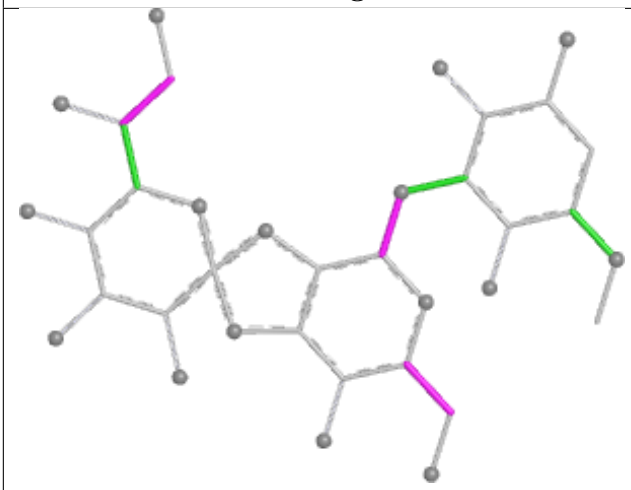
**Ligand HYG B 1953**



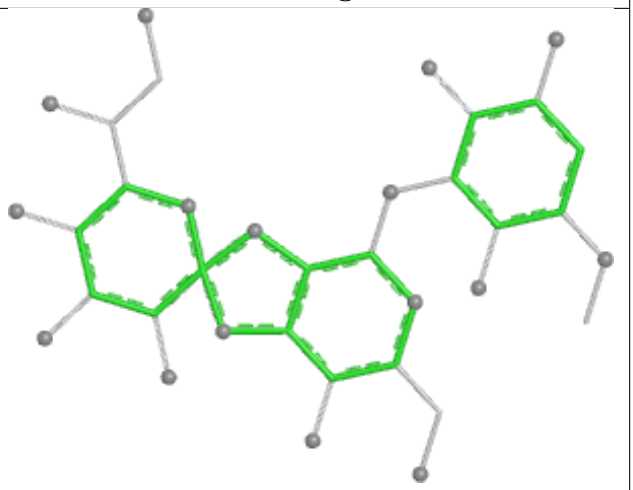
**Bond lengths**



**Bond angles**

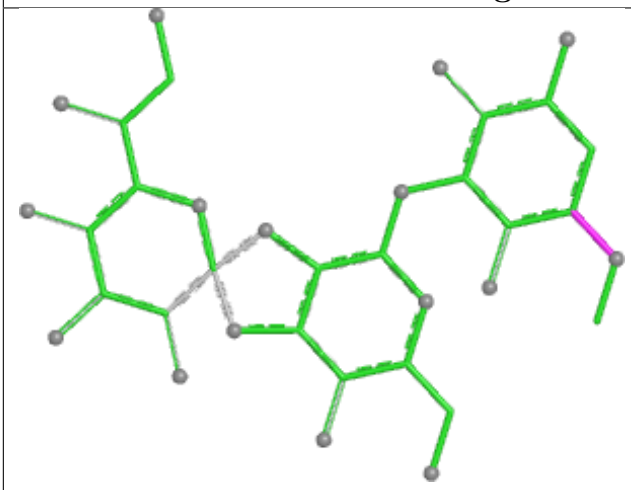


**Torsions**

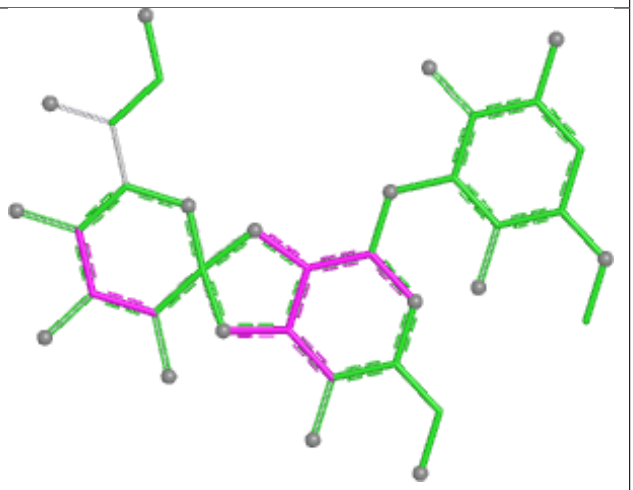


**Rings**

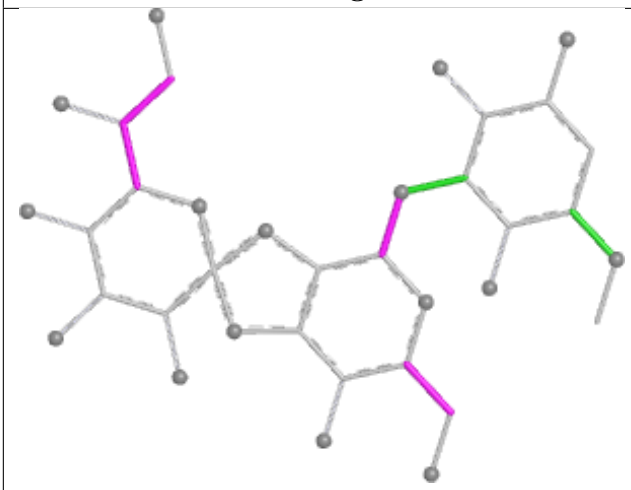
**Ligand HYG CM 1902**



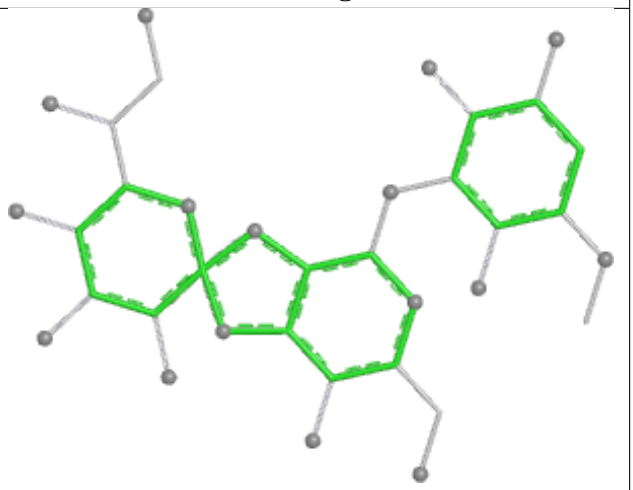
**Bond lengths**



**Bond angles**

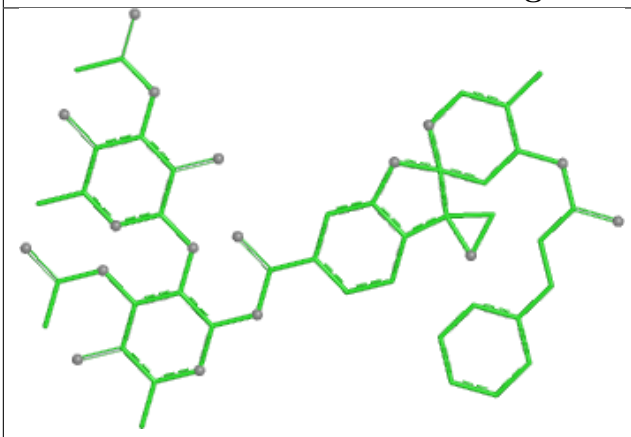


**Torsions**

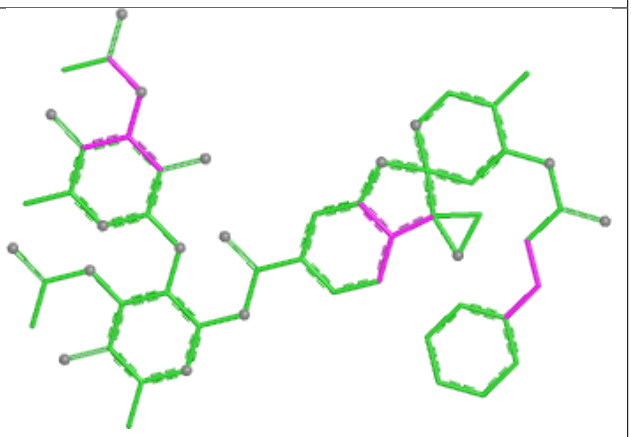


**Rings**

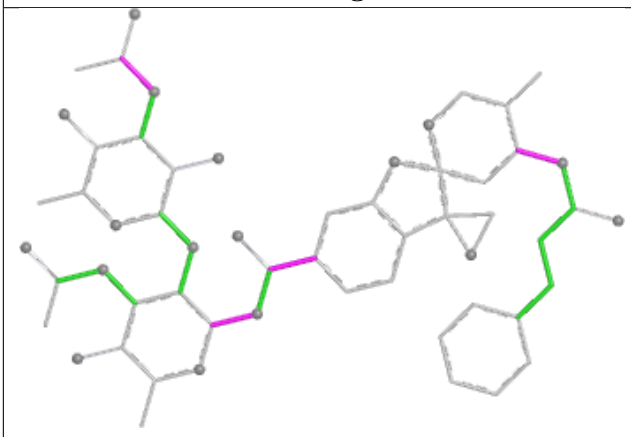
**Ligand 3K5 1 3402**



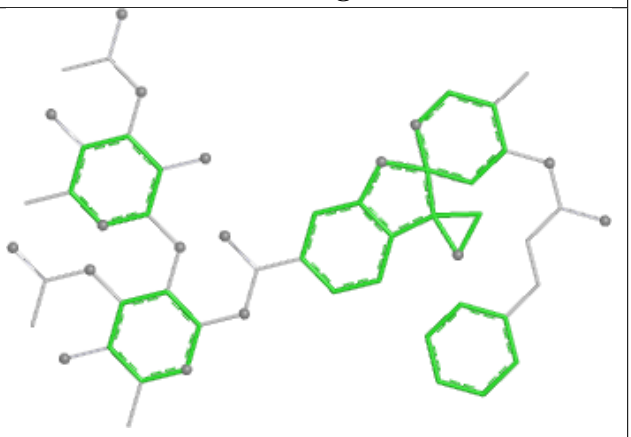
**Bond lengths**



**Bond angles**



**Torsions**



**Rings**

## 5.7 Other polymers

There are no such residues in this entry.

## 5.8 Polymer linkage issues

There are no chain breaks in this entry.

# 6 Fit of model and data

## 6.1 Protein, DNA and RNA chains

In the following table, the column labelled '#RSRZ> 2' contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, $95^{th}$ percentile and maximum values of the occupancy-weighted average B-factor per residue. The column labelled 'Q< 0.9' lists the number of (and percentage) of residues with an average occupancy less than 0.9.

| Mol | Chain | Analysed | <RSRZ> | #RSRZ>2 | OWAB(Å$^2$) | Q<0.9 |
|---|---|---|---|---|---|---|
| 1 | 1 | 3208/3359 (95%) | 0.31 | 78 (2%) 59 37 | 32, 64, 173, 334 | 0 |
| 1 | AS | 3227/3359 (96%) | 0.29 | 97 (3%) 52 30 | 34, 69, 204, 323 | 0 |
| 2 | 3 | 121/121 (100%) | 0.29 | 0 100 100 | 50, 78, 100, 136 | 0 |
| 2 | AT | 121/121 (100%) | 0.19 | 1 (0%) 82 63 | 39, 70, 93, 145 | 0 |
| 3 | 4 | 157/158 (99%) | 0.12 | 1 (0%) 85 69 | 46, 67, 117, 169 | 0 |
| 3 | AU | 157/158 (99%) | 0.44 | 6 (3%) 44 24 | 55, 89, 136, 219 | 0 |
| 4 | AW | 249/254 (98%) | 0.81 | 18 (7%) 21 11 | 37, 72, 95, 108 | 0 |
| 4 | j | 249/254 (98%) | 0.78 | 13 (5%) 33 16 | 28, 52, 74, 143 | 0 |
| 5 | AX | 386/389 (99%) | 0.49 | 11 (2%) 55 32 | 34, 56, 85, 150 | 0 |
| 5 | k | 386/389 (99%) | 0.63 | 14 (3%) 46 25 | 29, 58, 78, 116 | 0 |
| 6 | AY | 361/363 (99%) | 1.12 | 50 (13%) 6 4 | 44, 73, 101, 132 | 0 |
| 6 | l | 361/363 (99%) | 1.03 | 48 (13%) 7 4 | 35, 70, 105, 135 | 0 |
| 7 | AZ | 292/298 (97%) | 1.45 | 66 (22%) 2 1 | 44, 93, 124, 140 | 0 |
| 7 | m | 296/298 (99%) | 1.25 | 43 (14%) 6 3 | 50, 87, 119, 141 | 0 |
| 8 | BA | 153/176 (86%) | 0.82 | 10 (6%) 25 12 | 48, 68, 103, 132 | 0 |
| 8 | n | 157/176 (89%) | 0.85 | 12 (7%) 20 10 | 53, 75, 101, 138 | 0 |
| 9 | BB | 234/241 (97%) | 0.54 | 9 (3%) 44 24 | 35, 55, 113, 167 | 0 |
| 9 | o | 233/241 (96%) | 0.90 | 13 (5%) 30 15 | 38, 63, 123, 164 | 0 |
| 10 | BC | 229/262 (87%) | 1.44 | 54 (23%) 2 1 | 76, 117, 159, 188 | 0 |
| 10 | p | 233/262 (88%) | 1.08 | 34 (14%) 6 3 | 51, 76, 125, 148 | 0 |
| 11 | BD | 190/191 (99%) | 0.99 | 14 (7%) 20 10 | 48, 74, 106, 155 | 0 |
| 11 | q | 189/191 (98%) | 1.21 | 31 (16%) 4 2 | 52, 77, 97, 127 | 0 |
| 12 | BE | 208/220 (94%) | 0.56 | 9 (4%) 40 21 | 33, 51, 99, 134 | 0 |
| 12 | r | 208/220 (94%) | 0.89 | 18 (8%) 16 9 | 40, 65, 101, 119 | 0 |

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| Mol | Chain | Analysed | <RSRZ> | #RSRZ>2 | OWAB(Å$^2$) | Q<0.9 |
|---|---|---|---|---|---|---|
| 13 | BF | 171/174 (98%) | 1.02 | 16 (9%) 14 7 | 53, 81, 114, 127 | 0 |
| 13 | s | 171/174 (98%) | 1.34 | 28 (16%) 4 2 | 58, 92, 116, 131 | 0 |
| 14 | BG | 200/202 (99%) | 1.13 | 33 (16%) 4 2 | 48, 92, 133, 154 | 0 |
| 14 | t | 200/202 (99%) | 0.80 | 12 (6%) 27 14 | 43, 75, 110, 143 | 0 |
| 15 | BH | 130/131 (99%) | 0.70 | 8 (6%) 26 13 | 43, 65, 96, 128 | 0 |
| 15 | u | 130/131 (99%) | 0.83 | 8 (6%) 26 13 | 52, 70, 89, 103 | 0 |
| 16 | BI | 203/204 (99%) | 1.50 | 46 (22%) 2 1 | 54, 84, 106, 118 | 0 |
| 16 | v | 203/204 (99%) | 1.11 | 20 (9%) 13 6 | 36, 57, 71, 85 | 0 |
| 17 | BJ | 199/200 (99%) | 0.46 | 7 (3%) 47 26 | 34, 51, 86, 120 | 0 |
| 17 | w | 199/200 (99%) | 0.75 | 12 (6%) 27 14 | 33, 55, 82, 103 | 0 |
| 18 | BK | 176/185 (95%) | 1.00 | 14 (7%) 18 9 | 44, 63, 91, 123 | 0 |
| 18 | x | 173/185 (93%) | 0.90 | 13 (7%) 20 10 | 33, 59, 92, 120 | 0 |
| 19 | BL | 185/186 (99%) | 0.82 | 9 (4%) 35 17 | 45, 69, 85, 104 | 0 |
| 19 | y | 185/186 (99%) | 1.36 | 45 (24%) 2 1 | 41, 66, 85, 100 | 0 |
| 20 | BM | 179/190 (94%) | 0.92 | 17 (9%) 14 7 | 48, 77, 137, 169 | 0 |
| 20 | z | 179/190 (94%) | 0.84 | 6 (3%) 48 27 | 45, 68, 126, 145 | 0 |
| 21 | 0 | 170/172 (98%) | 0.92 | 15 (8%) 15 8 | 46, 64, 87, 137 | 0 |
| 21 | BN | 170/172 (98%) | 0.61 | 8 (4%) 36 19 | 39, 58, 77, 105 | 0 |
| 22 | 2 | 159/160 (99%) | 1.03 | 19 (11%) 9 5 | 44, 63, 111, 147 | 0 |
| 22 | BO | 159/160 (99%) | 0.97 | 20 (12%) 8 4 | 37, 60, 113, 147 | 0 |
| 23 | 5 | 102/124 (82%) | 1.00 | 9 (8%) 15 8 | 73, 109, 140, 160 | 0 |
| 23 | BP | 102/124 (82%) | 1.15 | 14 (13%) 6 4 | 89, 125, 151, 162 | 0 |
| 24 | 6 | 131/137 (95%) | 0.71 | 6 (4%) 37 19 | 37, 55, 76, 86 | 0 |
| 24 | BQ | 131/137 (95%) | 0.74 | 7 (5%) 32 16 | 32, 53, 77, 116 | 0 |
| 25 | 7 | 118/155 (76%) | 0.92 | 12 (10%) 12 6 | 38, 76, 126, 143 | 0 |
| 25 | BR | 98/155 (63%) | 1.00 | 15 (15%) 5 3 | 39, 70, 128, 138 | 0 |
| 26 | 8 | 120/142 (84%) | 0.89 | 10 (8%) 17 9 | 53, 71, 91, 98 | 0 |
| 26 | BS | 119/142 (83%) | 1.29 | 28 (23%) 2 1 | 62, 93, 113, 128 | 0 |
| 27 | 9 | 126/127 (99%) | 1.41 | 25 (19%) 3 1 | 55, 80, 98, 113 | 0 |
| 27 | BT | 126/127 (99%) | 1.09 | 16 (12%) 8 4 | 59, 91, 123, 140 | 0 |
| 28 | AA | 135/136 (99%) | 1.20 | 19 (14%) 6 3 | 56, 84, 111, 143 | 0 |

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| Mol | Chain | Analysed | <RSRZ> | #RSRZ>2 | OWAB(Å$^2$) | Q<0.9 |
|---|---|---|---|---|---|---|
| 28 | BU | 135/136 (99%) | 1.25 | 21 (15%) 5 2 | 78, 113, 137, 159 | 0 |
| 29 | AB | 148/149 (99%) | 1.06 | 14 (9%) 14 7 | 34, 63, 95, 123 | 0 |
| 29 | BV | 148/149 (99%) | 1.16 | 24 (16%) 4 2 | 44, 73, 96, 118 | 0 |
| 30 | AC | 62/63 (98%) | 1.60 | 21 (33%) 1 0 | 39, 77, 122, 143 | 0 |
| 30 | BW | 61/63 (96%) | 1.40 | 13 (21%) 2 1 | 38, 76, 112, 135 | 0 |
| 31 | AD | 96/106 (90%) | 0.72 | 6 (6%) 26 13 | 53, 73, 95, 108 | 0 |
| 31 | BX | 96/106 (90%) | 1.13 | 18 (18%) 3 2 | 78, 103, 128, 152 | 0 |
| 32 | AE | 110/112 (98%) | 0.66 | 4 (3%) 46 25 | 46, 64, 109, 134 | 0 |
| 32 | BY | 110/112 (98%) | 0.90 | 8 (7%) 21 10 | 42, 72, 120, 146 | 0 |
| 33 | AF | 124/131 (94%) | 1.09 | 16 (12%) 7 4 | 33, 65, 83, 94 | 0 |
| 33 | BZ | 124/131 (94%) | 0.80 | 7 (5%) 30 15 | 37, 63, 87, 107 | 0 |
| 34 | AG | 106/107 (99%) | 1.05 | 14 (13%) 7 4 | 45, 61, 78, 99 | 0 |
| 34 | CA | 106/107 (99%) | 0.56 | 3 (2%) 55 32 | 36, 51, 73, 91 | 0 |
| 35 | AH | 112/122 (91%) | 1.28 | 17 (15%) 5 3 | 46, 70, 113, 139 | 0 |
| 35 | CB | 112/122 (91%) | 1.44 | 30 (26%) 1 1 | 50, 95, 128, 158 | 0 |
| 36 | AI | 120/120 (100%) | 1.13 | 13 (10%) 11 5 | 60, 83, 106, 128 | 0 |
| 36 | CC | 118/120 (98%) | 1.45 | 29 (24%) 2 1 | 74, 100, 125, 135 | 0 |
| 37 | AJ | 97/99 (97%) | 1.04 | 13 (13%) 7 4 | 50, 70, 102, 166 | 0 |
| 37 | CD | 97/99 (97%) | 1.37 | 21 (21%) 2 1 | 77, 98, 125, 155 | 0 |
| 38 | AK | 86/90 (95%) | 0.87 | 6 (6%) 22 11 | 28, 54, 95, 109 | 0 |
| 38 | CE | 86/90 (95%) | 1.11 | 13 (15%) 5 3 | 48, 71, 100, 135 | 0 |
| 39 | AL | 77/78 (98%) | 1.17 | 9 (11%) 9 5 | 72, 94, 125, 153 | 0 |
| 39 | CF | 77/78 (98%) | 1.47 | 16 (20%) 2 1 | 83, 115, 157, 165 | 0 |
| 40 | AM | 50/51 (98%) | 1.01 | 4 (8%) 18 9 | 42, 61, 84, 95 | 0 |
| 40 | CG | 50/51 (98%) | 1.41 | 8 (16%) 5 2 | 55, 76, 97, 105 | 0 |
| 41 | AN | 52/52 (100%) | 2.11 | 21 (40%) 0 0 | 65, 96, 120, 128 | 0 |
| 41 | CH | 51/52 (98%) | 2.34 | 30 (58%) 0 0 | 60, 95, 115, 127 | 0 |
| 42 | AO | 25/25 (100%) | 1.74 | 10 (40%) 1 0 | 55, 66, 82, 88 | 0 |
| 42 | CI | 24/25 (96%) | 1.49 | 6 (25%) 2 1 | 43, 58, 68, 74 | 0 |
| 43 | AP | 103/106 (97%) | 0.85 | 13 (12%) 8 4 | 36, 62, 100, 118 | 0 |
| 43 | CJ | 103/106 (97%) | 0.98 | 14 (13%) 7 4 | 44, 72, 107, 121 | 0 |

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| Mol | Chain | Analysed | <RSRZ> | #RSRZ>2 | OWAB(Å$^2$) | Q<0.9 |
|---|---|---|---|---|---|---|
| 44 | AQ | 91/92 (98%) | 0.79 | 4 (4%) 39 20 | 39, 57, 97, 108 | 0 |
| 44 | CK | 91/92 (98%) | 0.84 | 6 (6%) 24 12 | 48, 72, 104, 123 | 0 |
| 45 | CL | 121/267 (45%) | 1.42 | 31 (25%) 1 1 | 59, 88, 120, 144 | 0 |
| 45 | i | 120/267 (44%) | 1.76 | 38 (31%) 1 1 | 59, 103, 135, 152 | 0 |
| 46 | B | 1741/1787 (97%) | 0.75 | 96 (5%) 30 16 | 48, 89, 173, 457 | 0 |
| 46 | CM | 1765/1787 (98%) | 0.62 | 75 (4%) 40 21 | 41, 79, 180, 457 | 0 |
| 47 | C | 208/261 (79%) | 1.25 | 41 (19%) 3 1 | 80, 109, 137, 148 | 0 |
| 47 | CN | 208/261 (79%) | 1.17 | 26 (12%) 8 4 | 53, 97, 127, 165 | 0 |
| 48 | CO | 214/256 (83%) | 1.42 | 51 (23%) 2 1 | 65, 113, 138, 164 | 0 |
| 48 | D | 214/256 (83%) | 1.04 | 27 (12%) 8 4 | 58, 92, 111, 131 | 0 |
| 49 | CP | 217/249 (87%) | 0.92 | 24 (11%) 10 5 | 42, 73, 102, 120 | 0 |
| 49 | E | 217/249 (87%) | 1.43 | 47 (21%) 2 1 | 69, 97, 121, 146 | 0 |
| 50 | CQ | 223/251 (88%) | 1.16 | 35 (15%) 5 2 | 49, 76, 133, 174 | 0 |
| 50 | F | 223/251 (88%) | 1.72 | 73 (32%) 1 0 | 70, 107, 152, 178 | 0 |
| 51 | CR | 260/262 (99%) | 1.54 | 63 (24%) 2 1 | 58, 88, 110, 151 | 0 |
| 51 | G | 259/262 (98%) | 1.67 | 85 (32%) 1 0 | 63, 96, 116, 156 | 0 |
| 52 | CS | 206/225 (91%) | 1.70 | 64 (31%) 1 1 | 65, 99, 137, 191 | 0 |
| 52 | H | 206/225 (91%) | 1.84 | 74 (35%) 1 0 | 67, 103, 143, 168 | 0 |
| 53 | CT | 236/236 (100%) | 1.24 | 35 (14%) 5 3 | 54, 94, 139, 159 | 0 |
| 53 | I | 226/236 (95%) | 1.21 | 42 (18%) 3 2 | 59, 96, 142, 175 | 0 |
| 54 | CU | 183/186 (98%) | 1.45 | 45 (24%) 2 1 | 67, 124, 165, 174 | 0 |
| 54 | J | 184/186 (98%) | 1.88 | 71 (38%) 1 0 | 76, 126, 156, 173 | 0 |
| 55 | CV | 203/206 (98%) | 1.29 | 41 (20%) 3 1 | 38, 70, 120, 148 | 0 |
| 55 | K | 203/206 (98%) | 1.15 | 37 (18%) 3 2 | 43, 79, 123, 140 | 0 |
| 56 | CW | 178/189 (94%) | 1.66 | 48 (26%) 1 1 | 59, 93, 121, 136 | 0 |
| 56 | L | 178/189 (94%) | 2.06 | 91 (51%) 0 0 | 74, 108, 129, 143 | 0 |
| 57 | CX | 94/118 (79%) | 1.02 | 9 (9%) 13 7 | 62, 85, 123, 142 | 0 |
| 57 | M | 98/118 (83%) | 1.70 | 36 (36%) 1 0 | 84, 117, 142, 158 | 0 |
| 58 | CY | 141/155 (90%) | 1.24 | 21 (14%) 5 3 | 39, 67, 95, 149 | 0 |
| 58 | N | 144/155 (92%) | 1.18 | 21 (14%) 6 3 | 48, 77, 113, 139 | 0 |
| 59 | CZ | 119/143 (83%) | 1.46 | 30 (25%) 1 1 | 124, 157, 177, 180 | 0 |

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| Mol | Chain | Analysed | <RSRZ> | #RSRZ>2 | | | OWAB(Å$^2$) | Q<0.9 |
|---|---|---|---|---|---|---|---|---|
| 59 | O | 116/143 (81%) | 1.69 | 38 (32%) | 1 | 0 | 136, 175, 196, 203 | 0 |
| 60 | DA | 150/151 (99%) | 1.52 | 41 (27%) | 1 | 1 | 54, 89, 117, 134 | 0 |
| 60 | P | 150/151 (99%) | 1.52 | 41 (27%) | 1 | 1 | 46, 88, 116, 122 | 0 |
| 61 | DB | 127/132 (96%) | 1.16 | 13 (10%) | 12 | 6 | 57, 97, 123, 132 | 0 |
| 61 | Q | 127/132 (96%) | 1.02 | 16 (12%) | 8 | 4 | 44, 79, 96, 107 | 0 |
| 62 | DC | 130/142 (91%) | 1.39 | 25 (19%) | 3 | 1 | 50, 89, 130, 144 | 0 |
| 62 | R | 129/142 (90%) | 1.77 | 45 (34%) | 1 | 0 | 63, 100, 137, 151 | 0 |
| 63 | DD | 140/142 (98%) | 2.15 | 74 (52%) | 0 | 0 | 58, 98, 130, 143 | 0 |
| 63 | S | 140/142 (98%) | 2.31 | 75 (53%) | 0 | 0 | 67, 112, 148, 152 | 0 |
| 64 | DE | 124/137 (90%) | 1.85 | 48 (38%) | 1 | 0 | 67, 108, 158, 166 | 0 |
| 64 | T | 124/137 (90%) | 2.04 | 52 (41%) | 0 | 0 | 80, 121, 166, 176 | 0 |
| 65 | DF | 141/145 (97%) | 1.36 | 27 (19%) | 3 | 1 | 54, 92, 124, 156 | 0 |
| 65 | U | 144/145 (99%) | 1.53 | 39 (27%) | 1 | 1 | 62, 90, 114, 157 | 0 |
| 66 | DG | 141/145 (97%) | 1.54 | 41 (29%) | 1 | 1 | 60, 90, 119, 148 | 0 |
| 66 | V | 141/145 (97%) | 1.88 | 48 (34%) | 1 | 0 | 79, 107, 140, 162 | 0 |
| 67 | DH | 97/119 (81%) | 1.64 | 29 (29%) | 1 | 1 | 49, 94, 122, 150 | 0 |
| 67 | W | 102/119 (85%) | 1.82 | 39 (38%) | 1 | 0 | 71, 121, 149, 158 | 0 |
| 68 | DI | 87/87 (100%) | 0.93 | 7 (8%) | 18 | 9 | 61, 83, 114, 149 | 0 |
| 68 | X | 87/87 (100%) | 1.14 | 12 (13%) | 6 | 4 | 76, 102, 126, 133 | 0 |
| 69 | DJ | 129/130 (99%) | 1.33 | 27 (20%) | 2 | 1 | 50, 69, 87, 96 | 0 |
| 69 | Y | 129/130 (99%) | 1.75 | 41 (31%) | 1 | 0 | 59, 84, 105, 113 | 0 |
| 70 | DK | 143/145 (98%) | 1.23 | 25 (17%) | 4 | 2 | 43, 64, 88, 116 | 0 |
| 70 | Z | 143/145 (98%) | 1.33 | 29 (20%) | 3 | 1 | 56, 78, 97, 115 | 0 |
| 71 | DL | 132/135 (97%) | 1.19 | 16 (12%) | 8 | 5 | 71, 110, 133, 174 | 0 |
| 71 | a | 134/135 (99%) | 1.48 | 33 (24%) | 2 | 1 | 68, 112, 130, 144 | 0 |
| 72 | DM | 71/105 (67%) | 1.19 | 10 (14%) | 6 | 3 | 89, 120, 143, 148 | 0 |
| 72 | b | 72/105 (68%) | 1.31 | 13 (18%) | 3 | 2 | 85, 111, 134, 154 | 0 |
| 73 | DN | 97/119 (81%) | 1.37 | 18 (18%) | 3 | 2 | 52, 75, 129, 137 | 0 |
| 73 | c | 98/119 (82%) | 1.46 | 24 (24%) | 2 | 1 | 53, 83, 123, 135 | 0 |
| 74 | DO | 81/82 (98%) | 1.46 | 18 (22%) | 2 | 1 | 73, 99, 160, 173 | 0 |
| 74 | d | 81/82 (98%) | 1.38 | 13 (16%) | 5 | 2 | 73, 99, 156, 170 | 0 |

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| Mol | Chain | Analysed | <RSRZ> | #RSRZ>2 | OWAB(Å$^2$) | Q<0.9 |
|---|---|---|---|---|---|---|
| 75 | DP | 61/67 (91%) | 1.07 | 9 (14%) 5 3 | 78, 101, 129, 148 | 0 |
| 75 | e | 62/67 (92%) | 1.45 | 13 (20%) 2 1 | 91, 111, 131, 138 | 0 |
| 76 | DQ | 54/56 (96%) | 1.38 | 12 (22%) 2 1 | 51, 65, 93, 103 | 0 |
| 76 | f | 55/56 (98%) | 1.82 | 17 (30%) 1 1 | 75, 92, 118, 141 | 0 |
| 77 | DR | 58/63 (92%) | 1.52 | 15 (25%) 1 1 | 63, 101, 161, 173 | 0 |
| 77 | g | 60/63 (95%) | 1.60 | 16 (26%) 1 1 | 75, 105, 154, 169 | 0 |
| 78 | DS | 70/193 (36%) | 2.33 | 36 (51%) 0 0 | 95, 163, 181, 196 | 0 |
| 78 | h | 70/193 (36%) | 1.88 | 28 (40%) 1 0 | 113, 160, 185, 191 | 0 |
| 79 | AR | 311/317 (98%) | 1.61 | 86 (27%) 1 1 | 114, 155, 178, 192 | 0 |
| 79 | DT | 306/317 (96%) | 1.72 | 103 (33%) 1 0 | 100, 145, 174, 196 | 0 |
| 80 | P0 | 107/312 (34%) | 1.52 | 30 (28%) 1 1 | 104, 127, 144, 157 | 0 |
| 80 | p0 | 79/312 (25%) | 2.19 | 37 (46%) 0 0 | 119, 138, 155, 161 | 0 |
| 81 | 12 | 63/165 (38%) | 0.98 | 6 (9%) 14 7 | 98, 132, 151, 157 | 0 |
| 82 | L1 | 217/217 (100%) | 1.00 | 28 (12%) 7 4 | 91, 127, 164, 224 | 0 |
| 82 | l1 | 217/217 (100%) | 1.36 | 51 (23%) 2 1 | 109, 137, 164, 197 | 0 |
| All | All | 33588/36349 (92%) | 0.97 | 4460 (13%) 7 4 | 28, 80, 154, 457 | 0 |

All (4460) RSRZ outliers are listed below:

| Mol | Chain | Res | Type | RSRZ |
|---|---|---|---|---|
| 67 | W | 81 | TYR | 9.5 |
| 51 | G | 110 | ALA | 9.5 |
| 50 | F | 206 | ALA | 9.0 |
| 1 | AS | 1263 | U | 8.2 |
| 66 | V | 18 | TYR | 7.9 |
| 45 | i | 64 | LEU | 7.3 |
| 62 | R | 109 | PRO | 7.3 |
| 78 | DS | 127 | TYR | 7.3 |
| 52 | H | 70 | VAL | 7.2 |
| 1 | AS | 1262 | G | 7.1 |
| 41 | AN | 16 | GLU | 7.0 |
| 63 | S | 50 | PRO | 6.9 |
| 64 | T | 68 | GLY | 6.9 |
| 56 | L | 138 | LYS | 6.9 |
| 52 | CS | 152 | SER | 6.8 |
| 79 | DT | 34 | LEU | 6.8 |
| 52 | CS | 151 | SER | 6.8 |

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| Mol | Chain | Res | Type | RSRZ |
|---|---|---|---|---|
| 54 | CU | 87 | VAL | 6.7 |
| 29 | BV | 20 | GLY | 6.5 |
| 27 | 9 | 4 | ILE | 6.3 |
| 74 | DO | 24 | LEU | 6.3 |
| 1 | AS | 3319 | U | 6.3 |
| 67 | DH | 81 | TYR | 6.2 |
| 51 | CR | 245 | ILE | 6.2 |
| 59 | O | 89 | ILE | 6.1 |
| 41 | CH | 16 | GLU | 6.1 |
| 63 | S | 67 | LYS | 5.9 |
| 67 | W | 79 | ASP | 5.9 |
| 63 | S | 120 | SER | 5.8 |
| 6 | AY | 361 | LEU | 5.8 |
| 5 | k | 12 | GLY | 5.8 |
| 65 | DF | 94 | ASP | 5.8 |
| 49 | E | 161 | ALA | 5.8 |
| 79 | AR | 80 | TYR | 5.8 |
| 49 | E | 86 | ARG | 5.7 |
| 52 | CS | 82 | PHE | 5.7 |
| 7 | AZ | 7 | PHE | 5.7 |
| 56 | L | 116 | LEU | 5.7 |
| 66 | V | 84 | LYS | 5.6 |
| 77 | g | 47 | VAL | 5.6 |
| 36 | CC | 107 | GLN | 5.6 |
| 54 | J | 77 | LEU | 5.6 |
| 80 | p0 | 74 | GLU | 5.6 |
| 80 | p0 | 59 | VAL | 5.6 |
| 73 | c | 29 | CYS | 5.5 |
| 6 | AY | 363 | ASN | 5.5 |
| 79 | DT | 290 | ALA | 5.5 |
| 80 | P0 | 85 | GLY | 5.5 |
| 48 | CO | 155 | TYR | 5.4 |
| 46 | CM | 1679 | A | 5.4 |
| 64 | DE | 91 | LEU | 5.4 |
| 79 | DT | 293 | ALA | 5.4 |
| 52 | H | 170 | GLN | 5.4 |
| 1 | AS | 1264 | G | 5.4 |
| 78 | DS | 125 | LYS | 5.4 |
| 76 | f | 34 | TYR | 5.4 |
| 4 | j | 250 | GLN | 5.4 |
| 14 | BG | 2 | ALA | 5.4 |
| 49 | E | 92 | ARG | 5.4 |

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| Mol | Chain | Res | Type | RSRZ |
|---|---|---|---|---|
| 1 | AS | 1261 | U | 5.3 |
| 64 | T | 51 | ALA | 5.3 |
| 64 | T | 12 | ALA | 5.3 |
| 37 | AJ | 96 | SER | 5.3 |
| 79 | DT | 80 | TYR | 5.3 |
| 67 | W | 66 | THR | 5.2 |
| 50 | CQ | 206 | ALA | 5.2 |
| 71 | DL | 88 | ALA | 5.2 |
| 50 | F | 168 | PHE | 5.2 |
| 56 | L | 35 | GLY | 5.2 |
| 69 | Y | 127 | GLY | 5.2 |
| 56 | L | 6 | ARG | 5.2 |
| 60 | P | 150 | VAL | 5.2 |
| 49 | E | 77 | LYS | 5.2 |
| 79 | AR | 260 | PHE | 5.2 |
| 52 | CS | 79 | SER | 5.2 |
| 79 | AR | 17 | ASN | 5.1 |
| 8 | n | 168 | GLY | 5.1 |
| 80 | p0 | 71 | PRO | 5.1 |
| 46 | B | 1339 | G | 5.1 |
| 50 | F | 154 | ALA | 5.1 |
| 80 | p0 | 73 | PHE | 5.1 |
| 1 | AS | 1265 | U | 5.1 |
| 52 | CS | 76 | LYS | 5.1 |
| 50 | F | 151 | GLN | 5.1 |
| 52 | H | 152 | SER | 5.1 |
| 54 | J | 179 | PHE | 5.1 |
| 79 | DT | 208 | CYS | 5.1 |
| 80 | p0 | 67 | LEU | 5.1 |
| 14 | t | 2 | ALA | 5.0 |
| 64 | T | 8 | THR | 5.0 |
| 48 | CO | 107 | SER | 5.0 |
| 40 | CG | 21 | ARG | 5.0 |
| 56 | CW | 62 | ARG | 5.0 |
| 45 | i | 108 | GLY | 5.0 |
| 16 | BI | 43 | SER | 5.0 |
| 52 | H | 130 | ILE | 5.0 |
| 51 | G | 39 | ARG | 5.0 |
| 71 | a | 23 | PHE | 5.0 |
| 59 | O | 118 | ALA | 5.0 |
| 27 | 9 | 44 | ASN | 5.0 |
| 63 | DD | 67 | LYS | 5.0 |

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| Mol | Chain | Res | Type | RSRZ |
|---|---|---|---|---|
| 58 | CY | 114 | ALA | 4.9 |
| 66 | V | 86 | ARG | 4.9 |
| 6 | AY | 73 | ALA | 4.9 |
| 79 | AR | 79 | ALA | 4.9 |
| 18 | BK | 66 | SER | 4.9 |
| 63 | S | 54 | VAL | 4.9 |
| 45 | CL | 95 | GLY | 4.9 |
| 79 | DT | 116 | ILE | 4.9 |
| 56 | L | 146 | PHE | 4.9 |
| 79 | DT | 299 | PHE | 4.9 |
| 79 | DT | 73 | THR | 4.9 |
| 66 | V | 116 | ILE | 4.9 |
| 63 | S | 66 | VAL | 4.9 |
| 15 | u | 131 | ALA | 4.9 |
| 53 | I | 135 | PRO | 4.9 |
| 51 | G | 109 | PHE | 4.9 |
| 1 | AS | 1244 | C | 4.9 |
| 46 | B | 1410 | A | 4.9 |
| 52 | H | 72 | HIS | 4.8 |
| 46 | CM | 1680 | A | 4.8 |
| 30 | AC | 21 | ILE | 4.8 |
| 54 | CU | 179 | PHE | 4.8 |
| 80 | p0 | 79 | PHE | 4.8 |
| 51 | CR | 44 | LEU | 4.8 |
| 73 | c | 16 | GLY | 4.8 |
| 68 | X | 56 | SER | 4.8 |
| 54 | J | 86 | VAL | 4.8 |
| 77 | g | 49 | LEU | 4.8 |
| 41 | AN | 12 | LYS | 4.8 |
| 61 | Q | 88 | THR | 4.8 |
| 46 | CM | 657 | C | 4.8 |
| 30 | BW | 10 | HIS | 4.7 |
| 79 | DT | 260 | PHE | 4.7 |
| 52 | H | 76 | LYS | 4.7 |
| 53 | I | 50 | PHE | 4.7 |
| 57 | M | 46 | LEU | 4.7 |
| 1 | 1 | 2436 | A | 4.7 |
| 63 | S | 119 | ASP | 4.7 |
| 10 | BC | 115 | ALA | 4.7 |
| 62 | R | 17 | PHE | 4.7 |
| 49 | E | 160 | VAL | 4.7 |
| 51 | CR | 246 | LYS | 4.7 |

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| Mol | Chain | Res | Type | RSRZ |
|---|---|---|---|---|
| 56 | L | 142 | ASN | 4.7 |
| 52 | CS | 26 | ALA | 4.7 |
| 67 | W | 80 | ALA | 4.7 |
| 61 | DB | 23 | VAL | 4.7 |
| 72 | b | 54 | VAL | 4.7 |
| 56 | CW | 18 | PRO | 4.7 |
| 1 | AS | 545 | G | 4.7 |
| 53 | CT | 169 | TYR | 4.7 |
| 56 | CW | 93 | LEU | 4.7 |
| 49 | CP | 95 | ALA | 4.7 |
| 60 | P | 7 | SER | 4.6 |
| 13 | s | 125 | MET | 4.6 |
| 75 | e | 50 | GLU | 4.6 |
| 7 | m | 150 | LEU | 4.6 |
| 43 | CJ | 72 | LEU | 4.6 |
| 64 | DE | 24 | LEU | 4.6 |
| 64 | T | 9 | VAL | 4.6 |
| 52 | CS | 99 | MET | 4.6 |
| 50 | F | 136 | GLU | 4.6 |
| 65 | DF | 22 | ILE | 4.6 |
| 62 | R | 116 | LEU | 4.6 |
| 54 | J | 87 | VAL | 4.6 |
| 50 | F | 149 | LYS | 4.6 |
| 76 | f | 43 | PHE | 4.6 |
| 66 | DG | 55 | TYR | 4.6 |
| 45 | i | 102 | LYS | 4.6 |
| 1 | AS | 1245 | G | 4.6 |
| 12 | BE | 114 | GLY | 4.6 |
| 82 | l1 | 167 | VAL | 4.6 |
| 6 | l | 184 | LYS | 4.5 |
| 64 | DE | 9 | VAL | 4.5 |
| 50 | F | 153 | TYR | 4.5 |
| 63 | DD | 131 | ARG | 4.5 |
| 55 | CV | 185 | CYS | 4.5 |
| 71 | a | 69 | SER | 4.5 |
| 45 | CL | 59 | GLY | 4.5 |
| 77 | DR | 4 | VAL | 4.5 |
| 10 | BC | 114 | ALA | 4.5 |
| 63 | S | 116 | LEU | 4.5 |
| 73 | c | 39 | VAL | 4.5 |
| 5 | k | 330 | GLY | 4.5 |
| 16 | BI | 108 | ARG | 4.5 |

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| Mol | Chain | Res | Type | RSRZ |
|---|---|---|---|---|
| 52 | CS | 154 | THR | 4.5 |
| 65 | U | 115 | ARG | 4.5 |
| 50 | F | 137 | VAL | 4.5 |
| 69 | Y | 79 | PHE | 4.5 |
| 18 | x | 128 | ARG | 4.5 |
| 7 | m | 9 | THR | 4.5 |
| 56 | CW | 118 | LEU | 4.5 |
| 79 | AR | 32 | LEU | 4.5 |
| 78 | DS | 179 | ASP | 4.4 |
| 34 | AG | 95 | GLY | 4.4 |
| 66 | DG | 50 | ALA | 4.4 |
| 68 | X | 54 | ALA | 4.4 |
| 78 | DS | 172 | ILE | 4.4 |
| 48 | CO | 156 | ALA | 4.4 |
| 59 | CZ | 118 | ALA | 4.4 |
| 61 | Q | 119 | ASP | 4.4 |
| 66 | DG | 119 | LYS | 4.4 |
| 73 | c | 90 | THR | 4.4 |
| 63 | S | 68 | VAL | 4.4 |
| 54 | CU | 55 | ALA | 4.4 |
| 56 | L | 130 | THR | 4.4 |
| 56 | CW | 74 | ASN | 4.4 |
| 63 | DD | 68 | VAL | 4.4 |
| 78 | h | 144 | VAL | 4.4 |
| 63 | DD | 118 | ALA | 4.4 |
| 25 | BR | 79 | GLN | 4.4 |
| 80 | p0 | 76 | LEU | 4.4 |
| 1 | 1 | 1552 | C | 4.4 |
| 63 | S | 79 | ALA | 4.3 |
| 7 | AZ | 171 | LEU | 4.3 |
| 55 | K | 80 | GLY | 4.3 |
| 29 | BV | 21 | ARG | 4.3 |
| 47 | C | 173 | ILE | 4.3 |
| 63 | S | 87 | GLY | 4.3 |
| 56 | L | 141 | VAL | 4.3 |
| 64 | DE | 12 | ALA | 4.3 |
| 79 | DT | 262 | LEU | 4.3 |
| 46 | B | 1 | U | 4.3 |
| 79 | AR | 96 | GLU | 4.3 |
| 7 | AZ | 125 | VAL | 4.3 |
| 23 | BP | 17 | VAL | 4.3 |
| 64 | T | 66 | VAL | 4.3 |

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| Mol | Chain | Res | Type | RSRZ |
|---|---|---|---|---|
| 51 | G | 44 | LEU | 4.3 |
| 54 | CU | 89 | LEU | 4.3 |
| 63 | S | 53 | LEU | 4.3 |
| 80 | p0 | 70 | LEU | 4.3 |
| 52 | H | 44 | ASN | 4.3 |
| 69 | Y | 75 | ILE | 4.3 |
| 1 | AS | 2472 | A | 4.3 |
| 1 | 1 | 2467 | C | 4.3 |
| 71 | a | 63 | GLN | 4.3 |
| 60 | DA | 16 | LEU | 4.3 |
| 79 | AR | 81 | ALA | 4.3 |
| 64 | T | 50 | ILE | 4.3 |
| 37 | CD | 65 | GLU | 4.3 |
| 50 | CQ | 40 | VAL | 4.3 |
| 1 | AS | 2470 | C | 4.2 |
| 35 | CB | 30 | LEU | 4.2 |
| 79 | AR | 62 | PHE | 4.2 |
| 63 | DD | 16 | THR | 4.2 |
| 16 | v | 6 | TYR | 4.2 |
| 74 | DO | 19 | HIS | 4.2 |
| 66 | V | 124 | ILE | 4.2 |
| 1 | 1 | 1099 | A | 4.2 |
| 54 | J | 148 | VAL | 4.2 |
| 47 | CN | 16 | LEU | 4.2 |
| 52 | H | 147 | THR | 4.2 |
| 64 | T | 55 | THR | 4.2 |
| 62 | R | 97 | TYR | 4.2 |
| 71 | a | 68 | LYS | 4.2 |
| 7 | AZ | 82 | GLU | 4.2 |
| 46 | CM | 1696 | U | 4.2 |
| 35 | CB | 39 | ALA | 4.2 |
| 54 | J | 145 | ILE | 4.2 |
| 78 | DS | 188 | LEU | 4.2 |
| 7 | m | 7 | PHE | 4.2 |
| 50 | F | 18 | PHE | 4.2 |
| 52 | H | 179 | ALA | 4.2 |
| 3 | AU | 21 | C | 4.2 |
| 10 | BC | 152 | VAL | 4.1 |
| 13 | s | 129 | VAL | 4.1 |
| 62 | DC | 49 | LEU | 4.1 |
| 80 | p0 | 15 | LEU | 4.1 |
| 12 | r | 162 | GLN | 4.1 |

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| Mol | Chain | Res | Type | RSRZ |
|---|---|---|---|---|
| 54 | J | 176 | GLN | 4.1 |
| 62 | R | 119 | PHE | 4.1 |
| 16 | BI | 117 | ASN | 4.1 |
| 10 | BC | 154 | ILE | 4.1 |
| 13 | s | 106 | ILE | 4.1 |
| 49 | E | 209 | ALA | 4.1 |
| 78 | DS | 133 | ILE | 4.1 |
| 36 | AI | 84 | LYS | 4.1 |
| 50 | F | 56 | THR | 4.1 |
| 64 | T | 25 | THR | 4.1 |
| 10 | p | 165 | VAL | 4.1 |
| 63 | DD | 18 | VAL | 4.1 |
| 6 | AY | 195 | LEU | 4.1 |
| 36 | CC | 116 | PHE | 4.1 |
| 70 | Z | 107 | PHE | 4.1 |
| 7 | AZ | 151 | GLN | 4.1 |
| 46 | CM | 1480 | G | 4.1 |
| 54 | J | 146 | GLN | 4.1 |
| 63 | DD | 80 | ILE | 4.1 |
| 6 | l | 363 | ASN | 4.1 |
| 15 | BH | 4 | THR | 4.1 |
| 62 | R | 34 | THR | 4.1 |
| 65 | DF | 46 | VAL | 4.1 |
| 80 | P0 | 26 | PHE | 4.1 |
| 14 | BG | 88 | LYS | 4.1 |
| 35 | CB | 21 | LYS | 4.1 |
| 69 | Y | 27 | ILE | 4.1 |
| 78 | DS | 123 | LYS | 4.1 |
| 64 | T | 62 | GLN | 4.1 |
| 13 | BF | 158 | ASP | 4.1 |
| 41 | AN | 26 | ARG | 4.1 |
| 47 | C | 127 | ARG | 4.1 |
| 54 | J | 125 | LEU | 4.1 |
| 74 | d | 24 | LEU | 4.1 |
| 79 | DT | 32 | LEU | 4.1 |
| 77 | DR | 35 | TYR | 4.1 |
| 54 | J | 57 | PHE | 4.1 |
| 70 | Z | 85 | ALA | 4.1 |
| 46 | CM | 1697 | C | 4.1 |
| 4 | j | 71 | LEU | 4.1 |
| 11 | q | 176 | LEU | 4.1 |
| 59 | O | 97 | LEU | 4.1 |

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| Mol | Chain | Res | Type | RSRZ |
|---|---|---|---|---|
| 42 | CI | 16 | LYS | 4.1 |
| 6 | AY | 55 | GLU | 4.1 |
| 45 | i | 88 | PHE | 4.1 |
| 52 | H | 43 | PHE | 4.1 |
| 10 | BC | 149 | ALA | 4.1 |
| 36 | CC | 114 | ARG | 4.1 |
| 79 | DT | 75 | SER | 4.0 |
| 60 | DA | 106 | ARG | 4.0 |
| 7 | AZ | 150 | LEU | 4.0 |
| 72 | b | 69 | LEU | 4.0 |
| 51 | G | 24 | SER | 4.0 |
| 7 | AZ | 219 | TYR | 4.0 |
| 61 | DB | 84 | THR | 4.0 |
| 71 | a | 64 | PHE | 4.0 |
| 30 | BW | 14 | ARG | 4.0 |
| 61 | Q | 12 | ALA | 4.0 |
| 63 | S | 19 | ALA | 4.0 |
| 47 | C | 16 | LEU | 4.0 |
| 52 | H | 104 | ASN | 4.0 |
| 71 | DL | 23 | PHE | 4.0 |
| 7 | AZ | 78 | ALA | 4.0 |
| 51 | G | 63 | ALA | 4.0 |
| 7 | m | 65 | VAL | 4.0 |
| 11 | q | 170 | LYS | 4.0 |
| 52 | H | 86 | GLN | 4.0 |
| 43 | CJ | 51 | GLY | 4.0 |
| 55 | K | 180 | GLY | 4.0 |
| 62 | R | 96 | VAL | 4.0 |
| 1 | AS | 1266 | A | 4.0 |
| 7 | AZ | 119 | TYR | 4.0 |
| 22 | 2 | 18 | ASP | 4.0 |
| 27 | BT | 21 | THR | 4.0 |
| 77 | g | 34 | ALA | 4.0 |
| 80 | p0 | 75 | LYS | 4.0 |
| 63 | S | 20 | HIS | 4.0 |
| 66 | DG | 53 | TRP | 4.0 |
| 7 | AZ | 109 | ALA | 4.0 |
| 39 | CF | 41 | THR | 4.0 |
| 41 | CH | 5 | SER | 4.0 |
| 47 | C | 155 | TYR | 4.0 |
| 64 | T | 21 | TYR | 4.0 |
| 64 | T | 90 | ALA | 4.0 |

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| Mol | Chain | Res | Type | RSRZ |
|---|---|---|---|---|
| 82 | l1 | 23 | THR | 4.0 |
| 66 | V | 119 | LYS | 4.0 |
| 79 | AR | 13 | LEU | 4.0 |
| 13 | s | 118 | PRO | 3.9 |
| 65 | U | 123 | ARG | 3.9 |
| 52 | CS | 187 | ILE | 3.9 |
| 56 | CW | 42 | ILE | 3.9 |
| 22 | 2 | 31 | LEU | 3.9 |
| 48 | CO | 120 | LEU | 3.9 |
| 51 | G | 78 | THR | 3.9 |
| 63 | DD | 14 | THR | 3.9 |
| 64 | T | 53 | TYR | 3.9 |
| 69 | DJ | 33 | VAL | 3.9 |
| 79 | DT | 155 | VAL | 3.9 |
| 33 | AF | 125 | GLY | 3.9 |
| 40 | AM | 28 | ARG | 3.9 |
| 46 | B | 131 | C | 3.9 |
| 20 | BM | 87 | ALA | 3.9 |
| 30 | AC | 22 | LYS | 3.9 |
| 7 | AZ | 92 | LEU | 3.9 |
| 36 | AI | 88 | LEU | 3.9 |
| 63 | S | 43 | LEU | 3.9 |
| 73 | c | 69 | ASN | 3.9 |
| 51 | CR | 76 | VAL | 3.9 |
| 6 | l | 352 | PRO | 3.9 |
| 46 | B | 1571 | G | 3.9 |
| 66 | V | 38 | LYS | 3.9 |
| 13 | s | 17 | LEU | 3.9 |
| 48 | D | 54 | LEU | 3.9 |
| 63 | DD | 90 | ALA | 3.9 |
| 77 | DR | 34 | ALA | 3.9 |
| 79 | AR | 76 | ALA | 3.9 |
| 51 | CR | 184 | THR | 3.9 |
| 6 | l | 353 | SER | 3.9 |
| 63 | DD | 50 | PRO | 3.9 |
| 78 | DS | 164 | PRO | 3.9 |
| 6 | AY | 66 | TRP | 3.9 |
| 26 | BS | 40 | LEU | 3.9 |
| 53 | I | 138 | ALA | 3.9 |
| 46 | CM | 1678 | G | 3.9 |
| 74 | DO | 15 | GLU | 3.9 |
| 10 | p | 237 | GLY | 3.9 |

