# Full wwPDB X-ray Structure Validation Report (i)

Mar 18, 2026 – 04:55 AM UTC

| | | |
|---|---|---|
| PDB ID | : | 4WZD / pdb_00004wzd |
| Title | : | Complex of 70S ribosome with cognate tRNA-Tyr in the P-site |
| Authors | : | Rozov, A.; Demeshkina, N.; Yusupov, M.; Yusupova, G. |
| Deposited on | : | 2014-11-19 |
| Resolution | : | 3.10 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 (i) 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 (i)) were used in the production of this report:

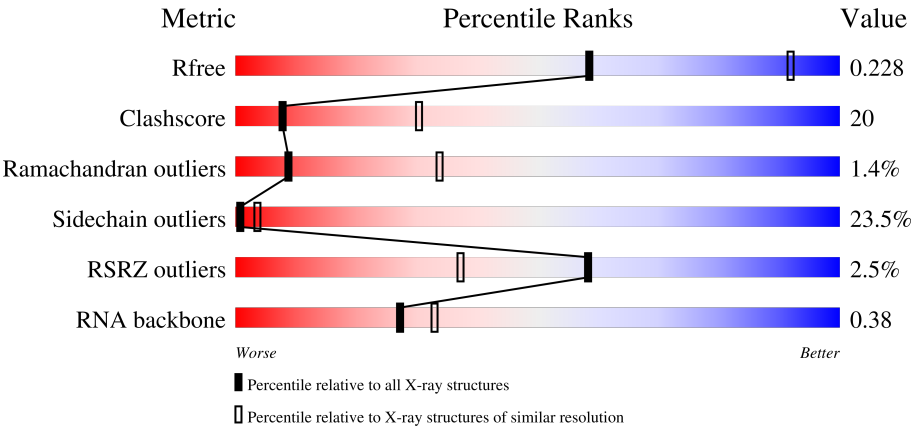
| | | |
|---|---|---|
| MolProbity | : | 4-5-2 with Phenix2.0 |
| Mogul | : | 2022.3.0, CSD as543be (2022) |
| Xtriage (Phenix) | : | 2.0 |
| EDS | : | 3.0 |
| Percentile statistics | : | 20250101.v01 (using entries in the PDB archive January 1st 2025) |
| CCP4 | : | 9.0.010 (Gargrove) |
| Density-Fitness | : | 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 3.10 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 | 1456 (3.10-3.10) |
| Clashscore | 190562 | 1539 (3.10-3.10) |
| Ramachandran outliers | 187476 | 1467 (3.10-3.10) |
| Sidechain outliers | 187428 | 1467 (3.10-3.10) |
| RSRZ outliers | 180081 | 1456 (3.10-3.10) |
| RNA backbone | 3983 | 1022 (3.32-2.88) |

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 | 13 | 1522 | 33% 50% 15% |
| 1 | 1G | 1522 | 36% 48% 15% |
| 2 | 12 | 256 | 4% 38% 41% 13% 7% |
| 2 | 1E | 256 | 2% 34% 42% 16% 7% |

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| Mol | Chain | Length | Quality of chain |
|---|---|---|---|
| 3 | 22 | 239 | 2% 38% 41% 8% 14% |
| 3 | 2E | 239 | % 41% 38% 6% 14% |
| 4 | 32 | 209 | 4% 40% 43% 16% |
| 4 | 3E | 209 | 3% 42% 46% 11% |
| 5 | 42 | 162 | % 39% 39% 15% 7% |
| 5 | 4E | 162 | % 46% 32% 15% 7% |
| 6 | 52 | 101 | 49% 41% 10% |
| 6 | 5E | 101 | % 45% 42% 13% |
| 7 | 62 | 156 | 2% 59% 29% 12% |
| 7 | 6E | 156 | 3% 50% 35% 13% |
| 8 | 72 | 138 | 2% 46% 44% 9% |
| 8 | 7E | 138 | 2% 39% 49% 12% |
| 9 | 82 | 128 | 12% 36% 52% 9% |
| 9 | 8E | 128 | 7% 48% 40% 12% |
| 10 | 1A | 105 | 15% 33% 45% 16% 6% |
| 10 | 1I | 105 | 4% 48% 34% 11% 6% |
| 11 | 2A | 129 | 2% 49% 37% 10% |
| 11 | 2I | 129 | 5% 43% 43% 5% 10% |
| 12 | 3A | 132 | 4% 52% 34% 7% 5% |
| 12 | 3I | 132 | 52% 33% 8% 5% |
| 13 | 4A | 126 | 10% 33% 44% 15% 7% |
| 13 | 4I | 126 | 6% 40% 44% 9% 8% |
| 14 | 5A | 61 | 18% 46% 48% 5% |
| 14 | 5I | 61 | 5% 31% 52% 15% |
| 15 | 6A | 89 | % 52% 39% 8% |

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| Mol | Chain | Length | Quality of chain |
|---|---|---|---|
| 15 | 6I | 89 | 47% 40% 11% |
| 16 | 7A | 88 | 41% 42% 11% 5% |
| 16 | 7I | 88 | 10% 36% 45% 13% 5% |
| 17 | 8A | 105 | 2% 44% 42% 10% 5% |
| 17 | 8I | 105 | 2% 37% 50% 9% 5% |
| 18 | 9A | 88 | 45% 32% 5% 18% |
| 18 | 9I | 88 | 45% 28% 8% 18% |
| 19 | AA | 93 | 8% 26% 42% 17% 15% |
| 19 | AI | 93 | 8% 35% 39% 10% 5% 11% |
| 20 | BA | 106 | 7% 40% 43% 9% 7% |
| 20 | BI | 106 | 7% 44% 35% 14% 7% |
| 21 | 1B | 27 | 41% 41% 48% 7% |
| 21 | 1F | 27 | 19% 44% 48% 7% |
| 22 | 2K | 85 | 27% 36% 29% |
| 22 | 2L | 85 | 29% 33% 25% 5% 8% |
| 22 | 3K | 85 | 2% 32% 38% 26% 5% |
| 22 | 3L | 85 | 34% 42% 19% 5% |
| 23 | 4K | 30 | 3% 20% 10% 20% 47% |
| 23 | 4L | 30 | 7% 13% 7% 7% 73% |
| 24 | 14 | 2917 | 41% 45% 14% |
| 24 | 1H | 2917 | 38% 46% 15% |
| 25 | 16 | 122 | 32% 48% 20% |
| 25 | 1J | 122 | 2% 25% 57% 18% |
| 26 | 71 | 229 | 3% 39% 19% 41% |
| 26 | 79 | 229 | 3% 34% 21% 41% |

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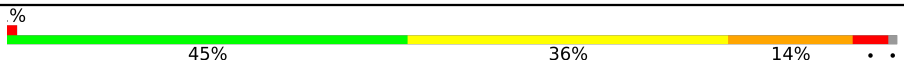
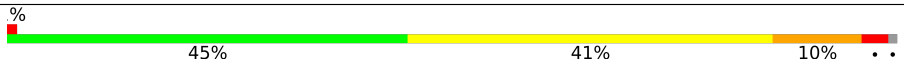
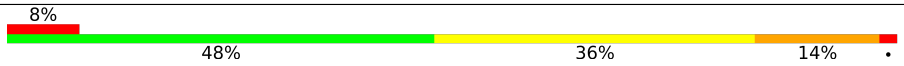
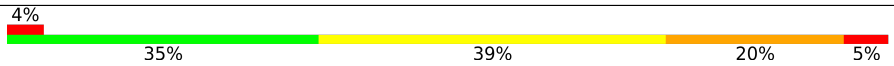
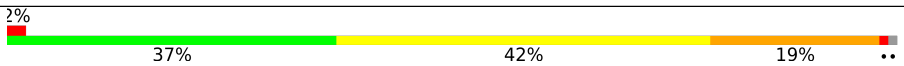
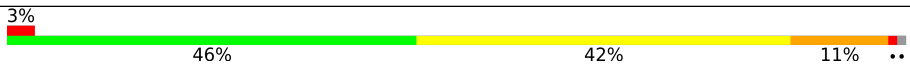
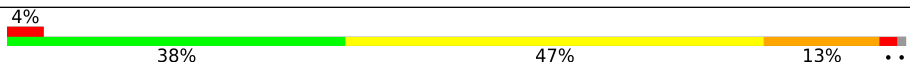
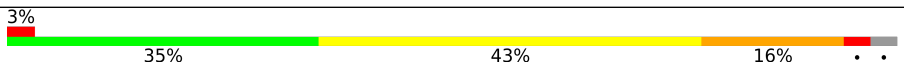
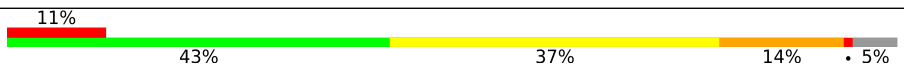
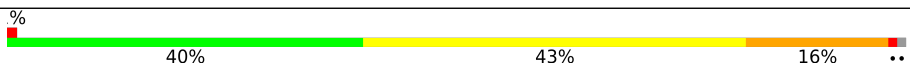
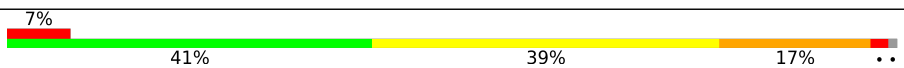
| Mol | Chain | Length | Quality of chain |
|---|---|---|---|
| 27 | 11 | 276 |   |
| 27 | 19 | 276 |   |
| 28 | 21 | 206 |   |
| 28 | 29 | 206 |   |
| 29 | 31 | 210 | |
| 29 | 39 | 210 |   |
| 30 | 41 | 182 |   |
| 30 | 49 | 182 |   |
| 31 | 51 | 180 |   |
| 31 | 59 | 180 |   |
| 32 | 61 | 148 |   |
| 32 | 69 | 148 |   |
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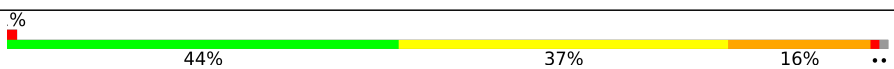
| 33 | 58 | 140 |   |
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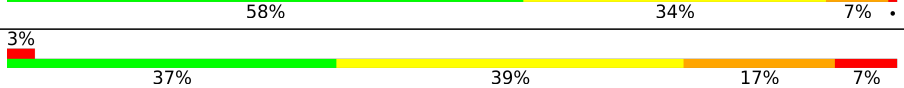
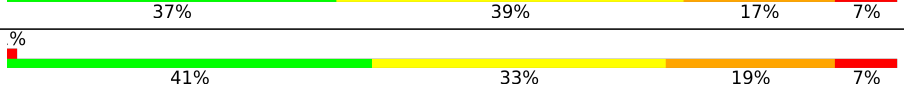
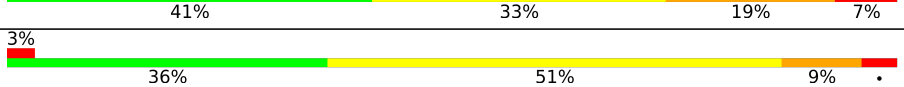
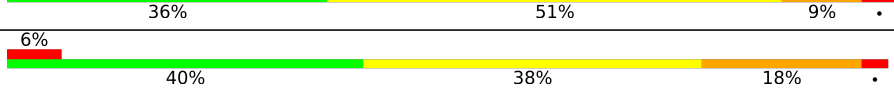
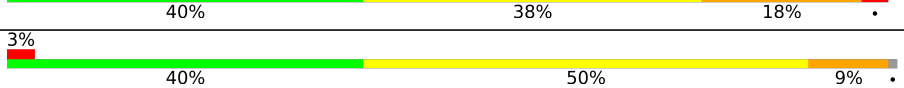
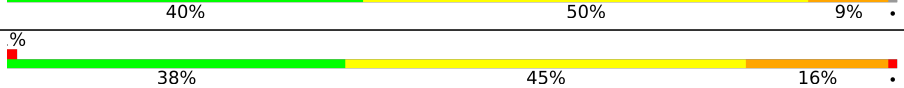
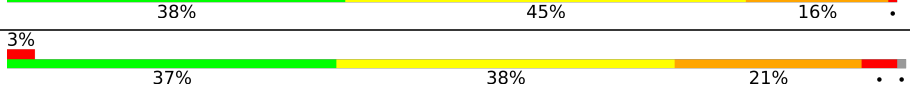
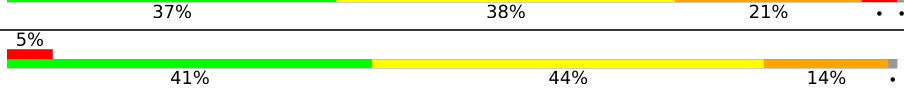
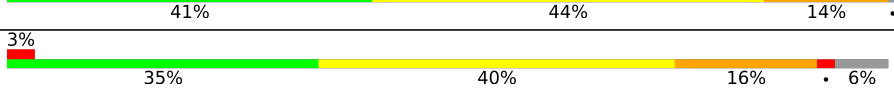
| 34 | 68 | 122 | |
| 35 | 35 | 150 |   |
| 35 | 78 | 150 |   |
| 36 | 45 | 141 |   |
| 36 | 88 | 141 |   |
| 37 | 55 | 118 |   |
| 37 | 98 | 118 |   |
| 38 | 65 | 112 |   |
| 38 | A8 | 112 |   |
| 39 | 75 | 146 |   |

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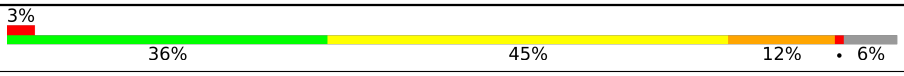
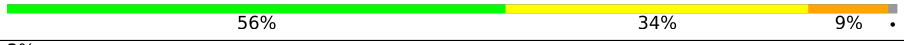
| Mol | Chain | Length | Quality of chain |
|---|---|---|---|
| 39 | B8 | 146 |   |
| 40 | 85 | 118 |   |
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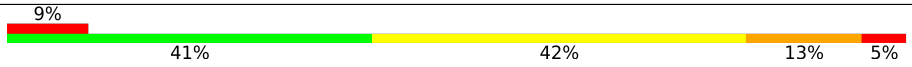
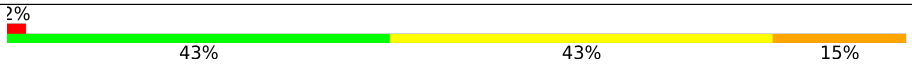
| 41 | 95 | 101 |   |
| 41 | D8 | 101 |   |
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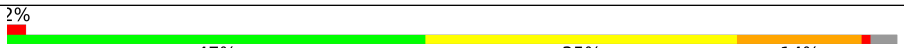
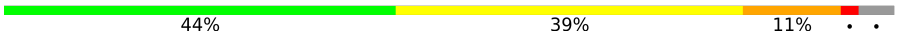
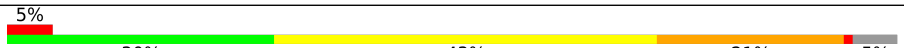
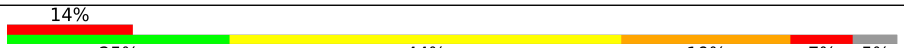
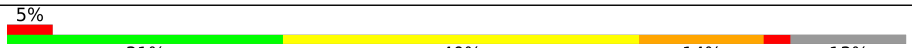
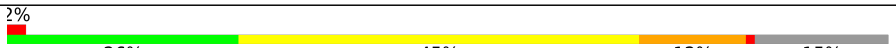
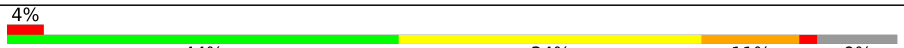
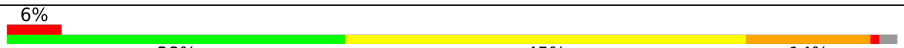
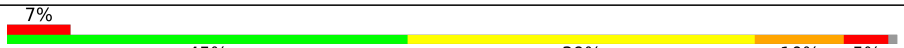
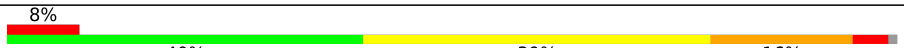
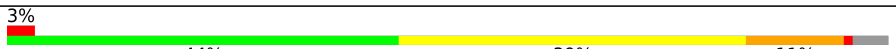
| 42 | E8 | 113 | |
| 43 | B5 | 96 |   |
| 43 | F8 | 96 |   |
| 44 | C5 | 110 |   |
| 44 | G8 | 110 |   |
| 45 | D5 | 206 |   |
| 45 | H8 | 206 |   |
| 46 | E5 | 85 |   |
| 46 | I8 | 85 |   |
| 47 | F5 | 98 |   |
| 47 | J8 | 98 |   |
| 48 | G5 | 72 |   |
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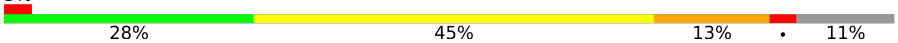
| 49 | H5 | 60 | |
| 49 | L8 | 60 | |
| 50 | I5 | 71 |   |
| 50 | M8 | 71 | |
| 51 | J5 | 60 | |
| 51 | N8 | 60 | |

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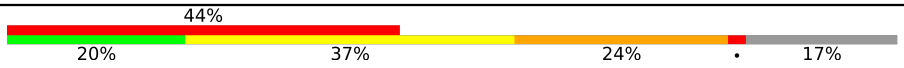
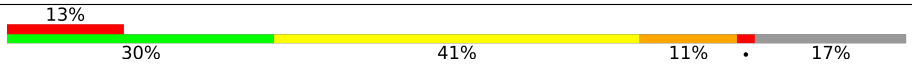
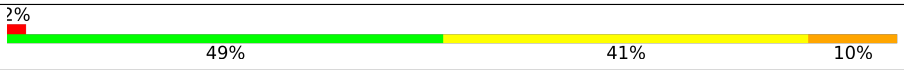
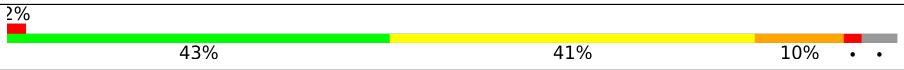
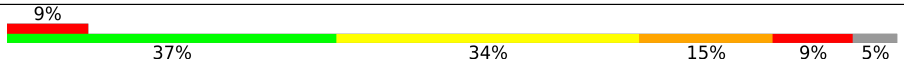
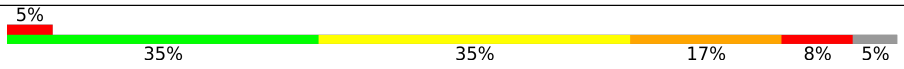
| Mol | Chain | Length | Quality of chain |
|---|---|---|---|
| 52 | K5 | 54 |   |
| 52 | O8 | 54 |   |
| 53 | L5 | 49 |   |
| 53 | P8 | 49 |   |
| 54 | M5 | 65 |   |
| 54 | Q8 | 65 |   |

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 |
|---|---|---|---|---|---|---|---|
| 55 | MG | 13 | 1624 | - | - | - | X |
| 55 | MG | 13 | 1668 | - | - | - | X |
| 55 | MG | 13 | 1681 | - | - | - | X |
| 55 | MG | 13 | 1684 | - | - | - | X |
| 55 | MG | 13 | 1688 | - | - | - | X |
| 55 | MG | 13 | 1689 | - | - | - | X |
| 55 | MG | 13 | 1692 | - | - | - | X |
| 55 | MG | 13 | 1700 | - | - | - | X |
| 55 | MG | 13 | 1708 | - | - | - | X |
| 55 | MG | 13 | 1714 | - | - | - | X |
| 55 | MG | 14 | 3105 | - | - | - | X |
| 55 | MG | 14 | 3119 | - | - | - | X |
| 55 | MG | 14 | 3157 | - | - | - | X |
| 55 | MG | 14 | 3287 | - | - | - | X |
| 55 | MG | 14 | 3314 | - | - | - | X |
| 55 | MG | 14 | 3324 | - | - | - | X |
| 55 | MG | 1G | 1610 | - | - | - | X |
| 55 | MG | 1G | 1656 | - | - | - | X |
| 55 | MG | 1G | 1674 | - | - | - | X |
| 55 | MG | 1G | 1691 | - | - | - | X |
| 55 | MG | 1G | 1700 | - | - | - | X |
| 55 | MG | 1G | 1721 | - | - | - | X |
| 55 | MG | 1G | 1727 | - | - | - | X |
| 55 | MG | 1H | 3044 | - | - | - | X |
| 55 | MG | 1H | 3168 | - | - | - | X |
| 55 | MG | 1H | 3203 | - | - | - | X |
| 55 | MG | 1H | 3209 | - | - | - | X |

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| Mol | Type | Chain | Res | Chirality | Geometry | Clashes | Electron density |
|---|---|---|---|---|---|---|---|
| 55 | MG | 1H | 3325 | - | - | - | X |
| 55 | MG | 1H | 3332 | - | - | - | X |
| 55 | MG | 1H | 3357 | - | - | - | X |
| 55 | MG | 1H | 3360 | - | - | - | X |
| 55 | MG | 1H | 3389 | - | - | - | X |
| 55 | MG | 4A | 201 | - | - | - | X |
| 55 | MG | I8 | 101 | - | - | - | X |

## 2 Entry composition (i)

There are 57 unique types of molecules in this entry. The entry contains 299705 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 16S ribosomal RNA.

| Mol | Chain | Residues | Atoms | | | | | ZeroOcc | AltConf | Trace |
|---|---|---|---|---|---|---|---|---|---|---|
| 1 | 13 | 1499 | Total | C | N | O | P | 0 | 5 | 0 |
| | | | 32337 | 14392 | 5999 | 10442 | 1504 | | | |
| 1 | 1G | 1503 | Total | C | N | O | P | 0 | 0 | 0 |
| | | | 32309 | 14381 | 5990 | 10436 | 1502 | | | |

- Molecule 2 is a protein called 30S ribosomal protein S2.

| Mol | Chain | Residues | Atoms | | | | | ZeroOcc | AltConf | Trace |
|---|---|---|---|---|---|---|---|---|---|---|
| 2 | 1E | 237 | Total | C | N | O | S | 0 | 0 | 0 |
| | | | 1924 | 1228 | 344 | 347 | 5 | | | |
| 2 | 12 | 237 | Total | C | N | O | S | 0 | 0 | 0 |
| | | | 1924 | 1228 | 344 | 347 | 5 | | | |

- Molecule 3 is a protein called 30S ribosomal protein S3.

| Mol | Chain | Residues | Atoms | | | | | ZeroOcc | AltConf | Trace |
|---|---|---|---|---|---|---|---|---|---|---|
| 3 | 2E | 205 | Total | C | N | O | S | 0 | 0 | 0 |
| | | | 1605 | 1011 | 313 | 280 | 1 | | | |
| 3 | 22 | 206 | Total | C | N | O | S | 0 | 0 | 0 |
| | | | 1612 | 1016 | 314 | 281 | 1 | | | |

- Molecule 4 is a protein called 30S ribosomal protein S4.

| Mol | Chain | Residues | Atoms | | | | | ZeroOcc | AltConf | Trace |
|---|---|---|---|---|---|---|---|---|---|---|
| 4 | 3E | 208 | Total | C | N | O | S | 0 | 0 | 0 |
| | | | 1702 | 1066 | 339 | 290 | 7 | | | |
| 4 | 32 | 208 | Total | C | N | O | S | 0 | 0 | 0 |
| | | | 1702 | 1066 | 339 | 290 | 7 | | | |

- Molecule 5 is a protein called 30S ribosomal protein S5.

| Mol | Chain | Residues | Atoms | | | | | ZeroOcc | AltConf | Trace |
|---|---|---|---|---|---|---|---|---|---|---|
| 5 | 4E | 151 | Total | C | N | O | S | 0 | 0 | 0 |
| | | | 1155 | 729 | 218 | 204 | 4 | | | |
| 5 | 42 | 151 | Total | C | N | O | S | 0 | 0 | 0 |
| | | | 1155 | 729 | 218 | 204 | 4 | | | |

- Molecule 6 is a protein called 30S ribosomal protein S6.

| Mol | Chain | Residues | Atoms | | | | | ZeroOcc | AltConf | Trace |
|---|---|---|---|---|---|---|---|---|---|---|
| 6 | 5E | 101 | Total | C | N | O | S | 0 | 0 | 0 |
| | | | 842 | 531 | 155 | 153 | 3 | | | |
| 6 | 52 | 101 | Total | C | N | O | S | 0 | 0 | 0 |
| | | | 842 | 531 | 155 | 153 | 3 | | | |

- Molecule 7 is a protein called 30S ribosomal protein S7.

| Mol | Chain | Residues | Atoms | | | | | ZeroOcc | AltConf | Trace |
|---|---|---|---|---|---|---|---|---|---|---|
| 7 | 6E | 155 | Total | C | N | O | S | 0 | 0 | 0 |
| | | | 1256 | 781 | 252 | 217 | 6 | | | |
| 7 | 62 | 155 | Total | C | N | O | S | 0 | 0 | 0 |
| | | | 1256 | 781 | 252 | 217 | 6 | | | |

- Molecule 8 is a protein called 30S ribosomal protein S8.

| Mol | Chain | Residues | Atoms | | | | | ZeroOcc | AltConf | Trace |
|---|---|---|---|---|---|---|---|---|---|---|
| 8 | 7E | 138 | Total | C | N | O | S | 0 | 0 | 0 |
| | | | 1115 | 705 | 215 | 192 | 3 | | | |
| 8 | 72 | 138 | Total | C | N | O | S | 0 | 0 | 0 |
| | | | 1115 | 705 | 215 | 192 | 3 | | | |

- Molecule 9 is a protein called 30S ribosomal protein S9.

| Mol | Chain | Residues | Atoms | | | | ZeroOcc | AltConf | Trace |
|---|---|---|---|---|---|---|---|---|---|
| 9 | 8E | 127 | Total | C | N | O | 0 | 0 | 0 |
| | | | 1009 | 639 | 197 | 173 | | | |
| 9 | 82 | 127 | Total | C | N | O | 0 | 0 | 0 |
| | | | 1009 | 639 | 197 | 173 | | | |

- Molecule 10 is a protein called 30S ribosomal protein S10.

| Mol | Chain | Residues | Atoms | | | | | ZeroOcc | AltConf | Trace |
|---|---|---|---|---|---|---|---|---|---|---|
| 10 | 1I | 99 | Total | C | N | O | S | 0 | 0 | 0 |
| | | | 801 | 504 | 157 | 139 | 1 | | | |

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| Mol | Chain | Residues | Atoms | | | | | ZeroOcc | AltConf | Trace |
|---|---|---|---|---|---|---|---|---|---|---|
| 10 | 1A | 99 | Total | C | N | O | S | 0 | 0 | 0 |
| | | | 801 | 504 | 157 | 139 | 1 | | | |

- Molecule 11 is a protein called 30S ribosomal protein S11.

| Mol | Chain | Residues | Atoms | | | | | ZeroOcc | AltConf | Trace |
|---|---|---|---|---|---|---|---|---|---|---|
| 11 | 2I | 116 | Total | C | N | O | S | 0 | 0 | 0 |
| | | | 864 | 537 | 164 | 160 | 3 | | | |
| 11 | 2A | 116 | Total | C | N | O | S | 0 | 0 | 0 |
| | | | 864 | 537 | 164 | 160 | 3 | | | |

- Molecule 12 is a protein called 30S ribosomal protein S12.

| Mol | Chain | Residues | Atoms | | | | | ZeroOcc | AltConf | Trace |
|---|---|---|---|---|---|---|---|---|---|---|
| 12 | 3I | 125 | Total | C | N | O | S | 0 | 0 | 0 |
| | | | 975 | 614 | 196 | 164 | 1 | | | |
| 12 | 3A | 125 | Total | C | N | O | S | 0 | 0 | 0 |
| | | | 975 | 614 | 196 | 164 | 1 | | | |

- Molecule 13 is a protein called 30S ribosomal protein S13.

| Mol | Chain | Residues | Atoms | | | | | ZeroOcc | AltConf | Trace |
|---|---|---|---|---|---|---|---|---|---|---|
| 13 | 4I | 116 | Total | C | N | O | S | 0 | 0 | 0 |
| | | | 928 | 574 | 191 | 161 | 2 | | | |
| 13 | 4A | 117 | Total | C | N | O | S | 0 | 0 | 0 |
| | | | 933 | 577 | 192 | 162 | 2 | | | |

- Molecule 14 is a protein called 30S ribosomal protein S14 type Z.

| Mol | Chain | Residues | Atoms | | | | | ZeroOcc | AltConf | Trace |
|---|---|---|---|---|---|---|---|---|---|---|
| 14 | 5I | 60 | Total | C | N | O | S | 0 | 0 | 0 |
| | | | 491 | 312 | 104 | 71 | 4 | | | |
| 14 | 5A | 60 | Total | C | N | O | S | 0 | 0 | 0 |
| | | | 491 | 312 | 104 | 71 | 4 | | | |

- Molecule 15 is a protein called 30S ribosomal protein S15.

| Mol | Chain | Residues | Atoms | | | | | ZeroOcc | AltConf | Trace |
|---|---|---|---|---|---|---|---|---|---|---|
| 15 | 6I | 88 | Total | C | N | O | S | 0 | 0 | 0 |
| | | | 733 | 459 | 147 | 125 | 2 | | | |
| 15 | 6A | 88 | Total | C | N | O | S | 0 | 0 | 0 |
| | | | 733 | 459 | 147 | 125 | 2 | | | |

- Molecule 16 is a protein called 30S ribosomal protein S16.

| Mol | Chain | Residues | Atoms | | | | | ZeroOcc | AltConf | Trace |
|---|---|---|---|---|---|---|---|---|---|---|
| 16 | 7I | 84 | Total | C | N | O | S | 0 | 0 | 0 |
| | | | 705 | 446 | 140 | 118 | 1 | | | |
| 16 | 7A | 84 | Total | C | N | O | S | 0 | 0 | 0 |
| | | | 705 | 446 | 140 | 118 | 1 | | | |

- Molecule 17 is a protein called 30S ribosomal protein S17.

| Mol | Chain | Residues | Atoms | | | | | ZeroOcc | AltConf | Trace |
|---|---|---|---|---|---|---|---|---|---|---|
| 17 | 8I | 100 | Total | C | N | O | S | 0 | 0 | 0 |
| | | | 834 | 534 | 155 | 143 | 2 | | | |
| 17 | 8A | 100 | Total | C | N | O | S | 0 | 0 | 0 |
| | | | 834 | 534 | 155 | 143 | 2 | | | |

- Molecule 18 is a protein called 30S ribosomal protein S18.

| Mol | Chain | Residues | Atoms | | | | ZeroOcc | AltConf | Trace |
|---|---|---|---|---|---|---|---|---|---|
| 18 | 9I | 72 | Total | C | N | O | 0 | 0 | 0 |
| | | | 590 | 376 | 117 | 97 | | | |
| 18 | 9A | 72 | Total | C | N | O | 0 | 0 | 0 |
| | | | 590 | 376 | 117 | 97 | | | |

- Molecule 19 is a protein called 30S ribosomal protein S19.

| Mol | Chain | Residues | Atoms | | | | | ZeroOcc | AltConf | Trace |
|---|---|---|---|---|---|---|---|---|---|---|
| 19 | AI | 83 | Total | C | N | O | S | 0 | 0 | 0 |
| | | | 665 | 424 | 124 | 115 | 2 | | | |
| 19 | AA | 79 | Total | C | N | O | S | 0 | 0 | 0 |
| | | | 633 | 404 | 117 | 110 | 2 | | | |

- Molecule 20 is a protein called 30S ribosomal protein S20.

| Mol | Chain | Residues | Atoms | | | | | ZeroOcc | AltConf | Trace |
|---|---|---|---|---|---|---|---|---|---|---|
| 20 | BI | 99 | Total | C | N | O | S | 0 | 0 | 0 |
| | | | 762 | 470 | 162 | 128 | 2 | | | |
| 20 | BA | 99 | Total | C | N | O | S | 0 | 0 | 0 |
| | | | 762 | 470 | 162 | 128 | 2 | | | |

- Molecule 21 is a protein called 30S ribosomal protein Thx.

| Mol | Chain | Residues | Atoms | | | | ZeroOcc | AltConf | Trace |
|---|---|---|---|---|---|---|---|---|---|
| 21 | 1F | 25 | Total | C | N | O | 0 | 0 | 0 |
| | | | 217 | 134 | 52 | 31 | | | |
| 21 | 1B | 25 | Total | C | N | O | 0 | 0 | 0 |
| | | | 217 | 134 | 52 | 31 | | | |

- Molecule 22 is a RNA chain called tRNA-Tyr.

| Mol | Chain | Residues | Atoms | | | | | | ZeroOcc | AltConf | Trace |
|---|---|---|---|---|---|---|---|---|---|---|---|
| 22 | 2K | 82 | Total | C | N | O | P | S | 0 | 0 | 0 |
| | | | 1765 | 795 | 315 | 571 | 82 | 2 | | | |
| 22 | 3K | 85 | Total | C | N | O | P | S | 0 | 0 | 0 |
| | | | 1824 | 822 | 323 | 592 | 85 | 2 | | | |
| 22 | 2L | 78 | Total | C | N | O | P | S | 0 | 0 | 0 |
| | | | 1678 | 756 | 297 | 545 | 78 | 2 | | | |
| 22 | 3L | 85 | Total | C | N | O | P | S | 0 | 0 | 0 |
| | | | 1825 | 822 | 323 | 593 | 85 | 2 | | | |

- Molecule 23 is a RNA chain called mRNA.

| Mol | Chain | Residues | Atoms | | | | | ZeroOcc | AltConf | Trace |
|---|---|---|---|---|---|---|---|---|---|---|
| 23 | 4K | 16 | Total | C | N | O | P | 0 | 0 | 0 |
| | | | 348 | 157 | 72 | 103 | 16 | | | |
| 23 | 4L | 8 | Total | C | N | O | P | 0 | 0 | 0 |
| | | | 170 | 77 | 32 | 53 | 8 | | | |

- Molecule 24 is a RNA chain called 23S ribosomal RNA.

| Mol | Chain | Residues | Atoms | | | | | ZeroOcc | AltConf | Trace |
|---|---|---|---|---|---|---|---|---|---|---|
| 24 | 1H | 2912 | Total | C | N | O | P | 0 | 0 | 0 |
| | | | 62707 | 27911 | 11722 | 20163 | 2911 | | | |
| 24 | 14 | 2909 | Total | C | N | O | P | 0 | 0 | 0 |
| | | | 62647 | 27884 | 11716 | 20139 | 2908 | | | |

There are 6 discrepancies between the modelled and reference sequences:

| Chain | Residue | Modelled | Actual | Comment | Reference |
|---|---|---|---|---|---|
| 1H | 161 | U | - | insertion | GB 48268 |
| 1H | 493 | G | - | insertion | GB 48268 |
| 1H | 1228 | G | - | insertion | GB 48268 |
| 14 | 161 | U | - | insertion | GB 48268 |
| 14 | 493 | G | - | insertion | GB 48268 |
| 14 | 1228 | G | - | insertion | GB 48268 |

- Molecule 25 is a RNA chain called 5S ribosomal RNA.

| Mol | Chain | Residues | Atoms | | | | | ZeroOcc | AltConf | Trace |
|---|---|---|---|---|---|---|---|---|---|---|
| 25 | 16 | 122 | Total | C | N | O | P | 0 | 0 | 0 |
| | | | 2617 | 1166 | 486 | 844 | 121 | | | |
| 25 | 1J | 122 | Total | C | N | O | P | 0 | 0 | 0 |
| | | | 2617 | 1166 | 486 | 844 | 121 | | | |

- Molecule 26 is a protein called 50S ribosomal protein L1.

| Mol | Chain | Residues | Atoms | | | | | ZeroOcc | AltConf | Trace |
|---|---|---|---|---|---|---|---|---|---|---|
| 26 | 71 | 135 | Total | C | N | O | S | 0 | 0 | 0 |
| | | | 1049 | 662 | 197 | 189 | 1 | | | |
| 26 | 79 | 135 | Total | C | N | O | S | 0 | 0 | 0 |
| | | | 1049 | 662 | 197 | 189 | 1 | | | |

- Molecule 27 is a protein called 50S ribosomal protein L2.

| Mol | Chain | Residues | Atoms | | | | | ZeroOcc | AltConf | Trace |
|---|---|---|---|---|---|---|---|---|---|---|
| 27 | 11 | 272 | Total | C | N | O | S | 0 | 0 | 0 |
| | | | 2115 | 1335 | 420 | 357 | 3 | | | |
| 27 | 19 | 273 | Total | C | N | O | S | 0 | 0 | 0 |
| | | | 2120 | 1338 | 421 | 358 | 3 | | | |

- Molecule 28 is a protein called 50S ribosomal protein L3.

| Mol | Chain | Residues | Atoms | | | | | ZeroOcc | AltConf | Trace |
|---|---|---|---|---|---|---|---|---|---|---|
| 28 | 21 | 205 | Total | C | N | O | S | 0 | 0 | 0 |
| | | | 1568 | 991 | 300 | 271 | 6 | | | |
| 28 | 29 | 205 | Total | C | N | O | S | 0 | 0 | 0 |
| | | | 1568 | 991 | 300 | 271 | 6 | | | |

- Molecule 29 is a protein called 50S ribosomal protein L4.

| Mol | Chain | Residues | Atoms | | | | | ZeroOcc | AltConf | Trace |
|---|---|---|---|---|---|---|---|---|---|---|
| 29 | 31 | 202 | Total | C | N | O | S | 0 | 0 | 0 |
| | | | 1585 | 1011 | 297 | 275 | 2 | | | |
| 29 | 39 | 208 | Total | C | N | O | S | 0 | 0 | 0 |
| | | | 1627 | 1037 | 304 | 283 | 3 | | | |

- Molecule 30 is a protein called 50S ribosomal protein L5.

| Mol | Chain | Residues | Atoms | | | | | ZeroOcc | AltConf | Trace |
|---|---|---|---|---|---|---|---|---|---|---|
| 30 | 41 | 181 | Total | C | N | O | S | 0 | 0 | 0 |
| | | | 1473 | 942 | 268 | 259 | 4 | | | |
| 30 | 49 | 181 | Total | C | N | O | S | 0 | 0 | 0 |
| | | | 1473 | 942 | 268 | 259 | 4 | | | |

- Molecule 31 is a protein called 50S ribosomal protein L6.

| Mol | Chain | Residues | Atoms | | | | | ZeroOcc | AltConf | Trace |
|---|---|---|---|---|---|---|---|---|---|---|
| 31 | 51 | 174 | Total | C | N | O | S | 0 | 0 | 0 |
| | | | 1336 | 848 | 251 | 236 | 1 | | | |
| 31 | 59 | 171 | Total | C | N | O | S | 0 | 0 | 0 |
| | | | 1312 | 832 | 246 | 233 | 1 | | | |

- Molecule 32 is a protein called 50S ribosomal protein L9.

| Mol | Chain | Residues | Atoms | | | | | ZeroOcc | AltConf | Trace |
|---|---|---|---|---|---|---|---|---|---|---|
| 32 | 61 | 146 | Total | C | N | O | S | 0 | 0 | 0 |
| | | | 1136 | 726 | 201 | 208 | 1 | | | |
| 32 | 69 | 146 | Total | C | N | O | S | 0 | 0 | 0 |
| | | | 1136 | 726 | 201 | 208 | 1 | | | |

- Molecule 33 is a protein called 50S ribosomal protein L13.

| Mol | Chain | Residues | Atoms | | | | | ZeroOcc | AltConf | Trace |
|---|---|---|---|---|---|---|---|---|---|---|
| 33 | 58 | 138 | Total | C | N | O | S | 0 | 0 | 0 |
| | | | 1104 | 712 | 206 | 182 | 4 | | | |
| 33 | 15 | 138 | Total | C | N | O | S | 0 | 0 | 0 |
| | | | 1104 | 712 | 206 | 182 | 4 | | | |

- Molecule 34 is a protein called 50S ribosomal protein L14.

| Mol | Chain | Residues | Atoms | | | | | ZeroOcc | AltConf | Trace |
|---|---|---|---|---|---|---|---|---|---|---|
| 34 | 68 | 122 | Total | C | N | O | S | 0 | 0 | 0 |
| | | | 932 | 588 | 171 | 169 | 4 | | | |
| 34 | 25 | 122 | Total | C | N | O | S | 0 | 0 | 0 |
| | | | 932 | 588 | 171 | 169 | 4 | | | |

- Molecule 35 is a protein called 50S ribosomal protein L15.

| Mol | Chain | Residues | Atoms | | | | | ZeroOcc | AltConf | Trace |
|---|---|---|---|---|---|---|---|---|---|---|
| 35 | 78 | 150 | Total | C | N | O | S | 0 | 0 | 0 |
| | | | 1144 | 712 | 232 | 197 | 3 | | | |

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| Mol | Chain | Residues | Atoms | | | | | ZeroOcc | AltConf | Trace |
|---|---|---|---|---|---|---|---|---|---|---|
| 35 | 35 | 150 | Total | C | N | O | S | 0 | 0 | 0 |
| | | | 1144 | 712 | 232 | 197 | 3 | | | |

- Molecule 36 is a protein called 50S ribosomal protein L16.

| Mol | Chain | Residues | Atoms | | | | | ZeroOcc | AltConf | Trace |
|---|---|---|---|---|---|---|---|---|---|---|
| 36 | 88 | 141 | Total | C | N | O | S | 0 | 0 | 0 |
| | | | 1121 | 715 | 212 | 187 | 7 | | | |
| 36 | 45 | 141 | Total | C | N | O | S | 0 | 0 | 0 |
| | | | 1121 | 715 | 212 | 187 | 7 | | | |

- Molecule 37 is a protein called 50S ribosomal protein L17.

| Mol | Chain | Residues | Atoms | | | | | ZeroOcc | AltConf | Trace |
|---|---|---|---|---|---|---|---|---|---|---|
| 37 | 98 | 118 | Total | C | N | O | S | 0 | 0 | 0 |
| | | | 967 | 604 | 203 | 159 | 1 | | | |
| 37 | 55 | 117 | Total | C | N | O | | 0 | 0 | 0 |
| | | | 959 | 599 | 202 | 158 | | | | |

- Molecule 38 is a protein called 50S ribosomal protein L18.

| Mol | Chain | Residues | Atoms | | | | ZeroOcc | AltConf | Trace |
|---|---|---|---|---|---|---|---|---|---|
| 38 | A8 | 111 | Total | C | N | O | 0 | 0 | 0 |
| | | | 881 | 556 | 176 | 149 | | | |
| 38 | 65 | 111 | Total | C | N | O | 0 | 0 | 0 |
| | | | 881 | 556 | 176 | 149 | | | |

- Molecule 39 is a protein called 50S ribosomal protein L19.

| Mol | Chain | Residues | Atoms | | | | | ZeroOcc | AltConf | Trace |
|---|---|---|---|---|---|---|---|---|---|---|
| 39 | B8 | 137 | Total | C | N | O | S | 0 | 0 | 0 |
| | | | 1141 | 710 | 234 | 196 | 1 | | | |
| 39 | 75 | 137 | Total | C | N | O | | 0 | 0 | 0 |
| | | | 1131 | 704 | 232 | 195 | | | | |

- Molecule 40 is a protein called 50S ribosomal protein L20.

| Mol | Chain | Residues | Atoms | | | | | ZeroOcc | AltConf | Trace |
|---|---|---|---|---|---|---|---|---|---|---|
| 40 | C8 | 117 | Total | C | N | O | S | 0 | 0 | 0 |
| | | | 963 | 610 | 202 | 150 | 1 | | | |
| 40 | 85 | 117 | Total | C | N | O | S | 0 | 0 | 0 |
| | | | 963 | 610 | 202 | 150 | 1 | | | |

- Molecule 41 is a protein called 50S ribosomal protein L21.

| Mol | Chain | Residues | Atoms | | | | | ZeroOcc | AltConf | Trace |
|---|---|---|---|---|---|---|---|---|---|---|
| 41 | D8 | 101 | Total | C | N | O | S | 0 | 0 | 0 |
| | | | 778 | 501 | 142 | 134 | 1 | | | |
| 41 | 95 | 101 | Total | C | N | O | S | 0 | 0 | 0 |
| | | | 778 | 501 | 142 | 134 | 1 | | | |

- Molecule 42 is a protein called 50S ribosomal protein L22.

| Mol | Chain | Residues | Atoms | | | | | ZeroOcc | AltConf | Trace |
|---|---|---|---|---|---|---|---|---|---|---|
| 42 | E8 | 113 | Total | C | N | O | S | 0 | 0 | 0 |
| | | | 899 | 566 | 177 | 154 | 2 | | | |
| 42 | A5 | 113 | Total | C | N | O | S | 0 | 0 | 0 |
| | | | 899 | 566 | 177 | 154 | 2 | | | |

- Molecule 43 is a protein called 50S ribosomal protein L23.

| Mol | Chain | Residues | Atoms | | | | ZeroOcc | AltConf | Trace |
|---|---|---|---|---|---|---|---|---|---|
| 43 | F8 | 92 | Total | C | N | O | 0 | 0 | 0 |
| | | | 725 | 471 | 131 | 123 | | | |
| 43 | B5 | 93 | Total | C | N | O | 0 | 0 | 0 |
| | | | 730 | 474 | 132 | 124 | | | |

- Molecule 44 is a protein called 50S ribosomal protein L24.

| Mol | Chain | Residues | Atoms | | | | | ZeroOcc | AltConf | Trace |
|---|---|---|---|---|---|---|---|---|---|---|
| 44 | G8 | 104 | Total | C | N | O | S | 0 | 0 | 0 |
| | | | 791 | 510 | 149 | 127 | 5 | | | |
| 44 | C5 | 104 | Total | C | N | O | S | 0 | 0 | 0 |
| | | | 794 | 510 | 152 | 127 | 5 | | | |

- Molecule 45 is a protein called 50S ribosomal protein L25.

| Mol | Chain | Residues | Atoms | | | | | ZeroOcc | AltConf | Trace |
|---|---|---|---|---|---|---|---|---|---|---|
| 45 | H8 | 175 | Total | C | N | O | S | 0 | 0 | 0 |
| | | | 1397 | 892 | 251 | 251 | 3 | | | |
| 45 | D5 | 179 | Total | C | N | O | S | 0 | 0 | 0 |
| | | | 1428 | 911 | 255 | 259 | 3 | | | |

- Molecule 46 is a protein called 50S ribosomal protein L27.

| Mol | Chain | Residues | Atoms | | | | | ZeroOcc | AltConf | Trace |
|---|---|---|---|---|---|---|---|---|---|---|
| 46 | I8 | 83 | Total | C | N | O | S | 0 | 0 | 0 |
| | | | 656 | 407 | 139 | 109 | 1 | | | |
| 46 | E5 | 77 | Total | C | N | O | S | 0 | 0 | 0 |
| | | | 612 | 379 | 129 | 103 | 1 | | | |

- Molecule 47 is a protein called 50S ribosomal protein L28.