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| Mol | Chain | Res | Type | RSRZ |
|---|---|---|---|---|
| 63 | S | 5 | SER | 3.9 |
| 64 | DE | 14 | LYS | 3.9 |
| 74 | DO | 18 | GLN | 3.9 |
| 65 | U | 17 | LEU | 3.9 |
| 48 | D | 57 | ALA | 3.9 |
| 49 | CP | 87 | ALA | 3.9 |
| 24 | BQ | 88 | ARG | 3.8 |
| 6 | l | 12 | VAL | 3.8 |
| 52 | H | 137 | ILE | 3.8 |
| 64 | DE | 102 | ILE | 3.8 |
| 46 | B | 1359 | U | 3.8 |
| 54 | CU | 77 | LEU | 3.8 |
| 68 | X | 55 | LEU | 3.8 |
| 69 | Y | 104 | LEU | 3.8 |
| 50 | CQ | 172 | ALA | 3.8 |
| 60 | P | 151 | ALA | 3.8 |
| 10 | BC | 165 | VAL | 3.8 |
| 38 | CE | 29 | VAL | 3.8 |
| 19 | y | 95 | GLU | 3.8 |
| 69 | Y | 52 | TYR | 3.8 |
| 54 | CU | 94 | ILE | 3.8 |
| 64 | T | 41 | ILE | 3.8 |
| 80 | P0 | 80 | ILE | 3.8 |
| 80 | p0 | 78 | PRO | 3.8 |
| 47 | CN | 184 | LEU | 3.8 |
| 48 | CO | 218 | LEU | 3.8 |
| 38 | CE | 57 | ARG | 3.8 |
| 74 | DO | 29 | ARG | 3.8 |
| 9 | o | 69 | ALA | 3.8 |
| 63 | S | 90 | ALA | 3.8 |
| 1 | 1 | 2476 | C | 3.8 |
| 49 | E | 178 | VAL | 3.8 |
| 1 | 1 | 1345 | G | 3.8 |
| 46 | B | 1480 | G | 3.8 |
| 56 | CW | 140 | ILE | 3.8 |
| 7 | AZ | 8 | ARG | 3.8 |
| 59 | O | 59 | LEU | 3.8 |
| 70 | DK | 27 | GLN | 3.8 |
| 59 | CZ | 101 | ALA | 3.8 |
| 45 | i | 83 | HIS | 3.8 |
| 7 | m | 37 | VAL | 3.8 |
| 50 | F | 40 | VAL | 3.8 |

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| Mol | Chain | Res | Type | RSRZ |
|---|---|---|---|---|
| 36 | CC | 84 | LYS | 3.8 |
| 52 | H | 67 | PRO | 3.8 |
| 79 | AR | 55 | TYR | 3.8 |
| 6 | l | 199 | ARG | 3.8 |
| 10 | p | 202 | THR | 3.8 |
| 56 | CW | 146 | PHE | 3.8 |
| 67 | W | 69 | THR | 3.8 |
| 69 | Y | 2 | THR | 3.8 |
| 16 | v | 153 | ASN | 3.8 |
| 31 | BX | 44 | VAL | 3.8 |
| 49 | E | 162 | VAL | 3.8 |
| 64 | T | 125 | SER | 3.8 |
| 75 | e | 45 | LYS | 3.8 |
| 79 | AR | 77 | ASP | 3.8 |
| 50 | F | 178 | MET | 3.8 |
| 48 | CO | 163 | GLU | 3.8 |
| 54 | CU | 109 | PRO | 3.8 |
| 75 | DP | 66 | LEU | 3.8 |
| 78 | DS | 166 | PRO | 3.8 |
| 79 | DT | 38 | ARG | 3.8 |
| 45 | i | 115 | LEU | 3.8 |
| 62 | DC | 56 | LEU | 3.8 |
| 78 | DS | 190 | LEU | 3.8 |
| 49 | E | 205 | THR | 3.8 |
| 70 | Z | 28 | ALA | 3.7 |
| 73 | DN | 48 | ALA | 3.7 |
| 16 | BI | 155 | VAL | 3.7 |
| 45 | i | 65 | LYS | 3.7 |
| 51 | CR | 192 | VAL | 3.7 |
| 57 | CX | 12 | HIS | 3.7 |
| 45 | i | 78 | SER | 3.7 |
| 38 | CE | 2 | GLY | 3.7 |
| 63 | DD | 87 | GLY | 3.7 |
| 73 | DN | 16 | GLY | 3.7 |
| 7 | AZ | 226 | TYR | 3.7 |
| 54 | J | 96 | PRO | 3.7 |
| 55 | CV | 109 | PHE | 3.7 |
| 56 | CW | 12 | TYR | 3.7 |
| 45 | CL | 81 | THR | 3.7 |
| 30 | BW | 38 | LYS | 3.7 |
| 47 | C | 99 | ALA | 3.7 |
| 50 | F | 187 | VAL | 3.7 |

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| Mol | Chain | Res | Type | RSRZ |
|---|---|---|---|---|
| 52 | H | 63 | GLN | 3.7 |
| 64 | T | 42 | GLN | 3.7 |
| 63 | S | 2 | SER | 3.7 |
| 63 | S | 64 | ILE | 3.7 |
| 65 | U | 15 | LEU | 3.7 |
| 57 | M | 30 | PRO | 3.7 |
| 43 | AP | 26 | THR | 3.7 |
| 75 | DP | 45 | LYS | 3.7 |
| 35 | AH | 32 | ALA | 3.7 |
| 48 | CO | 141 | ALA | 3.7 |
| 51 | G | 14 | ALA | 3.7 |
| 19 | y | 140 | VAL | 3.7 |
| 51 | CR | 219 | VAL | 3.7 |
| 22 | BO | 103 | GLN | 3.7 |
| 66 | DG | 70 | GLN | 3.7 |
| 6 | AY | 84 | HIS | 3.7 |
| 52 | H | 99 | MET | 3.7 |
| 70 | Z | 48 | HIS | 3.7 |
| 82 | l1 | 1 | MET | 3.7 |
| 52 | H | 92 | ARG | 3.7 |
| 48 | D | 29 | TRP | 3.7 |
| 67 | W | 85 | ILE | 3.7 |
| 72 | DM | 50 | ILE | 3.7 |
| 9 | BB | 139 | LEU | 3.7 |
| 37 | CD | 71 | LEU | 3.7 |
| 79 | AR | 82 | LEU | 3.7 |
| 79 | DT | 94 | ASP | 3.7 |
| 1 | AS | 2448 | C | 3.7 |
| 41 | AN | 47 | PRO | 3.7 |
| 77 | DR | 60 | PRO | 3.7 |
| 51 | G | 54 | TYR | 3.7 |
| 53 | CT | 163 | THR | 3.7 |
| 79 | DT | 154 | ALA | 3.7 |
| 28 | AA | 68 | VAL | 3.7 |
| 50 | F | 138 | VAL | 3.7 |
| 69 | Y | 74 | VAL | 3.7 |
| 79 | DT | 114 | VAL | 3.7 |
| 29 | AB | 65 | GLN | 3.7 |
| 78 | h | 122 | ARG | 3.7 |
| 14 | BG | 95 | ILE | 3.7 |
| 51 | CR | 228 | ILE | 3.7 |
| 64 | DE | 124 | ILE | 3.7 |

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| Mol | Chain | Res | Type | RSRZ |
|---|---|---|---|---|
| 43 | AP | 104 | LEU | 3.7 |
| 49 | E | 129 | LEU | 3.7 |
| 23 | 5 | 15 | PHE | 3.7 |
| 63 | S | 108 | PHE | 3.7 |
| 63 | DD | 13 | LYS | 3.7 |
| 69 | Y | 48 | GLY | 3.7 |
| 1 | AS | 1560 | U | 3.7 |
| 53 | I | 96 | SER | 3.7 |
| 64 | T | 70 | SER | 3.7 |
| 52 | H | 85 | ALA | 3.7 |
| 51 | G | 208 | VAL | 3.7 |
| 64 | DE | 8 | THR | 3.7 |
| 27 | 9 | 120 | GLN | 3.7 |
| 56 | L | 48 | GLN | 3.7 |
| 7 | AZ | 68 | HIS | 3.7 |
| 52 | CS | 199 | ILE | 3.7 |
| 56 | CW | 123 | HIS | 3.7 |
| 63 | S | 80 | ILE | 3.7 |
| 69 | Y | 61 | ILE | 3.7 |
| 75 | e | 54 | LEU | 3.7 |
| 51 | G | 134 | LYS | 3.7 |
| 19 | y | 169 | GLY | 3.7 |
| 55 | CV | 21 | PHE | 3.7 |
| 25 | BR | 88 | GLU | 3.6 |
| 45 | CL | 84 | SER | 3.6 |
| 55 | K | 66 | SER | 3.6 |
| 54 | J | 119 | ASP | 3.6 |
| 56 | CW | 55 | ALA | 3.6 |
| 51 | CR | 80 | THR | 3.6 |
| 54 | J | 42 | ILE | 3.6 |
| 54 | J | 94 | ILE | 3.6 |
| 33 | BZ | 27 | HIS | 3.6 |
| 56 | L | 160 | HIS | 3.6 |
| 71 | DL | 111 | LYS | 3.6 |
| 1 | AS | 1235 | C | 3.6 |
| 58 | CY | 60 | PHE | 3.6 |
| 41 | AN | 14 | ASN | 3.6 |
| 41 | CH | 8 | ALA | 3.6 |
| 56 | L | 152 | SER | 3.6 |
| 63 | S | 21 | VAL | 3.6 |
| 63 | DD | 120 | SER | 3.6 |
| 78 | DS | 146 | THR | 3.6 |

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| Mol | Chain | Res | Type | RSRZ |
|---|---|---|---|---|
| 19 | y | 94 | LEU | 3.6 |
| 47 | CN | 111 | ILE | 3.6 |
| 59 | CZ | 62 | LEU | 3.6 |
| 43 | AP | 15 | LYS | 3.6 |
| 46 | B | 491 | U | 3.6 |
| 52 | CS | 84 | LYS | 3.6 |
| 71 | a | 67 | GLY | 3.6 |
| 18 | BK | 89 | ASN | 3.6 |
| 45 | i | 43 | PRO | 3.6 |
| 47 | C | 76 | CYS | 3.6 |
| 63 | DD | 65 | ARG | 3.6 |
| 52 | H | 133 | VAL | 3.6 |
| 66 | DG | 71 | VAL | 3.6 |
| 67 | W | 61 | VAL | 3.6 |
| 7 | m | 217 | GLU | 3.6 |
| 29 | BV | 46 | ASP | 3.6 |
| 15 | u | 130 | LYS | 3.6 |
| 47 | CN | 173 | ILE | 3.6 |
| 61 | DB | 14 | ILE | 3.6 |
| 64 | T | 73 | LEU | 3.6 |
| 72 | b | 51 | LEU | 3.6 |
| 78 | h | 123 | LYS | 3.6 |
| 79 | AR | 101 | THR | 3.6 |
| 10 | BC | 62 | GLN | 3.6 |
| 49 | E | 210 | PHE | 3.6 |
| 56 | L | 137 | GLY | 3.6 |
| 82 | L1 | 69 | GLY | 3.6 |
| 50 | CQ | 207 | VAL | 3.6 |
| 49 | CP | 151 | CYS | 3.6 |
| 1 | AS | 1248 | A | 3.6 |
| 30 | BW | 33 | LYS | 3.6 |
| 63 | DD | 140 | SER | 3.6 |
| 64 | T | 38 | ILE | 3.6 |
| 67 | DH | 23 | ILE | 3.6 |
| 76 | DQ | 38 | LEU | 3.6 |
| 44 | AQ | 59 | SER | 3.6 |
| 1 | AS | 1552 | C | 3.6 |
| 46 | CM | 131 | C | 3.6 |
| 10 | p | 62 | GLN | 3.6 |
| 57 | M | 13 | GLN | 3.6 |
| 7 | m | 8 | ARG | 3.6 |
| 41 | CH | 30 | ARG | 3.6 |

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| Mol | Chain | Res | Type | RSRZ |
|---|---|---|---|---|
| 60 | P | 68 | GLY | 3.6 |
| 9 | o | 202 | PRO | 3.6 |
| 52 | CS | 67 | PRO | 3.6 |
| 66 | V | 62 | ALA | 3.6 |
| 45 | i | 33 | ASN | 3.6 |
| 75 | e | 51 | ASN | 3.6 |
| 10 | p | 201 | LEU | 3.6 |
| 49 | E | 220 | LEU | 3.6 |
| 11 | q | 172 | ILE | 3.6 |
| 63 | S | 84 | ILE | 3.6 |
| 19 | BL | 174 | ARG | 3.5 |
| 52 | CS | 170 | GLN | 3.5 |
| 63 | S | 39 | GLN | 3.5 |
| 59 | CZ | 48 | ALA | 3.5 |
| 45 | CL | 102 | LYS | 3.5 |
| 6 | AY | 259 | LEU | 3.5 |
| 50 | F | 22 | LEU | 3.5 |
| 62 | R | 49 | LEU | 3.5 |
| 14 | t | 11 | ASN | 3.5 |
| 82 | l1 | 30 | GLU | 3.5 |
| 52 | H | 96 | SER | 3.5 |
| 64 | T | 5 | ARG | 3.5 |
| 29 | BV | 68 | PHE | 3.5 |
| 57 | M | 27 | PHE | 3.5 |
| 27 | 9 | 6 | GLN | 3.5 |
| 52 | CS | 155 | VAL | 3.5 |
| 62 | DC | 101 | VAL | 3.5 |
| 82 | L1 | 13 | VAL | 3.5 |
| 6 | l | 166 | ALA | 3.5 |
| 52 | CS | 74 | ALA | 3.5 |
| 1 | AS | 1247 | A | 3.5 |
| 41 | CH | 9 | LEU | 3.5 |
| 59 | CZ | 97 | LEU | 3.5 |
| 80 | p0 | 52 | LEU | 3.5 |
| 62 | R | 84 | ILE | 3.5 |
| 63 | S | 28 | ILE | 3.5 |
| 63 | S | 141 | TYR | 3.5 |
| 28 | BU | 130 | PHE | 3.5 |
| 29 | BV | 65 | GLN | 3.5 |
| 41 | CH | 44 | GLN | 3.5 |
| 74 | DO | 30 | SER | 3.5 |
| 76 | f | 20 | GLN | 3.5 |

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| Mol | Chain | Res | Type | RSRZ |
|---|---|---|---|---|
| 82 | l1 | 2 | SER | 3.5 |
| 7 | AZ | 170 | GLY | 3.5 |
| 12 | r | 114 | GLY | 3.5 |
| 13 | BF | 4 | LYS | 3.5 |
| 56 | CW | 10 | LYS | 3.5 |
| 59 | CZ | 44 | GLY | 3.5 |
| 64 | DE | 15 | VAL | 3.5 |
| 22 | 2 | 100 | ALA | 3.5 |
| 51 | G | 84 | ALA | 3.5 |
| 33 | AF | 123 | PRO | 3.5 |
| 39 | CF | 14 | LEU | 3.5 |
| 50 | F | 204 | PRO | 3.5 |
| 56 | L | 59 | LEU | 3.5 |
| 77 | g | 39 | LEU | 3.5 |
| 62 | R | 57 | ILE | 3.5 |
| 49 | E | 79 | ARG | 3.5 |
| 52 | CS | 102 | ARG | 3.5 |
| 45 | i | 69 | PHE | 3.5 |
| 1 | AS | 1239 | G | 3.5 |
| 35 | AH | 45 | GLY | 3.5 |
| 52 | H | 155 | VAL | 3.5 |
| 63 | S | 75 | SER | 3.5 |
| 80 | p0 | 51 | VAL | 3.5 |
| 43 | CJ | 81 | ALA | 3.5 |
| 49 | E | 95 | ALA | 3.5 |
| 63 | S | 118 | ALA | 3.5 |
| 66 | DG | 62 | ALA | 3.5 |
| 7 | AZ | 212 | LEU | 3.5 |
| 54 | J | 109 | PRO | 3.5 |
| 65 | DF | 120 | ARG | 3.5 |
| 11 | q | 175 | PHE | 3.5 |
| 51 | G | 22 | LYS | 3.5 |
| 80 | P0 | 79 | PHE | 3.5 |
| 53 | CT | 179 | VAL | 3.5 |
| 56 | CW | 113 | VAL | 3.5 |
| 63 | DD | 66 | VAL | 3.5 |
| 66 | V | 39 | THR | 3.5 |
| 20 | BM | 73 | GLY | 3.5 |
| 46 | B | 504 | A | 3.5 |
| 71 | a | 12 | VAL | 3.5 |
| 60 | P | 16 | LEU | 3.5 |
| 6 | l | 216 | ILE | 3.5 |

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| Mol | Chain | Res | Type | RSRZ |
|---|---|---|---|---|
| 9 | o | 221 | ILE | 3.5 |
| 46 | B | 1270 | U | 3.5 |
| 79 | DT | 285 | GLU | 3.4 |
| 14 | BG | 131 | LYS | 3.4 |
| 66 | V | 55 | TYR | 3.4 |
| 70 | DK | 38 | PHE | 3.4 |
| 80 | p0 | 11 | TYR | 3.4 |
| 52 | H | 23 | VAL | 3.4 |
| 53 | I | 97 | VAL | 3.4 |
| 7 | m | 212 | LEU | 3.4 |
| 30 | BW | 2 | ALA | 3.4 |
| 48 | D | 47 | LEU | 3.4 |
| 63 | S | 51 | LEU | 3.4 |
| 63 | DD | 19 | ALA | 3.4 |
| 36 | CC | 118 | ILE | 3.4 |
| 51 | CR | 15 | PRO | 3.4 |
| 52 | H | 79 | SER | 3.4 |
| 55 | K | 177 | SER | 3.4 |
| 46 | CM | 658 | A | 3.4 |
| 58 | CY | 32 | LYS | 3.4 |
| 65 | U | 48 | LYS | 3.4 |
| 79 | AR | 44 | LYS | 3.4 |
| 76 | f | 45 | GLU | 3.4 |
| 64 | DE | 28 | PHE | 3.4 |
| 1 | AS | 1249 | U | 3.4 |
| 46 | CM | 132 | U | 3.4 |
| 51 | CR | 208 | VAL | 3.4 |
| 52 | H | 134 | VAL | 3.4 |
| 7 | AZ | 146 | LEU | 3.4 |
| 27 | BT | 76 | LEU | 3.4 |
| 50 | F | 203 | LEU | 3.4 |
| 54 | J | 133 | GLY | 3.4 |
| 56 | CW | 70 | LEU | 3.4 |
| 53 | I | 168 | THR | 3.4 |
| 56 | CW | 142 | ASN | 3.4 |
| 57 | CX | 2 | LEU | 3.4 |
| 6 | AY | 89 | ALA | 3.4 |
| 57 | CX | 23 | ALA | 3.4 |
| 48 | CO | 140 | ILE | 3.4 |
| 79 | AR | 116 | ILE | 3.4 |
| 79 | DT | 167 | ILE | 3.4 |
| 59 | O | 49 | SER | 3.4 |

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| Mol | Chain | Res | Type | RSRZ |
|---|---|---|---|---|
| 35 | CB | 29 | LYS | 3.4 |
| 47 | C | 174 | TRP | 3.4 |
| 50 | CQ | 168 | PHE | 3.4 |
| 54 | J | 66 | TYR | 3.4 |
| 73 | DN | 73 | TYR | 3.4 |
| 7 | AZ | 105 | VAL | 3.4 |
| 27 | 9 | 45 | VAL | 3.4 |
| 56 | L | 113 | VAL | 3.4 |
| 67 | DH | 55 | VAL | 3.4 |
| 7 | m | 92 | LEU | 3.4 |
| 59 | CZ | 32 | LEU | 3.4 |
| 79 | DT | 207 | LEU | 3.4 |
| 1 | AS | 3051 | C | 3.4 |
| 19 | y | 154 | GLY | 3.4 |
| 58 | CY | 47 | ALA | 3.4 |
| 78 | h | 164 | PRO | 3.4 |
| 61 | DB | 85 | LYS | 3.4 |
| 1 | AS | 1246 | G | 3.4 |
| 21 | 0 | 60 | SER | 3.4 |
| 12 | BE | 199 | PHE | 3.4 |
| 52 | H | 119 | GLU | 3.4 |
| 7 | AZ | 104 | LEU | 3.4 |
| 47 | C | 177 | LEU | 3.4 |
| 63 | S | 47 | VAL | 3.4 |
| 66 | V | 113 | VAL | 3.4 |
| 78 | h | 126 | VAL | 3.4 |
| 63 | S | 65 | ARG | 3.4 |
| 21 | 0 | 116 | ALA | 3.4 |
| 22 | 2 | 2 | GLY | 3.4 |
| 35 | CB | 50 | ALA | 3.4 |
| 51 | G | 25 | GLY | 3.4 |
| 67 | DH | 66 | THR | 3.4 |
| 68 | X | 34 | ILE | 3.4 |
| 4 | AW | 47 | GLN | 3.4 |
| 26 | BS | 25 | LYS | 3.4 |
| 63 | DD | 76 | GLN | 3.4 |
| 66 | V | 31 | PRO | 3.4 |
| 1 | AS | 2450 | U | 3.4 |
| 6 | AY | 353 | SER | 3.4 |
| 23 | BP | 74 | PHE | 3.4 |
| 53 | I | 27 | PHE | 3.4 |
| 53 | CT | 100 | CYS | 3.4 |

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| Mol | Chain | Res | Type | RSRZ |
|---|---|---|---|---|
| 16 | BI | 63 | ARG | 3.4 |
| 35 | CB | 57 | LEU | 3.4 |
| 54 | J | 56 | VAL | 3.4 |
| 67 | W | 62 | LEU | 3.4 |
| 72 | DM | 93 | LEU | 3.4 |
| 78 | h | 190 | LEU | 3.4 |
| 78 | DS | 142 | LEU | 3.4 |
| 11 | q | 60 | GLY | 3.4 |
| 60 | P | 15 | ALA | 3.4 |
| 60 | DA | 151 | ALA | 3.4 |
| 12 | r | 165 | ILE | 3.4 |
| 66 | V | 69 | LYS | 3.4 |
| 73 | DN | 4 | LYS | 3.4 |
| 80 | P0 | 87 | ILE | 3.4 |
| 7 | m | 38 | THR | 3.4 |
| 41 | CH | 32 | THR | 3.4 |
| 57 | M | 83 | PRO | 3.4 |
| 64 | T | 22 | PRO | 3.4 |
| 80 | P0 | 108 | PRO | 3.4 |
| 5 | k | 233 | TRP | 3.3 |
| 28 | BU | 92 | PHE | 3.3 |
| 51 | CR | 18 | TRP | 3.3 |
| 58 | N | 60 | PHE | 3.3 |
| 6 | AY | 9 | VAL | 3.3 |
| 7 | AZ | 65 | VAL | 3.3 |
| 19 | y | 124 | LEU | 3.3 |
| 41 | CH | 6 | LEU | 3.3 |
| 47 | C | 58 | VAL | 3.3 |
| 52 | H | 68 | VAL | 3.3 |
| 79 | AR | 210 | SER | 3.3 |
| 77 | DR | 61 | ALA | 3.3 |
| 18 | x | 183 | THR | 3.3 |
| 38 | AK | 87 | THR | 3.3 |
| 64 | T | 54 | THR | 3.3 |
| 66 | V | 90 | PRO | 3.3 |
| 72 | b | 55 | PRO | 3.3 |
| 79 | DT | 29 | HIS | 3.3 |
| 52 | CS | 100 | ASN | 3.3 |
| 28 | BU | 118 | PHE | 3.3 |
| 10 | p | 66 | LEU | 3.3 |
| 15 | BH | 115 | VAL | 3.3 |
| 56 | L | 118 | LEU | 3.3 |

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| Mol | Chain | Res | Type | RSRZ |
|---|---|---|---|---|
| 66 | V | 114 | LEU | 3.3 |
| 63 | DD | 124 | GLU | 3.3 |
| 10 | p | 80 | SER | 3.3 |
| 50 | CQ | 149 | LYS | 3.3 |
| 55 | CV | 45 | SER | 3.3 |
| 79 | AR | 35 | SER | 3.3 |
| 10 | BC | 199 | ALA | 3.3 |
| 52 | H | 77 | TYR | 3.3 |
| 54 | J | 131 | ILE | 3.3 |
| 66 | DG | 18 | TYR | 3.3 |
| 69 | Y | 101 | TYR | 3.3 |
| 3 | AU | 91 | C | 3.3 |
| 79 | AR | 58 | PRO | 3.3 |
| 18 | BK | 64 | ASN | 3.3 |
| 39 | CF | 57 | ASN | 3.3 |
| 51 | G | 47 | PHE | 3.3 |
| 52 | CS | 104 | ASN | 3.3 |
| 56 | L | 93 | LEU | 3.3 |
| 64 | T | 28 | PHE | 3.3 |
| 70 | DK | 89 | ASN | 3.3 |
| 28 | BU | 14 | VAL | 3.3 |
| 51 | G | 111 | VAL | 3.3 |
| 56 | CW | 14 | VAL | 3.3 |
| 57 | M | 42 | VAL | 3.3 |
| 82 | l1 | 148 | VAL | 3.3 |
| 6 | l | 192 | LYS | 3.3 |
| 35 | CB | 43 | LYS | 3.3 |
| 58 | CY | 118 | GLU | 3.3 |
| 12 | BE | 33 | ILE | 3.3 |
| 35 | CB | 20 | ILE | 3.3 |
| 48 | CO | 102 | GLY | 3.3 |
| 51 | CR | 233 | GLY | 3.3 |
| 56 | L | 145 | SER | 3.3 |
| 22 | 2 | 30 | TYR | 3.3 |
| 66 | V | 66 | TYR | 3.3 |
| 41 | CH | 47 | PRO | 3.3 |
| 4 | AW | 250 | GLN | 3.3 |
| 10 | BC | 122 | THR | 3.3 |
| 60 | DA | 36 | GLN | 3.3 |
| 70 | Z | 16 | ARG | 3.3 |
| 77 | g | 41 | THR | 3.3 |
| 21 | 0 | 162 | LEU | 3.3 |

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| Mol | Chain | Res | Type | RSRZ |
|---|---|---|---|---|
| 76 | DQ | 8 | PHE | 3.3 |
| 6 | l | 186 | LYS | 3.3 |
| 38 | CE | 10 | LYS | 3.3 |
| 52 | CS | 33 | VAL | 3.3 |
| 66 | V | 37 | VAL | 3.3 |
| 64 | T | 124 | ILE | 3.3 |
| 51 | CR | 107 | GLY | 3.3 |
| 79 | AR | 15 | GLY | 3.3 |
| 65 | U | 121 | SER | 3.3 |
| 7 | AZ | 59 | ASP | 3.3 |
| 11 | q | 171 | ASP | 3.3 |
| 48 | CO | 59 | ASP | 3.3 |
| 57 | M | 26 | ASP | 3.3 |
| 65 | U | 145 | ARG | 3.3 |
| 75 | e | 49 | ARG | 3.3 |
| 33 | AF | 53 | GLN | 3.3 |
| 49 | E | 91 | THR | 3.3 |
| 49 | CP | 89 | GLN | 3.3 |
| 51 | G | 247 | LEU | 3.3 |
| 53 | CT | 156 | PHE | 3.3 |
| 54 | J | 149 | LEU | 3.3 |
| 70 | DK | 18 | HIS | 3.3 |
| 66 | V | 14 | PHE | 3.3 |
| 36 | CC | 91 | LYS | 3.3 |
| 55 | CV | 102 | VAL | 3.3 |
| 56 | CW | 148 | VAL | 3.3 |
| 64 | T | 63 | LYS | 3.3 |
| 71 | a | 35 | VAL | 3.3 |
| 73 | c | 12 | LYS | 3.3 |
| 3 | AU | 22 | U | 3.3 |
| 6 | AY | 110 | TRP | 3.3 |
| 14 | BG | 12 | ASN | 3.3 |
| 78 | DS | 174 | MET | 3.3 |
| 1 | 1 | 2456 | C | 3.3 |
| 6 | AY | 52 | ALA | 3.3 |
| 28 | BU | 117 | ALA | 3.3 |
| 68 | DI | 54 | ALA | 3.3 |
| 19 | y | 14 | GLY | 3.3 |
| 66 | DG | 120 | GLY | 3.3 |
| 13 | s | 41 | SER | 3.2 |
| 39 | CF | 22 | SER | 3.2 |
| 61 | Q | 120 | SER | 3.2 |

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| Mol | Chain | Res | Type | RSRZ |
|---|---|---|---|---|
| 48 | CO | 190 | PRO | 3.2 |
| 8 | n | 42 | LEU | 3.2 |
| 6 | AY | 184 | LYS | 3.2 |
| 27 | 9 | 7 | ASP | 3.2 |
| 49 | E | 206 | LEU | 3.2 |
| 64 | T | 46 | LEU | 3.2 |
| 7 | m | 142 | PHE | 3.2 |
| 30 | BW | 23 | LYS | 3.2 |
| 16 | BI | 115 | VAL | 3.2 |
| 55 | K | 102 | VAL | 3.2 |
| 71 | a | 70 | THR | 3.2 |
| 50 | F | 185 | ILE | 3.2 |
| 52 | H | 74 | ALA | 3.2 |
| 52 | CS | 173 | ALA | 3.2 |
| 1 | 1 | 2743 | U | 3.2 |
| 46 | CM | 1339 | G | 3.2 |
| 24 | 6 | 88 | ARG | 3.2 |
| 46 | CM | 1694 | A | 3.2 |
| 64 | T | 3 | ARG | 3.2 |
| 6 | l | 5 | PRO | 3.2 |
| 41 | CH | 12 | LYS | 3.2 |
| 41 | CH | 29 | PRO | 3.2 |
| 43 | CJ | 15 | LYS | 3.2 |
| 45 | i | 37 | LYS | 3.2 |
| 45 | CL | 54 | LYS | 3.2 |
| 53 | CT | 190 | LEU | 3.2 |
| 55 | CV | 41 | LYS | 3.2 |
| 57 | M | 60 | SER | 3.2 |
| 62 | DC | 58 | LYS | 3.2 |
| 45 | CL | 69 | PHE | 3.2 |
| 52 | CS | 53 | VAL | 3.2 |
| 71 | a | 122 | GLN | 3.2 |
| 31 | BX | 26 | THR | 3.2 |
| 8 | n | 1 | MET | 3.2 |
| 52 | H | 64 | ILE | 3.2 |
| 71 | DL | 25 | ILE | 3.2 |
| 49 | E | 87 | ALA | 3.2 |
| 4 | AW | 53 | GLY | 3.2 |
| 16 | BI | 8 | GLU | 3.2 |
| 60 | P | 21 | ASN | 3.2 |
| 67 | W | 67 | ARG | 3.2 |
| 49 | E | 94 | LYS | 3.2 |

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| Mol | Chain | Res | Type | RSRZ |
|---|---|---|---|---|
| 54 | CU | 168 | LEU | 3.2 |
| 79 | AR | 34 | LEU | 3.2 |
| 46 | CM | 1698 | U | 3.2 |
| 62 | DC | 109 | PRO | 3.2 |
| 1 | 1 | 2452 | G | 3.2 |
| 7 | AZ | 162 | VAL | 3.2 |
| 16 | BI | 198 | SER | 3.2 |
| 56 | L | 148 | VAL | 3.2 |
| 62 | R | 94 | VAL | 3.2 |
| 7 | m | 283 | GLN | 3.2 |
| 18 | x | 7 | THR | 3.2 |
| 48 | CO | 46 | THR | 3.2 |
| 51 | G | 217 | THR | 3.2 |
| 55 | K | 43 | ILE | 3.2 |
| 29 | AB | 127 | ALA | 3.2 |
| 68 | X | 26 | ALA | 3.2 |
| 79 | DT | 28 | ALA | 3.2 |
| 6 | l | 174 | GLY | 3.2 |
| 16 | BI | 120 | TRP | 3.2 |
| 56 | L | 20 | GLU | 3.2 |
| 45 | CL | 50 | LYS | 3.2 |
| 54 | J | 107 | LYS | 3.2 |
| 51 | CR | 180 | LEU | 3.2 |
| 52 | H | 108 | LEU | 3.2 |
| 56 | L | 109 | LEU | 3.2 |
| 69 | Y | 26 | LEU | 3.2 |
| 78 | DS | 145 | LEU | 3.2 |
| 79 | DT | 13 | LEU | 3.2 |
| 27 | BT | 20 | PHE | 3.2 |
| 47 | C | 107 | PHE | 3.2 |
| 78 | DS | 130 | PRO | 3.2 |
| 79 | DT | 124 | VAL | 3.2 |
| 24 | BQ | 7 | SER | 3.2 |
| 28 | AA | 98 | SER | 3.2 |
| 41 | AN | 5 | SER | 3.2 |
| 46 | CM | 278 | U | 3.2 |
| 50 | F | 63 | GLN | 3.2 |
| 54 | J | 3 | SER | 3.2 |
| 65 | DF | 121 | SER | 3.2 |
| 53 | I | 226 | ILE | 3.2 |
| 73 | c | 82 | ARG | 3.2 |
| 79 | DT | 97 | THR | 3.2 |

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| Mol | Chain | Res | Type | RSRZ |
|---|---|---|---|---|
| 79 | DT | 123 | ILE | 3.2 |
| 1 | 1 | 2437 | A | 3.2 |
| 30 | AC | 9 | ALA | 3.2 |
| 59 | O | 120 | CYS | 3.2 |
| 35 | AH | 28 | GLY | 3.2 |
| 48 | CO | 152 | LYS | 3.2 |
| 52 | CS | 75 | GLY | 3.2 |
| 56 | L | 32 | GLY | 3.2 |
| 66 | V | 82 | GLY | 3.2 |
| 46 | CM | 1703 | C | 3.2 |
| 11 | BD | 144 | LEU | 3.2 |
| 79 | DT | 289 | LEU | 3.2 |
| 16 | BI | 149 | ASN | 3.2 |
| 7 | m | 31 | TYR | 3.2 |
| 50 | F | 26 | PHE | 3.2 |
| 51 | G | 43 | PRO | 3.2 |
| 58 | CY | 95 | PRO | 3.2 |
| 76 | f | 11 | PRO | 3.2 |
| 77 | DR | 5 | HIS | 3.2 |
| 80 | p0 | 64 | ARG | 3.2 |
| 54 | J | 164 | SER | 3.2 |
| 10 | BC | 155 | ALA | 3.2 |
| 20 | BM | 63 | ALA | 3.2 |
| 60 | P | 67 | THR | 3.2 |
| 64 | DE | 54 | THR | 3.2 |
| 79 | AR | 276 | ALA | 3.2 |
| 46 | CM | 1 | U | 3.1 |
| 46 | CM | 1270 | U | 3.1 |
| 52 | H | 80 | LYS | 3.1 |
| 63 | S | 127 | LYS | 3.1 |
| 63 | S | 24 | GLY | 3.1 |
| 63 | DD | 32 | GLY | 3.1 |
| 50 | CQ | 177 | LEU | 3.1 |
| 61 | Q | 78 | LEU | 3.1 |
| 82 | L1 | 16 | LEU | 3.1 |
| 4 | AW | 73 | GLU | 3.1 |
| 6 | AY | 91 | PHE | 3.1 |
| 29 | BV | 144 | VAL | 3.1 |
| 40 | CG | 33 | ASN | 3.1 |
| 41 | CH | 14 | ASN | 3.1 |
| 57 | M | 64 | TYR | 3.1 |
| 59 | CZ | 121 | VAL | 3.1 |

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| Mol | Chain | Res | Type | RSRZ |
|---|---|---|---|---|
| 64 | DE | 31 | ASN | 3.1 |
| 51 | G | 82 | TYR | 3.1 |
| 63 | S | 48 | TYR | 3.1 |
| 70 | DK | 124 | VAL | 3.1 |
| 76 | DQ | 52 | PHE | 3.1 |
| 78 | h | 148 | TYR | 3.1 |
| 1 | AS | 2453 | G | 3.1 |
| 49 | CP | 86 | ARG | 3.1 |
| 7 | AZ | 81 | HIS | 3.1 |
| 26 | BS | 88 | ILE | 3.1 |
| 37 | AJ | 89 | MET | 3.1 |
| 41 | CH | 2 | ILE | 3.1 |
| 35 | AH | 33 | GLN | 3.1 |
| 50 | F | 188 | LYS | 3.1 |
| 54 | J | 147 | LYS | 3.1 |
| 79 | DT | 63 | LYS | 3.1 |
| 5 | AX | 139 | THR | 3.1 |
| 7 | m | 70 | THR | 3.1 |
| 54 | J | 129 | THR | 3.1 |
| 79 | AR | 41 | THR | 3.1 |
| 79 | DT | 81 | ALA | 3.1 |
| 37 | CD | 49 | LEU | 3.1 |
| 45 | i | 47 | ASP | 3.1 |
| 48 | CO | 54 | LEU | 3.1 |
| 55 | CV | 68 | GLY | 3.1 |
| 56 | L | 151 | ASP | 3.1 |
| 63 | DD | 27 | LEU | 3.1 |
| 63 | DD | 132 | GLY | 3.1 |
| 1 | 1 | 1557 | U | 3.1 |
| 47 | CN | 139 | VAL | 3.1 |
| 49 | E | 125 | VAL | 3.1 |
| 52 | H | 160 | VAL | 3.1 |
| 69 | Y | 37 | PHE | 3.1 |
| 56 | L | 18 | PRO | 3.1 |
| 58 | N | 98 | ASN | 3.1 |
| 67 | W | 70 | PRO | 3.1 |
| 69 | Y | 66 | ASN | 3.1 |
| 16 | v | 142 | ILE | 3.1 |
| 18 | x | 133 | HIS | 3.1 |
| 45 | i | 85 | LYS | 3.1 |
| 52 | H | 122 | HIS | 3.1 |
| 63 | DD | 105 | LYS | 3.1 |

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| Mol | Chain | Res | Type | RSRZ |
|---|---|---|---|---|
| 65 | U | 119 | ILE | 3.1 |
| 71 | DL | 99 | LYS | 3.1 |
| 11 | q | 163 | GLN | 3.1 |
| 16 | BI | 146 | ALA | 3.1 |
| 1 | AS | 2468 | C | 3.1 |
| 10 | BC | 95 | LEU | 3.1 |
| 35 | AH | 30 | LEU | 3.1 |
| 52 | CS | 97 | LEU | 3.1 |
| 67 | W | 25 | LEU | 3.1 |
| 67 | DH | 75 | SER | 3.1 |
| 75 | e | 33 | LEU | 3.1 |
| 79 | AR | 271 | LEU | 3.1 |
| 82 | l1 | 124 | LEU | 3.1 |
| 1 | AS | 1238 | G | 3.1 |
| 46 | B | 1349 | G | 3.1 |
| 67 | DH | 110 | GLY | 3.1 |
| 55 | K | 28 | GLU | 3.1 |
| 12 | r | 190 | VAL | 3.1 |
| 28 | AA | 118 | PHE | 3.1 |
| 59 | O | 30 | VAL | 3.1 |
| 52 | H | 148 | ARG | 3.1 |
| 70 | DK | 107 | PHE | 3.1 |
| 72 | DM | 91 | PRO | 3.1 |
| 10 | BC | 144 | ILE | 3.1 |
| 10 | BC | 180 | ILE | 3.1 |
| 14 | t | 6 | ASN | 3.1 |
| 56 | CW | 51 | LYS | 3.1 |
| 59 | O | 111 | ASN | 3.1 |
| 6 | AY | 145 | GLN | 3.1 |
| 65 | U | 83 | ALA | 3.1 |
| 79 | DT | 24 | ALA | 3.1 |
| 8 | n | 39 | LEU | 3.1 |
| 10 | BC | 137 | LEU | 3.1 |
| 47 | CN | 177 | LEU | 3.1 |
| 51 | CR | 101 | LEU | 3.1 |
| 51 | CR | 247 | LEU | 3.1 |
| 56 | L | 70 | LEU | 3.1 |
| 59 | CZ | 59 | LEU | 3.1 |
| 60 | P | 80 | LEU | 3.1 |
| 70 | Z | 104 | LEU | 3.1 |
| 1 | AS | 1240 | A | 3.1 |
| 38 | CE | 87 | THR | 3.1 |

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| Mol | Chain | Res | Type | RSRZ |
|---|---|---|---|---|
| 60 | P | 79 | GLY | 3.1 |
| 60 | DA | 59 | GLY | 3.1 |
| 8 | n | 2 | SER | 3.1 |
| 79 | AR | 75 | SER | 3.1 |
| 1 | AS | 1197 | C | 3.1 |
| 23 | 5 | 66 | VAL | 3.1 |
| 47 | CN | 107 | PHE | 3.1 |
| 51 | G | 60 | GLU | 3.1 |
| 61 | Q | 25 | VAL | 3.1 |
| 65 | DF | 128 | PHE | 3.1 |
| 71 | DL | 92 | VAL | 3.1 |
| 73 | c | 30 | VAL | 3.1 |
| 78 | DS | 126 | VAL | 3.1 |
| 53 | I | 100 | CYS | 3.1 |
| 65 | U | 82 | PRO | 3.1 |
| 78 | h | 130 | PRO | 3.1 |
| 78 | DS | 178 | LYS | 3.1 |
| 1 | 1 | 2443 | G | 3.1 |
| 65 | DF | 79 | TYR | 3.1 |
| 47 | CN | 33 | ASN | 3.1 |
| 69 | Y | 84 | ASN | 3.1 |
| 78 | h | 170 | ALA | 3.1 |
| 31 | AD | 86 | LEU | 3.1 |
| 46 | B | 1399 | U | 3.1 |
| 46 | CM | 133 | U | 3.1 |
| 51 | G | 101 | LEU | 3.1 |
| 55 | CV | 111 | GLN | 3.1 |
| 66 | V | 52 | THR | 3.1 |
| 19 | y | 3 | ARG | 3.1 |
| 19 | y | 174 | ARG | 3.1 |
| 6 | l | 296 | VAL | 3.1 |
| 22 | BO | 89 | VAL | 3.1 |
| 33 | AF | 120 | VAL | 3.1 |
| 45 | i | 39 | SER | 3.1 |
| 52 | H | 168 | VAL | 3.1 |
| 59 | O | 123 | VAL | 3.1 |
| 62 | R | 92 | SER | 3.1 |
| 10 | p | 166 | PHE | 3.1 |
| 13 | BF | 78 | GLU | 3.1 |
| 18 | BK | 42 | GLU | 3.1 |
| 35 | AH | 21 | LYS | 3.1 |
| 36 | AI | 64 | GLU | 3.1 |

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| Mol | Chain | Res | Type | RSRZ |
|---|---|---|---|---|
| 41 | AN | 52 | LYS | 3.1 |
| 46 | CM | 712 | A | 3.1 |
| 78 | h | 131 | LYS | 3.1 |
| 80 | p0 | 55 | LYS | 3.1 |
| 10 | p | 144 | ILE | 3.1 |
| 53 | CT | 181 | PRO | 3.1 |
| 55 | CV | 189 | ILE | 3.1 |
| 68 | X | 23 | ILE | 3.1 |
| 47 | CN | 76 | CYS | 3.1 |
| 58 | N | 93 | TYR | 3.1 |
| 63 | DD | 23 | ALA | 3.0 |
| 64 | DE | 46 | LEU | 3.0 |
| 71 | a | 134 | ALA | 3.0 |
| 6 | l | 356 | GLN | 3.0 |
| 7 | m | 24 | GLN | 3.0 |
| 49 | E | 89 | GLN | 3.0 |
| 1 | 1 | 2444 | G | 3.0 |
| 1 | AS | 1222 | G | 3.0 |
| 50 | CQ | 134 | GLY | 3.0 |
| 29 | BV | 43 | THR | 3.0 |
| 46 | CM | 75 | U | 3.0 |
| 46 | CM | 1356 | U | 3.0 |
| 60 | P | 66 | VAL | 3.0 |
| 64 | DE | 119 | VAL | 3.0 |
| 66 | V | 71 | VAL | 3.0 |
| 66 | DG | 34 | VAL | 3.0 |
| 42 | AO | 19 | LYS | 3.0 |
| 49 | E | 114 | LYS | 3.0 |
| 57 | M | 5 | LYS | 3.0 |
| 67 | W | 68 | LYS | 3.0 |
| 82 | l1 | 28 | PHE | 3.0 |
| 52 | H | 151 | SER | 3.0 |
| 64 | T | 13 | SER | 3.0 |
| 27 | 9 | 99 | ILE | 3.0 |
| 56 | L | 156 | ILE | 3.0 |
| 56 | CW | 15 | PRO | 3.0 |
| 16 | BI | 62 | TYR | 3.0 |
| 52 | H | 61 | TYR | 3.0 |
| 30 | AC | 2 | ALA | 3.0 |
| 56 | L | 86 | LEU | 3.0 |
| 59 | O | 74 | LEU | 3.0 |
| 59 | O | 101 | ALA | 3.0 |

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| Mol | Chain | Res | Type | RSRZ |
|---|---|---|---|---|
| 63 | DD | 20 | HIS | 3.0 |
| 52 | CS | 112 | ARG | 3.0 |
| 65 | U | 41 | ARG | 3.0 |
| 69 | Y | 80 | ASN | 3.0 |
| 55 | CV | 32 | GLN | 3.0 |
| 60 | DA | 62 | GLN | 3.0 |
| 1 | 1 | 2448 | C | 3.0 |
| 46 | B | 1568 | C | 3.0 |
| 7 | m | 236 | VAL | 3.0 |
| 9 | o | 156 | LYS | 3.0 |
| 25 | BR | 83 | VAL | 3.0 |
| 45 | i | 86 | LYS | 3.0 |
| 49 | E | 58 | VAL | 3.0 |
| 50 | F | 207 | VAL | 3.0 |
| 65 | DF | 4 | VAL | 3.0 |
| 78 | DS | 129 | THR | 3.0 |
| 31 | BX | 12 | ILE | 3.0 |
| 45 | i | 45 | SER | 3.0 |
| 48 | CO | 204 | ILE | 3.0 |
| 54 | J | 182 | PRO | 3.0 |
| 56 | L | 5 | PRO | 3.0 |
| 69 | Y | 29 | PRO | 3.0 |
| 52 | H | 145 | ASP | 3.0 |
| 63 | DD | 53 | LEU | 3.0 |
| 70 | DK | 104 | LEU | 3.0 |
| 6 | l | 175 | ALA | 3.0 |
| 7 | m | 226 | TYR | 3.0 |
| 20 | z | 12 | ALA | 3.0 |
| 51 | G | 55 | ALA | 3.0 |
| 52 | CS | 61 | TYR | 3.0 |
| 55 | CV | 173 | ALA | 3.0 |
| 70 | Z | 12 | ALA | 3.0 |
| 44 | CK | 28 | LYS | 3.0 |
| 50 | F | 191 | LYS | 3.0 |
| 62 | R | 117 | GLY | 3.0 |
| 73 | c | 37 | LYS | 3.0 |
| 78 | h | 124 | LYS | 3.0 |
| 1 | AS | 402 | A | 3.0 |
| 39 | CF | 27 | VAL | 3.0 |
| 51 | G | 76 | VAL | 3.0 |
| 30 | AC | 8 | THR | 3.0 |
| 48 | CO | 205 | PHE | 3.0 |

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| Mol | Chain | Res | Type | RSRZ |
|---|---|---|---|---|
| 52 | H | 82 | PHE | 3.0 |
| 53 | CT | 144 | PHE | 3.0 |
| 54 | CU | 21 | PHE | 3.0 |
| 55 | CV | 97 | THR | 3.0 |
| 64 | DE | 25 | THR | 3.0 |
| 79 | AR | 12 | THR | 3.0 |
| 1 | AS | 240 | C | 3.0 |
| 50 | F | 171 | ILE | 3.0 |
| 59 | O | 100 | TRP | 3.0 |
| 62 | R | 111 | MET | 3.0 |
| 62 | DC | 84 | ILE | 3.0 |
| 64 | DE | 117 | ILE | 3.0 |
| 67 | DH | 117 | ILE | 3.0 |
| 82 | l1 | 43 | PRO | 3.0 |
| 4 | AW | 104 | LEU | 3.0 |
| 10 | BC | 151 | LEU | 3.0 |
| 13 | BF | 19 | LEU | 3.0 |
| 30 | AC | 62 | SER | 3.0 |
| 35 | AH | 49 | SER | 3.0 |
| 45 | i | 35 | SER | 3.0 |
| 51 | G | 123 | LEU | 3.0 |
| 60 | P | 14 | SER | 3.0 |
| 79 | DT | 7 | LEU | 3.0 |
| 10 | BC | 178 | TYR | 3.0 |
| 31 | BX | 61 | TYR | 3.0 |
| 51 | CR | 63 | ALA | 3.0 |
| 63 | DD | 48 | TYR | 3.0 |
| 64 | DE | 11 | ARG | 3.0 |
| 79 | DT | 84 | ALA | 3.0 |
| 46 | B | 1114 | U | 3.0 |
| 69 | Y | 9 | ASP | 3.0 |
| 10 | p | 134 | LYS | 3.0 |
| 45 | i | 54 | LYS | 3.0 |
| 1 | 1 | 545 | G | 3.0 |
| 1 | 1 | 2455 | G | 3.0 |
| 7 | m | 52 | VAL | 3.0 |
| 7 | m | 151 | GLN | 3.0 |
| 7 | AZ | 236 | VAL | 3.0 |
| 11 | q | 162 | GLN | 3.0 |
| 48 | CO | 63 | GLY | 3.0 |
| 16 | v | 115 | VAL | 3.0 |
| 48 | D | 43 | VAL | 3.0 |

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| Mol | Chain | Res | Type | RSRZ |
|---|---|---|---|---|
| 48 | CO | 20 | VAL | 3.0 |
| 52 | CS | 160 | VAL | 3.0 |
| 70 | DK | 92 | CYS | 3.0 |
| 60 | P | 69 | ASN | 3.0 |
| 82 | l1 | 12 | ASN | 3.0 |
| 26 | BS | 32 | PHE | 3.0 |
| 57 | M | 16 | PHE | 3.0 |
| 30 | BW | 8 | THR | 3.0 |
| 63 | S | 16 | THR | 3.0 |
| 78 | DS | 189 | THR | 3.0 |
| 26 | 8 | 88 | ILE | 3.0 |
| 27 | 9 | 119 | ILE | 3.0 |
| 58 | N | 49 | ILE | 3.0 |
| 1 | AS | 3166 | A | 3.0 |
| 33 | BZ | 76 | LEU | 3.0 |
| 41 | AN | 51 | LEU | 3.0 |
| 41 | CH | 28 | PRO | 3.0 |
| 41 | CH | 45 | LEU | 3.0 |
| 66 | V | 79 | LEU | 3.0 |
| 76 | f | 12 | ARG | 3.0 |
| 7 | AZ | 80 | ALA | 3.0 |
| 10 | BC | 67 | SER | 3.0 |
| 16 | BI | 166 | SER | 3.0 |
| 60 | DA | 148 | ALA | 3.0 |
| 79 | DT | 66 | SER | 3.0 |
| 79 | DT | 251 | ALA | 3.0 |
| 14 | BG | 119 | TYR | 3.0 |
| 19 | y | 72 | LYS | 3.0 |
| 50 | F | 208 | LYS | 3.0 |
| 60 | P | 70 | LYS | 3.0 |
| 73 | c | 73 | TYR | 3.0 |
| 43 | CJ | 44 | ASP | 3.0 |
| 52 | H | 161 | ASP | 3.0 |
| 63 | DD | 119 | ASP | 3.0 |
| 5 | k | 274 | HIS | 3.0 |
| 7 | m | 169 | GLY | 3.0 |
| 11 | q | 154 | VAL | 3.0 |
| 32 | AE | 95 | VAL | 3.0 |
| 45 | CL | 83 | HIS | 3.0 |
| 50 | CQ | 135 | VAL | 3.0 |
| 56 | L | 85 | VAL | 3.0 |
| 58 | CY | 68 | GLY | 3.0 |

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| Mol | Chain | Res | Type | RSRZ |
|---|---|---|---|---|
| 69 | Y | 113 | HIS | 3.0 |
| 1 | AS | 3165 | U | 3.0 |
| 6 | AY | 356 | GLN | 3.0 |
| 80 | p0 | 12 | PHE | 3.0 |
| 6 | AY | 317 | ASN | 3.0 |
| 23 | BP | 57 | THR | 3.0 |
| 50 | CQ | 85 | ILE | 3.0 |
| 51 | G | 228 | ILE | 3.0 |
| 55 | CV | 104 | ILE | 3.0 |
| 60 | P | 84 | ILE | 3.0 |
| 63 | S | 123 | MET | 3.0 |
| 71 | a | 75 | ILE | 3.0 |
| 79 | AR | 314 | THR | 3.0 |
| 13 | s | 19 | LEU | 2.9 |
| 59 | O | 78 | LEU | 2.9 |
| 70 | Z | 33 | LEU | 2.9 |
| 6 | AY | 109 | ARG | 2.9 |
| 19 | y | 170 | ARG | 2.9 |
| 26 | BS | 48 | ARG | 2.9 |
| 56 | CW | 64 | GLU | 2.9 |
| 67 | W | 78 | TRP | 2.9 |
| 10 | BC | 182 | LYS | 2.9 |
| 47 | C | 97 | ALA | 2.9 |
| 53 | I | 191 | LYS | 2.9 |
| 79 | DT | 59 | LYS | 2.9 |
| 79 | DT | 76 | ALA | 2.9 |
| 19 | y | 63 | SER | 2.9 |
| 59 | O | 119 | SER | 2.9 |
| 59 | CZ | 119 | SER | 2.9 |
| 1 | 1 | 1021 | A | 2.9 |
| 1 | 1 | 2464 | A | 2.9 |
| 22 | BO | 67 | VAL | 2.9 |
| 52 | H | 75 | GLY | 2.9 |
| 59 | CZ | 127 | GLY | 2.9 |
| 67 | DH | 79 | ASP | 2.9 |
| 71 | a | 135 | ASP | 2.9 |
| 80 | p0 | 65 | GLY | 2.9 |
| 6 | AY | 253 | GLN | 2.9 |
| 51 | CR | 109 | PHE | 2.9 |
| 52 | CS | 43 | PHE | 2.9 |
| 46 | CM | 674 | C | 2.9 |
| 19 | y | 57 | ILE | 2.9 |

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| Mol | Chain | Res | Type | RSRZ |
|---|---|---|---|---|
| 72 | DM | 100 | ILE | 2.9 |
| 1 | AS | 3162 | U | 2.9 |
| 30 | AC | 18 | ARG | 2.9 |
| 36 | CC | 108 | ARG | 2.9 |
| 43 | CJ | 83 | LEU | 2.9 |
| 47 | C | 17 | LEU | 2.9 |
| 50 | F | 6 | LEU | 2.9 |
| 79 | AR | 145 | LEU | 2.9 |
| 51 | CR | 243 | LYS | 2.9 |
| 66 | DG | 51 | GLU | 2.9 |
| 82 | l1 | 137 | PRO | 2.9 |
| 7 | AZ | 100 | ALA | 2.9 |
| 54 | J | 65 | ALA | 2.9 |
| 54 | CU | 90 | ALA | 2.9 |
| 70 | Z | 31 | ALA | 2.9 |
| 17 | w | 2 | SER | 2.9 |
| 79 | DT | 210 | SER | 2.9 |
| 79 | DT | 216 | VAL | 2.9 |
| 52 | H | 153 | GLY | 2.9 |
| 53 | I | 146 | GLY | 2.9 |
| 64 | DE | 2 | GLY | 2.9 |
| 1 | 1 | 2459 | G | 2.9 |
| 13 | s | 102 | PHE | 2.9 |
| 33 | AF | 21 | HIS | 2.9 |
| 48 | CO | 24 | PHE | 2.9 |
| 53 | CT | 145 | PHE | 2.9 |
| 54 | J | 21 | PHE | 2.9 |
| 70 | DK | 48 | HIS | 2.9 |
| 29 | AB | 46 | ASP | 2.9 |
| 6 | AY | 249 | ILE | 2.9 |
| 28 | AA | 25 | ILE | 2.9 |
| 55 | CV | 20 | GLN | 2.9 |
| 56 | CW | 45 | ILE | 2.9 |
| 59 | O | 71 | ILE | 2.9 |
| 63 | DD | 123 | MET | 2.9 |
| 67 | DH | 83 | MET | 2.9 |
| 7 | m | 146 | LEU | 2.9 |
| 16 | BI | 197 | LEU | 2.9 |
| 46 | CM | 1476 | A | 2.9 |
| 63 | DD | 37 | LEU | 2.9 |
| 63 | DD | 104 | LEU | 2.9 |
| 78 | h | 128 | THR | 2.9 |

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| Mol | Chain | Res | Type | RSRZ |
|---|---|---|---|---|
| 14 | BG | 194 | GLU | 2.9 |
| 41 | CH | 3 | GLU | 2.9 |
| 59 | O | 48 | ALA | 2.9 |
| 78 | h | 143 | ALA | 2.9 |
| 1 | AS | 2743 | U | 2.9 |
| 46 | B | 1356 | U | 2.9 |
| 10 | p | 204 | VAL | 2.9 |
| 22 | BO | 93 | VAL | 2.9 |
| 41 | CH | 13 | TYR | 2.9 |
| 50 | F | 7 | SER | 2.9 |
| 51 | G | 107 | GLY | 2.9 |
| 52 | CS | 153 | GLY | 2.9 |
| 53 | CT | 50 | PHE | 2.9 |
| 60 | P | 19 | SER | 2.9 |
| 77 | DR | 6 | GLY | 2.9 |
| 33 | BZ | 18 | PHE | 2.9 |
| 57 | M | 12 | HIS | 2.9 |
| 60 | DA | 58 | HIS | 2.9 |
| 14 | t | 125 | ILE | 2.9 |
| 7 | AZ | 275 | GLN | 2.9 |
| 25 | 7 | 47 | ARG | 2.9 |
| 26 | 8 | 108 | LEU | 2.9 |
| 41 | AN | 6 | LEU | 2.9 |
| 49 | E | 93 | MET | 2.9 |
| 52 | CS | 190 | ILE | 2.9 |
| 54 | CU | 131 | ILE | 2.9 |
| 62 | R | 121 | ILE | 2.9 |
| 64 | DE | 16 | LEU | 2.9 |
| 65 | U | 120 | ARG | 2.9 |
| 66 | V | 89 | ARG | 2.9 |
| 79 | DT | 307 | ILE | 2.9 |
| 55 | CV | 53 | GLN | 2.9 |
| 57 | M | 15 | LEU | 2.9 |
| 62 | R | 80 | LEU | 2.9 |
| 63 | S | 27 | LEU | 2.9 |
| 17 | w | 177 | LYS | 2.9 |
| 45 | CL | 96 | LYS | 2.9 |
| 36 | CC | 100 | GLU | 2.9 |
| 46 | B | 1184 | G | 2.9 |
| 51 | G | 31 | PRO | 2.9 |
| 53 | I | 197 | ASN | 2.9 |
| 63 | S | 83 | ALA | 2.9 |

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| Mol | Chain | Res | Type | RSRZ |
|---|---|---|---|---|
| 63 | DD | 79 | ALA | 2.9 |
| 82 | l1 | 212 | PRO | 2.9 |
| 1 | AS | 2186 | A | 2.9 |
| 41 | CH | 23 | CYS | 2.9 |
| 46 | B | 1407 | A | 2.9 |
| 51 | CR | 236 | TRP | 2.9 |
| 47 | C | 158 | VAL | 2.9 |
| 54 | J | 177 | VAL | 2.9 |
| 62 | R | 76 | VAL | 2.9 |
| 7 | m | 219 | TYR | 2.9 |
| 10 | BC | 98 | TYR | 2.9 |
| 16 | v | 62 | TYR | 2.9 |
| 26 | BS | 84 | PHE | 2.9 |
| 29 | BV | 30 | GLY | 2.9 |
| 42 | AO | 17 | ARG | 2.9 |
| 47 | CN | 127 | ARG | 2.9 |
| 48 | CO | 105 | PHE | 2.9 |
| 55 | K | 65 | PHE | 2.9 |
| 69 | DJ | 57 | ARG | 2.9 |
| 79 | AR | 38 | ARG | 2.9 |
| 11 | q | 136 | ILE | 2.9 |
| 22 | 2 | 85 | ILE | 2.9 |
| 35 | CB | 17 | SER | 2.9 |
| 53 | CT | 217 | HIS | 2.9 |
| 54 | J | 175 | LYS | 2.9 |
| 57 | M | 25 | LYS | 2.9 |
| 59 | O | 106 | LEU | 2.9 |
| 64 | T | 91 | LEU | 2.9 |
| 69 | DJ | 27 | ILE | 2.9 |
| 73 | c | 36 | ILE | 2.9 |
| 19 | y | 74 | LYS | 2.9 |
| 35 | CB | 36 | LYS | 2.9 |
| 76 | f | 54 | LYS | 2.9 |
| 78 | h | 125 | LYS | 2.9 |
| 78 | DS | 124 | LYS | 2.9 |
| 79 | AR | 46 | LYS | 2.9 |
| 79 | DT | 42 | LEU | 2.9 |
| 80 | P0 | 18 | LEU | 2.9 |
| 39 | AL | 40 | GLN | 2.9 |
| 15 | u | 22 | ASP | 2.9 |
| 65 | U | 51 | ASP | 2.9 |
| 6 | l | 163 | THR | 2.9 |

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| Mol | Chain | Res | Type | RSRZ |
|---|---|---|---|---|
| 39 | AL | 33 | ALA | 2.9 |
| 47 | C | 74 | ALA | 2.9 |
| 58 | N | 95 | PRO | 2.9 |
| 65 | U | 77 | THR | 2.9 |
| 69 | DJ | 29 | PRO | 2.9 |
| 79 | DT | 79 | ALA | 2.9 |
| 38 | CE | 20 | ASN | 2.9 |
| 52 | H | 66 | ASN | 2.9 |
| 60 | P | 142 | GLU | 2.9 |
| 78 | h | 162 | GLU | 2.9 |
| 10 | BC | 198 | VAL | 2.9 |
| 47 | CN | 86 | VAL | 2.9 |
| 56 | CW | 96 | VAL | 2.9 |
| 63 | S | 77 | VAL | 2.9 |
| 65 | DF | 93 | VAL | 2.9 |
| 79 | AR | 277 | VAL | 2.9 |
| 82 | l1 | 36 | VAL | 2.9 |
| 4 | AW | 64 | ARG | 2.9 |
| 6 | l | 157 | PHE | 2.9 |
| 35 | AH | 48 | GLY | 2.9 |
| 48 | CO | 213 | ARG | 2.9 |
| 52 | CS | 77 | TYR | 2.9 |
| 54 | CU | 88 | PHE | 2.9 |
| 55 | K | 8 | ARG | 2.9 |
| 55 | K | 183 | GLY | 2.9 |
| 56 | CW | 104 | PHE | 2.9 |
| 64 | DE | 47 | ARG | 2.9 |
| 66 | V | 42 | GLY | 2.9 |
| 71 | a | 73 | GLY | 2.9 |
| 1 | AS | 2062 | G | 2.9 |
| 16 | BI | 36 | ILE | 2.9 |
| 45 | CL | 115 | LEU | 2.9 |
| 54 | J | 43 | LYS | 2.9 |
| 54 | CU | 134 | LYS | 2.9 |
| 55 | CV | 171 | LEU | 2.9 |
| 63 | DD | 28 | ILE | 2.9 |
| 65 | U | 28 | ILE | 2.9 |
| 66 | DG | 22 | LEU | 2.9 |
| 66 | DG | 132 | LEU | 2.9 |
| 69 | DJ | 104 | LEU | 2.9 |
| 71 | a | 7 | ILE | 2.9 |
| 78 | h | 145 | LEU | 2.9 |

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| Mol | Chain | Res | Type | RSRZ |
|---|---|---|---|---|
| 7 | AZ | 244 | HIS | 2.8 |
| 56 | L | 124 | HIS | 2.8 |
| 1 | 1 | 1346 | U | 2.8 |
| 1 | 1 | 1760 | U | 2.8 |
| 4 | j | 47 | GLN | 2.8 |
| 22 | 2 | 103 | GLN | 2.8 |
| 46 | B | 1047 | U | 2.8 |
| 76 | DQ | 28 | SER | 2.8 |
| 52 | CS | 85 | ALA | 2.8 |
| 52 | CS | 27 | THR | 2.8 |
| 60 | DA | 137 | PRO | 2.8 |
| 63 | DD | 83 | ALA | 2.8 |
| 65 | DF | 51 | ASP | 2.8 |
| 65 | DF | 76 | PRO | 2.8 |
| 73 | DN | 6 | ALA | 2.8 |
| 48 | CO | 37 | THR | 2.8 |
| 16 | BI | 153 | ASN | 2.8 |
| 16 | BI | 99 | ARG | 2.8 |
| 64 | T | 45 | ARG | 2.8 |
| 64 | T | 67 | ARG | 2.8 |
| 68 | X | 22 | ARG | 2.8 |
| 41 | CH | 15 | CYS | 2.8 |
| 10 | BC | 184 | LYS | 2.8 |
| 6 | AY | 245 | LEU | 2.8 |
| 8 | BA | 63 | LEU | 2.8 |
| 10 | BC | 187 | LEU | 2.8 |
| 16 | BI | 21 | PHE | 2.8 |
| 50 | CQ | 58 | GLY | 2.8 |
| 52 | CS | 115 | LYS | 2.8 |
| 53 | CT | 79 | LYS | 2.8 |
| 67 | W | 60 | LYS | 2.8 |
| 67 | DH | 29 | LYS | 2.8 |
| 52 | CS | 177 | ILE | 2.8 |
| 57 | M | 65 | TYR | 2.8 |
| 63 | DD | 56 | LEU | 2.8 |
| 69 | DJ | 128 | PHE | 2.8 |
| 69 | Y | 83 | ILE | 2.8 |
| 70 | DK | 133 | LEU | 2.8 |
| 78 | h | 159 | LEU | 2.8 |
| 82 | l1 | 68 | PHE | 2.8 |
| 63 | DD | 84 | ILE | 2.8 |
| 67 | W | 57 | MET | 2.8 |

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| Mol | Chain | Res | Type | RSRZ |
|---|---|---|---|---|
| 79 | AR | 259 | ILE | 2.8 |
| 79 | AR | 238 | HIS | 2.8 |
| 13 | s | 47 | GLN | 2.8 |
| 74 | d | 51 | GLN | 2.8 |
| 1 | AS | 1236 | A | 2.8 |
| 1 | AS | 2185 | A | 2.8 |
| 76 | DQ | 25 | SER | 2.8 |
| 79 | AR | 164 | SER | 2.8 |
| 1 | 1 | 2068 | U | 2.8 |
| 1 | AS | 2442 | U | 2.8 |
| 46 | B | 1603 | G | 2.8 |
| 77 | g | 27 | PRO | 2.8 |
| 6 | l | 64 | GLU | 2.8 |
| 63 | DD | 36 | THR | 2.8 |
| 9 | o | 115 | VAL | 2.8 |
| 19 | BL | 180 | ARG | 2.8 |
| 23 | 5 | 17 | VAL | 2.8 |
| 35 | CB | 35 | VAL | 2.8 |
| 46 | CM | 1412 | C | 2.8 |
| 49 | CP | 97 | VAL | 2.8 |
| 51 | CR | 39 | ARG | 2.8 |
| 60 | DA | 42 | ARG | 2.8 |
| 61 | Q | 74 | VAL | 2.8 |
| 61 | Q | 116 | VAL | 2.8 |
| 61 | DB | 130 | ARG | 2.8 |
| 72 | DM | 92 | VAL | 2.8 |
| 42 | CI | 5 | TRP | 2.8 |
| 49 | CP | 111 | LYS | 2.8 |
| 56 | L | 154 | LYS | 2.8 |
| 63 | S | 105 | LYS | 2.8 |
| 65 | U | 44 | ASN | 2.8 |
| 78 | DS | 191 | LYS | 2.8 |
| 5 | AX | 387 | LEU | 2.8 |
| 15 | BH | 128 | LEU | 2.8 |
| 32 | BY | 50 | LEU | 2.8 |
| 47 | C | 50 | ILE | 2.8 |
| 50 | CQ | 47 | LEU | 2.8 |
| 56 | CW | 60 | LEU | 2.8 |
| 80 | P0 | 86 | PHE | 2.8 |
| 82 | l1 | 34 | LEU | 2.8 |
| 36 | CC | 75 | TYR | 2.8 |
| 63 | S | 91 | TYR | 2.8 |

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| Mol | Chain | Res | Type | RSRZ |
|---|---|---|---|---|
| 66 | DG | 66 | TYR | 2.8 |
| 55 | K | 32 | GLN | 2.8 |
| 55 | K | 53 | GLN | 2.8 |
| 64 | DE | 62 | GLN | 2.8 |
| 51 | G | 2 | ALA | 2.8 |
| 55 | CV | 79 | ALA | 2.8 |
| 58 | N | 114 | ALA | 2.8 |
| 59 | CZ | 42 | ALA | 2.8 |
| 44 | CK | 17 | ARG | 2.8 |
| 49 | CP | 92 | ARG | 2.8 |
| 51 | CR | 191 | ARG | 2.8 |
| 52 | CS | 92 | ARG | 2.8 |
| 64 | T | 65 | PRO | 2.8 |
| 73 | DN | 89 | ARG | 2.8 |
| 52 | CS | 111 | VAL | 2.8 |
| 7 | m | 25 | GLU | 2.8 |
| 52 | CS | 109 | LYS | 2.8 |
| 56 | L | 7 | THR | 2.8 |
| 63 | DD | 8 | THR | 2.8 |
| 74 | d | 23 | THR | 2.8 |
| 78 | DS | 128 | THR | 2.8 |
| 82 | L1 | 30 | GLU | 2.8 |
| 46 | CM | 1479 | A | 2.8 |
| 1 | AS | 1012 | U | 2.8 |
| 40 | AM | 51 | ILE | 2.8 |
| 46 | B | 75 | U | 2.8 |
| 46 | B | 1541 | U | 2.8 |
| 46 | CM | 1399 | U | 2.8 |
| 48 | CO | 38 | PHE | 2.8 |
| 55 | K | 55 | PHE | 2.8 |
| 55 | K | 199 | LEU | 2.8 |
| 60 | P | 149 | LEU | 2.8 |
| 66 | DG | 21 | PHE | 2.8 |
| 67 | DH | 107 | ILE | 2.8 |
| 71 | a | 72 | PHE | 2.8 |
| 78 | DS | 159 | LEU | 2.8 |
| 49 | E | 78 | ILE | 2.8 |
| 50 | F | 129 | GLY | 2.8 |
| 62 | DC | 57 | ILE | 2.8 |
| 64 | DE | 68 | GLY | 2.8 |
| 1 | AS | 249 | G | 2.8 |
| 29 | BV | 52 | TYR | 2.8 |

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| Mol | Chain | Res | Type | RSRZ |
|---|---|---|---|---|
| 46 | B | 636 | C | 2.8 |
| 46 | B | 753 | C | 2.8 |
| 55 | CV | 188 | TYR | 2.8 |
| 60 | P | 90 | TYR | 2.8 |
| 78 | DS | 147 | TYR | 2.8 |
| 5 | k | 182 | GLN | 2.8 |
| 21 | 0 | 138 | GLN | 2.8 |
| 54 | J | 64 | GLN | 2.8 |
| 54 | CU | 70 | GLN | 2.8 |
| 63 | S | 23 | ALA | 2.8 |
| 64 | T | 60 | ARG | 2.8 |
| 69 | Y | 57 | ARG | 2.8 |
| 6 | l | 143 | VAL | 2.8 |
| 10 | BC | 181 | VAL | 2.8 |
| 22 | BO | 70 | SER | 2.8 |
| 54 | J | 36 | PRO | 2.8 |
| 58 | CY | 15 | LYS | 2.8 |
| 65 | DF | 100 | VAL | 2.8 |
| 82 | l1 | 172 | VAL | 2.8 |
| 21 | BN | 34 | THR | 2.8 |
| 24 | 6 | 34 | LEU | 2.8 |
| 28 | BU | 134 | LEU | 2.8 |
| 45 | i | 34 | THR | 2.8 |
| 52 | H | 198 | LEU | 2.8 |
| 58 | N | 50 | GLU | 2.8 |
| 63 | DD | 88 | LEU | 2.8 |
| 64 | T | 6 | THR | 2.8 |
| 65 | U | 116 | LEU | 2.8 |
| 10 | BC | 117 | ILE | 2.8 |
| 18 | x | 166 | ILE | 2.8 |
| 20 | BM | 143 | ILE | 2.8 |
| 21 | 0 | 42 | TRP | 2.8 |
| 28 | AA | 71 | PHE | 2.8 |
| 42 | AO | 3 | ASP | 2.8 |
| 53 | CT | 113 | ILE | 2.8 |
| 54 | J | 88 | PHE | 2.8 |
| 54 | J | 151 | ASP | 2.8 |
| 19 | y | 2 | GLY | 2.8 |
| 50 | F | 122 | GLY | 2.8 |
| 50 | F | 190 | MET | 2.8 |
| 63 | S | 42 | ILE | 2.8 |
| 64 | DE | 38 | ILE | 2.8 |

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| Mol | Chain | Res | Type | RSRZ |
|---|---|---|---|---|
| 64 | DE | 41 | ILE | 2.8 |
| 65 | U | 35 | ILE | 2.8 |
| 79 | DT | 56 | GLY | 2.8 |
| 31 | AD | 77 | ASN | 2.8 |
| 1 | 1 | 239 | A | 2.8 |
| 46 | B | 492 | U | 2.8 |
| 46 | CM | 659 | U | 2.8 |
| 51 | CR | 27 | TYR | 2.8 |
| 77 | g | 35 | TYR | 2.8 |
| 40 | CG | 46 | ARG | 2.8 |
| 41 | CH | 37 | ARG | 2.8 |
| 50 | F | 212 | ALA | 2.8 |
| 51 | G | 49 | ARG | 2.8 |
| 54 | J | 108 | ARG | 2.8 |
| 60 | P | 148 | ALA | 2.8 |
| 64 | DE | 3 | ARG | 2.8 |
| 48 | CO | 55 | LYS | 2.8 |
| 51 | G | 6 | LYS | 2.8 |
| 51 | G | 133 | LYS | 2.8 |
| 1 | AS | 2447 | G | 2.8 |
| 5 | k | 264 | VAL | 2.8 |
| 46 | B | 750 | G | 2.8 |
| 63 | S | 40 | PRO | 2.8 |
| 65 | U | 2 | PRO | 2.8 |
| 66 | V | 9 | VAL | 2.8 |
| 80 | p0 | 50 | VAL | 2.8 |
| 37 | CD | 41 | SER | 2.8 |
| 45 | CL | 99 | SER | 2.8 |
| 47 | C | 184 | LEU | 2.8 |
| 50 | F | 12 | LEU | 2.8 |
| 55 | CV | 58 | LEU | 2.8 |
| 72 | DM | 69 | LEU | 2.8 |
| 79 | DT | 228 | LEU | 2.8 |
| 82 | L1 | 38 | LEU | 2.8 |
| 82 | L1 | 213 | SER | 2.8 |
| 16 | v | 160 | GLU | 2.8 |
| 23 | 5 | 57 | THR | 2.8 |
| 38 | AK | 59 | THR | 2.8 |
| 56 | L | 33 | GLU | 2.8 |
| 39 | CF | 43 | PHE | 2.7 |
| 52 | CS | 149 | ILE | 2.8 |
| 57 | CX | 27 | PHE | 2.7 |

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| Mol | Chain | Res | Type | RSRZ |
|---|---|---|---|---|
| 63 | S | 69 | THR | 2.8 |
| 64 | T | 71 | PHE | 2.7 |
| 66 | V | 21 | PHE | 2.7 |
| 79 | AR | 253 | THR | 2.8 |
| 80 | p0 | 63 | ILE | 2.8 |
| 82 | l1 | 4 | ILE | 2.8 |
| 38 | CE | 23 | GLY | 2.7 |
| 45 | i | 107 | TRP | 2.7 |
| 63 | DD | 130 | GLY | 2.7 |
| 30 | BW | 11 | ASN | 2.7 |
| 56 | L | 164 | TYR | 2.7 |
| 69 | Y | 68 | ARG | 2.7 |
| 7 | AZ | 77 | ALA | 2.7 |
| 14 | t | 187 | LYS | 2.7 |
| 27 | 9 | 126 | ALA | 2.7 |
| 39 | CF | 33 | ALA | 2.7 |
| 40 | CG | 34 | LYS | 2.7 |
| 41 | AN | 48 | LYS | 2.7 |
| 45 | i | 41 | ALA | 2.7 |
| 63 | DD | 12 | LYS | 2.7 |
| 79 | AR | 251 | ALA | 2.7 |
| 1 | 1 | 1758 | U | 2.7 |
| 15 | u | 35 | GLN | 2.7 |
| 46 | B | 1348 | U | 2.7 |
| 46 | CM | 1695 | U | 2.7 |
| 53 | CT | 157 | VAL | 2.7 |
| 54 | J | 178 | VAL | 2.7 |
| 56 | L | 153 | GLN | 2.7 |
| 62 | R | 37 | CYS | 2.7 |
| 50 | F | 176 | VAL | 2.7 |
| 59 | O | 75 | VAL | 2.7 |
| 80 | p0 | 9 | VAL | 2.7 |
| 6 | AY | 5 | PRO | 2.7 |
| 60 | DA | 85 | PRO | 2.7 |
| 10 | BC | 94 | LEU | 2.7 |
| 10 | BC | 163 | LEU | 2.7 |
| 23 | 5 | 108 | LEU | 2.7 |
| 23 | BP | 108 | LEU | 2.7 |
| 51 | G | 23 | LEU | 2.7 |
| 54 | J | 13 | LEU | 2.7 |
| 58 | N | 5 | LEU | 2.7 |
| 73 | DN | 67 | LEU | 2.7 |

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| Mol | Chain | Res | Type | RSRZ |
|---|---|---|---|---|
| 1 | 1 | 2474 | C | 2.7 |
| 1 | AS | 247 | C | 2.7 |
| 1 | AS | 1223 | C | 2.7 |
| 6 | AY | 75 | ILE | 2.7 |
| 36 | CC | 102 | GLU | 2.7 |
| 46 | CM | 695 | C | 2.7 |
| 47 | C | 98 | ILE | 2.7 |
| 48 | CO | 150 | ILE | 2.7 |
| 67 | W | 64 | ILE | 2.7 |
| 70 | Z | 57 | ILE | 2.7 |
| 78 | h | 133 | ILE | 2.7 |
| 79 | DT | 101 | THR | 2.7 |
| 78 | DS | 169 | GLY | 2.7 |
| 1 | 1 | 2447 | G | 2.7 |
| 5 | AX | 140 | ASP | 2.7 |
| 53 | CT | 166 | ASP | 2.7 |
| 55 | K | 11 | ARG | 2.7 |
| 19 | y | 159 | LYS | 2.7 |
| 29 | AB | 63 | LYS | 2.7 |
| 40 | CG | 12 | LYS | 2.7 |
| 44 | AQ | 28 | LYS | 2.7 |
| 45 | CL | 65 | LYS | 2.7 |
| 56 | L | 65 | LYS | 2.7 |
| 58 | CY | 141 | LYS | 2.7 |
| 73 | c | 8 | ASN | 2.7 |
| 6 | l | 129 | ALA | 2.7 |
| 6 | l | 211 | ALA | 2.7 |
| 50 | F | 135 | VAL | 2.7 |
| 51 | CR | 225 | VAL | 2.7 |
| 58 | CY | 16 | GLN | 2.7 |
| 82 | L1 | 162 | VAL | 2.7 |
| 5 | k | 96 | PRO | 2.7 |
| 9 | BB | 10 | LEU | 2.7 |
| 13 | BF | 74 | PRO | 2.7 |
| 39 | CF | 65 | LEU | 2.7 |
| 41 | CH | 27 | LEU | 2.7 |
| 52 | H | 175 | LEU | 2.7 |
| 54 | J | 150 | LEU | 2.7 |
| 55 | K | 190 | LEU | 2.7 |
| 57 | M | 89 | LEU | 2.7 |
| 59 | O | 45 | LEU | 2.7 |
| 59 | CZ | 104 | CYS | 2.7 |

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| Mol | Chain | Res | Type | RSRZ |
|---|---|---|---|---|
| 75 | e | 66 | LEU | 2.7 |
| 10 | p | 180 | ILE | 2.7 |
| 28 | BU | 25 | ILE | 2.7 |
| 36 | CC | 111 | PHE | 2.7 |
| 49 | CP | 120 | ILE | 2.7 |
| 50 | F | 198 | PHE | 2.7 |
| 51 | CR | 249 | ILE | 2.7 |
| 54 | CU | 132 | ILE | 2.7 |
| 61 | DB | 110 | ILE | 2.7 |
| 63 | S | 62 | ILE | 2.7 |
| 65 | U | 22 | ILE | 2.7 |
| 74 | DO | 32 | PHE | 2.7 |
| 80 | P0 | 73 | PHE | 2.7 |
| 6 | AY | 261 | SER | 2.7 |
| 18 | BK | 32 | THR | 2.7 |
| 19 | BL | 177 | GLY | 2.7 |
| 27 | 9 | 72 | SER | 2.7 |
| 46 | CM | 215 | A | 2.7 |
| 51 | CR | 26 | THR | 2.7 |
| 53 | CT | 233 | SER | 2.7 |
| 54 | CU | 164 | SER | 2.7 |
| 64 | DE | 30 | THR | 2.7 |
| 67 | W | 28 | THR | 2.7 |
| 82 | l1 | 211 | GLY | 2.7 |
| 14 | BG | 49 | ARG | 2.7 |
| 52 | H | 166 | ARG | 2.7 |
| 56 | CW | 54 | ARG | 2.7 |
| 67 | DH | 87 | LYS | 2.7 |
| 71 | DL | 102 | LYS | 2.7 |
| 46 | CM | 1362 | C | 2.7 |
| 65 | U | 23 | ASP | 2.7 |
| 65 | DF | 23 | ASP | 2.7 |
| 79 | DT | 161 | ASP | 2.7 |
| 12 | r | 11 | TYR | 2.7 |
| 47 | CN | 155 | TYR | 2.7 |
| 57 | M | 66 | TYR | 2.7 |
| 30 | AC | 63 | ALA | 2.7 |
| 43 | AP | 81 | ALA | 2.7 |
| 51 | G | 45 | VAL | 2.7 |
| 54 | J | 117 | VAL | 2.7 |
| 56 | L | 14 | VAL | 2.7 |
| 79 | DT | 277 | VAL | 2.7 |

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| Mol | Chain | Res | Type | RSRZ |
|---|---|---|---|---|
| 54 | J | 89 | LEU | 2.7 |
| 55 | CV | 96 | LEU | 2.7 |
| 57 | M | 76 | LEU | 2.7 |
| 67 | W | 92 | LEU | 2.7 |
| 67 | DH | 25 | LEU | 2.7 |
| 79 | AR | 249 | LEU | 2.7 |
| 7 | AZ | 4 | GLN | 2.7 |
| 14 | BG | 126 | PHE | 2.7 |
| 54 | CU | 57 | PHE | 2.7 |
| 56 | L | 140 | ILE | 2.7 |
| 60 | P | 11 | ILE | 2.7 |
| 64 | T | 69 | ILE | 2.7 |
| 69 | Y | 125 | ILE | 2.7 |
| 19 | y | 69 | ARG | 2.7 |
| 51 | CR | 221 | ARG | 2.7 |
| 78 | h | 171 | GLY | 2.7 |
| 6 | AY | 65 | SER | 2.7 |
| 7 | AZ | 58 | LYS | 2.7 |
| 45 | CL | 94 | THR | 2.7 |
| 41 | CH | 11 | SER | 2.7 |
| 61 | DB | 124 | LYS | 2.7 |
| 67 | DH | 60 | LYS | 2.7 |
| 46 | B | 617 | A | 2.7 |
| 11 | BD | 11 | ASP | 2.7 |
| 14 | BG | 98 | ASP | 2.7 |
| 21 | 0 | 91 | TYR | 2.7 |
| 29 | AB | 149 | ALA | 2.7 |
| 47 | C | 65 | ALA | 2.7 |
| 48 | CO | 230 | ALA | 2.7 |
| 52 | H | 195 | ALA | 2.7 |
| 53 | CT | 224 | ALA | 2.7 |
| 65 | U | 50 | ALA | 2.7 |
| 66 | V | 80 | TYR | 2.7 |
| 72 | b | 59 | TYR | 2.7 |
| 10 | BC | 153 | LEU | 2.7 |
| 20 | BM | 177 | LEU | 2.7 |
| 27 | 9 | 35 | LEU | 2.7 |
| 38 | AK | 70 | VAL | 2.7 |
| 48 | CO | 188 | LEU | 2.7 |
| 54 | CU | 86 | VAL | 2.7 |
| 56 | CW | 28 | LEU | 2.7 |
| 63 | DD | 116 | LEU | 2.7 |

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| Mol | Chain | Res | Type | RSRZ |
|---|---|---|---|---|
| 70 | Z | 74 | VAL | 2.7 |
| 73 | DN | 21 | VAL | 2.7 |
| 1 | 1 | 1011 | C | 2.7 |
| 1 | AS | 1224 | C | 2.7 |
| 1 | AS | 2474 | C | 2.7 |
| 7 | m | 275 | GLN | 2.7 |
| 14 | BG | 48 | PRO | 2.7 |
| 46 | B | 1340 | C | 2.7 |
| 25 | 7 | 63 | ILE | 2.7 |
| 16 | v | 59 | PHE | 2.7 |
| 63 | S | 59 | PHE | 2.7 |
| 67 | DH | 67 | ARG | 2.7 |
| 10 | BC | 236 | GLY | 2.7 |
| 17 | BJ | 188 | GLU | 2.7 |
| 41 | AN | 7 | LYS | 2.7 |
| 42 | AO | 8 | LYS | 2.7 |
| 42 | CI | 19 | LYS | 2.7 |
| 49 | E | 214 | GLY | 2.7 |
| 53 | I | 222 | GLU | 2.7 |
| 55 | CV | 89 | GLU | 2.7 |
| 56 | L | 84 | GLY | 2.7 |
| 56 | CW | 65 | LYS | 2.7 |
| 62 | R | 113 | GLY | 2.7 |
| 66 | DG | 110 | LYS | 2.7 |
| 67 | W | 87 | LYS | 2.7 |
| 76 | DQ | 54 | LYS | 2.7 |
| 80 | P0 | 81 | LYS | 2.7 |
| 6 | l | 201 | THR | 2.7 |
| 51 | G | 26 | THR | 2.7 |
| 54 | J | 115 | THR | 2.7 |
| 55 | K | 62 | THR | 2.7 |
| 77 | g | 48 | THR | 2.7 |
| 1 | AS | 2441 | G | 2.7 |
| 1 | AS | 2452 | G | 2.7 |
| 46 | B | 1135 | G | 2.7 |
| 7 | AZ | 10 | SER | 2.7 |
| 35 | AH | 66 | SER | 2.7 |
| 54 | J | 62 | SER | 2.7 |
| 19 | y | 103 | ALA | 2.7 |
| 47 | CN | 19 | ALA | 2.7 |
| 51 | CR | 213 | ALA | 2.7 |
| 56 | L | 135 | ALA | 2.7 |

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| Mol | Chain | Res | Type | RSRZ |
|---|---|---|---|---|
| 1 | AS | 1557 | U | 2.7 |
| 10 | BC | 158 | VAL | 2.7 |
| 14 | t | 9 | LEU | 2.7 |
| 50 | F | 182 | VAL | 2.7 |
| 52 | CS | 59 | VAL | 2.7 |
| 54 | CU | 66 | TYR | 2.7 |
| 59 | CZ | 30 | VAL | 2.7 |
| 61 | Q | 23 | VAL | 2.7 |
| 63 | S | 18 | VAL | 2.7 |
| 67 | DH | 111 | VAL | 2.7 |
| 68 | X | 32 | VAL | 2.7 |
| 71 | DL | 74 | LEU | 2.7 |
| 76 | f | 6 | VAL | 2.7 |
| 77 | DR | 40 | TYR | 2.7 |
| 79 | AR | 33 | LEU | 2.7 |
| 74 | DO | 49 | HIS | 2.7 |
| 24 | BQ | 98 | ASN | 2.7 |
| 7 | m | 231 | ILE | 2.6 |
| 25 | 7 | 79 | GLN | 2.6 |
| 56 | L | 15 | PRO | 2.6 |
| 66 | DG | 36 | ILE | 2.6 |
| 79 | DT | 74 | ILE | 2.6 |
| 80 | P0 | 63 | ILE | 2.6 |
| 47 | CN | 115 | PHE | 2.6 |
| 49 | E | 90 | ARG | 2.6 |
| 55 | CV | 25 | ARG | 2.6 |
| 63 | S | 44 | ARG | 2.6 |
| 63 | DD | 122 | ARG | 2.6 |
| 19 | y | 8 | LYS | 2.6 |
| 45 | CL | 100 | LYS | 2.6 |
| 47 | CN | 134 | LYS | 2.6 |
| 47 | CN | 165 | LYS | 2.6 |
| 53 | I | 193 | LYS | 2.6 |
| 53 | CT | 193 | LYS | 2.6 |
| 63 | DD | 25 | LYS | 2.6 |
| 77 | g | 23 | LYS | 2.6 |
| 45 | i | 59 | GLY | 2.6 |
| 46 | B | 1611 | C | 2.6 |
| 52 | CS | 147 | THR | 2.6 |
| 55 | CV | 107 | THR | 2.6 |
| 79 | DT | 41 | THR | 2.6 |
| 79 | DT | 291 | TRP | 2.6 |

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| Mol | Chain | Res | Type | RSRZ |
|---|---|---|---|---|
| 9 | o | 10 | LEU | 2.6 |
| 10 | BC | 132 | VAL | 2.6 |
| 25 | 7 | 99 | SER | 2.6 |
| 25 | 7 | 109 | LEU | 2.6 |
| 29 | BV | 127 | ALA | 2.6 |
| 31 | BX | 43 | LEU | 2.6 |
| 49 | E | 81 | VAL | 2.6 |
| 49 | CP | 218 | SER | 2.6 |
| 59 | O | 31 | VAL | 2.6 |
| 64 | DE | 90 | ALA | 2.6 |
| 67 | W | 37 | SER | 2.6 |
| 79 | DT | 6 | VAL | 2.6 |
| 12 | r | 218 | TYR | 2.6 |
| 62 | R | 123 | TYR | 2.6 |
| 1 | 1 | 1264 | G | 2.6 |
| 11 | BD | 61 | ASP | 2.6 |
| 37 | AJ | 51 | PRO | 2.6 |
| 41 | AN | 29 | PRO | 2.6 |
| 46 | B | 1185 | G | 2.6 |
| 66 | DG | 116 | ILE | 2.6 |
| 67 | DH | 90 | ILE | 2.6 |
| 1 | AS | 1758 | U | 2.6 |
| 7 | m | 160 | PHE | 2.6 |
| 11 | q | 174 | LYS | 2.6 |
| 12 | r | 102 | MET | 2.6 |
| 41 | AN | 36 | LYS | 2.6 |
| 70 | Z | 39 | LYS | 2.6 |
| 77 | g | 56 | MET | 2.6 |
| 77 | DR | 27 | PRO | 2.6 |
| 78 | h | 155 | ASN | 2.6 |
| 82 | L1 | 28 | PHE | 2.6 |
| 82 | l1 | 110 | PHE | 2.6 |
| 6 | AY | 82 | GLY | 2.6 |
| 7 | m | 201 | GLY | 2.6 |
| 19 | y | 183 | GLY | 2.6 |
| 51 | CR | 25 | GLY | 2.6 |
| 65 | DF | 144 | GLY | 2.6 |
| 69 | Y | 21 | GLY | 2.6 |
| 1 | AS | 2436 | A | 2.6 |
| 3 | AU | 111 | A | 2.6 |
| 46 | CM | 847 | A | 2.6 |
| 46 | CM | 1743 | A | 2.6 |

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| Mol | Chain | Res | Type | RSRZ |
|---|---|---|---|---|
| 47 | C | 108 | THR | 2.6 |
| 54 | CU | 129 | THR | 2.6 |
| 59 | CZ | 120 | CYS | 2.6 |
| 71 | DL | 70 | THR | 2.6 |
| 6 | AY | 112 | VAL | 2.6 |
| 7 | m | 100 | ALA | 2.6 |
| 11 | BD | 18 | VAL | 2.6 |
| 17 | w | 7 | VAL | 2.6 |
| 25 | 7 | 128 | ALA | 2.6 |
| 36 | AI | 21 | LEU | 2.6 |
| 51 | CR | 214 | LEU | 2.6 |
| 51 | CR | 239 | LEU | 2.6 |
| 54 | CU | 53 | ALA | 2.6 |
| 54 | CU | 158 | VAL | 2.6 |
| 56 | CW | 105 | LEU | 2.6 |
| 62 | R | 75 | VAL | 2.6 |
| 63 | S | 38 | VAL | 2.6 |
| 64 | T | 16 | LEU | 2.6 |
| 65 | DF | 17 | LEU | 2.6 |
| 77 | DR | 8 | LEU | 2.6 |
| 79 | DT | 201 | LEU | 2.6 |
| 80 | p0 | 77 | LEU | 2.6 |
| 1 | 1 | 1188 | C | 2.6 |
| 16 | v | 100 | SER | 2.6 |
| 52 | H | 71 | SER | 2.6 |
| 67 | DH | 27 | SER | 2.6 |
| 10 | BC | 147 | LYS | 2.6 |
| 10 | BC | 150 | LYS | 2.6 |
| 11 | q | 168 | ARG | 2.6 |
| 22 | BO | 98 | HIS | 2.6 |
| 51 | G | 103 | TYR | 2.6 |
| 60 | DA | 90 | TYR | 2.6 |
| 37 | CD | 60 | ILE | 2.6 |
| 51 | G | 169 | ILE | 2.6 |
| 55 | CV | 74 | ARG | 2.6 |
| 56 | L | 40 | ARG | 2.6 |
| 63 | S | 131 | ARG | 2.6 |
| 64 | DE | 116 | LYS | 2.6 |
| 12 | r | 199 | PHE | 2.6 |
| 45 | i | 87 | PRO | 2.6 |
| 58 | CY | 23 | PRO | 2.6 |
| 62 | R | 15 | PHE | 2.6 |

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| Mol | Chain | Res | Type | RSRZ |
|---|---|---|---|---|
| 71 | a | 60 | PHE | 2.6 |
| 22 | BO | 77 | ASN | 2.6 |
| 40 | CG | 17 | GLN | 2.6 |
| 56 | CW | 25 | ASP | 2.6 |
| 79 | DT | 70 | GLN | 2.6 |
| 79 | DT | 77 | ASP | 2.6 |
| 80 | p0 | 31 | ASP | 2.6 |
| 45 | i | 68 | ASN | 2.6 |
| 51 | CR | 244 | GLY | 2.6 |
| 1 | AS | 132 | U | 2.6 |
| 1 | AS | 772 | U | 2.6 |
| 16 | v | 104 | GLU | 2.6 |
| 36 | CC | 64 | GLU | 2.6 |
| 46 | CM | 1359 | U | 2.6 |
| 48 | CO | 90 | GLU | 2.6 |
| 22 | 2 | 11 | THR | 2.6 |
| 22 | BO | 31 | LEU | 2.6 |
| 24 | 6 | 15 | LEU | 2.6 |
| 25 | BR | 87 | LEU | 2.6 |
| 43 | CJ | 35 | LEU | 2.6 |
| 51 | G | 38 | LEU | 2.6 |
| 51 | G | 184 | THR | 2.6 |
| 63 | DD | 51 | LEU | 2.6 |
| 67 | DH | 33 | LEU | 2.6 |
| 74 | d | 8 | LEU | 2.6 |
| 23 | BP | 47 | VAL | 2.6 |
| 62 | R | 86 | VAL | 2.6 |
| 67 | DH | 94 | ALA | 2.6 |
| 80 | P0 | 104 | VAL | 2.6 |
| 4 | j | 147 | ARG | 2.6 |
| 6 | l | 18 | SER | 2.6 |
| 11 | q | 41 | ILE | 2.6 |
| 19 | BL | 168 | LYS | 2.6 |
| 41 | AN | 50 | LYS | 2.6 |
| 46 | CM | 1142 | A | 2.6 |
| 22 | 2 | 4 | SER | 2.6 |
| 26 | BS | 142 | ILE | 2.6 |
| 50 | F | 152 | LYS | 2.6 |
| 56 | L | 83 | ILE | 2.6 |
| 58 | N | 70 | ILE | 2.6 |
| 58 | N | 86 | ILE | 2.6 |
| 79 | AR | 59 | LYS | 2.6 |

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| Mol | Chain | Res | Type | RSRZ |
|---|---|---|---|---|
| 27 | 9 | 5 | SER | 2.6 |
| 63 | S | 95 | TYR | 2.6 |
| 81 | 12 | 109 | ILE | 2.6 |
| 50 | CQ | 178 | MET | 2.6 |
| 18 | BK | 59 | PRO | 2.6 |
| 56 | L | 144 | PRO | 2.6 |
| 46 | CM | 656 | C | 2.6 |
| 33 | AF | 40 | ASP | 2.6 |
| 51 | G | 259 | GLN | 2.6 |
| 56 | CW | 58 | ASP | 2.6 |
| 70 | Z | 75 | GLN | 2.6 |
| 79 | DT | 294 | ASP | 2.6 |
| 10 | BC | 237 | GLY | 2.6 |
| 54 | J | 141 | GLY | 2.6 |
| 69 | DJ | 92 | ASN | 2.6 |
| 7 | AZ | 113 | LEU | 2.6 |
| 27 | 9 | 127 | GLU | 2.6 |
| 39 | CF | 78 | LEU | 2.6 |
| 50 | F | 104 | GLU | 2.6 |
| 54 | J | 172 | LEU | 2.6 |
| 55 | K | 193 | GLU | 2.6 |
| 82 | l1 | 53 | LEU | 2.6 |
| 82 | l1 | 123 | LEU | 2.6 |
| 8 | n | 73 | VAL | 2.6 |
| 23 | BP | 64 | VAL | 2.6 |
| 27 | BT | 126 | ALA | 2.6 |
| 35 | AH | 75 | ALA | 2.6 |
| 63 | DD | 38 | VAL | 2.6 |
| 52 | H | 94 | THR | 2.6 |
| 54 | J | 90 | ALA | 2.6 |
| 65 | DF | 5 | VAL | 2.6 |
| 80 | P0 | 28 | VAL | 2.6 |
| 1 | 1 | 977 | U | 2.6 |
| 1 | 1 | 1817 | U | 2.6 |
| 1 | AS | 167 | U | 2.6 |
| 7 | AZ | 294 | LYS | 2.6 |
| 14 | BG | 129 | LYS | 2.6 |
| 20 | z | 136 | ARG | 2.6 |
| 26 | BS | 89 | LYS | 2.6 |
| 29 | BV | 69 | TRP | 2.6 |
| 46 | B | 490 | U | 2.6 |
| 48 | CO | 29 | TRP | 2.6 |

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| Mol | Chain | Res | Type | RSRZ |
|---|---|---|---|---|
| 66 | V | 53 | TRP | 2.6 |
| 8 | BA | 130 | ILE | 2.6 |
| 51 | CR | 195 | ILE | 2.6 |
| 59 | CZ | 89 | ILE | 2.6 |
| 60 | DA | 84 | ILE | 2.6 |
| 61 | Q | 76 | ILE | 2.6 |
| 26 | BS | 46 | TYR | 2.6 |
| 51 | CR | 205 | PHE | 2.6 |
| 56 | L | 8 | TYR | 2.6 |
| 67 | W | 83 | MET | 2.6 |
| 30 | AC | 7 | HIS | 2.6 |
| 30 | BW | 31 | SER | 2.6 |
| 46 | B | 1038 | G | 2.6 |
| 46 | CM | 724 | G | 2.6 |
| 50 | F | 157 | PHE | 2.6 |
| 37 | CD | 51 | PRO | 2.6 |
| 48 | CO | 35 | PRO | 2.6 |
| 53 | CT | 112 | SER | 2.6 |
| 55 | CV | 12 | SER | 2.6 |
| 56 | L | 9 | SER | 2.6 |
| 64 | DE | 123 | SER | 2.6 |
| 73 | c | 7 | SER | 2.6 |
| 78 | h | 166 | PRO | 2.6 |
| 82 | l1 | 213 | SER | 2.6 |
| 1 | AS | 1021 | A | 2.6 |
| 35 | AH | 61 | GLN | 2.6 |
| 46 | B | 1573 | A | 2.6 |
| 46 | CM | 1702 | A | 2.6 |
| 75 | DP | 27 | GLN | 2.6 |
| 22 | BO | 66 | ASN | 2.6 |
| 34 | CA | 84 | ASN | 2.6 |
| 51 | G | 88 | ASP | 2.6 |
| 61 | DB | 125 | GLY | 2.6 |
| 65 | U | 97 | ASP | 2.6 |
| 66 | V | 13 | ASP | 2.6 |
| 76 | DQ | 5 | ASN | 2.6 |
| 10 | p | 27 | LEU | 2.6 |
| 37 | CD | 76 | LEU | 2.6 |
| 48 | CO | 231 | LEU | 2.6 |
| 57 | M | 68 | LEU | 2.6 |
| 59 | CZ | 41 | LEU | 2.6 |
| 63 | S | 56 | LEU | 2.6 |

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| Mol | Chain | Res | Type | RSRZ |
|---|---|---|---|---|
| 63 | S | 88 | LEU | 2.6 |
| 70 | Z | 9 | LEU | 2.6 |
| 79 | DT | 92 | LEU | 2.6 |
| 1 | 1 | 240 | C | 2.6 |
| 1 | 1 | 1578 | C | 2.6 |
| 1 | AS | 1188 | C | 2.6 |
| 4 | AW | 24 | LYS | 2.6 |
| 6 | AY | 218 | LYS | 2.6 |
| 7 | AZ | 97 | ALA | 2.6 |
| 35 | CB | 42 | VAL | 2.6 |
| 35 | CB | 65 | VAL | 2.6 |
| 29 | BV | 34 | LYS | 2.6 |
| 39 | AL | 6 | LYS | 2.6 |
| 41 | CH | 50 | LYS | 2.6 |
| 54 | J | 32 | ALA | 2.6 |
| 57 | CX | 24 | LYS | 2.6 |
| 66 | DG | 41 | ALA | 2.6 |
| 78 | h | 191 | LYS | 2.6 |
| 13 | BF | 147 | THR | 2.6 |
| 79 | AR | 137 | THR | 2.6 |
| 26 | BS | 95 | ILE | 2.5 |
| 50 | F | 116 | ILE | 2.5 |
| 52 | CS | 137 | ILE | 2.5 |
| 54 | J | 132 | ILE | 2.5 |
| 55 | CV | 27 | PHE | 2.5 |
| 62 | R | 102 | PHE | 2.5 |
| 64 | T | 20 | PHE | 2.5 |
| 69 | DJ | 37 | PHE | 2.5 |
| 76 | DQ | 14 | PHE | 2.5 |
| 29 | BV | 48 | TYR | 2.5 |
| 46 | B | 1675 | U | 2.5 |
| 51 | G | 27 | TYR | 2.5 |
| 65 | U | 122 | HIS | 2.5 |
| 65 | DF | 42 | TYR | 2.5 |
| 6 | AY | 33 | PRO | 2.5 |
| 28 | BU | 39 | PRO | 2.5 |
| 58 | N | 23 | PRO | 2.5 |
| 66 | V | 2 | PRO | 2.5 |
| 66 | V | 118 | PRO | 2.5 |
| 79 | DT | 27 | PRO | 2.5 |
| 33 | BZ | 23 | SER | 2.5 |
| 62 | DC | 51 | SER | 2.5 |

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| Mol | Chain | Res | Type | RSRZ |
|---|---|---|---|---|
| 77 | DR | 7 | SER | 2.5 |
| 4 | AW | 81 | GLY | 2.5 |
| 18 | x | 34 | GLN | 2.5 |
| 29 | AB | 38 | GLN | 2.5 |
| 52 | H | 101 | GLY | 2.5 |
| 56 | L | 112 | GLN | 2.5 |
| 56 | L | 139 | GLN | 2.5 |
| 57 | M | 72 | GLY | 2.5 |
| 70 | DK | 111 | GLY | 2.5 |
| 79 | AR | 278 | GLY | 2.5 |
| 7 | m | 277 | LEU | 2.5 |
| 31 | BX | 16 | LEU | 2.5 |
| 43 | CJ | 104 | LEU | 2.5 |
| 72 | b | 75 | LEU | 2.5 |
| 82 | l1 | 165 | LEU | 2.5 |
| 1 | 1 | 2445 | G | 2.5 |
| 12 | BE | 101 | LYS | 2.5 |
| 19 | BL | 83 | VAL | 2.5 |
| 26 | BS | 64 | VAL | 2.5 |
| 27 | 9 | 29 | VAL | 2.5 |
| 28 | AA | 114 | VAL | 2.5 |
| 45 | CL | 82 | LYS | 2.5 |
| 46 | B | 1405 | G | 2.5 |
| 46 | B | 1472 | G | 2.5 |
| 46 | CM | 701 | G | 2.5 |
| 50 | F | 155 | ASP | 2.5 |
| 56 | L | 29 | LYS | 2.5 |
| 57 | M | 38 | ARG | 2.5 |
| 63 | S | 31 | ASN | 2.5 |
| 64 | DE | 67 | ARG | 2.5 |
| 66 | V | 92 | LYS | 2.5 |
| 70 | Z | 3 | LYS | 2.5 |
| 79 | DT | 17 | ASN | 2.5 |
| 80 | P0 | 51 | VAL | 2.5 |
| 5 | k | 179 | ALA | 2.5 |
| 24 | BQ | 54 | ALA | 2.5 |
| 46 | CM | 708 | A | 2.5 |
| 52 | H | 171 | ALA | 2.5 |
| 52 | H | 191 | ALA | 2.5 |
| 53 | I | 213 | ALA | 2.5 |
| 66 | DG | 59 | ALA | 2.5 |
| 73 | c | 6 | ALA | 2.5 |

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| Mol | Chain | Res | Type | RSRZ |
|---|---|---|---|---|
| 79 | DT | 169 | ALA | 2.5 |
| 12 | r | 191 | ILE | 2.5 |
| 29 | AB | 102 | ILE | 2.5 |
| 43 | CJ | 10 | THR | 2.5 |
| 50 | CQ | 5 | ILE | 2.5 |
| 79 | AR | 97 | THR | 2.5 |
| 82 | l1 | 198 | TRP | 2.5 |
| 7 | AZ | 208 | MET | 2.5 |
| 11 | q | 90 | MET | 2.5 |
| 51 | G | 87 | MET | 2.5 |
| 62 | R | 54 | MET | 2.5 |
| 1 | 1 | 1197 | C | 2.5 |
| 1 | AS | 2473 | C | 2.5 |
| 19 | y | 96 | PHE | 2.5 |
| 26 | BS | 60 | HIS | 2.5 |
| 56 | L | 67 | PRO | 2.5 |
| 1 | AS | 3316 | U | 2.5 |
| 16 | BI | 87 | GLN | 2.5 |
| 25 | BR | 89 | LEU | 2.5 |
| 30 | AC | 4 | SER | 2.5 |
| 33 | BZ | 125 | GLY | 2.5 |
| 36 | CC | 88 | LEU | 2.5 |
| 37 | CD | 26 | SER | 2.5 |
| 54 | CU | 30 | LEU | 2.5 |
| 56 | L | 76 | LEU | 2.5 |
| 60 | DA | 14 | SER | 2.5 |
| 46 | B | 493 | U | 2.5 |
| 64 | DE | 100 | LEU | 2.5 |
| 74 | d | 27 | GLN | 2.5 |
| 79 | AR | 42 | LEU | 2.5 |
| 18 | BK | 128 | ARG | 2.5 |
| 39 | AL | 36 | LYS | 2.5 |
| 53 | I | 223 | ARG | 2.5 |
| 56 | L | 51 | LYS | 2.5 |
| 60 | P | 109 | LYS | 2.5 |
| 67 | W | 20 | LYS | 2.5 |
| 70 | DK | 70 | LYS | 2.5 |
| 23 | BP | 19 | VAL | 2.5 |
| 60 | P | 34 | VAL | 2.5 |
| 82 | L1 | 201 | VAL | 2.5 |
| 8 | BA | 108 | GLU | 2.5 |
| 10 | BC | 123 | ALA | 2.5 |