| Mol | Chain | Residues | Atoms | | | | | ZeroOcc | AltConf | Trace |
|---|---|---|---|---|---|---|---|---|---|---|
| 47 | J8 | 97 | Total | C | N | O | S | 0 | 0 | 0 |
| | | | 762 | 481 | 150 | 130 | 1 | | | |
| 47 | F5 | 97 | Total | C | N | O | S | 0 | 0 | 0 |
| | | | 762 | 481 | 150 | 130 | 1 | | | |

- Molecule 48 is a protein called 50S ribosomal protein L29.

| Mol | Chain | Residues | Atoms | | | | | ZeroOcc | AltConf | Trace |
|---|---|---|---|---|---|---|---|---|---|---|
| 48 | K8 | 66 | Total | C | N | O | S | 0 | 0 | 0 |
| | | | 558 | 346 | 113 | 98 | 1 | | | |
| 48 | G5 | 69 | Total | C | N | O | S | 0 | 0 | 0 |
| | | | 580 | 358 | 118 | 103 | 1 | | | |

- Molecule 49 is a protein called 50S ribosomal protein L30.

| Mol | Chain | Residues | Atoms | | | | ZeroOcc | AltConf | Trace |
|---|---|---|---|---|---|---|---|---|---|
| 49 | L8 | 59 | Total | C | N | O | 0 | 0 | 0 |
| | | | 468 | 298 | 90 | 80 | | | |
| 49 | H5 | 59 | Total | C | N | O | 0 | 0 | 0 |
| | | | 468 | 298 | 90 | 80 | | | |

- Molecule 50 is a protein called 50S ribosomal protein L31.

| Mol | Chain | Residues | Atoms | | | | | ZeroOcc | AltConf | Trace |
|---|---|---|---|---|---|---|---|---|---|---|
| 50 | M8 | 66 | Total | C | N | O | S | 0 | 0 | 0 |
| | | | 533 | 335 | 96 | 97 | 5 | | | |
| 50 | I5 | 63 | Total | C | N | O | S | 0 | 0 | 0 |
| | | | 515 | 326 | 93 | 91 | 5 | | | |

- Molecule 51 is a protein called 50S ribosomal protein L32.

| Mol | Chain | Residues | Atoms | | | | | ZeroOcc | AltConf | Trace |
|---|---|---|---|---|---|---|---|---|---|---|
| 51 | N8 | 59 | Total | C | N | O | S | 0 | 0 | 0 |
| | | | 458 | 288 | 90 | 75 | 5 | | | |

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| Mol | Chain | Residues | Atoms | | | | | ZeroOcc | AltConf | Trace |
|---|---|---|---|---|---|---|---|---|---|---|
| 51 | J5 | 59 | Total | C | N | O | S | 0 | 0 | 0 |
| | | | 458 | 288 | 90 | 75 | 5 | | | |

- Molecule 52 is a protein called 50S ribosomal protein L33.

| Mol | Chain | Residues | Atoms | | | | | ZeroOcc | AltConf | Trace |
|---|---|---|---|---|---|---|---|---|---|---|
| 52 | O8 | 45 | Total | C | N | O | S | 0 | 0 | 0 |
| | | | 389 | 241 | 79 | 65 | 4 | | | |
| 52 | K5 | 45 | Total | C | N | O | S | 0 | 0 | 0 |
| | | | 389 | 241 | 79 | 65 | 4 | | | |

- Molecule 53 is a protein called 50S ribosomal protein L34.

| Mol | Chain | Residues | Atoms | | | | | ZeroOcc | AltConf | Trace |
|---|---|---|---|---|---|---|---|---|---|---|
| 53 | P8 | 47 | Total | C | N | O | S | 0 | 0 | 0 |
| | | | 409 | 251 | 102 | 54 | 2 | | | |
| 53 | L5 | 49 | Total | C | N | O | S | 0 | 0 | 0 |
| | | | 429 | 263 | 108 | 56 | 2 | | | |

- Molecule 54 is a protein called 50S ribosomal protein L35.

| Mol | Chain | Residues | Atoms | | | | | ZeroOcc | AltConf | Trace |
|---|---|---|---|---|---|---|---|---|---|---|
| 54 | Q8 | 62 | Total | C | N | O | S | 0 | 0 | 0 |
| | | | 483 | 308 | 98 | 75 | 2 | | | |
| 54 | M5 | 62 | Total | C | N | O | S | 0 | 0 | 0 |
| | | | 495 | 317 | 100 | 76 | 2 | | | |

- Molecule 55 is MAGNESIUM ION (CCD ID: MG) (formula: Mg).

| Mol | Chain | Residues | Atoms | | ZeroOcc | AltConf |
|---|---|---|---|---|---|---|
| 55 | 13 | 139 | Total | Mg | 0 | 0 |
| | | | 139 | 139 | | |
| 55 | 3E | 1 | Total | Mg | 0 | 0 |
| | | | 1 | 1 | | |
| 55 | 5E | 1 | Total | Mg | 0 | 0 |
| | | | 1 | 1 | | |
| 55 | 7E | 1 | Total | Mg | 0 | 0 |
| | | | 1 | 1 | | |
| 55 | 3I | 1 | Total | Mg | 0 | 0 |
| | | | 1 | 1 | | |
| 55 | 2K | 5 | Total | Mg | 0 | 0 |
| | | | 5 | 5 | | |

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| Mol | Chain | Residues | Atoms | ZeroOcc | AltConf |
|---|---|---|---|---|---|
| 55 | 4K | 1 | Total Mg<br>1 1 | 0 | 0 |
| 55 | 1H | 523 | Total Mg<br>523 523 | 0 | 0 |
| 55 | 16 | 15 | Total Mg<br>15 15 | 0 | 0 |
| 55 | 11 | 2 | Total Mg<br>2 2 | 0 | 0 |
| 55 | 21 | 2 | Total Mg<br>2 2 | 0 | 0 |
| 55 | 88 | 1 | Total Mg<br>1 1 | 0 | 0 |
| 55 | 98 | 1 | Total Mg<br>1 1 | 0 | 0 |
| 55 | G8 | 1 | Total Mg<br>1 1 | 0 | 0 |
| 55 | I8 | 3 | Total Mg<br>3 3 | 0 | 0 |
| 55 | Q8 | 2 | Total Mg<br>2 2 | 0 | 0 |
| 55 | 1G | 148 | Total Mg<br>148 148 | 0 | 0 |
| 55 | 32 | 1 | Total Mg<br>1 1 | 0 | 0 |
| 55 | 42 | 1 | Total Mg<br>1 1 | 0 | 0 |
| 55 | 52 | 1 | Total Mg<br>1 1 | 0 | 0 |
| 55 | 3A | 1 | Total Mg<br>1 1 | 0 | 0 |
| 55 | 4A | 1 | Total Mg<br>1 1 | 0 | 0 |
| 55 | 2L | 4 | Total Mg<br>4 4 | 0 | 0 |
| 55 | 3L | 1 | Total Mg<br>1 1 | 0 | 0 |
| 55 | 14 | 465 | Total Mg<br>465 465 | 0 | 0 |
| 55 | 1J | 10 | Total Mg<br>10 10 | 0 | 0 |
| 55 | 19 | 1 | Total Mg<br>1 1 | 0 | 0 |

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| Mol | Chain | Residues | Atoms | ZeroOcc | AltConf |
|---|---|---|---|---|---|
| 55 | 29 | 4 | Total Mg<br>4 4 | 0 | 0 |
| 55 | 39 | 1 | Total Mg<br>1 1 | 0 | 0 |
| 55 | 15 | 1 | Total Mg<br>1 1 | 0 | 0 |
| 55 | 25 | 1 | Total Mg<br>1 1 | 0 | 0 |
| 55 | 45 | 1 | Total Mg<br>1 1 | 0 | 0 |
| 55 | 55 | 1 | Total Mg<br>1 1 | 0 | 0 |
| 55 | C5 | 1 | Total Mg<br>1 1 | 0 | 0 |
| 55 | E5 | 1 | Total Mg<br>1 1 | 0 | 0 |
| 55 | F5 | 1 | Total Mg<br>1 1 | 0 | 0 |

- Molecule 56 is ZINC ION (CCD ID: ZN) (formula: Zn).

| Mol | Chain | Residues | Atoms | ZeroOcc | AltConf |
|---|---|---|---|---|---|
| 56 | 3E | 1 | Total Zn<br>1 1 | 0 | 0 |
| 56 | 5I | 1 | Total Zn<br>1 1 | 0 | 0 |
| 56 | G8 | 1 | Total Zn<br>1 1 | 0 | 0 |
| 56 | 32 | 1 | Total Zn<br>1 1 | 0 | 0 |
| 56 | 5A | 1 | Total Zn<br>1 1 | 0 | 0 |
| 56 | C5 | 1 | Total Zn<br>1 1 | 0 | 0 |

- Molecule 57 is water.

| Mol | Chain | Residues | Atoms | ZeroOcc | AltConf |
|---|---|---|---|---|---|
| 57 | 13 | 125 | Total O<br>125 125 | 0 | 0 |
| 57 | 5I | 1 | Total O<br>1 1 | 0 | 0 |

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| Mol | Chain | Residues | Atoms | ZeroOcc | AltConf |
|---|---|---|---|---|---|
| 57 | AI | 3 | Total O<br>3 3 | 0 | 0 |
| 57 | 2K | 2 | Total O<br>2 2 | 0 | 0 |
| 57 | 4K | 3 | Total O<br>3 3 | 0 | 0 |
| 57 | 1H | 652 | Total O<br>652 652 | 0 | 0 |
| 57 | 16 | 12 | Total O<br>12 12 | 0 | 0 |
| 57 | 11 | 8 | Total O<br>8 8 | 0 | 0 |
| 57 | 21 | 2 | Total O<br>2 2 | 0 | 0 |
| 57 | 31 | 5 | Total O<br>5 5 | 0 | 0 |
| 57 | 78 | 4 | Total O<br>4 4 | 0 | 0 |
| 57 | 98 | 1 | Total O<br>1 1 | 0 | 0 |
| 57 | C8 | 2 | Total O<br>2 2 | 0 | 0 |
| 57 | E8 | 1 | Total O<br>1 1 | 0 | 0 |
| 57 | F8 | 2 | Total O<br>2 2 | 0 | 0 |
| 57 | G8 | 2 | Total O<br>2 2 | 0 | 0 |
| 57 | 1G | 96 | Total O<br>96 96 | 0 | 0 |
| 57 | 32 | 1 | Total O<br>1 1 | 0 | 0 |
| 57 | 5A | 1 | Total O<br>1 1 | 0 | 0 |
| 57 | 7A | 2 | Total O<br>2 2 | 0 | 0 |
| 57 | BA | 1 | Total O<br>1 1 | 0 | 0 |
| 57 | 2L | 6 | Total O<br>6 6 | 0 | 0 |
| 57 | 14 | 523 | Total O<br>523 523 | 0 | 0 |

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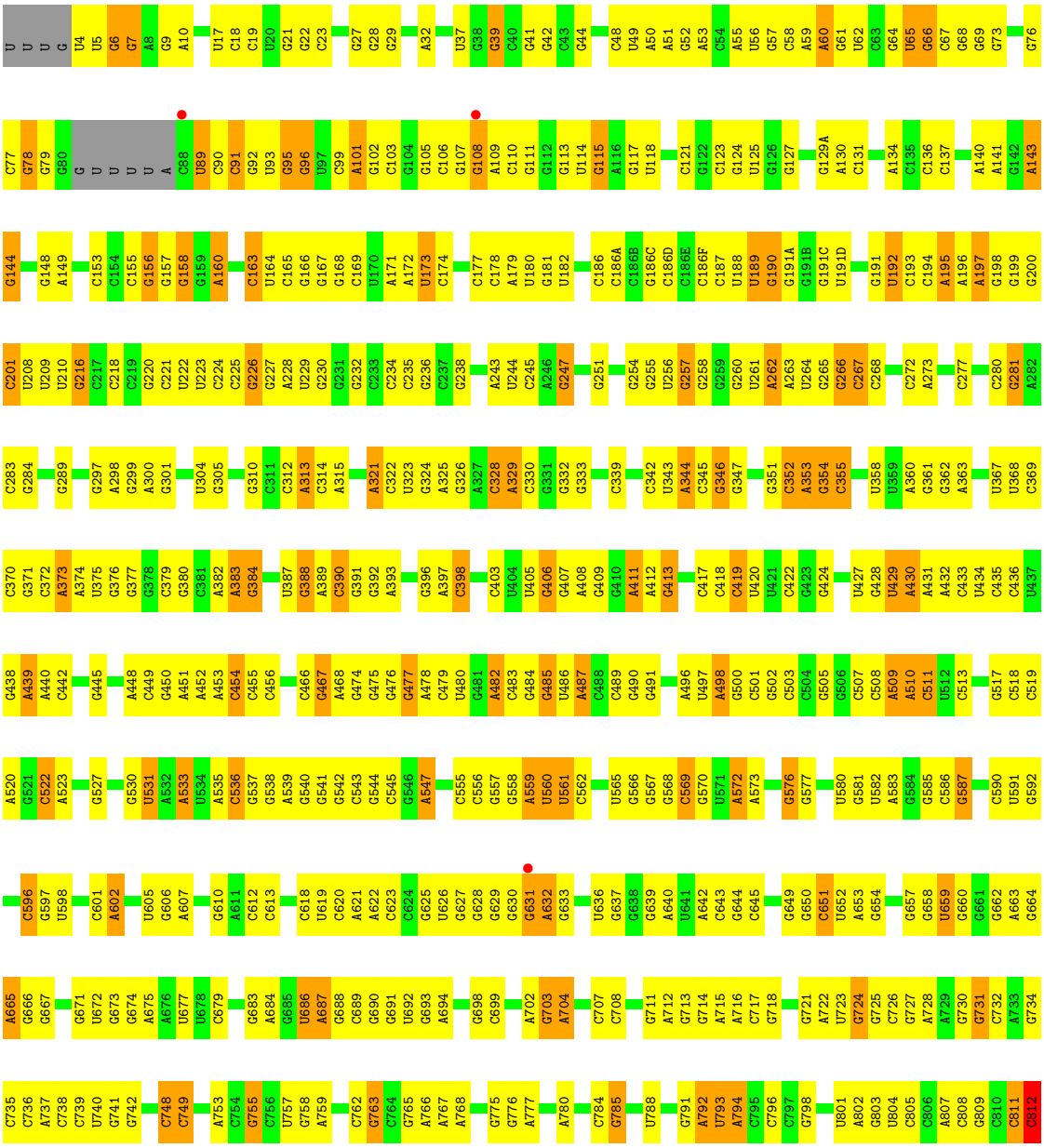
| Mol | Chain | Residues | Atoms | ZeroOcc | AltConf |
|---|---|---|---|---|---|
| 57 | 1J | 22 | Total O<br>22 22 | 0 | 0 |
| 57 | 19 | 11 | Total O<br>11 11 | 0 | 0 |
| 57 | 39 | 3 | Total O<br>3 3 | 0 | 0 |
| 57 | 25 | 6 | Total O<br>6 6 | 0 | 0 |
| 57 | 35 | 1 | Total O<br>1 1 | 0 | 0 |
| 57 | 75 | 1 | Total O<br>1 1 | 0 | 0 |
| 57 | 85 | 4 | Total O<br>4 4 | 0 | 0 |
| 57 | F5 | 1 | Total O<br>1 1 | 0 | 0 |
| 57 | H5 | 2 | Total O<br>2 2 | 0 | 0 |

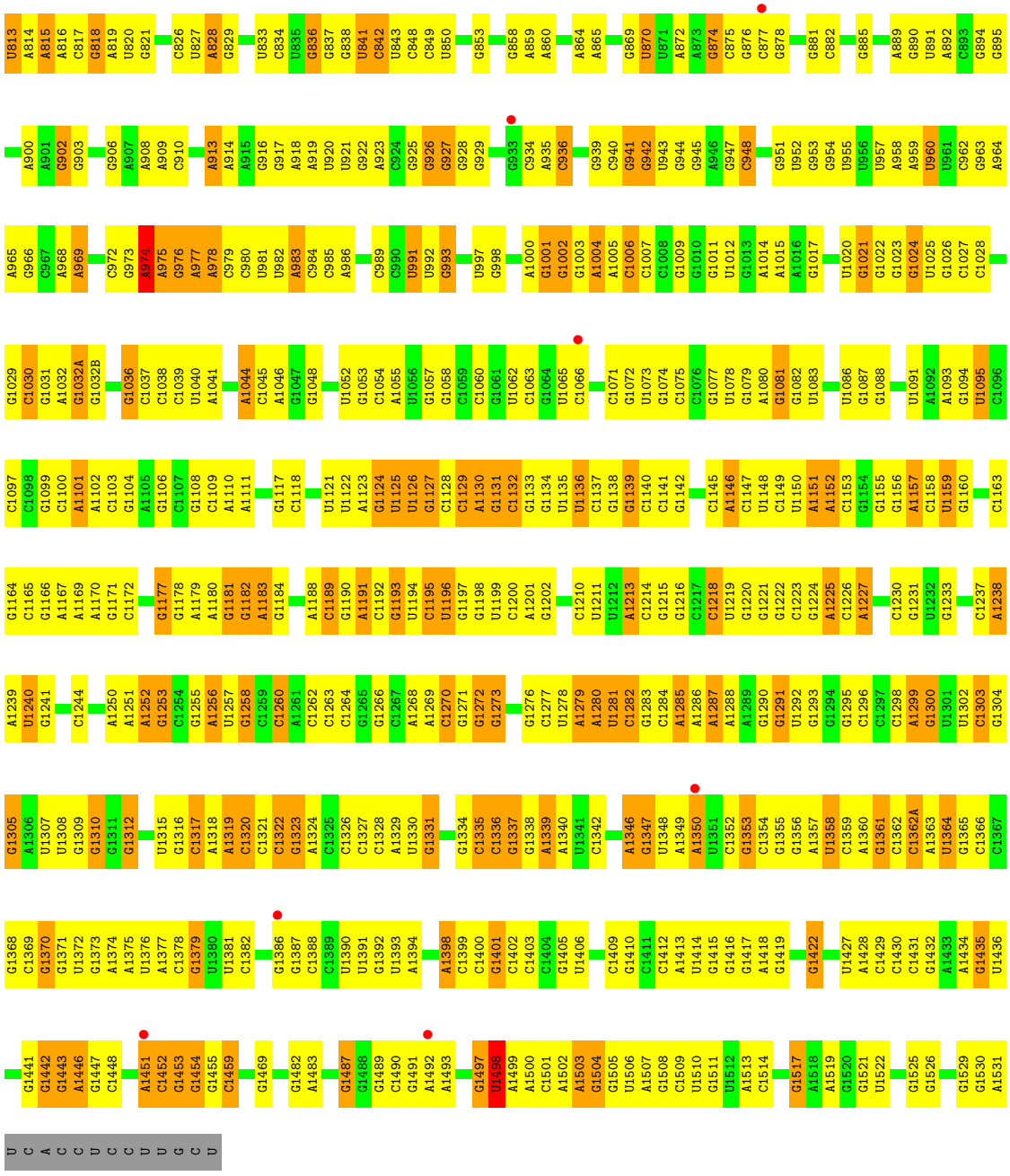
# 3 Residue-property plots (i)

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: 16S ribosomal RNA

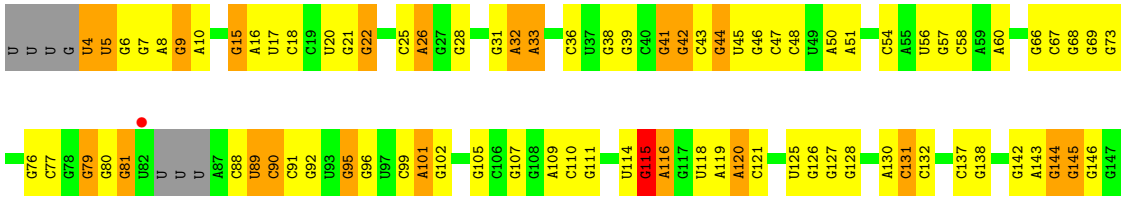
Chain 13:

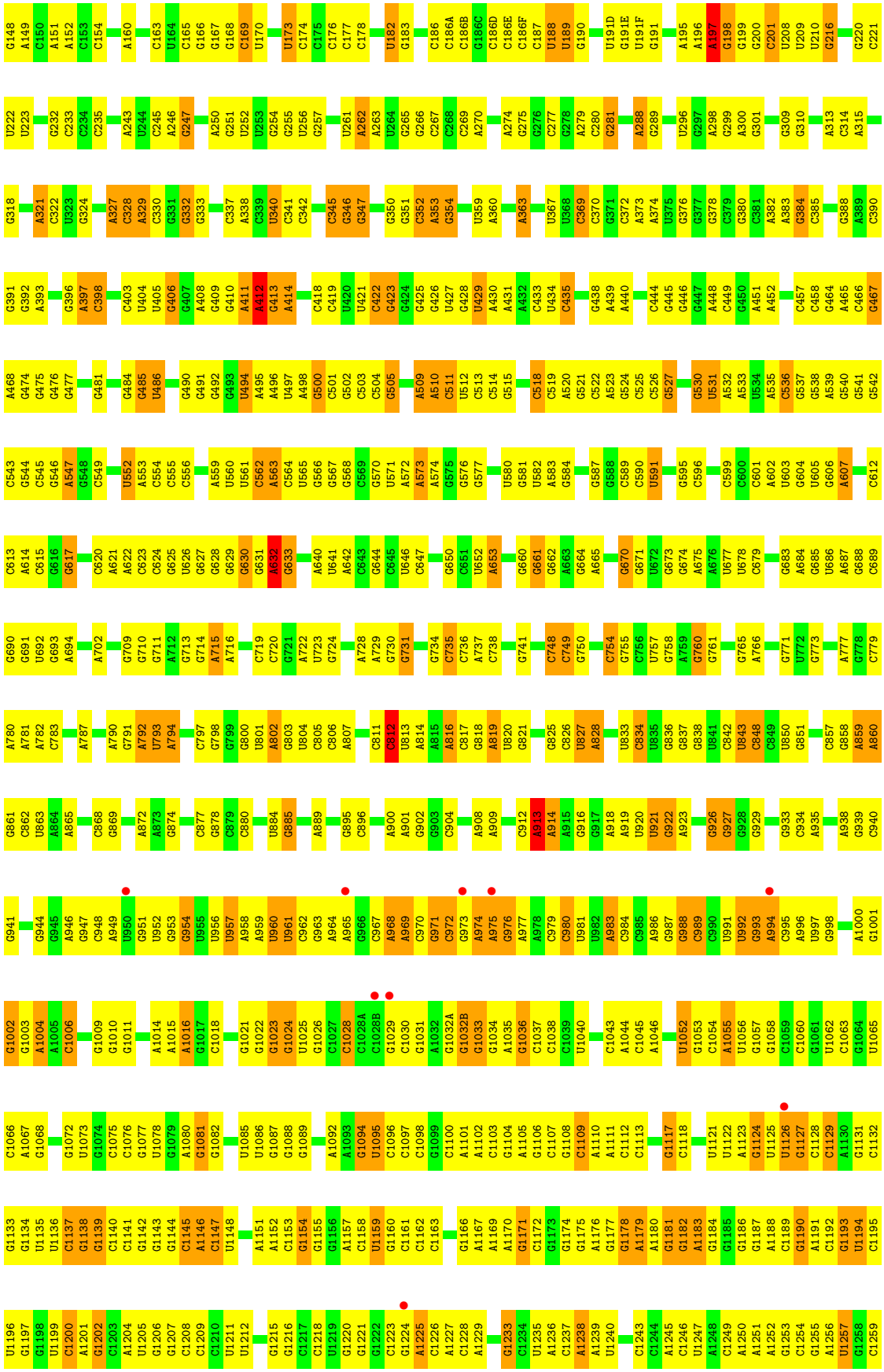


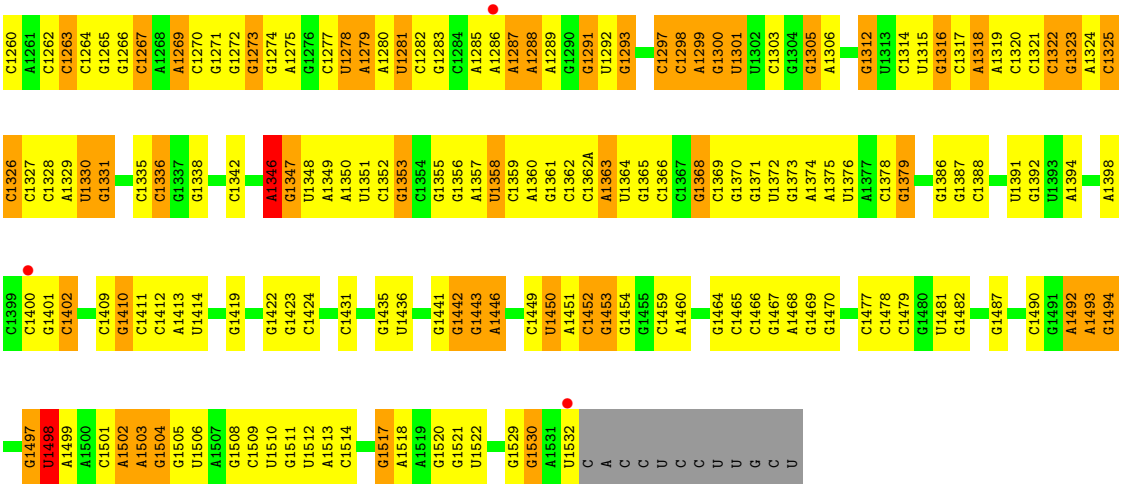


• Molecule 1: 16S ribosomal RNA

Chain 1G:

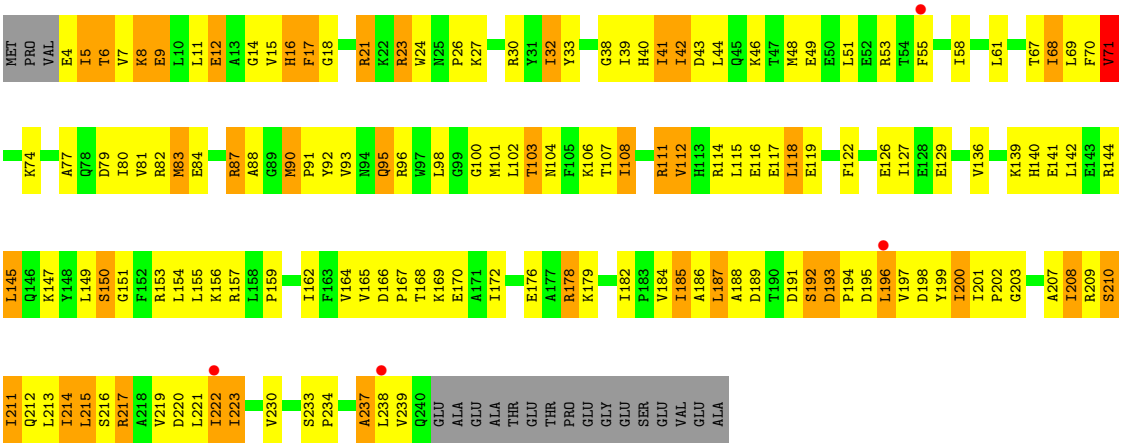






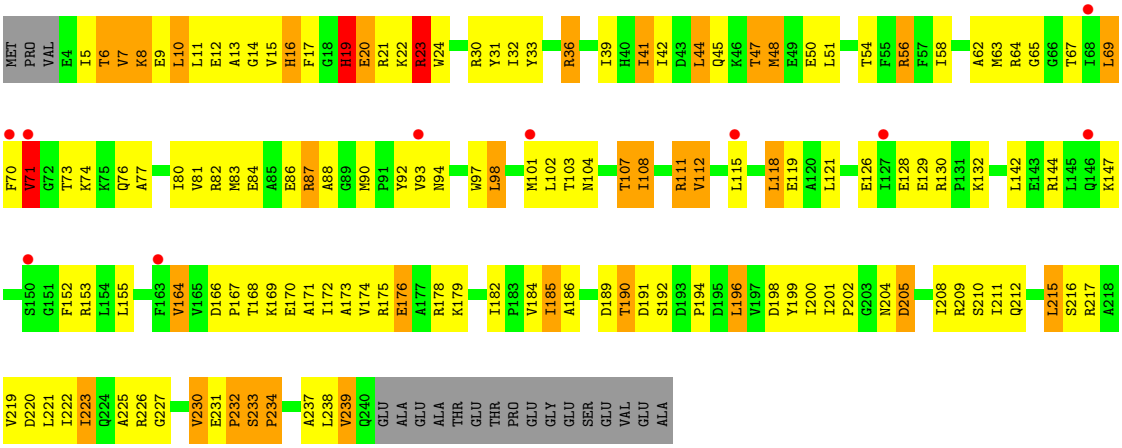
• Molecule 2: 30S ribosomal protein S2

Chain 1E:



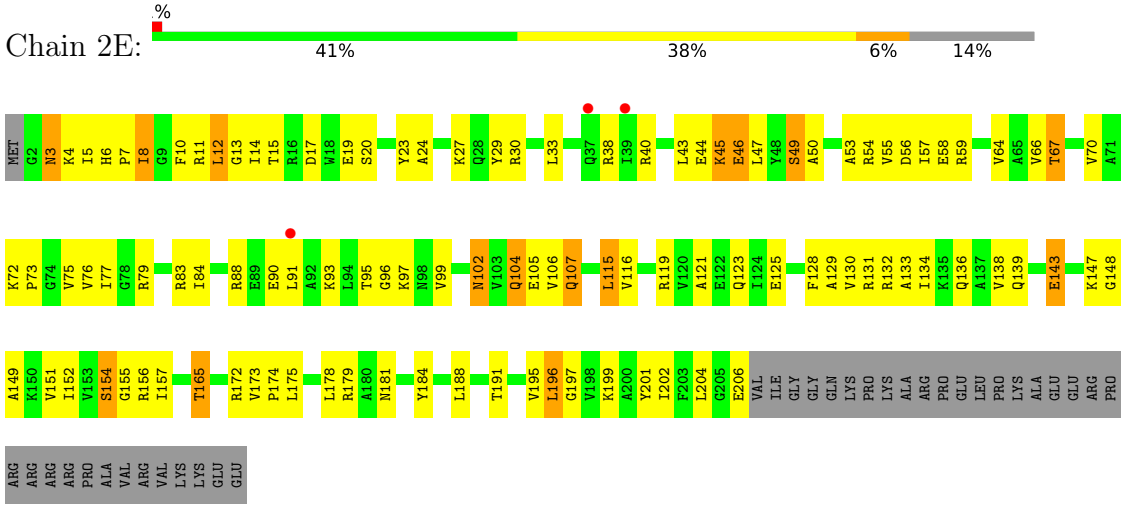
• Molecule 2: 30S ribosomal protein S2

Chain 12:



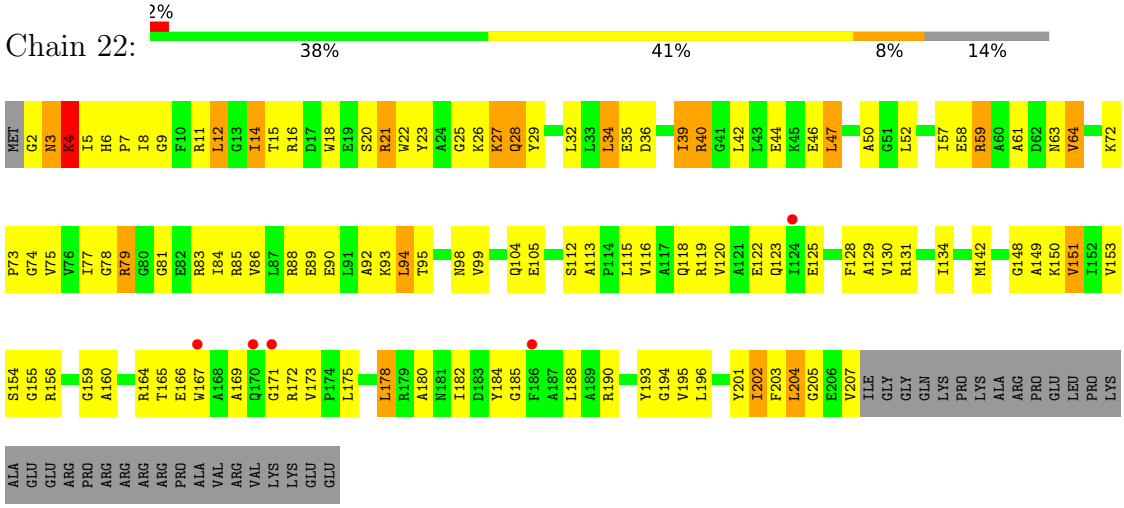
• Molecule 3: 30S ribosomal protein S3

Chain 2E:



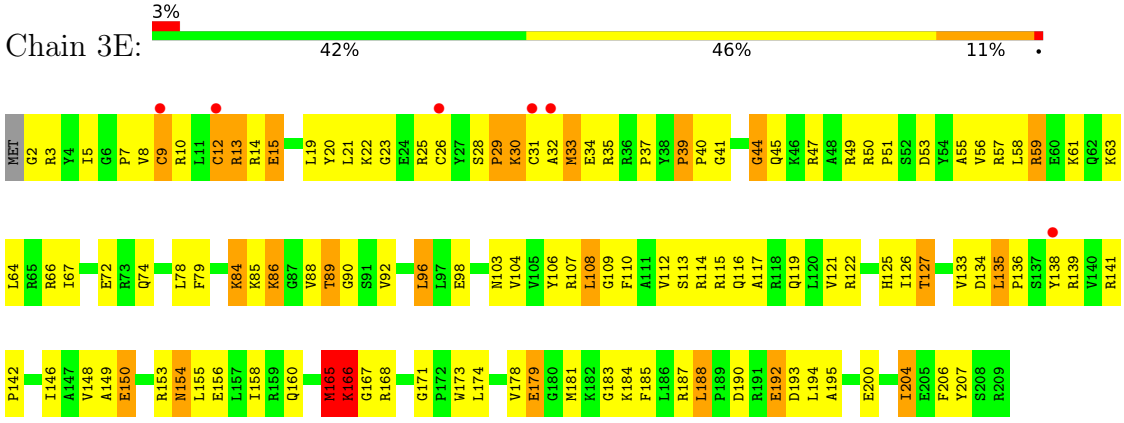

• Molecule 3: 30S ribosomal protein S3

Chain 22:



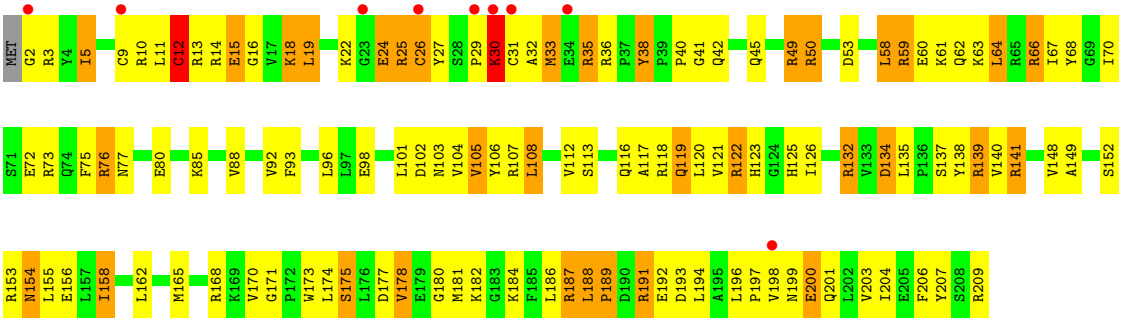

• Molecule 4: 30S ribosomal protein S4

Chain 3E:




• Molecule 4: 30S ribosomal protein S4

Chain 32:

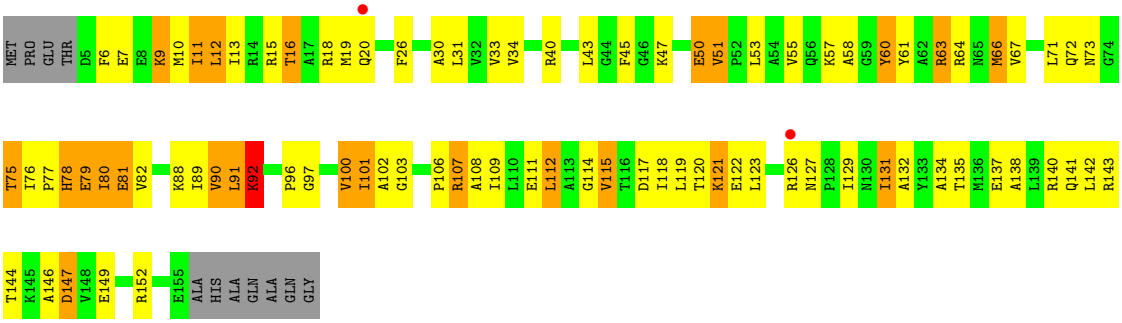



• Molecule 5: 30S ribosomal protein S5

Chain 4E:

• Molecule 5: 30S ribosomal protein S5

Chain 42:

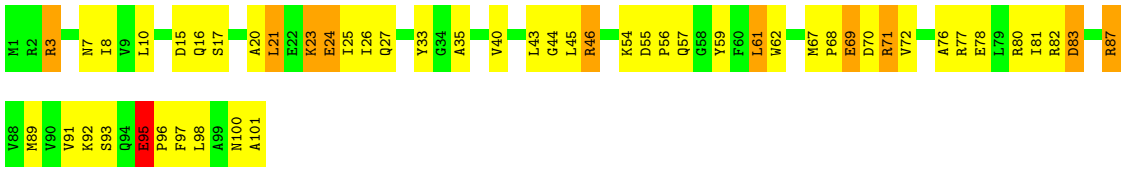



• Molecule 6: 30S ribosomal protein S6

Chain 5E:

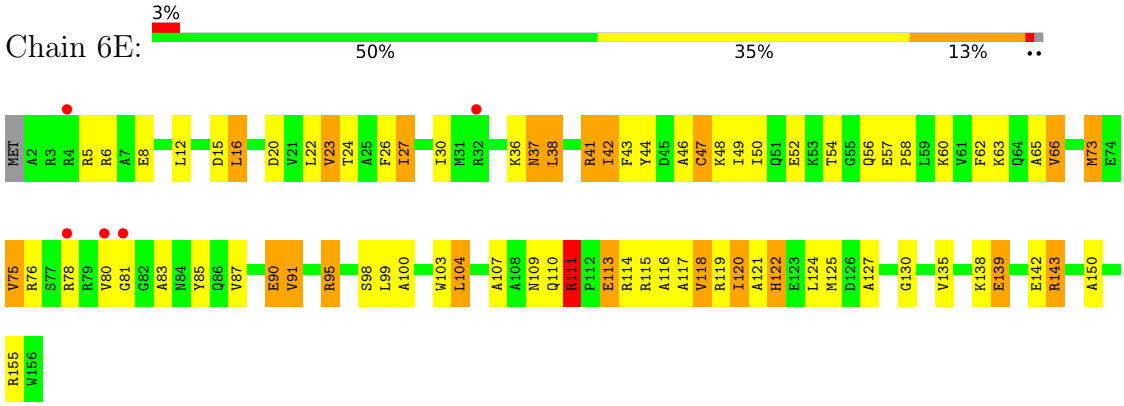
• Molecule 6: 30S ribosomal protein S6

Chain 52:



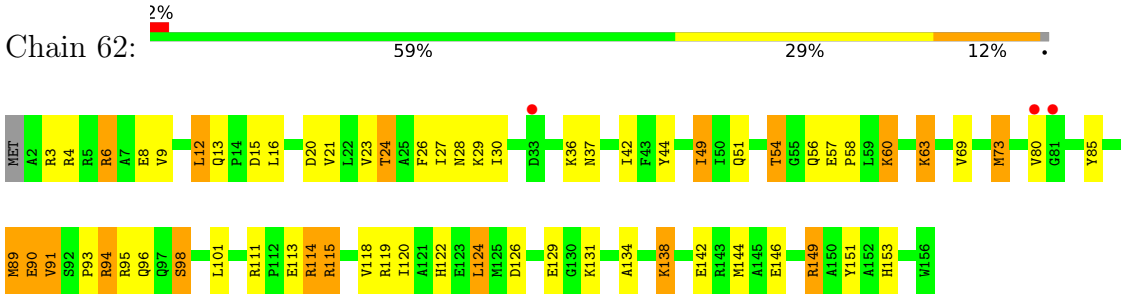

• Molecule 7: 30S ribosomal protein S7

Chain 6E:



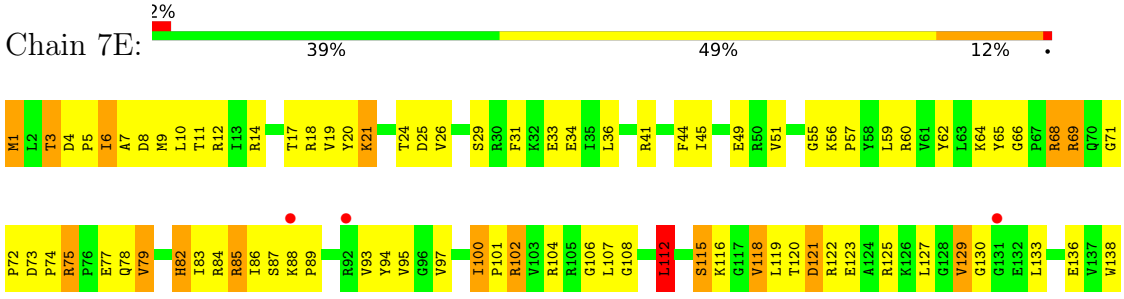

• Molecule 7: 30S ribosomal protein S7

Chain 62:



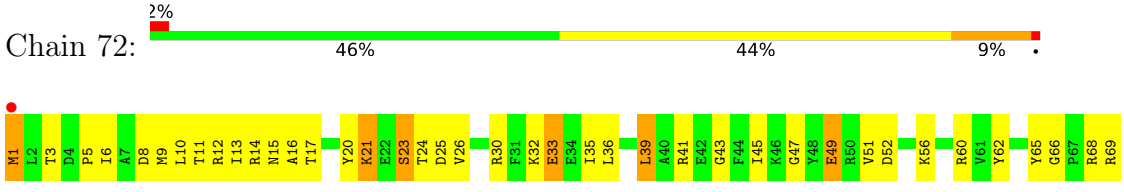

• Molecule 8: 30S ribosomal protein S8

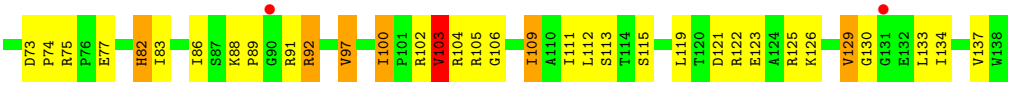
Chain 7E:




• Molecule 8: 30S ribosomal protein S8

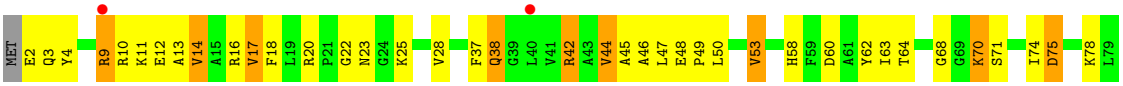
Chain 72:

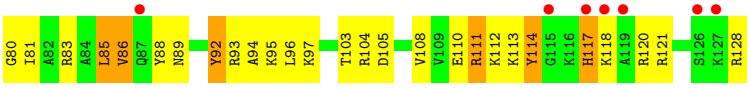





• Molecule 9: 30S ribosomal protein S9

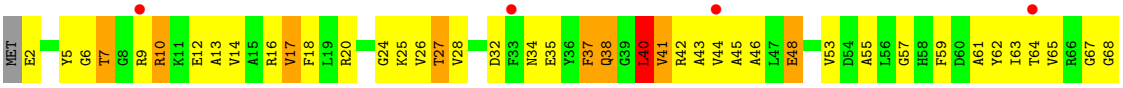
Chain 8E:

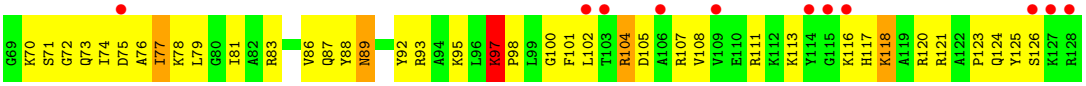



• Molecule 9: 30S ribosomal protein S9

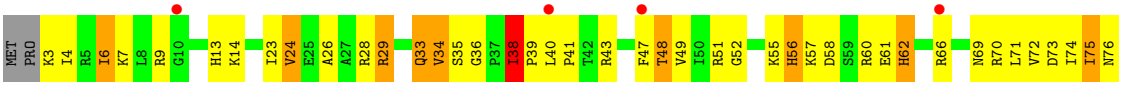
Chain 82:

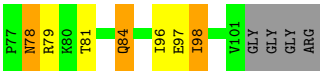



• Molecule 10: 30S ribosomal protein S10

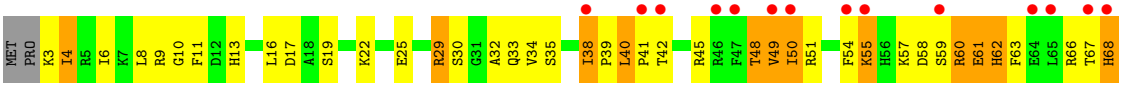
Chain 1I:

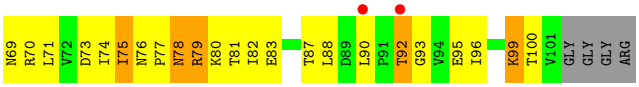



• Molecule 10: 30S ribosomal protein S10

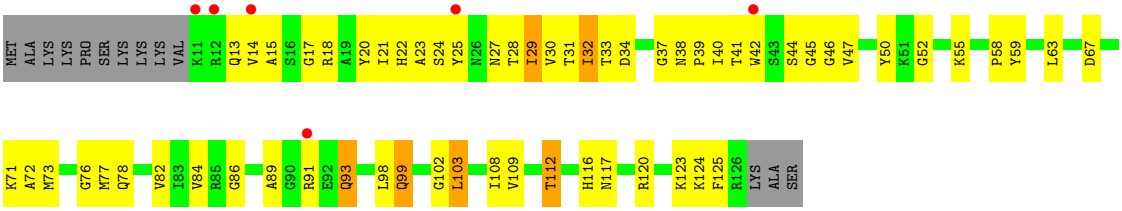
Chain 1A:




• Molecule 11: 30S ribosomal protein S11

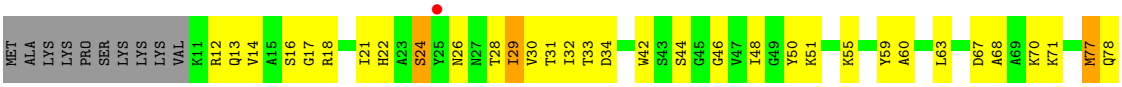
Chain 2I:





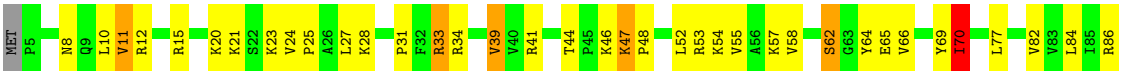
• Molecule 11: 30S ribosomal protein S11