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| Mol | Chain | Res | Type | RSRZ |
|---|---|---|---|---|
| 10 | BC | 197 | ALA | 2.5 |
| 13 | BF | 15 | GLU | 2.5 |
| 31 | BX | 11 | ASN | 2.5 |
| 45 | CL | 70 | ASN | 2.5 |
| 51 | G | 40 | GLU | 2.5 |
| 63 | S | 133 | ALA | 2.5 |
| 68 | X | 21 | ASN | 2.5 |
| 9 | BB | 125 | ILE | 2.5 |
| 53 | I | 175 | ILE | 2.5 |
| 54 | J | 121 | ILE | 2.5 |
| 60 | DA | 118 | ILE | 2.5 |
| 67 | W | 90 | ILE | 2.5 |
| 11 | q | 70 | THR | 2.5 |
| 12 | BE | 102 | MET | 2.5 |
| 38 | CE | 80 | THR | 2.5 |
| 48 | D | 25 | THR | 2.5 |
| 65 | DF | 84 | TRP | 2.5 |
| 82 | l1 | 127 | THR | 2.5 |
| 27 | 9 | 78 | PHE | 2.5 |
| 69 | DJ | 99 | PHE | 2.5 |
| 1 | 1 | 2439 | A | 2.5 |
| 46 | B | 1411 | A | 2.5 |
| 52 | H | 164 | PRO | 2.5 |
| 69 | Y | 77 | PRO | 2.5 |
| 78 | h | 127 | TYR | 2.5 |
| 79 | DT | 55 | TYR | 2.5 |
| 80 | P0 | 78 | PRO | 2.5 |
| 19 | BL | 124 | LEU | 2.5 |
| 27 | 9 | 68 | GLY | 2.5 |
| 31 | BX | 21 | LYS | 2.5 |
| 39 | AL | 42 | LYS | 2.5 |
| 40 | AM | 46 | ARG | 2.5 |
| 51 | CR | 4 | GLY | 2.5 |
| 51 | CR | 7 | LYS | 2.5 |
| 54 | CU | 147 | LYS | 2.5 |
| 64 | T | 34 | LEU | 2.5 |
| 64 | DE | 34 | LEU | 2.5 |
| 65 | U | 45 | LEU | 2.5 |
| 65 | DF | 68 | ARG | 2.5 |
| 65 | DF | 86 | LEU | 2.5 |
| 67 | W | 63 | LYS | 2.5 |
| 69 | Y | 19 | LYS | 2.5 |

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| Mol | Chain | Res | Type | RSRZ |
|---|---|---|---|---|
| 69 | DJ | 94 | LEU | 2.5 |
| 77 | DR | 49 | LEU | 2.5 |
| 50 | F | 181 | GLY | 2.5 |
| 63 | S | 10 | GLY | 2.5 |
| 82 | L1 | 3 | LYS | 2.5 |
| 34 | AG | 19 | SER | 2.5 |
| 38 | CE | 30 | GLN | 2.5 |
| 49 | CP | 176 | SER | 2.5 |
| 54 | CU | 176 | GLN | 2.5 |
| 79 | AR | 115 | SER | 2.5 |
| 6 | l | 146 | VAL | 2.5 |
| 10 | p | 140 | VAL | 2.5 |
| 21 | BN | 103 | VAL | 2.5 |
| 35 | AH | 23 | VAL | 2.5 |
| 51 | CR | 139 | VAL | 2.5 |
| 52 | CS | 70 | VAL | 2.5 |
| 71 | DL | 100 | VAL | 2.5 |
| 79 | DT | 105 | VAL | 2.5 |
| 10 | p | 197 | ALA | 2.5 |
| 37 | CD | 7 | ALA | 2.5 |
| 66 | V | 17 | ALA | 2.5 |
| 71 | a | 130 | ALA | 2.5 |
| 1 | 1 | 3127 | U | 2.5 |
| 46 | B | 1400 | U | 2.5 |
| 56 | L | 41 | GLU | 2.5 |
| 14 | BG | 184 | ILE | 2.5 |
| 19 | BL | 101 | ILE | 2.5 |
| 22 | BO | 160 | ILE | 2.5 |
| 28 | BU | 46 | ILE | 2.5 |
| 47 | CN | 170 | ILE | 2.5 |
| 54 | J | 181 | ILE | 2.5 |
| 82 | L1 | 70 | ASP | 2.5 |
| 82 | l1 | 100 | ILE | 2.5 |
| 4 | AW | 63 | PHE | 2.5 |
| 59 | CZ | 34 | THR | 2.5 |
| 7 | AZ | 139 | PRO | 2.5 |
| 4 | j | 70 | LYS | 2.5 |
| 7 | AZ | 207 | TYR | 2.5 |
| 16 | BI | 119 | TYR | 2.5 |
| 52 | CS | 116 | HIS | 2.5 |
| 57 | M | 88 | PRO | 2.5 |
| 28 | BU | 133 | LYS | 2.5 |

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| Mol | Chain | Res | Type | RSRZ |
|---|---|---|---|---|
| 43 | AP | 40 | LYS | 2.5 |
| 49 | E | 56 | LEU | 2.5 |
| 53 | I | 131 | LYS | 2.5 |
| 53 | I | 133 | LEU | 2.5 |
| 56 | L | 39 | LYS | 2.5 |
| 56 | L | 49 | LEU | 2.5 |
| 58 | CY | 43 | LYS | 2.5 |
| 64 | T | 49 | LYS | 2.5 |
| 65 | U | 42 | TYR | 2.5 |
| 65 | U | 86 | LEU | 2.5 |
| 1 | AS | 2518 | A | 2.5 |
| 19 | y | 75 | GLY | 2.5 |
| 19 | y | 118 | GLY | 2.5 |
| 46 | B | 577 | A | 2.5 |
| 46 | B | 1574 | A | 2.5 |
| 75 | e | 24 | GLY | 2.5 |
| 6 | l | 167 | VAL | 2.5 |
| 6 | AY | 313 | VAL | 2.5 |
| 9 | BB | 154 | VAL | 2.5 |
| 48 | D | 20 | VAL | 2.5 |
| 60 | DA | 33 | VAL | 2.5 |
| 63 | DD | 21 | VAL | 2.5 |
| 68 | DI | 39 | VAL | 2.5 |
| 79 | AR | 124 | VAL | 2.5 |
| 20 | BM | 33 | ALA | 2.5 |
| 42 | CI | 24 | SER | 2.5 |
| 46 | B | 494 | G | 2.5 |
| 46 | B | 1546 | G | 2.5 |
| 49 | E | 218 | SER | 2.5 |
| 56 | CW | 145 | SER | 2.5 |
| 62 | R | 6 | ALA | 2.5 |
| 63 | DD | 75 | SER | 2.5 |
| 67 | W | 75 | SER | 2.5 |
| 70 | DK | 85 | ALA | 2.5 |
| 73 | DN | 47 | ALA | 2.5 |
| 79 | AR | 290 | ALA | 2.5 |
| 79 | AR | 293 | ALA | 2.5 |
| 79 | DT | 153 | SER | 2.5 |
| 80 | p0 | 68 | SER | 2.5 |
| 14 | BG | 85 | ILE | 2.5 |
| 28 | AA | 5 | ILE | 2.5 |
| 33 | BZ | 97 | ILE | 2.5 |

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| Mol | Chain | Res | Type | RSRZ |
|---|---|---|---|---|
| 49 | CP | 124 | ILE | 2.5 |
| 52 | CS | 120 | ILE | 2.5 |
| 56 | L | 45 | ILE | 2.5 |
| 60 | DA | 119 | GLU | 2.5 |
| 62 | DC | 121 | ILE | 2.5 |
| 67 | W | 102 | ILE | 2.5 |
| 46 | B | 135 | C | 2.5 |
| 68 | DI | 1 | MET | 2.5 |
| 74 | d | 33 | MET | 2.5 |
| 77 | g | 36 | MET | 2.5 |
| 7 | AZ | 180 | PHE | 2.5 |
| 16 | BI | 181 | ASN | 2.5 |
| 48 | D | 24 | PHE | 2.5 |
| 51 | CR | 226 | PHE | 2.5 |
| 59 | CZ | 111 | ASN | 2.5 |
| 70 | Z | 99 | ASN | 2.5 |
| 1 | 1 | 2067 | U | 2.5 |
| 1 | 1 | 3163 | U | 2.5 |
| 1 | AS | 977 | U | 2.5 |
| 1 | AS | 1091 | U | 2.5 |
| 46 | B | 1338 | U | 2.5 |
| 46 | CM | 1673 | U | 2.5 |
| 51 | G | 18 | TRP | 2.5 |
| 55 | CV | 48 | THR | 2.5 |
| 79 | DT | 131 | THR | 2.5 |
| 4 | AW | 190 | LYS | 2.5 |
| 8 | BA | 131 | LYS | 2.5 |
| 10 | p | 147 | LYS | 2.5 |
| 37 | CD | 66 | LYS | 2.5 |
| 42 | AO | 16 | LYS | 2.5 |
| 52 | H | 83 | ARG | 2.5 |
| 69 | DJ | 19 | LYS | 2.5 |
| 6 | l | 151 | LEU | 2.5 |
| 6 | l | 245 | LEU | 2.5 |
| 11 | BD | 10 | LEU | 2.5 |
| 54 | CU | 37 | LEU | 2.5 |
| 59 | O | 88 | LEU | 2.5 |
| 78 | DS | 158 | ARG | 2.5 |
| 19 | y | 163 | PRO | 2.5 |
| 62 | R | 73 | PRO | 2.5 |
| 65 | U | 76 | PRO | 2.5 |
| 67 | W | 109 | PRO | 2.5 |

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| Mol | Chain | Res | Type | RSRZ |
|---|---|---|---|---|
| 72 | b | 91 | PRO | 2.5 |
| 79 | DT | 180 | LEU | 2.5 |
| 7 | m | 68 | HIS | 2.5 |
| 20 | BM | 58 | HIS | 2.5 |
| 27 | 9 | 123 | GLY | 2.5 |
| 80 | p0 | 82 | GLY | 2.5 |
| 27 | BT | 8 | VAL | 2.5 |
| 36 | CC | 57 | VAL | 2.5 |
| 43 | AP | 68 | VAL | 2.5 |
| 52 | CS | 168 | VAL | 2.5 |
| 26 | 8 | 47 | GLN | 2.5 |
| 35 | CB | 33 | GLN | 2.5 |
| 50 | CQ | 102 | GLN | 2.5 |
| 55 | K | 20 | GLN | 2.5 |
| 66 | DG | 109 | GLN | 2.5 |
| 17 | w | 191 | ALA | 2.4 |
| 30 | BW | 16 | ALA | 2.4 |
| 37 | AJ | 82 | ALA | 2.4 |
| 14 | t | 46 | ILE | 2.4 |
| 48 | CO | 186 | SER | 2.4 |
| 49 | CP | 159 | SER | 2.4 |
| 50 | F | 67 | ILE | 2.4 |
| 50 | CQ | 87 | ILE | 2.4 |
| 50 | CQ | 116 | ILE | 2.4 |
| 56 | L | 42 | ILE | 2.4 |
| 66 | V | 135 | ILE | 2.4 |
| 71 | a | 56 | SER | 2.4 |
| 82 | l1 | 66 | CYS | 2.4 |
| 46 | CM | 1701 | A | 2.4 |
| 51 | CR | 215 | GLU | 2.4 |
| 69 | DJ | 49 | GLU | 2.4 |
| 80 | p0 | 69 | GLU | 2.4 |
| 7 | AZ | 55 | PHE | 2.4 |
| 8 | n | 46 | PHE | 2.4 |
| 8 | BA | 46 | PHE | 2.4 |
| 13 | s | 127 | PHE | 2.4 |
| 48 | CO | 100 | PHE | 2.4 |
| 51 | G | 86 | PHE | 2.4 |
| 62 | R | 33 | PHE | 2.4 |
| 63 | DD | 9 | PHE | 2.4 |
| 6 | AY | 189 | ARG | 2.4 |
| 7 | AZ | 147 | ASP | 2.4 |

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| Mol | Chain | Res | Type | RSRZ |
|---|---|---|---|---|
| 19 | y | 185 | LYS | 2.4 |
| 54 | CU | 67 | ARG | 2.4 |
| 54 | CU | 101 | LYS | 2.4 |
| 60 | DA | 138 | ASN | 2.4 |
| 64 | T | 31 | ASN | 2.4 |
| 74 | DO | 22 | LYS | 2.4 |
| 1 | 1 | 2428 | G | 2.4 |
| 16 | v | 10 | LEU | 2.4 |
| 21 | BN | 98 | THR | 2.4 |
| 35 | CB | 56 | THR | 2.4 |
| 38 | AK | 51 | LEU | 2.4 |
| 48 | D | 98 | THR | 2.4 |
| 46 | B | 374 | C | 2.4 |
| 46 | B | 1385 | C | 2.4 |
| 48 | D | 225 | LEU | 2.4 |
| 56 | CW | 128 | LEU | 2.4 |
| 59 | O | 52 | LEU | 2.4 |
| 59 | O | 62 | LEU | 2.4 |
| 64 | DE | 55 | THR | 2.4 |
| 66 | V | 108 | LEU | 2.4 |
| 75 | e | 9 | LEU | 2.4 |
| 79 | DT | 231 | LEU | 2.4 |
| 51 | G | 5 | PRO | 2.4 |
| 56 | L | 2 | PRO | 2.4 |
| 1 | AS | 248 | U | 2.4 |
| 46 | CM | 1348 | U | 2.4 |
| 56 | CW | 160 | HIS | 2.4 |
| 80 | P0 | 11 | TYR | 2.4 |
| 6 | AY | 226 | VAL | 2.4 |
| 7 | AZ | 127 | GLY | 2.4 |
| 7 | AZ | 173 | VAL | 2.4 |
| 19 | y | 82 | VAL | 2.4 |
| 49 | CP | 140 | GLY | 2.4 |
| 50 | CQ | 187 | VAL | 2.4 |
| 64 | DE | 114 | GLY | 2.4 |
| 77 | g | 45 | VAL | 2.4 |
| 80 | P0 | 59 | VAL | 2.4 |
| 82 | l1 | 13 | VAL | 2.4 |
| 20 | BM | 147 | ALA | 2.4 |
| 45 | CL | 63 | ALA | 2.4 |
| 50 | CQ | 100 | ALA | 2.4 |
| 52 | H | 78 | ALA | 2.4 |

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| Mol | Chain | Res | Type | RSRZ |
|---|---|---|---|---|
| 63 | S | 76 | GLN | 2.4 |
| 11 | q | 79 | ILE | 2.4 |
| 36 | AI | 118 | ILE | 2.4 |
| 50 | F | 50 | ILE | 2.4 |
| 60 | P | 38 | ILE | 2.4 |
| 67 | DH | 102 | ILE | 2.4 |
| 79 | AR | 142 | MET | 2.4 |
| 5 | AX | 74 | GLU | 2.4 |
| 6 | AY | 95 | CYS | 2.4 |
| 48 | CO | 67 | GLU | 2.4 |
| 49 | E | 80 | SER | 2.4 |
| 52 | H | 181 | GLU | 2.4 |
| 57 | M | 6 | GLU | 2.4 |
| 60 | DA | 147 | SER | 2.4 |
| 6 | AY | 157 | PHE | 2.4 |
| 10 | p | 150 | LYS | 2.4 |
| 29 | AB | 68 | PHE | 2.4 |
| 51 | CR | 218 | PHE | 2.4 |
| 19 | y | 178 | ARG | 2.4 |
| 30 | AC | 58 | ARG | 2.4 |
| 56 | CW | 3 | ARG | 2.4 |
| 60 | DA | 9 | LYS | 2.4 |
| 62 | R | 72 | ARG | 2.4 |
| 69 | DJ | 3 | ARG | 2.4 |
| 72 | DM | 94 | LYS | 2.4 |
| 73 | c | 15 | ARG | 2.4 |
| 82 | L1 | 15 | LYS | 2.4 |
| 36 | CC | 36 | LEU | 2.4 |
| 49 | E | 108 | LEU | 2.4 |
| 50 | F | 177 | LEU | 2.4 |
| 65 | U | 109 | LEU | 2.4 |
| 10 | BC | 138 | ASN | 2.4 |
| 1 | AS | 2466 | A | 2.4 |
| 1 | AS | 2519 | A | 2.4 |
| 11 | BD | 28 | THR | 2.4 |
| 29 | BV | 66 | ASN | 2.4 |
| 39 | AL | 57 | ASN | 2.4 |
| 46 | CM | 1329 | A | 2.4 |
| 51 | CR | 220 | THR | 2.4 |
| 69 | DJ | 95 | PRO | 2.4 |
| 11 | BD | 64 | HIS | 2.4 |
| 15 | u | 13 | VAL | 2.4 |

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| Mol | Chain | Res | Type | RSRZ |
|---|---|---|---|---|
| 16 | v | 2 | GLY | 2.4 |
| 19 | y | 11 | VAL | 2.4 |
| 21 | BN | 97 | VAL | 2.4 |
| 28 | AA | 20 | GLY | 2.4 |
| 30 | AC | 27 | TYR | 2.4 |
| 35 | AH | 22 | VAL | 2.4 |
| 47 | CN | 110 | TYR | 2.4 |
| 48 | CO | 101 | HIS | 2.4 |
| 50 | CQ | 17 | VAL | 2.4 |
| 50 | CQ | 176 | VAL | 2.4 |
| 51 | G | 89 | VAL | 2.4 |
| 55 | CV | 80 | GLY | 2.4 |
| 58 | CY | 7 | VAL | 2.4 |
| 3 | 4 | 21 | C | 2.4 |
| 1 | 1 | 1560 | U | 2.4 |
| 1 | 1 | 2441 | G | 2.4 |
| 1 | 1 | 2449 | U | 2.4 |
| 1 | AS | 2429 | G | 2.4 |
| 7 | AZ | 69 | ILE | 2.4 |
| 18 | BK | 58 | ILE | 2.4 |
| 20 | BM | 7 | GLN | 2.4 |
| 26 | 8 | 139 | ILE | 2.4 |
| 41 | CH | 31 | ALA | 2.4 |
| 50 | F | 148 | ALA | 2.4 |
| 51 | CR | 258 | ALA | 2.4 |
| 54 | J | 45 | ILE | 2.4 |
| 56 | L | 129 | ILE | 2.4 |
| 57 | M | 23 | ALA | 2.4 |
| 57 | M | 45 | ALA | 2.4 |
| 58 | N | 61 | ALA | 2.4 |
| 28 | AA | 132 | GLN | 2.4 |
| 40 | CG | 4 | GLN | 2.4 |
| 46 | CM | 1047 | U | 2.4 |
| 59 | CZ | 71 | ILE | 2.4 |
| 80 | P0 | 25 | ILE | 2.4 |
| 20 | z | 89 | MET | 2.4 |
| 18 | x | 167 | ARG | 2.4 |
| 26 | 8 | 45 | LYS | 2.4 |
| 30 | AC | 33 | LYS | 2.4 |
| 33 | AF | 119 | LYS | 2.4 |
| 38 | CE | 63 | ARG | 2.4 |
| 40 | AM | 21 | ARG | 2.4 |

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| Mol | Chain | Res | Type | RSRZ |
|---|---|---|---|---|
| 41 | CH | 52 | LYS | 2.4 |
| 51 | CR | 198 | ARG | 2.4 |
| 63 | DD | 127 | LYS | 2.4 |
| 20 | BM | 31 | GLU | 2.4 |
| 66 | DG | 122 | ARG | 2.4 |
| 79 | AR | 299 | PHE | 2.4 |
| 80 | p0 | 26 | PHE | 2.4 |
| 19 | y | 68 | SER | 2.4 |
| 28 | BU | 98 | SER | 2.4 |
| 54 | J | 41 | SER | 2.4 |
| 55 | CV | 182 | SER | 2.4 |
| 69 | Y | 30 | SER | 2.4 |
| 17 | BJ | 53 | LEU | 2.4 |
| 26 | BS | 57 | LEU | 2.4 |
| 36 | AI | 92 | LEU | 2.4 |
| 50 | F | 114 | LEU | 2.4 |
| 51 | G | 12 | LEU | 2.4 |
| 51 | CR | 9 | LEU | 2.4 |
| 55 | K | 171 | LEU | 2.4 |
| 62 | DC | 116 | LEU | 2.4 |
| 75 | e | 55 | CYS | 2.4 |
| 80 | P0 | 52 | LEU | 2.4 |
| 13 | BF | 7 | ASN | 2.4 |
| 16 | BI | 101 | THR | 2.4 |
| 21 | 0 | 34 | THR | 2.4 |
| 23 | 5 | 22 | PRO | 2.4 |
| 30 | AC | 19 | ASN | 2.4 |
| 45 | CL | 68 | ASN | 2.4 |
| 64 | DE | 22 | PRO | 2.4 |
| 66 | DG | 52 | THR | 2.4 |
| 78 | h | 167 | THR | 2.4 |
| 79 | AR | 280 | THR | 2.4 |
| 11 | q | 27 | VAL | 2.4 |
| 28 | BU | 23 | VAL | 2.4 |
| 54 | J | 58 | VAL | 2.4 |
| 58 | N | 117 | VAL | 2.4 |
| 59 | O | 93 | ASP | 2.4 |
| 75 | e | 44 | VAL | 2.4 |
| 16 | BI | 148 | TYR | 2.4 |
| 31 | BX | 60 | TYR | 2.4 |
| 50 | F | 19 | TYR | 2.4 |
| 52 | CS | 101 | GLY | 2.4 |

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| Mol | Chain | Res | Type | RSRZ |
|---|---|---|---|---|
| 59 | CZ | 117 | GLY | 2.4 |
| 63 | DD | 91 | TYR | 2.4 |
| 70 | Z | 80 | GLY | 2.4 |
| 82 | L1 | 37 | GLY | 2.4 |
| 10 | p | 116 | ALA | 2.4 |
| 11 | q | 53 | ILE | 2.4 |
| 12 | r | 33 | ILE | 2.4 |
| 15 | BH | 131 | ALA | 2.4 |
| 20 | BM | 115 | ILE | 2.4 |
| 24 | 6 | 76 | ALA | 2.4 |
| 26 | BS | 124 | ILE | 2.4 |
| 34 | AG | 49 | ILE | 2.4 |
| 47 | C | 145 | ALA | 2.4 |
| 49 | E | 117 | ALA | 2.4 |
| 50 | F | 172 | ALA | 2.4 |
| 46 | B | 1403 | A | 2.4 |
| 51 | G | 90 | ILE | 2.4 |
| 56 | L | 143 | ILE | 2.4 |
| 69 | Y | 108 | ALA | 2.4 |
| 69 | Y | 110 | ILE | 2.4 |
| 9 | BB | 17 | GLN | 2.4 |
| 17 | BJ | 178 | LYS | 2.4 |
| 25 | BR | 27 | LYS | 2.4 |
| 27 | BT | 6 | GLN | 2.4 |
| 28 | AA | 22 | LYS | 2.4 |
| 30 | AC | 23 | LYS | 2.4 |
| 36 | CC | 115 | LYS | 2.4 |
| 37 | CD | 28 | ARG | 2.4 |
| 37 | CD | 69 | LYS | 2.4 |
| 37 | CD | 98 | ARG | 2.4 |
| 42 | CI | 14 | LYS | 2.4 |
| 50 | F | 102 | GLN | 2.4 |
| 50 | F | 186 | LYS | 2.4 |
| 65 | DF | 80 | LYS | 2.4 |
| 66 | DG | 69 | LYS | 2.4 |
| 79 | AR | 60 | LYS | 2.4 |
| 79 | DT | 122 | GLN | 2.4 |
| 6 | l | 200 | PHE | 2.4 |
| 23 | BP | 15 | PHE | 2.4 |
| 47 | C | 81 | PHE | 2.4 |
| 1 | AS | 1816 | U | 2.4 |
| 1 | AS | 2467 | C | 2.4 |

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| Mol | Chain | Res | Type | RSRZ |
|---|---|---|---|---|
| 10 | BC | 66 | LEU | 2.4 |
| 13 | BF | 40 | LEU | 2.4 |
| 16 | BI | 179 | LEU | 2.4 |
| 46 | B | 130 | C | 2.4 |
| 46 | B | 707 | C | 2.4 |
| 46 | B | 1406 | C | 2.4 |
| 51 | G | 52 | LEU | 2.4 |
| 54 | CU | 73 | LEU | 2.4 |
| 79 | AR | 201 | LEU | 2.4 |
| 79 | DT | 145 | LEU | 2.4 |
| 82 | l1 | 29 | LEU | 2.4 |
| 34 | AG | 97 | SER | 2.4 |
| 56 | L | 50 | SER | 2.4 |
| 66 | V | 5 | SER | 2.4 |
| 76 | f | 28 | SER | 2.4 |
| 76 | DQ | 18 | SER | 2.4 |
| 1 | 1 | 2313 | G | 2.4 |
| 1 | AS | 169 | G | 2.4 |
| 46 | B | 1358 | G | 2.4 |
| 6 | l | 107 | TRP | 2.4 |
| 4 | AW | 113 | VAL | 2.4 |
| 6 | l | 231 | VAL | 2.4 |
| 10 | BC | 130 | PRO | 2.4 |
| 26 | BS | 110 | VAL | 2.4 |
| 31 | BX | 68 | PRO | 2.4 |
| 35 | CB | 23 | VAL | 2.4 |
| 43 | AP | 75 | VAL | 2.4 |
| 43 | CJ | 21 | THR | 2.4 |
| 47 | C | 121 | VAL | 2.4 |
| 57 | CX | 90 | THR | 2.4 |
| 58 | N | 3 | THR | 2.4 |
| 62 | R | 104 | THR | 2.4 |
| 63 | DD | 114 | THR | 2.4 |
| 64 | DE | 40 | VAL | 2.4 |
| 70 | DK | 127 | VAL | 2.4 |
| 73 | c | 31 | PRO | 2.4 |
| 78 | h | 129 | THR | 2.4 |
| 82 | L1 | 212 | PRO | 2.4 |
| 12 | r | 132 | GLY | 2.4 |
| 6 | l | 10 | ILE | 2.4 |
| 7 | m | 280 | ALA | 2.4 |
| 8 | BA | 132 | ALA | 2.4 |

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| Mol | Chain | Res | Type | RSRZ |
|---|---|---|---|---|
| 13 | s | 52 | TYR | 2.4 |
| 14 | BG | 127 | ASP | 2.4 |
| 15 | BH | 68 | GLY | 2.4 |
| 67 | W | 71 | ASN | 2.4 |
| 79 | AR | 53 | ASN | 2.4 |
| 82 | l1 | 171 | ASN | 2.4 |
| 79 | DT | 67 | HIS | 2.4 |
| 26 | 8 | 23 | ALA | 2.4 |
| 27 | BT | 99 | ILE | 2.4 |
| 28 | AA | 46 | ILE | 2.4 |
| 34 | AG | 36 | ALA | 2.4 |
| 34 | AG | 44 | TYR | 2.4 |
| 55 | K | 189 | ILE | 2.4 |
| 57 | M | 43 | ILE | 2.4 |
| 62 | DC | 74 | ALA | 2.4 |
| 73 | c | 41 | ILE | 2.4 |
| 79 | DT | 276 | ALA | 2.4 |
| 80 | p0 | 25 | ILE | 2.4 |
| 82 | l1 | 111 | ILE | 2.4 |
| 14 | BG | 190 | LYS | 2.4 |
| 28 | AA | 9 | LYS | 2.4 |
| 42 | AO | 14 | LYS | 2.4 |
| 45 | i | 50 | LYS | 2.4 |
| 45 | CL | 37 | LYS | 2.4 |
| 57 | CX | 44 | LYS | 2.4 |
| 60 | DA | 112 | LYS | 2.4 |
| 82 | l1 | 24 | LYS | 2.4 |
| 26 | BS | 27 | ARG | 2.4 |
| 51 | G | 59 | ARG | 2.4 |
| 62 | R | 83 | MET | 2.4 |
| 62 | R | 127 | ARG | 2.4 |
| 13 | BF | 90 | GLN | 2.4 |
| 64 | DE | 74 | GLN | 2.4 |
| 13 | s | 163 | PHE | 2.4 |
| 29 | BV | 129 | PHE | 2.4 |
| 48 | CO | 30 | PHE | 2.4 |
| 50 | CQ | 18 | PHE | 2.4 |
| 7 | AZ | 36 | LEU | 2.4 |
| 14 | t | 123 | LEU | 2.4 |
| 21 | 0 | 45 | LEU | 2.4 |
| 37 | AJ | 71 | LEU | 2.4 |
| 53 | I | 212 | LEU | 2.4 |

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| Mol | Chain | Res | Type | RSRZ |
|---|---|---|---|---|
| 78 | h | 188 | LEU | 2.4 |
| 80 | p0 | 18 | LEU | 2.4 |
| 1 | 1 | 1217 | A | 2.4 |
| 46 | B | 847 | A | 2.4 |
| 46 | CM | 1331 | A | 2.4 |
| 60 | DA | 24 | SER | 2.4 |
| 60 | DA | 61 | SER | 2.4 |
| 1 | 1 | 1012 | U | 2.4 |
| 1 | 1 | 2471 | U | 2.4 |
| 1 | AS | 2475 | U | 2.4 |
| 10 | p | 152 | VAL | 2.4 |
| 22 | 2 | 79 | VAL | 2.4 |
| 23 | BP | 22 | PRO | 2.4 |
| 28 | BU | 96 | VAL | 2.4 |
| 42 | AO | 20 | VAL | 2.4 |
| 46 | B | 1614 | U | 2.4 |
| 49 | E | 40 | VAL | 2.4 |
| 52 | H | 123 | VAL | 2.4 |
| 55 | K | 81 | VAL | 2.4 |
| 62 | R | 126 | VAL | 2.4 |
| 75 | e | 47 | PRO | 2.4 |
| 79 | AR | 291 | TRP | 2.4 |
| 79 | AR | 309 | VAL | 2.4 |
| 82 | l1 | 135 | PRO | 2.4 |
| 46 | B | 674 | C | 2.3 |
| 27 | 9 | 124 | GLY | 2.3 |
| 60 | DA | 2 | GLY | 2.3 |
| 6 | AY | 175 | ALA | 2.3 |
| 12 | r | 208 | ALA | 2.3 |
| 14 | t | 42 | LYS | 2.3 |
| 32 | BY | 26 | LYS | 2.3 |
| 38 | AK | 10 | LYS | 2.3 |
| 38 | CE | 13 | ASN | 2.3 |
| 16 | BI | 30 | TYR | 2.3 |
| 16 | BI | 188 | ARG | 2.3 |
| 44 | AQ | 24 | ARG | 2.3 |
| 45 | i | 62 | ALA | 2.3 |
| 45 | CL | 80 | ALA | 2.3 |
| 48 | CO | 193 | ILE | 2.3 |
| 54 | CU | 145 | ILE | 2.3 |
| 54 | CU | 169 | TYR | 2.3 |
| 55 | CV | 137 | ALA | 2.3 |

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| Mol | Chain | Res | Type | RSRZ |
|---|---|---|---|---|
| 59 | O | 27 | ALA | 2.3 |
| 62 | DC | 59 | LYS | 2.3 |
| 63 | DD | 86 | LYS | 2.3 |
| 65 | U | 58 | ALA | 2.3 |
| 66 | V | 100 | ILE | 2.3 |
| 70 | DK | 140 | LYS | 2.3 |
| 69 | Y | 46 | TYR | 2.3 |
| 72 | b | 41 | ILE | 2.3 |
| 73 | DN | 19 | LYS | 2.3 |
| 77 | g | 42 | ARG | 2.3 |
| 79 | AR | 57 | ILE | 2.3 |
| 80 | p0 | 32 | ASN | 2.3 |
| 59 | O | 39 | ASP | 2.3 |
| 79 | AR | 294 | ASP | 2.3 |
| 65 | U | 73 | MET | 2.3 |
| 11 | q | 45 | PHE | 2.3 |
| 16 | BI | 134 | LEU | 2.3 |
| 17 | w | 27 | GLN | 2.3 |
| 20 | BM | 150 | LEU | 2.3 |
| 43 | AP | 27 | GLN | 2.3 |
| 48 | D | 157 | GLN | 2.3 |
| 49 | CP | 164 | LEU | 2.3 |
| 50 | CQ | 198 | PHE | 2.3 |
| 52 | CS | 37 | GLN | 2.3 |
| 54 | CU | 81 | PHE | 2.3 |
| 61 | DB | 78 | LEU | 2.3 |
| 61 | DB | 97 | LEU | 2.3 |
| 63 | DD | 137 | PHE | 2.3 |
| 65 | U | 32 | LEU | 2.3 |
| 66 | V | 28 | LEU | 2.3 |
| 66 | V | 70 | GLN | 2.3 |
| 66 | DG | 88 | PHE | 2.3 |
| 74 | DO | 8 | LEU | 2.3 |
| 78 | h | 142 | LEU | 2.3 |
| 82 | l1 | 119 | GLN | 2.3 |
| 10 | p | 113 | GLU | 2.3 |
| 13 | BF | 8 | VAL | 2.3 |
| 50 | CQ | 75 | VAL | 2.3 |
| 51 | G | 139 | VAL | 2.3 |
| 51 | G | 225 | VAL | 2.3 |
| 63 | S | 117 | VAL | 2.3 |
| 64 | DE | 110 | VAL | 2.3 |

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| Mol | Chain | Res | Type | RSRZ |
|---|---|---|---|---|
| 82 | l1 | 58 | VAL | 2.3 |
| 6 | l | 318 | PRO | 2.3 |
| 45 | CL | 110 | SER | 2.3 |
| 51 | G | 152 | PRO | 2.3 |
| 52 | CS | 30 | PRO | 2.3 |
| 54 | J | 128 | PRO | 2.3 |
| 56 | CW | 5 | PRO | 2.3 |
| 56 | CW | 101 | PRO | 2.3 |
| 58 | N | 59 | PRO | 2.3 |
| 6 | AY | 105 | LYS | 2.3 |
| 7 | AZ | 87 | GLY | 2.3 |
| 31 | AD | 84 | GLY | 2.3 |
| 46 | B | 215 | A | 2.3 |
| 46 | CM | 134 | A | 2.3 |
| 46 | CM | 1357 | A | 2.3 |
| 60 | P | 13 | SER | 2.3 |
| 60 | DA | 13 | SER | 2.3 |
| 48 | D | 116 | LYS | 2.3 |
| 51 | G | 108 | LYS | 2.3 |
| 54 | J | 153 | LYS | 2.3 |
| 52 | H | 112 | ARG | 2.3 |
| 53 | I | 154 | ARG | 2.3 |
| 54 | J | 135 | ARG | 2.3 |
| 58 | N | 145 | GLY | 2.3 |
| 60 | P | 121 | ARG | 2.3 |
| 63 | S | 8 | THR | 2.3 |
| 63 | S | 86 | LYS | 2.3 |
| 63 | DD | 11 | LYS | 2.3 |
| 70 | Z | 82 | LYS | 2.3 |
| 6 | l | 249 | ILE | 2.3 |
| 14 | BG | 46 | ILE | 2.3 |
| 17 | w | 99 | ALA | 2.3 |
| 49 | CP | 78 | ILE | 2.3 |
| 50 | CQ | 209 | ILE | 2.3 |
| 66 | V | 36 | ILE | 2.3 |
| 66 | V | 123 | ARG | 2.3 |
| 67 | W | 117 | ILE | 2.3 |
| 69 | Y | 4 | THR | 2.3 |
| 74 | d | 80 | ARG | 2.3 |
| 78 | DS | 122 | ARG | 2.3 |
| 53 | I | 103 | ALA | 2.3 |
| 62 | R | 4 | ALA | 2.3 |

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| Mol | Chain | Res | Type | RSRZ |
|---|---|---|---|---|
| 66 | DG | 96 | ALA | 2.3 |
| 73 | DN | 63 | ALA | 2.3 |
| 79 | AR | 154 | ALA | 2.3 |
| 82 | L1 | 183 | ILE | 2.3 |
| 1 | 1 | 1816 | U | 2.3 |
| 6 | l | 46 | ASN | 2.3 |
| 11 | BD | 1 | MET | 2.3 |
| 14 | t | 12 | ASN | 2.3 |
| 17 | BJ | 51 | ASN | 2.3 |
| 46 | B | 259 | U | 2.3 |
| 46 | CM | 259 | U | 2.3 |
| 46 | CM | 1363 | U | 2.3 |
| 53 | CT | 236 | ASN | 2.3 |
| 57 | CX | 66 | TYR | 2.3 |
| 72 | b | 101 | TYR | 2.3 |
| 80 | p0 | 58 | MET | 2.3 |
| 1 | 1 | 2457 | C | 2.3 |
| 1 | 1 | 3051 | C | 2.3 |
| 46 | B | 1317 | C | 2.3 |
| 50 | F | 205 | ASP | 2.3 |
| 66 | V | 8 | ASP | 2.3 |
| 6 | l | 137 | LEU | 2.3 |
| 8 | n | 75 | LEU | 2.3 |
| 17 | w | 20 | LEU | 2.3 |
| 27 | BT | 30 | LEU | 2.3 |
| 35 | CB | 51 | LEU | 2.3 |
| 36 | CC | 92 | LEU | 2.3 |
| 44 | CK | 86 | LEU | 2.3 |
| 51 | CR | 92 | LEU | 2.3 |
| 52 | CS | 20 | LEU | 2.3 |
| 52 | CS | 175 | LEU | 2.3 |
| 53 | CT | 75 | LEU | 2.3 |
| 54 | J | 73 | LEU | 2.3 |
| 74 | DO | 47 | PHE | 2.3 |
| 76 | f | 36 | LEU | 2.3 |
| 79 | AR | 7 | LEU | 2.3 |
| 79 | AR | 262 | LEU | 2.3 |
| 13 | s | 161 | GLN | 2.3 |
| 35 | CB | 64 | GLN | 2.3 |
| 52 | H | 37 | GLN | 2.3 |
| 54 | CU | 105 | GLN | 2.3 |
| 63 | DD | 93 | GLN | 2.3 |

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| Mol | Chain | Res | Type | RSRZ |
|---|---|---|---|---|
| 16 | v | 103 | GLU | 2.3 |
| 22 | BO | 86 | GLU | 2.3 |
| 50 | F | 29 | GLU | 2.3 |
| 1 | 1 | 2458 | G | 2.3 |
| 1 | AS | 2445 | G | 2.3 |
| 7 | AZ | 52 | VAL | 2.3 |
| 9 | o | 75 | VAL | 2.3 |
| 16 | BI | 60 | VAL | 2.3 |
| 28 | AA | 23 | VAL | 2.3 |
| 46 | B | 1131 | G | 2.3 |
| 46 | B | 1575 | G | 2.3 |
| 50 | F | 59 | VAL | 2.3 |
| 51 | CR | 160 | VAL | 2.3 |
| 56 | L | 81 | VAL | 2.3 |
| 79 | AR | 134 | VAL | 2.3 |
| 10 | BC | 63 | LYS | 2.3 |
| 13 | s | 174 | LYS | 2.3 |
| 35 | CB | 19 | LYS | 2.3 |
| 39 | CF | 21 | LYS | 2.3 |
| 50 | F | 8 | LYS | 2.3 |
| 63 | S | 13 | LYS | 2.3 |
| 64 | T | 23 | LYS | 2.3 |
| 7 | m | 181 | PRO | 2.3 |
| 14 | BG | 21 | ARG | 2.3 |
| 14 | BG | 41 | ARG | 2.3 |
| 52 | CS | 88 | PRO | 2.3 |
| 62 | DC | 10 | ARG | 2.3 |
| 13 | s | 132 | GLY | 2.3 |
| 19 | y | 81 | ILE | 2.3 |
| 28 | BU | 129 | TRP | 2.3 |
| 33 | AF | 97 | ILE | 2.3 |
| 34 | AG | 32 | ILE | 2.3 |
| 49 | E | 109 | GLY | 2.3 |
| 51 | G | 245 | ILE | 2.3 |
| 51 | CR | 94 | ALA | 2.3 |
| 52 | CS | 78 | ALA | 2.3 |
| 53 | I | 224 | ALA | 2.3 |
| 56 | CW | 21 | SER | 2.3 |
| 60 | P | 2 | GLY | 2.3 |
| 60 | DA | 11 | ILE | 2.3 |
| 61 | Q | 33 | THR | 2.3 |
| 63 | DD | 100 | SER | 2.3 |

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| Mol | Chain | Res | Type | RSRZ |
|---|---|---|---|---|
| 70 | Z | 2 | GLY | 2.3 |
| 75 | DP | 59 | SER | 2.3 |
| 76 | f | 29 | GLY | 2.3 |
| 79 | AR | 36 | GLY | 2.3 |
| 5 | k | 51 | ALA | 2.3 |
| 10 | p | 169 | ALA | 2.3 |
| 11 | q | 56 | THR | 2.3 |
| 26 | BS | 37 | THR | 2.3 |
| 49 | E | 193 | THR | 2.3 |
| 79 | DT | 211 | ALA | 2.3 |
| 79 | DT | 300 | ALA | 2.3 |
| 80 | p0 | 35 | SER | 2.3 |
| 82 | l1 | 208 | SER | 2.3 |
| 5 | AX | 256 | HIS | 2.3 |
| 35 | AH | 69 | HIS | 2.3 |
| 79 | DT | 238 | HIS | 2.3 |
| 22 | BO | 101 | CYS | 2.3 |
| 6 | AY | 93 | ASN | 2.3 |
| 45 | i | 103 | LEU | 2.3 |
| 52 | H | 100 | ASN | 2.3 |
| 56 | CW | 76 | LEU | 2.3 |
| 61 | DB | 28 | LEU | 2.3 |
| 79 | AR | 219 | LEU | 2.3 |
| 10 | BC | 79 | PHE | 2.3 |
| 16 | BI | 59 | PHE | 2.3 |
| 46 | CM | 673 | A | 2.3 |
| 51 | G | 99 | PHE | 2.3 |
| 79 | DT | 275 | PHE | 2.3 |
| 42 | CI | 3 | ASP | 2.3 |
| 50 | F | 192 | ASP | 2.3 |
| 54 | J | 154 | ASP | 2.3 |
| 46 | B | 480 | U | 2.3 |
| 52 | CS | 86 | GLN | 2.3 |
| 50 | F | 48 | GLU | 2.3 |
| 1 | 1 | 2468 | C | 2.3 |
| 6 | l | 164 | LYS | 2.3 |
| 6 | AY | 320 | LYS | 2.3 |
| 16 | BI | 152 | VAL | 2.3 |
| 17 | w | 37 | VAL | 2.3 |
| 17 | BJ | 52 | LYS | 2.3 |
| 22 | 2 | 97 | LYS | 2.3 |
| 25 | BR | 97 | LYS | 2.3 |

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| Mol | Chain | Res | Type | RSRZ |
|---|---|---|---|---|
| 28 | AA | 96 | VAL | 2.3 |
| 29 | AB | 27 | LYS | 2.3 |
| 42 | AO | 7 | LYS | 2.3 |
| 48 | D | 176 | VAL | 2.3 |
| 52 | H | 90 | VAL | 2.3 |
| 52 | H | 115 | LYS | 2.3 |
| 56 | L | 10 | LYS | 2.3 |
| 67 | W | 55 | VAL | 2.3 |
| 80 | p0 | 33 | VAL | 2.3 |
| 36 | AI | 10 | ARG | 2.3 |
| 56 | L | 132 | ARG | 2.3 |
| 60 | DA | 20 | ARG | 2.3 |
| 31 | BX | 94 | ILE | 2.3 |
| 48 | D | 193 | ILE | 2.3 |
| 52 | H | 178 | GLY | 2.3 |
| 53 | CT | 226 | ILE | 2.3 |
| 54 | J | 98 | PRO | 2.3 |
| 67 | W | 23 | ILE | 2.3 |
| 70 | DK | 91 | GLY | 2.3 |
| 71 | DL | 7 | ILE | 2.3 |
| 82 | L1 | 211 | GLY | 2.3 |
| 82 | l1 | 117 | ILE | 2.3 |
| 7 | AZ | 166 | ALA | 2.3 |
| 16 | BI | 3 | ALA | 2.3 |
| 28 | AA | 110 | ALA | 2.3 |
| 39 | CF | 59 | ALA | 2.3 |
| 55 | K | 161 | ALA | 2.3 |
| 55 | CV | 128 | ALA | 2.3 |
| 56 | CW | 56 | ALA | 2.3 |
| 63 | DD | 17 | ALA | 2.3 |
| 14 | BG | 130 | THR | 2.3 |
| 18 | BK | 79 | THR | 2.3 |
| 21 | BN | 60 | SER | 2.3 |
| 43 | CJ | 7 | THR | 2.3 |
| 45 | CL | 36 | SER | 2.3 |
| 50 | CQ | 150 | SER | 2.3 |
| 60 | P | 12 | SER | 2.3 |
| 68 | DI | 56 | SER | 2.3 |
| 79 | DT | 137 | THR | 2.3 |
| 53 | I | 75 | LEU | 2.3 |
| 54 | J | 186 | HIS | 2.3 |
| 55 | K | 44 | HIS | 2.3 |

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| Mol | Chain | Res | Type | RSRZ |
|---|---|---|---|---|
| 73 | c | 80 | HIS | 2.3 |
| 73 | DN | 17 | HIS | 2.3 |
| 79 | DT | 168 | SER | 2.3 |
| 10 | p | 94 | LEU | 2.3 |
| 20 | BM | 155 | LEU | 2.3 |
| 26 | BS | 38 | LEU | 2.3 |
| 48 | CO | 225 | LEU | 2.3 |
| 49 | E | 164 | LEU | 2.3 |
| 49 | CP | 235 | LEU | 2.3 |
| 51 | G | 42 | LEU | 2.3 |
| 59 | CZ | 36 | LEU | 2.3 |
| 59 | CZ | 74 | LEU | 2.3 |
| 80 | p0 | 93 | LEU | 2.3 |
| 1 | AS | 1281 | G | 2.3 |
| 7 | AZ | 272 | TYR | 2.3 |
| 9 | o | 73 | TYR | 2.3 |
| 46 | B | 1115 | G | 2.3 |
| 46 | CM | 1546 | G | 2.3 |
| 46 | CM | 1672 | G | 2.3 |
| 47 | C | 110 | TYR | 2.3 |
| 14 | BG | 138 | PHE | 2.3 |
| 32 | BY | 55 | ASN | 2.3 |
| 79 | AR | 208 | CYS | 2.3 |
| 25 | BR | 41 | GLN | 2.3 |
| 54 | CU | 146 | GLN | 2.3 |
| 55 | CV | 103 | GLN | 2.3 |
| 59 | O | 58 | GLN | 2.3 |
| 16 | v | 169 | LYS | 2.3 |
| 27 | 9 | 87 | LYS | 2.3 |
| 51 | G | 200 | LYS | 2.3 |
| 56 | L | 16 | LYS | 2.3 |
| 56 | L | 92 | LYS | 2.3 |
| 64 | T | 14 | LYS | 2.3 |
| 69 | DJ | 119 | LYS | 2.3 |
| 1 | 1 | 1541 | A | 2.3 |
| 1 | 1 | 2446 | A | 2.3 |
| 1 | AS | 1274 | A | 2.3 |
| 19 | y | 180 | ARG | 2.3 |
| 27 | 9 | 8 | VAL | 2.3 |
| 35 | CB | 22 | VAL | 2.3 |
| 47 | C | 181 | VAL | 2.3 |
| 48 | CO | 125 | VAL | 2.3 |

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| Mol | Chain | Res | Type | RSRZ |
|---|---|---|---|---|
| 49 | E | 96 | VAL | 2.3 |
| 53 | I | 102 | VAL | 2.3 |
| 54 | J | 67 | ARG | 2.3 |
| 56 | L | 72 | GLU | 2.3 |
| 57 | M | 21 | VAL | 2.3 |
| 58 | CY | 129 | ARG | 2.3 |
| 63 | DD | 47 | VAL | 2.3 |
| 69 | DJ | 97 | ARG | 2.3 |
| 3 | AU | 23 | U | 2.3 |
| 46 | B | 778 | U | 2.3 |
| 4 | AW | 49 | ILE | 2.3 |
| 11 | q | 75 | ILE | 2.3 |
| 11 | BD | 136 | ILE | 2.3 |
| 16 | BI | 45 | PRO | 2.3 |
| 47 | C | 142 | PRO | 2.3 |
| 69 | DJ | 110 | ILE | 2.3 |
| 73 | DN | 31 | PRO | 2.3 |
| 79 | DT | 157 | ILE | 2.3 |
| 29 | BV | 106 | ALA | 2.3 |
| 30 | AC | 20 | GLY | 2.3 |
| 30 | AC | 34 | GLY | 2.3 |
| 39 | CF | 2 | ALA | 2.3 |
| 41 | AN | 8 | ALA | 2.3 |
| 50 | F | 105 | ALA | 2.3 |
| 51 | CR | 186 | GLY | 2.3 |
| 54 | CU | 65 | ALA | 2.3 |
| 60 | P | 4 | MET | 2.3 |
| 71 | a | 80 | ALA | 2.3 |
| 79 | DT | 209 | ALA | 2.3 |
| 80 | p0 | 4 | ALA | 2.3 |
| 1 | 1 | 2157 | C | 2.3 |
| 1 | 1 | 2470 | C | 2.3 |
| 25 | BR | 109 | LEU | 2.3 |
| 6 | l | 84 | HIS | 2.3 |
| 9 | BB | 20 | THR | 2.3 |
| 10 | p | 95 | LEU | 2.3 |
| 10 | p | 137 | LEU | 2.3 |
| 27 | 9 | 85 | LEU | 2.3 |
| 35 | CB | 25 | THR | 2.3 |
| 42 | AO | 13 | LEU | 2.3 |
| 43 | CJ | 70 | LEU | 2.3 |
| 48 | D | 143 | THR | 2.3 |

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| Mol | Chain | Res | Type | RSRZ |
|---|---|---|---|---|
| 48 | CO | 96 | LEU | 2.3 |
| 51 | G | 131 | LEU | 2.3 |
| 52 | CS | 94 | THR | 2.3 |
| 63 | S | 104 | LEU | 2.3 |
| 73 | c | 53 | LEU | 2.3 |
| 67 | W | 86 | HIS | 2.3 |
| 67 | DH | 28 | THR | 2.3 |
| 76 | f | 30 | LEU | 2.3 |
| 16 | BI | 37 | HIS | 2.3 |
| 78 | DS | 140 | HIS | 2.3 |
| 6 | l | 154 | SER | 2.3 |
| 7 | m | 129 | PHE | 2.3 |
| 7 | AZ | 142 | PHE | 2.3 |
| 12 | r | 159 | PHE | 2.3 |
| 12 | BE | 219 | SER | 2.3 |
| 13 | BF | 5 | SER | 2.3 |
| 24 | BQ | 95 | PHE | 2.3 |
| 29 | AB | 129 | PHE | 2.3 |
| 35 | CB | 40 | SER | 2.3 |
| 53 | I | 144 | PHE | 2.3 |
| 60 | P | 61 | SER | 2.3 |
| 41 | AN | 24 | TYR | 2.3 |
| 69 | Y | 99 | PHE | 2.3 |
| 12 | r | 156 | ARG | 2.3 |
| 16 | BI | 26 | ARG | 2.3 |
| 16 | BI | 57 | GLN | 2.3 |
| 29 | BV | 38 | GLN | 2.3 |
| 36 | CC | 103 | LYS | 2.3 |
| 39 | CF | 36 | LYS | 2.3 |
| 55 | K | 35 | ASN | 2.3 |
| 60 | DA | 76 | LYS | 2.3 |
| 63 | S | 11 | LYS | 2.3 |
| 66 | DG | 78 | LYS | 2.3 |
| 66 | DG | 85 | ASN | 2.3 |
| 17 | w | 79 | ARG | 2.3 |
| 20 | BM | 71 | ARG | 2.3 |
| 49 | E | 163 | ARG | 2.3 |
| 55 | K | 201 | ARG | 2.3 |
| 56 | L | 3 | ARG | 2.3 |
| 56 | L | 120 | ARG | 2.3 |
| 58 | CY | 33 | ARG | 2.3 |
| 73 | c | 89 | ARG | 2.3 |

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| Mol | Chain | Res | Type | RSRZ |
|---|---|---|---|---|
| 75 | DP | 65 | ARG | 2.3 |
| 13 | s | 171 | VAL | 2.3 |
| 22 | BO | 72 | VAL | 2.3 |
| 26 | 8 | 87 | ASP | 2.3 |
| 48 | CO | 31 | ASP | 2.3 |
| 59 | O | 116 | VAL | 2.3 |
| 62 | DC | 2 | VAL | 2.3 |
| 64 | T | 15 | VAL | 2.3 |
| 65 | U | 100 | VAL | 2.3 |
| 67 | DH | 113 | VAL | 2.3 |
| 79 | AR | 155 | VAL | 2.3 |
| 82 | l1 | 138 | VAL | 2.3 |
| 20 | BM | 152 | GLU | 2.2 |
| 37 | CD | 53 | GLU | 2.2 |
| 45 | i | 116 | GLU | 2.2 |
| 56 | L | 88 | GLU | 2.2 |
| 1 | 1 | 2870 | G | 2.2 |
| 1 | AS | 2459 | G | 2.2 |
| 46 | B | 650 | G | 2.2 |
| 46 | B | 1213 | G | 2.2 |
| 46 | CM | 1431 | G | 2.2 |
| 46 | CM | 1671 | G | 2.2 |
| 11 | BD | 128 | ILE | 2.2 |
| 23 | BP | 56 | ILE | 2.2 |
| 27 | 9 | 97 | ILE | 2.2 |
| 57 | M | 86 | ILE | 2.2 |
| 67 | DH | 49 | ILE | 2.2 |
| 16 | BI | 107 | GLY | 2.2 |
| 19 | y | 160 | GLY | 2.2 |
| 47 | C | 100 | GLY | 2.2 |
| 47 | CN | 189 | PRO | 2.2 |
| 20 | z | 63 | ALA | 2.2 |
| 20 | z | 87 | ALA | 2.2 |
| 26 | BS | 98 | ALA | 2.2 |
| 36 | AI | 120 | ALA | 2.2 |
| 58 | CY | 145 | GLY | 2.2 |
| 59 | O | 94 | ALA | 2.2 |
| 65 | DF | 73 | MET | 2.2 |
| 69 | DJ | 73 | GLY | 2.2 |
| 70 | DK | 106 | GLY | 2.2 |
| 82 | l1 | 69 | GLY | 2.2 |
| 1 | 1 | 2434 | A | 2.2 |

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| Mol | Chain | Res | Type | RSRZ |
|---|---|---|---|---|
| 1 | 1 | 2475 | U | 2.2 |
| 1 | AS | 1267 | A | 2.2 |
| 1 | AS | 2469 | A | 2.2 |
| 19 | y | 49 | LEU | 2.2 |
| 38 | AK | 67 | LEU | 2.2 |
| 46 | B | 318 | U | 2.2 |
| 46 | B | 609 | U | 2.2 |
| 50 | CQ | 12 | LEU | 2.2 |
| 51 | G | 222 | LEU | 2.2 |
| 51 | CR | 56 | LEU | 2.2 |
| 58 | N | 140 | LEU | 2.2 |
| 62 | DC | 80 | LEU | 2.2 |
| 63 | S | 115 | LEU | 2.2 |
| 72 | b | 42 | LEU | 2.2 |
| 74 | DO | 3 | LEU | 2.2 |
| 80 | P0 | 15 | LEU | 2.2 |
| 79 | AR | 19 | TRP | 2.2 |
| 79 | DT | 248 | TRP | 2.2 |
| 6 | AY | 248 | PHE | 2.2 |
| 21 | 0 | 30 | PHE | 2.2 |
| 29 | BV | 53 | PHE | 2.2 |
| 35 | AH | 34 | HIS | 2.2 |
| 41 | AN | 41 | HIS | 2.2 |
| 47 | CN | 40 | THR | 2.2 |
| 54 | J | 127 | PHE | 2.2 |
| 56 | CW | 130 | THR | 2.2 |
| 58 | N | 20 | PHE | 2.2 |
| 71 | a | 9 | THR | 2.2 |
| 74 | DO | 23 | THR | 2.2 |
| 4 | j | 190 | LYS | 2.2 |
| 6 | AY | 177 | LYS | 2.2 |
| 6 | AY | 210 | TYR | 2.2 |
| 9 | o | 173 | LYS | 2.2 |
| 13 | BF | 52 | TYR | 2.2 |
| 18 | BK | 25 | SER | 2.2 |
| 21 | 0 | 85 | SER | 2.2 |
| 21 | BN | 160 | LYS | 2.2 |
| 25 | 7 | 127 | LYS | 2.2 |
| 26 | BS | 36 | LYS | 2.2 |
| 30 | BW | 22 | LYS | 2.2 |
| 47 | CN | 138 | TYR | 2.2 |
| 48 | D | 227 | SER | 2.2 |

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| Mol | Chain | Res | Type | RSRZ |
|---|---|---|---|---|
| 51 | CR | 250 | SER | 2.2 |
| 52 | CS | 96 | SER | 2.2 |
| 53 | I | 169 | TYR | 2.2 |
| 59 | CZ | 90 | LYS | 2.2 |
| 60 | P | 18 | TYR | 2.2 |
| 60 | P | 64 | LYS | 2.2 |
| 73 | DN | 32 | LYS | 2.2 |
| 76 | f | 18 | SER | 2.2 |
| 78 | DS | 139 | LYS | 2.2 |
| 79 | AR | 258 | LYS | 2.2 |
| 34 | AG | 54 | ARG | 2.2 |
| 55 | CV | 8 | ARG | 2.2 |
| 71 | DL | 20 | ARG | 2.2 |
| 4 | AW | 7 | ASN | 2.2 |
| 5 | AX | 143 | GLN | 2.2 |
| 7 | AZ | 144 | VAL | 2.2 |
| 15 | BH | 119 | GLN | 2.2 |
| 16 | v | 155 | VAL | 2.2 |
| 18 | BK | 55 | GLN | 2.2 |
| 27 | BT | 45 | VAL | 2.2 |
| 27 | BT | 104 | VAL | 2.2 |
| 36 | AI | 62 | GLN | 2.2 |
| 52 | CS | 44 | ASN | 2.2 |
| 53 | CT | 162 | VAL | 2.2 |
| 54 | CU | 177 | VAL | 2.2 |
| 55 | K | 185 | CYS | 2.2 |
| 59 | CZ | 60 | CYS | 2.2 |
| 63 | DD | 77 | VAL | 2.2 |
| 64 | T | 122 | VAL | 2.2 |
| 70 | Z | 27 | GLN | 2.2 |
| 79 | DT | 8 | VAL | 2.2 |
| 67 | DH | 82 | GLU | 2.2 |
| 12 | r | 167 | ILE | 2.2 |
| 37 | AJ | 6 | ILE | 2.2 |
| 37 | CD | 57 | ILE | 2.2 |
| 50 | F | 139 | ILE | 2.2 |
| 52 | CS | 172 | ILE | 2.2 |
| 5 | k | 15 | GLY | 2.2 |
| 14 | BG | 50 | PRO | 2.2 |
| 8 | n | 41 | LEU | 2.2 |
| 14 | BG | 123 | LEU | 2.2 |
| 16 | v | 134 | LEU | 2.2 |

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| Mol | Chain | Res | Type | RSRZ |
|---|---|---|---|---|
| 19 | y | 156 | GLY | 2.2 |
| 26 | 8 | 52 | PRO | 2.2 |
| 29 | BV | 2 | PRO | 2.2 |
| 31 | AD | 27 | LEU | 2.2 |
| 36 | CC | 104 | ALA | 2.2 |
| 48 | CO | 110 | LEU | 2.2 |
| 50 | CQ | 99 | ALA | 2.2 |
| 56 | CW | 137 | GLY | 2.2 |
| 59 | O | 40 | GLY | 2.2 |
| 60 | DA | 41 | ALA | 2.2 |
| 62 | R | 60 | LEU | 2.2 |
| 63 | DD | 129 | GLY | 2.2 |
| 64 | DE | 73 | LEU | 2.2 |
| 70 | Z | 91 | GLY | 2.2 |
| 74 | d | 28 | PRO | 2.2 |
| 77 | DR | 56 | MET | 2.2 |
| 79 | AR | 284 | PRO | 2.2 |
| 82 | L1 | 163 | LEU | 2.2 |
| 67 | DH | 78 | TRP | 2.2 |
| 79 | DT | 93 | TRP | 2.2 |
| 10 | p | 139 | HIS | 2.2 |
| 14 | t | 68 | LYS | 2.2 |
| 32 | AE | 101 | LYS | 2.2 |
| 36 | AI | 14 | LYS | 2.2 |
| 45 | CL | 67 | LYS | 2.2 |
| 49 | E | 83 | LYS | 2.2 |
| 51 | G | 241 | LYS | 2.2 |
| 55 | CV | 65 | PHE | 2.2 |
| 57 | CX | 16 | PHE | 2.2 |
| 60 | DA | 26 | PHE | 2.2 |
| 58 | N | 63 | THR | 2.2 |
| 58 | CY | 30 | LYS | 2.2 |
| 63 | S | 25 | LYS | 2.2 |
| 63 | DD | 3 | THR | 2.2 |
| 63 | DD | 126 | LYS | 2.2 |
| 63 | DD | 139 | LYS | 2.2 |
| 64 | DE | 115 | PHE | 2.2 |
| 51 | G | 36 | HIS | 2.2 |
| 64 | DE | 35 | THR | 2.2 |
| 66 | V | 93 | HIS | 2.2 |
| 74 | d | 19 | HIS | 2.2 |
| 79 | DT | 89 | THR | 2.2 |

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| Mol | Chain | Res | Type | RSRZ |
|---|---|---|---|---|
| 82 | l1 | 21 | THR | 2.2 |
| 1 | AS | 1204 | U | 2.2 |
| 1 | AS | 2471 | U | 2.2 |
| 1 | AS | 3320 | U | 2.2 |
| 25 | BR | 47 | ARG | 2.2 |
| 26 | BS | 103 | TYR | 2.2 |
| 36 | CC | 81 | ARG | 2.2 |
| 42 | AO | 6 | ARG | 2.2 |
| 46 | B | 675 | U | 2.2 |
| 46 | CM | 944 | U | 2.2 |
| 51 | G | 11 | ARG | 2.2 |
| 62 | R | 44 | ARG | 2.2 |
| 62 | R | 47 | ARG | 2.2 |
| 64 | T | 11 | ARG | 2.2 |
| 65 | U | 68 | ARG | 2.2 |
| 67 | W | 84 | ARG | 2.2 |
| 76 | f | 40 | ARG | 2.2 |
| 35 | CB | 49 | SER | 2.2 |
| 50 | F | 140 | SER | 2.2 |
| 79 | DT | 202 | SER | 2.2 |
| 36 | CC | 66 | VAL | 2.2 |
| 37 | AJ | 86 | VAL | 2.2 |
| 51 | G | 46 | VAL | 2.2 |
| 52 | CS | 90 | VAL | 2.2 |
| 56 | CW | 141 | VAL | 2.2 |
| 66 | DG | 4 | VAL | 2.2 |
| 14 | BG | 102 | GLN | 2.2 |
| 36 | CC | 113 | GLN | 2.2 |
| 64 | DE | 42 | GLN | 2.2 |
| 78 | DS | 181 | GLN | 2.2 |
| 16 | BI | 86 | ASN | 2.2 |
| 82 | L1 | 27 | ASN | 2.2 |
| 7 | AZ | 227 | ILE | 2.2 |
| 10 | BC | 162 | GLU | 2.2 |
| 13 | BF | 114 | ILE | 2.2 |
| 47 | C | 170 | ILE | 2.2 |
| 51 | CR | 231 | GLU | 2.2 |
| 60 | DA | 38 | ILE | 2.2 |
| 61 | Q | 110 | ILE | 2.2 |
| 64 | DE | 69 | ILE | 2.2 |
| 65 | U | 60 | GLU | 2.2 |
| 68 | DI | 41 | GLU | 2.2 |

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| Mol | Chain | Res | Type | RSRZ |
|---|---|---|---|---|
| 69 | DJ | 125 | ILE | 2.2 |
| 72 | b | 39 | ILE | 2.2 |
| 80 | P0 | 74 | GLU | 2.2 |
| 82 | L1 | 155 | ILE | 2.2 |
| 82 | L1 | 216 | ILE | 2.2 |
| 82 | l1 | 206 | ILE | 2.2 |
| 1 | AS | 2454 | C | 2.2 |
| 13 | s | 126 | ASP | 2.2 |
| 6 | l | 172 | ALA | 2.2 |
| 6 | l | 302 | PRO | 2.2 |
| 8 | n | 66 | GLY | 2.2 |
| 27 | BT | 111 | LEU | 2.2 |
| 30 | AC | 16 | ALA | 2.2 |
| 31 | BX | 97 | ALA | 2.2 |
| 37 | AJ | 76 | LEU | 2.2 |
| 41 | AN | 4 | PRO | 2.2 |
| 49 | E | 76 | MET | 2.2 |
| 50 | F | 194 | ALA | 2.2 |
| 51 | G | 150 | PRO | 2.2 |
| 51 | G | 258 | ALA | 2.2 |
| 52 | CS | 179 | ALA | 2.2 |
| 54 | J | 63 | LEU | 2.2 |
| 56 | L | 28 | LEU | 2.2 |
| 56 | L | 125 | ALA | 2.2 |
| 57 | M | 19 | GLY | 2.2 |
| 65 | DF | 54 | LEU | 2.2 |
| 71 | DL | 18 | LEU | 2.2 |
| 74 | DO | 73 | LEU | 2.2 |
| 77 | DR | 36 | MET | 2.2 |
| 78 | DS | 143 | ALA | 2.2 |
| 79 | AR | 56 | GLY | 2.2 |
| 79 | AR | 92 | LEU | 2.2 |
| 79 | DT | 244 | PRO | 2.2 |
| 80 | P0 | 65 | GLY | 2.2 |
| 5 | k | 5 | LYS | 2.2 |
| 6 | AY | 47 | LYS | 2.2 |
| 8 | BA | 156 | LYS | 2.2 |
| 9 | BB | 15 | LYS | 2.2 |
| 10 | p | 71 | LYS | 2.2 |
| 10 | BC | 71 | LYS | 2.2 |
| 52 | CS | 80 | LYS | 2.2 |
| 62 | R | 35 | LYS | 2.2 |

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| Mol | Chain | Res | Type | RSRZ |
|---|---|---|---|---|
| 62 | DC | 8 | LYS | 2.2 |
| 62 | DC | 108 | LYS | 2.2 |
| 67 | W | 76 | LYS | 2.2 |
| 69 | Y | 43 | LYS | 2.2 |
| 16 | v | 130 | PHE | 2.2 |
| 22 | 2 | 19 | PHE | 2.2 |
| 59 | O | 133 | ARG | 2.2 |
| 60 | P | 139 | TRP | 2.2 |
| 79 | AR | 275 | PHE | 2.2 |
| 82 | l1 | 157 | PHE | 2.2 |
| 16 | BI | 50 | ARG | 2.2 |
| 16 | BI | 143 | ARG | 2.2 |
| 45 | i | 113 | ARG | 2.2 |
| 70 | DK | 16 | ARG | 2.2 |
| 73 | DN | 15 | ARG | 2.2 |
| 18 | x | 32 | THR | 2.2 |
| 38 | CE | 47 | HIS | 2.2 |
| 56 | L | 147 | THR | 2.2 |
| 64 | T | 30 | THR | 2.2 |
| 79 | AR | 29 | HIS | 2.2 |
| 82 | l1 | 136 | THR | 2.2 |
| 77 | g | 40 | TYR | 2.2 |
| 11 | q | 188 | VAL | 2.2 |
| 39 | AL | 31 | VAL | 2.2 |
| 53 | I | 195 | VAL | 2.2 |
| 54 | CU | 148 | VAL | 2.2 |
| 59 | O | 91 | VAL | 2.2 |
| 66 | DG | 6 | VAL | 2.2 |
| 69 | Y | 121 | VAL | 2.2 |
| 70 | DK | 130 | VAL | 2.2 |
| 71 | a | 27 | VAL | 2.2 |
| 73 | c | 86 | VAL | 2.2 |
| 75 | DP | 41 | VAL | 2.2 |
| 81 | 12 | 162 | VAL | 2.2 |
| 26 | BS | 29 | SER | 2.2 |
| 28 | BU | 35 | SER | 2.2 |
| 44 | CK | 59 | SER | 2.2 |
| 62 | R | 16 | SER | 2.2 |
| 18 | BK | 165 | GLN | 2.2 |
| 46 | B | 672 | U | 2.2 |
| 46 | B | 1102 | U | 2.2 |
| 56 | CW | 139 | GLN | 2.2 |

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| Mol | Chain | Res | Type | RSRZ |
|---|---|---|---|---|
| 66 | V | 109 | GLN | 2.2 |
| 82 | l1 | 158 | GLN | 2.2 |
| 22 | BO | 63 | ILE | 2.2 |
| 27 | BT | 4 | ILE | 2.2 |
| 27 | BT | 80 | ILE | 2.2 |
| 33 | AF | 109 | ILE | 2.2 |
| 49 | E | 110 | ILE | 2.2 |
| 51 | G | 64 | ILE | 2.2 |
| 72 | b | 71 | ILE | 2.2 |
| 1 | 1 | 2089 | G | 2.2 |
| 1 | 1 | 2429 | G | 2.2 |
| 4 | j | 215 | ASN | 2.2 |
| 19 | y | 91 | ASN | 2.2 |
| 24 | BQ | 9 | ASN | 2.2 |
| 7 | AZ | 195 | LEU | 2.2 |
| 8 | n | 58 | GLU | 2.2 |
| 24 | 6 | 17 | LEU | 2.2 |
| 31 | AD | 43 | LEU | 2.2 |
| 46 | B | 1479 | A | 2.2 |
| 46 | CM | 216 | A | 2.2 |
| 48 | D | 61 | LEU | 2.2 |
| 48 | CO | 191 | GLU | 2.2 |
| 50 | CQ | 97 | LEU | 2.2 |
| 51 | CR | 48 | LEU | 2.2 |
| 53 | I | 216 | LEU | 2.2 |
| 66 | DG | 140 | LEU | 2.2 |
| 69 | Y | 7 | LEU | 2.2 |
| 67 | W | 96 | ALA | 2.2 |
| 69 | Y | 41 | MET | 2.2 |
| 69 | Y | 93 | LEU | 2.2 |
| 18 | BK | 57 | ALA | 2.2 |
| 19 | y | 99 | ALA | 2.2 |
| 24 | 6 | 16 | ALA | 2.2 |
| 27 | 9 | 117 | ALA | 2.2 |
| 41 | CH | 4 | PRO | 2.2 |
| 45 | i | 63 | ALA | 2.2 |
| 47 | C | 91 | ALA | 2.2 |
| 51 | CR | 2 | ALA | 2.2 |
| 61 | Q | 89 | PRO | 2.2 |
| 63 | DD | 10 | GLY | 2.2 |
| 66 | DG | 19 | ALA | 2.2 |
| 66 | DG | 31 | PRO | 2.2 |

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| Mol | Chain | Res | Type | RSRZ |
|---|---|---|---|---|
| 68 | X | 14 | PRO | 2.2 |
| 73 | DN | 29 | CYS | 2.2 |
| 77 | DR | 32 | GLY | 2.2 |
| 7 | AZ | 262 | LYS | 2.2 |
| 13 | BF | 174 | LYS | 2.2 |
| 15 | BH | 117 | LYS | 2.2 |
| 19 | y | 161 | LYS | 2.2 |
| 29 | BV | 111 | LYS | 2.2 |
| 32 | BY | 30 | LYS | 2.2 |
| 41 | CH | 7 | LYS | 2.2 |
| 48 | CO | 108 | ASP | 2.2 |
| 53 | CT | 220 | LYS | 2.2 |
| 50 | F | 144 | ARG | 2.2 |
| 56 | L | 104 | PHE | 2.2 |
| 56 | CW | 71 | PHE | 2.2 |
| 57 | M | 75 | PHE | 2.2 |
| 1 | AS | 1352 | C | 2.2 |
| 16 | BI | 200 | TRP | 2.2 |
| 69 | DJ | 89 | TRP | 2.2 |
| 11 | q | 64 | HIS | 2.2 |
| 13 | s | 139 | THR | 2.2 |
| 35 | CB | 6 | THR | 2.2 |
| 37 | AJ | 90 | THR | 2.2 |
| 67 | W | 59 | THR | 2.2 |
| 10 | BC | 133 | VAL | 2.2 |
| 13 | s | 128 | TYR | 2.2 |
| 21 | 0 | 51 | VAL | 2.2 |
| 23 | BP | 23 | VAL | 2.2 |
| 26 | BS | 109 | TYR | 2.2 |
| 29 | BV | 125 | VAL | 2.2 |
| 50 | CQ | 153 | TYR | 2.2 |
| 58 | CY | 53 | TYR | 2.2 |
| 66 | V | 34 | VAL | 2.2 |
| 13 | s | 43 | GLN | 2.2 |
| 19 | BL | 27 | GLN | 2.2 |
| 31 | BX | 93 | SER | 2.2 |
| 37 | AJ | 93 | ILE | 2.2 |
| 38 | CE | 36 | SER | 2.2 |
| 50 | CQ | 139 | ILE | 2.2 |
| 51 | CR | 248 | SER | 2.2 |
| 52 | CS | 130 | ILE | 2.2 |
| 60 | P | 147 | SER | 2.2 |

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| Mol | Chain | Res | Type | RSRZ |
|---|---|---|---|---|
| 63 | DD | 107 | ILE | 2.2 |
| 79 | DT | 257 | ILE | 2.2 |
| 9 | o | 161 | LEU | 2.2 |
| 10 | BC | 110 | LEU | 2.2 |
| 13 | s | 40 | LEU | 2.2 |
| 34 | AG | 102 | LEU | 2.2 |
| 52 | H | 174 | LEU | 2.2 |
| 66 | DG | 114 | LEU | 2.2 |
| 80 | P0 | 76 | LEU | 2.2 |
| 82 | L1 | 190 | LEU | 2.2 |
| 11 | BD | 125 | GLU | 2.2 |
| 6 | l | 187 | LYS | 2.2 |
| 15 | BH | 23 | ASN | 2.2 |
| 22 | BO | 100 | ALA | 2.2 |
| 28 | AA | 49 | ALA | 2.2 |
| 36 | CC | 120 | ALA | 2.2 |
| 37 | CD | 8 | ALA | 2.2 |
| 45 | i | 61 | GLU | 2.2 |
| 53 | I | 122 | GLU | 2.2 |
| 54 | J | 55 | ALA | 2.2 |
| 55 | CV | 34 | ALA | 2.2 |
| 64 | DE | 51 | ALA | 2.2 |
| 64 | DE | 79 | GLU | 2.2 |
| 25 | 7 | 97 | LYS | 2.2 |
| 26 | BS | 96 | LYS | 2.2 |
| 48 | CO | 45 | LYS | 2.2 |
| 69 | Y | 70 | ASN | 2.2 |
| 69 | DJ | 10 | ALA | 2.2 |
| 70 | DK | 28 | ALA | 2.2 |
| 71 | a | 34 | ASN | 2.2 |
| 80 | P0 | 44 | ALA | 2.2 |
| 1 | 1 | 2832 | U | 2.2 |
| 1 | AS | 544 | U | 2.2 |
| 1 | AS | 1561 | U | 2.2 |
| 46 | B | 278 | U | 2.2 |
| 46 | B | 944 | U | 2.2 |
| 46 | B | 1364 | U | 2.2 |
| 46 | CM | 778 | U | 2.2 |
| 51 | CR | 240 | PRO | 2.2 |
| 53 | CT | 173 | PRO | 2.2 |
| 66 | DG | 46 | PRO | 2.2 |
| 79 | DT | 30 | PRO | 2.2 |

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| Mol | Chain | Res | Type | RSRZ |
|---|---|---|---|---|
| 81 | 12 | 140 | GLY | 2.2 |
| 4 | AW | 184 | ARG | 2.2 |
| 4 | AW | 247 | ARG | 2.2 |
| 12 | BE | 49 | CYS | 2.2 |
| 37 | CD | 55 | ARG | 2.2 |
| 41 | AN | 37 | ARG | 2.2 |
| 45 | i | 90 | ARG | 2.2 |
| 59 | CZ | 43 | ARG | 2.2 |
| 60 | P | 114 | ARG | 2.2 |
| 71 | a | 61 | ARG | 2.2 |
| 7 | AZ | 200 | PHE | 2.2 |
| 23 | 5 | 74 | PHE | 2.2 |
| 31 | BX | 99 | ASP | 2.2 |
| 43 | AP | 44 | ASP | 2.2 |
| 47 | C | 72 | ASP | 2.2 |
| 53 | I | 145 | PHE | 2.2 |
| 56 | L | 47 | PHE | 2.2 |
| 56 | CW | 63 | ASP | 2.2 |
| 58 | CY | 13 | PHE | 2.2 |
| 63 | DD | 63 | ASP | 2.2 |
| 66 | V | 35 | ASP | 2.2 |
| 79 | AR | 269 | ASP | 2.2 |
| 80 | P0 | 88 | PHE | 2.2 |
| 46 | B | 705 | G | 2.2 |
| 46 | B | 921 | G | 2.2 |
| 46 | B | 1099 | G | 2.2 |
| 46 | CM | 142 | G | 2.2 |
| 60 | P | 25 | TRP | 2.2 |
| 76 | DQ | 7 | TRP | 2.2 |
| 79 | DT | 178 | TRP | 2.2 |
| 7 | m | 244 | HIS | 2.2 |
| 13 | s | 68 | HIS | 2.2 |
| 53 | CT | 69 | HIS | 2.2 |
| 72 | b | 38 | HIS | 2.2 |
| 10 | BC | 204 | VAL | 2.1 |
| 11 | q | 57 | VAL | 2.1 |
| 22 | 2 | 93 | VAL | 2.1 |
| 51 | G | 194 | VAL | 2.1 |
| 53 | I | 148 | THR | 2.1 |
| 55 | CV | 46 | VAL | 2.1 |
| 55 | CV | 60 | VAL | 2.1 |
| 62 | R | 11 | THR | 2.1 |

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| Mol | Chain | Res | Type | RSRZ |
|---|---|---|---|---|
| 62 | DC | 94 | VAL | 2.1 |
| 67 | DH | 89 | VAL | 2.1 |
| 69 | DJ | 40 | VAL | 2.1 |
| 78 | h | 156 | VAL | 2.1 |
| 79 | DT | 309 | VAL | 2.1 |
| 7 | m | 240 | TYR | 2.1 |
| 35 | CB | 62 | TYR | 2.1 |
| 57 | M | 63 | TYR | 2.1 |
| 79 | DT | 247 | TYR | 2.1 |
| 1 | AS | 487 | C | 2.1 |
| 7 | AZ | 290 | ILE | 2.1 |
| 10 | BC | 161 | ILE | 2.1 |
| 11 | BD | 55 | ILE | 2.1 |
| 26 | 8 | 135 | ILE | 2.1 |
| 28 | BU | 5 | ILE | 2.1 |
| 46 | B | 1081 | C | 2.1 |
| 46 | B | 1141 | C | 2.1 |
| 47 | CN | 144 | ILE | 2.1 |
| 50 | F | 5 | ILE | 2.1 |
| 50 | F | 87 | ILE | 2.1 |
| 52 | CS | 121 | ILE | 2.1 |
| 59 | CZ | 72 | ILE | 2.1 |
| 6 | l | 195 | LEU | 2.1 |
| 6 | l | 234 | LEU | 2.1 |
| 10 | p | 151 | LEU | 2.1 |
| 12 | r | 113 | GLN | 2.1 |
| 19 | y | 93 | LEU | 2.1 |
| 20 | z | 94 | LEU | 2.1 |
| 26 | BS | 108 | LEU | 2.1 |
| 49 | CP | 66 | LEU | 2.1 |
| 53 | CT | 184 | LEU | 2.1 |
| 68 | X | 79 | LEU | 2.1 |
| 68 | DI | 79 | LEU | 2.1 |
| 70 | DK | 93 | LEU | 2.1 |
| 74 | d | 73 | LEU | 2.1 |
| 74 | DO | 5 | GLN | 2.1 |
| 80 | P0 | 19 | LEU | 2.1 |
| 6 | l | 3 | SER | 2.1 |
| 6 | l | 54 | ALA | 2.1 |
| 6 | AY | 229 | ALA | 2.1 |
| 7 | m | 77 | ALA | 2.1 |
| 10 | p | 206 | SER | 2.1 |

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| Mol | Chain | Res | Type | RSRZ |
|---|---|---|---|---|
| 29 | BV | 63 | LYS | 2.1 |
| 36 | CC | 32 | LYS | 2.1 |
| 45 | CL | 71 | LYS | 2.1 |
| 50 | F | 133 | LYS | 2.1 |
| 52 | CS | 71 | SER | 2.1 |
| 54 | CU | 104 | LYS | 2.1 |
| 59 | O | 70 | SER | 2.1 |
| 62 | R | 9 | LYS | 2.1 |
| 64 | DE | 58 | MET | 2.1 |
| 67 | W | 29 | LYS | 2.1 |
| 14 | BG | 86 | ALA | 2.1 |
| 21 | BN | 82 | GLU | 2.1 |
| 25 | 7 | 126 | GLU | 2.1 |
| 48 | D | 163 | GLU | 2.1 |
| 50 | F | 53 | ALA | 2.1 |
| 51 | G | 215 | GLU | 2.1 |
| 53 | CT | 138 | ALA | 2.1 |
| 53 | CT | 172 | ALA | 2.1 |
| 55 | K | 34 | ALA | 2.1 |
| 70 | Z | 128 | SER | 2.1 |
| 71 | DL | 104 | SER | 2.1 |
| 79 | AR | 113 | SER | 2.1 |
| 11 | q | 30 | PRO | 2.1 |
| 25 | BR | 57 | ARG | 2.1 |
| 31 | BX | 39 | GLY | 2.1 |
| 34 | AG | 79 | GLY | 2.1 |
| 37 | AJ | 75 | ARG | 2.1 |
| 53 | I | 142 | ARG | 2.1 |
| 53 | CT | 123 | GLY | 2.1 |
| 63 | S | 121 | ARG | 2.1 |
| 63 | DD | 49 | GLU | 2.1 |
| 63 | DD | 81 | ARG | 2.1 |
| 66 | V | 63 | ARG | 2.1 |
| 66 | DG | 2 | PRO | 2.1 |
| 71 | a | 16 | PRO | 2.1 |
| 75 | DP | 18 | ARG | 2.1 |
| 79 | DT | 159 | PRO | 2.1 |
| 80 | P0 | 83 | ASN | 2.1 |
| 22 | BO | 19 | PHE | 2.1 |
| 62 | DC | 45 | PHE | 2.1 |
| 78 | DS | 173 | PHE | 2.1 |
| 1 | 1 | 2847 | U | 2.1 |

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| Mol | Chain | Res | Type | RSRZ |
|---|---|---|---|---|
| 1 | 1 | 3284 | U | 2.1 |
| 3 | AU | 157 | U | 2.1 |
| 8 | n | 169 | ASP | 2.1 |
| 25 | BR | 100 | ASP | 2.1 |
| 41 | CH | 34 | CYS | 2.1 |
| 46 | CM | 1591 | U | 2.1 |
| 64 | T | 27 | ASP | 2.1 |
| 74 | d | 64 | CYS | 2.1 |
| 74 | DO | 64 | CYS | 2.1 |
| 7 | m | 173 | VAL | 2.1 |
| 29 | BV | 112 | VAL | 2.1 |
| 32 | BY | 95 | VAL | 2.1 |
| 47 | C | 123 | VAL | 2.1 |
| 47 | CN | 158 | VAL | 2.1 |
| 47 | CN | 174 | TRP | 2.1 |
| 20 | BM | 141 | HIS | 2.1 |
| 51 | G | 69 | HIS | 2.1 |
| 52 | CS | 133 | VAL | 2.1 |
| 53 | I | 179 | VAL | 2.1 |
| 55 | CV | 44 | HIS | 2.1 |
| 56 | L | 136 | VAL | 2.1 |
| 78 | DS | 187 | HIS | 2.1 |
| 4 | AW | 249 | THR | 2.1 |
| 14 | BG | 171 | THR | 2.1 |
| 47 | C | 147 | THR | 2.1 |
| 49 | CP | 91 | THR | 2.1 |
| 79 | AR | 26 | THR | 2.1 |
| 79 | DT | 48 | THR | 2.1 |
| 82 | l1 | 209 | THR | 2.1 |
| 10 | p | 227 | TYR | 2.1 |
| 15 | u | 32 | ILE | 2.1 |
| 39 | CF | 24 | ILE | 2.1 |
| 40 | CG | 27 | ILE | 2.1 |
| 48 | D | 32 | ILE | 2.1 |
| 55 | CV | 43 | ILE | 2.1 |
| 58 | CY | 86 | ILE | 2.1 |
| 62 | R | 115 | TYR | 2.1 |
| 73 | DN | 41 | ILE | 2.1 |
| 76 | f | 50 | ILE | 2.1 |
| 82 | l1 | 217 | TYR | 2.1 |
| 7 | m | 194 | LEU | 2.1 |
| 13 | s | 80 | LEU | 2.1 |

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| Mol | Chain | Res | Type | RSRZ |
|---|---|---|---|---|
| 24 | BQ | 64 | LYS | 2.1 |
| 43 | AP | 35 | LEU | 2.1 |
| 47 | C | 120 | LEU | 2.1 |
| 47 | C | 134 | LYS | 2.1 |
| 47 | CN | 87 | LEU | 2.1 |
| 48 | D | 27 | LYS | 2.1 |
| 53 | CT | 77 | LEU | 2.1 |
| 60 | P | 75 | LEU | 2.1 |
| 61 | Q | 97 | LEU | 2.1 |
| 62 | R | 108 | LYS | 2.1 |
| 65 | U | 49 | LYS | 2.1 |
| 70 | DK | 132 | LEU | 2.1 |
| 71 | a | 44 | LEU | 2.1 |
| 1 | 1 | 1556 | G | 2.1 |
| 14 | BG | 19 | GLN | 2.1 |
| 18 | x | 165 | GLN | 2.1 |
| 10 | BC | 257 | ALA | 2.1 |
| 14 | BG | 91 | ARG | 2.1 |
| 32 | BY | 18 | ARG | 2.1 |
| 46 | B | 1466 | G | 2.1 |
| 50 | F | 180 | GLN | 2.1 |
| 51 | CR | 260 | GLN | 2.1 |
| 57 | M | 1 | MET | 2.1 |
| 50 | F | 195 | ALA | 2.1 |
| 54 | J | 157 | ALA | 2.1 |
| 56 | L | 26 | ALA | 2.1 |
| 62 | DC | 61 | ARG | 2.1 |
| 71 | DL | 130 | ALA | 2.1 |
| 5 | AX | 125 | SER | 2.1 |
| 7 | m | 114 | GLY | 2.1 |
| 12 | r | 194 | GLY | 2.1 |
| 16 | v | 168 | GLY | 2.1 |
| 18 | BK | 75 | GLU | 2.1 |
| 22 | BO | 144 | GLU | 2.1 |
| 1 | AS | 2476 | C | 2.1 |
| 7 | AZ | 84 | PRO | 2.1 |
| 28 | BU | 16 | GLY | 2.1 |
| 48 | CO | 119 | SER | 2.1 |
| 51 | G | 74 | GLY | 2.1 |
| 46 | B | 25 | C | 2.1 |
| 46 | B | 1365 | C | 2.1 |
| 48 | D | 23 | PRO | 2.1 |

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| Mol | Chain | Res | Type | RSRZ |
|---|---|---|---|---|
| 52 | H | 105 | GLY | 2.1 |
| 53 | CT | 161 | GLU | 2.1 |
| 53 | CT | 225 | GLU | 2.1 |
| 54 | J | 185 | SER | 2.1 |
| 63 | S | 26 | GLY | 2.1 |
| 63 | DD | 2 | SER | 2.1 |
| 65 | DF | 7 | GLU | 2.1 |
| 79 | DT | 115 | SER | 2.1 |
| 82 | L1 | 20 | SER | 2.1 |
| 9 | o | 207 | ASN | 2.1 |
| 33 | BZ | 47 | PHE | 2.1 |
| 41 | CH | 43 | ASN | 2.1 |
| 43 | CJ | 36 | PHE | 2.1 |
| 47 | C | 115 | PHE | 2.1 |
| 56 | L | 71 | PHE | 2.1 |
| 63 | S | 9 | PHE | 2.1 |
| 66 | DG | 54 | PHE | 2.1 |
| 8 | BA | 8 | TRP | 2.1 |
| 14 | BG | 24 | VAL | 2.1 |
| 15 | u | 34 | ASP | 2.1 |
| 16 | v | 150 | TRP | 2.1 |
| 18 | x | 113 | VAL | 2.1 |
| 26 | BS | 105 | VAL | 2.1 |
| 30 | BW | 35 | VAL | 2.1 |
| 36 | CC | 79 | ASP | 2.1 |
| 49 | E | 70 | ASP | 2.1 |
| 51 | CR | 183 | VAL | 2.1 |
| 54 | CU | 151 | ASP | 2.1 |
| 59 | O | 60 | CYS | 2.1 |
| 62 | DC | 50 | ASP | 2.1 |
| 63 | S | 96 | VAL | 2.1 |
| 64 | T | 105 | ASP | 2.1 |
| 69 | DJ | 54 | ASP | 2.1 |
| 69 | DJ | 74 | VAL | 2.1 |
| 75 | DP | 48 | VAL | 2.1 |
| 79 | DT | 220 | TRP | 2.1 |
| 82 | l1 | 82 | VAL | 2.1 |
| 7 | m | 13 | HIS | 2.1 |
| 19 | y | 5 | HIS | 2.1 |
| 25 | BR | 78 | HIS | 2.1 |
| 53 | I | 22 | HIS | 2.1 |
| 4 | j | 22 | LEU | 2.1 |

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| Mol | Chain | Res | Type | RSRZ |
|---|---|---|---|---|
| 4 | j | 104 | LEU | 2.1 |
| 5 | k | 328 | ILE | 2.1 |
| 7 | m | 104 | LEU | 2.1 |
| 11 | q | 4 | ILE | 2.1 |
| 11 | q | 72 | LYS | 2.1 |
| 13 | s | 112 | LEU | 2.1 |
| 14 | BG | 125 | ILE | 2.1 |
| 16 | BI | 10 | LEU | 2.1 |
| 19 | y | 32 | LEU | 2.1 |
| 19 | y | 138 | LEU | 2.1 |
| 22 | 2 | 21 | LYS | 2.1 |
| 22 | 2 | 106 | LEU | 2.1 |
| 30 | AC | 25 | LYS | 2.1 |
| 31 | BX | 102 | ILE | 2.1 |
| 34 | AG | 86 | LYS | 2.1 |
| 36 | AI | 28 | LEU | 2.1 |
| 37 | CD | 52 | TYR | 2.1 |
| 46 | CM | 711 | U | 2.1 |
| 52 | H | 31 | LEU | 2.1 |
| 52 | H | 89 | ILE | 2.1 |
| 52 | H | 107 | LYS | 2.1 |
| 53 | I | 16 | ILE | 2.1 |
| 54 | J | 97 | LYS | 2.1 |
| 55 | K | 58 | LEU | 2.1 |
| 55 | K | 75 | LYS | 2.1 |
| 55 | K | 202 | LEU | 2.1 |
| 56 | L | 134 | ILE | 2.1 |
| 56 | L | 12 | TYR | 2.1 |
| 56 | L | 95 | TYR | 2.1 |
| 57 | M | 24 | LYS | 2.1 |
| 59 | O | 135 | ILE | 2.1 |
| 50 | F | 121 | TYR | 2.1 |
| 59 | CZ | 103 | LEU | 2.1 |
| 61 | Q | 28 | LEU | 2.1 |
| 63 | S | 126 | LYS | 2.1 |
| 70 | Z | 29 | TYR | 2.1 |
| 79 | DT | 47 | LEU | 2.1 |
| 70 | Z | 23 | ARG | 2.1 |
| 4 | j | 154 | ALA | 2.1 |
| 5 | AX | 138 | ALA | 2.1 |
| 6 | AY | 334 | ALA | 2.1 |
| 27 | BT | 120 | GLN | 2.1 |

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| Mol | Chain | Res | Type | RSRZ |
|---|---|---|---|---|
| 28 | BU | 19 | ALA | 2.1 |
| 36 | CC | 110 | ALA | 2.1 |
| 37 | CD | 2 | ALA | 2.1 |
| 63 | DD | 82 | GLN | 2.1 |
| 1 | 1 | 2668 | A | 2.1 |
| 1 | AS | 239 | A | 2.1 |
| 1 | AS | 1219 | A | 2.1 |
| 7 | AZ | 114 | GLY | 2.1 |
| 12 | BE | 132 | GLY | 2.1 |
| 17 | w | 90 | PRO | 2.1 |
| 49 | CP | 172 | GLY | 2.1 |
| 69 | Y | 123 | GLY | 2.1 |
| 69 | DJ | 67 | GLY | 2.1 |
| 69 | DJ | 127 | GLY | 2.1 |
| 7 | AZ | 269 | SER | 2.1 |
| 16 | BI | 16 | SER | 2.1 |
| 21 | BN | 143 | PHE | 2.1 |
| 23 | BP | 28 | PHE | 2.1 |
| 34 | AG | 85 | PHE | 2.1 |
| 37 | CD | 38 | PHE | 2.1 |
| 48 | CO | 112 | SER | 2.1 |
| 54 | CU | 111 | SER | 2.1 |
| 59 | CZ | 49 | SER | 2.1 |
| 63 | S | 137 | PHE | 2.1 |
| 79 | AR | 266 | SER | 2.1 |
| 12 | BE | 205 | ASN | 2.1 |
| 56 | L | 74 | ASN | 2.1 |
| 1 | 1 | 1503 | G | 2.1 |
| 1 | AS | 368 | G | 2.1 |
| 1 | AS | 1242 | G | 2.1 |
| 10 | BC | 131 | VAL | 2.1 |
| 17 | w | 127 | VAL | 2.1 |
| 46 | B | 495 | G | 2.1 |
| 46 | B | 1404 | G | 2.1 |
| 46 | CM | 723 | G | 2.1 |
| 47 | C | 139 | VAL | 2.1 |
| 48 | D | 91 | VAL | 2.1 |
| 51 | G | 140 | VAL | 2.1 |
| 58 | N | 7 | VAL | 2.1 |
| 64 | DE | 88 | VAL | 2.1 |
| 71 | a | 55 | VAL | 2.1 |
| 75 | e | 7 | VAL | 2.1 |

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| Mol | Chain | Res | Type | RSRZ |
|---|---|---|---|---|
| 78 | DS | 150 | VAL | 2.1 |
| 79 | DT | 166 | VAL | 2.1 |
| 1 | AS | 1234 | C | 2.1 |
| 46 | CM | 296 | C | 2.1 |
| 17 | w | 68 | LYS | 2.1 |
| 4 | AW | 180 | LEU | 2.1 |
| 8 | BA | 75 | LEU | 2.1 |
| 9 | o | 177 | LEU | 2.1 |
| 10 | p | 59 | LEU | 2.1 |
| 12 | r | 166 | ILE | 2.1 |
| 25 | 7 | 100 | ASP | 2.1 |
| 26 | BS | 49 | LYS | 2.1 |
| 28 | AA | 111 | LYS | 2.1 |
| 39 | CF | 6 | LYS | 2.1 |
| 36 | AI | 51 | ILE | 2.1 |
| 45 | i | 124 | ASP | 2.1 |
| 47 | C | 146 | LEU | 2.1 |
| 47 | C | 201 | LEU | 2.1 |
| 48 | CO | 197 | ILE | 2.1 |
| 50 | CQ | 192 | ASP | 2.1 |
| 51 | G | 10 | LYS | 2.1 |
| 66 | DG | 92 | LYS | 2.1 |
| 77 | g | 29 | LYS | 2.1 |
| 78 | DS | 132 | LYS | 2.1 |
| 26 | BS | 139 | ILE | 2.1 |
| 51 | G | 48 | LEU | 2.1 |
| 52 | H | 172 | ILE | 2.1 |
| 54 | CU | 150 | LEU | 2.1 |
| 55 | K | 38 | ILE | 2.1 |
| 59 | CZ | 28 | LEU | 2.1 |
| 60 | P | 92 | ILE | 2.1 |
| 60 | DA | 72 | LEU | 2.1 |
| 65 | DF | 35 | ILE | 2.1 |
| 70 | DK | 52 | ILE | 2.1 |
| 72 | DM | 80 | LEU | 2.1 |
| 76 | f | 38 | LEU | 2.1 |
| 79 | AR | 298 | LEU | 2.1 |
| 79 | DT | 249 | LEU | 2.1 |
| 80 | P0 | 48 | ASP | 2.1 |
| 81 | 12 | 112 | ILE | 2.1 |
| 82 | L1 | 206 | ILE | 2.1 |
| 82 | l1 | 179 | LEU | 2.1 |

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| Mol | Chain | Res | Type | RSRZ |
|---|---|---|---|---|
| 7 | AZ | 9 | THR | 2.1 |
| 10 | BC | 186 | ARG | 2.1 |
| 16 | BI | 144 | ARG | 2.1 |
| 18 | x | 135 | ARG | 2.1 |
| 19 | y | 113 | ARG | 2.1 |
| 19 | y | 176 | ARG | 2.1 |
| 41 | CH | 26 | ARG | 2.1 |
| 44 | CK | 24 | ARG | 2.1 |
| 66 | DG | 39 | THR | 2.1 |
| 67 | W | 98 | THR | 2.1 |
| 74 | d | 81 | ARG | 2.1 |
| 60 | DA | 40 | TYR | 2.1 |
| 68 | X | 53 | TYR | 2.1 |
| 76 | DQ | 55 | TYR | 2.1 |
| 79 | DT | 12 | THR | 2.1 |
| 6 | l | 190 | ALA | 2.1 |
| 6 | l | 219 | ALA | 2.1 |
| 52 | H | 182 | ALA | 2.1 |
| 1 | 1 | 1759 | U | 2.1 |
| 1 | AS | 2847 | U | 2.1 |
| 9 | BB | 108 | GLN | 2.1 |
| 46 | CM | 697 | U | 2.1 |
| 46 | CM | 1335 | U | 2.1 |
| 48 | CO | 208 | GLN | 2.1 |
| 51 | G | 68 | GLN | 2.1 |
| 72 | DM | 37 | GLN | 2.1 |
| 5 | AX | 253 | GLY | 2.1 |
| 35 | CB | 27 | GLY | 2.1 |
| 70 | Z | 35 | GLY | 2.1 |
| 13 | BF | 163 | PHE | 2.1 |
| 21 | 0 | 20 | PRO | 2.1 |
| 25 | BR | 8 | PHE | 2.1 |
| 33 | AF | 54 | PRO | 2.1 |
| 48 | CO | 122 | GLU | 2.1 |
| 56 | L | 158 | PHE | 2.1 |
| 56 | CW | 2 | PRO | 2.1 |
| 63 | DD | 108 | PHE | 2.1 |
| 81 | 12 | 163 | PRO | 2.1 |
| 11 | q | 182 | SER | 2.1 |
| 27 | BT | 10 | SER | 2.1 |
| 49 | CP | 80 | SER | 2.1 |
| 60 | P | 143 | SER | 2.1 |

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| Mol | Chain | Res | Type | RSRZ |
|---|---|---|---|---|
| 60 | DA | 7 | SER | 2.1 |
| 7 | AZ | 37 | VAL | 2.1 |
| 10 | p | 198 | VAL | 2.1 |
| 23 | 5 | 19 | VAL | 2.1 |
| 25 | 7 | 131 | VAL | 2.1 |
| 32 | BY | 48 | VAL | 2.1 |
| 50 | F | 92 | VAL | 2.1 |
| 51 | CR | 45 | VAL | 2.1 |
| 59 | O | 115 | VAL | 2.1 |
| 75 | DP | 28 | VAL | 2.1 |
| 1 | 1 | 2419 | A | 2.1 |
| 1 | AS | 1221 | A | 2.1 |
| 7 | AZ | 276 | LYS | 2.1 |
| 9 | BB | 156 | LYS | 2.1 |
| 10 | BC | 97 | LYS | 2.1 |
| 11 | BD | 157 | ASN | 2.1 |
| 30 | BW | 25 | LYS | 2.1 |
| 39 | CF | 30 | LYS | 2.1 |
| 43 | AP | 100 | LYS | 2.1 |
| 46 | CM | 1411 | A | 2.1 |
| 55 | K | 88 | ASN | 2.1 |
| 60 | DA | 43 | LYS | 2.1 |
| 71 | a | 83 | LYS | 2.1 |
| 79 | AR | 282 | LYS | 2.1 |
| 6 | AY | 199 | ARG | 2.1 |
| 16 | BI | 164 | LEU | 2.1 |
| 17 | BJ | 20 | LEU | 2.1 |
| 26 | 8 | 40 | LEU | 2.1 |
| 7 | m | 81 | HIS | 2.1 |
| 22 | 2 | 54 | HIS | 2.1 |
| 27 | 9 | 28 | ARG | 2.1 |
| 27 | 9 | 118 | LEU | 2.1 |
| 29 | AB | 22 | ILE | 2.1 |
| 29 | AB | 42 | ARG | 2.1 |
| 33 | AF | 87 | LEU | 2.1 |
| 35 | AH | 54 | ILE | 2.1 |
| 36 | CC | 60 | LEU | 2.1 |
| 43 | CJ | 18 | ARG | 2.1 |
| 51 | G | 154 | ILE | 2.1 |
| 51 | CR | 253 | ARG | 2.1 |
| 51 | CR | 256 | ARG | 2.1 |
| 56 | L | 99 | LEU | 2.1 |

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| Mol | Chain | Res | Type | RSRZ |
|---|---|---|---|---|
| 57 | M | 2 | LEU | 2.1 |
| 57 | M | 92 | LEU | 2.1 |
| 60 | DA | 45 | LEU | 2.1 |
| 63 | DD | 62 | ILE | 2.1 |
| 65 | U | 129 | TRP | 2.1 |
| 71 | a | 28 | LEU | 2.1 |
| 79 | AR | 289 | LEU | 2.1 |
| 79 | DT | 68 | ILE | 2.1 |
| 79 | DT | 271 | LEU | 2.1 |
| 80 | p0 | 19 | LEU | 2.1 |
| 45 | CL | 98 | ASP | 2.1 |
| 47 | C | 13 | ASP | 2.1 |
| 34 | AG | 8 | TYR | 2.1 |
| 49 | E | 201 | THR | 2.1 |
| 53 | I | 128 | THR | 2.1 |
| 58 | N | 97 | TYR | 2.1 |
| 59 | O | 67 | THR | 2.1 |
| 1 | AS | 486 | C | 2.1 |
| 2 | AT | 73 | C | 2.1 |
| 5 | AX | 374 | ALA | 2.1 |
| 28 | AA | 11 | ALA | 2.1 |
| 45 | i | 49 | ALA | 2.1 |
| 46 | B | 379 | C | 2.1 |
| 46 | B | 1610 | C | 2.1 |
| 46 | CM | 277 | G | 2.1 |
| 47 | C | 95 | ALA | 2.1 |
| 49 | E | 113 | ALA | 2.1 |
| 49 | E | 175 | ALA | 2.1 |
| 49 | CP | 123 | ALA | 2.1 |
| 77 | g | 61 | ALA | 2.1 |
| 10 | BC | 81 | GLN | 2.1 |
| 35 | CB | 45 | GLY | 2.1 |
| 36 | CC | 16 | GLN | 2.1 |
| 56 | CW | 153 | GLN | 2.1 |
| 63 | DD | 26 | GLY | 2.1 |
| 79 | AR | 122 | GLN | 2.1 |
| 4 | j | 66 | PRO | 2.1 |
| 6 | AY | 257 | GLU | 2.1 |
| 14 | BG | 139 | GLU | 2.1 |
| 30 | AC | 30 | PRO | 2.1 |
| 34 | AG | 94 | PHE | 2.1 |
| 35 | CB | 87 | GLU | 2.1 |

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| Mol | Chain | Res | Type | RSRZ |
|---|---|---|---|---|
| 43 | AP | 16 | GLU | 2.1 |
| 48 | D | 38 | PHE | 2.1 |
| 54 | J | 184 | GLU | 2.1 |
| 62 | DC | 7 | PRO | 2.1 |
| 62 | DC | 87 | PRO | 2.1 |
| 76 | f | 52 | PHE | 2.1 |
| 79 | AR | 14 | GLU | 2.1 |
| 82 | l1 | 214 | PHE | 2.1 |
| 1 | 1 | 1263 | U | 2.0 |
| 1 | 1 | 1815 | U | 2.0 |
| 4 | AW | 120 | VAL | 2.0 |
| 10 | p | 133 | VAL | 2.0 |
| 11 | BD | 126 | VAL | 2.0 |
| 14 | t | 88 | LYS | 2.0 |
| 16 | BI | 56 | LYS | 2.0 |
| 18 | x | 2 | VAL | 2.0 |
| 19 | y | 83 | VAL | 2.0 |
| 20 | BM | 85 | LYS | 2.0 |
| 25 | 7 | 120 | LYS | 2.0 |
| 45 | CL | 55 | LYS | 2.0 |
| 46 | B | 556 | U | 2.0 |
| 48 | D | 125 | VAL | 2.0 |
| 49 | E | 153 | VAL | 2.0 |
| 50 | CQ | 101 | VAL | 2.0 |
| 50 | CQ | 186 | LYS | 2.0 |
| 52 | H | 51 | VAL | 2.0 |
| 54 | J | 68 | LYS | 2.0 |
| 54 | J | 158 | VAL | 2.0 |
| 54 | CU | 80 | LYS | 2.0 |
| 56 | L | 96 | VAL | 2.0 |
| 57 | M | 56 | LYS | 2.0 |
| 60 | DA | 96 | VAL | 2.0 |
| 63 | S | 106 | LYS | 2.0 |
| 70 | Z | 125 | VAL | 2.0 |
| 71 | a | 127 | LYS | 2.0 |
| 71 | DL | 24 | VAL | 2.0 |
| 4 | j | 14 | SER | 2.0 |
| 6 | AY | 86 | SER | 2.0 |
| 16 | v | 118 | SER | 2.0 |
| 21 | 0 | 65 | SER | 2.0 |
| 49 | CP | 194 | SER | 2.0 |
| 70 | Z | 40 | SER | 2.0 |

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| Mol | Chain | Res | Type | RSRZ |
|---|---|---|---|---|
| 11 | q | 99 | ILE | 2.0 |
| 13 | s | 65 | ILE | 2.0 |
| 19 | BL | 49 | LEU | 2.0 |
| 23 | BP | 52 | ASN | 2.0 |
| 27 | BT | 31 | LEU | 2.0 |
| 30 | AC | 32 | LEU | 2.0 |
| 33 | AF | 83 | LEU | 2.0 |
| 39 | AL | 78 | LEU | 2.0 |
| 45 | CL | 64 | LEU | 2.0 |
| 45 | CL | 90 | ARG | 2.0 |
| 47 | C | 59 | LEU | 2.0 |
| 47 | CN | 146 | LEU | 2.0 |
| 48 | D | 188 | LEU | 2.0 |
| 48 | D | 207 | LEU | 2.0 |
| 51 | G | 56 | LEU | 2.0 |
| 52 | H | 65 | ARG | 2.0 |
| 52 | H | 190 | ILE | 2.0 |
| 55 | K | 158 | ILE | 2.0 |
| 56 | L | 17 | ARG | 2.0 |
| 60 | DA | 21 | ASN | 2.0 |
| 64 | DE | 45 | ARG | 2.0 |
| 65 | DF | 18 | LEU | 2.0 |
| 66 | DG | 28 | LEU | 2.0 |
| 67 | DH | 64 | ILE | 2.0 |
| 79 | DT | 33 | LEU | 2.0 |
| 15 | u | 10 | TRP | 2.0 |
| 19 | y | 15 | HIS | 2.0 |
| 60 | DA | 25 | TRP | 2.0 |
| 64 | T | 56 | HIS | 2.0 |
| 64 | T | 95 | HIS | 2.0 |
| 69 | Y | 89 | TRP | 2.0 |
| 72 | DM | 38 | HIS | 2.0 |
| 1 | 1 | 2078 | A | 2.0 |
| 1 | 1 | 2185 | A | 2.0 |
| 1 | 1 | 2518 | A | 2.0 |
| 1 | 1 | 3050 | A | 2.0 |
| 1 | AS | 664 | A | 2.0 |
| 4 | j | 176 | ASP | 2.0 |
| 5 | AX | 103 | THR | 2.0 |
| 7 | m | 12 | TYR | 2.0 |
| 22 | 2 | 84 | TYR | 2.0 |
| 22 | BO | 24 | ALA | 2.0 |