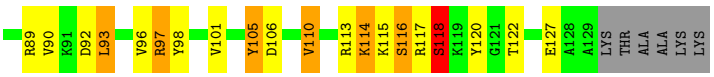
Chain 2A:



• Molecule 12: 30S ribosomal protein S12

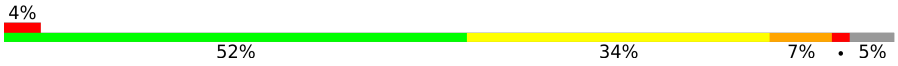
Chain 3I:

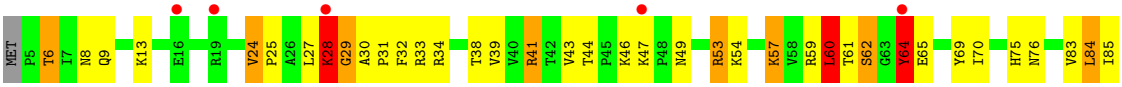


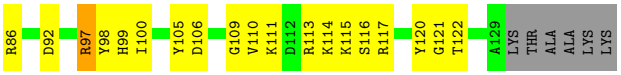


• Molecule 12: 30S ribosomal protein S12

Chain 3A:

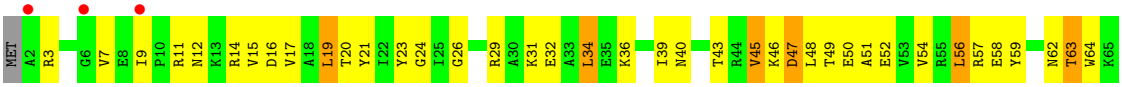


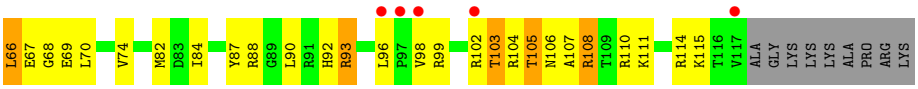





• Molecule 13: 30S ribosomal protein S13

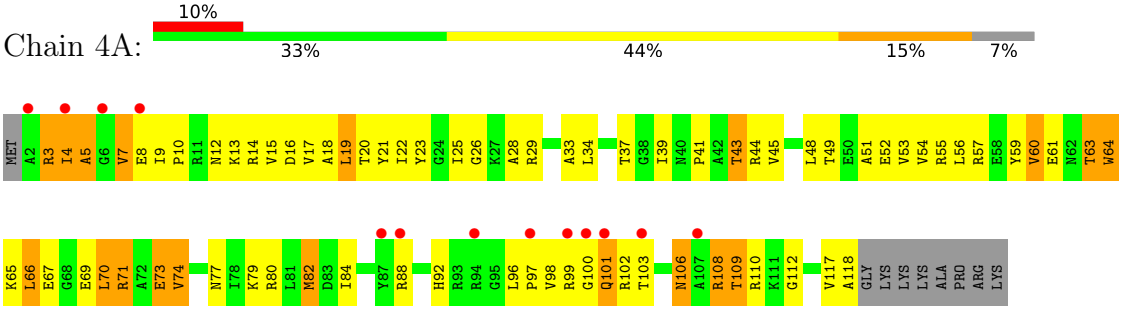
Chain 4I:





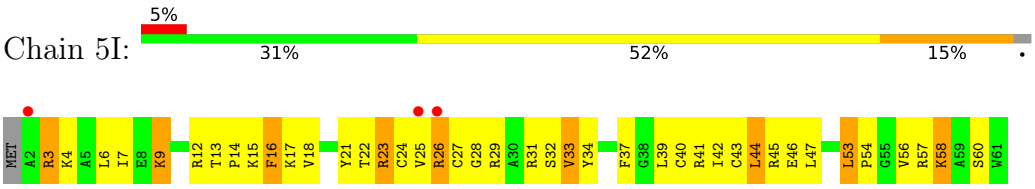
• Molecule 13: 30S ribosomal protein S13

Chain 4A:



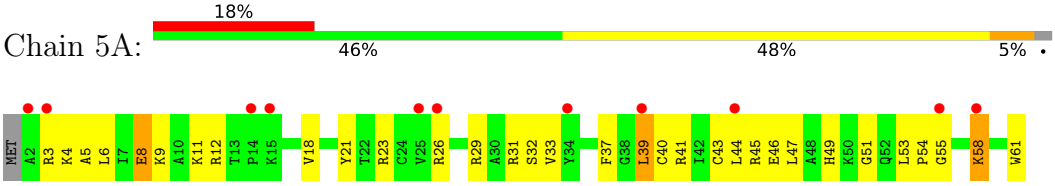

• Molecule 14: 30S ribosomal protein S14 type Z

Chain 5I:



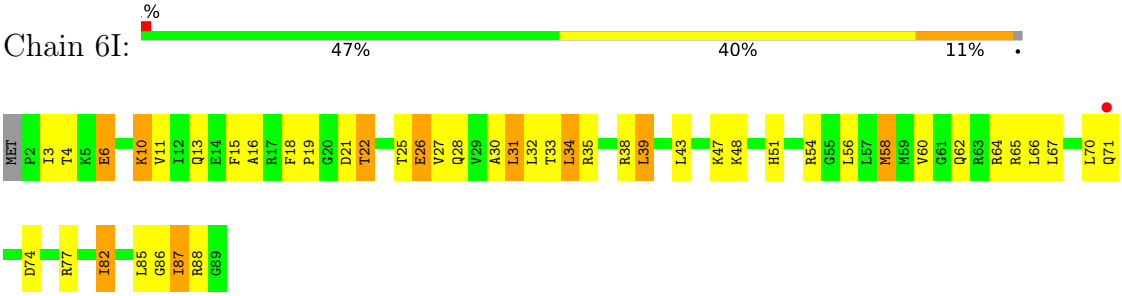

• Molecule 14: 30S ribosomal protein S14 type Z

Chain 5A:



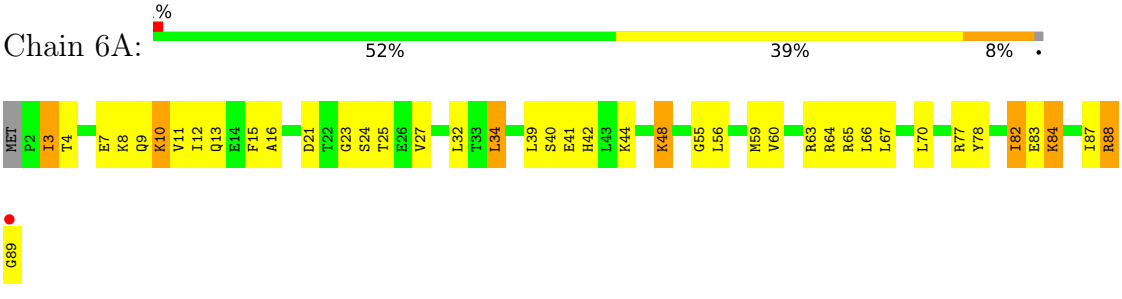

• Molecule 15: 30S ribosomal protein S15

Chain 6I:



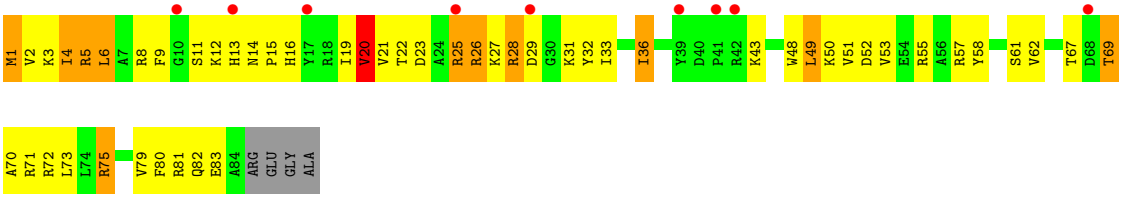

• Molecule 15: 30S ribosomal protein S15

Chain 6A:




• Molecule 16: 30S ribosomal protein S16

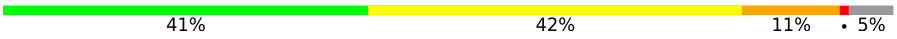
Chain 7I:

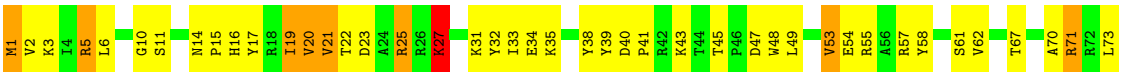


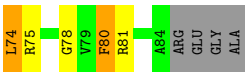


• Molecule 16: 30S ribosomal protein S16

Chain 7A:

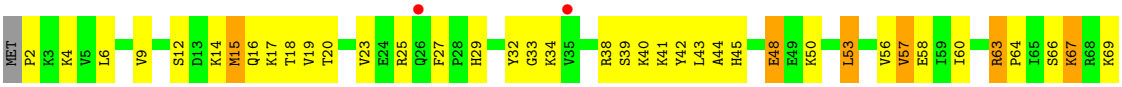




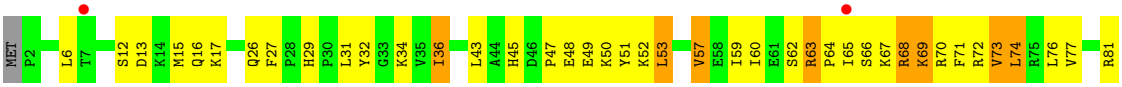
• Molecule 17: 30S ribosomal protein S17

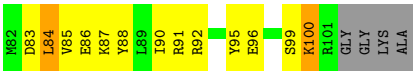
Chain 8I:



• Molecule 17: 30S ribosomal protein S17

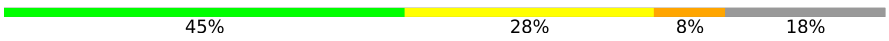
Chain 8A:

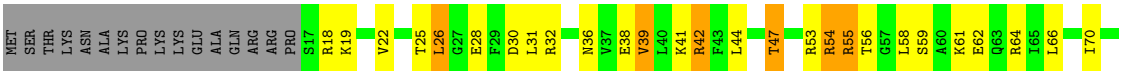


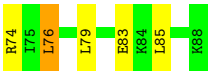


• Molecule 18: 30S ribosomal protein S18

Chain 9I:

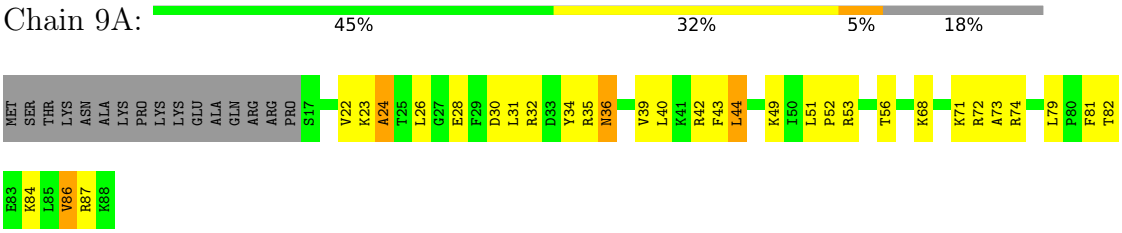




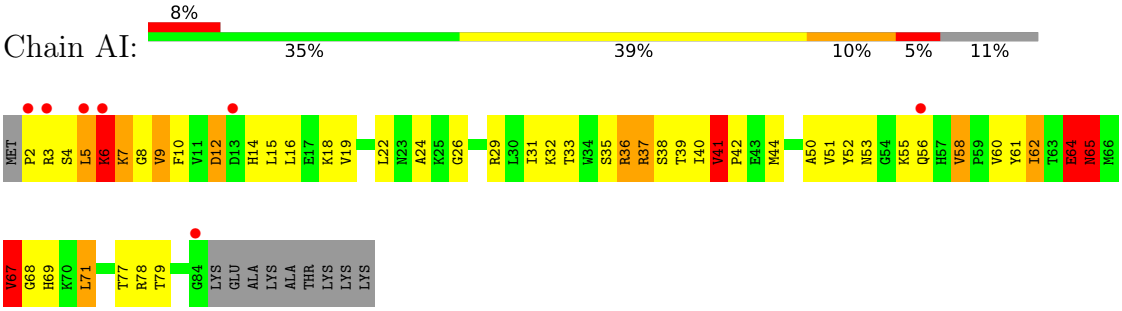
• Molecule 18: 30S ribosomal protein S18

Chain 9A:



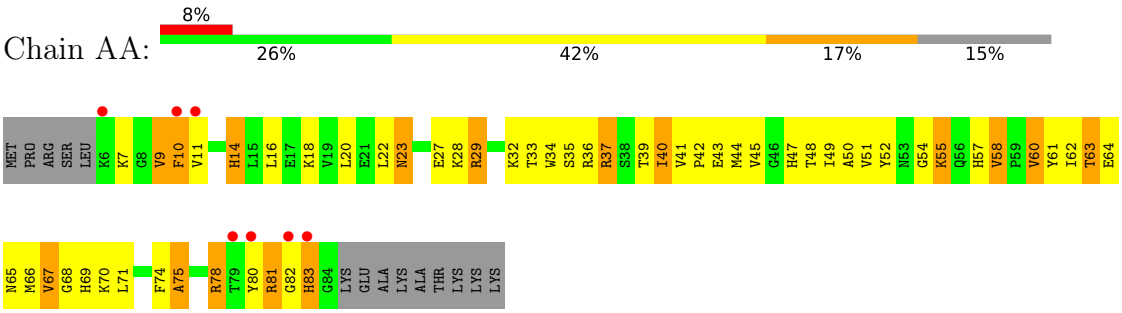

• Molecule 19: 30S ribosomal protein S19

Chain AI:



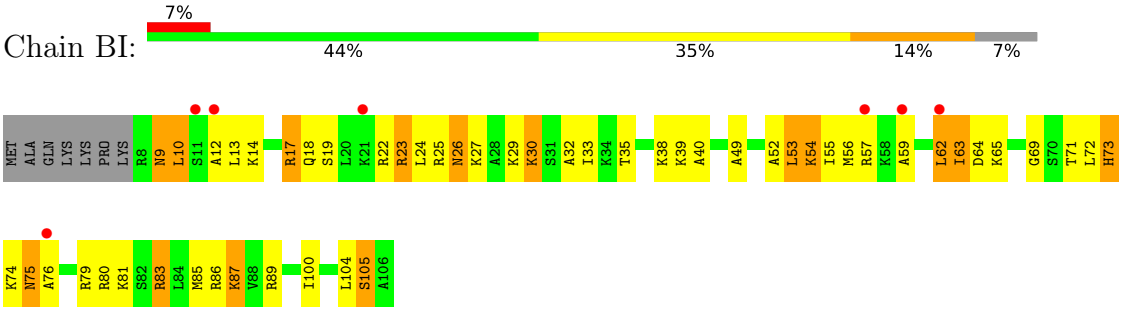

• Molecule 19: 30S ribosomal protein S19

Chain AA:



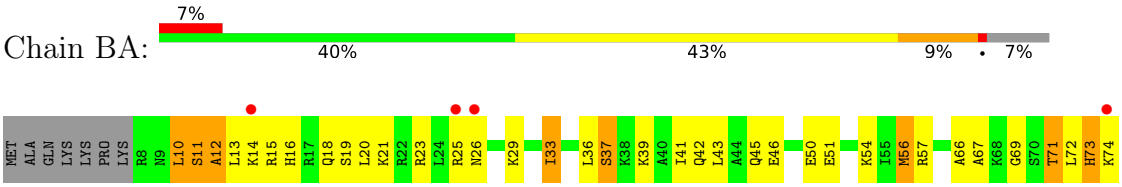

• Molecule 20: 30S ribosomal protein S20

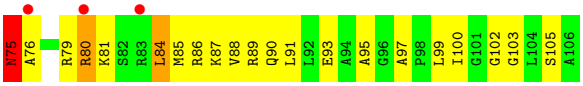
Chain BI:




• Molecule 20: 30S ribosomal protein S20

Chain BA:



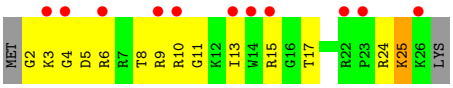



• Molecule 21: 30S ribosomal protein Thx

Chain 1F:

• Molecule 21: 30S ribosomal protein Thx

Chain 1B:

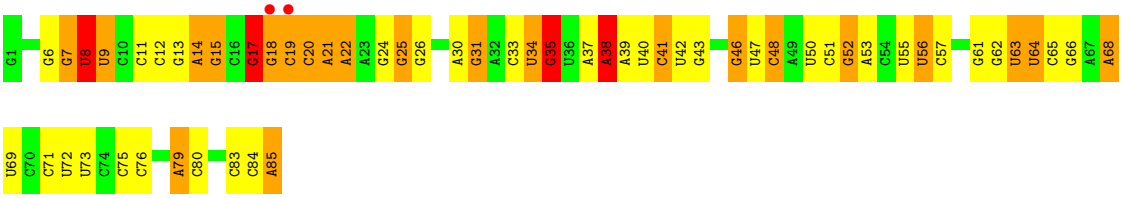



• Molecule 22: tRNA-Tyr

Chain 2K:

• Molecule 22: tRNA-Tyr

Chain 3K:

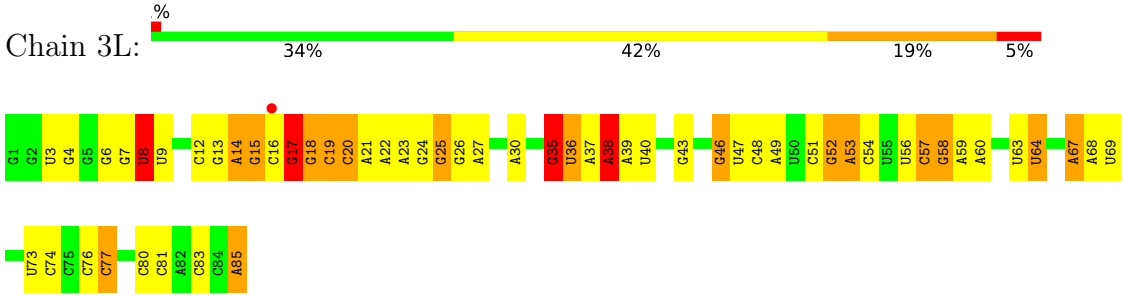



• Molecule 22: tRNA-Tyr

Chain 2L:

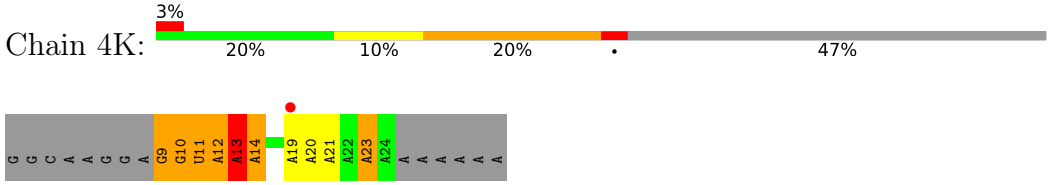
• Molecule 22: tRNA-Tyr

Chain 3L:



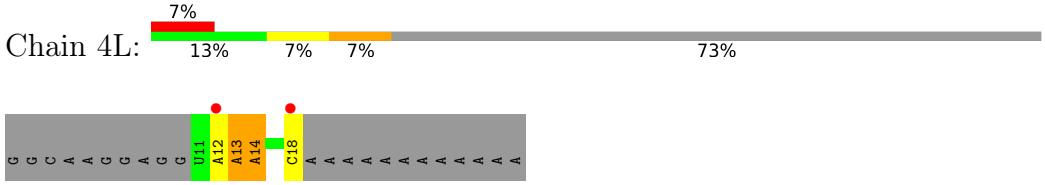

• Molecule 23: mRNA

Chain 4K:



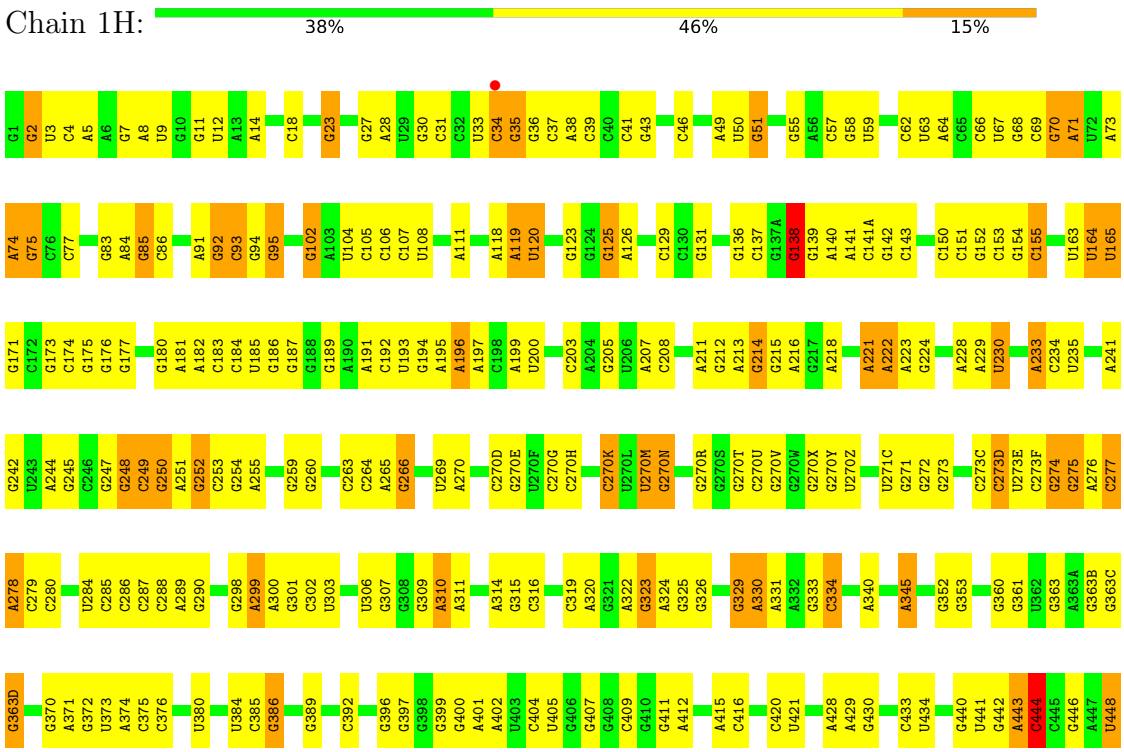

• Molecule 23: mRNA

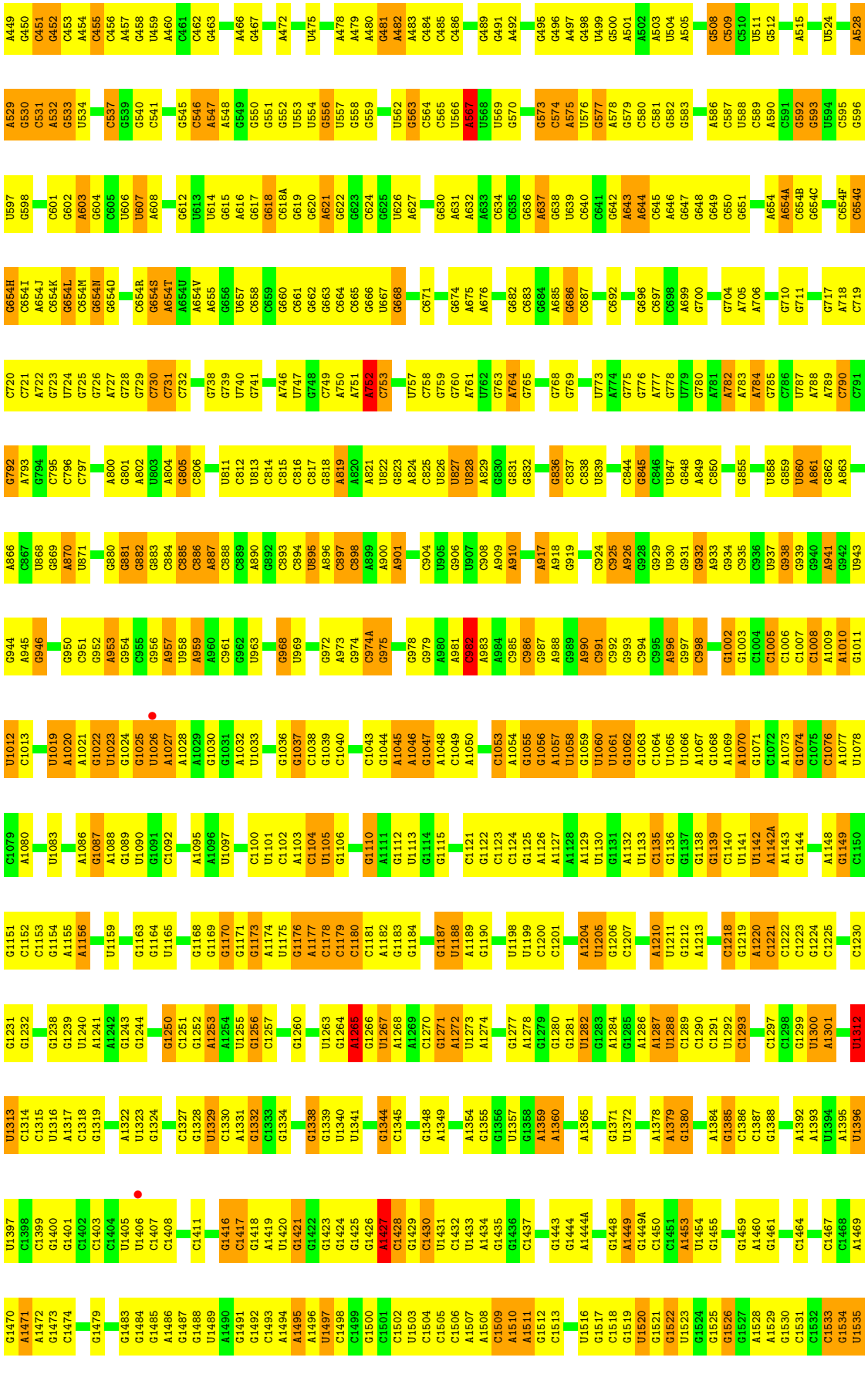
Chain 4L:

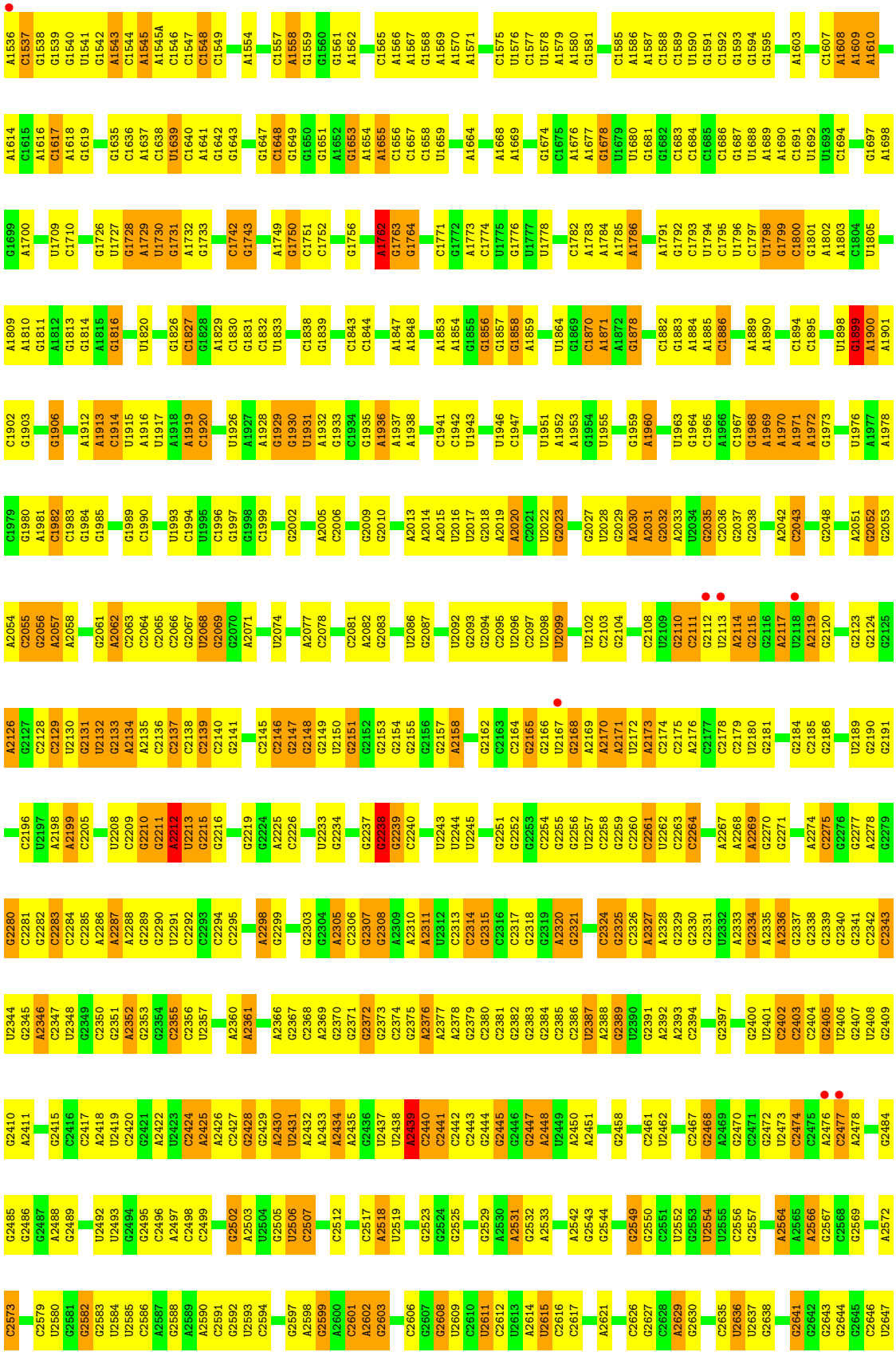


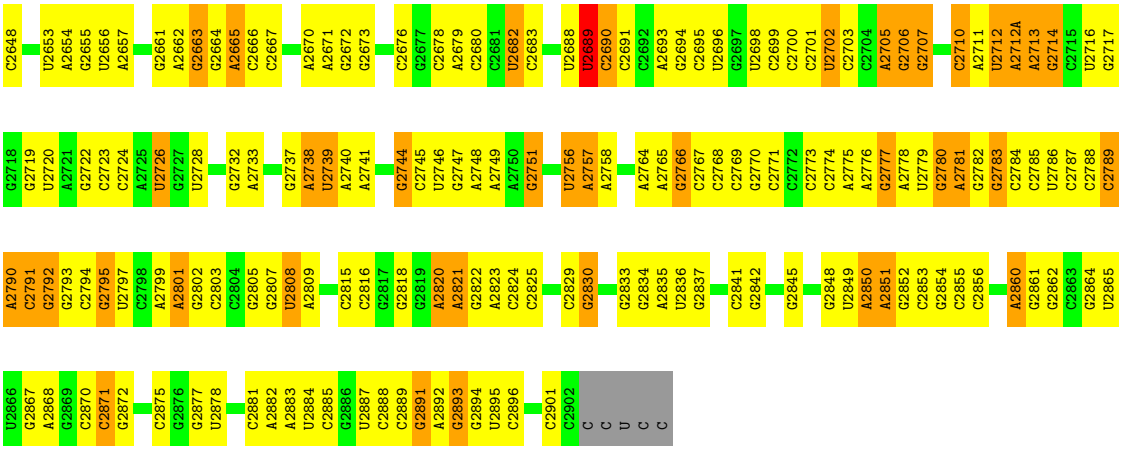

• Molecule 24: 23S ribosomal RNA

Chain 1H:



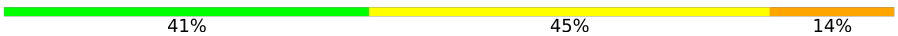


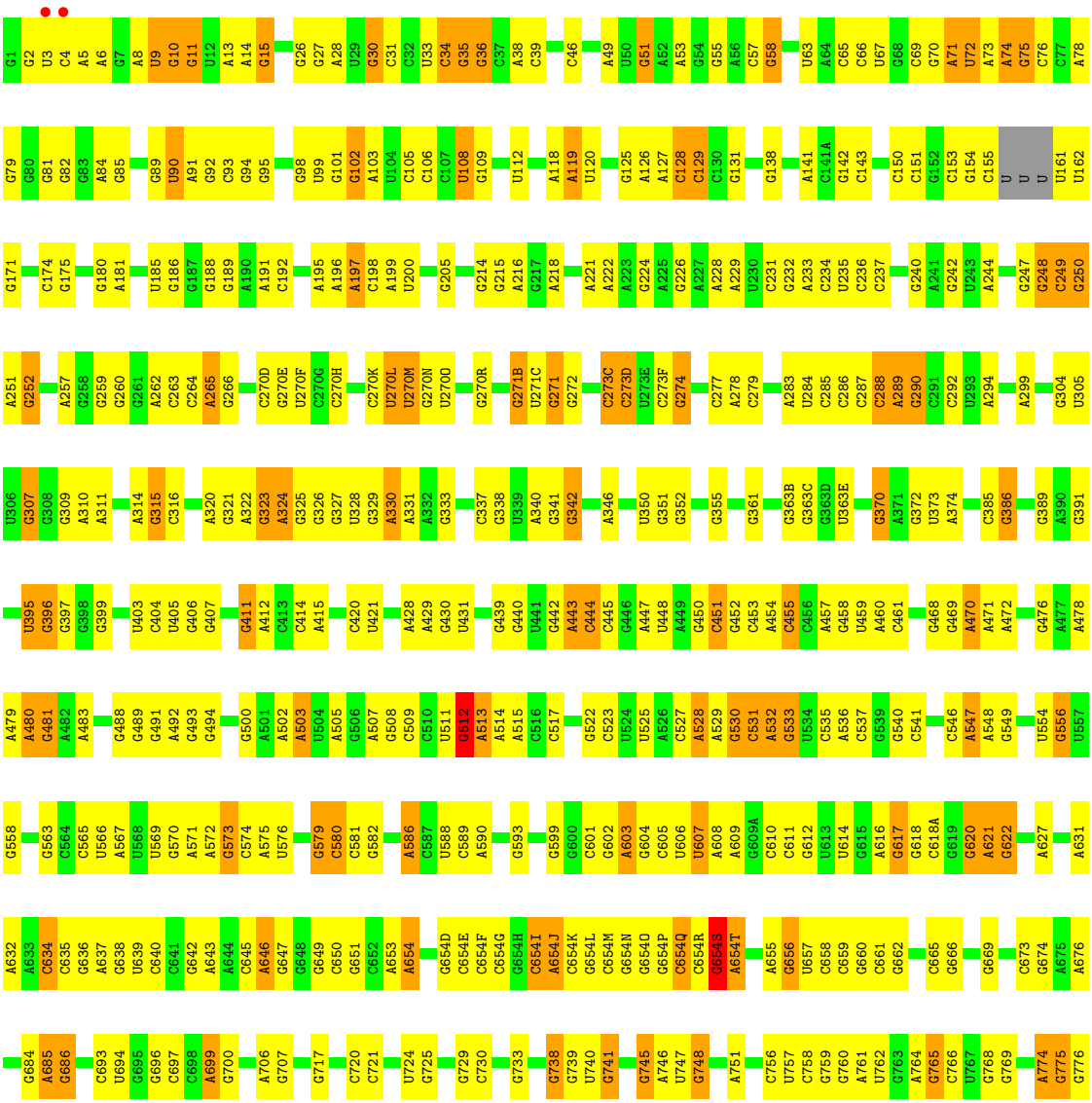


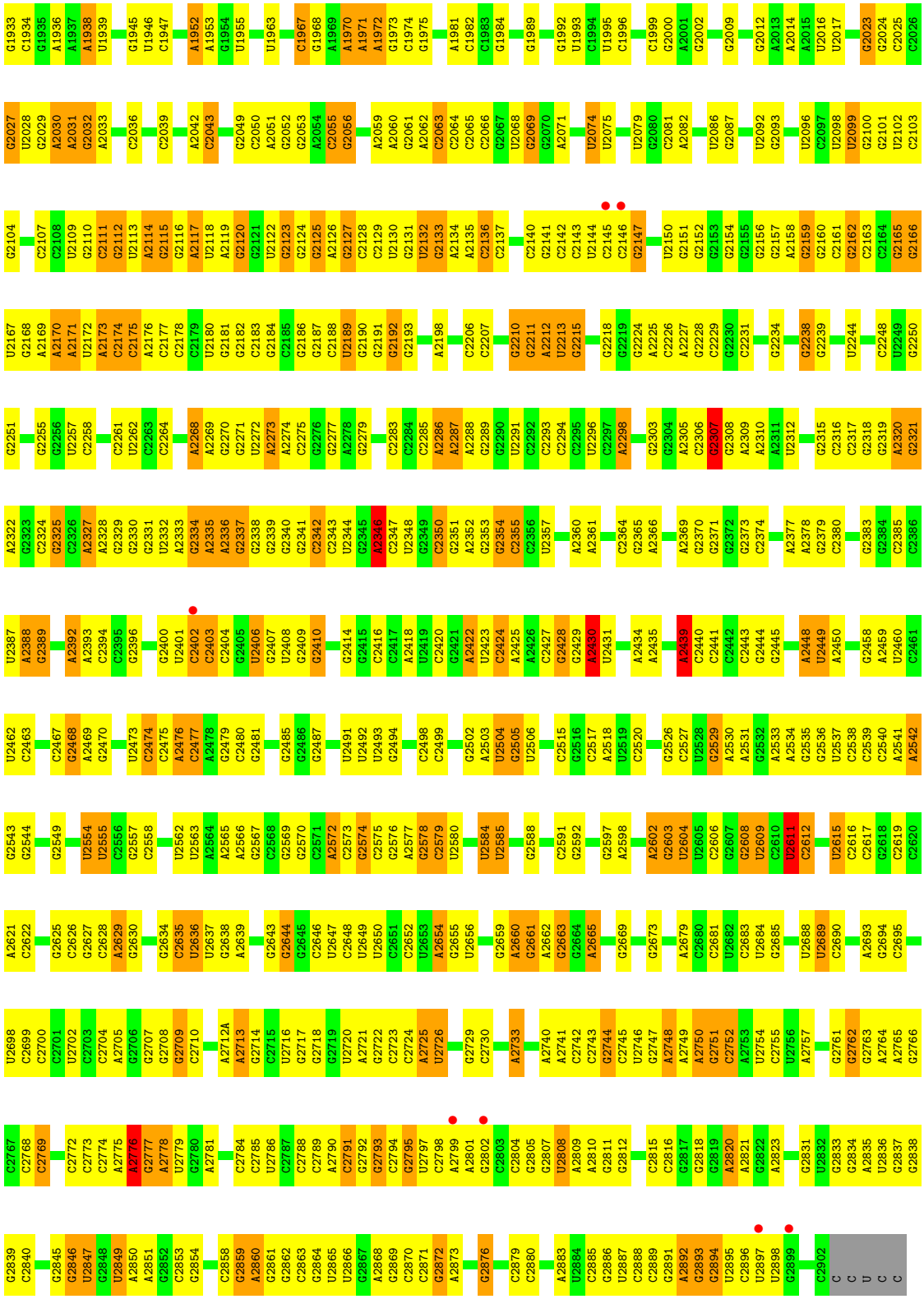


• Molecule 24: 23S ribosomal RNA

Chain 14:

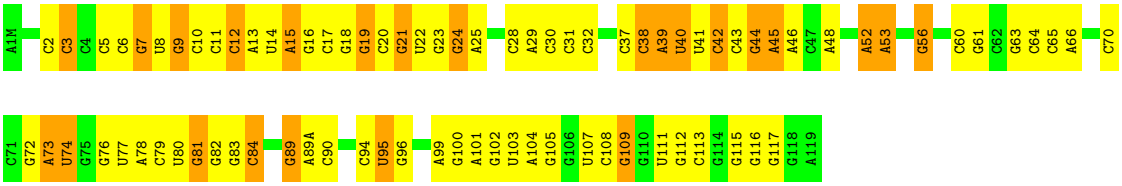


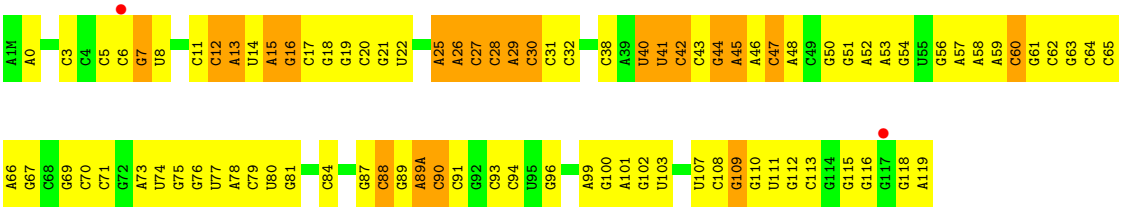





• Molecule 25: 5S ribosomal RNA

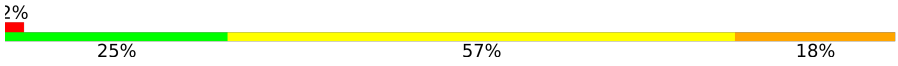
Chain 16:





• Molecule 25: 5S ribosomal RNA

Chain 1J:

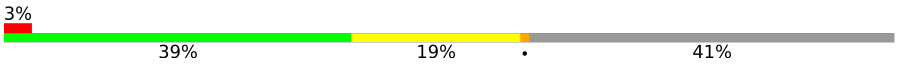


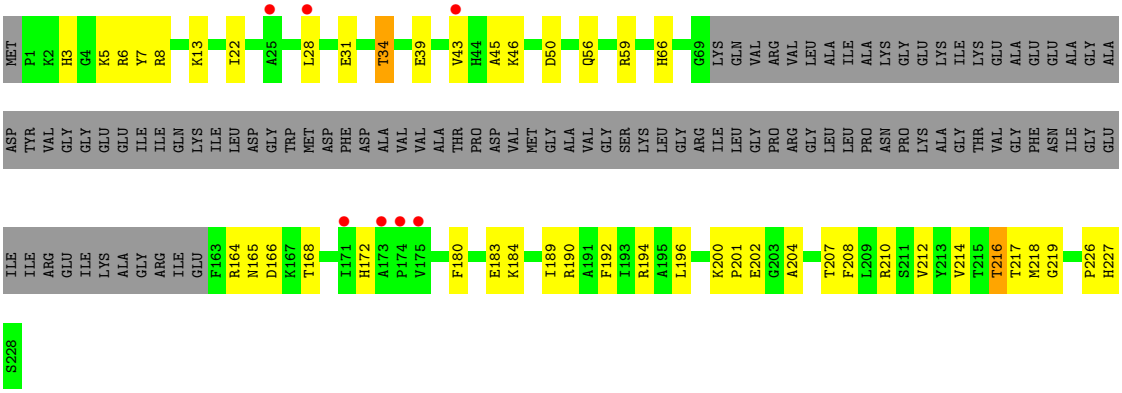





• Molecule 26: 50S ribosomal protein L1

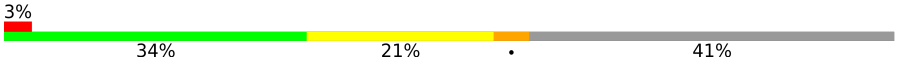
Chain 71:

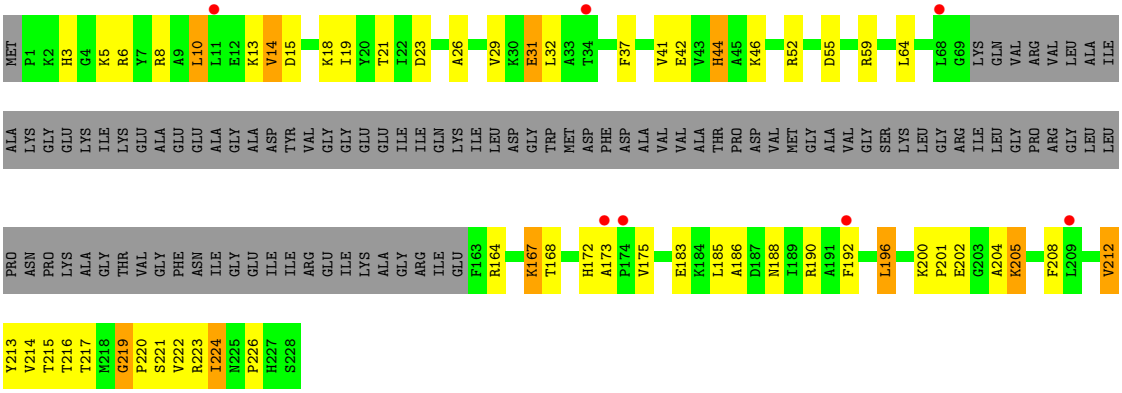


• Molecule 26: 50S ribosomal protein L1

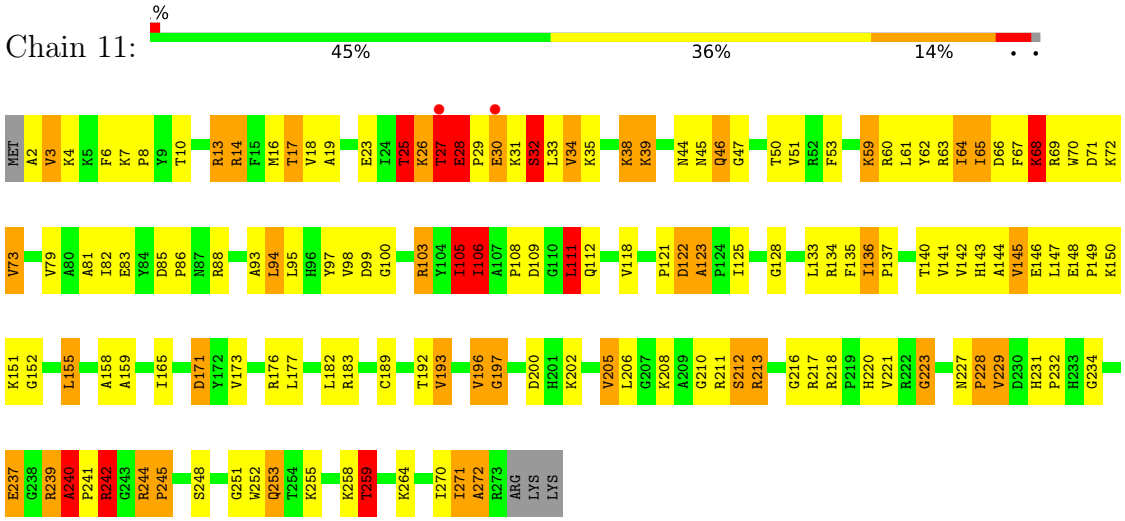
Chain 79:



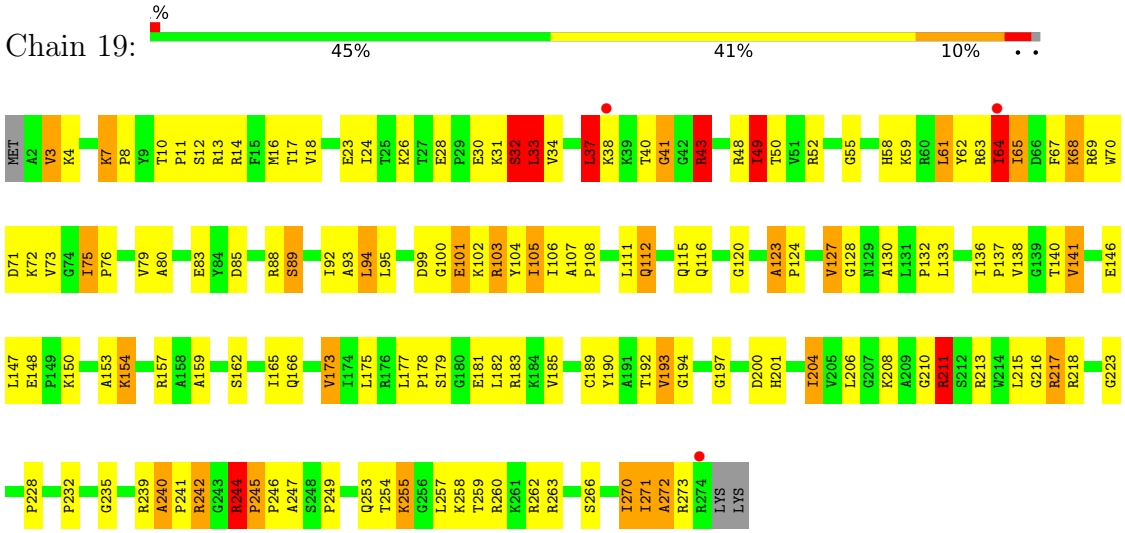
• Molecule 27: 50S ribosomal protein L2

Chain 11:



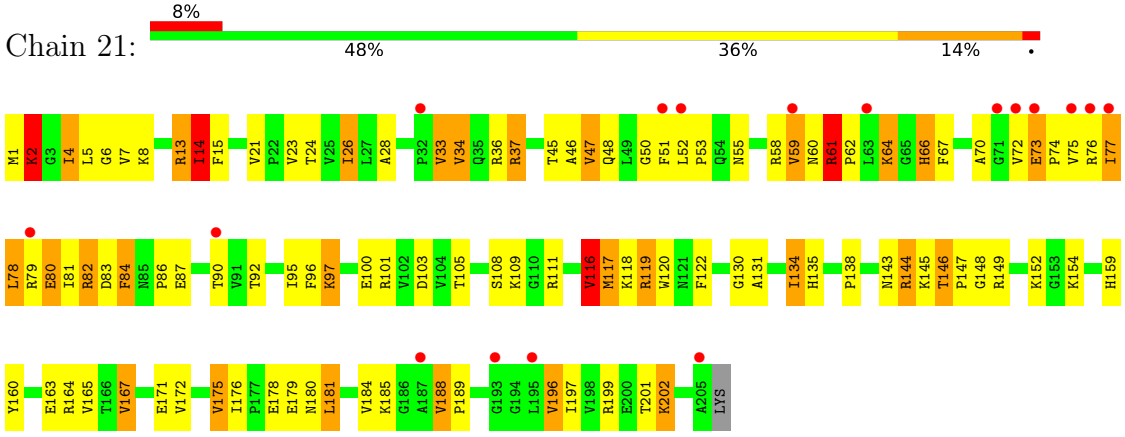

• Molecule 27: 50S ribosomal protein L2

Chain 19:



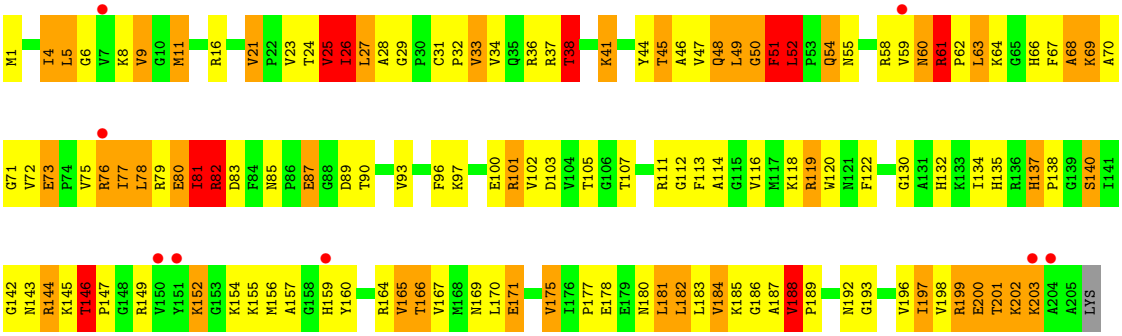

• Molecule 28: 50S ribosomal protein L3

Chain 21:



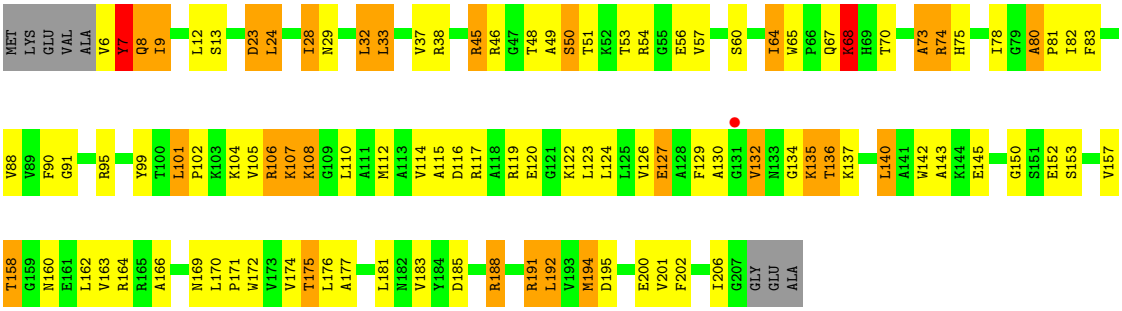

• Molecule 28: 50S ribosomal protein L3

Chain 29:



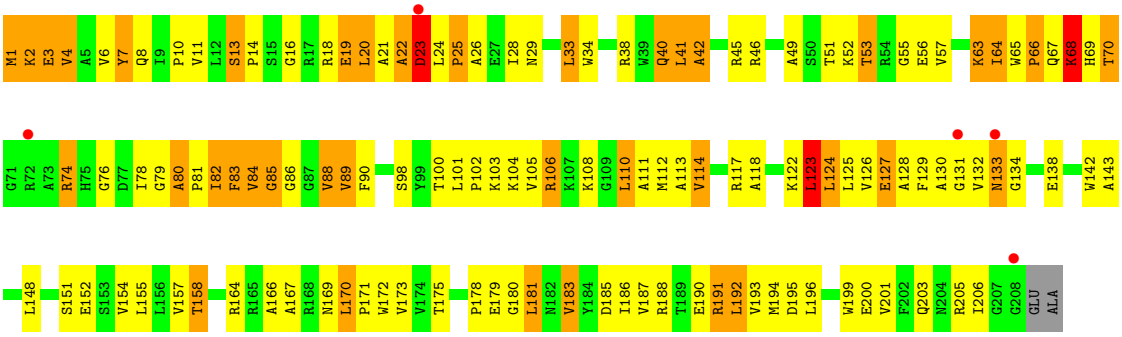
• Molecule 29: 50S ribosomal protein L4

Chain 31:



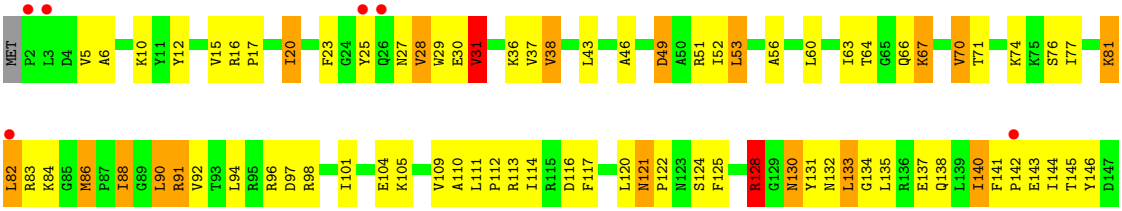
• Molecule 29: 50S ribosomal protein L4

Chain 39:

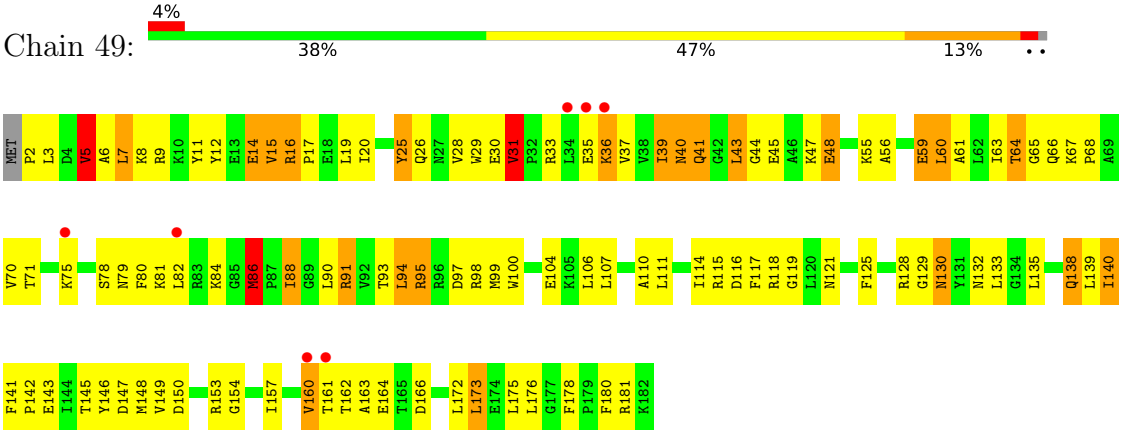


• Molecule 30: 50S ribosomal protein L5

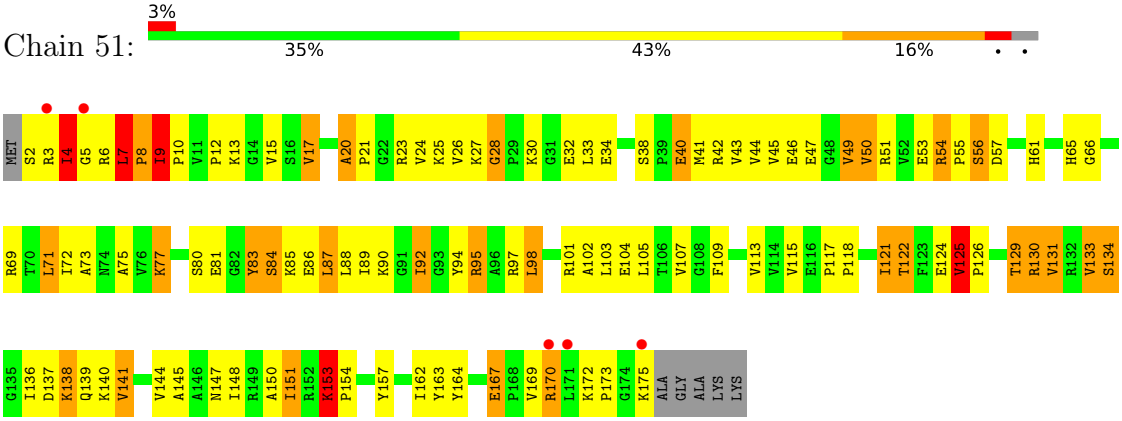
Chain 41:



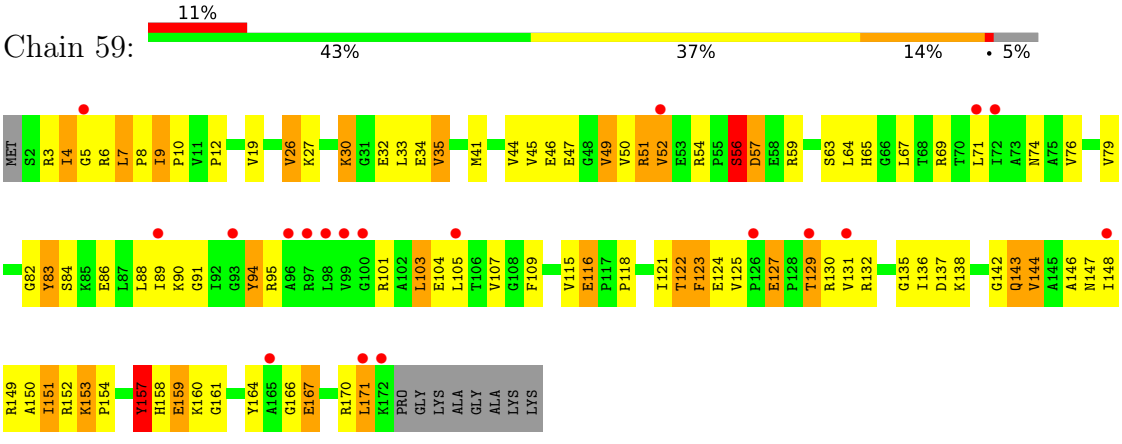
• Molecule 30: 50S ribosomal protein L5



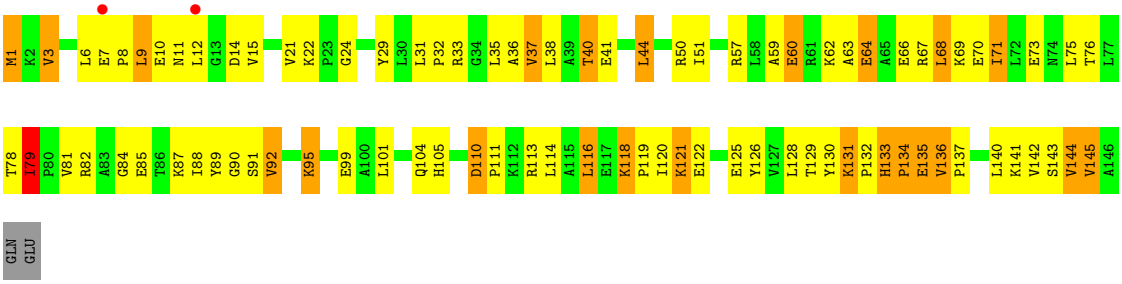

• Molecule 31: 50S ribosomal protein L6




• Molecule 31: 50S ribosomal protein L6



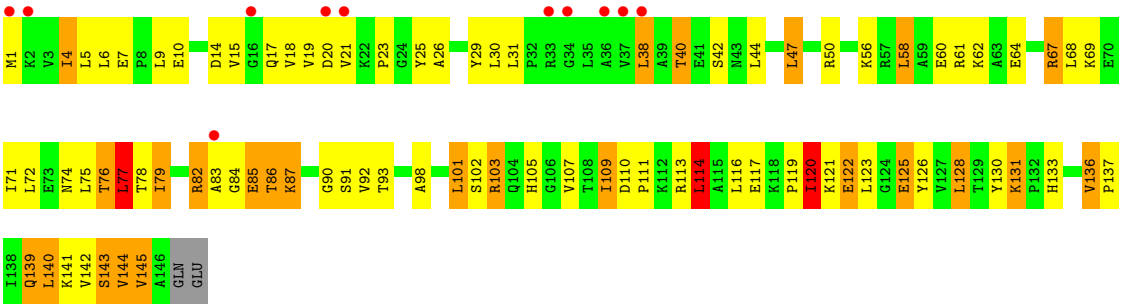

• Molecule 32: 50S ribosomal protein L9





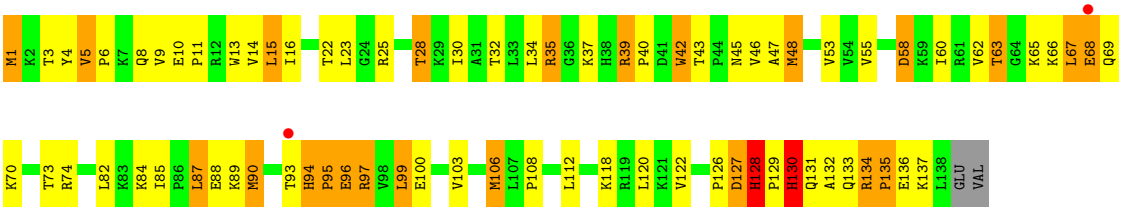
• Molecule 32: 50S ribosomal protein L9

Chain 69:



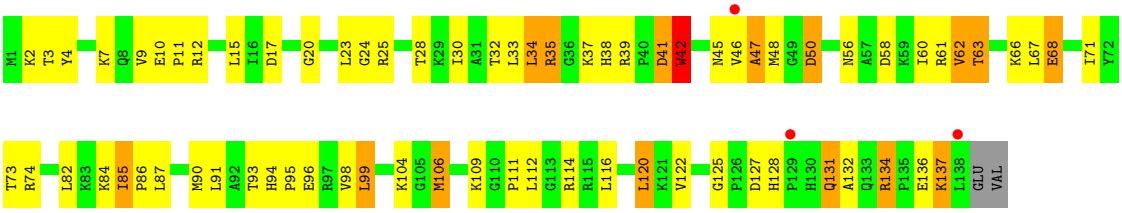
• Molecule 33: 50S ribosomal protein L13

Chain 58:



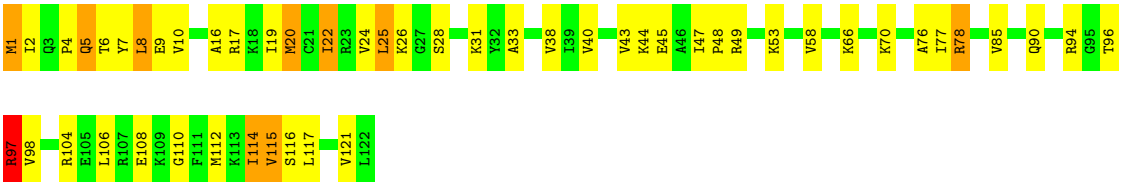
• Molecule 33: 50S ribosomal protein L13

Chain 15:



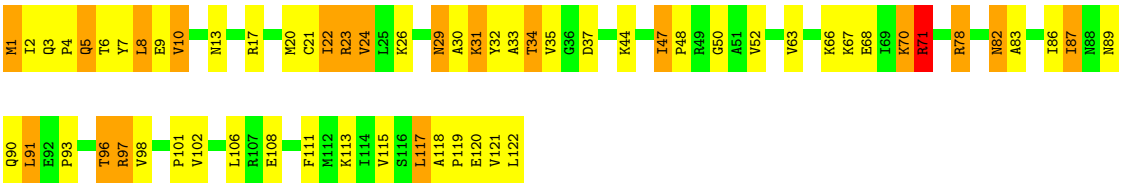
• Molecule 34: 50S ribosomal protein L14

Chain 68:



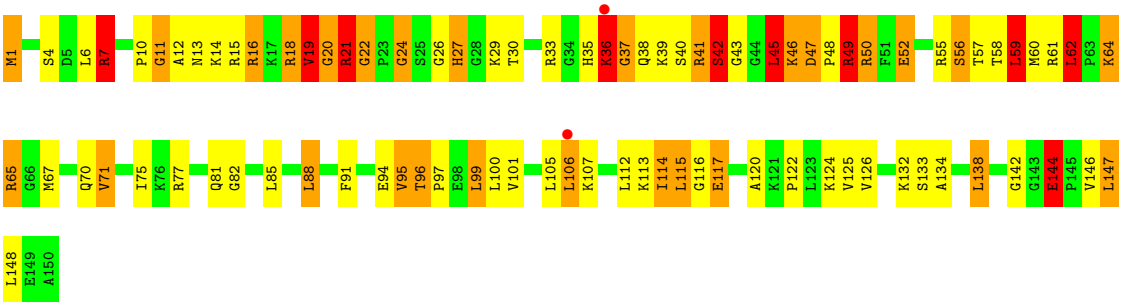
• Molecule 34: 50S ribosomal protein L14

Chain 25:



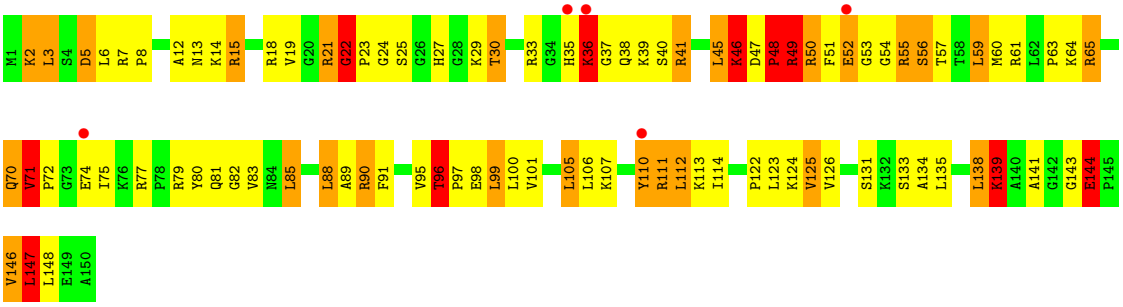
• Molecule 35: 50S ribosomal protein L15

Chain 78:



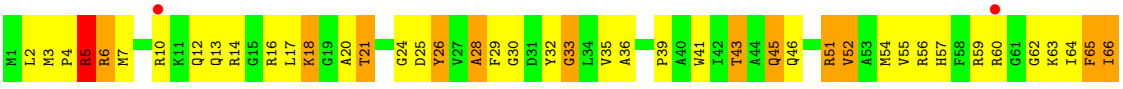
• Molecule 35: 50S ribosomal protein L15

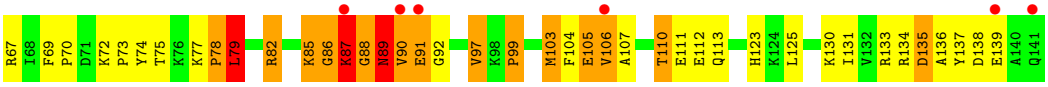
Chain 35:



• Molecule 36: 50S ribosomal protein L16

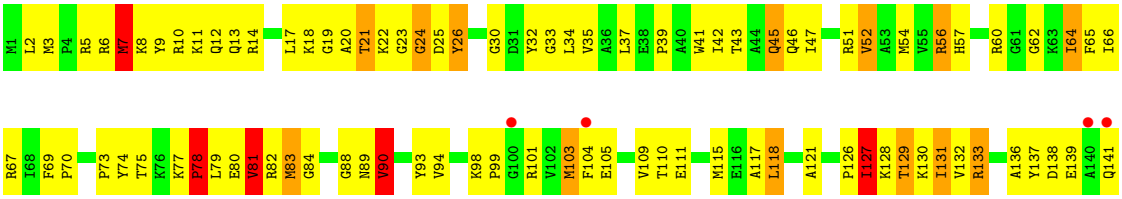
Chain 88:





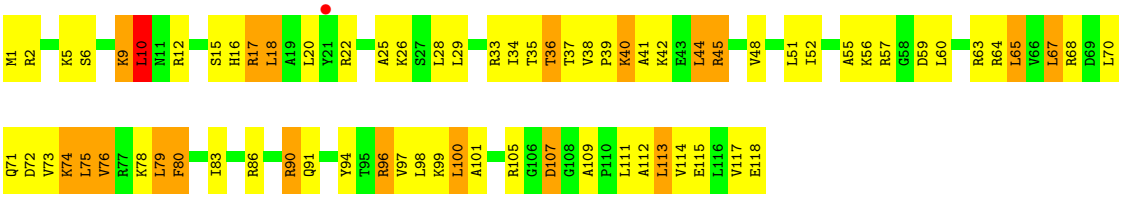
• Molecule 36: 50S ribosomal protein L16

Chain 45:



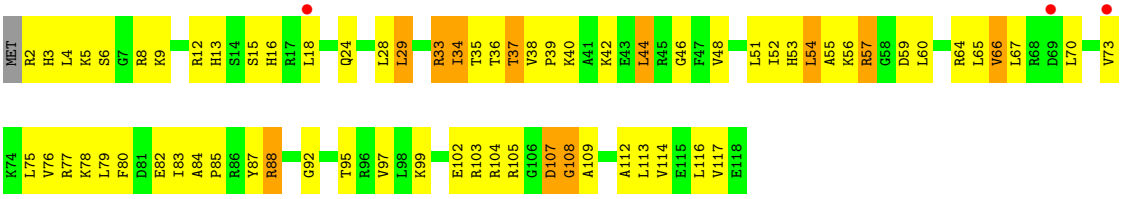
• Molecule 37: 50S ribosomal protein L17

Chain 98:



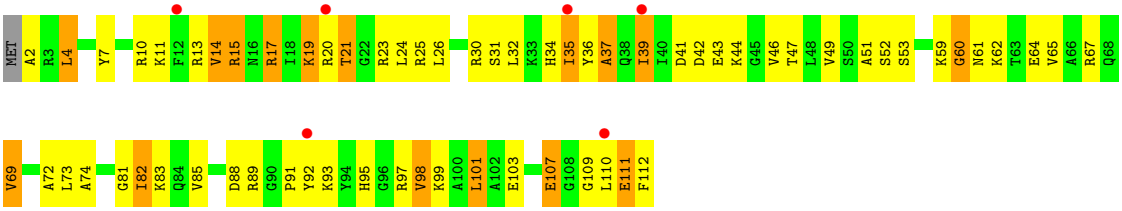
• Molecule 37: 50S ribosomal protein L17

Chain 55:



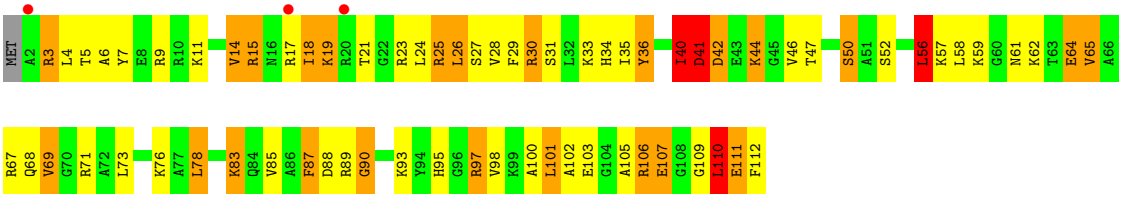
• Molecule 38: 50S ribosomal protein L18

Chain A8:



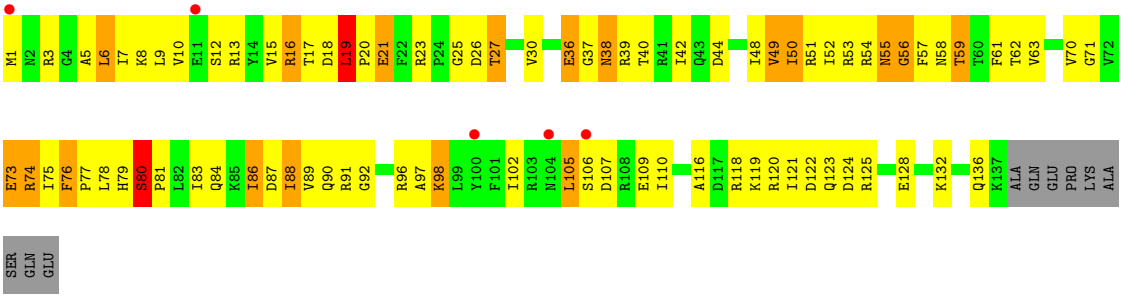
• Molecule 38: 50S ribosomal protein L18

Chain 65:



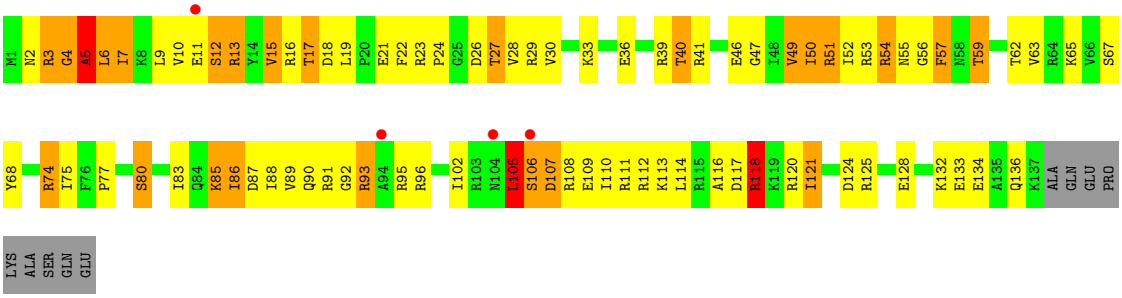

• Molecule 39: 50S ribosomal protein L19

Chain B8:



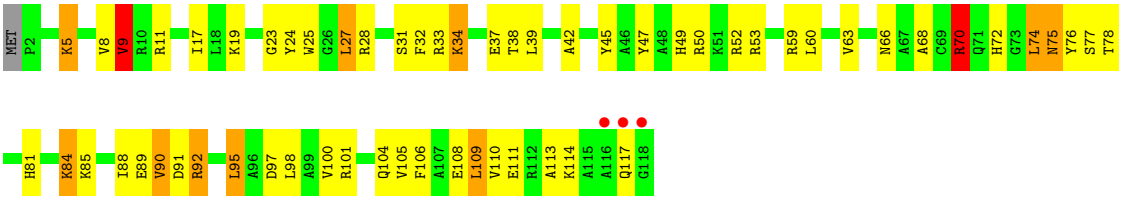

• Molecule 39: 50S ribosomal protein L19

Chain 75:




• Molecule 40: 50S ribosomal protein L20

Chain C8:

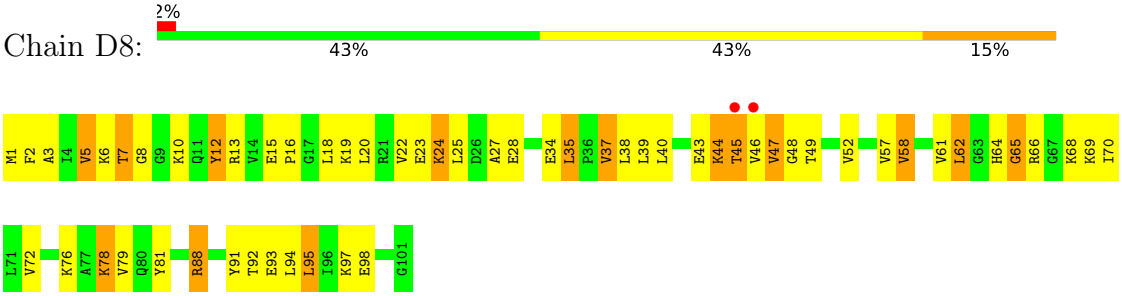



• Molecule 40: 50S ribosomal protein L20

Chain 85:

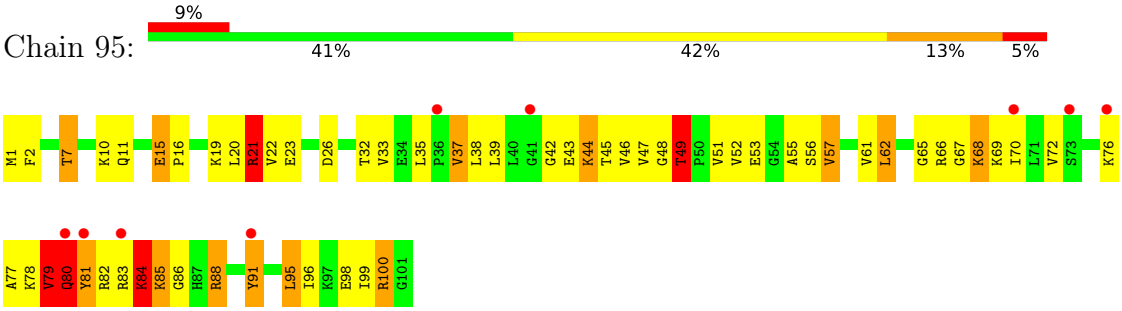
• Molecule 41: 50S ribosomal protein L21

Chain D8:



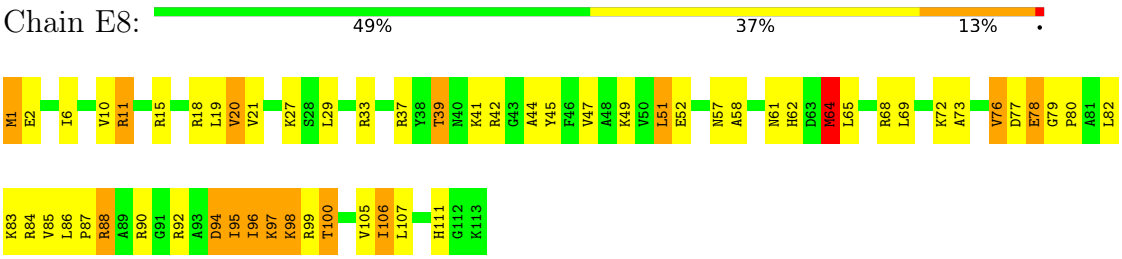

• Molecule 41: 50S ribosomal protein L21

Chain 95:



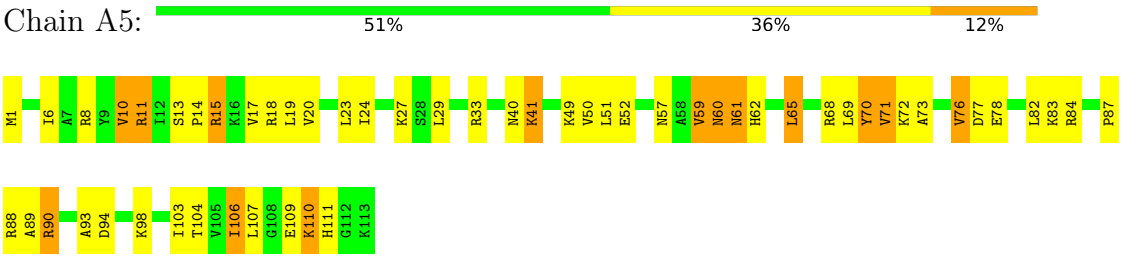

• Molecule 42: 50S ribosomal protein L22

Chain E8:



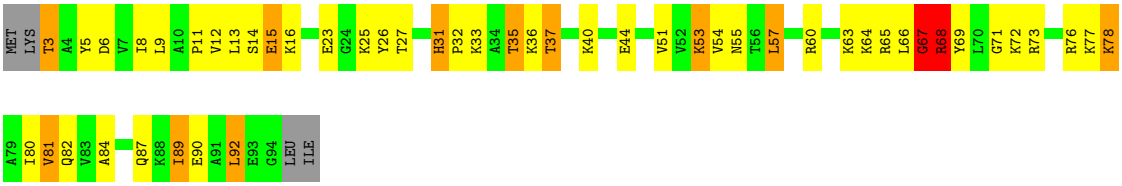

• Molecule 42: 50S ribosomal protein L22

Chain A5:



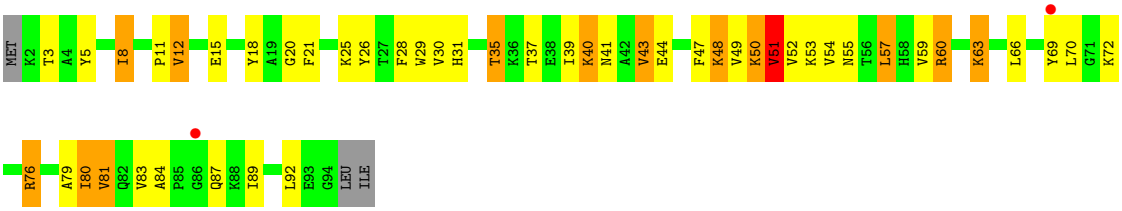

• Molecule 43: 50S ribosomal protein L23

Chain F8:



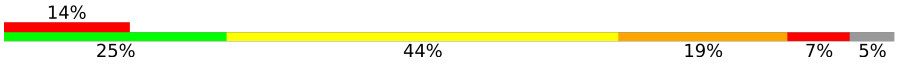
• Molecule 43: 50S ribosomal protein L23

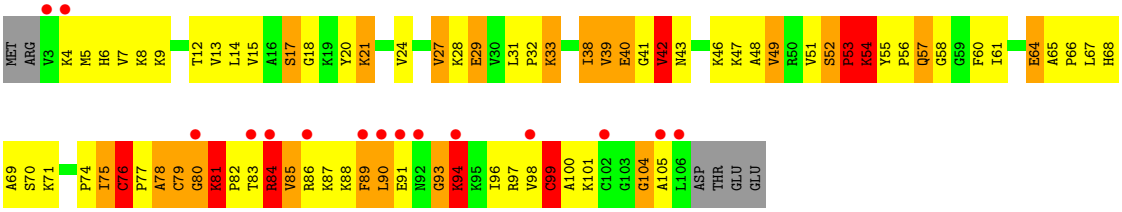
Chain B5:



• Molecule 44: 50S ribosomal protein L24

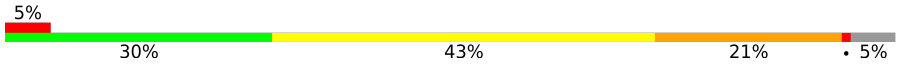
Chain G8:

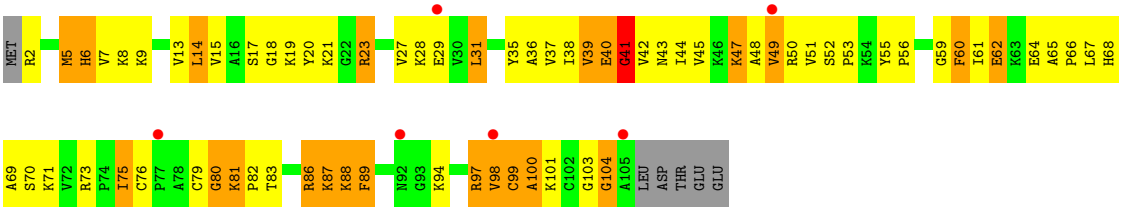


• Molecule 44: 50S ribosomal protein L24

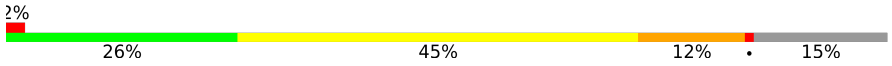
Chain C5:

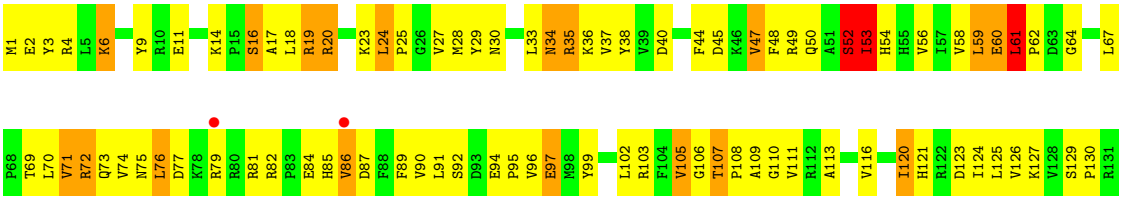


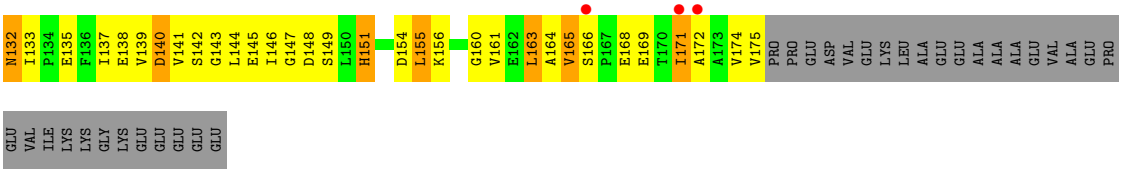



• Molecule 45: 50S ribosomal protein L25

Chain H8:



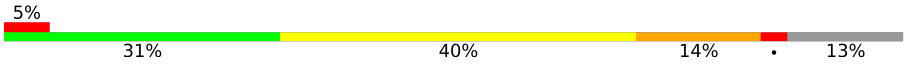



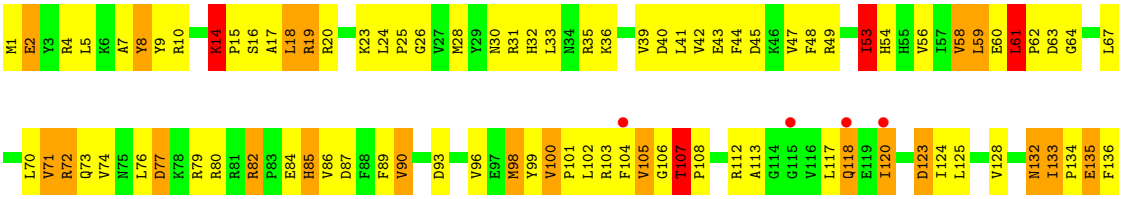


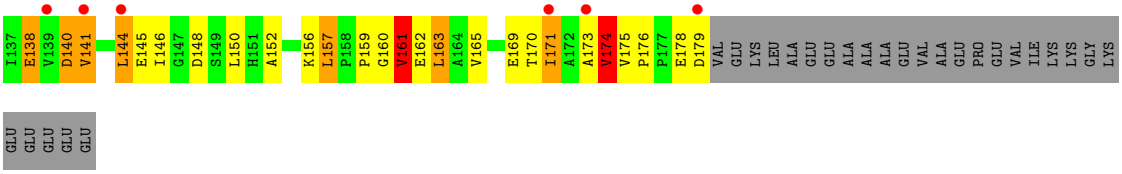


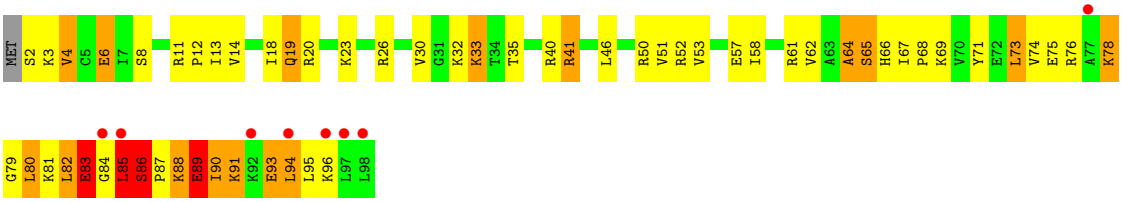
• Molecule 45: 50S ribosomal protein L25

Chain D5:

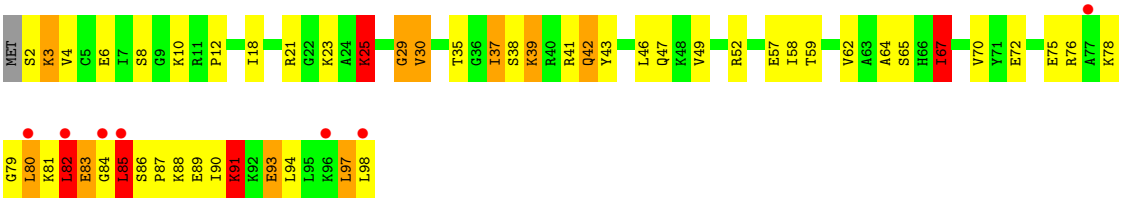


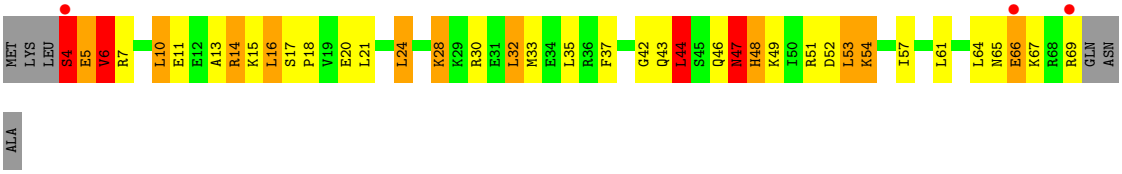




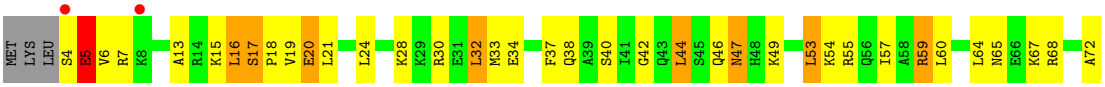

• Molecule 47: 50S ribosomal protein L28



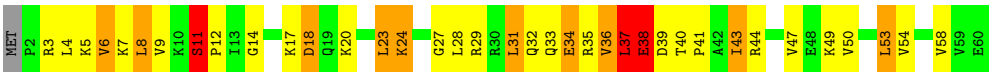

• Molecule 48: 50S ribosomal protein L29



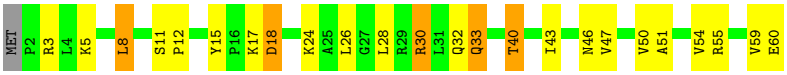

• Molecule 48: 50S ribosomal protein L29




• Molecule 49: 50S ribosomal protein L30

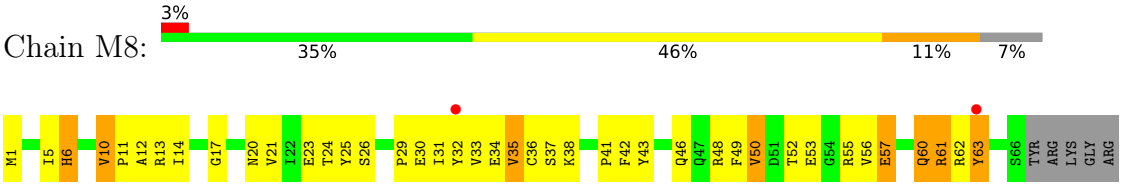



• Molecule 49: 50S ribosomal protein L30



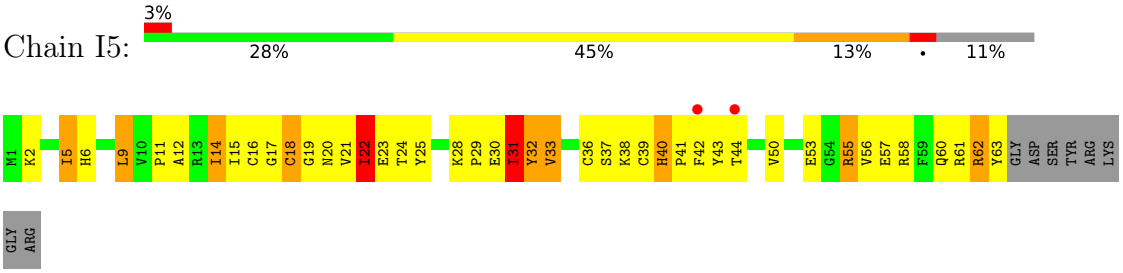

• Molecule 50: 50S ribosomal protein L31

Chain M8:



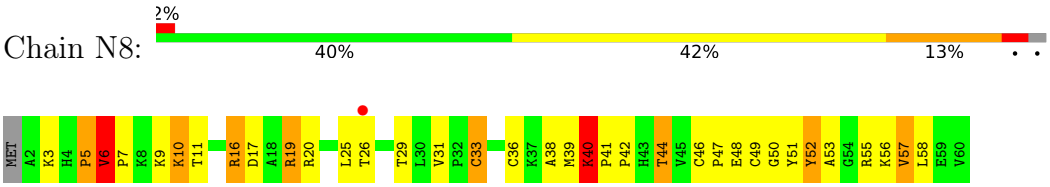

• Molecule 50: 50S ribosomal protein L31

Chain I5:



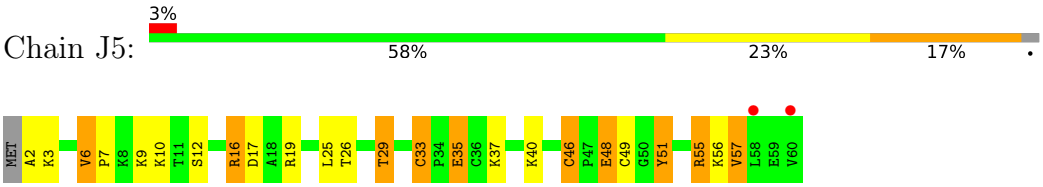

• Molecule 51: 50S ribosomal protein L32

Chain N8:



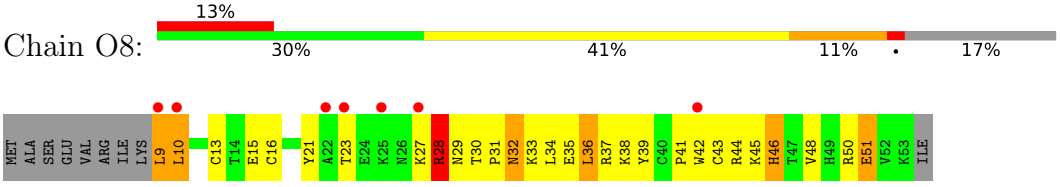

• Molecule 51: 50S ribosomal protein L32

Chain J5:



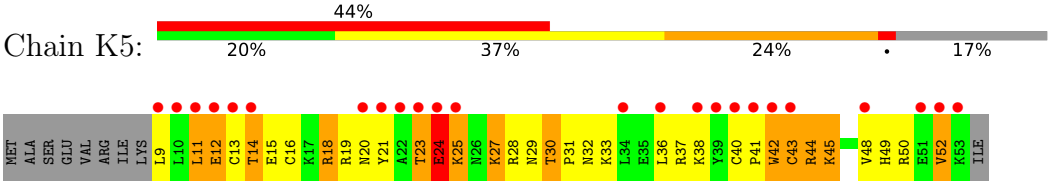

• Molecule 52: 50S ribosomal protein L33

Chain O8:



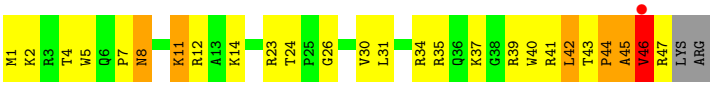

• Molecule 52: 50S ribosomal protein L33

Chain K5:




• Molecule 53: 50S ribosomal protein L34

Chain P8:

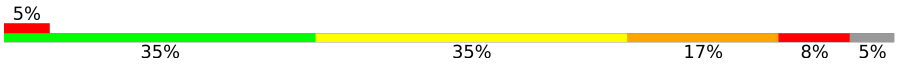



• Molecule 53: 50S ribosomal protein L34

Chain L5:

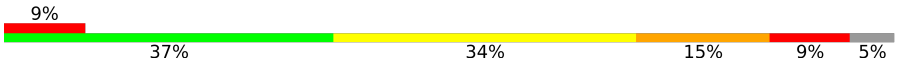
• Molecule 54: 50S ribosomal protein L35

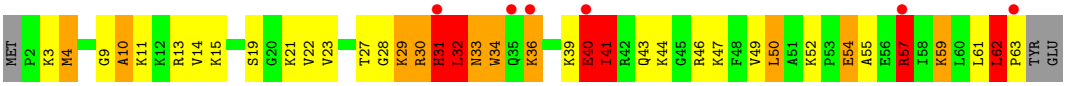
Chain Q8:



• Molecule 54: 50S ribosomal protein L35

Chain M5:



# 4 Data and refinement statistics (i)

| Property | Value | Source |
|---|---|---|
| Space group | P 21 21 21 | Depositor |
| Cell constants<br>a, b, c, $\alpha$, $\beta$, $\gamma$ | 210.70Å 448.40Å 616.30Å<br>90.00° 90.00° 90.00° | Depositor |
| Resolution (Å) | 153.54 – 3.10<br>153.54 – 3.10 | Depositor<br>EDS |
| % Data completeness<br>(in resolution range) | 99.8 (153.54-3.10)<br>91.1 (153.54-3.10) | Depositor<br>EDS |
| $R_{merge}$ | 0.22 | Depositor |
| $R_{sym}$ | (Not available) | Depositor |
| $< I/\sigma(I) >$ [1] | 0.83 (at 3.07Å) | Xtriage |
| Refinement program | PHENIX | Depositor |
| R, $R_{free}$ | 0.227 , 0.193<br>0.194 , 0.228 | Depositor<br>DCC |
| $R_{free}$ test set | 2000 reflections (0.19%) | wwPDB-VP |
| Wilson B-factor (Å$^2$) | 84.3 | Xtriage |
| Anisotropy | 0.119 | Xtriage |
| Bulk solvent $k_{sol}$(e/Å$^3$), $B_{sol}$(Å$^2$) | 0.28 , 69.5 | EDS |
| L-test for twinning[2] | $< \|L\| > = 0.47$, $< L^2 > = 0.30$ | Xtriage |
| Estimated twinning fraction | No twinning to report. | Xtriage |
| $F_o$,$F_c$ correlation | 0.95 | EDS |
| Total number of atoms | 299705 | wwPDB-VP |
| Average B, all atoms (Å$^2$) | 114.0 | wwPDB-VP |

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 1.48% 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: MG, PSU, MIA, 5MU, 4SU, QUO, OMG, ZN

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

| Mol | Chain | Bond lengths | | Bond angles | |
|---|---|---|---|---|---|
| | | RMSZ | #$\|Z\|$ >5 | RMSZ | #$\|Z\|$ >5 |
| 1 | 13 | 0.45 | 0/36199 | 0.70 | 4/56498 (0.0%) |
| 1 | 1G | 0.45 | 0/36167 | 0.71 | 12/56448 (0.0%) |
| 2 | 12 | 0.53 | 0/1959 | 1.02 | 9/2642 (0.3%) |
| 2 | 1E | 0.56 | 0/1959 | 0.98 | 4/2642 (0.2%) |
| 3 | 22 | 0.62 | 0/1636 | 0.98 | 2/2205 (0.1%) |
| 3 | 2E | 0.61 | 0/1629 | 0.96 | 1/2195 (0.0%) |
| 4 | 32 | 0.69 | 1/1732 (0.1%) | 1.16 | 12/2318 (0.5%) |
| 4 | 3E | 0.76 | 1/1732 (0.1%) | 1.19 | 13/2318 (0.6%) |
| 5 | 42 | 0.72 | 0/1171 | 1.21 | 9/1576 (0.6%) |
| 5 | 4E | 0.72 | 0/1171 | 1.11 | 7/1576 (0.4%) |
| 6 | 52 | 0.73 | 0/855 | 1.08 | 3/1154 (0.3%) |
| 6 | 5E | 0.68 | 0/855 | 1.08 | 2/1154 (0.2%) |
| 7 | 62 | 0.61 | 0/1275 | 1.03 | 3/1709 (0.2%) |
| 7 | 6E | 0.59 | 0/1275 | 1.01 | 5/1709 (0.3%) |
| 8 | 72 | 0.68 | 0/1135 | 1.10 | 2/1527 (0.1%) |
| 8 | 7E | 0.67 | 0/1135 | 1.27 | 12/1527 (0.8%) |
| 9 | 82 | 0.59 | 0/1028 | 1.04 | 5/1379 (0.4%) |
| 9 | 8E | 0.57 | 0/1028 | 0.94 | 0/1379 |
| 10 | 1A | 0.57 | 0/814 | 0.98 | 2/1095 (0.2%) |
| 10 | 1I | 0.61 | 0/814 | 1.08 | 8/1095 (0.7%) |
| 11 | 2A | 0.74 | 0/879 | 1.17 | 6/1187 (0.5%) |
| 11 | 2I | 0.73 | 0/879 | 1.15 | 2/1187 (0.2%) |
| 12 | 3A | 0.84 | 0/991 | 1.21 | 9/1327 (0.7%) |
| 12 | 3I | 0.85 | 0/991 | 1.31 | 6/1327 (0.5%) |
| 13 | 4A | 0.54 | 0/943 | 0.94 | 3/1265 (0.2%) |
| 13 | 4I | 0.54 | 0/938 | 1.09 | 4/1258 (0.3%) |
| 14 | 5A | 0.60 | 0/500 | 1.09 | 1/664 (0.2%) |
| 14 | 5I | 0.68 | 1/500 (0.2%) | 1.12 | 3/664 (0.5%) |
| 15 | 6A | 0.77 | 0/744 | 1.02 | 1/992 (0.1%) |
| 15 | 6I | 0.76 | 0/744 | 1.08 | 0/992 |
| 16 | 7A | 0.75 | 0/721 | 1.10 | 3/970 (0.3%) |
| 16 | 7I | 0.67 | 0/721 | 1.12 | 3/970 (0.3%) |

| Mol | Chain | Bond lengths | | Bond angles | |
|---|---|---|---|---|---|
| | | RMSZ | #\|Z\| >5 | RMSZ | #\|Z\| >5 |
| 17 | 8A | 0.70 | 0/847 | 1.13 | 4/1131 (0.4%) |
| 17 | 8I | 0.65 | 0/847 | 1.06 | 1/1131 (0.1%) |
| 18 | 9A | 0.71 | 0/595 | 1.11 | 1/790 (0.1%) |
| 18 | 9I | 0.69 | 0/595 | 1.05 | 3/790 (0.4%) |
| 19 | AA | 0.61 | 0/647 | 1.12 | 3/871 (0.3%) |
| 19 | AI | 0.55 | 0/680 | 1.17 | 6/915 (0.7%) |
| 20 | BA | 0.73 | 0/764 | 1.19 | 5/1007 (0.5%) |
| 20 | BI | 0.59 | 0/764 | 1.07 | 1/1007 (0.1%) |
| 21 | 1B | 0.54 | 0/221 | 0.97 | 0/288 |
| 21 | 1F | 0.52 | 0/221 | 0.96 | 0/288 |
| 22 | 2K | 0.47 | 1/1784 (0.1%) | 0.80 | 1/2771 (0.0%) |
| 22 | 2L | 0.47 | 0/1686 | 0.75 | 0/2618 |
| 22 | 3K | 0.29 | 0/1850 | 0.49 | 0/2875 |
| 22 | 3L | 0.31 | 0/1851 | 0.51 | 0/2877 |
| 23 | 4K | 0.68 | 0/392 | 0.87 | 1/609 (0.2%) |
| 23 | 4L | 0.56 | 0/190 | 0.83 | 0/293 |
| 24 | 14 | 0.59 | 0/70167 | 0.82 | 20/109541 (0.0%) |
| 24 | 1H | 0.63 | 0/70233 | 0.86 | 36/109643 (0.0%) |
| 25 | 16 | 0.48 | 0/2928 | 0.74 | 0/4568 |
| 25 | 1J | 0.48 | 0/2928 | 0.78 | 0/4568 |
| 26 | 71 | 0.39 | 0/1072 | 0.84 | 2/1447 (0.1%) |
| 26 | 79 | 0.40 | 0/1072 | 0.90 | 6/1447 (0.4%) |
| 27 | 11 | 1.17 | 8/2165 (0.4%) | 1.63 | 43/2919 (1.5%) |
| 27 | 19 | 1.06 | 3/2170 (0.1%) | 1.45 | 26/2926 (0.9%) |
| 28 | 21 | 0.93 | 1/1601 (0.1%) | 1.43 | 18/2160 (0.8%) |
| 28 | 29 | 0.97 | 1/1601 (0.1%) | 1.49 | 25/2160 (1.2%) |
| 29 | 31 | 1.01 | 1/1620 (0.1%) | 1.38 | 17/2194 (0.8%) |
| 29 | 39 | 0.89 | 0/1662 | 1.38 | 15/2249 (0.7%) |
| 30 | 41 | 0.57 | 0/1498 | 1.01 | 6/2016 (0.3%) |
| 30 | 49 | 0.55 | 0/1498 | 1.02 | 5/2016 (0.2%) |
| 31 | 51 | 0.85 | 0/1362 | 1.46 | 27/1841 (1.5%) |
| 31 | 59 | 0.55 | 0/1337 | 1.19 | 17/1809 (0.9%) |
| 32 | 61 | 0.73 | 0/1151 | 1.15 | 11/1558 (0.7%) |
| 32 | 69 | 0.69 | 0/1151 | 1.12 | 9/1558 (0.6%) |
| 33 | 15 | 0.75 | 0/1131 | 1.21 | 8/1525 (0.5%) |
| 33 | 58 | 0.83 | 0/1131 | 1.20 | 6/1525 (0.4%) |
| 34 | 25 | 1.04 | 1/942 (0.1%) | 1.28 | 7/1269 (0.6%) |
| 34 | 68 | 0.95 | 0/942 | 1.25 | 2/1269 (0.2%) |
| 35 | 35 | 0.92 | 0/1161 | 1.60 | 21/1544 (1.4%) |
| 35 | 78 | 1.04 | 2/1161 (0.2%) | 1.53 | 17/1544 (1.1%) |
| 36 | 45 | 0.87 | 1/1142 (0.1%) | 1.36 | 7/1527 (0.5%) |
| 36 | 88 | 0.98 | 1/1142 (0.1%) | 1.38 | 15/1527 (1.0%) |
| 37 | 55 | 0.94 | 0/973 | 1.26 | 1/1302 (0.1%) |

| Mol | Chain | Bond lengths | | Bond angles | |
|---|---|---|---|---|---|
| | | RMSZ | #\|Z\| >5 | RMSZ | #\|Z\| >5 |
| 37 | 98 | 0.91 | 1/981 (0.1%) | 1.30 | 7/1312 (0.5%) |
| 38 | 65 | 0.76 | 0/891 | 1.22 | 9/1187 (0.8%) |
| 38 | A8 | 0.77 | 0/891 | 1.19 | 3/1187 (0.3%) |
| 39 | 75 | 0.94 | 0/1145 | 1.28 | 8/1531 (0.5%) |
| 39 | B8 | 0.87 | 0/1155 | 1.31 | 13/1542 (0.8%) |
| 40 | 85 | 0.85 | 0/981 | 1.16 | 3/1306 (0.2%) |
| 40 | C8 | 0.94 | 0/981 | 1.20 | 2/1306 (0.2%) |
| 41 | 95 | 2.58 | 9/789 (1.1%) | 1.66 | 17/1057 (1.6%) |
| 41 | D8 | 0.88 | 0/789 | 1.23 | 3/1057 (0.3%) |
| 42 | A5 | 0.96 | 0/910 | 1.23 | 6/1220 (0.5%) |
| 42 | E8 | 1.02 | 0/910 | 1.28 | 4/1220 (0.3%) |
| 43 | B5 | 0.99 | 0/744 | 1.19 | 3/1000 (0.3%) |
| 43 | F8 | 1.06 | 1/739 (0.1%) | 1.27 | 2/993 (0.2%) |
| 44 | C5 | 0.89 | 1/807 (0.1%) | 1.33 | 12/1076 (1.1%) |
| 44 | G8 | 1.13 | 2/804 (0.2%) | 1.63 | 19/1073 (1.8%) |
| 45 | D5 | 0.61 | 0/1460 | 1.14 | 15/1982 (0.8%) |
| 45 | H8 | 0.61 | 0/1427 | 1.15 | 10/1935 (0.5%) |
| 46 | E5 | 0.88 | 0/620 | 1.30 | 6/827 (0.7%) |
| 46 | I8 | 1.01 | 0/665 | 1.30 | 2/885 (0.2%) |
| 47 | F5 | 0.89 | 1/769 (0.1%) | 1.29 | 7/1022 (0.7%) |
| 47 | J8 | 0.91 | 0/769 | 1.39 | 8/1022 (0.8%) |
| 48 | G5 | 0.75 | 0/582 | 1.25 | 2/771 (0.3%) |
| 48 | K8 | 1.02 | 1/560 (0.2%) | 1.39 | 5/741 (0.7%) |
| 49 | H5 | 0.79 | 0/473 | 1.26 | 2/635 (0.3%) |
| 49 | L8 | 0.88 | 1/473 (0.2%) | 1.44 | 8/635 (1.3%) |
| 50 | I5 | 0.65 | 0/527 | 1.06 | 3/709 (0.4%) |
| 50 | M8 | 0.51 | 0/545 | 0.92 | 0/733 |
| 51 | J5 | 0.87 | 0/472 | 1.24 | 4/639 (0.6%) |
| 51 | N8 | 1.05 | 1/472 (0.2%) | 1.32 | 7/639 (1.1%) |
| 52 | K5 | 0.78 | 0/396 | 1.24 | 6/529 (1.1%) |
| 52 | O8 | 0.74 | 0/396 | 1.22 | 4/529 (0.8%) |
| 53 | L5 | 1.08 | 1/437 (0.2%) | 1.31 | 2/575 (0.3%) |
| 53 | P8 | 1.18 | 0/417 | 1.34 | 1/550 (0.2%) |
| 54 | M5 | 1.20 | 1/502 (0.2%) | 1.63 | 12/661 (1.8%) |
| 54 | Q8 | 1.26 | 2/488 (0.4%) | 1.68 | 6/641 (0.9%) |
| All | All | 0.65 | 45/321962 (0.0%) | 0.93 | 770/481589 (0.2%) |

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

| Mol | Chain | #Chirality outliers | #Planarity outliers |
|---|---|---|---|
| 2 | 12 | 0 | 2 |
| 2 | 1E | 0 | 1 |
| 3 | 22 | 0 | 1 |
| 4 | 3E | 0 | 3 |
| 9 | 82 | 0 | 2 |
| 12 | 3A | 0 | 4 |
| 14 | 5I | 0 | 1 |
| 19 | AA | 0 | 1 |
| 19 | AI | 0 | 3 |
| 20 | BA | 0 | 2 |
| 27 | 11 | 0 | 4 |
| 27 | 19 | 0 | 5 |
| 28 | 29 | 0 | 7 |
| 29 | 31 | 0 | 1 |
| 29 | 39 | 0 | 1 |
| 30 | 49 | 0 | 1 |
| 31 | 59 | 0 | 1 |
| 32 | 61 | 0 | 1 |
| 33 | 15 | 0 | 1 |
| 34 | 25 | 0 | 1 |
| 35 | 35 | 0 | 7 |
| 35 | 78 | 0 | 7 |
| 36 | 45 | 0 | 1 |
| 36 | 88 | 0 | 3 |
| 38 | 65 | 0 | 1 |
| 38 | A8 | 0 | 2 |
| 39 | 75 | 0 | 3 |
| 39 | B8 | 0 | 1 |
| 40 | 85 | 0 | 1 |
| 41 | 95 | 0 | 2 |
| 43 | F8 | 0 | 1 |
| 44 | C5 | 0 | 3 |
| 44 | G8 | 0 | 5 |
| 45 | D5 | 0 | 3 |
| 47 | F5 | 0 | 2 |
| 47 | J8 | 0 | 2 |
| 48 | K8 | 0 | 2 |
| 49 | L8 | 0 | 1 |
| 51 | J5 | 0 | 1 |
| 52 | K5 | 0 | 1 |
| 53 | P8 | 0 | 2 |
| 54 | M5 | 0 | 2 |
| 54 | Q8 | 0 | 4 |

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| Mol | Chain | #Chirality outliers | #Planarity outliers |
|---|---|---|---|
| All | All | 0 | 100 |

All (45) bond length outliers are listed below:

| Mol | Chain | Res | Type | Atoms | Z | Observed(Å) | Ideal(Å) |
|---|---|---|---|---|---|---|---|
| 41 | 95 | 91 | TYR | CD1-CE1 | 30.02 | 2.28 | 1.38 |
| 41 | 95 | 91 | TYR | CD2-CE2 | 29.01 | 2.25 | 1.38 |
| 41 | 95 | 21 | ARG | CD-NE | 28.53 | 1.86 | 1.46 |
| 41 | 95 | 91 | TYR | CE2-CZ | 22.59 | 1.92 | 1.38 |
| 41 | 95 | 91 | TYR | CE1-CZ | 21.76 | 1.90 | 1.38 |
| 41 | 95 | 91 | TYR | CG-CD2 | 19.29 | 1.79 | 1.39 |
| 41 | 95 | 91 | TYR | CG-CD1 | 19.14 | 1.79 | 1.39 |
| 41 | 95 | 21 | ARG | NE-CZ | 17.79 | 1.52 | 1.33 |
| 27 | 19 | 64 | ILE | CA-CB | 8.76 | 1.64 | 1.54 |
| 35 | 78 | 19 | VAL | CA-CB | 7.86 | 1.64 | 1.55 |
| 41 | 95 | 80 | GLN | CA-C | 7.63 | 1.64 | 1.53 |
| 51 | N8 | 6 | VAL | CA-C | 7.35 | 1.60 | 1.52 |
| 27 | 11 | 27 | THR | CA-CB | 6.95 | 1.65 | 1.53 |
| 27 | 11 | 271 | ILE | CA-C | 6.37 | 1.61 | 1.52 |
| 54 | Q8 | 62 | LEU | CA-C | 6.26 | 1.60 | 1.52 |
| 34 | 25 | 34 | THR | CA-CB | -6.13 | 1.44 | 1.53 |
| 27 | 11 | 30 | GLU | CG-CD | 6.07 | 1.67 | 1.52 |
| 36 | 45 | 90 | VAL | CA-CB | 5.80 | 1.62 | 1.54 |
| 27 | 11 | 32 | SER | CA-CB | -5.75 | 1.46 | 1.53 |
| 54 | M5 | 32 | LEU | CA-C | 5.61 | 1.60 | 1.52 |
| 27 | 11 | 272 | ALA | CA-C | 5.59 | 1.59 | 1.53 |
| 48 | K8 | 5 | GLU | CB-CG | 5.58 | 1.69 | 1.52 |
| 47 | F5 | 49 | VAL | CA-CB | -5.58 | 1.47 | 1.54 |
| 44 | G8 | 83 | THR | CA-CB | 5.52 | 1.62 | 1.53 |
| 27 | 11 | 122 | ASP | CB-CG | 5.51 | 1.65 | 1.52 |
| 27 | 19 | 107 | ALA | CA-C | -5.50 | 1.46 | 1.52 |
| 54 | Q8 | 58 | ILE | CA-CB | 5.45 | 1.61 | 1.54 |
| 27 | 11 | 106 | ILE | CA-CB | 5.42 | 1.60 | 1.54 |
| 14 | 5I | 26 | ARG | CA-C | 5.40 | 1.56 | 1.52 |
| 28 | 21 | 134 | ILE | CA-CB | -5.39 | 1.47 | 1.54 |
| 27 | 11 | 45 | ASN | C-O | -5.35 | 1.17 | 1.24 |
| 43 | F8 | 9 | LEU | CA-C | -5.33 | 1.47 | 1.53 |
| 27 | 19 | 240 | ALA | CA-C | -5.29 | 1.46 | 1.52 |
| 44 | C5 | 98 | VAL | CA-CB | 5.26 | 1.60 | 1.54 |
| 37 | 98 | 10 | LEU | CA-C | -5.25 | 1.46 | 1.53 |
| 35 | 78 | 18 | ARG | CA-C | -5.25 | 1.46 | 1.52 |
| 22 | 2K | 8 | 4SU | O3'-P | 5.23 | 1.61 | 1.56 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(Å) | Ideal(Å) |
|---|---|---|---|---|---|---|---|
| 28 | 29 | 146 | THR | CA-C | -5.18 | 1.48 | 1.52 |
| 49 | L8 | 38 | GLU | CA-C | 5.10 | 1.55 | 1.52 |
| 44 | G8 | 79 | CYS | CA-C | 5.10 | 1.59 | 1.52 |
| 36 | 88 | 105 | GLU | CA-C | 5.07 | 1.59 | 1.52 |
| 4 | 3E | 56 | VAL | CA-CB | -5.06 | 1.49 | 1.54 |
| 53 | L5 | 30 | VAL | CA-CB | -5.05 | 1.48 | 1.54 |
| 29 | 31 | 73 | ALA | CA-CB | -5.04 | 1.45 | 1.53 |
| 4 | 32 | 26 | CYS | CA-C | -5.04 | 1.47 | 1.53 |

All (770) bond angle outliers are listed below:

| Mol | Chain | Res | Type | Atoms | Z | Observed($^o$) | Ideal($^o$) |
|---|---|---|---|---|---|---|---|
| 41 | 95 | 21 | ARG | CD-NE-CZ | 22.47 | 155.86 | 124.40 |
| 54 | Q8 | 41 | ILE | N-CA-C | -17.43 | 97.85 | 111.62 |
| 27 | 11 | 28 | GLU | CA-C-N | -15.72 | 104.47 | 120.03 |
| 27 | 11 | 28 | GLU | C-N-CA | -15.72 | 104.47 | 120.03 |
| 31 | 51 | 9 | ILE | CA-C-N | -13.16 | 107.00 | 120.03 |
| 31 | 51 | 9 | ILE | C-N-CA | -13.16 | 107.00 | 120.03 |
| 36 | 45 | 62 | GLY | N-CA-C | -12.18 | 94.00 | 110.56 |
| 28 | 29 | 80 | GLU | N-CA-C | 12.14 | 127.53 | 112.23 |
| 28 | 21 | 61 | ARG | CA-C-N | -12.12 | 105.33 | 120.23 |
| 28 | 21 | 61 | ARG | C-N-CA | -12.12 | 105.33 | 120.23 |
| 27 | 11 | 272 | ALA | N-CA-C | 11.80 | 123.41 | 108.19 |
| 35 | 35 | 144 | GLU | CA-C-N | 11.55 | 131.63 | 120.31 |
| 35 | 35 | 144 | GLU | C-N-CA | 11.55 | 131.63 | 120.31 |
| 27 | 11 | 271 | ILE | N-CA-C | 11.27 | 123.72 | 112.90 |
| 28 | 29 | 52 | LEU | CA-C-N | 11.26 | 132.15 | 119.32 |
| 28 | 29 | 52 | LEU | C-N-CA | 11.26 | 132.15 | 119.32 |
| 49 | H5 | 11 | SER | CA-C-N | 11.01 | 130.68 | 119.56 |
| 49 | H5 | 11 | SER | C-N-CA | 11.01 | 130.68 | 119.56 |
| 45 | H8 | 61 | LEU | CA-C-N | 10.85 | 130.46 | 119.82 |
| 45 | H8 | 61 | LEU | C-N-CA | 10.85 | 130.46 | 119.82 |
| 44 | G8 | 98 | VAL | N-CA-C | -10.35 | 102.56 | 112.29 |
| 31 | 51 | 7 | LEU | CA-C-N | -10.24 | 107.04 | 119.84 |
| 31 | 51 | 7 | LEU | C-N-CA | -10.24 | 107.04 | 119.84 |
| 41 | 95 | 21 | ARG | NE-CZ-NH1 | 10.01 | 131.51 | 121.50 |
| 44 | G8 | 93 | GLY | CA-C-O | -9.94 | 115.76 | 122.22 |
| 44 | G8 | 76 | CYS | CA-C-N | -9.74 | 107.66 | 119.84 |
| 44 | G8 | 76 | CYS | C-N-CA | -9.74 | 107.66 | 119.84 |
| 49 | L8 | 38 | GLU | N-CA-C | 9.64 | 123.44 | 108.12 |
| 28 | 29 | 26 | ILE | N-CA-C | 9.60 | 121.46 | 111.00 |
| 42 | E8 | 64 | MET | N-CA-C | 9.51 | 125.15 | 112.88 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed($^o$) | Ideal($^o$) |
|---|---|---|---|---|---|---|---|
| 12 | 3I | 115 | LYS | CA-C-N | -9.47 | 108.76 | 122.77 |
| 12 | 3I | 115 | LYS | C-N-CA | -9.47 | 108.76 | 122.77 |
| 27 | 19 | 272 | ALA | N-CA-C | 9.39 | 130.81 | 110.80 |
| 37 | 55 | 108 | GLY | N-CA-C | -9.37 | 102.73 | 114.92 |
| 28 | 29 | 73 | GLU | CA-C-N | 9.31 | 129.25 | 120.03 |
| 28 | 29 | 73 | GLU | C-N-CA | 9.31 | 129.25 | 120.03 |
| 47 | J8 | 89 | GLU | N-CA-C | -9.31 | 101.93 | 113.28 |
| 8 | 72 | 66 | GLY | CA-C-N | 9.25 | 129.33 | 119.89 |
| 8 | 72 | 66 | GLY | C-N-CA | 9.25 | 129.33 | 119.89 |
| 54 | Q8 | 58 | ILE | N-CA-C | -9.09 | 101.35 | 110.62 |
| 27 | 19 | 85 | ASP | CA-C-N | 9.09 | 128.72 | 119.82 |
| 27 | 19 | 85 | ASP | C-N-CA | 9.09 | 128.72 | 119.82 |
| 41 | 95 | 81 | TYR | N-CA-C | 8.99 | 121.94 | 109.18 |
| 36 | 45 | 89 | ASN | N-CA-C | 8.87 | 123.83 | 112.92 |
| 49 | L8 | 37 | LEU | CA-C-N | -8.84 | 110.05 | 121.98 |
| 49 | L8 | 37 | LEU | C-N-CA | -8.84 | 110.05 | 121.98 |
| 46 | E5 | 44 | ARG | N-CA-C | -8.75 | 100.92 | 111.69 |
| 41 | 95 | 49 | THR | N-CA-C | -8.74 | 97.33 | 110.01 |
| 1 | 1G | 1498 | U | C2'-C3'-O3' | 8.72 | 122.58 | 109.50 |
| 54 | M5 | 29 | LYS | N-CA-C | -8.64 | 102.28 | 113.17 |
| 4 | 3E | 28 | SER | CA-C-N | -8.64 | 108.78 | 120.96 |
| 4 | 3E | 28 | SER | C-N-CA | -8.64 | 108.78 | 120.96 |
| 4 | 3E | 12 | CYS | N-CA-C | -8.63 | 100.75 | 111.11 |
| 27 | 19 | 68 | LYS | CA-C-N | -8.63 | 108.54 | 122.26 |
| 27 | 19 | 68 | LYS | C-N-CA | -8.63 | 108.54 | 122.26 |
| 20 | BA | 12 | ALA | N-CA-C | -8.60 | 102.33 | 113.17 |
| 35 | 35 | 22 | GLY | CA-C-N | -8.59 | 110.01 | 119.98 |
| 35 | 35 | 22 | GLY | C-N-CA | -8.59 | 110.01 | 119.98 |
| 8 | 7E | 75 | ARG | CA-C-N | 8.58 | 130.56 | 119.84 |
| 8 | 7E | 75 | ARG | C-N-CA | 8.58 | 130.56 | 119.84 |
| 29 | 39 | 89 | VAL | CA-C-N | -8.50 | 111.05 | 123.11 |
| 29 | 39 | 89 | VAL | C-N-CA | -8.50 | 111.05 | 123.11 |
| 24 | 1H | 750 | A | OP1-P-O3' | -8.47 | 82.58 | 108.00 |
| 2 | 12 | 23 | ARG | N-CA-C | -8.43 | 102.55 | 113.17 |
| 39 | B8 | 19 | LEU | CA-C-N | 8.39 | 128.33 | 120.03 |
| 39 | B8 | 19 | LEU | C-N-CA | 8.39 | 128.33 | 120.03 |
| 29 | 39 | 68 | LYS | CA-C-N | -8.32 | 108.25 | 122.56 |
| 29 | 39 | 68 | LYS | C-N-CA | -8.32 | 108.25 | 122.56 |
| 39 | B8 | 13 | ARG | N-CA-C | -8.30 | 102.86 | 113.16 |
| 52 | O8 | 48 | VAL | N-CA-C | 8.28 | 118.84 | 110.23 |
| 4 | 3E | 9 | CYS | N-CA-C | -8.23 | 102.68 | 112.89 |
| 4 | 32 | 171 | GLY | CA-C-N | 8.19 | 128.96 | 119.47 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed($^o$) | Ideal($^o$) |
|---|---|---|---|---|---|---|---|
| 4 | 32 | 171 | GLY | C-N-CA | 8.19 | 128.96 | 119.47 |
| 29 | 39 | 69 | HIS | N-CA-C | 8.18 | 122.83 | 113.02 |
| 31 | 51 | 125 | VAL | CA-C-N | 8.15 | 130.02 | 119.84 |
| 31 | 51 | 125 | VAL | C-N-CA | 8.15 | 130.02 | 119.84 |
| 49 | L8 | 11 | SER | CA-C-N | 8.11 | 128.31 | 119.87 |
| 49 | L8 | 11 | SER | C-N-CA | 8.11 | 128.31 | 119.87 |
| 27 | 11 | 237 | GLU | CA-C-N | -8.01 | 113.78 | 120.98 |
| 27 | 11 | 237 | GLU | C-N-CA | -8.01 | 113.78 | 120.98 |
| 45 | H8 | 166 | SER | CA-C-N | -8.00 | 113.57 | 121.65 |
| 45 | H8 | 166 | SER | C-N-CA | -8.00 | 113.57 | 121.65 |
| 36 | 88 | 65 | PHE | N-CA-C | 7.97 | 123.31 | 113.50 |
| 39 | B8 | 76 | PHE | CA-C-N | 7.97 | 129.80 | 119.84 |
| 39 | B8 | 76 | PHE | C-N-CA | 7.97 | 129.80 | 119.84 |
| 29 | 39 | 83 | PHE | N-CA-C | 7.94 | 121.78 | 112.72 |
| 35 | 35 | 71 | VAL | CA-C-N | -7.93 | 111.62 | 119.87 |
| 35 | 35 | 71 | VAL | C-N-CA | -7.93 | 111.62 | 119.87 |
| 2 | 1E | 193 | ASP | CA-C-N | 7.92 | 129.73 | 119.84 |
| 2 | 1E | 193 | ASP | C-N-CA | 7.92 | 129.73 | 119.84 |
| 12 | 3I | 118 | SER | N-CA-C | -7.86 | 102.66 | 111.07 |
| 40 | C8 | 9 | VAL | N-CA-C | 7.85 | 118.40 | 110.23 |
| 48 | G5 | 17 | SER | N-CA-C | 7.83 | 127.12 | 109.81 |
| 48 | K8 | 5 | GLU | N-CA-C | -7.82 | 102.07 | 111.69 |
| 19 | AI | 65 | ASN | N-CA-C | -7.76 | 102.89 | 113.30 |
| 32 | 69 | 79 | ILE | CA-C-N | 7.75 | 127.51 | 119.76 |
| 32 | 69 | 79 | ILE | C-N-CA | 7.75 | 127.51 | 119.76 |
| 37 | 98 | 9 | LYS | CA-C-N | -7.72 | 111.11 | 123.23 |
| 37 | 98 | 9 | LYS | C-N-CA | -7.72 | 111.11 | 123.23 |
| 31 | 59 | 167 | GLU | CA-C-N | 7.71 | 129.48 | 119.84 |
| 31 | 59 | 167 | GLU | C-N-CA | 7.71 | 129.48 | 119.84 |
| 39 | 75 | 118 | ARG | N-CA-C | -7.71 | 103.32 | 112.89 |
| 10 | 1I | 76 | ASN | CA-C-N | 7.69 | 129.45 | 119.84 |
| 10 | 1I | 76 | ASN | C-N-CA | 7.69 | 129.45 | 119.84 |
| 8 | 7E | 100 | ILE | CA-C-N | 7.68 | 127.84 | 120.31 |
| 8 | 7E | 100 | ILE | C-N-CA | 7.68 | 127.84 | 120.31 |
| 4 | 32 | 30 | LYS | CA-C-N | -7.67 | 111.46 | 123.12 |
| 4 | 32 | 30 | LYS | C-N-CA | -7.67 | 111.46 | 123.12 |
| 41 | 95 | 80 | GLN | N-CA-C | 7.62 | 121.53 | 109.65 |
| 35 | 78 | 62 | LEU | CA-C-N | -7.59 | 112.66 | 120.85 |
| 35 | 78 | 62 | LEU | C-N-CA | -7.59 | 112.66 | 120.85 |
| 31 | 51 | 86 | GLU | N-CA-C | 7.57 | 119.43 | 111.03 |
| 4 | 3E | 31 | CYS | N-CA-C | -7.56 | 103.94 | 113.02 |
| 34 | 25 | 29 | ASN | N-CA-C | 7.56 | 122.22 | 112.92 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed($^o$) | Ideal($^o$) |
|---|---|---|---|---|---|---|---|
| 54 | M5 | 34 | TRP | N-CA-C | 7.56 | 122.51 | 107.62 |
| 35 | 78 | 144 | GLU | N-CA-C | 7.53 | 120.43 | 108.23 |
| 16 | 7I | 20 | VAL | N-CA-C | 7.52 | 119.17 | 108.42 |
| 46 | E5 | 22 | GLY | N-CA-C | 7.52 | 121.33 | 111.70 |
| 36 | 88 | 88 | GLY | N-CA-C | -7.49 | 95.44 | 113.18 |
| 31 | 51 | 54 | ARG | CA-C-N | 7.48 | 127.12 | 119.56 |
| 31 | 51 | 54 | ARG | C-N-CA | 7.48 | 127.12 | 119.56 |
| 36 | 88 | 87 | LYS | N-CA-C | -7.48 | 90.06 | 111.00 |
| 47 | J8 | 83 | GLU | N-CA-C | 7.46 | 119.74 | 107.73 |
| 38 | A8 | 111 | GLU | N-CA-C | 7.43 | 121.92 | 112.86 |
| 48 | G5 | 5 | GLU | N-CA-C | -7.43 | 104.22 | 113.28 |
| 44 | G8 | 89 | PHE | CB-CA-C | -7.42 | 108.00 | 116.54 |
| 45 | D5 | 157 | LEU | CA-C-N | -7.41 | 112.75 | 120.38 |
| 45 | D5 | 157 | LEU | C-N-CA | -7.41 | 112.75 | 120.38 |
| 28 | 21 | 58 | ARG | N-CA-C | -7.38 | 103.84 | 112.92 |
| 11 | 2I | 112 | THR | CA-C-N | 7.37 | 127.64 | 119.90 |
| 11 | 2I | 112 | THR | C-N-CA | 7.37 | 127.64 | 119.90 |
| 16 | 7A | 71 | ARG | N-CA-C | -7.34 | 102.98 | 112.23 |
| 32 | 61 | 79 | ILE | CA-C-N | 7.34 | 127.61 | 119.90 |
| 32 | 61 | 79 | ILE | C-N-CA | 7.34 | 127.61 | 119.90 |
| 35 | 78 | 37 | GLY | N-CA-C | -7.33 | 99.11 | 110.77 |
| 36 | 88 | 106 | VAL | N-CA-C | 7.32 | 119.53 | 109.80 |
| 1 | 13 | 1498 | U | C2'-C3'-O3' | 7.31 | 120.46 | 109.50 |
| 2 | 1E | 23 | ARG | N-CA-C | -7.30 | 104.25 | 113.02 |
| 31 | 59 | 116 | GLU | CA-C-N | 7.30 | 127.90 | 120.38 |
| 31 | 59 | 116 | GLU | C-N-CA | 7.30 | 127.90 | 120.38 |
| 28 | 21 | 77 | ILE | N-CA-C | -7.29 | 105.44 | 112.29 |
| 12 | 3I | 70 | ILE | CA-C-N | 7.29 | 127.21 | 119.85 |
| 12 | 3I | 70 | ILE | C-N-CA | 7.29 | 127.21 | 119.85 |
| 44 | G8 | 89 | PHE | N-CA-C | 7.27 | 119.37 | 108.31 |
| 27 | 19 | 194 | GLY | N-CA-C | -7.27 | 100.07 | 110.46 |
| 6 | 5E | 55 | ASP | CA-C-N | 7.25 | 126.92 | 119.82 |
| 6 | 5E | 55 | ASP | C-N-CA | 7.25 | 126.92 | 119.82 |
| 31 | 51 | 4 | ILE | N-CA-C | 7.23 | 119.53 | 109.55 |
| 10 | 1I | 38 | ILE | CA-C-N | 7.22 | 128.87 | 119.84 |
| 10 | 1I | 38 | ILE | C-N-CA | 7.22 | 128.87 | 119.84 |
| 36 | 88 | 106 | VAL | CB-CA-C | -7.21 | 101.33 | 111.28 |
| 2 | 12 | 10 | LEU | N-CA-C | -7.20 | 104.49 | 113.28 |
| 31 | 59 | 170 | ARG | N-CA-C | 7.20 | 117.75 | 108.24 |
| 28 | 21 | 14 | ILE | N-CA-C | 7.20 | 117.30 | 111.62 |
| 32 | 61 | 9 | LEU | N-CA-C | 7.17 | 122.13 | 112.88 |
| 18 | 9I | 18 | ARG | N-CA-C | 7.13 | 117.44 | 108.45 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed($^o$) | Ideal($^o$) |
|---|---|---|---|---|---|---|---|
| 5 | 42 | 127 | ASN | CA-C-N | 7.12 | 126.38 | 118.97 |
| 5 | 42 | 127 | ASN | C-N-CA | 7.12 | 126.38 | 118.97 |
| 24 | 1H | 2439 | A | C2'-C3'-O3' | 7.10 | 120.15 | 109.50 |
| 36 | 88 | 21 | THR | N-CA-C | 7.10 | 117.24 | 107.73 |
| 47 | J8 | 32 | LYS | N-CA-C | 7.10 | 120.00 | 110.35 |
| 28 | 21 | 2 | LYS | N-CA-C | 7.07 | 119.44 | 110.24 |
| 12 | 3A | 47 | LYS | CA-C-N | -7.07 | 111.00 | 119.84 |
| 12 | 3A | 47 | LYS | C-N-CA | -7.07 | 111.00 | 119.84 |
| 44 | G8 | 81 | LYS | CA-C-N | 7.07 | 143.96 | 127.00 |
| 44 | G8 | 81 | LYS | C-N-CA | 7.07 | 143.96 | 127.00 |
| 35 | 35 | 54 | GLY | N-CA-C | -7.06 | 104.76 | 114.64 |
| 35 | 78 | 42 | SER | CA-C-N | -7.04 | 112.16 | 119.98 |
| 35 | 78 | 42 | SER | C-N-CA | -7.04 | 112.16 | 119.98 |
| 54 | M5 | 31 | HIS | CB-CA-C | 7.04 | 124.42 | 110.42 |
| 27 | 11 | 223 | GLY | N-CA-C | -7.04 | 103.77 | 112.77 |
| 29 | 31 | 91 | GLY | CA-C-N | 7.02 | 127.44 | 119.93 |
| 29 | 31 | 91 | GLY | C-N-CA | 7.02 | 127.44 | 119.93 |
| 1 | 13 | 812 | C | C4'-C3'-O3' | 7.01 | 119.91 | 109.40 |
| 43 | F8 | 31 | HIS | CA-C-N | 6.98 | 126.61 | 119.56 |
| 43 | F8 | 31 | HIS | C-N-CA | 6.98 | 126.61 | 119.56 |
| 27 | 11 | 240 | ALA | CA-C-N | 6.97 | 128.55 | 119.84 |
| 27 | 11 | 240 | ALA | C-N-CA | 6.97 | 128.55 | 119.84 |
| 35 | 78 | 21 | ARG | N-CA-C | 6.97 | 125.65 | 110.80 |
| 1 | 13 | 974 | A | O4'-C1'-N9 | 6.95 | 118.93 | 108.50 |
| 52 | K5 | 14 | THR | N-CA-C | 6.95 | 119.81 | 108.55 |
| 35 | 78 | 71 | VAL | CA-C-N | -6.93 | 112.66 | 119.87 |
| 35 | 78 | 71 | VAL | C-N-CA | -6.93 | 112.66 | 119.87 |
| 31 | 59 | 124 | GLU | N-CA-C | 6.92 | 120.00 | 110.24 |
| 45 | D5 | 107 | THR | CA-C-N | -6.92 | 111.85 | 119.19 |
| 45 | D5 | 107 | THR | C-N-CA | -6.92 | 111.85 | 119.19 |
| 24 | 1H | 1799 | G | C2'-C3'-O3' | 6.92 | 119.88 | 109.50 |
| 5 | 4E | 67 | VAL | N-CA-C | 6.92 | 117.48 | 108.35 |
| 44 | G8 | 79 | CYS | N-CA-C | 6.92 | 125.53 | 110.80 |
| 1 | 1G | 812 | C | C2'-C3'-O3' | 6.89 | 119.84 | 109.50 |
| 41 | 95 | 37 | VAL | N-CA-C | 6.88 | 117.98 | 110.21 |
| 20 | BA | 73 | HIS | CB-CA-C | -6.88 | 107.61 | 115.79 |
| 24 | 1H | 1653 | G | C2'-C3'-O3' | 6.87 | 119.80 | 109.50 |
| 8 | 7E | 112 | LEU | N-CA-C | 6.86 | 119.64 | 108.26 |
| 27 | 11 | 245 | PRO | CA-C-N | 6.84 | 127.25 | 119.93 |
| 27 | 11 | 245 | PRO | C-N-CA | 6.84 | 127.25 | 119.93 |
| 24 | 1H | 2689 | U | C4'-C3'-O3' | 6.82 | 119.63 | 109.40 |
| 27 | 11 | 145 | VAL | N-CA-C | 6.81 | 118.65 | 108.23 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed($^o$) | Ideal($^o$) |
|---|---|---|---|---|---|---|---|
| 8 | 7E | 66 | GLY | CA-C-N | 6.81 | 126.72 | 119.85 |
| 8 | 7E | 66 | GLY | C-N-CA | 6.81 | 126.72 | 119.85 |
| 41 | 95 | 15 | GLU | CA-C-N | -6.79 | 113.31 | 120.03 |
| 41 | 95 | 15 | GLU | C-N-CA | -6.79 | 113.31 | 120.03 |
| 54 | M5 | 57 | ARG | N-CA-C | 6.76 | 118.34 | 110.97 |
| 35 | 35 | 36 | LYS | CB-CA-C | -6.76 | 106.88 | 116.34 |
| 35 | 78 | 116 | GLY | N-CA-C | 6.75 | 123.79 | 110.77 |
| 29 | 31 | 130 | ALA | CA-C-N | 6.74 | 127.04 | 120.98 |
| 29 | 31 | 130 | ALA | C-N-CA | 6.74 | 127.04 | 120.98 |
| 29 | 39 | 42 | ALA | N-CA-C | -6.73 | 96.46 | 110.80 |
| 28 | 29 | 68 | ALA | CA-C-N | 6.73 | 133.81 | 121.70 |
| 28 | 29 | 68 | ALA | C-N-CA | 6.73 | 133.81 | 121.70 |
| 31 | 51 | 38 | SER | CA-C-N | 6.72 | 126.51 | 119.05 |
| 31 | 51 | 38 | SER | C-N-CA | 6.72 | 126.51 | 119.05 |
| 24 | 14 | 2776 | A | C2'-C3'-O3' | 6.72 | 119.58 | 109.50 |
| 31 | 59 | 159 | GLU | N-CA-C | 6.71 | 117.93 | 108.00 |
| 1 | 1G | 812 | C | P-O3'-C3' | 6.69 | 130.23 | 120.20 |
| 7 | 6E | 118 | VAL | N-CA-C | -6.68 | 103.21 | 112.50 |
| 54 | M5 | 33 | ASN | N-CA-C | 6.68 | 125.03 | 110.80 |
| 11 | 2A | 112 | THR | CA-C-N | 6.68 | 128.19 | 119.84 |
| 11 | 2A | 112 | THR | C-N-CA | 6.68 | 128.19 | 119.84 |
| 27 | 19 | 75 | ILE | CA-C-N | -6.68 | 113.84 | 120.98 |
| 27 | 19 | 75 | ILE | C-N-CA | -6.68 | 113.84 | 120.98 |
| 27 | 19 | 154 | LYS | N-CA-C | 6.67 | 122.39 | 113.72 |
| 2 | 12 | 19 | HIS | N-CA-C | 6.67 | 118.99 | 108.79 |
| 45 | D5 | 174 | VAL | N-CA-C | 6.66 | 118.12 | 107.73 |
| 5 | 4E | 105 | VAL | CA-C-N | -6.65 | 112.85 | 119.56 |
| 5 | 4E | 105 | VAL | C-N-CA | -6.65 | 112.85 | 119.56 |
| 48 | K8 | 44 | LEU | N-CA-C | -6.64 | 104.80 | 113.17 |
| 32 | 61 | 110 | ASP | CA-C-N | 6.63 | 142.91 | 127.00 |
| 32 | 61 | 110 | ASP | C-N-CA | 6.63 | 142.91 | 127.00 |
| 29 | 31 | 135 | LYS | N-CA-C | -6.62 | 98.61 | 109.40 |
| 24 | 1H | 668 | G | OP2-P-O3' | -6.61 | 88.16 | 108.00 |
| 24 | 14 | 2611 | U | O5'-C5'-C4' | 6.61 | 121.42 | 111.50 |
| 48 | K8 | 6 | VAL | N-CA-C | 6.61 | 118.15 | 110.62 |
| 30 | 41 | 128 | ARG | N-CA-C | -6.60 | 104.80 | 112.92 |
| 41 | 95 | 33 | VAL | N-CA-C | 6.60 | 116.98 | 107.88 |
| 30 | 49 | 86 | MET | N-CA-C | 6.58 | 117.66 | 109.57 |
| 27 | 11 | 196 | VAL | N-CA-C | 6.57 | 117.32 | 110.62 |
| 27 | 11 | 105 | ILE | CA-C-N | -6.57 | 112.05 | 120.98 |
| 27 | 11 | 105 | ILE | C-N-CA | -6.57 | 112.05 | 120.98 |
| 4 | 3E | 39 | PRO | O-C-N | 6.57 | 124.23 | 121.15 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed($^o$) | Ideal($^o$) |
|---|---|---|---|---|---|---|---|
| 27 | 11 | 68 | LYS | CA-C-N | -6.57 | 111.71 | 122.54 |
| 27 | 11 | 68 | LYS | C-N-CA | -6.57 | 111.71 | 122.54 |
| 28 | 29 | 51 | PHE | N-CA-C | 6.56 | 124.77 | 110.80 |
| 44 | C5 | 103 | GLY | N-CA-C | 6.54 | 127.17 | 115.80 |
| 31 | 51 | 170 | ARG | N-CA-C | 6.53 | 120.05 | 109.40 |
| 54 | Q8 | 29 | LYS | CA-C-N | 6.53 | 133.46 | 121.70 |
| 54 | Q8 | 29 | LYS | C-N-CA | 6.53 | 133.46 | 121.70 |
| 30 | 41 | 31 | VAL | CA-C-N | 6.53 | 126.92 | 119.93 |
| 30 | 41 | 31 | VAL | C-N-CA | 6.53 | 126.92 | 119.93 |
| 24 | 1H | 222 | A | P-O3'-C3' | 6.50 | 129.95 | 120.20 |
| 12 | 3I | 105 | TYR | CB-CA-C | -6.50 | 109.09 | 116.63 |
| 44 | G8 | 81 | LYS | C-N-CD | -6.50 | 106.31 | 120.60 |
| 5 | 42 | 67 | VAL | N-CA-C | 6.49 | 118.05 | 108.45 |
| 28 | 29 | 44 | TYR | N-CA-C | 6.49 | 121.81 | 113.18 |
| 42 | A5 | 61 | ASN | N-CA-C | 6.49 | 119.67 | 111.69 |
| 39 | B8 | 80 | SER | N-CA-C | 6.48 | 117.54 | 109.57 |
| 40 | 85 | 94 | ASN | N-CA-C | -6.45 | 104.17 | 111.14 |
| 27 | 19 | 245 | PRO | CA-C-N | 6.45 | 126.83 | 119.93 |
| 27 | 19 | 245 | PRO | C-N-CA | 6.45 | 126.83 | 119.93 |
| 45 | D5 | 67 | LEU | CA-C-N | 6.43 | 127.88 | 119.84 |
| 45 | D5 | 67 | LEU | C-N-CA | 6.43 | 127.88 | 119.84 |
| 32 | 61 | 135 | GLU | N-CA-C | 6.43 | 116.72 | 108.24 |
| 28 | 29 | 38 | THR | CA-C-N | 6.42 | 126.92 | 119.47 |
| 28 | 29 | 38 | THR | C-N-CA | 6.42 | 126.92 | 119.47 |
| 2 | 12 | 17 | PHE | N-CA-C | 6.41 | 119.86 | 110.17 |
| 34 | 25 | 118 | ALA | CA-C-N | 6.41 | 126.10 | 119.56 |
| 34 | 25 | 118 | ALA | C-N-CA | 6.41 | 126.10 | 119.56 |
| 54 | M5 | 41 | ILE | N-CA-C | -6.41 | 96.01 | 109.34 |
| 20 | BA | 75 | ASN | N-CA-C | -6.41 | 105.10 | 113.17 |
| 48 | K8 | 14 | ARG | N-CA-C | -6.40 | 102.09 | 110.53 |
| 24 | 14 | 1022 | G | C2'-C3'-O3' | 6.40 | 119.10 | 109.50 |
| 53 | L5 | 6 | GLN | CA-C-N | 6.38 | 126.73 | 119.83 |
| 53 | L5 | 6 | GLN | C-N-CA | 6.38 | 126.73 | 119.83 |
| 27 | 11 | 259 | THR | N-CA-C | 6.38 | 121.34 | 113.50 |
| 28 | 29 | 61 | ARG | CA-C-N | -6.37 | 113.97 | 120.85 |
| 28 | 29 | 61 | ARG | C-N-CA | -6.37 | 113.97 | 120.85 |
| 24 | 14 | 1786 | A | N9-C1'-C2' | 6.37 | 123.55 | 114.00 |
| 28 | 21 | 73 | GLU | CA-C-N | 6.36 | 126.33 | 120.03 |
| 28 | 21 | 73 | GLU | C-N-CA | 6.36 | 126.33 | 120.03 |
| 36 | 45 | 26 | TYR | N-CA-C | 6.36 | 119.97 | 112.72 |
| 31 | 51 | 56 | SER | N-CA-C | 6.36 | 116.96 | 108.38 |
| 34 | 25 | 71 | ARG | CA-C-N | 6.36 | 126.05 | 119.82 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed($^o$) | Ideal($^o$) |
|---|---|---|---|---|---|---|---|
| 34 | 25 | 71 | ARG | C-N-CA | 6.36 | 126.05 | 119.82 |
| 19 | AI | 8 | GLY | N-CA-C | 6.35 | 123.42 | 114.85 |
| 31 | 51 | 87 | LEU | N-CA-C | 6.34 | 124.31 | 110.80 |
| 41 | 95 | 37 | VAL | CB-CA-C | -6.32 | 104.37 | 111.45 |
| 33 | 58 | 69 | GLN | N-CA-C | 6.32 | 118.17 | 111.28 |
| 28 | 29 | 137 | HIS | N-CA-C | 6.32 | 119.86 | 110.39 |
| 35 | 35 | 33 | ARG | N-CA-C | -6.31 | 105.58 | 113.28 |
| 27 | 11 | 13 | ARG | N-CA-C | -6.31 | 105.06 | 112.89 |
| 39 | 75 | 5 | ALA | N-CA-C | -6.30 | 97.38 | 110.80 |
| 47 | F5 | 29 | GLY | N-CA-C | 6.29 | 122.78 | 112.84 |
| 32 | 61 | 131 | LYS | C-N-CD | -6.28 | 106.78 | 120.60 |
| 24 | 1H | 1786 | A | N9-C1'-C2' | 6.27 | 123.41 | 114.00 |
| 27 | 19 | 273 | ARG | N-CA-C | 6.27 | 124.16 | 110.80 |
| 29 | 39 | 4 | VAL | N-CA-C | 6.26 | 116.40 | 106.88 |
| 24 | 1H | 138 | G | N9-C1'-C2' | 6.23 | 121.34 | 112.00 |
| 44 | C5 | 80 | GLY | N-CA-C | 6.22 | 123.35 | 114.64 |
| 7 | 62 | 13 | GLN | CA-C-N | 6.22 | 126.57 | 119.92 |
| 7 | 62 | 13 | GLN | C-N-CA | 6.22 | 126.57 | 119.92 |
| 39 | B8 | 36 | GLU | N-CA-C | 6.21 | 118.18 | 110.91 |
| 24 | 14 | 654(S) | G | P-O3'-C3' | 6.21 | 127.15 | 119.70 |
| 8 | 7E | 71 | GLY | CA-C-N | -6.20 | 114.25 | 120.21 |
| 8 | 7E | 71 | GLY | C-N-CA | -6.20 | 114.25 | 120.21 |
| 20 | BI | 9 | ASN | N-CA-C | 6.20 | 116.62 | 107.88 |
| 35 | 35 | 36 | LYS | N-CA-C | 6.20 | 117.17 | 108.00 |
| 45 | D5 | 14 | LYS | CA-C-N | 6.19 | 125.88 | 119.56 |
| 45 | D5 | 14 | LYS | C-N-CA | 6.19 | 125.88 | 119.56 |
| 5 | 4E | 48 | ALA | CA-C-N | 6.19 | 126.65 | 119.47 |
| 5 | 4E | 48 | ALA | C-N-CA | 6.19 | 126.65 | 119.47 |
| 35 | 35 | 139 | LYS | N-CA-C | -6.19 | 104.99 | 112.54 |
| 34 | 68 | 90 | GLN | N-CA-C | -6.18 | 105.60 | 113.02 |
| 44 | C5 | 41 | GLY | N-CA-C | -6.18 | 103.85 | 112.13 |
| 27 | 11 | 220 | HIS | CA-C-N | -6.18 | 114.08 | 122.91 |
| 27 | 11 | 220 | HIS | C-N-CA | -6.18 | 114.08 | 122.91 |
| 33 | 15 | 2 | LYS | N-CA-C | 6.17 | 120.43 | 113.02 |
| 3 | 22 | 4 | LYS | N-CA-C | 6.17 | 118.74 | 110.35 |
| 27 | 11 | 242 | ARG | N-CA-C | -6.17 | 104.10 | 111.69 |
| 43 | B5 | 3 | THR | N-CA-C | 6.17 | 117.94 | 109.18 |
| 31 | 59 | 7 | LEU | N-CA-C | 6.15 | 122.00 | 113.45 |
| 35 | 35 | 96 | THR | CA-C-N | -6.14 | 113.24 | 120.11 |
| 35 | 35 | 96 | THR | C-N-CA | -6.14 | 113.24 | 120.11 |
| 22 | 2K | 34 | U | C2'-C3'-O3' | 6.13 | 122.90 | 113.70 |
| 19 | AA | 75 | ALA | CA-C-N | 6.13 | 126.34 | 119.90 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed($^o$) | Ideal($^o$) |
|---|---|---|---|---|---|---|---|
| 19 | AA | 75 | ALA | C-N-CA | 6.13 | 126.34 | 119.90 |
| 52 | K5 | 24 | GLU | N-CA-C | 6.13 | 117.07 | 108.00 |
| 37 | 98 | 80 | PHE | N-CA-C | 6.12 | 117.62 | 111.07 |
| 44 | C5 | 79 | CYS | N-CA-C | 6.12 | 123.83 | 110.80 |
| 51 | N8 | 3 | LYS | N-CA-C | 6.11 | 119.33 | 107.71 |
| 41 | D8 | 44 | LYS | CB-CA-C | -6.11 | 107.79 | 116.34 |
| 52 | K5 | 40 | CYS | CA-C-N | 6.11 | 126.29 | 120.31 |
| 52 | K5 | 40 | CYS | C-N-CA | 6.11 | 126.29 | 120.31 |
| 29 | 31 | 74 | ARG | CG-CD-NE | 6.10 | 125.42 | 112.00 |
| 39 | B8 | 55 | ASN | N-CA-C | 6.10 | 121.47 | 113.30 |
| 33 | 58 | 46 | VAL | N-CA-C | 6.09 | 116.80 | 111.56 |
| 38 | A8 | 60 | GLY | N-CA-C | 6.09 | 127.60 | 113.18 |
| 35 | 35 | 46 | LYS | CA-C-N | -6.08 | 106.96 | 121.80 |
| 35 | 35 | 46 | LYS | C-N-CA | -6.08 | 106.96 | 121.80 |
| 35 | 78 | 19 | VAL | N-CA-C | -6.08 | 100.28 | 108.06 |
| 11 | 2A | 34 | ASP | CA-C-N | -6.08 | 113.55 | 119.87 |
| 11 | 2A | 34 | ASP | C-N-CA | -6.08 | 113.55 | 119.87 |
| 29 | 31 | 177 | ALA | CA-C-N | -6.06 | 112.77 | 119.19 |
| 29 | 31 | 177 | ALA | C-N-CA | -6.06 | 112.77 | 119.19 |
| 51 | J5 | 46 | CYS | CA-C-N | 6.06 | 125.68 | 119.56 |
| 51 | J5 | 46 | CYS | C-N-CA | 6.06 | 125.68 | 119.56 |
| 32 | 61 | 131 | LYS | CA-C-N | 6.05 | 141.53 | 127.00 |
| 32 | 61 | 131 | LYS | C-N-CA | 6.05 | 141.53 | 127.00 |
| 44 | C5 | 86 | ARG | N-CA-C | 6.05 | 118.72 | 110.55 |
| 44 | G8 | 83 | THR | N-CA-C | -6.05 | 97.92 | 110.80 |
| 26 | 79 | 219 | GLY | CA-C-N | 6.04 | 127.39 | 119.84 |
| 26 | 79 | 219 | GLY | C-N-CA | 6.04 | 127.39 | 119.84 |
| 18 | 9A | 24 | ALA | N-CA-C | -6.04 | 105.56 | 113.17 |
| 4 | 3E | 165 | MET | CA-C-N | -6.04 | 114.46 | 122.85 |
| 4 | 3E | 165 | MET | C-N-CA | -6.04 | 114.46 | 122.85 |
| 27 | 11 | 227 | ASN | CA-C-N | -6.04 | 112.64 | 119.28 |
| 27 | 11 | 227 | ASN | C-N-CA | -6.04 | 112.64 | 119.28 |
| 39 | 75 | 80 | SER | CA-C-N | 6.03 | 125.51 | 119.24 |
| 39 | 75 | 80 | SER | C-N-CA | 6.03 | 125.51 | 119.24 |
| 8 | 7E | 71 | GLY | N-CA-C | -6.03 | 100.04 | 112.34 |
| 31 | 59 | 84 | SER | N-CA-C | 6.03 | 116.92 | 108.00 |
| 24 | 14 | 2439 | A | P-O3'-C3' | 6.03 | 129.24 | 120.20 |
| 41 | 95 | 21 | ARG | CG-CD-NE | 6.03 | 125.26 | 112.00 |
| 44 | G8 | 42 | VAL | CA-C-N | -6.02 | 114.56 | 123.11 |
| 44 | G8 | 42 | VAL | C-N-CA | -6.02 | 114.56 | 123.11 |
| 37 | 98 | 90 | ARG | CA-C-N | -6.02 | 113.48 | 122.74 |
| 37 | 98 | 90 | ARG | C-N-CA | -6.02 | 113.48 | 122.74 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed($^o$) | Ideal($^o$) |
|---|---|---|---|---|---|---|---|
| 28 | 29 | 188 | VAL | CA-C-N | 6.02 | 127.36 | 119.84 |
| 28 | 29 | 188 | VAL | C-N-CA | 6.02 | 127.36 | 119.84 |
| 2 | 1E | 200 | ILE | N-CA-C | 6.01 | 117.13 | 108.48 |
| 13 | 4I | 106 | ASN | N-CA-C | 6.01 | 119.68 | 111.39 |
| 27 | 11 | 16 | MET | CB-CG-SD | -6.01 | 94.67 | 112.70 |
| 31 | 51 | 20 | ALA | CA-C-N | -6.00 | 112.30 | 118.85 |
| 31 | 51 | 20 | ALA | C-N-CA | -6.00 | 112.30 | 118.85 |
| 13 | 4A | 112 | GLY | CA-C-N | 6.00 | 126.01 | 119.89 |
| 13 | 4A | 112 | GLY | C-N-CA | 6.00 | 126.01 | 119.89 |
| 42 | A5 | 77 | ASP | N-CA-C | -6.00 | 100.84 | 110.14 |
| 5 | 42 | 103 | GLY | N-CA-C | -6.00 | 104.54 | 112.82 |
| 39 | B8 | 80 | SER | CA-C-N | 5.99 | 127.32 | 119.84 |
| 39 | B8 | 80 | SER | C-N-CA | 5.99 | 127.32 | 119.84 |
| 10 | 1A | 60 | ARG | N-CA-C | 5.98 | 119.33 | 109.94 |
| 11 | 2A | 114 | VAL | CA-C-N | 5.97 | 126.47 | 120.14 |
| 11 | 2A | 114 | VAL | C-N-CA | 5.97 | 126.47 | 120.14 |
| 24 | 1H | 1899 | G | C8-N9-C1' | 5.97 | 144.91 | 127.00 |
| 24 | 1H | 752 | A | C4'-C3'-O3' | 5.95 | 118.33 | 109.40 |
| 54 | M5 | 39 | LYS | N-CA-C | -5.95 | 101.67 | 110.48 |
| 45 | D5 | 82 | ARG | CA-C-N | 5.94 | 126.14 | 119.90 |
| 45 | D5 | 82 | ARG | C-N-CA | 5.94 | 126.14 | 119.90 |
| 32 | 61 | 110 | ASP | C-N-CD | -5.93 | 107.55 | 120.60 |
| 14 | 5I | 25 | VAL | N-CA-C | -5.92 | 105.99 | 112.80 |
| 41 | 95 | 49 | THR | CA-C-N | -5.92 | 112.44 | 119.84 |
| 41 | 95 | 49 | THR | C-N-CA | -5.92 | 112.44 | 119.84 |
| 45 | H8 | 52 | SER | N-CA-C | 5.92 | 118.42 | 111.02 |
| 27 | 19 | 244 | ARG | CA-C-N | -5.91 | 114.29 | 120.38 |
| 27 | 19 | 244 | ARG | C-N-CA | -5.91 | 114.29 | 120.38 |
| 50 | I5 | 40 | HIS | CA-C-N | -5.91 | 113.87 | 120.14 |
| 50 | I5 | 40 | HIS | C-N-CA | -5.91 | 113.87 | 120.14 |
| 24 | 1H | 1427 | A | C4'-C3'-O3' | 5.91 | 118.27 | 109.40 |
| 46 | I8 | 11 | ARG | N-CA-C | -5.91 | 106.07 | 113.28 |
| 39 | 75 | 28 | VAL | N-CA-C | 5.91 | 118.70 | 108.90 |
| 27 | 11 | 270 | ILE | N-CA-C | 5.90 | 117.08 | 108.53 |
| 24 | 14 | 1427 | A | P-O3'-C3' | 5.89 | 129.04 | 120.20 |
| 4 | 3E | 168 | ARG | N-CA-C | 5.88 | 119.14 | 109.72 |
| 12 | 3A | 64 | TYR | N-CA-C | 5.88 | 117.50 | 111.14 |
| 26 | 79 | 173 | ALA | CA-C-N | 5.88 | 126.08 | 119.90 |
| 26 | 79 | 173 | ALA | C-N-CA | 5.88 | 126.08 | 119.90 |
| 27 | 11 | 73 | VAL | CB-CA-C | -5.88 | 101.64 | 111.29 |
| 44 | C5 | 82 | PRO | N-CA-C | 5.88 | 120.56 | 111.21 |
| 35 | 78 | 49 | ARG | CG-CD-NE | 5.88 | 124.93 | 112.00 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed($^o$) | Ideal($^o$) |
|---|---|---|---|---|---|---|---|
| 29 | 39 | 78 | ILE | CA-C-N | -5.88 | 113.52 | 122.28 |
| 29 | 39 | 78 | ILE | C-N-CA | -5.88 | 113.52 | 122.28 |
| 28 | 21 | 116 | VAL | N-CA-C | -5.87 | 101.12 | 109.51 |
| 4 | 32 | 33 | MET | N-CA-C | -5.87 | 102.08 | 110.59 |
| 27 | 11 | 46 | GLN | N-CA-C | -5.86 | 100.64 | 109.79 |
| 29 | 39 | 170 | LEU | CA-C-N | 5.86 | 126.26 | 119.47 |
| 29 | 39 | 170 | LEU | C-N-CA | 5.86 | 126.26 | 119.47 |
| 44 | C5 | 39 | VAL | N-CA-C | 5.85 | 115.25 | 106.42 |
| 38 | 65 | 41 | ASP | CA-C-N | -5.85 | 114.12 | 122.77 |
| 38 | 65 | 41 | ASP | C-N-CA | -5.85 | 114.12 | 122.77 |
| 36 | 45 | 126 | PRO | CA-C-O | -5.85 | 116.98 | 121.31 |
| 1 | 1G | 1346 | A | P-O3'-C3' | 5.84 | 128.96 | 120.20 |
| 4 | 32 | 188 | LEU | CA-C-N | 5.84 | 127.14 | 119.84 |
| 4 | 32 | 188 | LEU | C-N-CA | 5.84 | 127.14 | 119.84 |
| 8 | 7E | 55 | GLY | N-CA-C | -5.84 | 107.74 | 114.69 |
| 44 | C5 | 83 | THR | N-CA-C | -5.83 | 101.33 | 110.36 |
| 24 | 1H | 222 | A | C2'-C3'-O3' | 5.82 | 118.23 | 109.50 |
| 38 | 65 | 87 | PHE | N-CA-C | 5.81 | 117.77 | 108.41 |
| 10 | 1I | 33 | GLN | N-CA-C | 5.81 | 118.43 | 110.24 |
| 41 | D8 | 65 | GLY | N-CA-C | 5.81 | 118.42 | 110.69 |
| 14 | 5A | 39 | LEU | N-CA-C | 5.81 | 118.94 | 110.17 |
| 31 | 59 | 84 | SER | CB-CA-C | -5.80 | 108.21 | 116.34 |
| 33 | 58 | 130 | HIS | N-CA-C | 5.80 | 120.48 | 113.17 |
| 19 | AI | 6 | LYS | N-CA-C | 5.79 | 118.47 | 109.60 |
| 31 | 59 | 83 | TYR | N-CA-C | 5.79 | 115.50 | 107.73 |
| 44 | C5 | 49 | VAL | N-CA-C | -5.79 | 104.71 | 110.62 |
| 24 | 1H | 2506 | U | P-O3'-C3' | 5.79 | 128.89 | 120.20 |
| 45 | D5 | 56 | VAL | N-CA-C | 5.79 | 116.92 | 108.53 |
| 45 | D5 | 85 | HIS | N-CA-C | 5.79 | 117.90 | 108.76 |
| 35 | 35 | 88 | LEU | CA-C-N | -5.78 | 114.15 | 123.23 |
| 35 | 35 | 88 | LEU | C-N-CA | -5.78 | 114.15 | 123.23 |
| 12 | 3A | 29 | GLY | N-CA-C | -5.78 | 105.60 | 115.08 |
| 46 | E5 | 35 | ASN | CA-C-N | -5.77 | 114.66 | 122.91 |
| 46 | E5 | 35 | ASN | C-N-CA | -5.77 | 114.66 | 122.91 |
| 54 | M5 | 34 | TRP | CA-C-N | 5.77 | 131.88 | 122.65 |
| 54 | M5 | 34 | TRP | C-N-CA | 5.77 | 131.88 | 122.65 |
| 2 | 12 | 11 | LEU | N-CA-C | -5.77 | 104.68 | 110.97 |
| 10 | 1I | 52 | GLY | CA-C-N | 5.76 | 125.45 | 119.05 |
| 10 | 1I | 52 | GLY | C-N-CA | 5.76 | 125.45 | 119.05 |
| 51 | N8 | 5 | PRO | N-CA-C | 5.76 | 123.11 | 113.78 |
| 17 | 8I | 67 | LYS | N-CA-C | -5.74 | 102.80 | 110.55 |
| 45 | H8 | 120 | ILE | N-CA-C | 5.74 | 115.90 | 107.75 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed($^o$) | Ideal($^o$) |
|---|---|---|---|---|---|---|---|
| 24 | 1H | 2712 | U | P-O3'-C3' | 5.74 | 126.59 | 119.70 |
| 1 | 1G | 197 | A | P-O3'-C3' | 5.74 | 128.81 | 120.20 |
| 30 | 49 | 31 | VAL | CA-C-N | 5.73 | 125.75 | 119.90 |
| 30 | 49 | 31 | VAL | C-N-CA | 5.73 | 125.75 | 119.90 |
| 1 | 1G | 115 | G | C4'-C3'-O3' | 5.73 | 118.00 | 109.40 |
| 28 | 29 | 50 | GLY | N-CA-C | 5.73 | 126.76 | 113.18 |
| 24 | 14 | 784 | A | C4'-C3'-O3' | -5.72 | 104.41 | 113.00 |
| 27 | 11 | 118 | VAL | N-CA-C | 5.72 | 115.88 | 107.75 |
| 33 | 58 | 94 | HIS | CA-C-N | 5.72 | 126.99 | 119.84 |
| 33 | 58 | 94 | HIS | C-N-CA | 5.72 | 126.99 | 119.84 |
| 4 | 3E | 167 | GLY | N-CA-C | -5.72 | 99.63 | 113.18 |
| 35 | 35 | 147 | LEU | CA-CB-CG | 5.71 | 136.30 | 116.30 |
| 24 | 14 | 2346 | A | O4'-C1'-N9 | 5.71 | 116.76 | 108.20 |
| 28 | 29 | 90 | THR | N-CA-C | 5.71 | 118.15 | 111.02 |
| 32 | 69 | 114 | LEU | N-CA-C | 5.71 | 119.42 | 112.23 |
| 24 | 1H | 1653 | G | P-O3'-C3' | 5.70 | 128.75 | 120.20 |
| 24 | 1H | 1265 | A | O5'-P-OP1 | -5.70 | 90.91 | 108.00 |
| 24 | 14 | 2430 | A | O5'-P-OP2 | -5.70 | 90.91 | 108.00 |
| 9 | 82 | 17 | VAL | N-CA-C | 5.69 | 115.80 | 107.37 |
| 27 | 11 | 244 | ARG | CA-C-N | -5.68 | 114.53 | 120.38 |
| 27 | 11 | 244 | ARG | C-N-CA | -5.68 | 114.53 | 120.38 |
| 1 | 1G | 632 | A | P-O3'-C3' | 5.68 | 128.72 | 120.20 |
| 17 | 8A | 29 | HIS | CA-C-N | 5.68 | 126.94 | 119.84 |
| 17 | 8A | 29 | HIS | C-N-CA | 5.68 | 126.94 | 119.84 |
| 40 | 85 | 3 | ARG | CA-C-N | -5.68 | 114.95 | 122.85 |
| 40 | 85 | 3 | ARG | C-N-CA | -5.68 | 114.95 | 122.85 |
| 35 | 78 | 59 | LEU | N-CA-C | -5.68 | 103.15 | 110.19 |
| 27 | 19 | 259 | THR | N-CA-C | 5.68 | 120.36 | 113.38 |
| 26 | 79 | 64 | LEU | CA-C-N | 5.67 | 125.35 | 119.05 |
| 26 | 79 | 64 | LEU | C-N-CA | 5.67 | 125.35 | 119.05 |
| 31 | 51 | 89 | ILE | N-CA-C | 5.67 | 116.91 | 108.23 |
| 24 | 14 | 917 | A | O5'-P-OP1 | -5.67 | 90.99 | 108.00 |
| 36 | 88 | 103 | MET | N-CA-C | -5.66 | 101.82 | 110.14 |
| 44 | G8 | 80 | GLY | CA-C-O | 5.66 | 124.98 | 119.27 |
| 35 | 35 | 51 | PHE | N-CA-C | 5.65 | 118.44 | 109.96 |
| 49 | L8 | 9 | VAL | N-CA-C | 5.65 | 118.32 | 112.90 |
| 47 | J8 | 64 | ALA | N-CA-C | -5.65 | 105.27 | 111.82 |
| 31 | 59 | 171 | LEU | N-CA-C | 5.64 | 122.82 | 110.80 |
| 31 | 59 | 153 | LYS | CB-CA-C | -5.64 | 107.20 | 111.20 |
| 37 | 98 | 109 | ALA | CA-C-N | 5.64 | 125.96 | 119.93 |
| 37 | 98 | 109 | ALA | C-N-CA | 5.64 | 125.96 | 119.93 |
| 24 | 1H | 567 | A | O5'-P-OP1 | -5.63 | 91.10 | 108.00 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed($^o$) | Ideal($^o$) |
|---|---|---|---|---|---|---|---|
| 47 | F5 | 79 | GLY | N-CA-C | 5.62 | 126.50 | 113.18 |
| 47 | F5 | 82 | LEU | N-CA-C | 5.62 | 117.29 | 109.31 |
| 31 | 51 | 28 | GLY | CA-C-N | 5.62 | 126.86 | 119.84 |
| 31 | 51 | 28 | GLY | C-N-CA | 5.62 | 126.86 | 119.84 |
| 27 | 19 | 49 | ILE | N-CA-CB | 5.62 | 117.06 | 110.82 |
| 24 | 1H | 1204 | A | N9-C1'-C2' | 5.62 | 122.42 | 114.00 |
| 16 | 7A | 27 | LYS | N-CA-C | -5.61 | 103.23 | 110.19 |
| 1 | 1G | 1498 | U | P-O3'-C3' | 5.61 | 128.61 | 120.20 |
| 27 | 19 | 43 | ARG | CG-CD-NE | 5.61 | 124.34 | 112.00 |
| 24 | 14 | 1252 | G | O4'-C1'-N9 | -5.61 | 99.79 | 108.20 |
| 24 | 1H | 2212 | A | C2'-C3'-O3' | 5.60 | 117.90 | 109.50 |
| 24 | 14 | 2307 | G | O4'-C1'-N9 | 5.60 | 116.89 | 108.50 |
| 44 | G8 | 17 | SER | N-CA-C | 5.60 | 117.58 | 109.07 |
| 5 | 4E | 18 | ARG | N-CA-C | -5.59 | 101.69 | 110.36 |
| 33 | 15 | 47 | ALA | N-CA-C | 5.59 | 117.45 | 110.91 |
| 32 | 61 | 122 | GLU | CB-CA-C | -5.59 | 108.51 | 115.89 |
| 36 | 88 | 24 | GLY | N-CA-C | -5.59 | 102.06 | 111.73 |
| 28 | 21 | 131 | ALA | CB-CA-C | -5.59 | 109.63 | 117.23 |
| 38 | 65 | 90 | GLY | CA-C-N | 5.58 | 125.68 | 119.87 |
| 38 | 65 | 90 | GLY | C-N-CA | 5.58 | 125.68 | 119.87 |
| 35 | 78 | 45 | LEU | N-CA-C | 5.58 | 118.51 | 109.86 |
| 28 | 21 | 84 | PHE | CA-C-N | -5.58 | 116.40 | 123.15 |
| 28 | 21 | 84 | PHE | C-N-CA | -5.58 | 116.40 | 123.15 |
| 36 | 88 | 33 | GLY | N-CA-C | 5.58 | 121.47 | 111.03 |
| 32 | 69 | 131 | LYS | CA-C-N | 5.58 | 140.38 | 127.00 |
| 32 | 69 | 131 | LYS | C-N-CA | 5.58 | 140.38 | 127.00 |
| 14 | 5I | 53 | LEU | CA-C-N | 5.57 | 125.89 | 119.93 |
| 14 | 5I | 53 | LEU | C-N-CA | 5.57 | 125.89 | 119.93 |
| 24 | 1H | 444 | C | O5'-P-OP1 | 5.55 | 124.65 | 108.00 |
| 51 | N8 | 40 | LYS | CA-C-N | -5.54 | 114.67 | 120.38 |
| 51 | N8 | 40 | LYS | C-N-CA | -5.54 | 114.67 | 120.38 |
| 7 | 6E | 111 | ARG | CA-C-N | 5.54 | 125.16 | 119.56 |
| 7 | 6E | 111 | ARG | C-N-CA | 5.54 | 125.16 | 119.56 |
| 33 | 15 | 46 | VAL | N-CA-C | 5.54 | 117.46 | 111.58 |
| 41 | 95 | 44 | LYS | CB-CA-C | -5.54 | 109.20 | 115.79 |
| 4 | 3E | 171 | GLY | CA-C-N | 5.54 | 125.63 | 119.32 |
| 4 | 3E | 171 | GLY | C-N-CA | 5.54 | 125.63 | 119.32 |
| 39 | B8 | 56 | GLY | N-CA-C | -5.54 | 100.06 | 113.18 |
| 44 | G8 | 52 | SER | CA-C-N | 5.54 | 126.76 | 119.84 |
| 44 | G8 | 52 | SER | C-N-CA | 5.54 | 126.76 | 119.84 |
| 42 | A5 | 72 | LYS | N-CA-C | -5.54 | 105.33 | 111.36 |
| 12 | 3A | 6 | THR | N-CA-C | -5.53 | 101.00 | 109.41 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed($^o$) | Ideal($^o$) |
|---|---|---|---|---|---|---|---|
| 24 | 1H | 2439 | A | P-O3'-C3' | 5.53 | 128.50 | 120.20 |
| 1 | 1G | 913 | A | C2'-C3'-O3' | 5.53 | 117.79 | 109.50 |
| 27 | 11 | 111 | LEU | CA-CB-CG | 5.52 | 135.60 | 116.30 |
| 45 | H8 | 86 | VAL | CA-C-N | -5.51 | 114.25 | 122.74 |
| 45 | H8 | 86 | VAL | C-N-CA | -5.51 | 114.25 | 122.74 |
| 29 | 39 | 106 | ARG | N-CA-C | -5.51 | 105.19 | 111.14 |
| 48 | K8 | 6 | VAL | CB-CA-C | -5.50 | 104.83 | 112.04 |
| 4 | 3E | 44 | GLY | N-CA-C | 5.50 | 119.54 | 112.83 |
| 19 | AI | 64 | GLU | N-CA-C | 5.50 | 117.98 | 107.75 |
| 32 | 69 | 120 | ILE | N-CA-C | 5.50 | 115.64 | 110.30 |
| 38 | 65 | 5 | THR | N-CA-C | 5.50 | 117.42 | 110.33 |
| 31 | 51 | 89 | ILE | CB-CA-C | -5.50 | 104.31 | 110.96 |
| 27 | 19 | 31 | LYS | CA-C-O | -5.49 | 114.98 | 120.96 |
| 27 | 11 | 32 | SER | CA-CB-OG | -5.48 | 100.13 | 111.10 |
| 36 | 88 | 10 | ARG | N-CA-C | -5.48 | 103.15 | 110.55 |
| 9 | 82 | 48 | GLU | CA-C-N | -5.48 | 113.25 | 119.28 |
| 9 | 82 | 48 | GLU | C-N-CA | -5.48 | 113.25 | 119.28 |
| 31 | 59 | 159 | GLU | CB-CA-C | -5.48 | 108.67 | 116.34 |
| 36 | 88 | 86 | GLY | CA-C-N | 5.47 | 131.55 | 121.70 |
| 36 | 88 | 86 | GLY | C-N-CA | 5.47 | 131.55 | 121.70 |
| 23 | 4K | 13 | A | C2'-C3'-O3' | 5.46 | 117.69 | 109.50 |
| 31 | 59 | 157 | TYR | N-CA-C | -5.45 | 104.75 | 111.40 |
| 46 | E5 | 11 | ARG | CA-C-N | -5.44 | 115.11 | 122.95 |
| 46 | E5 | 11 | ARG | C-N-CA | -5.44 | 115.11 | 122.95 |
| 5 | 42 | 11 | ILE | N-CA-C | 5.44 | 116.10 | 110.82 |
| 31 | 51 | 153 | LYS | CA-C-N | 5.43 | 125.74 | 119.93 |
| 31 | 51 | 153 | LYS | C-N-CA | 5.43 | 125.74 | 119.93 |
| 29 | 31 | 80 | ALA | CA-C-N | 5.43 | 126.63 | 119.84 |
| 29 | 31 | 80 | ALA | C-N-CA | 5.43 | 126.63 | 119.84 |
| 27 | 19 | 211 | ARG | N-CA-C | -5.43 | 105.52 | 111.82 |
| 4 | 32 | 188 | LEU | N-CA-C | 5.42 | 116.50 | 109.72 |
| 54 | M5 | 33 | ASN | CB-CA-C | -5.42 | 99.64 | 110.42 |
| 39 | B8 | 59 | THR | N-CA-C | -5.41 | 102.38 | 110.23 |
| 24 | 1H | 2689 | U | P-O3'-C3' | 5.41 | 128.31 | 120.20 |
| 38 | 65 | 34 | HIS | N-CA-C | 5.41 | 118.08 | 109.81 |
| 38 | A8 | 37 | ALA | N-CA-C | 5.40 | 117.15 | 107.80 |
| 12 | 3A | 13 | LYS | N-CA-C | 5.40 | 120.03 | 113.38 |
| 27 | 11 | 216 | GLY | N-CA-C | -5.40 | 107.82 | 115.43 |
| 19 | AA | 58 | VAL | N-CA-C | 5.40 | 112.47 | 107.56 |
| 6 | 52 | 95 | GLU | CA-C-N | 5.40 | 126.59 | 119.84 |
| 6 | 52 | 95 | GLU | C-N-CA | 5.40 | 126.59 | 119.84 |
| 16 | 7A | 80 | PHE | N-CA-C | 5.40 | 118.33 | 111.69 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed($^o$) | Ideal($^o$) |
|---|---|---|---|---|---|---|---|
| 24 | 1H | 2238 | G | OP1-P-OP2 | 5.39 | 135.77 | 119.60 |
| 36 | 45 | 81 | VAL | N-CA-C | -5.39 | 100.58 | 108.99 |
| 27 | 11 | 25 | THR | N-CA-C | -5.39 | 103.51 | 110.19 |
| 28 | 21 | 64 | LYS | N-CA-C | -5.39 | 106.56 | 113.02 |
| 4 | 32 | 201 | GLN | N-CA-C | -5.39 | 105.06 | 111.69 |
| 34 | 25 | 30 | ALA | N-CA-C | 5.39 | 118.16 | 110.24 |
| 24 | 1H | 974(A) | C | C4'-C3'-O3' | 5.38 | 117.47 | 109.40 |
| 52 | K5 | 24 | GLU | CB-CA-C | -5.38 | 108.81 | 116.34 |
| 9 | 82 | 97 | LYS | CA-C-N | -5.37 | 114.13 | 119.56 |
| 9 | 82 | 97 | LYS | C-N-CA | -5.37 | 114.13 | 119.56 |
| 1 | 13 | 812 | C | P-O3'-C3' | 5.37 | 128.26 | 120.20 |
| 45 | H8 | 160 | GLY | N-CA-C | -5.37 | 102.75 | 110.38 |
| 20 | BA | 33 | ILE | CB-CA-C | -5.37 | 105.00 | 111.88 |
| 29 | 39 | 70 | THR | N-CA-C | 5.37 | 117.14 | 111.28 |
| 49 | L8 | 36 | VAL | N-CA-C | 5.37 | 115.82 | 107.28 |
| 31 | 51 | 88 | LEU | N-CA-C | 5.36 | 118.56 | 109.76 |
| 16 | 7I | 5 | ARG | N-CA-C | 5.36 | 115.32 | 108.24 |
| 51 | N8 | 6 | VAL | N-CA-C | 5.36 | 120.46 | 108.88 |
| 36 | 88 | 135 | ASP | N-CA-C | 5.36 | 117.21 | 109.07 |
| 36 | 88 | 5 | ARG | N-CA-C | -5.35 | 103.56 | 110.19 |
| 31 | 51 | 40 | GLU | N-CA-C | -5.34 | 103.56 | 110.19 |
| 47 | F5 | 25 | LYS | N-CA-C | -5.34 | 105.46 | 111.28 |
| 12 | 3A | 60 | LEU | CA-C-N | -5.34 | 115.00 | 123.12 |
| 12 | 3A | 60 | LEU | C-N-CA | -5.34 | 115.00 | 123.12 |
| 30 | 49 | 118 | ARG | N-CA-C | -5.34 | 103.48 | 110.53 |
| 33 | 15 | 85 | ILE | N-CA-C | 5.34 | 113.31 | 107.60 |
| 38 | 65 | 19 | LYS | N-CA-C | -5.34 | 102.99 | 110.35 |
| 41 | 95 | 21 | ARG | NH1-CZ-NH2 | -5.34 | 112.36 | 119.30 |
| 29 | 31 | 101 | LEU | CA-C-N | -5.33 | 114.27 | 119.76 |
| 29 | 31 | 101 | LEU | C-N-CA | -5.33 | 114.27 | 119.76 |
| 24 | 1H | 982 | C | OP1-P-O3' | 5.33 | 123.99 | 108.00 |
| 29 | 31 | 68 | LYS | N-CA-C | 5.33 | 117.08 | 109.14 |
| 12 | 3A | 62 | SER | N-CA-C | -5.33 | 105.62 | 113.61 |
| 45 | H8 | 64 | GLY | N-CA-C | -5.32 | 100.56 | 113.18 |
| 19 | AI | 67 | VAL | N-CA-C | 5.32 | 115.95 | 110.36 |
| 32 | 69 | 131 | LYS | C-N-CD | -5.32 | 108.89 | 120.60 |
| 39 | 75 | 75 | ILE | CB-CA-C | -5.32 | 103.21 | 110.77 |
| 33 | 15 | 42 | TRP | N-CA-C | 5.31 | 117.54 | 110.53 |
| 35 | 35 | 90 | ARG | N-CA-C | -5.31 | 106.81 | 113.72 |
| 13 | 4I | 40 | ASN | CA-C-N | 5.31 | 124.92 | 119.56 |
| 13 | 4I | 40 | ASN | C-N-CA | 5.31 | 124.92 | 119.56 |
| 42 | E8 | 98 | LYS | N-CA-C | -5.31 | 101.13 | 109.25 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed($^o$) | Ideal($^o$) |
|---|---|---|---|---|---|---|---|
| 53 | P8 | 11 | LYS | N-CA-C | -5.31 | 104.74 | 111.11 |
| 24 | 14 | 1022 | G | P-O3'-C3' | 5.31 | 128.16 | 120.20 |
| 18 | 9I | 19 | LYS | N-CA-C | 5.30 | 115.85 | 108.00 |
| 19 | AI | 4 | SER | N-CA-C | 5.30 | 116.50 | 108.07 |
| 24 | 14 | 856 | C | C2'-C3'-O3' | 5.29 | 121.64 | 113.70 |
| 31 | 51 | 138 | LYS | N-CA-C | -5.29 | 105.03 | 112.12 |
| 32 | 69 | 77 | LEU | CB-CA-C | -5.29 | 110.49 | 116.63 |
| 28 | 29 | 146 | THR | N-CA-C | -5.29 | 98.25 | 108.45 |
| 42 | A5 | 69 | LEU | N-CA-C | 5.29 | 116.93 | 108.41 |
| 54 | M5 | 10 | ALA | N-CA-C | -5.29 | 105.60 | 111.36 |
| 17 | 8A | 99 | SER | N-CA-C | 5.27 | 117.67 | 109.60 |
| 7 | 6E | 42 | ILE | N-CA-C | 5.27 | 115.90 | 110.36 |
| 24 | 1H | 1427 | A | P-O3'-C3' | 5.27 | 128.10 | 120.20 |
| 6 | 52 | 24 | GLU | N-CA-C | -5.27 | 105.43 | 111.07 |
| 51 | J5 | 40 | LYS | CA-C-N | -5.27 | 114.95 | 120.38 |
| 51 | J5 | 40 | LYS | C-N-CA | -5.27 | 114.95 | 120.38 |
| 39 | B8 | 123 | GLN | N-CA-C | -5.26 | 101.58 | 109.79 |
| 24 | 1H | 2566 | A | P-O3'-C3' | 5.26 | 128.09 | 120.20 |
| 3 | 22 | 131 | ARG | N-CA-C | -5.25 | 106.38 | 112.89 |
| 7 | 6E | 37 | ASN | N-CA-C | -5.25 | 105.47 | 111.14 |
| 24 | 1H | 654(S) | G | P-O3'-C3' | 5.25 | 126.00 | 119.70 |
| 35 | 78 | 36 | LYS | O-C-N | 5.25 | 129.58 | 122.59 |
| 32 | 69 | 143 | SER | N-CA-C | 5.25 | 115.99 | 108.74 |
| 27 | 11 | 229 | VAL | CB-CA-C | -5.25 | 104.39 | 112.05 |
| 52 | K5 | 25 | LYS | N-CA-C | 5.25 | 115.28 | 107.88 |
| 5 | 4E | 120 | THR | N-CA-C | 5.24 | 117.16 | 109.24 |
| 13 | 4A | 67 | GLU | CB-CA-C | -5.24 | 110.55 | 116.63 |
| 27 | 11 | 264 | LYS | CA-C-N | 5.24 | 124.91 | 119.56 |
| 27 | 11 | 264 | LYS | C-N-CA | 5.24 | 124.91 | 119.56 |
| 2 | 12 | 201 | ILE | CA-C-N | 5.24 | 126.39 | 119.84 |
| 2 | 12 | 201 | ILE | C-N-CA | 5.24 | 126.39 | 119.84 |
| 1 | 1G | 913 | A | P-O3'-C3' | 5.23 | 128.05 | 120.20 |
| 24 | 1H | 2387 | U | OP2-P-O3' | 5.23 | 123.68 | 108.00 |
| 30 | 41 | 137 | GLU | N-CA-C | 5.23 | 115.25 | 107.88 |
| 40 | C8 | 70 | ARG | N-CA-C | -5.22 | 106.86 | 113.18 |
| 27 | 19 | 223 | GLY | N-CA-C | -5.22 | 106.46 | 112.73 |
| 30 | 41 | 46 | ALA | N-CA-C | -5.22 | 106.59 | 113.17 |
| 16 | 7I | 83 | GLU | CB-CA-C | -5.22 | 110.13 | 117.23 |
| 54 | M5 | 32 | LEU | N-CA-C | 5.22 | 121.91 | 110.80 |
| 24 | 1H | 1762 | A | O5'-P-OP2 | -5.21 | 92.36 | 108.00 |
| 49 | L8 | 24 | LYS | N-CA-C | -5.21 | 105.25 | 111.03 |
| 46 | I8 | 40 | GLN | N-CA-C | 5.21 | 116.76 | 108.79 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed($^o$) | Ideal($^o$) |
|---|---|---|---|---|---|---|---|
| 27 | 11 | 152 | GLY | CA-C-O | -5.21 | 118.07 | 122.29 |
| 27 | 19 | 41 | GLY | N-CA-C | -5.21 | 100.84 | 113.18 |
| 51 | N8 | 5 | PRO | CA-C-O | -5.21 | 111.83 | 120.05 |
| 10 | 1A | 49 | VAL | N-CA-C | 5.21 | 116.20 | 108.65 |
| 29 | 31 | 9 | ILE | CA-C-N | 5.20 | 125.49 | 119.93 |
| 29 | 31 | 9 | ILE | C-N-CA | 5.20 | 125.49 | 119.93 |
| 36 | 88 | 28 | ALA | N-CA-C | 5.20 | 119.52 | 112.04 |
| 2 | 12 | 16 | HIS | N-CA-C | 5.19 | 119.72 | 113.17 |
| 39 | 75 | 17 | THR | N-CA-C | -5.19 | 106.63 | 113.17 |
| 52 | O8 | 21 | TYR | CB-CA-C | -5.19 | 109.04 | 115.89 |
| 44 | C5 | 39 | VAL | N-CA-CB | -5.19 | 107.46 | 112.65 |
| 1 | 1G | 412 | A | C2'-C3'-O3' | 5.18 | 117.27 | 109.50 |
| 27 | 11 | 53 | PHE | N-CA-C | 5.18 | 118.90 | 112.58 |
| 42 | A5 | 10 | VAL | CA-C-N | -5.17 | 114.06 | 122.34 |
| 42 | A5 | 10 | VAL | C-N-CA | -5.17 | 114.06 | 122.34 |
| 13 | 4I | 105 | THR | N-CA-C | 5.17 | 115.36 | 108.38 |
| 27 | 19 | 48 | ARG | CA-C-N | -5.17 | 113.42 | 121.18 |
| 27 | 19 | 48 | ARG | C-N-CA | -5.17 | 113.42 | 121.18 |
| 42 | E8 | 10 | VAL | CA-C-N | -5.17 | 114.81 | 122.41 |
| 42 | E8 | 10 | VAL | C-N-CA | -5.17 | 114.81 | 122.41 |
| 15 | 6A | 48 | LYS | N-CA-C | -5.17 | 106.75 | 113.16 |
| 4 | 32 | 19 | LEU | CA-C-N | -5.17 | 114.08 | 122.34 |
| 4 | 32 | 19 | LEU | C-N-CA | -5.17 | 114.08 | 122.34 |
| 28 | 21 | 61 | ARG | N-CA-C | 5.16 | 121.22 | 109.81 |
| 41 | D8 | 34 | GLU | N-CA-C | -5.16 | 102.04 | 110.20 |
| 27 | 11 | 212 | SER | N-CA-C | -5.16 | 106.25 | 112.54 |
| 38 | 65 | 40 | ILE | N-CA-C | 5.15 | 115.89 | 108.48 |
| 10 | 1I | 58 | ASP | N-CA-C | -5.15 | 103.25 | 110.35 |
| 30 | 41 | 38 | VAL | N-CA-C | 5.15 | 115.38 | 108.17 |
| 17 | 8A | 67 | LYS | N-CA-C | -5.15 | 103.35 | 110.35 |
| 28 | 21 | 59 | VAL | N-CA-C | 5.14 | 120.04 | 109.34 |
| 51 | N8 | 19 | ARG | N-CA-C | -5.14 | 105.76 | 111.36 |
| 44 | G8 | 99 | CYS | CA-C-N | 5.14 | 130.94 | 121.70 |
| 44 | G8 | 99 | CYS | C-N-CA | 5.14 | 130.94 | 121.70 |
| 54 | Q8 | 21 | LYS | CA-C-N | -5.13 | 116.44 | 123.12 |
| 54 | Q8 | 21 | LYS | C-N-CA | -5.13 | 116.44 | 123.12 |
| 24 | 14 | 1899 | G | N1-C2-N2 | -5.13 | 100.80 | 116.20 |
| 44 | C5 | 101 | LYS | N-CA-C | 5.13 | 121.74 | 110.80 |
| 27 | 11 | 271 | ILE | N-CA-CB | -5.13 | 105.64 | 112.26 |
| 43 | B5 | 50 | LYS | N-CA-C | 5.13 | 119.58 | 112.45 |
| 27 | 11 | 34 | VAL | CB-CA-C | -5.12 | 105.95 | 111.59 |
| 34 | 25 | 50 | GLY | N-CA-C | -5.12 | 105.75 | 112.81 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed($^o$) | Ideal($^o$) |
|---|---|---|---|---|---|---|---|
| 4 | 32 | 12 | CYS | N-CA-C | -5.12 | 104.97 | 111.11 |
| 47 | J8 | 33 | LYS | CA-C-N | -5.11 | 115.97 | 122.77 |
| 47 | J8 | 33 | LYS | C-N-CA | -5.11 | 115.97 | 122.77 |
| 24 | 14 | 1899 | G | C4'-C3'-O3' | -5.11 | 105.33 | 113.00 |
| 5 | 42 | 92 | LYS | CA-C-N | 5.11 | 125.35 | 119.83 |
| 5 | 42 | 92 | LYS | C-N-CA | 5.11 | 125.35 | 119.83 |
| 5 | 42 | 100 | VAL | CA-C-N | -5.11 | 116.16 | 123.11 |
| 5 | 42 | 100 | VAL | C-N-CA | -5.11 | 116.16 | 123.11 |
| 28 | 29 | 132 | HIS | N-CA-C | 5.11 | 116.89 | 110.91 |
| 44 | C5 | 104 | GLY | CA-C-O | -5.10 | 116.99 | 121.58 |
| 7 | 62 | 49 | ILE | N-CA-C | -5.10 | 106.71 | 111.45 |
| 8 | 7E | 79 | VAL | N-CA-C | -5.10 | 105.57 | 110.72 |
| 24 | 1H | 1799 | G | C4'-C3'-O3' | 5.09 | 117.04 | 109.40 |
| 24 | 14 | 512 | G | C5'-C4'-C3' | -5.09 | 107.56 | 115.20 |
| 47 | J8 | 85 | LEU | CA-C-N | 5.09 | 130.86 | 121.70 |
| 47 | J8 | 85 | LEU | C-N-CA | 5.09 | 130.86 | 121.70 |
| 36 | 45 | 78 | PRO | CA-C-O | -5.09 | 111.34 | 120.60 |
| 18 | 9I | 19 | LYS | CB-CA-C | -5.09 | 109.22 | 116.34 |
| 41 | 95 | 79 | VAL | CA-C-N | -5.09 | 113.22 | 123.09 |
| 41 | 95 | 79 | VAL | C-N-CA | -5.09 | 113.22 | 123.09 |
| 31 | 59 | 56 | SER | N-CA-C | 5.08 | 114.95 | 108.24 |
| 24 | 1H | 1312 | U | C2'-C3'-O3' | 5.08 | 117.12 | 109.50 |
| 29 | 31 | 7 | TYR | N-CA-C | 5.08 | 121.62 | 110.80 |
| 33 | 15 | 134 | ARG | CA-C-N | -5.08 | 114.57 | 119.90 |
| 33 | 15 | 134 | ARG | C-N-CA | -5.08 | 114.57 | 119.90 |
| 29 | 31 | 75 | HIS | N-CA-C | 5.07 | 116.90 | 109.24 |
| 28 | 21 | 97 | LYS | CA-C-N | -5.07 | 114.49 | 119.92 |
| 28 | 21 | 97 | LYS | C-N-CA | -5.07 | 114.49 | 119.92 |
| 43 | B5 | 81 | VAL | N-CA-C | 5.07 | 116.83 | 108.97 |
| 30 | 49 | 15 | VAL | N-CA-C | 5.07 | 116.53 | 111.00 |
| 20 | BA | 103 | GLY | N-CA-C | 5.07 | 121.71 | 110.66 |
| 52 | O8 | 28 | ARG | N-CA-C | 5.07 | 116.98 | 109.69 |
| 39 | 75 | 57 | PHE | N-CA-C | -5.07 | 106.88 | 113.16 |
| 26 | 71 | 180 | PHE | CA-C-N | 5.06 | 123.35 | 119.66 |
| 26 | 71 | 180 | PHE | C-N-CA | 5.06 | 123.35 | 119.66 |
| 24 | 1H | 750 | A | OP2-P-O3' | 5.05 | 123.15 | 108.00 |
| 24 | 14 | 1342 | A | N9-C1'-C2' | 5.05 | 121.57 | 114.00 |
| 28 | 29 | 21 | VAL | CA-C-N | 5.05 | 125.20 | 119.90 |
| 28 | 29 | 21 | VAL | C-N-CA | 5.05 | 125.20 | 119.90 |
| 27 | 19 | 123 | ALA | CA-C-N | 5.05 | 125.04 | 119.89 |
| 27 | 19 | 123 | ALA | C-N-CA | 5.05 | 125.04 | 119.89 |
| 3 | 2E | 96 | GLY | N-CA-C | -5.05 | 107.31 | 115.08 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed($^o$) | Ideal($^o$) |
|---|---|---|---|---|---|---|---|
| 24 | 1H | 790 | C | P-O3'-C3' | -5.04 | 112.64 | 120.20 |
| 35 | 35 | 99 | LEU | N-CA-C | -5.04 | 105.49 | 111.69 |
| 50 | I5 | 30 | GLU | N-CA-C | 5.04 | 116.73 | 108.76 |
| 31 | 51 | 44 | VAL | N-CA-C | 5.04 | 115.30 | 107.28 |
| 47 | F5 | 67 | ILE | CB-CA-C | -5.04 | 108.91 | 113.70 |
| 28 | 21 | 82 | ARG | N-CA-C | 5.04 | 121.53 | 110.80 |
| 52 | O8 | 46 | HIS | N-CA-C | 5.04 | 121.53 | 110.80 |
| 24 | 1H | 537 | C | C5'-C4'-C3' | -5.04 | 108.44 | 116.00 |
| 34 | 68 | 96 | THR | N-CA-C | -5.03 | 102.56 | 110.36 |
| 47 | F5 | 75 | GLU | CA-C-N | -5.03 | 116.31 | 122.84 |
| 47 | F5 | 75 | GLU | C-N-CA | -5.03 | 116.31 | 122.84 |
| 24 | 14 | 2611 | U | C5'-C4'-C3' | 5.02 | 123.53 | 116.00 |
| 33 | 58 | 129 | PRO | N-CA-C | 5.02 | 118.38 | 110.80 |
| 28 | 29 | 81 | ILE | N-CA-C | 5.02 | 119.79 | 109.34 |
| 33 | 15 | 35 | ARG | N-CA-C | -5.02 | 103.90 | 110.53 |
| 1 | 1G | 115 | G | P-O3'-C3' | 5.02 | 127.73 | 120.20 |
| 2 | 12 | 190 | THR | N-CA-C | -5.02 | 103.17 | 110.24 |
| 29 | 39 | 80 | ALA | N-CA-C | -5.02 | 103.83 | 109.60 |
| 27 | 19 | 247 | ALA | N-CA-C | 5.01 | 117.29 | 109.52 |
| 36 | 45 | 133 | ARG | N-CA-C | 5.01 | 119.54 | 113.38 |
| 31 | 59 | 94 | TYR | N-CA-C | 5.01 | 119.48 | 113.17 |
| 35 | 78 | 77 | ARG | CA-C-N | 5.00 | 125.29 | 119.93 |
| 35 | 78 | 77 | ARG | C-N-CA | 5.00 | 125.29 | 119.93 |
| 45 | D5 | 61 | LEU | CA-C-N | 5.00 | 126.09 | 119.84 |
| 45 | D5 | 61 | LEU | C-N-CA | 5.00 | 126.09 | 119.84 |
| 28 | 29 | 198 | VAL | N-CA-C | 5.00 | 115.53 | 107.73 |