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| Mol | Chain | Res | Type | RSRZ |
|---|---|---|---|---|
| 33 | AF | 58 | TYR | 2.0 |
| 33 | AF | 70 | ALA | 2.0 |
| 36 | AI | 82 | ALA | 2.0 |
| 43 | AP | 10 | THR | 2.0 |
| 44 | CK | 11 | THR | 2.0 |
| 46 | CM | 1361 | A | 2.0 |
| 50 | F | 71 | THR | 2.0 |
| 51 | G | 213 | ALA | 2.0 |
| 53 | I | 163 | THR | 2.0 |
| 56 | L | 4 | ALA | 2.0 |
| 56 | L | 119 | ALA | 2.0 |
| 58 | CY | 35 | TYR | 2.0 |
| 60 | P | 129 | TYR | 2.0 |
| 63 | S | 63 | ASP | 2.0 |
| 65 | U | 98 | TYR | 2.0 |
| 71 | a | 38 | ASP | 2.0 |
| 73 | c | 91 | ASP | 2.0 |
| 73 | DN | 68 | TYR | 2.0 |
| 82 | L1 | 109 | ALA | 2.0 |
| 6 | l | 69 | GLY | 2.0 |
| 10 | p | 183 | GLY | 2.0 |
| 14 | BG | 152 | PRO | 2.0 |
| 22 | 2 | 159 | PHE | 2.0 |
| 29 | AB | 114 | GLY | 2.0 |
| 34 | CA | 31 | GLN | 2.0 |
| 35 | AH | 59 | PRO | 2.0 |
| 39 | AL | 38 | PHE | 2.0 |
| 48 | CO | 220 | GLN | 2.0 |
| 50 | F | 25 | PHE | 2.0 |
| 55 | CV | 118 | GLY | 2.0 |
| 56 | CW | 177 | GLN | 2.0 |
| 62 | R | 48 | GLY | 2.0 |
| 51 | CR | 43 | PRO | 2.0 |
| 62 | DC | 102 | PHE | 2.0 |
| 65 | DF | 6 | GLN | 2.0 |
| 70 | Z | 51 | GLY | 2.0 |
| 70 | Z | 119 | GLY | 2.0 |
| 76 | DQ | 43 | PHE | 2.0 |
| 80 | P0 | 47 | GLY | 2.0 |
| 51 | G | 35 | PRO | 2.0 |
| 82 | L1 | 43 | PRO | 2.0 |
| 8 | BA | 139 | LYS | 2.0 |

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| Mol | Chain | Res | Type | RSRZ |
|---|---|---|---|---|
| 14 | BG | 20 | GLU | 2.0 |
| 16 | v | 192 | LYS | 2.0 |
| 28 | BU | 47 | GLU | 2.0 |
| 33 | AF | 12 | LYS | 2.0 |
| 35 | CB | 24 | LYS | 2.0 |
| 37 | AJ | 69 | LYS | 2.0 |
| 37 | CD | 80 | LYS | 2.0 |
| 44 | AQ | 58 | LYS | 2.0 |
| 45 | CL | 101 | LYS | 2.0 |
| 49 | E | 189 | GLU | 2.0 |
| 55 | K | 191 | GLU | 2.0 |
| 56 | L | 179 | LYS | 2.0 |
| 62 | DC | 31 | GLU | 2.0 |
| 63 | S | 12 | LYS | 2.0 |
| 66 | V | 115 | GLU | 2.0 |
| 13 | s | 71 | VAL | 2.0 |
| 28 | BU | 53 | VAL | 2.0 |
| 37 | AJ | 43 | VAL | 2.0 |
| 46 | B | 1113 | C | 2.0 |
| 46 | CM | 720 | C | 2.0 |
| 74 | DO | 17 | LYS | 2.0 |
| 79 | DT | 258 | LYS | 2.0 |
| 51 | G | 102 | VAL | 2.0 |
| 51 | G | 192 | VAL | 2.0 |
| 54 | CU | 178 | VAL | 2.0 |
| 60 | DA | 34 | VAL | 2.0 |
| 61 | DB | 8 | VAL | 2.0 |
| 69 | Y | 40 | VAL | 2.0 |
| 74 | d | 35 | VAL | 2.0 |
| 79 | AR | 8 | VAL | 2.0 |
| 1 | 1 | 2435 | G | 2.0 |
| 5 | k | 387 | LEU | 2.0 |
| 6 | AY | 220 | LEU | 2.0 |
| 10 | BC | 83 | LEU | 2.0 |
| 17 | BJ | 175 | LEU | 2.0 |
| 21 | 0 | 124 | LEU | 2.0 |
| 45 | i | 93 | ARG | 2.0 |
| 45 | i | 165 | LEU | 2.0 |
| 46 | B | 1597 | G | 2.0 |
| 46 | CM | 1135 | G | 2.0 |
| 53 | I | 111 | LEU | 2.0 |
| 53 | I | 190 | LEU | 2.0 |

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| Mol | Chain | Res | Type | RSRZ |
|---|---|---|---|---|
| 53 | CT | 216 | LEU | 2.0 |
| 62 | R | 40 | ARG | 2.0 |
| 66 | DG | 45 | LEU | 2.0 |
| 71 | a | 41 | ARG | 2.0 |
| 78 | DS | 161 | ARG | 2.0 |
| 5 | k | 207 | SER | 2.0 |
| 7 | AZ | 88 | ILE | 2.0 |
| 9 | o | 72 | SER | 2.0 |
| 10 | BC | 196 | SER | 2.0 |
| 13 | s | 48 | SER | 2.0 |
| 18 | x | 110 | SER | 2.0 |
| 22 | 2 | 48 | ILE | 2.0 |
| 31 | BX | 100 | SER | 2.0 |
| 32 | AE | 35 | ILE | 2.0 |
| 32 | BY | 99 | SER | 2.0 |
| 34 | CA | 32 | ILE | 2.0 |
| 55 | CV | 158 | ILE | 2.0 |
| 64 | T | 117 | ILE | 2.0 |
| 68 | DI | 24 | ILE | 2.0 |
| 70 | DK | 128 | SER | 2.0 |
| 71 | a | 78 | SER | 2.0 |
| 79 | AR | 138 | ILE | 2.0 |
| 1 | AS | 1013 | U | 2.0 |
| 22 | BO | 45 | ASN | 2.0 |
| 31 | AD | 13 | ASN | 2.0 |
| 46 | CM | 258 | U | 2.0 |
| 46 | CM | 491 | U | 2.0 |
| 46 | CM | 675 | U | 2.0 |
| 51 | G | 188 | ASN | 2.0 |
| 60 | P | 78 | ASN | 2.0 |
| 11 | q | 58 | HIS | 2.0 |
| 51 | G | 17 | HIS | 2.0 |
| 65 | U | 99 | HIS | 2.0 |
| 79 | DT | 19 | TRP | 2.0 |
| 82 | L1 | 210 | MET | 2.0 |
| 16 | BI | 196 | THR | 2.0 |
| 33 | AF | 98 | ALA | 2.0 |
| 45 | i | 156 | ALA | 2.0 |
| 47 | C | 130 | ALA | 2.0 |
| 29 | AB | 48 | TYR | 2.0 |
| 48 | D | 153 | THR | 2.0 |
| 52 | H | 176 | THR | 2.0 |

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| Mol | Chain | Res | Type | RSRZ |
|---|---|---|---|---|
| 54 | J | 99 | ALA | 2.0 |
| 54 | CU | 71 | THR | 2.0 |
| 55 | K | 14 | THR | 2.0 |
| 55 | K | 97 | THR | 2.0 |
| 61 | Q | 45 | ALA | 2.0 |
| 73 | c | 40 | THR | 2.0 |
| 79 | DT | 25 | THR | 2.0 |
| 80 | P0 | 62 | ALA | 2.0 |
| 82 | l1 | 52 | THR | 2.0 |
| 82 | l1 | 71 | ALA | 2.0 |
| 53 | I | 155 | ASP | 2.0 |
| 54 | CU | 154 | ASP | 2.0 |
| 79 | AR | 39 | ASP | 2.0 |
| 79 | DT | 31 | ASP | 2.0 |
| 6 | AY | 98 | GLY | 2.0 |
| 7 | AZ | 201 | GLY | 2.0 |
| 23 | 5 | 45 | GLY | 2.0 |
| 28 | AA | 128 | LYS | 2.0 |
| 29 | BV | 132 | LYS | 2.0 |
| 41 | AN | 22 | LYS | 2.0 |
| 41 | AN | 34 | CYS | 2.0 |
| 50 | F | 134 | GLY | 2.0 |
| 50 | CQ | 181 | GLY | 2.0 |
| 53 | I | 165 | GLY | 2.0 |
| 61 | DB | 108 | GLY | 2.0 |
| 67 | W | 110 | GLY | 2.0 |
| 74 | DO | 79 | PHE | 2.0 |
| 79 | DT | 104 | PHE | 2.0 |
| 82 | L1 | 68 | PHE | 2.0 |
| 7 | AZ | 274 | GLN | 2.0 |
| 36 | CC | 62 | GLN | 2.0 |
| 45 | CL | 163 | GLN | 2.0 |
| 51 | CR | 62 | LYS | 2.0 |
| 60 | DA | 39 | LYS | 2.0 |
| 63 | S | 22 | LYS | 2.0 |
| 67 | DH | 76 | LYS | 2.0 |
| 70 | DK | 6 | PRO | 2.0 |
| 79 | AR | 296 | GLN | 2.0 |
| 80 | p0 | 7 | LYS | 2.0 |
| 1 | 1 | 1022 | A | 2.0 |
| 1 | 1 | 2117 | A | 2.0 |
| 1 | AS | 2379 | A | 2.0 |

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| Mol | Chain | Res | Type | RSRZ |
|---|---|---|---|---|
| 10 | p | 131 | VAL | 2.0 |
| 22 | BO | 96 | VAL | 2.0 |
| 23 | BP | 99 | VAL | 2.0 |
| 28 | BU | 75 | VAL | 2.0 |
| 46 | B | 298 | A | 2.0 |
| 46 | B | 299 | A | 2.0 |
| 46 | B | 682 | A | 2.0 |
| 46 | B | 1316 | A | 2.0 |
| 46 | B | 1361 | A | 2.0 |
| 46 | CM | 1410 | A | 2.0 |
| 25 | BR | 93 | ARG | 2.0 |
| 35 | CB | 16 | ARG | 2.0 |
| 49 | CP | 174 | VAL | 2.0 |
| 53 | CT | 230 | ARG | 2.0 |
| 56 | L | 57 | ARG | 2.0 |
| 56 | L | 126 | ARG | 2.0 |
| 69 | DJ | 117 | ARG | 2.0 |
| 73 | c | 18 | VAL | 2.0 |
| 79 | AR | 105 | VAL | 2.0 |
| 10 | BC | 27 | LEU | 2.0 |
| 13 | s | 30 | LEU | 2.0 |
| 21 | 0 | 110 | LEU | 2.0 |
| 31 | BX | 86 | LEU | 2.0 |
| 59 | O | 28 | LEU | 2.0 |
| 82 | L1 | 165 | LEU | 2.0 |
| 7 | AZ | 231 | ILE | 2.0 |
| 11 | q | 48 | ILE | 2.0 |
| 32 | AE | 58 | ILE | 2.0 |
| 56 | L | 77 | ILE | 2.0 |
| 81 | 12 | 132 | ILE | 2.0 |
| 1 | AS | 3193 | C | 2.0 |
| 46 | B | 1467 | C | 2.0 |
| 46 | CM | 261 | C | 2.0 |

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

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

## 6.3 Carbohydrates (i)

There are no oligosaccharides in this entry.

## 6.4 Ligands (i)

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, $95^{th}$ percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

| Mol | Type | Chain | Res | Atoms | RSCC | RSR | B-factors(Å$^2$) | Q<0.9 |
|---|---|---|---|---|---|---|---|---|
| 83 | MG | 1 | 3715 | 1/1 | -0.02 | 0.38 | 76,76,76,76 | 0 |
| 83 | MG | 1 | 3921 | 1/1 | 0.15 | 0.20 | 67,67,67,67 | 0 |
| 83 | MG | B | 1928 | 1/1 | 0.16 | 0.32 | 108,108,108,108 | 0 |
| 83 | MG | J | 201 | 1/1 | 0.31 | 0.16 | 129,129,129,129 | 0 |
| 83 | MG | 1 | 3841 | 1/1 | 0.36 | 0.18 | 73,73,73,73 | 0 |
| 83 | MG | CM | 1819 | 1/1 | 0.41 | 0.24 | 74,74,74,74 | 0 |
| 83 | MG | 8 | 201 | 1/1 | 0.43 | 0.26 | 62,62,62,62 | 0 |
| 83 | MG | 8 | 202 | 1/1 | 0.46 | 0.61 | 79,79,79,79 | 0 |
| 83 | MG | 1 | 3868 | 1/1 | 0.50 | 0.18 | 54,54,54,54 | 0 |
| 83 | MG | B | 1898 | 1/1 | 0.52 | 0.31 | 60,60,60,60 | 0 |
| 83 | MG | B | 1851 | 1/1 | 0.52 | 0.19 | 53,53,53,53 | 0 |
| 83 | MG | 9 | 202 | 1/1 | 0.53 | 0.23 | 81,81,81,81 | 0 |
| 83 | MG | 1 | 3651 | 1/1 | 0.53 | 0.36 | 77,77,77,77 | 0 |
| 85 | ZN | d | 101 | 1/1 | 0.53 | 0.17 | 285,285,285,285 | 0 |
| 83 | MG | AS | 3676 | 1/1 | 0.54 | 0.17 | 72,72,72,72 | 0 |
| 83 | MG | u | 202 | 1/1 | 0.54 | 0.12 | 51,51,51,51 | 0 |
| 83 | MG | 1 | 3630 | 1/1 | 0.54 | 0.34 | 59,59,59,59 | 0 |
| 83 | MG | 1 | 3669 | 1/1 | 0.56 | 0.33 | 76,76,76,76 | 0 |
| 83 | MG | AJ | 101 | 1/1 | 0.57 | 0.22 | 82,82,82,82 | 0 |
| 83 | MG | CM | 1876 | 1/1 | 0.57 | 0.21 | 51,51,51,51 | 0 |
| 83 | MG | 1 | 3930 | 1/1 | 0.57 | 0.23 | 81,81,81,81 | 0 |
| 83 | MG | 1 | 3803 | 1/1 | 0.58 | 0.27 | 92,92,92,92 | 0 |
| 83 | MG | 1 | 3527 | 1/1 | 0.58 | 0.32 | 72,72,72,72 | 0 |
| 83 | MG | CL | 301 | 1/1 | 0.59 | 0.17 | 40,40,40,40 | 0 |
| 83 | MG | AS | 3601 | 1/1 | 0.59 | 0.15 | 124,124,124,124 | 0 |
| 83 | MG | B | 1924 | 1/1 | 0.60 | 0.30 | 69,69,69,69 | 0 |
| 83 | MG | 4 | 207 | 1/1 | 0.61 | 0.27 | 64,64,64,64 | 0 |
| 83 | MG | f | 102 | 1/1 | 0.61 | 0.14 | 81,81,81,81 | 0 |
| 83 | MG | 1 | 3776 | 1/1 | 0.61 | 0.38 | 57,57,57,57 | 0 |
| 83 | MG | B | 1941 | 1/1 | 0.61 | 0.13 | 58,58,58,58 | 0 |
| 83 | MG | AS | 3631 | 1/1 | 0.62 | 0.16 | 66,66,66,66 | 0 |
| 83 | MG | 1 | 3856 | 1/1 | 0.62 | 0.15 | 66,66,66,66 | 0 |
| 83 | MG | 4 | 203 | 1/1 | 0.62 | 0.16 | 57,57,57,57 | 0 |
| 83 | MG | Y | 201 | 1/1 | 0.63 | 0.12 | 58,58,58,58 | 0 |
| 83 | MG | AG | 201 | 1/1 | 0.63 | 0.25 | 86,86,86,86 | 0 |
| 83 | MG | DG | 201 | 1/1 | 0.63 | 0.30 | 52,52,52,52 | 0 |
| 83 | MG | 1 | 3688 | 1/1 | 0.63 | 0.35 | 82,82,82,82 | 0 |

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| Mol | Type | Chain | Res | Atoms | RSCC | RSR | B-factors(Å$^2$) | Q<0.9 |
|---|---|---|---|---|---|---|---|---|
| 83 | MG | 1 | 3716 | 1/1 | 0.64 | 0.14 | 77,77,77,77 | 0 |
| 83 | MG | s | 201 | 1/1 | 0.64 | 0.20 | 62,62,62,62 | 0 |
| 83 | MG | 1 | 3867 | 1/1 | 0.64 | 0.18 | 51,51,51,51 | 0 |
| 83 | MG | 1 | 3470 | 1/1 | 0.64 | 0.27 | 53,53,53,53 | 0 |
| 83 | MG | 1 | 3722 | 1/1 | 0.65 | 0.19 | 61,61,61,61 | 0 |
| 83 | MG | CM | 1859 | 1/1 | 0.65 | 0.18 | 60,60,60,60 | 0 |
| 83 | MG | B | 1890 | 1/1 | 0.65 | 0.16 | 53,53,53,53 | 0 |
| 83 | MG | a | 201 | 1/1 | 0.65 | 0.12 | 76,76,76,76 | 0 |
| 83 | MG | B | 1829 | 1/1 | 0.65 | 0.14 | 64,64,64,64 | 0 |
| 83 | MG | 1 | 3713 | 1/1 | 0.66 | 0.13 | 51,51,51,51 | 0 |
| 83 | MG | G | 302 | 1/1 | 0.66 | 0.32 | 63,63,63,63 | 0 |
| 83 | MG | 1 | 3890 | 1/1 | 0.66 | 0.19 | 46,46,46,46 | 0 |
| 83 | MG | 1 | 3796 | 1/1 | 0.66 | 0.15 | 84,84,84,84 | 0 |
| 83 | MG | B | 1875 | 1/1 | 0.66 | 0.31 | 75,75,75,75 | 0 |
| 83 | MG | 1 | 3476 | 1/1 | 0.67 | 0.15 | 58,58,58,58 | 0 |
| 83 | MG | DB | 203 | 1/1 | 0.67 | 0.14 | 52,52,52,52 | 0 |
| 83 | MG | B | 1939 | 1/1 | 0.68 | 0.14 | 78,78,78,78 | 0 |
| 83 | MG | I | 301 | 1/1 | 0.68 | 0.25 | 99,99,99,99 | 0 |
| 83 | MG | CM | 1880 | 1/1 | 0.68 | 0.18 | 66,66,66,66 | 0 |
| 83 | MG | 1 | 3699 | 1/1 | 0.68 | 0.21 | 54,54,54,54 | 0 |
| 83 | MG | AS | 3519 | 1/1 | 0.68 | 0.24 | 42,42,42,42 | 0 |
| 83 | MG | AS | 3597 | 1/1 | 0.68 | 0.10 | 28,28,28,28 | 0 |
| 83 | MG | 1 | 3681 | 1/1 | 0.69 | 0.21 | 52,52,52,52 | 0 |
| 83 | MG | 1 | 3914 | 1/1 | 0.69 | 0.18 | 57,57,57,57 | 0 |
| 83 | MG | CM | 1864 | 1/1 | 0.69 | 0.18 | 73,73,73,73 | 0 |
| 83 | MG | B | 1896 | 1/1 | 0.69 | 0.09 | 61,61,61,61 | 0 |
| 83 | MG | 1 | 3797 | 1/1 | 0.69 | 0.18 | 77,77,77,77 | 0 |
| 83 | MG | B | 1922 | 1/1 | 0.69 | 0.20 | 66,66,66,66 | 0 |
| 83 | MG | 1 | 3598 | 1/1 | 0.69 | 0.20 | 56,56,56,56 | 0 |
| 83 | MG | 1 | 3837 | 1/1 | 0.69 | 0.13 | 34,34,34,34 | 0 |
| 83 | MG | 1 | 3432 | 1/1 | 0.70 | 0.14 | 48,48,48,48 | 0 |
| 83 | MG | 1 | 3923 | 1/1 | 0.70 | 0.20 | 64,64,64,64 | 0 |
| 83 | MG | 1 | 3694 | 1/1 | 0.70 | 0.14 | 39,39,39,39 | 0 |
| 83 | MG | 1 | 3931 | 1/1 | 0.70 | 0.16 | 61,61,61,61 | 0 |
| 83 | MG | 1 | 3517 | 1/1 | 0.70 | 0.15 | 58,58,58,58 | 0 |
| 83 | MG | B | 1856 | 1/1 | 0.70 | 0.15 | 47,47,47,47 | 0 |
| 83 | MG | BF | 201 | 1/1 | 0.70 | 0.14 | 44,44,44,44 | 0 |
| 83 | MG | B | 1862 | 1/1 | 0.70 | 0.16 | 68,68,68,68 | 0 |
| 83 | MG | 1 | 3438 | 1/1 | 0.71 | 0.19 | 31,31,31,31 | 0 |
| 83 | MG | 1 | 3483 | 1/1 | 0.71 | 0.13 | 38,38,38,38 | 0 |
| 83 | MG | o | 303 | 1/1 | 0.71 | 0.17 | 57,57,57,57 | 0 |
| 83 | MG | 1 | 3842 | 1/1 | 0.71 | 0.11 | 63,63,63,63 | 0 |

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| Mol | Type | Chain | Res | Atoms | RSCC | RSR | B-factors(Å$^2$) | Q<0.9 |
|---|---|---|---|---|---|---|---|---|
| 83 | MG | AS | 3493 | 1/1 | 0.72 | 0.19 | 51,51,51,51 | 0 |
| 83 | MG | B | 1810 | 1/1 | 0.72 | 0.23 | 45,45,45,45 | 0 |
| 83 | MG | k | 404 | 1/1 | 0.72 | 0.17 | 79,79,79,79 | 0 |
| 83 | MG | CM | 1882 | 1/1 | 0.72 | 0.22 | 66,66,66,66 | 0 |
| 83 | MG | 1 | 3584 | 1/1 | 0.72 | 0.14 | 41,41,41,41 | 0 |
| 83 | MG | CM | 1822 | 1/1 | 0.72 | 0.19 | 44,44,44,44 | 0 |
| 83 | MG | 1 | 3876 | 1/1 | 0.72 | 0.14 | 42,42,42,42 | 0 |
| 83 | MG | 1 | 3655 | 1/1 | 0.73 | 0.18 | 54,54,54,54 | 0 |
| 83 | MG | j | 302 | 1/1 | 0.73 | 0.12 | 53,53,53,53 | 0 |
| 83 | MG | BZ | 202 | 1/1 | 0.73 | 0.13 | 66,66,66,66 | 0 |
| 83 | MG | 1 | 3543 | 1/1 | 0.73 | 0.21 | 62,62,62,62 | 0 |
| 83 | MG | CM | 1816 | 1/1 | 0.73 | 0.20 | 27,27,27,27 | 0 |
| 83 | MG | 1 | 3854 | 1/1 | 0.74 | 0.27 | 61,61,61,61 | 0 |
| 83 | MG | CM | 1821 | 1/1 | 0.74 | 0.15 | 35,35,35,35 | 0 |
| 83 | MG | AS | 3602 | 1/1 | 0.74 | 0.15 | 59,59,59,59 | 0 |
| 83 | MG | CM | 1836 | 1/1 | 0.74 | 0.15 | 48,48,48,48 | 0 |
| 83 | MG | AS | 3622 | 1/1 | 0.74 | 0.09 | 47,47,47,47 | 0 |
| 83 | MG | AS | 3627 | 1/1 | 0.74 | 0.15 | 57,57,57,57 | 0 |
| 83 | MG | 1 | 3891 | 1/1 | 0.74 | 0.18 | 65,65,65,65 | 0 |
| 83 | MG | 1 | 3648 | 1/1 | 0.74 | 0.12 | 44,44,44,44 | 0 |
| 83 | MG | 1 | 3783 | 1/1 | 0.74 | 0.18 | 48,48,48,48 | 0 |
| 83 | MG | 1 | 3468 | 1/1 | 0.74 | 0.21 | 38,38,38,38 | 0 |
| 83 | MG | 1 | 3871 | 1/1 | 0.74 | 0.18 | 67,67,67,67 | 0 |
| 83 | MG | 1 | 3597 | 1/1 | 0.74 | 0.34 | 60,60,60,60 | 0 |
| 83 | MG | 1 | 3618 | 1/1 | 0.75 | 0.13 | 34,34,34,34 | 0 |
| 83 | MG | 1 | 3700 | 1/1 | 0.75 | 0.22 | 47,47,47,47 | 0 |
| 83 | MG | 1 | 3545 | 1/1 | 0.75 | 0.23 | 51,51,51,51 | 0 |
| 83 | MG | 1 | 3674 | 1/1 | 0.75 | 0.17 | 83,83,83,83 | 0 |
| 83 | MG | 1 | 3631 | 1/1 | 0.75 | 0.25 | 64,64,64,64 | 0 |
| 83 | MG | AS | 3646 | 1/1 | 0.75 | 0.12 | 35,35,35,35 | 0 |
| 83 | MG | AS | 3652 | 1/1 | 0.75 | 0.11 | 51,51,51,51 | 0 |
| 83 | MG | 1 | 3547 | 1/1 | 0.75 | 0.11 | 42,42,42,42 | 0 |
| 83 | MG | 1 | 3746 | 1/1 | 0.75 | 0.13 | 66,66,66,66 | 0 |
| 83 | MG | 1 | 3909 | 1/1 | 0.75 | 0.18 | 79,79,79,79 | 0 |
| 83 | MG | 1 | 3553 | 1/1 | 0.75 | 0.24 | 54,54,54,54 | 0 |
| 83 | MG | r | 302 | 1/1 | 0.75 | 0.18 | 50,50,50,50 | 0 |
| 83 | MG | 1 | 3913 | 1/1 | 0.76 | 0.18 | 55,55,55,55 | 0 |
| 83 | MG | V | 201 | 1/1 | 0.76 | 0.28 | 48,48,48,48 | 0 |
| 83 | MG | 1 | 3524 | 1/1 | 0.76 | 0.24 | 44,44,44,44 | 0 |
| 83 | MG | B | 1926 | 1/1 | 0.76 | 0.20 | 41,41,41,41 | 0 |
| 83 | MG | 3 | 202 | 1/1 | 0.76 | 0.11 | 59,59,59,59 | 0 |
| 83 | MG | 3 | 214 | 1/1 | 0.76 | 0.14 | 82,82,82,82 | 0 |

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| Mol | Type | Chain | Res | Atoms | RSCC | RSR | B-factors(Å$^2$) | Q<0.9 |
|---|---|---|---|---|---|---|---|---|
| 83 | MG | 1 | 3587 | 1/1 | 0.76 | 0.13 | 58,58,58,58 | 0 |
| 83 | MG | AS | 3562 | 1/1 | 0.76 | 0.13 | 50,50,50,50 | 0 |
| 83 | MG | B | 1944 | 1/1 | 0.76 | 0.10 | 76,76,76,76 | 0 |
| 83 | MG | 1 | 3583 | 1/1 | 0.76 | 0.21 | 52,52,52,52 | 0 |
| 83 | MG | 0 | 201 | 1/1 | 0.76 | 0.19 | 70,70,70,70 | 0 |
| 83 | MG | 1 | 3652 | 1/1 | 0.77 | 0.18 | 43,43,43,43 | 0 |
| 83 | MG | AS | 3580 | 1/1 | 0.77 | 0.12 | 42,42,42,42 | 0 |
| 83 | MG | CM | 1853 | 1/1 | 0.77 | 0.25 | 72,72,72,72 | 0 |
| 83 | MG | B | 1877 | 1/1 | 0.77 | 0.22 | 53,53,53,53 | 0 |
| 83 | MG | CM | 1860 | 1/1 | 0.77 | 0.21 | 41,41,41,41 | 0 |
| 83 | MG | B | 1827 | 1/1 | 0.77 | 0.13 | 37,37,37,37 | 0 |
| 83 | MG | 1 | 3671 | 1/1 | 0.77 | 0.20 | 52,52,52,52 | 0 |
| 83 | MG | 5 | 201 | 1/1 | 0.77 | 0.12 | 64,64,64,64 | 0 |
| 83 | MG | 1 | 3732 | 1/1 | 0.77 | 0.12 | 26,26,26,26 | 0 |
| 83 | MG | CM | 1818 | 1/1 | 0.77 | 0.18 | 38,38,38,38 | 0 |
| 83 | MG | B | 1806 | 1/1 | 0.77 | 0.13 | 67,67,67,67 | 0 |
| 83 | MG | AS | 3637 | 1/1 | 0.77 | 0.24 | 97,97,97,97 | 0 |
| 83 | MG | 1 | 3838 | 1/1 | 0.78 | 0.14 | 61,61,61,61 | 0 |
| 83 | MG | 6 | 203 | 1/1 | 0.78 | 0.16 | 42,42,42,42 | 0 |
| 83 | MG | 1 | 3564 | 1/1 | 0.78 | 0.14 | 57,57,57,57 | 0 |
| 83 | MG | 1 | 3502 | 1/1 | 0.78 | 0.13 | 41,41,41,41 | 0 |
| 83 | MG | 1 | 3591 | 1/1 | 0.78 | 0.14 | 58,58,58,58 | 0 |
| 83 | MG | 1 | 3622 | 1/1 | 0.78 | 0.23 | 42,42,42,42 | 0 |
| 83 | MG | AS | 3641 | 1/1 | 0.78 | 0.28 | 48,48,48,48 | 0 |
| 83 | MG | AH | 202 | 1/1 | 0.78 | 0.14 | 55,55,55,55 | 0 |
| 83 | MG | 1 | 3861 | 1/1 | 0.78 | 0.12 | 56,56,56,56 | 0 |
| 83 | MG | 1 | 3747 | 1/1 | 0.78 | 0.08 | 45,45,45,45 | 0 |
| 83 | MG | AT | 207 | 1/1 | 0.78 | 0.19 | 68,68,68,68 | 0 |
| 83 | MG | 1 | 3830 | 1/1 | 0.78 | 0.23 | 43,43,43,43 | 0 |
| 83 | MG | DA | 201 | 1/1 | 0.78 | 0.26 | 57,57,57,57 | 0 |
| 83 | MG | 1 | 3832 | 1/1 | 0.78 | 0.18 | 56,56,56,56 | 0 |
| 83 | MG | 1 | 3754 | 1/1 | 0.78 | 0.22 | 61,61,61,61 | 0 |
| 83 | MG | 0 | 204 | 1/1 | 0.78 | 0.18 | 45,45,45,45 | 0 |
| 83 | MG | 1 | 3677 | 1/1 | 0.79 | 0.19 | 55,55,55,55 | 0 |
| 83 | MG | 1 | 3554 | 1/1 | 0.79 | 0.09 | 40,40,40,40 | 0 |
| 83 | MG | B | 1943 | 1/1 | 0.79 | 0.07 | 68,68,68,68 | 0 |
| 83 | MG | 1 | 3555 | 1/1 | 0.79 | 0.10 | 46,46,46,46 | 0 |
| 83 | MG | 1 | 3781 | 1/1 | 0.79 | 0.12 | 82,82,82,82 | 0 |
| 83 | MG | AS | 3673 | 1/1 | 0.79 | 0.13 | 45,45,45,45 | 0 |
| 83 | MG | AS | 3581 | 1/1 | 0.79 | 0.11 | 46,46,46,46 | 0 |
| 83 | MG | B | 1850 | 1/1 | 0.79 | 0.10 | 24,24,24,24 | 0 |
| 83 | MG | 0 | 202 | 1/1 | 0.79 | 0.10 | 39,39,39,39 | 0 |

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| Mol | Type | Chain | Res | Atoms | RSCC | RSR | B-factors(Å$^2$) | Q<0.9 |
|---|---|---|---|---|---|---|---|---|
| 83 | MG | BN | 201 | 1/1 | 0.79 | 0.11 | 59,59,59,59 | 0 |
| 83 | MG | 1 | 3858 | 1/1 | 0.79 | 0.15 | 48,48,48,48 | 0 |
| 83 | MG | CM | 1898 | 1/1 | 0.79 | 0.12 | 44,44,44,44 | 0 |
| 83 | MG | CM | 1899 | 1/1 | 0.79 | 0.17 | 31,31,31,31 | 0 |
| 83 | MG | CO | 301 | 1/1 | 0.79 | 0.25 | 34,34,34,34 | 0 |
| 83 | MG | AS | 3615 | 1/1 | 0.79 | 0.16 | 50,50,50,50 | 0 |
| 83 | MG | CL | 303 | 1/1 | 0.79 | 0.19 | 41,41,41,41 | 0 |
| 83 | MG | 3 | 210 | 1/1 | 0.79 | 0.19 | 59,59,59,59 | 0 |
| 83 | MG | B | 1866 | 1/1 | 0.79 | 0.20 | 78,78,78,78 | 0 |
| 83 | MG | 1 | 3563 | 1/1 | 0.80 | 0.21 | 50,50,50,50 | 0 |
| 83 | MG | CM | 1808 | 1/1 | 0.80 | 0.21 | 58,58,58,58 | 0 |
| 83 | MG | 1 | 3466 | 1/1 | 0.80 | 0.19 | 43,43,43,43 | 0 |
| 83 | MG | B | 1927 | 1/1 | 0.80 | 0.11 | 57,57,57,57 | 0 |
| 83 | MG | 9 | 201 | 1/1 | 0.80 | 0.76 | 70,70,70,70 | 0 |
| 83 | MG | 1 | 3873 | 1/1 | 0.80 | 0.09 | 40,40,40,40 | 0 |
| 83 | MG | 1 | 3848 | 1/1 | 0.80 | 0.18 | 78,78,78,78 | 0 |
| 83 | MG | 1 | 3595 | 1/1 | 0.80 | 0.14 | 42,42,42,42 | 0 |
| 83 | MG | CM | 1837 | 1/1 | 0.80 | 0.19 | 39,39,39,39 | 0 |
| 83 | MG | 1 | 3686 | 1/1 | 0.80 | 0.18 | 60,60,60,60 | 0 |
| 83 | MG | 1 | 3893 | 1/1 | 0.80 | 0.17 | 52,52,52,52 | 0 |
| 83 | MG | B | 1893 | 1/1 | 0.80 | 0.30 | 43,43,43,43 | 0 |
| 83 | MG | 1 | 3530 | 1/1 | 0.80 | 0.18 | 52,52,52,52 | 0 |
| 83 | MG | 1 | 3559 | 1/1 | 0.80 | 0.16 | 46,46,46,46 | 0 |
| 83 | MG | B | 1902 | 1/1 | 0.80 | 0.32 | 60,60,60,60 | 0 |
| 83 | MG | B | 1907 | 1/1 | 0.80 | 0.10 | 44,44,44,44 | 0 |
| 83 | MG | AS | 3675 | 1/1 | 0.80 | 0.12 | 55,55,55,55 | 0 |
| 83 | MG | B | 1909 | 1/1 | 0.80 | 0.16 | 35,35,35,35 | 0 |
| 83 | MG | AS | 3427 | 1/1 | 0.80 | 0.10 | 43,43,43,43 | 0 |
| 83 | MG | AS | 3491 | 1/1 | 0.80 | 0.17 | 64,64,64,64 | 0 |
| 83 | MG | B | 1911 | 1/1 | 0.80 | 0.23 | 60,60,60,60 | 0 |
| 83 | MG | B | 1916 | 1/1 | 0.80 | 0.17 | 69,69,69,69 | 0 |
| 83 | MG | 1 | 3727 | 1/1 | 0.80 | 0.09 | 38,38,38,38 | 0 |
| 83 | MG | 1 | 3902 | 1/1 | 0.81 | 0.23 | 51,51,51,51 | 0 |
| 83 | MG | 1 | 3607 | 1/1 | 0.81 | 0.12 | 51,51,51,51 | 0 |
| 83 | MG | 1 | 3866 | 1/1 | 0.81 | 0.08 | 62,62,62,62 | 0 |
| 83 | MG | 1 | 3645 | 1/1 | 0.81 | 0.22 | 47,47,47,47 | 0 |
| 83 | MG | 1 | 3625 | 1/1 | 0.81 | 0.38 | 95,95,95,95 | 0 |
| 83 | MG | 1 | 3518 | 1/1 | 0.81 | 0.25 | 57,57,57,57 | 0 |
| 83 | MG | B | 1934 | 1/1 | 0.81 | 0.14 | 102,102,102,102 | 0 |
| 83 | MG | 1 | 3928 | 1/1 | 0.81 | 0.21 | 59,59,59,59 | 0 |
| 83 | MG | AS | 3662 | 1/1 | 0.81 | 0.08 | 57,57,57,57 | 0 |
| 83 | MG | AS | 3666 | 1/1 | 0.81 | 0.11 | 53,53,53,53 | 0 |

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| Mol | Type | Chain | Res | Atoms | RSCC | RSR | B-factors(Å$^2$) | Q<0.9 |
|---|---|---|---|---|---|---|---|---|
| 83 | MG | AS | 3560 | 1/1 | 0.81 | 0.10 | 52,52,52,52 | 0 |
| 83 | MG | 1 | 3800 | 1/1 | 0.81 | 0.17 | 62,62,62,62 | 0 |
| 83 | MG | AS | 3573 | 1/1 | 0.81 | 0.14 | 30,30,30,30 | 0 |
| 83 | MG | 1 | 3849 | 1/1 | 0.81 | 0.24 | 47,47,47,47 | 0 |
| 83 | MG | BB | 301 | 1/1 | 0.81 | 0.12 | 28,28,28,28 | 0 |
| 83 | MG | BE | 302 | 1/1 | 0.81 | 0.10 | 48,48,48,48 | 0 |
| 83 | MG | 1 | 3714 | 1/1 | 0.81 | 0.19 | 43,43,43,43 | 0 |
| 83 | MG | BJ | 303 | 1/1 | 0.81 | 0.11 | 30,30,30,30 | 0 |
| 83 | MG | AS | 3585 | 1/1 | 0.81 | 0.20 | 44,44,44,44 | 0 |
| 83 | MG | 3 | 206 | 1/1 | 0.81 | 0.12 | 47,47,47,47 | 0 |
| 83 | MG | 1 | 3672 | 1/1 | 0.81 | 0.11 | 57,57,57,57 | 0 |
| 83 | MG | 1 | 3692 | 1/1 | 0.81 | 0.13 | 176,176,176,176 | 0 |
| 83 | MG | 1 | 3442 | 1/1 | 0.82 | 0.30 | 52,52,52,52 | 0 |
| 83 | MG | AE | 202 | 1/1 | 0.82 | 0.07 | 63,63,63,63 | 0 |
| 83 | MG | 1 | 3720 | 1/1 | 0.82 | 0.18 | 23,23,23,23 | 0 |
| 83 | MG | B | 1938 | 1/1 | 0.82 | 0.26 | 70,70,70,70 | 0 |
| 83 | MG | 1 | 3639 | 1/1 | 0.82 | 0.16 | 54,54,54,54 | 0 |
| 83 | MG | 1 | 3726 | 1/1 | 0.82 | 0.19 | 43,43,43,43 | 0 |
| 83 | MG | CL | 302 | 1/1 | 0.82 | 0.37 | 59,59,59,59 | 0 |
| 83 | MG | B | 1942 | 1/1 | 0.82 | 0.16 | 67,67,67,67 | 0 |
| 83 | MG | 1 | 3798 | 1/1 | 0.82 | 0.13 | 41,41,41,41 | 0 |
| 83 | MG | 1 | 3419 | 1/1 | 0.82 | 0.15 | 47,47,47,47 | 0 |
| 83 | MG | B | 1949 | 1/1 | 0.82 | 0.17 | 47,47,47,47 | 0 |
| 83 | MG | B | 1899 | 1/1 | 0.82 | 0.18 | 73,73,73,73 | 0 |
| 83 | MG | CM | 1820 | 1/1 | 0.82 | 0.21 | 27,27,27,27 | 0 |
| 83 | MG | B | 1817 | 1/1 | 0.82 | 0.24 | 45,45,45,45 | 0 |
| 83 | MG | AS | 3629 | 1/1 | 0.82 | 0.14 | 38,38,38,38 | 0 |
| 83 | MG | AS | 3630 | 1/1 | 0.82 | 0.07 | 50,50,50,50 | 0 |
| 83 | MG | 1 | 3489 | 1/1 | 0.82 | 0.13 | 49,49,49,49 | 0 |
| 83 | MG | 1 | 3594 | 1/1 | 0.82 | 0.23 | 72,72,72,72 | 0 |
| 83 | MG | B | 1846 | 1/1 | 0.82 | 0.10 | 57,57,57,57 | 0 |
| 83 | MG | B | 1912 | 1/1 | 0.82 | 0.12 | 81,81,81,81 | 0 |
| 83 | MG | 1 | 3911 | 1/1 | 0.82 | 0.12 | 63,63,63,63 | 0 |
| 83 | MG | CM | 1874 | 1/1 | 0.82 | 0.15 | 66,66,66,66 | 0 |
| 83 | MG | AS | 3414 | 1/1 | 0.82 | 0.27 | 47,47,47,47 | 0 |
| 83 | MG | B | 1918 | 1/1 | 0.82 | 0.14 | 59,59,59,59 | 0 |
| 83 | MG | AS | 3490 | 1/1 | 0.82 | 0.12 | 35,35,35,35 | 0 |
| 83 | MG | 1 | 3568 | 1/1 | 0.82 | 0.23 | 44,44,44,44 | 0 |
| 83 | MG | 1 | 3683 | 1/1 | 0.82 | 0.12 | 104,104,104,104 | 0 |
| 83 | MG | AT | 202 | 1/1 | 0.82 | 0.25 | 55,55,55,55 | 0 |
| 83 | MG | AT | 203 | 1/1 | 0.82 | 0.20 | 57,57,57,57 | 0 |
| 83 | MG | 1 | 3495 | 1/1 | 0.82 | 0.22 | 68,68,68,68 | 0 |

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| Mol | Type | Chain | Res | Atoms | RSCC | RSR | B-factors(Å$^2$) | Q<0.9 |
|---|---|---|---|---|---|---|---|---|
| 83 | MG | AW | 304 | 1/1 | 0.82 | 0.25 | 84,84,84,84 | 0 |
| 83 | MG | AS | 3538 | 1/1 | 0.82 | 0.11 | 32,32,32,32 | 0 |
| 83 | MG | AS | 3616 | 1/1 | 0.83 | 0.15 | 45,45,45,45 | 0 |
| 83 | MG | AS | 3621 | 1/1 | 0.83 | 0.14 | 53,53,53,53 | 0 |
| 83 | MG | 1 | 3428 | 1/1 | 0.83 | 0.30 | 47,47,47,47 | 0 |
| 83 | MG | AS | 3624 | 1/1 | 0.83 | 0.10 | 41,41,41,41 | 0 |
| 83 | MG | 1 | 3523 | 1/1 | 0.83 | 0.18 | 42,42,42,42 | 0 |
| 83 | MG | CM | 1806 | 1/1 | 0.83 | 0.10 | 28,28,28,28 | 0 |
| 83 | MG | AS | 3628 | 1/1 | 0.83 | 0.15 | 33,33,33,33 | 0 |
| 83 | MG | 4 | 206 | 1/1 | 0.83 | 0.15 | 24,24,24,24 | 0 |
| 83 | MG | 1 | 3661 | 1/1 | 0.83 | 0.09 | 33,33,33,33 | 0 |
| 83 | MG | AS | 3455 | 1/1 | 0.83 | 0.10 | 29,29,29,29 | 0 |
| 83 | MG | AS | 3482 | 1/1 | 0.83 | 0.13 | 67,67,67,67 | 0 |
| 83 | MG | AS | 3638 | 1/1 | 0.83 | 0.18 | 59,59,59,59 | 0 |
| 83 | MG | 1 | 3444 | 1/1 | 0.83 | 0.25 | 45,45,45,45 | 0 |
| 83 | MG | 1 | 3766 | 1/1 | 0.83 | 0.15 | 44,44,44,44 | 0 |
| 83 | MG | 1 | 3455 | 1/1 | 0.83 | 0.28 | 32,32,32,32 | 0 |
| 83 | MG | AS | 3661 | 1/1 | 0.83 | 0.19 | 64,64,64,64 | 0 |
| 83 | MG | AS | 3516 | 1/1 | 0.83 | 0.25 | 40,40,40,40 | 0 |
| 83 | MG | B | 1886 | 1/1 | 0.83 | 0.15 | 95,95,95,95 | 0 |
| 83 | MG | 1 | 3877 | 1/1 | 0.83 | 0.10 | 52,52,52,52 | 0 |
| 83 | MG | AH | 203 | 1/1 | 0.83 | 0.14 | 29,29,29,29 | 0 |
| 83 | MG | 1 | 3929 | 1/1 | 0.83 | 0.10 | 77,77,77,77 | 0 |
| 83 | MG | CM | 1877 | 1/1 | 0.83 | 0.12 | 47,47,47,47 | 0 |
| 83 | MG | B | 1802 | 1/1 | 0.83 | 0.25 | 45,45,45,45 | 0 |
| 83 | MG | 1 | 3552 | 1/1 | 0.83 | 0.17 | 50,50,50,50 | 0 |
| 83 | MG | AT | 204 | 1/1 | 0.83 | 0.20 | 64,64,64,64 | 0 |
| 83 | MG | 1 | 3836 | 1/1 | 0.83 | 0.16 | 31,31,31,31 | 0 |
| 83 | MG | 1 | 3729 | 1/1 | 0.83 | 0.35 | 50,50,50,50 | 0 |
| 83 | MG | 1 | 3895 | 1/1 | 0.83 | 0.12 | 44,44,44,44 | 0 |
| 83 | MG | 0 | 205 | 1/1 | 0.83 | 0.34 | 55,55,55,55 | 0 |
| 83 | MG | B | 1833 | 1/1 | 0.83 | 0.26 | 32,32,32,32 | 0 |
| 83 | MG | 1 | 3862 | 1/1 | 0.83 | 0.15 | 80,80,80,80 | 0 |
| 83 | MG | BH | 201 | 1/1 | 0.84 | 0.08 | 43,43,43,43 | 0 |
| 83 | MG | 1 | 3853 | 1/1 | 0.84 | 0.13 | 33,33,33,33 | 0 |
| 83 | MG | B | 1836 | 1/1 | 0.84 | 0.19 | 51,51,51,51 | 0 |
| 83 | MG | AS | 3618 | 1/1 | 0.84 | 0.18 | 45,45,45,45 | 0 |
| 83 | MG | Z | 202 | 1/1 | 0.84 | 0.15 | 58,58,58,58 | 0 |
| 83 | MG | 1 | 3433 | 1/1 | 0.84 | 0.28 | 45,45,45,45 | 0 |
| 83 | MG | 1 | 3855 | 1/1 | 0.84 | 0.11 | 43,43,43,43 | 0 |
| 83 | MG | 1 | 3721 | 1/1 | 0.84 | 0.18 | 43,43,43,43 | 0 |
| 83 | MG | 1 | 3908 | 1/1 | 0.84 | 0.09 | 23,23,23,23 | 0 |

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| Mol | Type | Chain | Res | Atoms | RSCC | RSR | B-factors(Å$^2$) | Q<0.9 |
|---|---|---|---|---|---|---|---|---|
| 83 | MG | CM | 1811 | 1/1 | 0.84 | 0.21 | 59,59,59,59 | 0 |
| 83 | MG | 1 | 3812 | 1/1 | 0.84 | 0.20 | 46,46,46,46 | 0 |
| 83 | MG | AS | 3473 | 1/1 | 0.84 | 0.11 | 16,16,16,16 | 0 |
| 83 | MG | AB | 202 | 1/1 | 0.84 | 0.21 | 76,76,76,76 | 0 |
| 83 | MG | AS | 3632 | 1/1 | 0.84 | 0.16 | 38,38,38,38 | 0 |
| 83 | MG | 1 | 3603 | 1/1 | 0.84 | 0.13 | 50,50,50,50 | 0 |
| 83 | MG | 1 | 3724 | 1/1 | 0.84 | 0.16 | 49,49,49,49 | 0 |
| 83 | MG | 1 | 3491 | 1/1 | 0.84 | 0.17 | 32,32,32,32 | 0 |
| 83 | MG | AS | 3642 | 1/1 | 0.84 | 0.16 | 46,46,46,46 | 0 |
| 83 | MG | CM | 1848 | 1/1 | 0.84 | 0.28 | 52,52,52,52 | 0 |
| 83 | MG | AS | 3512 | 1/1 | 0.84 | 0.17 | 20,20,20,20 | 0 |
| 83 | MG | CM | 1858 | 1/1 | 0.84 | 0.14 | 42,42,42,42 | 0 |
| 83 | MG | 1 | 3668 | 1/1 | 0.84 | 0.11 | 32,32,32,32 | 0 |
| 83 | MG | AS | 3518 | 1/1 | 0.84 | 0.19 | 43,43,43,43 | 0 |
| 83 | MG | B | 1940 | 1/1 | 0.84 | 0.15 | 76,76,76,76 | 0 |
| 83 | MG | 1 | 3793 | 1/1 | 0.84 | 0.11 | 18,18,18,18 | 0 |
| 83 | MG | AS | 3539 | 1/1 | 0.84 | 0.19 | 59,59,59,59 | 0 |
| 83 | MG | AS | 3540 | 1/1 | 0.84 | 0.19 | 37,37,37,37 | 0 |
| 83 | MG | 1 | 3839 | 1/1 | 0.84 | 0.08 | 55,55,55,55 | 0 |
| 83 | MG | B | 1897 | 1/1 | 0.84 | 0.12 | 42,42,42,42 | 0 |
| 83 | MG | w | 303 | 1/1 | 0.84 | 0.14 | 56,56,56,56 | 0 |
| 83 | MG | B | 1946 | 1/1 | 0.84 | 0.21 | 32,32,32,32 | 0 |
| 83 | MG | 1 | 3794 | 1/1 | 0.84 | 0.22 | 68,68,68,68 | 0 |
| 83 | MG | B | 1952 | 1/1 | 0.84 | 0.22 | 48,48,48,48 | 0 |
| 83 | MG | 1 | 3569 | 1/1 | 0.84 | 0.24 | 38,38,38,38 | 0 |
| 83 | MG | 1 | 3537 | 1/1 | 0.84 | 0.17 | 51,51,51,51 | 0 |
| 83 | MG | 1 | 3525 | 1/1 | 0.84 | 0.19 | 44,44,44,44 | 0 |
| 83 | MG | 1 | 3423 | 1/1 | 0.85 | 0.15 | 42,42,42,42 | 0 |
| 83 | MG | 1 | 3918 | 1/1 | 0.85 | 0.12 | 43,43,43,43 | 0 |
| 83 | MG | k | 401 | 1/1 | 0.85 | 0.11 | 58,58,58,58 | 0 |
| 83 | MG | B | 1919 | 1/1 | 0.85 | 0.26 | 50,50,50,50 | 0 |
| 83 | MG | AS | 3600 | 1/1 | 0.85 | 0.14 | 46,46,46,46 | 0 |
| 83 | MG | 1 | 3719 | 1/1 | 0.85 | 0.07 | 27,27,27,27 | 0 |
| 83 | MG | AE | 201 | 1/1 | 0.85 | 0.11 | 62,62,62,62 | 0 |
| 83 | MG | AS | 3426 | 1/1 | 0.85 | 0.17 | 30,30,30,30 | 0 |
| 83 | MG | B | 1864 | 1/1 | 0.85 | 0.18 | 42,42,42,42 | 0 |
| 83 | MG | B | 1865 | 1/1 | 0.85 | 0.13 | 25,25,25,25 | 0 |
| 83 | MG | 1 | 3881 | 1/1 | 0.85 | 0.18 | 25,25,25,25 | 0 |
| 83 | MG | 1 | 3924 | 1/1 | 0.85 | 0.14 | 69,69,69,69 | 0 |
| 83 | MG | 1 | 3675 | 1/1 | 0.85 | 0.20 | 52,52,52,52 | 0 |
| 83 | MG | 1 | 3575 | 1/1 | 0.85 | 0.16 | 28,28,28,28 | 0 |
| 83 | MG | w | 302 | 1/1 | 0.85 | 0.31 | 52,52,52,52 | 0 |

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| Mol | Type | Chain | Res | Atoms | RSCC | RSR | B-factors(Å$^2$) | Q<0.9 |
|---|---|---|---|---|---|---|---|---|
| 83 | MG | 1 | 3753 | 1/1 | 0.85 | 0.26 | 55,55,55,55 | 0 |
| 83 | MG | 1 | 3580 | 1/1 | 0.85 | 0.19 | 61,61,61,61 | 0 |
| 83 | MG | B | 1807 | 1/1 | 0.85 | 0.20 | 40,40,40,40 | 0 |
| 83 | MG | CM | 1883 | 1/1 | 0.85 | 0.12 | 45,45,45,45 | 0 |
| 83 | MG | CM | 1891 | 1/1 | 0.85 | 0.20 | 26,26,26,26 | 0 |
| 83 | MG | 1 | 3896 | 1/1 | 0.85 | 0.16 | 43,43,43,43 | 0 |
| 83 | MG | 1 | 3503 | 1/1 | 0.85 | 0.09 | 32,32,32,32 | 0 |
| 83 | MG | 1 | 3434 | 1/1 | 0.85 | 0.22 | 41,41,41,41 | 0 |
| 83 | MG | 1 | 3807 | 1/1 | 0.85 | 0.09 | 54,54,54,54 | 0 |
| 83 | MG | 1 | 3585 | 1/1 | 0.85 | 0.19 | 44,44,44,44 | 0 |
| 83 | MG | B | 1910 | 1/1 | 0.85 | 0.10 | 54,54,54,54 | 0 |
| 83 | MG | DG | 202 | 1/1 | 0.85 | 0.11 | 63,63,63,63 | 0 |
| 83 | MG | 1 | 3815 | 1/1 | 0.85 | 0.17 | 30,30,30,30 | 0 |
| 85 | ZN | CB | 201 | 1/1 | 0.85 | 0.14 | 202,202,202,202 | 0 |
| 83 | MG | AS | 3605 | 1/1 | 0.86 | 0.22 | 38,38,38,38 | 0 |
| 83 | MG | 1 | 3925 | 1/1 | 0.86 | 0.10 | 37,37,37,37 | 0 |
| 83 | MG | B | 1835 | 1/1 | 0.86 | 0.18 | 21,21,21,21 | 0 |
| 83 | MG | 1 | 3926 | 1/1 | 0.86 | 0.23 | 53,53,53,53 | 0 |
| 83 | MG | B | 1844 | 1/1 | 0.86 | 0.13 | 55,55,55,55 | 0 |
| 83 | MG | AS | 3449 | 1/1 | 0.86 | 0.14 | 40,40,40,40 | 0 |
| 83 | MG | AS | 3450 | 1/1 | 0.86 | 0.18 | 38,38,38,38 | 0 |
| 83 | MG | AS | 3626 | 1/1 | 0.86 | 0.19 | 40,40,40,40 | 0 |
| 83 | MG | 1 | 3401 | 1/1 | 0.86 | 0.29 | 30,30,30,30 | 0 |
| 83 | MG | 1 | 3885 | 1/1 | 0.86 | 0.09 | 53,53,53,53 | 0 |
| 83 | MG | 1 | 3804 | 1/1 | 0.86 | 0.12 | 30,30,30,30 | 0 |
| 83 | MG | 1 | 3579 | 1/1 | 0.86 | 0.09 | 36,36,36,36 | 0 |
| 83 | MG | 1 | 3892 | 1/1 | 0.86 | 0.10 | 53,53,53,53 | 0 |
| 83 | MG | 3 | 203 | 1/1 | 0.86 | 0.15 | 31,31,31,31 | 0 |
| 83 | MG | AS | 3500 | 1/1 | 0.86 | 0.10 | 32,32,32,32 | 0 |
| 83 | MG | CM | 1823 | 1/1 | 0.86 | 0.16 | 34,34,34,34 | 0 |
| 83 | MG | CM | 1827 | 1/1 | 0.86 | 0.21 | 34,34,34,34 | 0 |
| 83 | MG | CM | 1835 | 1/1 | 0.86 | 0.22 | 54,54,54,54 | 0 |
| 83 | MG | 1 | 3693 | 1/1 | 0.86 | 0.10 | 37,37,37,37 | 0 |
| 83 | MG | 1 | 3894 | 1/1 | 0.86 | 0.15 | 57,57,57,57 | 0 |
| 83 | MG | CM | 1845 | 1/1 | 0.86 | 0.13 | 29,29,29,29 | 0 |
| 83 | MG | 1 | 3778 | 1/1 | 0.86 | 0.19 | 57,57,57,57 | 0 |
| 83 | MG | CM | 1850 | 1/1 | 0.86 | 0.12 | 58,58,58,58 | 0 |
| 83 | MG | AS | 3643 | 1/1 | 0.86 | 0.16 | 39,39,39,39 | 0 |
| 83 | MG | 1 | 3593 | 1/1 | 0.86 | 0.17 | 35,35,35,35 | 0 |
| 83 | MG | 1 | 3457 | 1/1 | 0.86 | 0.10 | 20,20,20,20 | 0 |
| 83 | MG | AS | 3653 | 1/1 | 0.86 | 0.15 | 68,68,68,68 | 0 |
| 83 | MG | B | 1887 | 1/1 | 0.86 | 0.23 | 47,47,47,47 | 0 |

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| Mol | Type | Chain | Res | Atoms | RSCC | RSR | B-factors(Å$^2$) | Q<0.9 |
|---|---|---|---|---|---|---|---|---|
| 83 | MG | CM | 1868 | 1/1 | 0.86 | 0.18 | 64,64,64,64 | 0 |
| 83 | MG | CM | 1872 | 1/1 | 0.86 | 0.19 | 45,45,45,45 | 0 |
| 83 | MG | 1 | 3906 | 1/1 | 0.86 | 0.13 | 27,27,27,27 | 0 |
| 83 | MG | AS | 3544 | 1/1 | 0.86 | 0.12 | 28,28,28,28 | 0 |
| 83 | MG | AS | 3671 | 1/1 | 0.86 | 0.13 | 32,32,32,32 | 0 |
| 83 | MG | AS | 3547 | 1/1 | 0.86 | 0.11 | 35,35,35,35 | 0 |
| 83 | MG | 4 | 209 | 1/1 | 0.86 | 0.07 | 54,54,54,54 | 0 |
| 83 | MG | 1 | 3835 | 1/1 | 0.86 | 0.08 | 25,25,25,25 | 0 |
| 83 | MG | AS | 3678 | 1/1 | 0.86 | 0.12 | 42,42,42,42 | 0 |
| 83 | MG | 1 | 3515 | 1/1 | 0.86 | 0.20 | 21,21,21,21 | 0 |
| 83 | MG | 1 | 3653 | 1/1 | 0.86 | 0.07 | 39,39,39,39 | 0 |
| 83 | MG | 1 | 3498 | 1/1 | 0.86 | 0.21 | 39,39,39,39 | 0 |
| 83 | MG | 1 | 3657 | 1/1 | 0.86 | 0.15 | 22,22,22,22 | 0 |
| 83 | MG | DB | 201 | 1/1 | 0.86 | 0.13 | 38,38,38,38 | 0 |
| 83 | MG | 1 | 3526 | 1/1 | 0.86 | 0.12 | 48,48,48,48 | 0 |
| 83 | MG | AS | 3599 | 1/1 | 0.86 | 0.28 | 50,50,50,50 | 0 |
| 83 | MG | 1 | 3875 | 1/1 | 0.86 | 0.11 | 42,42,42,42 | 0 |
| 83 | MG | 1 | 3799 | 1/1 | 0.86 | 0.10 | 33,33,33,33 | 0 |
| 83 | MG | 1 | 3664 | 1/1 | 0.86 | 0.20 | 32,32,32,32 | 0 |
| 86 | HYG | B | 1953 | 36/36 | 0.86 | 0.14 | 49,77,94,99 | 0 |
| 83 | MG | 1 | 3827 | 1/1 | 0.87 | 0.14 | 50,50,50,50 | 0 |
| 83 | MG | B | 1892 | 1/1 | 0.87 | 0.15 | 40,40,40,40 | 0 |
| 83 | MG | B | 1823 | 1/1 | 0.87 | 0.14 | 31,31,31,31 | 0 |
| 83 | MG | B | 1824 | 1/1 | 0.87 | 0.21 | 26,26,26,26 | 0 |
| 83 | MG | B | 1825 | 1/1 | 0.87 | 0.15 | 32,32,32,32 | 0 |
| 83 | MG | AS | 3644 | 1/1 | 0.87 | 0.13 | 59,59,59,59 | 0 |
| 83 | MG | 1 | 3500 | 1/1 | 0.87 | 0.16 | 37,37,37,37 | 0 |
| 83 | MG | AS | 3648 | 1/1 | 0.87 | 0.17 | 32,32,32,32 | 0 |
| 83 | MG | 1 | 3879 | 1/1 | 0.87 | 0.11 | 39,39,39,39 | 0 |
| 83 | MG | B | 1830 | 1/1 | 0.87 | 0.21 | 46,46,46,46 | 0 |
| 83 | MG | B | 1905 | 1/1 | 0.87 | 0.13 | 38,38,38,38 | 0 |
| 83 | MG | Q | 201 | 1/1 | 0.87 | 0.20 | 49,49,49,49 | 0 |
| 83 | MG | 1 | 3880 | 1/1 | 0.87 | 0.21 | 58,58,58,58 | 0 |
| 83 | MG | B | 1908 | 1/1 | 0.87 | 0.19 | 46,46,46,46 | 0 |
| 83 | MG | 1 | 3765 | 1/1 | 0.87 | 0.13 | 38,38,38,38 | 0 |
| 83 | MG | AS | 3596 | 1/1 | 0.87 | 0.08 | 37,37,37,37 | 0 |
| 83 | MG | 1 | 3920 | 1/1 | 0.87 | 0.20 | 49,49,49,49 | 0 |
| 83 | MG | 1 | 3884 | 1/1 | 0.87 | 0.10 | 65,65,65,65 | 0 |
| 83 | MG | AS | 3412 | 1/1 | 0.87 | 0.16 | 23,23,23,23 | 0 |
| 83 | MG | B | 1845 | 1/1 | 0.87 | 0.18 | 35,35,35,35 | 0 |
| 83 | MG | 1 | 3617 | 1/1 | 0.87 | 0.08 | 37,37,37,37 | 0 |
| 83 | MG | AS | 3603 | 1/1 | 0.87 | 0.16 | 38,38,38,38 | 0 |

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| Mol | Type | Chain | Res | Atoms | RSCC | RSR | B-factors(Å$^2$) | Q<0.9 |
|---|---|---|---|---|---|---|---|---|
| 83 | MG | 1 | 3643 | 1/1 | 0.87 | 0.12 | 27,27,27,27 | 0 |
| 83 | MG | AS | 3606 | 1/1 | 0.87 | 0.07 | 32,32,32,32 | 0 |
| 83 | MG | 1 | 3540 | 1/1 | 0.87 | 0.23 | 42,42,42,42 | 0 |
| 83 | MG | 1 | 3740 | 1/1 | 0.87 | 0.18 | 53,53,53,53 | 0 |
| 83 | MG | B | 1859 | 1/1 | 0.87 | 0.16 | 34,34,34,34 | 0 |
| 83 | MG | AS | 3467 | 1/1 | 0.87 | 0.12 | 57,57,57,57 | 0 |
| 83 | MG | 1 | 3647 | 1/1 | 0.87 | 0.14 | 45,45,45,45 | 0 |
| 83 | MG | 1 | 3789 | 1/1 | 0.87 | 0.15 | 21,21,21,21 | 0 |
| 83 | MG | CK | 102 | 1/1 | 0.87 | 0.14 | 32,32,32,32 | 0 |
| 83 | MG | 1 | 3680 | 1/1 | 0.87 | 0.08 | 30,30,30,30 | 0 |
| 83 | MG | 1 | 3845 | 1/1 | 0.87 | 0.15 | 37,37,37,37 | 0 |
| 83 | MG | 1 | 3872 | 1/1 | 0.87 | 0.12 | 48,48,48,48 | 0 |
| 83 | MG | 1 | 3725 | 1/1 | 0.87 | 0.17 | 40,40,40,40 | 0 |
| 83 | MG | AS | 3504 | 1/1 | 0.87 | 0.24 | 50,50,50,50 | 0 |
| 83 | MG | 1 | 3817 | 1/1 | 0.87 | 0.10 | 32,32,32,32 | 0 |
| 85 | ZN | DQ | 102 | 1/1 | 0.87 | 0.27 | 118,118,118,118 | 0 |
| 83 | MG | B | 1815 | 1/1 | 0.87 | 0.25 | 51,51,51,51 | 0 |
| 83 | MG | B | 1931 | 1/1 | 0.88 | 0.17 | 47,47,47,47 | 0 |
| 83 | MG | AS | 3474 | 1/1 | 0.88 | 0.21 | 41,41,41,41 | 0 |
| 83 | MG | B | 1814 | 1/1 | 0.88 | 0.13 | 53,53,53,53 | 0 |
| 83 | MG | B | 1882 | 1/1 | 0.88 | 0.20 | 49,49,49,49 | 0 |
| 83 | MG | 1 | 3734 | 1/1 | 0.88 | 0.15 | 14,14,14,14 | 0 |
| 83 | MG | 1 | 3844 | 1/1 | 0.88 | 0.12 | 48,48,48,48 | 0 |
| 83 | MG | 1 | 3464 | 1/1 | 0.88 | 0.23 | 48,48,48,48 | 0 |
| 83 | MG | 1 | 3682 | 1/1 | 0.88 | 0.19 | 85,85,85,85 | 0 |
| 83 | MG | AS | 3507 | 1/1 | 0.88 | 0.13 | 20,20,20,20 | 0 |
| 83 | MG | 1 | 3887 | 1/1 | 0.88 | 0.07 | 58,58,58,58 | 0 |
| 83 | MG | AS | 3515 | 1/1 | 0.88 | 0.14 | 31,31,31,31 | 0 |
| 83 | MG | CM | 1824 | 1/1 | 0.88 | 0.08 | 28,28,28,28 | 0 |
| 83 | MG | 1 | 3539 | 1/1 | 0.88 | 0.09 | 24,24,24,24 | 0 |
| 83 | MG | CM | 1833 | 1/1 | 0.88 | 0.24 | 42,42,42,42 | 0 |
| 83 | MG | B | 1828 | 1/1 | 0.88 | 0.17 | 39,39,39,39 | 0 |
| 83 | MG | B | 1947 | 1/1 | 0.88 | 0.15 | 63,63,63,63 | 0 |
| 83 | MG | 1 | 3611 | 1/1 | 0.88 | 0.26 | 24,24,24,24 | 0 |
| 83 | MG | AS | 3649 | 1/1 | 0.88 | 0.13 | 48,48,48,48 | 0 |
| 83 | MG | 1 | 3718 | 1/1 | 0.88 | 0.12 | 35,35,35,35 | 0 |
| 83 | MG | B | 1900 | 1/1 | 0.88 | 0.25 | 50,50,50,50 | 0 |
| 83 | MG | AS | 3657 | 1/1 | 0.88 | 0.18 | 17,17,17,17 | 0 |
| 83 | MG | 1 | 3763 | 1/1 | 0.88 | 0.17 | 28,28,28,28 | 0 |
| 83 | MG | 1 | 3548 | 1/1 | 0.88 | 0.13 | 43,43,43,43 | 0 |
| 83 | MG | K | 301 | 1/1 | 0.88 | 0.06 | 27,27,27,27 | 0 |
| 83 | MG | AS | 3667 | 1/1 | 0.88 | 0.11 | 92,92,92,92 | 0 |

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| Mol | Type | Chain | Res | Atoms | RSCC | RSR | B-factors(Å$^2$) | Q<0.9 |
|---|---|---|---|---|---|---|---|---|
| 83 | MG | 1 | 3691 | 1/1 | 0.88 | 0.20 | 22,22,22,22 | 0 |
| 83 | MG | 1 | 3824 | 1/1 | 0.88 | 0.12 | 47,47,47,47 | 0 |
| 83 | MG | 1 | 3529 | 1/1 | 0.88 | 0.08 | 38,38,38,38 | 0 |
| 83 | MG | 1 | 3829 | 1/1 | 0.88 | 0.12 | 25,25,25,25 | 0 |
| 83 | MG | 1 | 3413 | 1/1 | 0.88 | 0.21 | 31,31,31,31 | 0 |
| 83 | MG | 1 | 3663 | 1/1 | 0.88 | 0.14 | 54,54,54,54 | 0 |
| 83 | MG | AR | 401 | 1/1 | 0.88 | 0.18 | 48,48,48,48 | 0 |
| 83 | MG | AS | 3404 | 1/1 | 0.88 | 0.27 | 19,19,19,19 | 0 |
| 83 | MG | CM | 1884 | 1/1 | 0.88 | 0.17 | 54,54,54,54 | 0 |
| 83 | MG | CM | 1890 | 1/1 | 0.88 | 0.11 | 24,24,24,24 | 0 |
| 83 | MG | AT | 206 | 1/1 | 0.88 | 0.14 | 61,61,61,61 | 0 |
| 83 | MG | 1 | 3833 | 1/1 | 0.88 | 0.19 | 41,41,41,41 | 0 |
| 83 | MG | AS | 3413 | 1/1 | 0.88 | 0.17 | 24,24,24,24 | 0 |
| 83 | MG | 1 | 3697 | 1/1 | 0.88 | 0.09 | 50,50,50,50 | 0 |
| 83 | MG | AS | 3420 | 1/1 | 0.88 | 0.11 | 15,15,15,15 | 0 |
| 83 | MG | 1 | 3679 | 1/1 | 0.88 | 0.13 | 27,27,27,27 | 0 |
| 83 | MG | 1 | 3599 | 1/1 | 0.88 | 0.16 | 36,36,36,36 | 0 |
| 83 | MG | AS | 3428 | 1/1 | 0.88 | 0.23 | 37,37,37,37 | 0 |
| 83 | MG | AS | 3441 | 1/1 | 0.88 | 0.21 | 29,29,29,29 | 0 |
| 83 | MG | 1 | 3705 | 1/1 | 0.88 | 0.11 | 34,34,34,34 | 0 |
| 83 | MG | 1 | 3731 | 1/1 | 0.88 | 0.10 | 37,37,37,37 | 0 |
| 83 | MG | B | 1868 | 1/1 | 0.88 | 0.09 | 59,59,59,59 | 0 |
| 83 | MG | 1 | 3706 | 1/1 | 0.88 | 0.12 | 36,36,36,36 | 0 |
| 83 | MG | r | 301 | 1/1 | 0.89 | 0.19 | 34,34,34,34 | 0 |
| 83 | MG | B | 1805 | 1/1 | 0.89 | 0.17 | 57,57,57,57 | 0 |
| 83 | MG | Y | 202 | 1/1 | 0.89 | 0.18 | 71,71,71,71 | 0 |
| 83 | MG | 1 | 3717 | 1/1 | 0.89 | 0.17 | 42,42,42,42 | 0 |
| 83 | MG | AS | 3524 | 1/1 | 0.89 | 0.19 | 27,27,27,27 | 0 |
| 83 | MG | AS | 3537 | 1/1 | 0.89 | 0.20 | 41,41,41,41 | 0 |
| 83 | MG | 1 | 3889 | 1/1 | 0.89 | 0.11 | 69,69,69,69 | 0 |
| 83 | MG | 1 | 3600 | 1/1 | 0.89 | 0.13 | 35,35,35,35 | 0 |
| 83 | MG | B | 1923 | 1/1 | 0.89 | 0.15 | 57,57,57,57 | 0 |
| 83 | MG | 1 | 3558 | 1/1 | 0.89 | 0.13 | 47,47,47,47 | 0 |
| 83 | MG | CM | 1825 | 1/1 | 0.89 | 0.25 | 31,31,31,31 | 0 |
| 83 | MG | 1 | 3658 | 1/1 | 0.89 | 0.10 | 39,39,39,39 | 0 |
| 83 | MG | AS | 3550 | 1/1 | 0.89 | 0.20 | 19,19,19,19 | 0 |
| 83 | MG | B | 1879 | 1/1 | 0.89 | 0.20 | 46,46,46,46 | 0 |
| 83 | MG | AS | 3658 | 1/1 | 0.89 | 0.10 | 28,28,28,28 | 0 |
| 83 | MG | 1 | 3863 | 1/1 | 0.89 | 0.12 | 29,29,29,29 | 0 |
| 83 | MG | AS | 3565 | 1/1 | 0.89 | 0.23 | 31,31,31,31 | 0 |
| 83 | MG | AS | 3665 | 1/1 | 0.89 | 0.12 | 51,51,51,51 | 0 |
| 83 | MG | CM | 1849 | 1/1 | 0.89 | 0.14 | 50,50,50,50 | 0 |

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| Mol | Type | Chain | Res | Atoms | RSCC | RSR | B-factors(Å$^2$) | Q<0.9 |
|---|---|---|---|---|---|---|---|---|
| 83 | MG | AS | 3417 | 1/1 | 0.89 | 0.21 | 23,23,23,23 | 0 |
| 83 | MG | AS | 3419 | 1/1 | 0.89 | 0.12 | 27,27,27,27 | 0 |
| 83 | MG | 1 | 3684 | 1/1 | 0.89 | 0.25 | 54,54,54,54 | 0 |
| 83 | MG | 1 | 3701 | 1/1 | 0.89 | 0.18 | 59,59,59,59 | 0 |
| 83 | MG | AS | 3674 | 1/1 | 0.89 | 0.18 | 44,44,44,44 | 0 |
| 83 | MG | B | 1935 | 1/1 | 0.89 | 0.17 | 56,56,56,56 | 0 |
| 83 | MG | 1 | 3723 | 1/1 | 0.89 | 0.06 | 16,16,16,16 | 0 |
| 83 | MG | AS | 3677 | 1/1 | 0.89 | 0.14 | 45,45,45,45 | 0 |
| 83 | MG | 2 | 203 | 1/1 | 0.89 | 0.08 | 37,37,37,37 | 0 |
| 83 | MG | AS | 3442 | 1/1 | 0.89 | 0.22 | 45,45,45,45 | 0 |
| 83 | MG | AS | 3447 | 1/1 | 0.89 | 0.35 | 48,48,48,48 | 0 |
| 83 | MG | 1 | 3759 | 1/1 | 0.89 | 0.08 | 49,49,49,49 | 0 |
| 83 | MG | 1 | 3621 | 1/1 | 0.89 | 0.10 | 54,54,54,54 | 0 |
| 83 | MG | 1 | 3662 | 1/1 | 0.89 | 0.15 | 42,42,42,42 | 0 |
| 83 | MG | AT | 209 | 1/1 | 0.89 | 0.15 | 52,52,52,52 | 0 |
| 83 | MG | 1 | 3690 | 1/1 | 0.89 | 0.08 | 25,25,25,25 | 0 |
| 83 | MG | AS | 3468 | 1/1 | 0.89 | 0.10 | 37,37,37,37 | 0 |
| 83 | MG | 1 | 3773 | 1/1 | 0.89 | 0.12 | 32,32,32,32 | 0 |
| 83 | MG | 1 | 3774 | 1/1 | 0.89 | 0.10 | 29,29,29,29 | 0 |
| 83 | MG | AS | 3481 | 1/1 | 0.89 | 0.13 | 25,25,25,25 | 0 |
| 83 | MG | BJ | 302 | 1/1 | 0.89 | 0.16 | 58,58,58,58 | 0 |
| 83 | MG | 1 | 3775 | 1/1 | 0.89 | 0.14 | 32,32,32,32 | 0 |
| 83 | MG | B | 1903 | 1/1 | 0.89 | 0.17 | 87,87,87,87 | 0 |
| 83 | MG | 4 | 212 | 1/1 | 0.89 | 0.08 | 60,60,60,60 | 0 |
| 83 | MG | 1 | 3463 | 1/1 | 0.89 | 0.16 | 18,18,18,18 | 0 |
| 83 | MG | 1 | 3818 | 1/1 | 0.89 | 0.11 | 38,38,38,38 | 0 |
| 83 | MG | k | 403 | 1/1 | 0.89 | 0.13 | 57,57,57,57 | 0 |
| 83 | MG | 1 | 3562 | 1/1 | 0.89 | 0.15 | 48,48,48,48 | 0 |
| 83 | MG | 1 | 3654 | 1/1 | 0.89 | 0.13 | 70,70,70,70 | 0 |
| 83 | MG | B | 1839 | 1/1 | 0.90 | 0.30 | 48,48,48,48 | 0 |
| 83 | MG | B | 1842 | 1/1 | 0.90 | 0.15 | 25,25,25,25 | 0 |
| 83 | MG | 1 | 3628 | 1/1 | 0.90 | 0.22 | 48,48,48,48 | 0 |
| 83 | MG | 1 | 3429 | 1/1 | 0.90 | 0.23 | 24,24,24,24 | 0 |
| 83 | MG | 1 | 3851 | 1/1 | 0.90 | 0.08 | 19,19,19,19 | 0 |
| 83 | MG | CM | 1801 | 1/1 | 0.90 | 0.21 | 41,41,41,41 | 0 |
| 83 | MG | CM | 1805 | 1/1 | 0.90 | 0.13 | 18,18,18,18 | 0 |
| 83 | MG | B | 1847 | 1/1 | 0.90 | 0.13 | 35,35,35,35 | 0 |
| 83 | MG | 1 | 3809 | 1/1 | 0.90 | 0.07 | 57,57,57,57 | 0 |
| 83 | MG | 1 | 3577 | 1/1 | 0.90 | 0.14 | 12,12,12,12 | 0 |
| 83 | MG | B | 1855 | 1/1 | 0.90 | 0.16 | 79,79,79,79 | 0 |
| 83 | MG | 1 | 3770 | 1/1 | 0.90 | 0.12 | 46,46,46,46 | 0 |
| 83 | MG | B | 1858 | 1/1 | 0.90 | 0.12 | 66,66,66,66 | 0 |

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| Mol | Type | Chain | Res | Atoms | RSCC | RSR | B-factors(Å$^2$) | Q<0.9 |
|---|---|---|---|---|---|---|---|---|
| 83 | MG | 1 | 3771 | 1/1 | 0.90 | 0.10 | 38,38,38,38 | 0 |
| 83 | MG | 3 | 212 | 1/1 | 0.90 | 0.15 | 59,59,59,59 | 0 |
| 83 | MG | 1 | 3608 | 1/1 | 0.90 | 0.32 | 67,67,67,67 | 0 |
| 83 | MG | 1 | 3860 | 1/1 | 0.90 | 0.11 | 46,46,46,46 | 0 |
| 83 | MG | 1 | 3497 | 1/1 | 0.90 | 0.17 | 11,11,11,11 | 0 |
| 83 | MG | AG | 202 | 1/1 | 0.90 | 0.12 | 52,52,52,52 | 0 |
| 83 | MG | B | 1869 | 1/1 | 0.90 | 0.17 | 41,41,41,41 | 0 |
| 83 | MG | B | 1870 | 1/1 | 0.90 | 0.10 | 42,42,42,42 | 0 |
| 83 | MG | 1 | 3901 | 1/1 | 0.90 | 0.09 | 29,29,29,29 | 0 |
| 83 | MG | 1 | 3484 | 1/1 | 0.90 | 0.12 | 34,34,34,34 | 0 |
| 83 | MG | B | 1950 | 1/1 | 0.90 | 0.08 | 40,40,40,40 | 0 |
| 83 | MG | CM | 1843 | 1/1 | 0.90 | 0.10 | 26,26,26,26 | 0 |
| 83 | MG | 1 | 3904 | 1/1 | 0.90 | 0.14 | 32,32,32,32 | 0 |
| 83 | MG | G | 301 | 1/1 | 0.90 | 0.11 | 72,72,72,72 | 0 |
| 83 | MG | AM | 101 | 1/1 | 0.90 | 0.16 | 54,54,54,54 | 0 |
| 83 | MG | AS | 3536 | 1/1 | 0.90 | 0.12 | 35,35,35,35 | 0 |
| 83 | MG | 1 | 3905 | 1/1 | 0.90 | 0.10 | 27,27,27,27 | 0 |
| 83 | MG | CM | 1857 | 1/1 | 0.90 | 0.11 | 48,48,48,48 | 0 |
| 83 | MG | B | 1803 | 1/1 | 0.90 | 0.17 | 28,28,28,28 | 0 |
| 83 | MG | j | 303 | 1/1 | 0.90 | 0.10 | 19,19,19,19 | 0 |
| 83 | MG | 1 | 3730 | 1/1 | 0.90 | 0.22 | 55,55,55,55 | 0 |
| 83 | MG | k | 402 | 1/1 | 0.90 | 0.12 | 54,54,54,54 | 0 |
| 83 | MG | 1 | 3427 | 1/1 | 0.90 | 0.23 | 16,16,16,16 | 0 |
| 83 | MG | CM | 1871 | 1/1 | 0.90 | 0.15 | 22,22,22,22 | 0 |
| 83 | MG | 1 | 3619 | 1/1 | 0.90 | 0.11 | 33,33,33,33 | 0 |
| 83 | MG | AS | 3552 | 1/1 | 0.90 | 0.16 | 27,27,27,27 | 0 |
| 83 | MG | Y | 203 | 1/1 | 0.90 | 0.23 | 41,41,41,41 | 0 |
| 83 | MG | 1 | 3620 | 1/1 | 0.90 | 0.13 | 21,21,21,21 | 0 |
| 83 | MG | 1 | 3735 | 1/1 | 0.90 | 0.24 | 33,33,33,33 | 0 |
| 83 | MG | B | 1821 | 1/1 | 0.90 | 0.20 | 31,31,31,31 | 0 |
| 83 | MG | AT | 201 | 1/1 | 0.90 | 0.11 | 21,21,21,21 | 0 |
| 83 | MG | AS | 3575 | 1/1 | 0.90 | 0.09 | 33,33,33,33 | 0 |
| 83 | MG | 1 | 3739 | 1/1 | 0.90 | 0.17 | 28,28,28,28 | 0 |
| 83 | MG | 1 | 3411 | 1/1 | 0.90 | 0.15 | 10,10,10,10 | 0 |
| 83 | MG | CM | 1897 | 1/1 | 0.90 | 0.18 | 41,41,41,41 | 0 |
| 83 | MG | AS | 3408 | 1/1 | 0.90 | 0.09 | 28,28,28,28 | 0 |
| 83 | MG | AS | 3588 | 1/1 | 0.90 | 0.09 | 21,21,21,21 | 0 |
| 83 | MG | AT | 208 | 1/1 | 0.90 | 0.13 | 27,27,27,27 | 0 |
| 83 | MG | CP | 301 | 1/1 | 0.90 | 0.24 | 32,32,32,32 | 0 |
| 83 | MG | 1 | 3673 | 1/1 | 0.90 | 0.14 | 47,47,47,47 | 0 |
| 83 | MG | v | 303 | 1/1 | 0.90 | 0.10 | 72,72,72,72 | 0 |
| 83 | MG | 1 | 3494 | 1/1 | 0.90 | 0.17 | 13,13,13,13 | 0 |

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| Mol | Type | Chain | Res | Atoms | RSCC | RSR | B-factors(Å$^2$) | Q<0.9 |
|---|---|---|---|---|---|---|---|---|
| 83 | MG | 1 | 3623 | 1/1 | 0.90 | 0.08 | 40,40,40,40 | 0 |
| 83 | MG | 1 | 3508 | 1/1 | 0.90 | 0.16 | 33,33,33,33 | 0 |
| 84 | 3K5 | 1 | 3402 | 57/57 | 0.90 | 0.17 | 26,53,74,90 | 0 |
| 84 | 3K5 | AS | 3401 | 57/57 | 0.90 | 0.15 | 41,66,88,90 | 0 |
| 85 | ZN | AH | 201 | 1/1 | 0.90 | 0.10 | 138,138,138,138 | 0 |
| 83 | MG | 1 | 3843 | 1/1 | 0.90 | 0.27 | 62,62,62,62 | 0 |
| 85 | ZN | h | 201 | 1/1 | 0.90 | 0.09 | 209,209,209,209 | 0 |
| 83 | MG | AS | 3421 | 1/1 | 0.90 | 0.33 | 19,19,19,19 | 0 |
| 83 | MG | 1 | 3698 | 1/1 | 0.90 | 0.18 | 58,58,58,58 | 0 |
| 83 | MG | 1 | 3762 | 1/1 | 0.90 | 0.13 | 31,31,31,31 | 0 |
| 86 | HYG | CM | 1902 | 36/36 | 0.90 | 0.12 | 34,53,79,89 | 0 |
| 83 | MG | CM | 1813 | 1/1 | 0.91 | 0.24 | 35,35,35,35 | 0 |
| 83 | MG | 1 | 3542 | 1/1 | 0.91 | 0.16 | 28,28,28,28 | 0 |
| 83 | MG | 1 | 3487 | 1/1 | 0.91 | 0.05 | 11,11,11,11 | 0 |
| 83 | MG | 1 | 3567 | 1/1 | 0.91 | 0.07 | 20,20,20,20 | 0 |
| 83 | MG | 1 | 3430 | 1/1 | 0.91 | 0.10 | 50,50,50,50 | 0 |
| 83 | MG | B | 1818 | 1/1 | 0.91 | 0.09 | 33,33,33,33 | 0 |
| 83 | MG | 0 | 203 | 1/1 | 0.91 | 0.11 | 75,75,75,75 | 0 |
| 83 | MG | 1 | 3490 | 1/1 | 0.91 | 0.15 | 44,44,44,44 | 0 |
| 83 | MG | B | 1933 | 1/1 | 0.91 | 0.10 | 57,57,57,57 | 0 |
| 83 | MG | 1 | 3473 | 1/1 | 0.91 | 0.18 | 13,13,13,13 | 0 |
| 83 | MG | 1 | 3626 | 1/1 | 0.91 | 0.16 | 46,46,46,46 | 0 |
| 83 | MG | 1 | 3507 | 1/1 | 0.91 | 0.17 | 9,9,9,9 | 0 |
| 83 | MG | 1 | 3736 | 1/1 | 0.91 | 0.17 | 39,39,39,39 | 0 |
| 83 | MG | 1 | 3780 | 1/1 | 0.91 | 0.18 | 32,32,32,32 | 0 |
| 83 | MG | AS | 3567 | 1/1 | 0.91 | 0.09 | 45,45,45,45 | 0 |
| 83 | MG | CM | 1839 | 1/1 | 0.91 | 0.17 | 36,36,36,36 | 0 |
| 83 | MG | CM | 1841 | 1/1 | 0.91 | 0.27 | 45,45,45,45 | 0 |
| 83 | MG | AS | 3434 | 1/1 | 0.91 | 0.18 | 18,18,18,18 | 0 |
| 83 | MG | B | 1891 | 1/1 | 0.91 | 0.10 | 41,41,41,41 | 0 |
| 83 | MG | 1 | 3446 | 1/1 | 0.91 | 0.10 | 71,71,71,71 | 0 |
| 83 | MG | AS | 3672 | 1/1 | 0.91 | 0.08 | 29,29,29,29 | 0 |
| 83 | MG | 1 | 3514 | 1/1 | 0.91 | 0.17 | 30,30,30,30 | 0 |
| 83 | MG | CM | 1851 | 1/1 | 0.91 | 0.12 | 28,28,28,28 | 0 |
| 83 | MG | 1 | 3787 | 1/1 | 0.91 | 0.22 | 23,23,23,23 | 0 |
| 83 | MG | CM | 1855 | 1/1 | 0.91 | 0.17 | 29,29,29,29 | 0 |
| 83 | MG | 1 | 3907 | 1/1 | 0.91 | 0.18 | 74,74,74,74 | 0 |
| 83 | MG | AS | 3591 | 1/1 | 0.91 | 0.16 | 52,52,52,52 | 0 |
| 83 | MG | AS | 3593 | 1/1 | 0.91 | 0.07 | 16,16,16,16 | 0 |
| 83 | MG | AD | 201 | 1/1 | 0.91 | 0.14 | 59,59,59,59 | 0 |
| 83 | MG | AS | 3465 | 1/1 | 0.91 | 0.14 | 19,19,19,19 | 0 |
| 83 | MG | CM | 1865 | 1/1 | 0.91 | 0.17 | 45,45,45,45 | 0 |

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| Mol | Type | Chain | Res | Atoms | RSCC | RSR | B-factors(Å$^2$) | Q<0.9 |
|---|---|---|---|---|---|---|---|---|
| 83 | MG | 1 | 3637 | 1/1 | 0.91 | 0.09 | 49,49,49,49 | 0 |
| 83 | MG | 1 | 3790 | 1/1 | 0.91 | 0.10 | 49,49,49,49 | 0 |
| 83 | MG | AS | 3469 | 1/1 | 0.91 | 0.25 | 25,25,25,25 | 0 |
| 83 | MG | AS | 3472 | 1/1 | 0.91 | 0.24 | 36,36,36,36 | 0 |
| 83 | MG | B | 1951 | 1/1 | 0.91 | 0.11 | 29,29,29,29 | 0 |
| 83 | MG | 1 | 3535 | 1/1 | 0.91 | 0.14 | 34,34,34,34 | 0 |
| 83 | MG | AS | 3476 | 1/1 | 0.91 | 0.24 | 34,34,34,34 | 0 |
| 83 | MG | AU | 202 | 1/1 | 0.91 | 0.18 | 31,31,31,31 | 0 |
| 83 | MG | 1 | 3425 | 1/1 | 0.91 | 0.12 | 36,36,36,36 | 0 |
| 83 | MG | 1 | 3840 | 1/1 | 0.91 | 0.06 | 14,14,14,14 | 0 |
| 83 | MG | CM | 1885 | 1/1 | 0.91 | 0.10 | 26,26,26,26 | 0 |
| 83 | MG | BB | 302 | 1/1 | 0.91 | 0.12 | 53,53,53,53 | 0 |
| 83 | MG | BE | 301 | 1/1 | 0.91 | 0.17 | 33,33,33,33 | 0 |
| 83 | MG | 1 | 3496 | 1/1 | 0.91 | 0.11 | 31,31,31,31 | 0 |
| 83 | MG | 1 | 3755 | 1/1 | 0.91 | 0.14 | 34,34,34,34 | 0 |
| 83 | MG | 1 | 3758 | 1/1 | 0.91 | 0.14 | 33,33,33,33 | 0 |
| 83 | MG | AS | 3623 | 1/1 | 0.91 | 0.21 | 32,32,32,32 | 0 |
| 83 | MG | AS | 3496 | 1/1 | 0.91 | 0.21 | 40,40,40,40 | 0 |
| 83 | MG | 1 | 3922 | 1/1 | 0.91 | 0.24 | 42,42,42,42 | 0 |
| 83 | MG | AS | 3502 | 1/1 | 0.91 | 0.18 | 34,34,34,34 | 0 |
| 83 | MG | CJ | 202 | 1/1 | 0.91 | 0.09 | 21,21,21,21 | 0 |
| 83 | MG | 1 | 3614 | 1/1 | 0.91 | 0.19 | 86,86,86,86 | 0 |
| 83 | MG | 1 | 3760 | 1/1 | 0.91 | 0.09 | 55,55,55,55 | 0 |
| 83 | MG | B | 1913 | 1/1 | 0.91 | 0.11 | 49,49,49,49 | 0 |
| 83 | MG | B | 1914 | 1/1 | 0.91 | 0.07 | 47,47,47,47 | 0 |
| 83 | MG | B | 1860 | 1/1 | 0.91 | 0.08 | 78,78,78,78 | 0 |
| 85 | ZN | AP | 201 | 1/1 | 0.91 | 0.09 | 181,181,181,181 | 0 |
| 83 | MG | CM | 1804 | 1/1 | 0.91 | 0.21 | 25,25,25,25 | 0 |
| 83 | MG | AS | 3634 | 1/1 | 0.91 | 0.07 | 52,52,52,52 | 0 |
| 83 | MG | 1 | 3586 | 1/1 | 0.91 | 0.12 | 47,47,47,47 | 0 |
| 83 | MG | CM | 1807 | 1/1 | 0.91 | 0.20 | 37,37,37,37 | 0 |
| 83 | MG | 1 | 3443 | 1/1 | 0.91 | 0.18 | 44,44,44,44 | 0 |
| 83 | MG | AS | 3640 | 1/1 | 0.91 | 0.15 | 46,46,46,46 | 0 |
| 83 | MG | AS | 3435 | 1/1 | 0.92 | 0.21 | 30,30,30,30 | 0 |
| 83 | MG | 1 | 3459 | 1/1 | 0.92 | 0.07 | 20,20,20,20 | 0 |
| 83 | MG | B | 1930 | 1/1 | 0.92 | 0.13 | 60,60,60,60 | 0 |
| 83 | MG | 1 | 3741 | 1/1 | 0.92 | 0.22 | 18,18,18,18 | 0 |
| 83 | MG | 1 | 3821 | 1/1 | 0.92 | 0.20 | 43,43,43,43 | 0 |
| 83 | MG | 4 | 205 | 1/1 | 0.92 | 0.07 | 33,33,33,33 | 0 |
| 83 | MG | 1 | 3900 | 1/1 | 0.92 | 0.15 | 29,29,29,29 | 0 |
| 83 | MG | AS | 3457 | 1/1 | 0.92 | 0.09 | 23,23,23,23 | 0 |
| 83 | MG | AS | 3460 | 1/1 | 0.92 | 0.14 | 51,51,51,51 | 0 |

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| Mol | Type | Chain | Res | Atoms | RSCC | RSR | B-factors(Å$^2$) | Q<0.9 |
|---|---|---|---|---|---|---|---|---|
| 83 | MG | AS | 3612 | 1/1 | 0.92 | 0.11 | 25,25,25,25 | 0 |
| 83 | MG | AS | 3462 | 1/1 | 0.92 | 0.24 | 31,31,31,31 | 0 |
| 83 | MG | B | 1937 | 1/1 | 0.92 | 0.17 | 47,47,47,47 | 0 |
| 83 | MG | 1 | 3859 | 1/1 | 0.92 | 0.11 | 77,77,77,77 | 0 |
| 83 | MG | CM | 1814 | 1/1 | 0.92 | 0.11 | 19,19,19,19 | 0 |
| 83 | MG | CM | 1815 | 1/1 | 0.92 | 0.15 | 28,28,28,28 | 0 |
| 83 | MG | 1 | 3744 | 1/1 | 0.92 | 0.17 | 23,23,23,23 | 0 |
| 83 | MG | AP | 203 | 1/1 | 0.92 | 0.13 | 73,73,73,73 | 0 |
| 83 | MG | 4 | 210 | 1/1 | 0.92 | 0.07 | 34,34,34,34 | 0 |
| 83 | MG | 1 | 3825 | 1/1 | 0.92 | 0.09 | 39,39,39,39 | 0 |
| 83 | MG | 1 | 3576 | 1/1 | 0.92 | 0.16 | 31,31,31,31 | 0 |
| 83 | MG | 1 | 3644 | 1/1 | 0.92 | 0.08 | 20,20,20,20 | 0 |
| 83 | MG | AS | 3480 | 1/1 | 0.92 | 0.10 | 29,29,29,29 | 0 |
| 83 | MG | B | 1945 | 1/1 | 0.92 | 0.19 | 56,56,56,56 | 0 |
| 83 | MG | B | 1884 | 1/1 | 0.92 | 0.08 | 97,97,97,97 | 0 |
| 83 | MG | CM | 1826 | 1/1 | 0.92 | 0.10 | 34,34,34,34 | 0 |
| 83 | MG | 1 | 3864 | 1/1 | 0.92 | 0.14 | 41,41,41,41 | 0 |
| 83 | MG | CM | 1828 | 1/1 | 0.92 | 0.23 | 22,22,22,22 | 0 |
| 83 | MG | CM | 1832 | 1/1 | 0.92 | 0.18 | 14,14,14,14 | 0 |
| 83 | MG | 1 | 3510 | 1/1 | 0.92 | 0.11 | 23,23,23,23 | 0 |
| 83 | MG | 1 | 3788 | 1/1 | 0.92 | 0.17 | 23,23,23,23 | 0 |
| 83 | MG | AS | 3635 | 1/1 | 0.92 | 0.21 | 44,44,44,44 | 0 |
| 83 | MG | AS | 3495 | 1/1 | 0.92 | 0.21 | 33,33,33,33 | 0 |
| 83 | MG | 1 | 3513 | 1/1 | 0.92 | 0.17 | 23,23,23,23 | 0 |
| 83 | MG | AS | 3497 | 1/1 | 0.92 | 0.11 | 26,26,26,26 | 0 |
| 83 | MG | 1 | 3462 | 1/1 | 0.92 | 0.14 | 19,19,19,19 | 0 |
| 83 | MG | D | 301 | 1/1 | 0.92 | 0.14 | 38,38,38,38 | 0 |
| 83 | MG | 1 | 3792 | 1/1 | 0.92 | 0.14 | 32,32,32,32 | 0 |
| 83 | MG | 1 | 3915 | 1/1 | 0.92 | 0.06 | 17,17,17,17 | 0 |
| 83 | MG | 1 | 3649 | 1/1 | 0.92 | 0.17 | 38,38,38,38 | 0 |
| 83 | MG | u | 201 | 1/1 | 0.92 | 0.11 | 28,28,28,28 | 0 |
| 83 | MG | 1 | 3403 | 1/1 | 0.92 | 0.20 | 25,25,25,25 | 0 |
| 83 | MG | B | 1826 | 1/1 | 0.92 | 0.13 | 43,43,43,43 | 0 |
| 83 | MG | B | 1901 | 1/1 | 0.92 | 0.12 | 43,43,43,43 | 0 |
| 83 | MG | AS | 3523 | 1/1 | 0.92 | 0.19 | 29,29,29,29 | 0 |
| 83 | MG | 1 | 3451 | 1/1 | 0.92 | 0.10 | 26,26,26,26 | 0 |
| 83 | MG | AS | 3660 | 1/1 | 0.92 | 0.08 | 27,27,27,27 | 0 |
| 83 | MG | AS | 3525 | 1/1 | 0.92 | 0.23 | 32,32,32,32 | 0 |
| 83 | MG | AS | 3528 | 1/1 | 0.92 | 0.13 | 41,41,41,41 | 0 |
| 83 | MG | AS | 3529 | 1/1 | 0.92 | 0.09 | 55,55,55,55 | 0 |
| 83 | MG | CM | 1870 | 1/1 | 0.92 | 0.13 | 30,30,30,30 | 0 |
| 83 | MG | AS | 3533 | 1/1 | 0.92 | 0.18 | 40,40,40,40 | 0 |

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| Mol | Type | Chain | Res | Atoms | RSCC | RSR | B-factors(Å$^2$) | Q<0.9 |
|---|---|---|---|---|---|---|---|---|
| 83 | MG | AS | 3534 | 1/1 | 0.92 | 0.17 | 38,38,38,38 | 0 |
| 83 | MG | AS | 3535 | 1/1 | 0.92 | 0.19 | 27,27,27,27 | 0 |
| 83 | MG | 1 | 3601 | 1/1 | 0.92 | 0.09 | 61,61,61,61 | 0 |
| 83 | MG | B | 1904 | 1/1 | 0.92 | 0.07 | 36,36,36,36 | 0 |
| 83 | MG | 1 | 3407 | 1/1 | 0.92 | 0.30 | 23,23,23,23 | 0 |
| 83 | MG | CM | 1881 | 1/1 | 0.92 | 0.09 | 11,11,11,11 | 0 |
| 83 | MG | x | 201 | 1/1 | 0.92 | 0.18 | 16,16,16,16 | 0 |
| 83 | MG | 1 | 3551 | 1/1 | 0.92 | 0.09 | 36,36,36,36 | 0 |
| 83 | MG | 1 | 3424 | 1/1 | 0.92 | 0.17 | 14,14,14,14 | 0 |
| 83 | MG | AS | 3546 | 1/1 | 0.92 | 0.14 | 15,15,15,15 | 0 |
| 83 | MG | CM | 1888 | 1/1 | 0.92 | 0.08 | 47,47,47,47 | 0 |
| 83 | MG | AS | 3403 | 1/1 | 0.92 | 0.19 | 5,5,5,5 | 0 |
| 83 | MG | 1 | 3883 | 1/1 | 0.92 | 0.07 | 28,28,28,28 | 0 |
| 83 | MG | CM | 1895 | 1/1 | 0.92 | 0.19 | 21,21,21,21 | 0 |
| 83 | MG | AS | 3405 | 1/1 | 0.92 | 0.23 | 16,16,16,16 | 0 |
| 83 | MG | AS | 3556 | 1/1 | 0.92 | 0.16 | 37,37,37,37 | 0 |
| 83 | MG | 1 | 3769 | 1/1 | 0.92 | 0.12 | 21,21,21,21 | 0 |
| 83 | MG | 1 | 3609 | 1/1 | 0.92 | 0.06 | 20,20,20,20 | 0 |
| 83 | MG | 1 | 3846 | 1/1 | 0.92 | 0.09 | 44,44,44,44 | 0 |
| 83 | MG | 1 | 3660 | 1/1 | 0.92 | 0.07 | 25,25,25,25 | 0 |
| 83 | MG | AS | 3568 | 1/1 | 0.92 | 0.17 | 39,39,39,39 | 0 |
| 83 | MG | 1 | 3538 | 1/1 | 0.92 | 0.14 | 48,48,48,48 | 0 |
| 83 | MG | 1 | 3810 | 1/1 | 0.92 | 0.12 | 20,20,20,20 | 0 |
| 83 | MG | AS | 3577 | 1/1 | 0.92 | 0.22 | 30,30,30,30 | 0 |
| 83 | MG | DQ | 101 | 1/1 | 0.92 | 0.09 | 42,42,42,42 | 0 |
| 83 | MG | AS | 3578 | 1/1 | 0.92 | 0.19 | 27,27,27,27 | 0 |
| 83 | MG | 3 | 204 | 1/1 | 0.92 | 0.19 | 32,32,32,32 | 0 |
| 83 | MG | 1 | 3612 | 1/1 | 0.92 | 0.09 | 27,27,27,27 | 0 |
| 83 | MG | AS | 3584 | 1/1 | 0.92 | 0.18 | 37,37,37,37 | 0 |
| 83 | MG | BJ | 301 | 1/1 | 0.92 | 0.14 | 22,22,22,22 | 0 |
| 83 | MG | 3 | 208 | 1/1 | 0.92 | 0.09 | 47,47,47,47 | 0 |
| 83 | MG | 3 | 209 | 1/1 | 0.92 | 0.18 | 48,48,48,48 | 0 |
| 83 | MG | 1 | 3687 | 1/1 | 0.92 | 0.12 | 39,39,39,39 | 0 |
| 83 | MG | BZ | 201 | 1/1 | 0.92 | 0.17 | 41,41,41,41 | 0 |
| 83 | MG | 3 | 211 | 1/1 | 0.92 | 0.15 | 34,34,34,34 | 0 |
| 83 | MG | 1 | 3516 | 1/1 | 0.93 | 0.15 | 30,30,30,30 | 0 |
| 83 | MG | AS | 3614 | 1/1 | 0.93 | 0.09 | 16,16,16,16 | 0 |
| 83 | MG | B | 1888 | 1/1 | 0.93 | 0.21 | 52,52,52,52 | 0 |
| 83 | MG | B | 1808 | 1/1 | 0.93 | 0.14 | 29,29,29,29 | 0 |
| 83 | MG | 1 | 3590 | 1/1 | 0.93 | 0.12 | 17,17,17,17 | 0 |
| 83 | MG | CM | 1810 | 1/1 | 0.93 | 0.12 | 46,46,46,46 | 0 |
| 83 | MG | 1 | 3431 | 1/1 | 0.93 | 0.18 | 20,20,20,20 | 0 |

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| Mol | Type | Chain | Res | Atoms | RSCC | RSR | B-factors(Å$^2$) | Q<0.9 |
|---|---|---|---|---|---|---|---|---|
| 83 | MG | 1 | 3565 | 1/1 | 0.93 | 0.15 | 44,44,44,44 | 0 |
| 83 | MG | o | 301 | 1/1 | 0.93 | 0.06 | 21,21,21,21 | 0 |
| 83 | MG | AS | 3503 | 1/1 | 0.93 | 0.15 | 21,21,21,21 | 0 |
| 83 | MG | 1 | 3436 | 1/1 | 0.93 | 0.14 | 23,23,23,23 | 0 |
| 83 | MG | AS | 3505 | 1/1 | 0.93 | 0.07 | 12,12,12,12 | 0 |
| 83 | MG | R | 201 | 1/1 | 0.93 | 0.11 | 83,83,83,83 | 0 |
| 83 | MG | AS | 3508 | 1/1 | 0.93 | 0.06 | 46,46,46,46 | 0 |
| 83 | MG | B | 1820 | 1/1 | 0.93 | 0.11 | 22,22,22,22 | 0 |
| 83 | MG | AS | 3514 | 1/1 | 0.93 | 0.16 | 22,22,22,22 | 0 |
| 83 | MG | 1 | 3478 | 1/1 | 0.93 | 0.12 | 20,20,20,20 | 0 |
| 83 | MG | 1 | 3820 | 1/1 | 0.93 | 0.06 | 29,29,29,29 | 0 |
| 83 | MG | 1 | 3916 | 1/1 | 0.93 | 0.08 | 45,45,45,45 | 0 |
| 83 | MG | AS | 3636 | 1/1 | 0.93 | 0.10 | 42,42,42,42 | 0 |
| 83 | MG | Z | 201 | 1/1 | 0.93 | 0.29 | 54,54,54,54 | 0 |
| 83 | MG | AS | 3520 | 1/1 | 0.93 | 0.14 | 20,20,20,20 | 0 |
| 83 | MG | AS | 3639 | 1/1 | 0.93 | 0.12 | 37,37,37,37 | 0 |
| 83 | MG | AS | 3522 | 1/1 | 0.93 | 0.11 | 30,30,30,30 | 0 |
| 83 | MG | 1 | 3445 | 1/1 | 0.93 | 0.16 | 25,25,25,25 | 0 |
| 83 | MG | 1 | 3919 | 1/1 | 0.93 | 0.32 | 51,51,51,51 | 0 |
| 83 | MG | v | 302 | 1/1 | 0.93 | 0.08 | 19,19,19,19 | 0 |
| 83 | MG | AS | 3526 | 1/1 | 0.93 | 0.07 | 27,27,27,27 | 0 |
| 83 | MG | 1 | 3624 | 1/1 | 0.93 | 0.19 | 24,24,24,24 | 0 |
| 83 | MG | AS | 3647 | 1/1 | 0.93 | 0.13 | 45,45,45,45 | 0 |
| 83 | MG | 1 | 3574 | 1/1 | 0.93 | 0.11 | 22,22,22,22 | 0 |
| 83 | MG | CM | 1847 | 1/1 | 0.93 | 0.15 | 27,27,27,27 | 0 |
| 83 | MG | AS | 3532 | 1/1 | 0.93 | 0.26 | 23,23,23,23 | 0 |
| 83 | MG | AS | 3651 | 1/1 | 0.93 | 0.07 | 17,17,17,17 | 0 |
| 83 | MG | 1 | 3418 | 1/1 | 0.93 | 0.13 | 33,33,33,33 | 0 |
| 83 | MG | 1 | 3439 | 1/1 | 0.93 | 0.17 | 20,20,20,20 | 0 |
| 83 | MG | AS | 3654 | 1/1 | 0.93 | 0.05 | 17,17,17,17 | 0 |
| 83 | MG | AS | 3655 | 1/1 | 0.93 | 0.18 | 55,55,55,55 | 0 |
| 83 | MG | x | 202 | 1/1 | 0.93 | 0.06 | 20,20,20,20 | 0 |
| 83 | MG | 1 | 3505 | 1/1 | 0.93 | 0.05 | 22,22,22,22 | 0 |
| 83 | MG | 1 | 3831 | 1/1 | 0.93 | 0.15 | 80,80,80,80 | 0 |
| 83 | MG | 1 | 3578 | 1/1 | 0.93 | 0.19 | 27,27,27,27 | 0 |
| 83 | MG | CM | 1861 | 1/1 | 0.93 | 0.07 | 24,24,24,24 | 0 |
| 83 | MG | CM | 1862 | 1/1 | 0.93 | 0.12 | 29,29,29,29 | 0 |
| 83 | MG | 1 | 3665 | 1/1 | 0.93 | 0.05 | 24,24,24,24 | 0 |
| 83 | MG | 1 | 3667 | 1/1 | 0.93 | 0.05 | 16,16,16,16 | 0 |
| 83 | MG | CM | 1866 | 1/1 | 0.93 | 0.07 | 25,25,25,25 | 0 |
| 83 | MG | 1 | 3733 | 1/1 | 0.93 | 0.20 | 11,11,11,11 | 0 |
| 83 | MG | CM | 1869 | 1/1 | 0.93 | 0.12 | 17,17,17,17 | 0 |