There are no chirality outliers.

All (100) planarity outliers are listed below:

| Mol | Chain | Res | Type | Group |
|---|---|---|---|---|
| 27 | 11 | 197 | GLY | Peptide |
| 27 | 11 | 239 | ARG | Peptide |
| 27 | 11 | 27 | THR | Peptide |
| 27 | 11 | 32 | SER | Peptide |
| 2 | 12 | 233 | SER | Peptide |
| 2 | 12 | 71 | VAL | Peptide |
| 33 | 15 | 41 | ASP | Peptide |
| 27 | 19 | 197 | GLY | Peptide |
| 27 | 19 | 270 | ILE | Peptide |
| 27 | 19 | 271 | ILE | Peptide |
| 27 | 19 | 32 | SER | Peptide |

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| Mol | Chain | Res | Type | Group |
|---|---|---|---|---|
| 27 | 19 | 37 | LEU | Peptide |
| 2 | 1E | 71 | VAL | Peptide |
| 3 | 22 | 166 | GLU | Peptide |
| 34 | 25 | 97 | ARG | Peptide |
| 28 | 29 | 130 | GLY | Peptide |
| 28 | 29 | 186 | GLY | Peptide |
| 28 | 29 | 202 | LYS | Peptide |
| 28 | 29 | 54 | GLN | Peptide |
| 28 | 29 | 61 | ARG | Peptide |
| 28 | 29 | 76 | ARG | Peptide |
| 28 | 29 | 81 | ILE | Peptide |
| 29 | 31 | 132 | VAL | Peptide |
| 35 | 35 | 110 | TYR | Peptide |
| 35 | 35 | 22 | GLY | Peptide |
| 35 | 35 | 24 | GLY | Peptide |
| 35 | 35 | 36 | LYS | Peptide |
| 35 | 35 | 48 | PRO | Peptide |
| 35 | 35 | 70 | GLN | Peptide |
| 35 | 35 | 89 | ALA | Peptide |
| 29 | 39 | 128 | ALA | Peptide |
| 12 | 3A | 28 | LYS | Peptide |
| 12 | 3A | 46 | LYS | Peptide |
| 12 | 3A | 60 | LEU | Peptide |
| 12 | 3A | 61 | THR | Peptide |
| 4 | 3E | 166 | LYS | Peptide |
| 4 | 3E | 193 | ASP | Peptide |
| 4 | 3E | 29 | PRO | Peptide |
| 36 | 45 | 24 | GLY | Peptide |
| 30 | 49 | 117 | PHE | Peptide |
| 31 | 59 | 123 | PHE | Peptide |
| 14 | 5I | 13 | THR | Peptide |
| 32 | 61 | 134 | PRO | Peptide |
| 38 | 65 | 56 | LEU | Peptide |
| 39 | 75 | 105 | LEU | Peptide |
| 39 | 75 | 4 | GLY | Peptide |
| 39 | 75 | 6 | LEU | Peptide |
| 35 | 78 | 11 | GLY | Peptide |
| 35 | 78 | 147 | LEU | Peptide |
| 35 | 78 | 20 | GLY | Peptide |
| 35 | 78 | 22 | GLY | Peptide |
| 35 | 78 | 24 | GLY | Peptide |
| 35 | 78 | 45 | LEU | Peptide |

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| Mol | Chain | Res | Type | Group |
|---|---|---|---|---|
| 35 | 78 | 65 | ARG | Peptide |
| 9 | 82 | 40 | LEU | Peptide |
| 9 | 82 | 87 | GLN | Peptide |
| 40 | 85 | 96 | ALA | Peptide |
| 36 | 88 | 21 | THR | Peptide |
| 36 | 88 | 78 | PRO | Peptide |
| 36 | 88 | 89 | ASN | Peptide |
| 41 | 95 | 48 | GLY | Peptide |
| 41 | 95 | 49 | THR | Peptide |
| 38 | A8 | 2 | ALA | Peptide |
| 38 | A8 | 81 | GLY | Peptide |
| 19 | AA | 10 | PHE | Peptide |
| 19 | AI | 5 | LEU | Peptide |
| 19 | AI | 6 | LYS | Peptide |
| 19 | AI | 64 | GLU | Peptide |
| 39 | B8 | 58 | ASN | Peptide |
| 20 | BA | 102 | GLY | Peptide |
| 20 | BA | 11 | SER | Peptide |
| 44 | C5 | 100 | ALA | Peptide |
| 44 | C5 | 41 | GLY | Peptide |
| 44 | C5 | 81 | LYS | Peptide |
| 45 | D5 | 107 | THR | Peptide |
| 45 | D5 | 174 | VAL | Peptide |
| 45 | D5 | 61 | LEU | Peptide |
| 47 | F5 | 85 | LEU | Peptide |
| 47 | F5 | 91 | LYS | Peptide |
| 43 | F8 | 67 | GLY | Peptide |
| 44 | G8 | 104 | GLY | Peptide |
| 44 | G8 | 53 | PRO | Peptide |
| 44 | G8 | 54 | LYS | Peptide |
| 44 | G8 | 77 | PRO | Peptide |
| 44 | G8 | 78 | ALA | Peptide |
| 51 | J5 | 51 | TYR | Peptide |
| 47 | J8 | 86 | SER | Peptide |
| 47 | J8 | 88 | LYS | Peptide |
| 52 | K5 | 44 | ARG | Peptide |
| 48 | K8 | 4 | SER | Peptide |
| 48 | K8 | 46 | GLN | Peptide |
| 49 | L8 | 39 | ASP | Peptide |
| 54 | M5 | 40 | GLU | Peptide |
| 54 | M5 | 54 | GLU | Peptide |
| 53 | P8 | 42 | LEU | Peptide |

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| Mol | Chain | Res | Type | Group |
|---|---|---|---|---|
| 53 | P8 | 44 | PRO | Peptide |
| 54 | Q8 | 32 | LEU | Peptide |
| 54 | Q8 | 34 | TRP | Peptide |
| 54 | Q8 | 40 | GLU | Peptide |
| 54 | Q8 | 54 | GLU | Peptide |

## 5.2 Too-close contacts (i)

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

| Mol | Chain | Non-H | H(model) | H(added) | Clashes | Symm-Clashes |
|---|---|---|---|---|---|---|
| 1 | 13 | 32337 | 0 | 16321 | 895 | 0 |
| 1 | 1G | 32309 | 0 | 16307 | 842 | 0 |
| 2 | 12 | 1924 | 0 | 1975 | 102 | 0 |
| 2 | 1E | 1924 | 0 | 1975 | 123 | 0 |
| 3 | 22 | 1612 | 0 | 1677 | 96 | 0 |
| 3 | 2E | 1605 | 0 | 1668 | 72 | 0 |
| 4 | 32 | 1702 | 0 | 1763 | 117 | 1 |
| 4 | 3E | 1702 | 0 | 1763 | 83 | 0 |
| 5 | 42 | 1155 | 0 | 1213 | 75 | 0 |
| 5 | 4E | 1155 | 0 | 1213 | 58 | 0 |
| 6 | 52 | 842 | 0 | 857 | 39 | 0 |
| 6 | 5E | 842 | 0 | 857 | 47 | 1 |
| 7 | 62 | 1256 | 0 | 1296 | 42 | 0 |
| 7 | 6E | 1256 | 0 | 1296 | 60 | 0 |
| 8 | 72 | 1115 | 0 | 1177 | 52 | 0 |
| 8 | 7E | 1115 | 0 | 1177 | 74 | 0 |
| 9 | 82 | 1009 | 0 | 1037 | 77 | 0 |
| 9 | 8E | 1009 | 0 | 1037 | 67 | 0 |
| 10 | 1A | 801 | 0 | 849 | 55 | 0 |
| 10 | 1I | 801 | 0 | 849 | 44 | 0 |
| 11 | 2A | 864 | 0 | 881 | 28 | 0 |
| 11 | 2I | 864 | 0 | 881 | 40 | 0 |
| 12 | 3A | 975 | 0 | 1062 | 39 | 0 |
| 12 | 3I | 975 | 0 | 1062 | 43 | 0 |
| 13 | 4A | 933 | 0 | 992 | 58 | 0 |
| 13 | 4I | 928 | 0 | 987 | 52 | 0 |
| 14 | 5A | 491 | 0 | 529 | 38 | 0 |
| 14 | 5I | 491 | 0 | 529 | 46 | 0 |

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| Mol | Chain | Non-H | H(model) | H(added) | Clashes | Symm-Clashes |
|---|---|---|---|---|---|---|
| 15 | 6A | 733 | 0 | 771 | 28 | 0 |
| 15 | 6I | 733 | 0 | 771 | 36 | 0 |
| 16 | 7A | 705 | 0 | 725 | 35 | 0 |
| 16 | 7I | 705 | 0 | 725 | 51 | 0 |
| 17 | 8A | 834 | 0 | 904 | 47 | 0 |
| 17 | 8I | 834 | 0 | 904 | 49 | 0 |
| 18 | 9A | 590 | 0 | 662 | 27 | 0 |
| 18 | 9I | 590 | 0 | 662 | 22 | 0 |
| 19 | AA | 633 | 0 | 649 | 48 | 0 |
| 19 | AI | 665 | 0 | 686 | 38 | 0 |
| 20 | BA | 762 | 0 | 861 | 38 | 0 |
| 20 | BI | 762 | 0 | 861 | 55 | 0 |
| 21 | 1B | 217 | 0 | 234 | 16 | 0 |
| 21 | 1F | 217 | 0 | 234 | 12 | 0 |
| 22 | 2K | 1765 | 0 | 916 | 67 | 0 |
| 22 | 2L | 1678 | 0 | 872 | 65 | 0 |
| 22 | 3K | 1824 | 0 | 945 | 58 | 0 |
| 22 | 3L | 1825 | 0 | 946 | 51 | 0 |
| 23 | 4K | 348 | 0 | 175 | 9 | 0 |
| 23 | 4L | 170 | 0 | 87 | 3 | 0 |
| 24 | 14 | 62647 | 0 | 31572 | 1465 | 0 |
| 24 | 1H | 62707 | 0 | 31606 | 1615 | 0 |
| 25 | 16 | 2617 | 0 | 1328 | 87 | 0 |
| 25 | 1J | 2617 | 0 | 1328 | 93 | 0 |
| 26 | 71 | 1049 | 0 | 1071 | 32 | 0 |
| 26 | 79 | 1049 | 0 | 1071 | 42 | 0 |
| 27 | 11 | 2115 | 0 | 2195 | 136 | 0 |
| 27 | 19 | 2120 | 0 | 2197 | 116 | 0 |
| 28 | 21 | 1568 | 0 | 1634 | 98 | 0 |
| 28 | 29 | 1568 | 0 | 1634 | 127 | 0 |
| 29 | 31 | 1585 | 0 | 1632 | 86 | 0 |
| 29 | 39 | 1627 | 0 | 1680 | 107 | 0 |
| 30 | 41 | 1473 | 0 | 1535 | 75 | 0 |
| 30 | 49 | 1473 | 0 | 1535 | 90 | 0 |
| 31 | 51 | 1336 | 0 | 1418 | 92 | 0 |
| 31 | 59 | 1312 | 0 | 1384 | 65 | 0 |
| 32 | 61 | 1136 | 0 | 1223 | 56 | 0 |
| 32 | 69 | 1136 | 0 | 1223 | 68 | 0 |
| 33 | 15 | 1104 | 0 | 1180 | 50 | 0 |
| 33 | 58 | 1104 | 0 | 1180 | 55 | 0 |
| 34 | 25 | 932 | 0 | 996 | 45 | 0 |
| 34 | 68 | 932 | 0 | 996 | 34 | 0 |

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| Mol | Chain | Non-H | H(model) | H(added) | Clashes | Symm-Clashes |
|---|---|---|---|---|---|---|
| 35 | 35 | 1144 | 0 | 1228 | 84 | 0 |
| 35 | 78 | 1144 | 0 | 1228 | 92 | 0 |
| 36 | 45 | 1121 | 0 | 1179 | 75 | 0 |
| 36 | 88 | 1121 | 0 | 1179 | 87 | 0 |
| 37 | 55 | 959 | 0 | 1021 | 54 | 0 |
| 37 | 98 | 967 | 0 | 1033 | 69 | 0 |
| 38 | 65 | 881 | 0 | 943 | 77 | 0 |
| 38 | A8 | 881 | 0 | 943 | 49 | 0 |
| 39 | 75 | 1131 | 0 | 1180 | 89 | 0 |
| 39 | B8 | 1141 | 0 | 1202 | 58 | 0 |
| 40 | 85 | 963 | 0 | 1022 | 58 | 0 |
| 40 | C8 | 963 | 0 | 1022 | 61 | 0 |
| 41 | 95 | 778 | 0 | 852 | 87 | 0 |
| 41 | D8 | 778 | 0 | 852 | 33 | 0 |
| 42 | A5 | 899 | 0 | 964 | 36 | 0 |
| 42 | E8 | 899 | 0 | 964 | 41 | 0 |
| 43 | B5 | 730 | 0 | 780 | 41 | 0 |
| 43 | F8 | 725 | 0 | 778 | 47 | 0 |
| 44 | C5 | 794 | 0 | 884 | 58 | 0 |
| 44 | G8 | 791 | 0 | 880 | 68 | 0 |
| 45 | D5 | 1428 | 0 | 1454 | 92 | 0 |
| 45 | H8 | 1397 | 0 | 1430 | 89 | 0 |
| 46 | E5 | 612 | 0 | 633 | 39 | 0 |
| 46 | I8 | 656 | 0 | 683 | 56 | 0 |
| 47 | F5 | 762 | 0 | 848 | 36 | 0 |
| 47 | J8 | 762 | 0 | 848 | 49 | 0 |
| 48 | G5 | 580 | 0 | 629 | 28 | 0 |
| 48 | K8 | 558 | 0 | 610 | 33 | 0 |
| 49 | H5 | 468 | 0 | 518 | 14 | 0 |
| 49 | L8 | 468 | 0 | 518 | 36 | 0 |
| 50 | I5 | 515 | 0 | 514 | 44 | 0 |
| 50 | M8 | 533 | 0 | 526 | 41 | 0 |
| 51 | J5 | 458 | 0 | 480 | 19 | 0 |
| 51 | N8 | 458 | 0 | 480 | 36 | 0 |
| 52 | K5 | 389 | 0 | 404 | 25 | 0 |
| 52 | O8 | 389 | 0 | 404 | 26 | 0 |
| 53 | L5 | 429 | 0 | 480 | 33 | 0 |
| 53 | P8 | 409 | 0 | 454 | 20 | 0 |
| 54 | M5 | 495 | 0 | 567 | 37 | 0 |
| 54 | Q8 | 483 | 0 | 555 | 43 | 0 |
| 55 | 11 | 2 | 0 | 0 | 0 | 0 |
| 55 | 13 | 139 | 0 | 0 | 0 | 0 |

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| Mol | Chain | Non-H | H(model) | H(added) | Clashes | Symm-Clashes |
|---|---|---|---|---|---|---|
| 55 | 14 | 465 | 0 | 0 | 0 | 0 |
| 55 | 15 | 1 | 0 | 0 | 0 | 0 |
| 55 | 16 | 15 | 0 | 0 | 0 | 0 |
| 55 | 19 | 1 | 0 | 0 | 0 | 0 |
| 55 | 1G | 148 | 0 | 0 | 0 | 0 |
| 55 | 1H | 523 | 0 | 0 | 0 | 0 |
| 55 | 1J | 10 | 0 | 0 | 0 | 0 |
| 55 | 21 | 2 | 0 | 0 | 0 | 0 |
| 55 | 25 | 1 | 0 | 0 | 0 | 0 |
| 55 | 29 | 4 | 0 | 0 | 0 | 0 |
| 55 | 2K | 5 | 0 | 0 | 0 | 0 |
| 55 | 2L | 4 | 0 | 0 | 0 | 0 |
| 55 | 32 | 1 | 0 | 0 | 0 | 0 |
| 55 | 39 | 1 | 0 | 0 | 0 | 0 |
| 55 | 3A | 1 | 0 | 0 | 0 | 0 |
| 55 | 3E | 1 | 0 | 0 | 0 | 0 |
| 55 | 3I | 1 | 0 | 0 | 0 | 0 |
| 55 | 3L | 1 | 0 | 0 | 0 | 0 |
| 55 | 42 | 1 | 0 | 0 | 0 | 0 |
| 55 | 45 | 1 | 0 | 0 | 0 | 0 |
| 55 | 4A | 1 | 0 | 0 | 0 | 0 |
| 55 | 4K | 1 | 0 | 0 | 0 | 0 |
| 55 | 52 | 1 | 0 | 0 | 0 | 0 |
| 55 | 55 | 1 | 0 | 0 | 0 | 0 |
| 55 | 5E | 1 | 0 | 0 | 0 | 0 |
| 55 | 7E | 1 | 0 | 0 | 0 | 0 |
| 55 | 88 | 1 | 0 | 0 | 0 | 0 |
| 55 | 98 | 1 | 0 | 0 | 0 | 0 |
| 55 | C5 | 1 | 0 | 0 | 0 | 0 |
| 55 | E5 | 1 | 0 | 0 | 0 | 0 |
| 55 | F5 | 1 | 0 | 0 | 0 | 0 |
| 55 | G8 | 1 | 0 | 0 | 0 | 0 |
| 55 | I8 | 3 | 0 | 0 | 0 | 0 |
| 55 | Q8 | 2 | 0 | 0 | 0 | 0 |
| 56 | 32 | 1 | 0 | 0 | 0 | 0 |
| 56 | 3E | 1 | 0 | 0 | 0 | 0 |
| 56 | 5A | 1 | 0 | 0 | 0 | 0 |
| 56 | 5I | 1 | 0 | 0 | 0 | 0 |
| 56 | C5 | 1 | 0 | 0 | 0 | 0 |
| 56 | G8 | 1 | 0 | 0 | 0 | 0 |
| 57 | 11 | 8 | 0 | 0 | 2 | 0 |
| 57 | 13 | 125 | 0 | 0 | 23 | 0 |

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| Mol | Chain | Non-H | H(model) | H(added) | Clashes | Symm-Clashes |
|---|---|---|---|---|---|---|
| 57 | 14 | 523 | 0 | 0 | 116 | 0 |
| 57 | 16 | 12 | 0 | 0 | 3 | 0 |
| 57 | 19 | 11 | 0 | 0 | 3 | 0 |
| 57 | 1G | 96 | 0 | 0 | 18 | 0 |
| 57 | 1H | 652 | 0 | 0 | 172 | 0 |
| 57 | 1J | 22 | 0 | 0 | 2 | 0 |
| 57 | 21 | 2 | 0 | 0 | 2 | 0 |
| 57 | 25 | 6 | 0 | 0 | 0 | 0 |
| 57 | 2K | 2 | 0 | 0 | 0 | 0 |
| 57 | 2L | 6 | 0 | 0 | 0 | 0 |
| 57 | 31 | 5 | 0 | 0 | 0 | 0 |
| 57 | 32 | 1 | 0 | 0 | 0 | 0 |
| 57 | 35 | 1 | 0 | 0 | 0 | 0 |
| 57 | 39 | 3 | 0 | 0 | 0 | 0 |
| 57 | 4K | 3 | 0 | 0 | 0 | 0 |
| 57 | 5A | 1 | 0 | 0 | 0 | 0 |
| 57 | 5I | 1 | 0 | 0 | 0 | 0 |
| 57 | 75 | 1 | 0 | 0 | 0 | 0 |
| 57 | 78 | 4 | 0 | 0 | 2 | 0 |
| 57 | 7A | 2 | 0 | 0 | 0 | 0 |
| 57 | 85 | 4 | 0 | 0 | 0 | 0 |
| 57 | 98 | 1 | 0 | 0 | 2 | 0 |
| 57 | AI | 3 | 0 | 0 | 0 | 0 |
| 57 | BA | 1 | 0 | 0 | 0 | 0 |
| 57 | C8 | 2 | 0 | 0 | 0 | 0 |
| 57 | E8 | 1 | 0 | 0 | 0 | 0 |
| 57 | F5 | 1 | 0 | 0 | 0 | 0 |
| 57 | F8 | 2 | 0 | 0 | 0 | 0 |
| 57 | G8 | 2 | 0 | 0 | 1 | 0 |
| 57 | H5 | 2 | 0 | 0 | 0 | 0 |
| All | All | 299705 | 0 | 201607 | 9522 | 1 |

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 20.