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| Mol | Type | Chain | Res | Atoms | RSCC | RSR | B-factors(Å$^2$) | Q<0.9 |
|---|---|---|---|---|---|---|---|---|
| 83 | MG | 1 | 3784 | 1/1 | 0.93 | 0.16 | 30,30,30,30 | 0 |
| 83 | MG | B | 1848 | 1/1 | 0.93 | 0.14 | 30,30,30,30 | 0 |
| 83 | MG | 1 | 3633 | 1/1 | 0.93 | 0.10 | 40,40,40,40 | 0 |
| 83 | MG | 1 | 3453 | 1/1 | 0.93 | 0.12 | 33,33,33,33 | 0 |
| 83 | MG | 1 | 3454 | 1/1 | 0.93 | 0.06 | 9,9,9,9 | 0 |
| 83 | MG | 1 | 3702 | 1/1 | 0.93 | 0.14 | 33,33,33,33 | 0 |
| 83 | MG | B | 1857 | 1/1 | 0.93 | 0.14 | 37,37,37,37 | 0 |
| 83 | MG | B | 1929 | 1/1 | 0.93 | 0.09 | 37,37,37,37 | 0 |
| 83 | MG | AS | 3566 | 1/1 | 0.93 | 0.13 | 26,26,26,26 | 0 |
| 83 | MG | 1 | 3703 | 1/1 | 0.93 | 0.21 | 48,48,48,48 | 0 |
| 83 | MG | 1 | 3704 | 1/1 | 0.93 | 0.12 | 30,30,30,30 | 0 |
| 83 | MG | 1 | 3469 | 1/1 | 0.93 | 0.15 | 28,28,28,28 | 0 |
| 83 | MG | CM | 1886 | 1/1 | 0.93 | 0.20 | 40,40,40,40 | 0 |
| 83 | MG | CM | 1887 | 1/1 | 0.93 | 0.18 | 16,16,16,16 | 0 |
| 83 | MG | AS | 3574 | 1/1 | 0.93 | 0.06 | 17,17,17,17 | 0 |
| 83 | MG | 1 | 3795 | 1/1 | 0.93 | 0.14 | 37,37,37,37 | 0 |
| 83 | MG | 1 | 3493 | 1/1 | 0.93 | 0.19 | 30,30,30,30 | 0 |
| 83 | MG | AS | 3459 | 1/1 | 0.93 | 0.13 | 50,50,50,50 | 0 |
| 83 | MG | AS | 3579 | 1/1 | 0.93 | 0.17 | 38,38,38,38 | 0 |
| 83 | MG | 1 | 3847 | 1/1 | 0.93 | 0.06 | 36,36,36,36 | 0 |
| 83 | MG | 1 | 3709 | 1/1 | 0.93 | 0.14 | 25,25,25,25 | 0 |
| 83 | MG | B | 1867 | 1/1 | 0.93 | 0.08 | 49,49,49,49 | 0 |
| 83 | MG | 4 | 204 | 1/1 | 0.93 | 0.14 | 25,25,25,25 | 0 |
| 83 | MG | 1 | 3749 | 1/1 | 0.93 | 0.13 | 20,20,20,20 | 0 |
| 83 | MG | AS | 3589 | 1/1 | 0.93 | 0.16 | 21,21,21,21 | 0 |
| 83 | MG | AS | 3590 | 1/1 | 0.93 | 0.15 | 33,33,33,33 | 0 |
| 83 | MG | 1 | 3898 | 1/1 | 0.93 | 0.05 | 16,16,16,16 | 0 |
| 83 | MG | AS | 3470 | 1/1 | 0.93 | 0.19 | 31,31,31,31 | 0 |
| 83 | MG | B | 1874 | 1/1 | 0.93 | 0.16 | 37,37,37,37 | 0 |
| 83 | MG | 1 | 3850 | 1/1 | 0.93 | 0.06 | 22,22,22,22 | 0 |
| 83 | MG | 1 | 3710 | 1/1 | 0.93 | 0.09 | 38,38,38,38 | 0 |
| 83 | MG | B | 1878 | 1/1 | 0.93 | 0.16 | 14,14,14,14 | 0 |
| 83 | MG | 1 | 3426 | 1/1 | 0.93 | 0.13 | 24,24,24,24 | 0 |
| 83 | MG | 1 | 3646 | 1/1 | 0.93 | 0.19 | 48,48,48,48 | 0 |
| 83 | MG | 1 | 3471 | 1/1 | 0.93 | 0.13 | 21,21,21,21 | 0 |
| 83 | MG | AS | 3604 | 1/1 | 0.93 | 0.22 | 46,46,46,46 | 0 |
| 85 | ZN | CJ | 201 | 1/1 | 0.93 | 0.10 | 211,211,211,211 | 0 |
| 83 | MG | AS | 3486 | 1/1 | 0.93 | 0.11 | 28,28,28,28 | 0 |
| 83 | MG | 1 | 3615 | 1/1 | 0.93 | 0.15 | 51,51,51,51 | 0 |
| 83 | MG | AS | 3607 | 1/1 | 0.93 | 0.10 | 37,37,37,37 | 0 |
| 83 | MG | B | 1811 | 1/1 | 0.94 | 0.16 | 27,27,27,27 | 0 |
| 83 | MG | B | 1813 | 1/1 | 0.94 | 0.12 | 19,19,19,19 | 0 |

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| Mol | Type | Chain | Res | Atoms | RSCC | RSR | B-factors(Å$^2$) | Q<0.9 |
|---|---|---|---|---|---|---|---|---|
| 83 | MG | B | 1883 | 1/1 | 0.94 | 0.16 | 23,23,23,23 | 0 |
| 83 | MG | 1 | 3415 | 1/1 | 0.94 | 0.23 | 23,23,23,23 | 0 |
| 83 | MG | 1 | 3482 | 1/1 | 0.94 | 0.23 | 23,23,23,23 | 0 |
| 83 | MG | AS | 3659 | 1/1 | 0.94 | 0.09 | 18,18,18,18 | 0 |
| 83 | MG | AS | 3471 | 1/1 | 0.94 | 0.21 | 51,51,51,51 | 0 |
| 83 | MG | 1 | 3557 | 1/1 | 0.94 | 0.14 | 34,34,34,34 | 0 |
| 83 | MG | 1 | 3659 | 1/1 | 0.94 | 0.10 | 24,24,24,24 | 0 |
| 83 | MG | 1 | 3602 | 1/1 | 0.94 | 0.06 | 28,28,28,28 | 0 |
| 83 | MG | 1 | 3504 | 1/1 | 0.94 | 0.10 | 21,21,21,21 | 0 |
| 83 | MG | 1 | 3886 | 1/1 | 0.94 | 0.09 | 27,27,27,27 | 0 |
| 83 | MG | AS | 3669 | 1/1 | 0.94 | 0.19 | 56,56,56,56 | 0 |
| 83 | MG | 1 | 3604 | 1/1 | 0.94 | 0.14 | 25,25,25,25 | 0 |
| 83 | MG | 1 | 3801 | 1/1 | 0.94 | 0.08 | 29,29,29,29 | 0 |
| 83 | MG | 1 | 3606 | 1/1 | 0.94 | 0.13 | 58,58,58,58 | 0 |
| 83 | MG | y | 201 | 1/1 | 0.94 | 0.09 | 12,12,12,12 | 0 |
| 83 | MG | 1 | 3519 | 1/1 | 0.94 | 0.13 | 41,41,41,41 | 0 |
| 83 | MG | 1 | 3634 | 1/1 | 0.94 | 0.10 | 43,43,43,43 | 0 |
| 83 | MG | 3 | 205 | 1/1 | 0.94 | 0.15 | 27,27,27,27 | 0 |
| 83 | MG | 1 | 3696 | 1/1 | 0.94 | 0.10 | 19,19,19,19 | 0 |
| 83 | MG | 1 | 3666 | 1/1 | 0.94 | 0.10 | 27,27,27,27 | 0 |
| 83 | MG | 2 | 201 | 1/1 | 0.94 | 0.16 | 75,75,75,75 | 0 |
| 83 | MG | AS | 3501 | 1/1 | 0.94 | 0.10 | 40,40,40,40 | 0 |
| 83 | MG | 2 | 202 | 1/1 | 0.94 | 0.10 | 34,34,34,34 | 0 |
| 83 | MG | 1 | 3560 | 1/1 | 0.94 | 0.14 | 24,24,24,24 | 0 |
| 83 | MG | B | 1843 | 1/1 | 0.94 | 0.16 | 21,21,21,21 | 0 |
| 83 | MG | 1 | 3814 | 1/1 | 0.94 | 0.07 | 33,33,33,33 | 0 |
| 83 | MG | 1 | 3520 | 1/1 | 0.94 | 0.16 | 25,25,25,25 | 0 |
| 83 | MG | AU | 201 | 1/1 | 0.94 | 0.08 | 40,40,40,40 | 0 |
| 83 | MG | 1 | 3610 | 1/1 | 0.94 | 0.17 | 47,47,47,47 | 0 |
| 83 | MG | AW | 303 | 1/1 | 0.94 | 0.08 | 34,34,34,34 | 0 |
| 83 | MG | 3 | 213 | 1/1 | 0.94 | 0.13 | 49,49,49,49 | 0 |
| 83 | MG | 1 | 3458 | 1/1 | 0.94 | 0.19 | 8,8,8,8 | 0 |
| 83 | MG | CM | 1873 | 1/1 | 0.94 | 0.18 | 40,40,40,40 | 0 |
| 83 | MG | 1 | 3412 | 1/1 | 0.94 | 0.24 | 19,19,19,19 | 0 |
| 83 | MG | CM | 1875 | 1/1 | 0.94 | 0.08 | 18,18,18,18 | 0 |
| 83 | MG | 1 | 3777 | 1/1 | 0.94 | 0.17 | 21,21,21,21 | 0 |
| 83 | MG | B | 1852 | 1/1 | 0.94 | 0.11 | 26,26,26,26 | 0 |
| 83 | MG | CM | 1878 | 1/1 | 0.94 | 0.17 | 33,33,33,33 | 0 |
| 83 | MG | AC | 101 | 1/1 | 0.94 | 0.08 | 41,41,41,41 | 0 |
| 83 | MG | 1 | 3485 | 1/1 | 0.94 | 0.11 | 37,37,37,37 | 0 |
| 83 | MG | 1 | 3779 | 1/1 | 0.94 | 0.20 | 33,33,33,33 | 0 |
| 83 | MG | 1 | 3546 | 1/1 | 0.94 | 0.11 | 36,36,36,36 | 0 |

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| Mol | Type | Chain | Res | Atoms | RSCC | RSR | B-factors(Å$^2$) | Q<0.9 |
|---|---|---|---|---|---|---|---|---|
| 83 | MG | 1 | 3828 | 1/1 | 0.94 | 0.08 | 36,36,36,36 | 0 |
| 83 | MG | AS | 3425 | 1/1 | 0.94 | 0.17 | 17,17,17,17 | 0 |
| 83 | MG | 1 | 3592 | 1/1 | 0.94 | 0.21 | 43,43,43,43 | 0 |
| 83 | MG | AS | 3527 | 1/1 | 0.94 | 0.08 | 35,35,35,35 | 0 |
| 83 | MG | 4 | 211 | 1/1 | 0.94 | 0.08 | 11,11,11,11 | 0 |
| 83 | MG | B | 1863 | 1/1 | 0.94 | 0.17 | 58,58,58,58 | 0 |
| 83 | MG | 1 | 3910 | 1/1 | 0.94 | 0.08 | 64,64,64,64 | 0 |
| 83 | MG | 1 | 3486 | 1/1 | 0.94 | 0.16 | 18,18,18,18 | 0 |
| 83 | MG | AS | 3437 | 1/1 | 0.94 | 0.15 | 33,33,33,33 | 0 |
| 83 | MG | 1 | 3678 | 1/1 | 0.94 | 0.15 | 19,19,19,19 | 0 |
| 83 | MG | CM | 1802 | 1/1 | 0.94 | 0.24 | 15,15,15,15 | 0 |
| 83 | MG | CM | 1901 | 1/1 | 0.94 | 0.08 | 20,20,20,20 | 0 |
| 83 | MG | CM | 1903 | 1/1 | 0.94 | 0.08 | 38,38,38,38 | 0 |
| 83 | MG | 1 | 3467 | 1/1 | 0.94 | 0.17 | 37,37,37,37 | 0 |
| 83 | MG | AS | 3444 | 1/1 | 0.94 | 0.13 | 15,15,15,15 | 0 |
| 83 | MG | 1 | 3712 | 1/1 | 0.94 | 0.10 | 41,41,41,41 | 0 |
| 83 | MG | 1 | 3488 | 1/1 | 0.94 | 0.24 | 9,9,9,9 | 0 |
| 83 | MG | DB | 202 | 1/1 | 0.94 | 0.14 | 57,57,57,57 | 0 |
| 83 | MG | 1 | 3414 | 1/1 | 0.94 | 0.20 | 20,20,20,20 | 0 |
| 83 | MG | AS | 3541 | 1/1 | 0.94 | 0.09 | 49,49,49,49 | 0 |
| 83 | MG | AS | 3542 | 1/1 | 0.94 | 0.15 | 37,37,37,37 | 0 |
| 83 | MG | CM | 1812 | 1/1 | 0.94 | 0.13 | 41,41,41,41 | 0 |
| 83 | MG | B | 1873 | 1/1 | 0.94 | 0.14 | 48,48,48,48 | 0 |
| 83 | MG | AS | 3545 | 1/1 | 0.94 | 0.20 | 15,15,15,15 | 0 |
| 83 | MG | 1 | 3531 | 1/1 | 0.94 | 0.16 | 39,39,39,39 | 0 |
| 83 | MG | o | 302 | 1/1 | 0.94 | 0.12 | 16,16,16,16 | 0 |
| 83 | MG | AS | 3548 | 1/1 | 0.94 | 0.11 | 26,26,26,26 | 0 |
| 83 | MG | AS | 3549 | 1/1 | 0.94 | 0.31 | 33,33,33,33 | 0 |
| 83 | MG | 1 | 3751 | 1/1 | 0.94 | 0.17 | 43,43,43,43 | 0 |
| 83 | MG | 1 | 3878 | 1/1 | 0.94 | 0.15 | 34,34,34,34 | 0 |
| 83 | MG | AS | 3553 | 1/1 | 0.94 | 0.09 | 46,46,46,46 | 0 |
| 83 | MG | AS | 3554 | 1/1 | 0.94 | 0.15 | 18,18,18,18 | 0 |
| 83 | MG | AS | 3463 | 1/1 | 0.94 | 0.16 | 34,34,34,34 | 0 |
| 83 | MG | B | 1832 | 1/1 | 0.95 | 0.17 | 19,19,19,19 | 0 |
| 83 | MG | 1 | 3650 | 1/1 | 0.95 | 0.11 | 34,34,34,34 | 0 |
| 83 | MG | 1 | 3441 | 1/1 | 0.95 | 0.21 | 29,29,29,29 | 0 |
| 83 | MG | AS | 3650 | 1/1 | 0.95 | 0.08 | 7,7,7,7 | 0 |
| 83 | MG | 1 | 3571 | 1/1 | 0.95 | 0.14 | 15,15,15,15 | 0 |
| 83 | MG | B | 1838 | 1/1 | 0.95 | 0.14 | 20,20,20,20 | 0 |
| 83 | MG | CM | 1829 | 1/1 | 0.95 | 0.13 | 25,25,25,25 | 0 |
| 83 | MG | CM | 1830 | 1/1 | 0.95 | 0.17 | 25,25,25,25 | 0 |
| 83 | MG | AS | 3475 | 1/1 | 0.95 | 0.09 | 22,22,22,22 | 0 |

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| Mol | Type | Chain | Res | Atoms | RSCC | RSR | B-factors(Å$^2$) | Q<0.9 |
|---|---|---|---|---|---|---|---|---|
| 83 | MG | 1 | 3813 | 1/1 | 0.95 | 0.11 | 27,27,27,27 | 0 |
| 83 | MG | CM | 1834 | 1/1 | 0.95 | 0.22 | 28,28,28,28 | 0 |
| 83 | MG | 1 | 3511 | 1/1 | 0.95 | 0.18 | 14,14,14,14 | 0 |
| 83 | MG | 1 | 3549 | 1/1 | 0.95 | 0.17 | 32,32,32,32 | 0 |
| 83 | MG | 1 | 3897 | 1/1 | 0.95 | 0.15 | 52,52,52,52 | 0 |
| 83 | MG | AS | 3569 | 1/1 | 0.95 | 0.13 | 33,33,33,33 | 0 |
| 83 | MG | AS | 3571 | 1/1 | 0.95 | 0.16 | 14,14,14,14 | 0 |
| 83 | MG | 1 | 3816 | 1/1 | 0.95 | 0.15 | 28,28,28,28 | 0 |
| 83 | MG | CM | 1844 | 1/1 | 0.95 | 0.13 | 26,26,26,26 | 0 |
| 83 | MG | AS | 3487 | 1/1 | 0.95 | 0.14 | 20,20,20,20 | 0 |
| 83 | MG | AS | 3663 | 1/1 | 0.95 | 0.15 | 42,42,42,42 | 0 |
| 83 | MG | 1 | 3737 | 1/1 | 0.95 | 0.15 | 15,15,15,15 | 0 |
| 83 | MG | AS | 3576 | 1/1 | 0.95 | 0.14 | 24,24,24,24 | 0 |
| 83 | MG | 1 | 3857 | 1/1 | 0.95 | 0.08 | 40,40,40,40 | 0 |
| 83 | MG | 1 | 3738 | 1/1 | 0.95 | 0.11 | 21,21,21,21 | 0 |
| 83 | MG | CM | 1852 | 1/1 | 0.95 | 0.06 | 24,24,24,24 | 0 |
| 83 | MG | AS | 3494 | 1/1 | 0.95 | 0.15 | 31,31,31,31 | 0 |
| 83 | MG | 1 | 3903 | 1/1 | 0.95 | 0.12 | 56,56,56,56 | 0 |
| 83 | MG | 1 | 3512 | 1/1 | 0.95 | 0.17 | 49,49,49,49 | 0 |
| 83 | MG | 1 | 3437 | 1/1 | 0.95 | 0.18 | 19,19,19,19 | 0 |
| 83 | MG | 1 | 3823 | 1/1 | 0.95 | 0.11 | 34,34,34,34 | 0 |
| 83 | MG | AS | 3586 | 1/1 | 0.95 | 0.16 | 15,15,15,15 | 0 |
| 83 | MG | AS | 3587 | 1/1 | 0.95 | 0.09 | 14,14,14,14 | 0 |
| 83 | MG | 1 | 3474 | 1/1 | 0.95 | 0.25 | 21,21,21,21 | 0 |
| 83 | MG | CM | 1863 | 1/1 | 0.95 | 0.11 | 44,44,44,44 | 0 |
| 83 | MG | j | 301 | 1/1 | 0.95 | 0.06 | 15,15,15,15 | 0 |
| 83 | MG | AS | 3406 | 1/1 | 0.95 | 0.21 | 17,17,17,17 | 0 |
| 83 | MG | 1 | 3782 | 1/1 | 0.95 | 0.10 | 28,28,28,28 | 0 |
| 83 | MG | 1 | 3448 | 1/1 | 0.95 | 0.16 | 14,14,14,14 | 0 |
| 83 | MG | AS | 3594 | 1/1 | 0.95 | 0.10 | 34,34,34,34 | 0 |
| 83 | MG | 1 | 3532 | 1/1 | 0.95 | 0.16 | 15,15,15,15 | 0 |
| 83 | MG | 1 | 3450 | 1/1 | 0.95 | 0.17 | 32,32,32,32 | 0 |
| 83 | MG | AS | 3509 | 1/1 | 0.95 | 0.09 | 29,29,29,29 | 0 |
| 83 | MG | AS | 3511 | 1/1 | 0.95 | 0.23 | 50,50,50,50 | 0 |
| 83 | MG | B | 1801 | 1/1 | 0.95 | 0.07 | 69,69,69,69 | 0 |
| 83 | MG | AW | 301 | 1/1 | 0.95 | 0.11 | 30,30,30,30 | 0 |
| 83 | MG | AS | 3418 | 1/1 | 0.95 | 0.24 | 19,19,19,19 | 0 |
| 83 | MG | 1 | 3748 | 1/1 | 0.95 | 0.14 | 28,28,28,28 | 0 |
| 83 | MG | 1 | 3869 | 1/1 | 0.95 | 0.07 | 37,37,37,37 | 0 |
| 83 | MG | 1 | 3870 | 1/1 | 0.95 | 0.13 | 43,43,43,43 | 0 |
| 83 | MG | 1 | 3479 | 1/1 | 0.95 | 0.15 | 35,35,35,35 | 0 |
| 83 | MG | 1 | 3481 | 1/1 | 0.95 | 0.11 | 12,12,12,12 | 0 |

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| Mol | Type | Chain | Res | Atoms | RSCC | RSR | B-factors(Å$^2$) | Q<0.9 |
|---|---|---|---|---|---|---|---|---|
| 83 | MG | AS | 3610 | 1/1 | 0.95 | 0.06 | 35,35,35,35 | 0 |
| 83 | MG | AS | 3611 | 1/1 | 0.95 | 0.12 | 29,29,29,29 | 0 |
| 83 | MG | B | 1932 | 1/1 | 0.95 | 0.07 | 18,18,18,18 | 0 |
| 83 | MG | AS | 3613 | 1/1 | 0.95 | 0.11 | 28,28,28,28 | 0 |
| 83 | MG | 1 | 3406 | 1/1 | 0.95 | 0.22 | 26,26,26,26 | 0 |
| 83 | MG | AS | 3430 | 1/1 | 0.95 | 0.27 | 31,31,31,31 | 0 |
| 83 | MG | AS | 3432 | 1/1 | 0.95 | 0.13 | 12,12,12,12 | 0 |
| 83 | MG | 1 | 3834 | 1/1 | 0.95 | 0.19 | 21,21,21,21 | 0 |
| 83 | MG | 1 | 3638 | 1/1 | 0.95 | 0.14 | 9,9,9,9 | 0 |
| 83 | MG | AS | 3436 | 1/1 | 0.95 | 0.16 | 10,10,10,10 | 0 |
| 83 | MG | B | 1936 | 1/1 | 0.95 | 0.08 | 25,25,25,25 | 0 |
| 83 | MG | AS | 3530 | 1/1 | 0.95 | 0.15 | 34,34,34,34 | 0 |
| 83 | MG | AS | 3625 | 1/1 | 0.95 | 0.17 | 42,42,42,42 | 0 |
| 83 | MG | AS | 3531 | 1/1 | 0.95 | 0.11 | 45,45,45,45 | 0 |
| 83 | MG | 1 | 3561 | 1/1 | 0.95 | 0.07 | 26,26,26,26 | 0 |
| 83 | MG | 1 | 3506 | 1/1 | 0.95 | 0.07 | 26,26,26,26 | 0 |
| 83 | MG | 1 | 3695 | 1/1 | 0.95 | 0.16 | 32,32,32,32 | 0 |
| 83 | MG | 1 | 3541 | 1/1 | 0.95 | 0.07 | 34,34,34,34 | 0 |
| 83 | MG | w | 301 | 1/1 | 0.95 | 0.08 | 22,22,22,22 | 0 |
| 83 | MG | 1 | 3521 | 1/1 | 0.95 | 0.13 | 26,26,26,26 | 0 |
| 83 | MG | CM | 1809 | 1/1 | 0.95 | 0.12 | 67,67,67,67 | 0 |
| 83 | MG | 1 | 3882 | 1/1 | 0.95 | 0.12 | 39,39,39,39 | 0 |
| 83 | MG | B | 1822 | 1/1 | 0.95 | 0.18 | 22,22,22,22 | 0 |
| 83 | MG | 1 | 3670 | 1/1 | 0.95 | 0.09 | 47,47,47,47 | 0 |
| 83 | MG | 1 | 3616 | 1/1 | 0.95 | 0.16 | 22,22,22,22 | 0 |
| 83 | MG | AS | 3461 | 1/1 | 0.95 | 0.17 | 23,23,23,23 | 0 |
| 83 | MG | 1 | 3522 | 1/1 | 0.95 | 0.06 | 24,24,24,24 | 0 |
| 83 | MG | 1 | 3768 | 1/1 | 0.95 | 0.07 | 27,27,27,27 | 0 |
| 83 | MG | CM | 1817 | 1/1 | 0.95 | 0.11 | 19,19,19,19 | 0 |
| 83 | MG | AS | 3464 | 1/1 | 0.95 | 0.16 | 21,21,21,21 | 0 |
| 83 | MG | 1 | 3460 | 1/1 | 0.95 | 0.15 | 15,15,15,15 | 0 |
| 83 | MG | 1 | 3888 | 1/1 | 0.95 | 0.16 | 28,28,28,28 | 0 |
| 83 | MG | 1 | 3410 | 1/1 | 0.95 | 0.18 | 7,7,7,7 | 0 |
| 83 | MG | 1 | 3808 | 1/1 | 0.95 | 0.11 | 28,28,28,28 | 0 |
| 83 | MG | AS | 3620 | 1/1 | 0.96 | 0.15 | 26,26,26,26 | 0 |
| 83 | MG | B | 1917 | 1/1 | 0.96 | 0.11 | 24,24,24,24 | 0 |
| 83 | MG | AS | 3424 | 1/1 | 0.96 | 0.18 | 15,15,15,15 | 0 |
| 83 | MG | B | 1853 | 1/1 | 0.96 | 0.19 | 27,27,27,27 | 0 |
| 83 | MG | 1 | 3536 | 1/1 | 0.96 | 0.15 | 15,15,15,15 | 0 |
| 83 | MG | B | 1921 | 1/1 | 0.96 | 0.08 | 24,24,24,24 | 0 |
| 83 | MG | AK | 102 | 1/1 | 0.96 | 0.05 | 12,12,12,12 | 0 |
| 83 | MG | AS | 3429 | 1/1 | 0.96 | 0.15 | 17,17,17,17 | 0 |

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| Mol | Type | Chain | Res | Atoms | RSCC | RSR | B-factors(Å$^2$) | Q<0.9 |
|---|---|---|---|---|---|---|---|---|
| 83 | MG | 1 | 3743 | 1/1 | 0.96 | 0.10 | 25,25,25,25 | 0 |
| 83 | MG | AS | 3431 | 1/1 | 0.96 | 0.18 | 8,8,8,8 | 0 |
| 83 | MG | 1 | 3589 | 1/1 | 0.96 | 0.12 | 16,16,16,16 | 0 |
| 83 | MG | 1 | 3745 | 1/1 | 0.96 | 0.14 | 30,30,30,30 | 0 |
| 83 | MG | 1 | 3573 | 1/1 | 0.96 | 0.10 | 23,23,23,23 | 0 |
| 83 | MG | AS | 3633 | 1/1 | 0.96 | 0.05 | 43,43,43,43 | 0 |
| 83 | MG | B | 1861 | 1/1 | 0.96 | 0.08 | 45,45,45,45 | 0 |
| 83 | MG | 1 | 3509 | 1/1 | 0.96 | 0.17 | 20,20,20,20 | 0 |
| 83 | MG | AS | 3439 | 1/1 | 0.96 | 0.13 | 32,32,32,32 | 0 |
| 83 | MG | 1 | 3447 | 1/1 | 0.96 | 0.12 | 10,10,10,10 | 0 |
| 83 | MG | 1 | 3416 | 1/1 | 0.96 | 0.14 | 25,25,25,25 | 0 |
| 83 | MG | AS | 3443 | 1/1 | 0.96 | 0.19 | 11,11,11,11 | 0 |
| 83 | MG | 1 | 3927 | 1/1 | 0.96 | 0.06 | 22,22,22,22 | 0 |
| 83 | MG | AS | 3446 | 1/1 | 0.96 | 0.21 | 22,22,22,22 | 0 |
| 83 | MG | 1 | 3461 | 1/1 | 0.96 | 0.13 | 13,13,13,13 | 0 |
| 83 | MG | B | 1809 | 1/1 | 0.96 | 0.06 | 79,79,79,79 | 0 |
| 83 | MG | 1 | 3752 | 1/1 | 0.96 | 0.11 | 39,39,39,39 | 0 |
| 83 | MG | 1 | 3819 | 1/1 | 0.96 | 0.19 | 13,13,13,13 | 0 |
| 83 | MG | B | 1812 | 1/1 | 0.96 | 0.10 | 17,17,17,17 | 0 |
| 83 | MG | B | 1871 | 1/1 | 0.96 | 0.11 | 63,63,63,63 | 0 |
| 83 | MG | CM | 1842 | 1/1 | 0.96 | 0.09 | 45,45,45,45 | 0 |
| 83 | MG | B | 1872 | 1/1 | 0.96 | 0.12 | 40,40,40,40 | 0 |
| 83 | MG | 1 | 3785 | 1/1 | 0.96 | 0.13 | 20,20,20,20 | 0 |
| 83 | MG | 1 | 3786 | 1/1 | 0.96 | 0.06 | 24,24,24,24 | 0 |
| 83 | MG | CM | 1846 | 1/1 | 0.96 | 0.08 | 18,18,18,18 | 0 |
| 83 | MG | 1 | 3822 | 1/1 | 0.96 | 0.05 | 23,23,23,23 | 0 |
| 83 | MG | B | 1876 | 1/1 | 0.96 | 0.11 | 54,54,54,54 | 0 |
| 83 | MG | AS | 3555 | 1/1 | 0.96 | 0.15 | 11,11,11,11 | 0 |
| 83 | MG | 1 | 3422 | 1/1 | 0.96 | 0.22 | 14,14,14,14 | 0 |
| 83 | MG | AS | 3558 | 1/1 | 0.96 | 0.05 | 25,25,25,25 | 0 |
| 83 | MG | AS | 3466 | 1/1 | 0.96 | 0.13 | 25,25,25,25 | 0 |
| 83 | MG | AS | 3561 | 1/1 | 0.96 | 0.18 | 18,18,18,18 | 0 |
| 83 | MG | CM | 1854 | 1/1 | 0.96 | 0.20 | 27,27,27,27 | 0 |
| 83 | MG | 1 | 3632 | 1/1 | 0.96 | 0.12 | 20,20,20,20 | 0 |
| 83 | MG | AS | 3563 | 1/1 | 0.96 | 0.13 | 17,17,17,17 | 0 |
| 83 | MG | B | 1819 | 1/1 | 0.96 | 0.19 | 16,16,16,16 | 0 |
| 83 | MG | B | 1881 | 1/1 | 0.96 | 0.12 | 51,51,51,51 | 0 |
| 83 | MG | x | 203 | 1/1 | 0.96 | 0.13 | 24,24,24,24 | 0 |
| 83 | MG | 1 | 3656 | 1/1 | 0.96 | 0.11 | 28,28,28,28 | 0 |
| 83 | MG | 3 | 207 | 1/1 | 0.96 | 0.09 | 51,51,51,51 | 0 |
| 83 | MG | B | 1885 | 1/1 | 0.96 | 0.07 | 45,45,45,45 | 0 |
| 83 | MG | AS | 3572 | 1/1 | 0.96 | 0.14 | 16,16,16,16 | 0 |

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| Mol | Type | Chain | Res | Atoms | RSCC | RSR | B-factors(Å$^2$) | Q<0.9 |
|---|---|---|---|---|---|---|---|---|
| 83 | MG | 1 | 3757 | 1/1 | 0.96 | 0.23 | 19,19,19,19 | 0 |
| 83 | MG | 1 | 3899 | 1/1 | 0.96 | 0.16 | 31,31,31,31 | 0 |
| 83 | MG | 1 | 3613 | 1/1 | 0.96 | 0.16 | 24,24,24,24 | 0 |
| 83 | MG | AS | 3478 | 1/1 | 0.96 | 0.11 | 16,16,16,16 | 0 |
| 83 | MG | 1 | 3596 | 1/1 | 0.96 | 0.10 | 36,36,36,36 | 0 |
| 83 | MG | I | 302 | 1/1 | 0.96 | 0.06 | 31,31,31,31 | 0 |
| 83 | MG | 1 | 3456 | 1/1 | 0.96 | 0.07 | 6,6,6,6 | 0 |
| 83 | MG | AS | 3484 | 1/1 | 0.96 | 0.04 | 22,22,22,22 | 0 |
| 83 | MG | 1 | 3405 | 1/1 | 0.96 | 0.21 | 21,21,21,21 | 0 |
| 83 | MG | AS | 3582 | 1/1 | 0.96 | 0.15 | 16,16,16,16 | 0 |
| 83 | MG | AS | 3583 | 1/1 | 0.96 | 0.22 | 30,30,30,30 | 0 |
| 83 | MG | AT | 205 | 1/1 | 0.96 | 0.15 | 22,22,22,22 | 0 |
| 83 | MG | 1 | 3581 | 1/1 | 0.96 | 0.08 | 24,24,24,24 | 0 |
| 83 | MG | AS | 3489 | 1/1 | 0.96 | 0.08 | 29,29,29,29 | 0 |
| 83 | MG | B | 1894 | 1/1 | 0.96 | 0.11 | 27,27,27,27 | 0 |
| 83 | MG | B | 1895 | 1/1 | 0.96 | 0.10 | 37,37,37,37 | 0 |
| 83 | MG | 4 | 201 | 1/1 | 0.96 | 0.23 | 41,41,41,41 | 0 |
| 83 | MG | 1 | 3641 | 1/1 | 0.96 | 0.15 | 7,7,7,7 | 0 |
| 83 | MG | 1 | 3642 | 1/1 | 0.96 | 0.17 | 16,16,16,16 | 0 |
| 83 | MG | AW | 302 | 1/1 | 0.96 | 0.07 | 29,29,29,29 | 0 |
| 83 | MG | B | 1834 | 1/1 | 0.96 | 0.10 | 29,29,29,29 | 0 |
| 83 | MG | AS | 3592 | 1/1 | 0.96 | 0.10 | 20,20,20,20 | 0 |
| 83 | MG | 1 | 3711 | 1/1 | 0.96 | 0.05 | 22,22,22,22 | 0 |
| 83 | MG | 1 | 3544 | 1/1 | 0.96 | 0.26 | 19,19,19,19 | 0 |
| 83 | MG | AS | 3595 | 1/1 | 0.96 | 0.18 | 31,31,31,31 | 0 |
| 83 | MG | CM | 1896 | 1/1 | 0.96 | 0.05 | 4,4,4,4 | 0 |
| 83 | MG | B | 1837 | 1/1 | 0.96 | 0.13 | 26,26,26,26 | 0 |
| 83 | MG | 1 | 3556 | 1/1 | 0.96 | 0.06 | 35,35,35,35 | 0 |
| 83 | MG | AS | 3598 | 1/1 | 0.96 | 0.04 | 24,24,24,24 | 0 |
| 83 | MG | AB | 201 | 1/1 | 0.96 | 0.07 | 9,9,9,9 | 0 |
| 83 | MG | 1 | 3874 | 1/1 | 0.96 | 0.10 | 45,45,45,45 | 0 |
| 83 | MG | B | 1906 | 1/1 | 0.96 | 0.11 | 12,12,12,12 | 0 |
| 83 | MG | BK | 201 | 1/1 | 0.96 | 0.16 | 11,11,11,11 | 0 |
| 83 | MG | 1 | 3802 | 1/1 | 0.96 | 0.13 | 19,19,19,19 | 0 |
| 83 | MG | 1 | 3912 | 1/1 | 0.96 | 0.06 | 26,26,26,26 | 0 |
| 83 | MG | AS | 3410 | 1/1 | 0.96 | 0.18 | 26,26,26,26 | 0 |
| 83 | MG | CA | 201 | 1/1 | 0.96 | 0.08 | 33,33,33,33 | 0 |
| 83 | MG | AS | 3510 | 1/1 | 0.96 | 0.15 | 28,28,28,28 | 0 |
| 83 | MG | 1 | 3689 | 1/1 | 0.96 | 0.07 | 33,33,33,33 | 0 |
| 83 | MG | 1 | 3452 | 1/1 | 0.96 | 0.15 | 19,19,19,19 | 0 |
| 83 | MG | AS | 3609 | 1/1 | 0.96 | 0.06 | 8,8,8,8 | 0 |
| 83 | MG | AS | 3513 | 1/1 | 0.96 | 0.13 | 28,28,28,28 | 0 |

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| Mol | Type | Chain | Res | Atoms | RSCC | RSR | B-factors(Å$^2$) | Q<0.9 |
|---|---|---|---|---|---|---|---|---|
| 83 | MG | AF | 201 | 1/1 | 0.96 | 0.12 | 23,23,23,23 | 0 |
| 83 | MG | AS | 3415 | 1/1 | 0.96 | 0.22 | 22,22,22,22 | 0 |
| 85 | ZN | AQ | 101 | 1/1 | 0.96 | 0.05 | 65,65,65,65 | 0 |
| 83 | MG | 1 | 3805 | 1/1 | 0.96 | 0.07 | 27,27,27,27 | 0 |
| 83 | MG | 1 | 3806 | 1/1 | 0.96 | 0.06 | 32,32,32,32 | 0 |
| 83 | MG | 1 | 3917 | 1/1 | 0.96 | 0.07 | 79,79,79,79 | 0 |
| 83 | MG | 1 | 3570 | 1/1 | 0.96 | 0.17 | 28,28,28,28 | 0 |
| 83 | MG | AS | 3617 | 1/1 | 0.96 | 0.07 | 25,25,25,25 | 0 |
| 83 | MG | AS | 3521 | 1/1 | 0.96 | 0.21 | 28,28,28,28 | 0 |
| 83 | MG | AS | 3619 | 1/1 | 0.96 | 0.08 | 20,20,20,20 | 0 |
| 83 | MG | 1 | 3640 | 1/1 | 0.97 | 0.20 | 27,27,27,27 | 0 |
| 83 | MG | 1 | 3756 | 1/1 | 0.97 | 0.13 | 31,31,31,31 | 0 |
| 83 | MG | AS | 3485 | 1/1 | 0.97 | 0.15 | 15,15,15,15 | 0 |
| 83 | MG | 1 | 3421 | 1/1 | 0.97 | 0.21 | 3,3,3,3 | 0 |
| 83 | MG | 1 | 3629 | 1/1 | 0.97 | 0.09 | 25,25,25,25 | 0 |
| 83 | MG | AS | 3488 | 1/1 | 0.97 | 0.25 | 15,15,15,15 | 0 |
| 83 | MG | AS | 3438 | 1/1 | 0.97 | 0.18 | 17,17,17,17 | 0 |
| 83 | MG | 1 | 3742 | 1/1 | 0.97 | 0.10 | 32,32,32,32 | 0 |
| 83 | MG | AS | 3543 | 1/1 | 0.97 | 0.08 | 23,23,23,23 | 0 |
| 83 | MG | AS | 3440 | 1/1 | 0.97 | 0.16 | 17,17,17,17 | 0 |
| 83 | MG | AS | 3492 | 1/1 | 0.97 | 0.10 | 16,16,16,16 | 0 |
| 83 | MG | 1 | 3728 | 1/1 | 0.97 | 0.17 | 18,18,18,18 | 0 |
| 83 | MG | AS | 3402 | 1/1 | 0.97 | 0.05 | 46,46,46,46 | 0 |
| 83 | MG | 1 | 3761 | 1/1 | 0.97 | 0.06 | 18,18,18,18 | 0 |
| 83 | MG | 1 | 3533 | 1/1 | 0.97 | 0.13 | 25,25,25,25 | 0 |
| 83 | MG | AS | 3445 | 1/1 | 0.97 | 0.06 | 22,22,22,22 | 0 |
| 83 | MG | AS | 3499 | 1/1 | 0.97 | 0.07 | 6,6,6,6 | 0 |
| 83 | MG | 1 | 3480 | 1/1 | 0.97 | 0.16 | 16,16,16,16 | 0 |
| 83 | MG | B | 1915 | 1/1 | 0.97 | 0.09 | 31,31,31,31 | 0 |
| 83 | MG | CM | 1879 | 1/1 | 0.97 | 0.12 | 26,26,26,26 | 0 |
| 83 | MG | AS | 3448 | 1/1 | 0.97 | 0.10 | 33,33,33,33 | 0 |
| 83 | MG | 1 | 3404 | 1/1 | 0.97 | 0.13 | 30,30,30,30 | 0 |
| 83 | MG | AS | 3557 | 1/1 | 0.97 | 0.09 | 20,20,20,20 | 0 |
| 83 | MG | AS | 3409 | 1/1 | 0.97 | 0.11 | 9,9,9,9 | 0 |
| 83 | MG | AS | 3451 | 1/1 | 0.97 | 0.12 | 26,26,26,26 | 0 |
| 83 | MG | AS | 3506 | 1/1 | 0.97 | 0.09 | 18,18,18,18 | 0 |
| 83 | MG | AS | 3453 | 1/1 | 0.97 | 0.13 | 14,14,14,14 | 0 |
| 83 | MG | AS | 3454 | 1/1 | 0.97 | 0.08 | 20,20,20,20 | 0 |
| 83 | MG | AS | 3564 | 1/1 | 0.97 | 0.04 | 12,12,12,12 | 0 |
| 83 | MG | CM | 1889 | 1/1 | 0.97 | 0.12 | 33,33,33,33 | 0 |
| 83 | MG | B | 1889 | 1/1 | 0.97 | 0.15 | 37,37,37,37 | 0 |
| 83 | MG | AS | 3411 | 1/1 | 0.97 | 0.18 | 13,13,13,13 | 0 |

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| Mol | Type | Chain | Res | Atoms | RSCC | RSR | B-factors(Å$^2$) | Q<0.9 |
|---|---|---|---|---|---|---|---|---|
| 83 | MG | CM | 1893 | 1/1 | 0.97 | 0.09 | 17,17,17,17 | 0 |
| 83 | MG | B | 1948 | 1/1 | 0.97 | 0.17 | 22,22,22,22 | 0 |
| 83 | MG | 6 | 201 | 1/1 | 0.97 | 0.12 | 23,23,23,23 | 0 |
| 83 | MG | 6 | 202 | 1/1 | 0.97 | 0.13 | 27,27,27,27 | 0 |
| 83 | MG | AS | 3570 | 1/1 | 0.97 | 0.13 | 16,16,16,16 | 0 |
| 83 | MG | 4 | 202 | 1/1 | 0.97 | 0.17 | 10,10,10,10 | 0 |
| 83 | MG | CM | 1900 | 1/1 | 0.97 | 0.11 | 35,35,35,35 | 0 |
| 83 | MG | 1 | 3492 | 1/1 | 0.97 | 0.09 | 31,31,31,31 | 0 |
| 83 | MG | 1 | 3477 | 1/1 | 0.97 | 0.09 | 14,14,14,14 | 0 |
| 83 | MG | AS | 3517 | 1/1 | 0.97 | 0.09 | 22,22,22,22 | 0 |
| 83 | MG | 1 | 3501 | 1/1 | 0.97 | 0.14 | 12,12,12,12 | 0 |
| 83 | MG | CM | 1838 | 1/1 | 0.97 | 0.11 | 32,32,32,32 | 0 |
| 83 | MG | v | 301 | 1/1 | 0.97 | 0.07 | 21,21,21,21 | 0 |
| 83 | MG | 1 | 3750 | 1/1 | 0.97 | 0.14 | 39,39,39,39 | 0 |
| 83 | MG | AS | 3422 | 1/1 | 0.97 | 0.06 | 20,20,20,20 | 0 |
| 83 | MG | AS | 3423 | 1/1 | 0.97 | 0.13 | 25,25,25,25 | 0 |
| 83 | MG | 1 | 3707 | 1/1 | 0.97 | 0.04 | 3,3,3,3 | 0 |
| 83 | MG | 4 | 208 | 1/1 | 0.97 | 0.11 | 8,8,8,8 | 0 |
| 83 | MG | 1 | 3791 | 1/1 | 0.97 | 0.11 | 46,46,46,46 | 0 |
| 83 | MG | L | 201 | 1/1 | 0.97 | 0.18 | 41,41,41,41 | 0 |
| 83 | MG | B | 1816 | 1/1 | 0.97 | 0.21 | 17,17,17,17 | 0 |
| 83 | MG | 1 | 3417 | 1/1 | 0.97 | 0.08 | 13,13,13,13 | 0 |
| 83 | MG | 1 | 3852 | 1/1 | 0.97 | 0.13 | 24,24,24,24 | 0 |
| 83 | MG | AS | 3477 | 1/1 | 0.97 | 0.12 | 14,14,14,14 | 0 |
| 85 | ZN | f | 101 | 1/1 | 0.97 | 0.07 | 71,71,71,71 | 0 |
| 83 | MG | 1 | 3627 | 1/1 | 0.97 | 0.14 | 11,11,11,11 | 0 |
| 83 | MG | BQ | 201 | 1/1 | 0.97 | 0.13 | 14,14,14,14 | 0 |
| 85 | ZN | CH | 101 | 1/1 | 0.97 | 0.10 | 75,75,75,75 | 0 |
| 83 | MG | AS | 3645 | 1/1 | 0.97 | 0.10 | 26,26,26,26 | 0 |
| 83 | MG | AS | 3479 | 1/1 | 0.97 | 0.12 | 30,30,30,30 | 0 |
| 85 | ZN | DS | 201 | 1/1 | 0.97 | 0.06 | 134,134,134,134 | 0 |
| 83 | MG | 1 | 3685 | 1/1 | 0.97 | 0.14 | 33,33,33,33 | 0 |
| 83 | MG | AS | 3433 | 1/1 | 0.97 | 0.20 | 17,17,17,17 | 0 |
| 83 | MG | AS | 3608 | 1/1 | 0.98 | 0.04 | 21,21,21,21 | 0 |
| 83 | MG | 1 | 3572 | 1/1 | 0.98 | 0.10 | 11,11,11,11 | 0 |
| 83 | MG | CM | 1803 | 1/1 | 0.98 | 0.13 | 13,13,13,13 | 0 |
| 83 | MG | B | 1854 | 1/1 | 0.98 | 0.05 | 58,58,58,58 | 0 |
| 83 | MG | 1 | 3449 | 1/1 | 0.98 | 0.15 | 11,11,11,11 | 0 |
| 83 | MG | AS | 3458 | 1/1 | 0.98 | 0.13 | 1,1,1,1 | 0 |
| 83 | MG | 1 | 3472 | 1/1 | 0.98 | 0.10 | 10,10,10,10 | 0 |
| 83 | MG | 1 | 3605 | 1/1 | 0.98 | 0.05 | 22,22,22,22 | 0 |
| 83 | MG | B | 1880 | 1/1 | 0.98 | 0.12 | 20,20,20,20 | 0 |

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| Mol | Type | Chain | Res | Atoms | RSCC | RSR | B-factors(Å$^2$) | Q<0.9 |
|---|---|---|---|---|---|---|---|---|
| 83 | MG | AS | 3551 | 1/1 | 0.98 | 0.11 | 23,23,23,23 | 0 |
| 83 | MG | CM | 1894 | 1/1 | 0.98 | 0.25 | 16,16,16,16 | 0 |
| 83 | MG | AS | 3407 | 1/1 | 0.98 | 0.05 | 0,0,0,0 | 0 |
| 83 | MG | 1 | 3826 | 1/1 | 0.98 | 0.05 | 36,36,36,36 | 0 |
| 83 | MG | 1 | 3811 | 1/1 | 0.98 | 0.04 | 6,6,6,6 | 0 |
| 83 | MG | 1 | 3566 | 1/1 | 0.98 | 0.10 | 3,3,3,3 | 0 |
| 83 | MG | 1 | 3409 | 1/1 | 0.98 | 0.04 | 12,12,12,12 | 0 |
| 83 | MG | CM | 1856 | 1/1 | 0.98 | 0.12 | 24,24,24,24 | 0 |
| 83 | MG | B | 1840 | 1/1 | 0.98 | 0.14 | 38,38,38,38 | 0 |
| 83 | MG | B | 1841 | 1/1 | 0.98 | 0.18 | 36,36,36,36 | 0 |
| 83 | MG | AS | 3559 | 1/1 | 0.98 | 0.09 | 8,8,8,8 | 0 |
| 83 | MG | AS | 3498 | 1/1 | 0.98 | 0.10 | 26,26,26,26 | 0 |
| 83 | MG | CQ | 301 | 1/1 | 0.98 | 0.06 | 3,3,3,3 | 0 |
| 83 | MG | 1 | 3420 | 1/1 | 0.98 | 0.12 | 17,17,17,17 | 0 |
| 83 | MG | B | 1804 | 1/1 | 0.98 | 0.14 | 14,14,14,14 | 0 |
| 83 | MG | AS | 3416 | 1/1 | 0.98 | 0.05 | 47,47,47,47 | 0 |
| 83 | MG | 1 | 3588 | 1/1 | 0.98 | 0.10 | 26,26,26,26 | 0 |
| 83 | MG | AS | 3664 | 1/1 | 0.98 | 0.09 | 29,29,29,29 | 0 |
| 83 | MG | 1 | 3435 | 1/1 | 0.98 | 0.08 | 0,0,0,0 | 0 |
| 83 | MG | CM | 1867 | 1/1 | 0.98 | 0.10 | 34,34,34,34 | 0 |
| 83 | MG | 1 | 3865 | 1/1 | 0.98 | 0.03 | 25,25,25,25 | 0 |
| 83 | MG | 1 | 3465 | 1/1 | 0.98 | 0.09 | 10,10,10,10 | 0 |
| 83 | MG | AS | 3668 | 1/1 | 0.98 | 0.05 | 63,63,63,63 | 0 |
| 85 | ZN | AK | 101 | 1/1 | 0.98 | 0.07 | 55,55,55,55 | 0 |
| 85 | ZN | AN | 101 | 1/1 | 0.98 | 0.06 | 73,73,73,73 | 0 |
| 83 | MG | 1 | 3534 | 1/1 | 0.98 | 0.05 | 15,15,15,15 | 0 |
| 83 | MG | BV | 201 | 1/1 | 0.98 | 0.19 | 25,25,25,25 | 0 |
| 83 | MG | CM | 1831 | 1/1 | 0.98 | 0.08 | 44,44,44,44 | 0 |
| 83 | MG | AS | 3670 | 1/1 | 0.98 | 0.08 | 11,11,11,11 | 0 |
| 83 | MG | B | 1849 | 1/1 | 0.98 | 0.13 | 32,32,32,32 | 0 |
| 83 | MG | 1 | 3635 | 1/1 | 0.98 | 0.07 | 37,37,37,37 | 0 |
| 83 | MG | 1 | 3636 | 1/1 | 0.98 | 0.04 | 22,22,22,22 | 0 |
| 83 | MG | B | 1920 | 1/1 | 0.98 | 0.06 | 68,68,68,68 | 0 |
| 85 | ZN | DN | 201 | 1/1 | 0.98 | 0.03 | 59,59,59,59 | 0 |
| 83 | MG | AS | 3452 | 1/1 | 0.98 | 0.14 | 19,19,19,19 | 0 |
| 83 | MG | 1 | 3676 | 1/1 | 0.98 | 0.09 | 41,41,41,41 | 0 |
| 83 | MG | AS | 3483 | 1/1 | 0.98 | 0.11 | 13,13,13,13 | 0 |
| 83 | MG | CM | 1840 | 1/1 | 0.98 | 0.18 | 24,24,24,24 | 0 |
| 83 | MG | 1 | 3440 | 1/1 | 0.99 | 0.17 | 2,2,2,2 | 0 |
| 83 | MG | 1 | 3499 | 1/1 | 0.99 | 0.16 | 13,13,13,13 | 0 |
| 83 | MG | 1 | 3528 | 1/1 | 0.99 | 0.09 | 32,32,32,32 | 0 |
| 83 | MG | 1 | 3475 | 1/1 | 0.99 | 0.16 | 3,3,3,3 | 0 |

*Continued on next page...*

*Continued from previous page...*

| Mol | Type | Chain | Res | Atoms | RSCC | RSR | B-factors(Å$^2$) | Q<0.9 |
|---|---|---|---|---|---|---|---|---|
| 83 | MG | B | 1831 | 1/1 | 0.99 | 0.14 | 23,23,23,23 | 0 |
| 83 | MG | 3 | 201 | 1/1 | 0.99 | 0.10 | 0,0,0,0 | 0 |
| 83 | MG | AS | 3679 | 1/1 | 0.99 | 0.06 | 28,28,28,28 | 0 |
| 85 | ZN | c | 201 | 1/1 | 0.99 | 0.03 | 51,51,51,51 | 0 |
| 83 | MG | 1 | 3772 | 1/1 | 0.99 | 0.12 | 18,18,18,18 | 0 |
| 83 | MG | B | 1925 | 1/1 | 0.99 | 0.06 | 28,28,28,28 | 0 |
| 83 | MG | 1 | 3550 | 1/1 | 0.99 | 0.12 | 9,9,9,9 | 0 |
| 83 | MG | 1 | 3764 | 1/1 | 0.99 | 0.13 | 18,18,18,18 | 0 |
| 85 | ZN | CE | 101 | 1/1 | 0.99 | 0.03 | 66,66,66,66 | 0 |
| 83 | MG | AS | 3456 | 1/1 | 0.99 | 0.15 | 7,7,7,7 | 0 |
| 83 | MG | AP | 202 | 1/1 | 0.99 | 0.03 | 12,12,12,12 | 0 |
| 85 | ZN | CK | 101 | 1/1 | 0.99 | 0.03 | 84,84,84,84 | 0 |
| 83 | MG | 1 | 3408 | 1/1 | 0.99 | 0.03 | 47,47,47,47 | 0 |
| 83 | MG | 1 | 3582 | 1/1 | 0.99 | 0.18 | 31,31,31,31 | 0 |
| 83 | MG | CM | 1892 | 1/1 | 0.99 | 0.14 | 9,9,9,9 | 0 |
| 83 | MG | 1 | 3767 | 1/1 | 0.99 | 0.03 | 26,26,26,26 | 0 |
| 83 | MG | AS | 3656 | 1/1 | 0.99 | 0.04 | 45,45,45,45 | 0 |
| 83 | MG | 1 | 3708 | 1/1 | 1.00 | 0.07 | 11,11,11,11 | 0 |

## 6.5 Other polymers (i)

There are no such residues in this entry.