All (9522) 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) |
|---|---|---|---|
| 41:95:91:TYR:CG | 41:95:91:TYR:CD1 | 1.79 | 1.67 |
| 41:95:91:TYR:CG | 41:95:91:TYR:CD2 | 1.79 | 1.65 |
| 41:95:91:TYR:CE1 | 41:95:91:TYR:CZ | 1.90 | 1.56 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 41:95:91:TYR:CZ | 41:95:91:TYR:CE2 | 1.92 | 1.55 |
| 22:2K:35:QUO:C4 | 22:2K:35:QUO:N3 | 1.68 | 1.55 |
| 22:3K:35:QUO:C4 | 22:3K:35:QUO:N3 | 1.71 | 1.53 |
| 22:3L:35:QUO:N3 | 22:3L:35:QUO:C4 | 1.71 | 1.50 |
| 22:2L:35:QUO:C4 | 22:2L:35:QUO:N3 | 1.71 | 1.49 |
| 41:95:21:ARG:NE | 41:95:91:TYR:CD1 | 1.86 | 1.38 |
| 41:95:21:ARG:NE | 41:95:21:ARG:CD | 1.86 | 1.36 |
| 41:95:21:ARG:NE | 41:95:91:TYR:CD2 | 1.97 | 1.30 |
| 41:95:21:ARG:NE | 41:95:91:TYR:CE1 | 1.98 | 1.29 |
| 41:95:21:ARG:NE | 41:95:91:TYR:CG | 1.96 | 1.27 |
| 41:95:91:TYR:CD2 | 41:95:91:TYR:CE2 | 2.25 | 1.25 |
| 41:95:91:TYR:CD1 | 41:95:91:TYR:CE1 | 2.28 | 1.19 |
| 41:95:21:ARG:NE | 41:95:91:TYR:CE2 | 2.11 | 1.19 |
| 41:95:21:ARG:NE | 41:95:91:TYR:CZ | 2.12 | 1.17 |
| 24:1H:2711:A:OP2 | 57:1H:3601:HOH:O | 1.66 | 1.12 |
| 24:1H:1774:C:OP1 | 57:1H:3602:HOH:O | 1.68 | 1.11 |
| 24:1H:2714:G:OP2 | 57:1H:3601:HOH:O | 1.69 | 1.08 |
| 24:1H:730:C:OP2 | 57:1H:3603:HOH:O | 1.70 | 1.06 |
| 14:5I:24:CYS:SG | 14:5I:40:CYS:HB3 | 1.95 | 1.06 |
| 24:14:1632:A:N7 | 57:14:3511:HOH:O | 1.91 | 1.04 |
| 24:14:1899:G:H21 | 24:14:1902:C:N4 | 1.55 | 1.04 |
| 41:95:21:ARG:CD | 41:95:91:TYR:CE2 | 2.41 | 1.03 |
| 41:95:21:ARG:CD | 41:95:91:TYR:CZ | 2.42 | 1.03 |
| 24:14:192:C:N3 | 57:14:3515:HOH:O | 1.92 | 1.02 |
| 24:1H:1268:A:OP1 | 57:1H:3604:HOH:O | 1.76 | 1.02 |
| 47:J8:85:LEU:N | 47:J8:86:SER:O | 1.93 | 1.01 |
| 4:3E:12:CYS:HB3 | 4:3E:33:MET:HE1 | 1.40 | 1.01 |
| 24:14:1664:A:OP2 | 57:14:3501:HOH:O | 1.78 | 1.01 |
| 33:15:47:ALA:HB2 | 33:15:112:LEU:HD11 | 1.43 | 1.01 |
| 41:95:37:VAL:HG21 | 41:95:56:SER:HA | 1.39 | 1.01 |
| 24:14:574:C:OP2 | 57:14:3503:HOH:O | 1.80 | 1.00 |
| 40:85:90:VAL:HG22 | 41:95:39:LEU:HB3 | 1.43 | 1.00 |
| 24:14:2576:G:OP1 | 57:14:3502:HOH:O | 1.79 | 0.99 |
| 24:14:2074:U:OP1 | 57:14:3504:HOH:O | 1.81 | 0.99 |
| 24:14:323:G:HO2' | 24:14:1205:U:H3 | 1.12 | 0.98 |
| 41:95:21:ARG:CZ | 41:95:91:TYR:CE2 | 2.47 | 0.97 |
| 24:1H:945:A:OP1 | 57:1H:3606:HOH:O | 1.82 | 0.97 |
| 20:BI:22:ARG:O | 20:BI:26:ASN:ND2 | 1.98 | 0.97 |
| 24:1H:67:U:H3 | 24:1H:74:A:H2 | 1.07 | 0.97 |
| 24:14:676:A:H8 | 24:14:2069:G:H21 | 1.08 | 0.96 |
| 24:1H:49:A:N7 | 24:1H:120:U:H5 | 1.63 | 0.96 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 6:52:87:ARG:HH11 | 6:52:87:ARG:HG3 | 1.26 | 0.96 |
| 1:13:1502:A:H2 | 1:13:1505:G:H1 | 1.12 | 0.96 |
| 41:95:21:ARG:CZ | 41:95:91:TYR:CZ | 2.47 | 0.96 |
| 24:1H:2:G:H22 | 24:1H:2901:C:H42 | 1.10 | 0.96 |
| 41:95:21:ARG:HD2 | 41:95:91:TYR:CE2 | 2.01 | 0.96 |
| 24:1H:2006:C:OP1 | 57:1H:3605:HOH:O | 1.81 | 0.96 |
| 24:14:2499:C:OP2 | 57:14:3505:HOH:O | 1.82 | 0.96 |
| 24:14:1771:C:HO2' | 24:14:1786:A:H8 | 0.98 | 0.95 |
| 24:14:960:A:H61 | 36:45:83:MET:HE2 | 1.31 | 0.95 |
| 35:35:23:PRO:HB3 | 41:95:80:GLN:HG2 | 1.46 | 0.95 |
| 25:1J:5:C:H42 | 25:1J:115:G:H1 | 1.02 | 0.95 |
| 24:1H:450:G:OP2 | 57:1H:3608:HOH:O | 1.83 | 0.95 |
| 24:1H:2419:U:O4 | 54:Q8:30:ARG:NE | 1.99 | 0.95 |
| 1:13:1348:U:H3 | 1:13:1374:A:H2 | 1.14 | 0.94 |
| 24:1H:1658:C:OP1 | 57:1H:3607:HOH:O | 1.83 | 0.94 |
| 24:14:2420:C:H41 | 54:M5:31:HIS:HB3 | 1.33 | 0.94 |
| 1:13:686:U:H1' | 11:2I:42:TRP:HE1 | 1.32 | 0.94 |
| 24:1H:2588:G:OP2 | 57:1H:3610:HOH:O | 1.85 | 0.94 |
| 24:1H:2392:A:H8 | 35:78:61:ARG:HG2 | 1.32 | 0.94 |
| 1:1G:1348:U:H3 | 1:1G:1374:A:H2 | 1.13 | 0.94 |
| 24:1H:1771:C:HO2' | 24:1H:1786:A:H8 | 1.03 | 0.93 |
| 29:31:6:VAL:HG21 | 29:31:119:ARG:HB2 | 1.50 | 0.93 |
| 43:F8:67:GLY:O | 43:F8:69:TYR:N | 2.01 | 0.93 |
| 24:1H:741:G:OP1 | 57:1H:3609:HOH:O | 1.84 | 0.93 |
| 24:14:2448:A:OP2 | 57:14:3505:HOH:O | 1.87 | 0.93 |
| 24:14:2681:C:H5 | 24:14:2725:A:H62 | 1.15 | 0.93 |
| 1:1G:1502:A:H2 | 1:1G:1505:G:H1 | 1.12 | 0.93 |
| 25:1J:80:U:H2' | 25:1J:81:G:H21 | 1.32 | 0.93 |
| 24:1H:1479:G:N7 | 24:1H:1510:A:N6 | 2.16 | 0.93 |
| 24:14:1022:G:H22 | 24:14:1142(A):A:H2 | 1.15 | 0.93 |
| 33:58:96:GLU:HG2 | 33:58:97:ARG:H | 1.33 | 0.92 |
| 24:14:1614:A:OP1 | 57:14:3506:HOH:O | 1.87 | 0.92 |
| 28:29:1:MET:N | 28:29:200:GLU:OE2 | 2.01 | 0.92 |
| 47:J8:86:SER:HA | 47:J8:88:LYS:HB2 | 1.50 | 0.92 |
| 1:1G:406:G:H21 | 4:32:119:GLN:HE22 | 1.15 | 0.92 |
| 24:14:259:G:H21 | 24:14:621:A:H8 | 1.13 | 0.92 |
| 24:1H:2035:G:OP1 | 57:1H:3611:HOH:O | 1.85 | 0.92 |
| 24:14:617:G:OP1 | 29:39:40:GLN:NE2 | 2.02 | 0.92 |
| 25:1J:15:A:H5' | 25:1J:16:G:C8 | 2.05 | 0.92 |
| 10:1I:48:THR:HG23 | 10:1I:62:HIS:HB3 | 1.52 | 0.92 |
| 24:1H:676:A:H8 | 24:1H:2069:G:H21 | 1.13 | 0.92 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 41:95:21:ARG:CZ | 41:95:91:TYR:CE1 | 2.52 | 0.92 |
| 4:32:29:PRO:HG2 | 4:32:30:LYS:HG3 | 1.51 | 0.91 |
| 41:95:21:ARG:HD2 | 41:95:91:TYR:CZ | 2.04 | 0.91 |
| 24:14:1891:G:O6 | 57:14:3508:HOH:O | 1.89 | 0.91 |
| 38:A8:11:LYS:HD3 | 38:A8:91:PRO:HD3 | 1.52 | 0.91 |
| 22:3L:20:C:H5" | 22:3L:68:A:H62 | 1.36 | 0.91 |
| 24:14:2016:U:OP1 | 57:14:3507:HOH:O | 1.87 | 0.91 |
| 25:16:100:G:OP2 | 57:16:301:HOH:O | 1.87 | 0.91 |
| 24:14:1855:G:N7 | 57:14:3531:HOH:O | 2.02 | 0.91 |
| 30:49:161:THR:HG22 | 30:49:163:ALA:H | 1.33 | 0.91 |
| 2:12:185:ILE:HG22 | 2:12:199:TYR:HB2 | 1.53 | 0.90 |
| 19:AA:50:ALA:HB1 | 19:AA:57:HIS:HB3 | 1.53 | 0.90 |
| 24:1H:409:C:OP1 | 57:1H:3612:HOH:O | 1.88 | 0.90 |
| 52:O8:31:PRO:HB2 | 52:O8:35:GLU:HG2 | 1.53 | 0.90 |
| 1:13:1329:A:H5' | 13:4I:29:ARG:HD2 | 1.53 | 0.90 |
| 22:2L:62:G:O6 | 22:2L:70:C:N4 | 2.03 | 0.90 |
| 1:1G:448:A:OP2 | 1:1G:485:G:N2 | 2.05 | 0.89 |
| 24:1H:567:A:OP1 | 57:1H:3613:HOH:O | 1.89 | 0.89 |
| 24:1H:1187:G:OP2 | 57:1H:3614:HOH:O | 1.90 | 0.89 |
| 24:14:249:C:OP1 | 57:14:3510:HOH:O | 1.90 | 0.89 |
| 36:45:19:GLY:H | 36:45:98:LYS:HZ3 | 1.21 | 0.89 |
| 24:14:1012:U:H3 | 24:14:1143:A:H2 | 1.21 | 0.89 |
| 24:1H:1265:A:OP2 | 57:1H:3616:HOH:O | 1.91 | 0.88 |
| 27:11:242:ARG:O | 57:11:401:HOH:O | 1.90 | 0.88 |
| 24:14:1332:G:N2 | 24:14:1609:A:O2' | 2.06 | 0.88 |
| 24:1H:2062:A:N6 | 24:1H:2503:A:N7 | 2.20 | 0.88 |
| 24:14:2577:A:OP1 | 57:14:3513:HOH:O | 1.92 | 0.88 |
| 24:14:192:C:OP1 | 57:14:3514:HOH:O | 1.92 | 0.88 |
| 24:14:2269:A:OP1 | 57:14:3512:HOH:O | 1.91 | 0.88 |
| 1:13:339:C:OP2 | 34:68:97:ARG:NH1 | 2.07 | 0.88 |
| 24:1H:252:G:OP2 | 35:78:50:ARG:NH1 | 2.07 | 0.88 |
| 24:1H:2305:A:H5" | 30:41:134:GLY:HA3 | 1.56 | 0.88 |
| 24:1H:2447:G:OP2 | 57:1H:3615:HOH:O | 1.91 | 0.88 |
| 24:14:800:A:OP1 | 57:14:3517:HOH:O | 1.92 | 0.88 |
| 1:1G:1128:C:H1' | 1:1G:1146:A:H61 | 1.40 | 0.87 |
| 39:75:92:GLY:HA2 | 39:75:116:ALA:HA | 1.55 | 0.87 |
| 24:1H:2056:G:N7 | 57:1H:3650:HOH:O | 2.05 | 0.87 |
| 31:51:8:PRO:HG2 | 31:51:69:ARG:HH21 | 1.37 | 0.87 |
| 24:14:751:A:OP1 | 57:14:3509:HOH:O | 1.89 | 0.87 |
| 38:65:107:GLU:H | 38:65:110:LEU:HD21 | 1.37 | 0.87 |
| 4:3E:7:PRO:HB2 | 4:3E:10:ARG:HD2 | 1.55 | 0.87 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 24:1H:1280:G:N7 | 57:1H:3649:HOH:O | 2.05 | 0.87 |
| 1:1G:971:G:N2 | 1:1G:1363:A:OP2 | 2.06 | 0.87 |
| 24:1H:1525:G:H2' | 24:1H:1526:G:H8 | 1.37 | 0.87 |
| 1:1G:353:A:H5' | 1:1G:353:A:H8 | 1.37 | 0.87 |
| 1:1G:537:G:N7 | 57:1G:1804:HOH:O | 2.06 | 0.87 |
| 1:13:631:G:H2' | 1:13:632:A:H8 | 1.39 | 0.87 |
| 22:3K:20:C:H5" | 22:3K:68:A:H62 | 1.39 | 0.87 |
| 27:11:182:LEU:H | 27:11:272:ALA:HB3 | 1.37 | 0.87 |
| 24:1H:2582:G:OP2 | 57:1H:3618:HOH:O | 1.93 | 0.87 |
| 19:AA:11:VAL:HG22 | 19:AA:39:THR:HB | 1.57 | 0.87 |
| 24:14:2287:A:H62 | 24:14:2344:U:H3 | 1.22 | 0.87 |
| 30:49:47:LYS:HG3 | 30:49:81:LYS:HG2 | 1.56 | 0.87 |
| 24:1H:1678:G:N2 | 24:1H:1989:G:H22 | 1.72 | 0.86 |
| 25:16:40:U:O2 | 25:16:45:A:N6 | 2.08 | 0.86 |
| 24:14:1861:G:H5' | 26:79:205:LYS:HZ1 | 1.36 | 0.86 |
| 25:16:19:G:H1 | 25:16:64:C:H42 | 1.23 | 0.86 |
| 24:1H:2032:G:N7 | 57:1H:3652:HOH:O | 2.06 | 0.86 |
| 24:14:741:G:OP1 | 57:14:3516:HOH:O | 1.92 | 0.86 |
| 24:1H:932:G:N7 | 57:1H:3655:HOH:O | 2.07 | 0.86 |
| 2:12:118:LEU:HB3 | 2:12:142:LEU:HD12 | 1.57 | 0.86 |
| 24:1H:102:G:OP1 | 48:K8:7:ARG:NH2 | 2.07 | 0.86 |
| 37:98:55:ALA:HA | 37:98:80:PHE:HE1 | 1.38 | 0.86 |
| 1:1G:711:G:OP1 | 6:52:54:LYS:NZ | 2.09 | 0.86 |
| 24:14:2178:C:H4' | 26:79:46:LYS:HD3 | 1.57 | 0.86 |
| 28:29:32:PRO:HD2 | 28:29:50:GLY:HA3 | 1.55 | 0.86 |
| 45:H8:19:ARG:NH1 | 45:H8:84:GLU:O | 2.09 | 0.86 |
| 44:G8:15:VAL:HG21 | 44:G8:42:VAL:HG21 | 1.58 | 0.86 |
| 1:1G:963:G:N3 | 10:1A:55:LYS:NZ | 2.23 | 0.86 |
| 43:B5:63:LYS:H | 43:B5:63:LYS:HE3 | 1.40 | 0.86 |
| 31:51:15:VAL:HG12 | 31:51:28:GLY:HA3 | 1.58 | 0.86 |
| 24:1H:2707:G:H5' | 37:98:68:ARG:HH21 | 1.40 | 0.85 |
| 24:1H:574:C:OP2 | 57:1H:3617:HOH:O | 1.92 | 0.85 |
| 53:L5:47:ARG:HH11 | 53:L5:47:ARG:HG3 | 1.41 | 0.85 |
| 1:13:1453:G:O2' | 20:BI:39:LYS:NZ | 2.10 | 0.85 |
| 24:14:1729:A:O2' | 24:14:1731:G:N2 | 2.09 | 0.85 |
| 22:3K:24:G:H2' | 22:3K:25:G:H8 | 1.40 | 0.85 |
| 24:14:2268:A:OP1 | 57:14:3512:HOH:O | 1.93 | 0.85 |
| 24:1H:764:A:N3 | 27:11:213:ARG:NH1 | 2.25 | 0.85 |
| 44:G8:28:LYS:NZ | 44:G8:64:GLU:OE2 | 2.09 | 0.85 |
| 4:32:31:CYS:C | 4:32:33:MET:H | 1.84 | 0.85 |
| 8:7E:33:GLU:HA | 8:7E:36:LEU:HD12 | 1.57 | 0.85 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 22:2K:15:G:H21 | 22:2K:20:C:H41 | 1.22 | 0.85 |
| 25:16:101:A:OP2 | 57:16:302:HOH:O | 1.95 | 0.85 |
| 22:3K:21:A:N6 | 22:3K:55:U:O4 | 2.09 | 0.85 |
| 24:14:2709:G:O6 | 57:14:3520:HOH:O | 1.94 | 0.85 |
| 1:13:1368:G:H5" | 9:8E:112:LYS:HB3 | 1.59 | 0.85 |
| 24:1H:1250:G:N7 | 35:78:18:ARG:NH2 | 2.24 | 0.85 |
| 24:1H:1496:A:H8 | 24:1H:1577:C:HO2' | 0.89 | 0.85 |
| 52:K5:19:ARG:HH21 | 52:K5:52:VAL:HG11 | 1.42 | 0.85 |
| 2:1E:21:ARG:HD3 | 2:1E:39:ILE:HG12 | 1.57 | 0.85 |
| 15:6I:16:ALA:HB1 | 15:6I:21:ASP:HB3 | 1.57 | 0.85 |
| 24:1H:860:U:H5 | 24:1H:917:A:C2 | 1.95 | 0.84 |
| 54:M5:62:LEU:HB2 | 54:M5:63:PRO:HD2 | 1.57 | 0.84 |
| 1:13:509:A:OP2 | 57:13:1801:HOH:O | 1.94 | 0.84 |
| 24:1H:946:G:OP2 | 57:1H:3623:HOH:O | 1.95 | 0.84 |
| 24:1H:2313:C:H4' | 30:41:91:ARG:HG3 | 1.59 | 0.84 |
| 13:4A:97:PRO:HB2 | 13:4A:101:GLN:HE21 | 1.41 | 0.84 |
| 24:14:31:C:OP1 | 57:14:3518:HOH:O | 1.93 | 0.84 |
| 24:14:2684:U:O4 | 57:14:3519:HOH:O | 1.94 | 0.84 |
| 24:1H:761:A:N7 | 57:1H:3665:HOH:O | 2.09 | 0.84 |
| 24:14:2068:U:H3 | 24:14:2430:A:H2 | 1.25 | 0.84 |
| 24:14:2776:A:O2' | 57:14:3521:HOH:O | 1.95 | 0.84 |
| 24:14:994:C:OP2 | 40:85:54:LYS:NZ | 2.09 | 0.84 |
| 41:95:21:ARG:CD | 41:95:91:TYR:CE1 | 2.61 | 0.84 |
| 41:95:21:ARG:CZ | 41:95:91:TYR:CD2 | 2.60 | 0.84 |
| 24:1H:1997:G:OP2 | 57:1H:3620:HOH:O | 1.94 | 0.84 |
| 28:21:119:ARG:HH11 | 28:21:119:ARG:HG3 | 1.42 | 0.84 |
| 51:N8:40:LYS:NZ | 51:N8:46:CYS:SG | 2.50 | 0.84 |
| 9:82:89:ASN:HB3 | 9:82:92:TYR:HB2 | 1.60 | 0.84 |
| 2:1E:69:LEU:HB3 | 2:1E:162:ILE:HG22 | 1.60 | 0.84 |
| 1:1G:363:A:OP2 | 12:3A:34:ARG:NH2 | 2.11 | 0.84 |
| 24:1H:453:C:OP1 | 57:1H:3622:HOH:O | 1.95 | 0.84 |
| 1:1G:81:G:H1 | 1:1G:88:C:H42 | 1.23 | 0.84 |
| 5:42:101:ILE:HD11 | 5:42:119:LEU:HD23 | 1.60 | 0.84 |
| 29:39:53:THR:HG23 | 29:39:55:GLY:H | 1.43 | 0.84 |
| 2:12:8:LYS:HG2 | 2:12:217:ARG:HE | 1.42 | 0.84 |
| 24:14:67:U:H3 | 24:14:74:A:H2 | 1.22 | 0.84 |
| 24:1H:1324:G:O6 | 57:1H:3621:HOH:O | 1.95 | 0.83 |
| 45:H8:17:ALA:HA | 45:H8:20:ARG:HD2 | 1.60 | 0.83 |
| 1:13:1320:C:OP2 | 19:AI:3:ARG:NH2 | 2.10 | 0.83 |
| 24:1H:654(C):G:N2 | 24:1H:654(R):C:O2 | 2.10 | 0.83 |
| 34:68:98:VAL:HG21 | 34:68:114:ILE:HG23 | 1.61 | 0.83 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 24:14:2343:C:O2' | 24:14:2373:G:O2' | 1.96 | 0.83 |
| 1:13:1500:A:OP1 | 57:13:1802:HOH:O | 1.97 | 0.83 |
| 24:14:138:G:N2 | 43:B5:44:GLU:OE2 | 2.10 | 0.83 |
| 45:D5:157:LEU:HB3 | 45:D5:161:VAL:HA | 1.57 | 0.83 |
| 1:13:201:C:H42 | 1:13:216:G:H1 | 1.26 | 0.83 |
| 4:3E:14:ARG:HB2 | 4:3E:40:PRO:HD2 | 1.59 | 0.83 |
| 24:1H:1264:G:OP1 | 51:N8:19:ARG:NH2 | 2.11 | 0.83 |
| 24:1H:1313:U:OP1 | 57:1H:3619:HOH:O | 1.94 | 0.83 |
| 22:3L:15:G:N1 | 22:3L:57:C:O2 | 2.12 | 0.83 |
| 24:14:761:A:N7 | 57:14:3552:HOH:O | 2.10 | 0.83 |
| 24:14:2306:C:H3' | 24:14:2307:G:H5" | 1.61 | 0.83 |
| 36:45:78:PRO:HB2 | 36:45:81:VAL:HG11 | 1.60 | 0.83 |
| 27:11:17:THR:HG22 | 27:11:205:VAL:H | 1.42 | 0.83 |
| 27:19:255:LYS:H | 27:19:255:LYS:NZ | 1.76 | 0.83 |
| 24:1H:1386:C:H2' | 24:1H:1387:C:H6 | 1.44 | 0.83 |
| 30:41:112:PRO:HG3 | 50:M8:38:LYS:HB2 | 1.61 | 0.83 |
| 41:95:21:ARG:CD | 41:95:91:TYR:CD2 | 2.62 | 0.83 |
| 2:1E:84:GLU:HB3 | 2:1E:219:VAL:HG21 | 1.61 | 0.82 |
| 24:1H:2580:U:H4' | 28:21:130:GLY:HA3 | 1.60 | 0.82 |
| 24:1H:839:U:N3 | 24:1H:939:G:O6 | 2.10 | 0.82 |
| 24:14:2786:U:O2' | 28:29:63:LEU:N | 2.10 | 0.82 |
| 24:1H:249:C:OP1 | 57:1H:3625:HOH:O | 1.95 | 0.82 |
| 36:88:14:ARG:HG2 | 36:88:41:TRP:HH2 | 1.41 | 0.82 |
| 44:G8:94:LYS:HA | 44:G8:94:LYS:HZ2 | 1.42 | 0.82 |
| 24:1H:1776:G:OP2 | 57:1H:3626:HOH:O | 1.97 | 0.82 |
| 24:14:833:U:O2 | 35:35:55:ARG:NH1 | 2.12 | 0.82 |
| 24:1H:805:G:OP1 | 57:1H:3624:HOH:O | 1.95 | 0.82 |
| 34:25:7:TYR:HE1 | 34:25:20:MET:HE3 | 1.45 | 0.82 |
| 24:14:2807:G:N1 | 24:14:2893:G:O6 | 2.11 | 0.82 |
| 29:39:148:LEU:HD21 | 29:39:191:ARG:HH11 | 1.42 | 0.82 |
| 1:13:738:C:H2' | 1:13:739:C:H6 | 1.44 | 0.82 |
| 45:H8:139:VAL:HG22 | 45:H8:155:LEU:HD21 | 1.61 | 0.82 |
| 46:I8:72:ARG:HB2 | 46:I8:75:LEU:HB2 | 1.61 | 0.82 |
| 15:6A:87:ILE:HG22 | 15:6A:88:ARG:H | 1.43 | 0.82 |
| 24:14:2102:U:O2 | 24:14:2187:G:N2 | 2.13 | 0.82 |
| 24:1H:2789:C:O2 | 24:1H:2894:G:N2 | 2.12 | 0.81 |
| 24:1H:1669:A:OP2 | 57:1H:3629:HOH:O | 1.98 | 0.81 |
| 1:1G:664:G:H22 | 1:1G:741:G:H1 | 1.28 | 0.81 |
| 24:14:1141:U:OP2 | 33:15:63:THR:OG1 | 1.97 | 0.81 |
| 40:85:92:ARG:NH1 | 41:95:11:GLN:O | 2.13 | 0.81 |
| 24:1H:2210:G:H3' | 24:1H:2211:G:C8 | 2.15 | 0.81 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 1:1G:827:U:H3 | 1:1G:872:A:H62 | 1.24 | 0.81 |
| 24:14:1364:G:OP2 | 47:F5:2:SER:N | 2.13 | 0.81 |
| 24:1H:804:A:OP1 | 57:1H:3627:HOH:O | 1.97 | 0.81 |
| 22:2K:1:G:H2' | 22:2K:2:G:H8 | 1.45 | 0.81 |
| 24:1H:2057:A:OP2 | 57:1H:3628:HOH:O | 1.97 | 0.81 |
| 1:1G:536:C:OP2 | 57:1G:1802:HOH:O | 1.99 | 0.81 |
| 24:14:660:G:H21 | 35:35:12:ALA:HA | 1.43 | 0.81 |
| 4:32:98:GLU:OE2 | 4:32:103:ASN:ND2 | 2.14 | 0.81 |
| 24:14:2357:U:OP1 | 46:E5:20:ARG:NH1 | 2.14 | 0.81 |
| 38:65:7:TYR:HE2 | 38:65:11:LYS:HZ3 | 1.28 | 0.81 |
| 24:14:452:G:OP2 | 57:14:3524:HOH:O | 1.98 | 0.81 |
| 24:14:1970:A:OP2 | 57:14:3522:HOH:O | 1.97 | 0.81 |
| 24:14:2638:G:HO2' | 24:14:2639:A:H8 | 1.27 | 0.81 |
| 39:75:7:ILE:HA | 39:75:11:GLU:HG3 | 1.59 | 0.81 |
| 1:13:39:G:N2 | 1:13:403:C:O2 | 2.14 | 0.81 |
| 22:2K:15:G:H22 | 22:2K:57:C:H5 | 1.28 | 0.81 |
| 37:55:57:ARG:HH11 | 37:55:57:ARG:HG3 | 1.45 | 0.81 |
| 45:H8:147:GLY:H | 45:H8:174:VAL:HB | 1.45 | 0.81 |
| 1:1G:962:C:H42 | 1:1G:973:G:H1 | 1.29 | 0.81 |
| 24:14:192:C:OP2 | 57:14:3523:HOH:O | 1.97 | 0.81 |
| 50:I5:16:CYS:SG | 50:I5:17:GLY:N | 2.52 | 0.81 |
| 1:13:263:A:OP2 | 20:BI:79:ARG:NH1 | 2.14 | 0.81 |
| 25:16:17:C:N4 | 25:16:108:C:O2 | 2.13 | 0.81 |
| 45:H8:24:LEU:HD11 | 45:H8:86:VAL:HG23 | 1.61 | 0.81 |
| 24:14:2294:C:P | 38:65:89:ARG:HH22 | 2.04 | 0.81 |
| 8:7E:69:ARG:NH2 | 8:7E:73:ASP:O | 2.12 | 0.80 |
| 24:14:2157:G:H2' | 24:14:2158:A:H8 | 1.45 | 0.80 |
| 1:1G:315:A:OP1 | 57:1G:1801:HOH:O | 1.98 | 0.80 |
| 24:1H:993:G:OP1 | 40:C8:50:ARG:NH2 | 2.14 | 0.80 |
| 24:1H:2615:U:OP1 | 57:1H:3616:HOH:O | 1.98 | 0.80 |
| 24:14:654(D):G:H1 | 24:14:654(Q):C:H42 | 1.28 | 0.80 |
| 45:D5:33:LEU:HD23 | 45:D5:90:VAL:HG21 | 1.63 | 0.80 |
| 5:42:126:ARG:HG2 | 5:42:126:ARG:HH11 | 1.44 | 0.80 |
| 9:82:28:VAL:HG22 | 9:82:63:ILE:HB | 1.64 | 0.80 |
| 1:1G:324:G:N7 | 57:1G:1805:HOH:O | 2.13 | 0.80 |
| 1:1G:957:U:OP1 | 19:AA:81:ARG:NH2 | 2.14 | 0.80 |
| 1:1G:974:A:OP2 | 14:5A:41:ARG:NH1 | 2.15 | 0.80 |
| 14:5A:40:CYS:H | 14:5A:43:CYS:HB2 | 1.45 | 0.80 |
| 41:95:21:ARG:NH1 | 41:95:91:TYR:CZ | 2.49 | 0.80 |
| 17:8I:66:SER:HB3 | 17:8I:69:LYS:HB3 | 1.63 | 0.80 |
| 37:98:55:ALA:HA | 37:98:80:PHE:CE1 | 2.14 | 0.80 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 37:55:78:LYS:HE2 | 37:55:83:ILE:HD11 | 1.61 | 0.80 |
| 1:13:507:C:OP2 | 57:13:1805:HOH:O | 2.00 | 0.80 |
| 48:K8:47:ASN:C | 48:K8:49:LYS:H | 1.90 | 0.80 |
| 22:2L:8:4SU:H6 | 22:2L:8:4SU:H5' | 1.64 | 0.80 |
| 24:14:2597:G:O3' | 57:14:3525:HOH:O | 1.99 | 0.80 |
| 25:1J:18:G:H1 | 25:1J:65:C:H42 | 1.28 | 0.80 |
| 24:1H:446:G:OP2 | 57:1H:3634:HOH:O | 2.00 | 0.80 |
| 24:1H:2154:G:H2' | 24:1H:2155:G:H8 | 1.47 | 0.80 |
| 44:G8:39:VAL:HB | 44:G8:42:VAL:HG13 | 1.62 | 0.80 |
| 1:1G:617:G:N7 | 57:1G:1809:HOH:O | 2.14 | 0.80 |
| 24:1H:1856:G:OP2 | 57:1H:3635:HOH:O | 2.00 | 0.80 |
| 44:G8:76:CYS:SG | 44:G8:97:ARG:HG3 | 2.22 | 0.80 |
| 1:1G:963:G:H21 | 10:1A:55:LYS:HE2 | 1.46 | 0.80 |
| 24:14:450:G:N7 | 57:14:3558:HOH:O | 2.14 | 0.80 |
| 24:14:784:A:OP1 | 57:14:3527:HOH:O | 2.00 | 0.80 |
| 24:14:1828:G:OP1 | 57:14:3528:HOH:O | 2.00 | 0.80 |
| 35:35:85:LEU:HA | 35:35:88:LEU:HB2 | 1.63 | 0.80 |
| 16:7I:53:VAL:HG13 | 16:7I:79:VAL:HG22 | 1.64 | 0.79 |
| 42:E8:65:LEU:HD12 | 42:E8:68:ARG:HH11 | 1.47 | 0.79 |
| 13:4A:80:ARG:NH1 | 19:AA:66:MET:SD | 2.55 | 0.79 |
| 1:1G:1243:C:OP2 | 21:1B:10:ARG:NH2 | 2.13 | 0.79 |
| 3:22:204:LEU:HD12 | 3:22:205:GLY:H | 1.46 | 0.79 |
| 33:15:42:TRP:O | 40:85:64:ARG:NH2 | 2.15 | 0.79 |
| 8:7E:51:VAL:HG11 | 8:7E:60:ARG:HD2 | 1.65 | 0.79 |
| 1:13:21:G:OP1 | 57:13:1804:HOH:O | 2.00 | 0.79 |
| 24:1H:1265:A:OP2 | 57:1H:3633:HOH:O | 2.00 | 0.79 |
| 35:35:47:ASP:HB3 | 35:35:48:PRO:O | 1.81 | 0.79 |
| 24:1H:1267:U:O3' | 57:1H:3631:HOH:O | 2.00 | 0.79 |
| 49:L8:12:PRO:O | 49:L8:20:LYS:NZ | 2.15 | 0.79 |
| 50:M8:37:SER:HA | 50:M8:41:PRO:HG2 | 1.64 | 0.79 |
| 27:19:206:LEU:HD22 | 27:19:211:ARG:HG2 | 1.65 | 0.79 |
| 15:6I:87:ILE:HG22 | 15:6I:88:ARG:H | 1.47 | 0.79 |
| 24:1H:598:G:H5' | 35:78:11:GLY:HA3 | 1.64 | 0.79 |
| 1:1G:1256:A:H62 | 1:1G:1277:C:H3' | 1.47 | 0.79 |
| 24:14:2227:A:OP2 | 57:14:3526:HOH:O | 1.99 | 0.79 |
| 6:5E:23:LYS:HZ3 | 6:5E:23:LYS:HB2 | 1.46 | 0.79 |
| 24:1H:1007:C:OP1 | 33:58:35:ARG:NH1 | 2.15 | 0.79 |
| 24:1H:1970:A:OP2 | 57:1H:3632:HOH:O | 2.00 | 0.79 |
| 42:E8:1:MET:HB3 | 42:E8:64:MET:HE2 | 1.64 | 0.79 |
| 1:1G:1224:G:C6 | 1:1G:1322:C:H1' | 2.18 | 0.79 |
| 10:1A:34:VAL:HG22 | 10:1A:74:ILE:HG12 | 1.65 | 0.79 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 24:14:1007:C:OP1 | 33:15:35:ARG:NH1 | 2.15 | 0.79 |
| 39:75:24:PRO:HD3 | 39:75:52:ILE:HD12 | 1.64 | 0.79 |
| 4:3E:29:PRO:HA | 4:3E:34:GLU:HG3 | 1.63 | 0.79 |
| 24:1H:1495:A:OP2 | 57:1H:3637:HOH:O | 2.01 | 0.79 |
| 24:1H:2392:A:H2 | 24:1H:2424:C:H42 | 1.30 | 0.79 |
| 27:19:69:ARG:NH2 | 27:19:128:GLY:O | 2.14 | 0.79 |
| 24:1H:397:G:N7 | 57:1H:3681:HOH:O | 2.15 | 0.79 |
| 29:39:53:THR:HG22 | 29:39:56:GLU:HG3 | 1.64 | 0.79 |
| 1:13:330:C:O2 | 57:13:1803:HOH:O | 1.98 | 0.78 |
| 1:13:1147:C:O2 | 9:8E:16:ARG:NH1 | 2.16 | 0.78 |
| 1:13:1149:C:H2' | 1:13:1150:U:H6 | 1.48 | 0.78 |
| 2:12:167:PRO:O | 2:12:171:ALA:N | 2.16 | 0.78 |
| 24:14:1327:C:OP2 | 57:14:3529:HOH:O | 2.00 | 0.78 |
| 1:13:673:G:H2' | 1:13:674:G:C8 | 2.18 | 0.78 |
| 24:1H:270(K):C:O2 | 24:1H:270(N):G:N1 | 2.14 | 0.78 |
| 24:1H:956:G:OP2 | 36:88:14:ARG:NH2 | 2.16 | 0.78 |
| 46:I8:38:VAL:HG12 | 46:I8:40:GLN:HG2 | 1.64 | 0.78 |
| 4:32:125:HIS:HD1 | 4:32:152:SER:HG | 0.78 | 0.78 |
| 24:14:259:G:N2 | 24:14:621:A:H8 | 1.81 | 0.78 |
| 24:14:1249:U:OP1 | 57:14:3530:HOH:O | 2.01 | 0.78 |
| 24:14:1171:G:OP2 | 24:14:1173:G:N2 | 2.17 | 0.78 |
| 5:4E:148:VAL:HA | 5:4E:151:LEU:HD12 | 1.65 | 0.78 |
| 24:1H:811:U:H2' | 35:78:21:ARG:HA | 1.65 | 0.78 |
| 24:1H:963:U:OP1 | 57:1H:3636:HOH:O | 2.01 | 0.78 |
| 5:42:31:LEU:HD12 | 5:42:45:PHE:HB2 | 1.65 | 0.78 |
| 24:14:593:G:H4' | 54:M5:62:LEU:HD22 | 1.62 | 0.78 |
| 24:1H:1664:A:OP2 | 57:1H:3630:HOH:O | 1.99 | 0.78 |
| 57:1H:3607:HOH:O | 28:21:135:HIS:NE2 | 2.17 | 0.78 |
| 24:14:620:G:N3 | 24:14:620:G:H5" | 1.99 | 0.78 |
| 2:1E:69:LEU:HD22 | 2:1E:155:LEU:HD21 | 1.65 | 0.78 |
| 1:1G:1435:G:H2' | 1:1G:1436:U:C6 | 2.19 | 0.78 |
| 24:14:1041:C:O2 | 24:14:1114:G:N2 | 2.17 | 0.78 |
| 54:Q8:29:LYS:HB3 | 54:Q8:31:HIS:N | 1.99 | 0.78 |
| 3:22:90:GLU:HG3 | 3:22:93:LYS:HD2 | 1.66 | 0.78 |
| 44:C5:19:LYS:HG3 | 44:C5:20:TYR:H | 1.49 | 0.78 |
| 1:13:396:G:O2' | 1:13:398:C:OP1 | 2.00 | 0.78 |
| 7:6E:42:ILE:HG23 | 7:6E:117:ALA:HB2 | 1.65 | 0.78 |
| 1:13:736:C:H2' | 1:13:737:A:C8 | 2.18 | 0.77 |
| 24:1H:583:G:N7 | 57:1H:3690:HOH:O | 2.17 | 0.77 |
| 24:1H:2017:U:OP2 | 57:1H:3640:HOH:O | 2.01 | 0.77 |
| 24:1H:2867:G:OP2 | 39:B8:119:LYS:NZ | 2.13 | 0.77 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 17:8A:45:HIS:CD2 | 17:8A:47:PRO:HG3 | 2.19 | 0.77 |
| 42:A5:59:VAL:HG12 | 42:A5:60:ASN:HD22 | 1.50 | 0.77 |
| 45:D5:161:VAL:HG23 | 45:D5:162:GLU:HG2 | 1.66 | 0.77 |
| 24:1H:563:G:OP2 | 57:1H:3639:HOH:O | 2.01 | 0.77 |
| 36:88:16:ARG:HH21 | 36:88:18:LYS:HD3 | 1.48 | 0.77 |
| 24:14:910:A:C5 | 36:45:13:GLN:HG3 | 2.20 | 0.77 |
| 24:14:2477:C:H2' | 24:14:2529:G:H22 | 1.49 | 0.77 |
| 25:1J:28:C:H42 | 25:1J:56:G:H1 | 1.31 | 0.77 |
| 7:6E:143:ARG:NH2 | 22:3K:43:G:OP1 | 2.17 | 0.77 |
| 16:7I:26:ARG:HG2 | 16:7I:26:ARG:HH11 | 1.49 | 0.77 |
| 24:1H:1141:U:H2' | 33:58:63:THR:HG21 | 1.66 | 0.77 |
| 1:1G:1006:C:O2 | 1:1G:1023:G:N1 | 2.16 | 0.77 |
| 1:1G:1286:A:C8 | 1:1G:1287:A:H4' | 2.20 | 0.77 |
| 28:29:167:VAL:HG12 | 28:29:170:LEU:HD11 | 1.66 | 0.77 |
| 1:1G:998:G:N2 | 1:1G:1043:C:O2 | 2.17 | 0.77 |
| 13:4A:3:ARG:HE | 13:4A:9:ILE:HD11 | 1.48 | 0.77 |
| 22:2L:22:A:N6 | 22:2L:57:C:N3 | 2.32 | 0.77 |
| 33:58:96:GLU:HG2 | 33:58:97:ARG:N | 2.00 | 0.77 |
| 1:1G:1204:A:OP1 | 14:5A:3:ARG:NH1 | 2.18 | 0.77 |
| 2:12:178:ARG:NH1 | 2:12:196:LEU:O | 2.17 | 0.77 |
| 24:14:248:G:OP1 | 57:14:3532:HOH:O | 2.03 | 0.77 |
| 45:D5:105:VAL:HG22 | 45:D5:107:THR:H | 1.50 | 0.77 |
| 17:8I:15:MET:HB3 | 17:8I:18:THR:HB | 1.67 | 0.77 |
| 24:1H:192:C:N3 | 57:1H:3696:HOH:O | 2.18 | 0.77 |
| 37:98:33:ARG:HH22 | 51:N8:55:ARG:HG2 | 1.49 | 0.77 |
| 1:1G:816:A:OP2 | 57:1G:1803:HOH:O | 2.03 | 0.77 |
| 24:14:2475:C:O2 | 24:14:2477:C:N4 | 2.18 | 0.77 |
| 24:1H:452:G:OP2 | 57:1H:3638:HOH:O | 2.01 | 0.77 |
| 24:1H:1399:C:OP1 | 43:F8:25:LYS:NZ | 2.17 | 0.77 |
| 24:1H:1614:A:OP1 | 57:1H:3644:HOH:O | 2.03 | 0.77 |
| 24:1H:2256:G:N7 | 57:1H:3694:HOH:O | 2.18 | 0.77 |
| 24:14:2588:G:OP2 | 57:14:3533:HOH:O | 2.03 | 0.77 |
| 1:13:1159:U:O4' | 1:13:1182:G:N2 | 2.17 | 0.77 |
| 22:2K:60:A:O2' | 22:2K:61:G:O5' | 2.03 | 0.77 |
| 24:1H:592:G:O6 | 24:1H:665:C:N4 | 2.16 | 0.77 |
| 1:1G:1205:U:H4' | 3:22:195:VAL:HG11 | 1.66 | 0.77 |
| 24:14:1105:U:H2' | 24:14:1106:G:H8 | 1.49 | 0.77 |
| 1:13:766:A:OP2 | 57:13:1806:HOH:O | 2.02 | 0.77 |
| 24:1H:2048:G:N7 | 57:1H:3691:HOH:O | 2.17 | 0.77 |
| 25:16:19:G:N2 | 25:16:64:C:N3 | 2.33 | 0.77 |
| 27:11:33:LEU:O | 27:11:64:ILE:HG23 | 1.85 | 0.77 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 5:42:143:ARG:NH1 | 8:72:77:GLU:OE1 | 2.18 | 0.77 |
| 24:14:1073:A:OP2 | 24:14:1094:U:N3 | 2.18 | 0.77 |
| 24:14:2808:U:O2 | 24:14:2892:A:N6 | 2.17 | 0.77 |
| 24:1H:792:G:H5" | 24:1H:793:A:H5' | 1.67 | 0.77 |
| 24:14:493:G:N7 | 57:14:3564:HOH:O | 2.16 | 0.77 |
| 44:C5:39:VAL:O | 44:C5:41:GLY:N | 2.17 | 0.77 |
| 34:68:76:ALA:HB3 | 39:B8:75:ILE:HB | 1.65 | 0.76 |
| 27:19:17:THR:O | 27:19:211:ARG:NH2 | 2.18 | 0.76 |
| 28:29:37:ARG:HB2 | 28:29:46:ALA:H | 1.50 | 0.76 |
| 4:3E:98:GLU:O | 4:3E:103:ASN:ND2 | 2.18 | 0.76 |
| 24:1H:392:C:OP1 | 57:1H:3641:HOH:O | 2.02 | 0.76 |
| 38:A8:25:ARG:NH1 | 38:A8:42:ASP:OD2 | 2.17 | 0.76 |
| 3:2E:13:GLY:HA3 | 14:5I:57:ARG:HE | 1.49 | 0.76 |
| 17:8I:18:THR:OG1 | 17:8I:69:LYS:NZ | 2.17 | 0.76 |
| 8:72:45:ILE:HG22 | 8:72:47:GLY:H | 1.50 | 0.76 |
| 1:13:1346:A:OP1 | 9:8E:120:ARG:NH1 | 2.18 | 0.76 |
| 2:1E:16:HIS:HD2 | 2:1E:210:SER:HA | 1.50 | 0.76 |
| 24:1H:910:A:H62 | 36:88:12:GLN:HA | 1.49 | 0.76 |
| 51:N8:41:PRO:O | 51:N8:44:THR:OG1 | 2.01 | 0.76 |
| 24:14:1416:G:O2' | 24:14:1417:C:O5' | 2.02 | 0.76 |
| 24:14:888:C:H4' | 24:14:889:C:H5' | 1.66 | 0.76 |
| 45:D5:10:ARG:NH2 | 45:D5:26:GLY:O | 2.18 | 0.76 |
| 47:F5:64:ALA:HA | 47:F5:67:ILE:HD12 | 1.67 | 0.76 |
| 24:1H:2788:C:O2' | 24:1H:2809:A:N3 | 2.19 | 0.76 |
| 4:32:139:ARG:HH11 | 4:32:139:ARG:HG3 | 1.50 | 0.76 |
| 26:79:201:PRO:HG2 | 26:79:204:ALA:HB2 | 1.67 | 0.76 |
| 35:35:122:PRO:HB3 | 35:35:141:ALA:HB1 | 1.68 | 0.76 |
| 24:1H:1030:G:O6 | 24:1H:1124:C:N4 | 2.15 | 0.76 |
| 24:1H:2392:A:C8 | 35:78:61:ARG:HG2 | 2.18 | 0.76 |
| 2:1E:7:VAL:HG21 | 2:1E:11:LEU:HD22 | 1.67 | 0.76 |
| 2:1E:21:ARG:HB3 | 2:1E:39:ILE:HA | 1.66 | 0.76 |
| 47:J8:41:ARG:HH11 | 47:J8:41:ARG:HG3 | 1.48 | 0.76 |
| 5:42:50:GLU:HB3 | 5:42:53:LEU:HD13 | 1.64 | 0.76 |
| 19:AA:9:VAL:HG11 | 50:I5:63:TYR:HB3 | 1.65 | 0.76 |
| 22:3L:17:OMG:N2 | 22:3L:67:A:OP2 | 2.19 | 0.76 |
| 35:35:47:ASP:OD2 | 35:35:50:ARG:NH1 | 2.19 | 0.76 |
| 1:13:1157:A:O2' | 1:13:1181:G:N2 | 2.18 | 0.76 |
| 27:11:65:ILE:HD11 | 27:11:67:PHE:CZ | 2.20 | 0.76 |
| 35:78:88:LEU:HD12 | 35:78:95:VAL:HG11 | 1.68 | 0.76 |
| 36:88:86:GLY:HA3 | 36:88:87:LYS:HG3 | 1.67 | 0.76 |
| 1:1G:771:G:N7 | 57:1G:1813:HOH:O | 2.17 | 0.76 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 24:14:1084:A:O2' | 24:14:1105:U:O2' | 2.03 | 0.76 |
| 25:1J:40:U:O2 | 25:1J:45:A:N6 | 2.18 | 0.76 |
| 1:13:454:C:OP1 | 16:7I:75:ARG:NH1 | 2.19 | 0.76 |
| 2:1E:111:ARG:HG2 | 2:1E:111:ARG:HH11 | 1.51 | 0.76 |
| 24:1H:751:A:OP1 | 57:1H:3642:HOH:O | 2.02 | 0.76 |
| 24:1H:751:A:OP1 | 57:1H:3645:HOH:O | 2.04 | 0.76 |
| 1:1G:957:U:H1' | 1:1G:960:U:C5 | 2.20 | 0.76 |
| 45:D5:59:LEU:O | 45:D5:61:LEU:N | 2.17 | 0.76 |
| 1:13:511:C:OP2 | 4:3E:49:ARG:NH2 | 2.20 | 0.75 |
| 24:1H:1334:G:N7 | 57:1H:3701:HOH:O | 2.20 | 0.75 |
| 24:14:399:G:OP2 | 57:14:3535:HOH:O | 2.04 | 0.75 |
| 38:65:14:VAL:HG21 | 38:65:89:ARG:HG2 | 1.67 | 0.75 |
| 38:65:106:ARG:NH1 | 38:65:106:ARG:O | 2.19 | 0.75 |
| 45:D5:128:VAL:HG23 | 45:D5:160:GLY:HA3 | 1.67 | 0.75 |
| 24:1H:450:G:O6 | 57:1H:3643:HOH:O | 2.03 | 0.75 |
| 24:1H:1803:A:O2' | 27:11:259:THR:HG21 | 1.86 | 0.75 |
| 24:1H:2327:A:H2' | 24:1H:2328:A:C8 | 2.21 | 0.75 |
| 27:19:242:ARG:O | 57:19:401:HOH:O | 2.03 | 0.75 |
| 40:85:92:ARG:HD3 | 40:85:95:LEU:HD12 | 1.68 | 0.75 |
| 24:1H:2635:C:H5" | 28:21:78:LEU:HA | 1.67 | 0.75 |
| 26:79:19:ILE:HG12 | 26:79:223:ARG:HG2 | 1.67 | 0.75 |
| 4:3E:85:LYS:O | 4:3E:89:THR:OG1 | 2.02 | 0.75 |
| 8:7E:41:ARG:NH1 | 8:7E:123:GLU:OE2 | 2.17 | 0.75 |
| 10:1I:33:GLN:HB2 | 10:1I:75:ILE:HG12 | 1.69 | 0.75 |
| 24:1H:1728:G:H8 | 24:1H:1732:A:H62 | 1.32 | 0.75 |
| 34:68:4:PRO:O | 34:68:5:GLN:HB2 | 1.84 | 0.75 |
| 39:B8:51:ARG:HG3 | 39:B8:98:LYS:HE3 | 1.68 | 0.75 |
| 1:1G:929:G:N2 | 1:1G:1388:C:O2 | 2.19 | 0.75 |
| 1:1G:1315:U:O2' | 1:1G:1360:A:O2' | 2.05 | 0.75 |
| 3:22:27:LYS:NZ | 3:22:28:GLN:OE1 | 2.17 | 0.75 |
| 48:G5:17:SER:HB2 | 48:G5:20:GLU:H | 1.50 | 0.75 |
| 2:1E:17:PHE:HA | 2:1E:44:LEU:HD11 | 1.68 | 0.75 |
| 24:1H:1021:A:H3' | 24:1H:1022:G:H5" | 1.69 | 0.75 |
| 1:1G:448:A:H62 | 1:1G:486:U:H3 | 1.35 | 0.75 |
| 14:5A:23:ARG:NH1 | 14:5A:29:ARG:O | 2.19 | 0.75 |
| 5:4E:126:ARG:HG3 | 5:4E:126:ARG:HH11 | 1.51 | 0.75 |
| 24:1H:2032:G:H21 | 28:21:146:THR:HG23 | 1.49 | 0.75 |
| 24:14:1047:G:H21 | 24:14:1111:A:H62 | 1.35 | 0.75 |
| 37:55:37:THR:HG22 | 37:55:39:PRO:HD2 | 1.69 | 0.75 |
| 1:13:321:A:N7 | 1:13:328:C:O2' | 2.19 | 0.75 |
| 1:13:376:G:H5" | 16:7I:5:ARG:HG3 | 1.69 | 0.75 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 1:13:407:G:OP1 | 4:3E:115:ARG:NH1 | 2.20 | 0.75 |
| 24:1H:1403:C:H5" | 24:1H:1471:A:H1' | 1.67 | 0.75 |
| 33:58:58:ASP:N | 33:58:58:ASP:OD1 | 2.17 | 0.75 |
| 24:14:1012:U:OP2 | 40:85:70:ARG:NH2 | 2.19 | 0.75 |
| 8:7E:64:LYS:HB3 | 8:7E:79:VAL:HG21 | 1.67 | 0.75 |
| 24:1H:881:G:O6 | 24:1H:882:G:N2 | 2.20 | 0.75 |
| 24:1H:2213:U:O2 | 47:J8:52:ARG:NH2 | 2.20 | 0.75 |
| 28:21:55:ASN:ND2 | 28:21:73:GLU:O | 2.19 | 0.75 |
| 39:75:50:ILE:HD11 | 39:75:102:ILE:HD11 | 1.66 | 0.75 |
| 1:13:881:G:OP2 | 12:3I:12:ARG:NH2 | 2.19 | 0.74 |
| 1:13:1378:C:O2 | 7:6E:76:ARG:NH1 | 2.20 | 0.74 |
| 24:1H:2287:A:H62 | 24:1H:2344:U:H3 | 1.33 | 0.74 |
| 27:11:228:PRO:O | 57:11:402:HOH:O | 2.03 | 0.74 |
| 39:B8:107:ASP:OD1 | 39:B8:107:ASP:N | 2.20 | 0.74 |
| 4:32:73:ARG:O | 4:32:77:ASN:ND2 | 2.20 | 0.74 |
| 24:14:1250:G:OP2 | 35:35:21:ARG:NH1 | 2.20 | 0.74 |
| 24:1H:1614:A:OP1 | 57:1H:3646:HOH:O | 2.05 | 0.74 |
| 1:1G:512:U:H2' | 1:1G:513:C:H6 | 1.52 | 0.74 |
| 24:14:1022:G:O2' | 24:14:1023:U:OP2 | 2.05 | 0.74 |
| 31:59:30:LYS:NZ | 31:59:79:VAL:O | 2.19 | 0.74 |
| 1:13:1077:G:N2 | 1:13:1080:A:OP2 | 2.19 | 0.74 |
| 24:1H:1138:G:H21 | 33:58:106:MET:HE3 | 1.51 | 0.74 |
| 24:1H:1430:C:H2' | 24:1H:1431:U:C6 | 2.21 | 0.74 |
| 24:1H:2485:G:H5" | 36:88:46:GLN:HE21 | 1.51 | 0.74 |
| 1:1G:895:G:H1 | 1:1G:904:C:H42 | 1.35 | 0.74 |
| 22:2L:12:C:H5 | 22:2L:24:G:H1 | 1.35 | 0.74 |
| 24:14:2656:U:H3 | 24:14:2665:A:H2 | 1.34 | 0.74 |
| 24:1H:2074:U:OP1 | 57:1H:3651:HOH:O | 2.06 | 0.74 |
| 25:16:52:A:OP2 | 38:A8:59:LYS:NZ | 2.17 | 0.74 |
| 1:1G:1187:G:N7 | 57:1G:1815:HOH:O | 2.20 | 0.74 |
| 27:19:89:SER:HB2 | 27:19:159:ALA:H | 1.51 | 0.74 |
| 1:13:812:C:N3 | 57:13:1812:HOH:O | 2.19 | 0.74 |
| 7:6E:111:ARG:NH1 | 7:6E:113:GLU:OE2 | 2.19 | 0.74 |
| 21:1F:9:ARG:NH2 | 21:1F:21:TYR:O | 2.20 | 0.74 |
| 34:68:2:ILE:HD12 | 34:68:6:THR:HG21 | 1.68 | 0.74 |
| 24:14:1975:G:OP2 | 57:14:3536:HOH:O | 2.05 | 0.74 |
| 38:65:25:ARG:HD2 | 38:65:88:ASP:HB2 | 1.68 | 0.74 |
| 1:13:748:C:H4' | 1:13:749:C:O5' | 1.88 | 0.74 |
| 24:1H:307:G:N7 | 57:1H:3703:HOH:O | 2.20 | 0.74 |
| 38:A8:35:ILE:HD11 | 38:A8:101:LEU:HD23 | 1.69 | 0.74 |
| 43:F8:60:ARG:HH22 | 53:P8:47:ARG:HH22 | 1.35 | 0.74 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 1:1G:750:G:N3 | 15:6A:23:GLY:HA3 | 2.03 | 0.74 |
| 3:22:79:ARG:HH22 | 3:22:83:ARG:HB3 | 1.51 | 0.74 |
| 24:14:330:A:H2 | 24:14:1210:A:HO2' | 1.35 | 0.74 |
| 24:14:1525:G:H2' | 24:14:1526:G:H8 | 1.52 | 0.74 |
| 24:14:2592:G:N7 | 57:14:3567:HOH:O | 2.19 | 0.74 |
| 1:13:4:U:O2' | 8:7E:102:ARG:NH1 | 2.19 | 0.74 |
| 31:51:8:PRO:HD2 | 31:51:69:ARG:HE | 1.52 | 0.74 |
| 24:14:995:C:O2 | 33:15:3:THR:OG1 | 2.05 | 0.74 |
| 24:14:2102:U:H3 | 24:14:2187:G:H1 | 1.36 | 0.74 |
| 24:14:2392:A:H8 | 35:35:61:ARG:HB3 | 1.53 | 0.74 |
| 25:1J:7:G:H4' | 38:65:29:PHE:CD2 | 2.22 | 0.74 |
| 34:25:13:ASN:ND2 | 34:25:97:ARG:H | 1.84 | 0.74 |
| 41:95:21:ARG:CZ | 41:95:91:TYR:CD1 | 2.69 | 0.74 |
| 28:21:135:HIS:NE2 | 57:21:401:HOH:O | 2.19 | 0.74 |
| 41:D8:19:LYS:HG3 | 41:D8:95:LEU:HD23 | 1.70 | 0.74 |
| 19:AA:49:ILE:HD13 | 19:AA:62:ILE:HD13 | 1.70 | 0.74 |
| 24:14:9:U:N3 | 24:14:2629:A:N1 | 2.35 | 0.74 |
| 1:13:1058:G:OP1 | 3:2E:199:LYS:NZ | 2.21 | 0.74 |
| 4:3E:98:GLU:OE2 | 4:3E:103:ASN:ND2 | 2.20 | 0.74 |
| 24:1H:249:C:O5' | 57:1H:3625:HOH:O | 2.04 | 0.74 |
| 24:1H:2331:G:H4' | 46:I8:43:THR:H | 1.52 | 0.74 |
| 24:1H:2597:G:O3' | 57:1H:3653:HOH:O | 2.06 | 0.74 |
| 10:1A:61:GLU:OE2 | 14:5A:45:ARG:NH1 | 2.21 | 0.74 |
| 24:14:49:A:H5" | 24:14:51:G:O4' | 1.87 | 0.74 |
| 30:49:98:ARG:HH21 | 50:I5:2:LYS:HE2 | 1.51 | 0.74 |
| 1:13:136:C:N4 | 1:13:227:G:O6 | 2.18 | 0.74 |
| 24:1H:298:G:N7 | 57:1H:3702:HOH:O | 2.20 | 0.74 |
| 1:1G:1228:C:H2' | 1:1G:1229:A:H8 | 1.51 | 0.74 |
| 24:1H:1728:G:H3' | 24:1H:1729:A:H5" | 1.70 | 0.73 |
| 24:1H:2243:U:OP1 | 57:1H:3648:HOH:O | 2.05 | 0.73 |
| 10:1A:48:THR:OG1 | 10:1A:62:HIS:ND1 | 2.18 | 0.73 |
| 24:14:2685:G:O6 | 57:14:3519:HOH:O | 2.06 | 0.73 |
| 32:69:74:ASN:O | 32:69:139:GLN:NE2 | 2.21 | 0.73 |
| 6:5E:36:ARG:NH2 | 6:5E:38:GLU:OE2 | 2.22 | 0.73 |
| 11:2I:21:ILE:HB | 11:2I:84:VAL:HG12 | 1.69 | 0.73 |
| 20:BI:73:HIS:HB3 | 20:BI:74:LYS:HG2 | 1.70 | 0.73 |
| 24:1H:2713:A:OP2 | 57:1H:3647:HOH:O | 2.05 | 0.73 |
| 37:55:107:ASP:HB3 | 37:55:109:ALA:H | 1.52 | 0.73 |
| 43:B5:44:GLU:HG3 | 43:B5:51:VAL:HG23 | 1.70 | 0.73 |
| 1:13:468:A:H5" | 16:7I:80:PHE:HB3 | 1.70 | 0.73 |
| 1:13:677:U:H3 | 1:13:713:G:H22 | 1.34 | 0.73 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 1:13:1023:G:OP2 | 1:13:1024:G:N2 | 2.21 | 0.73 |
| 24:1H:1175:U:O2 | 24:1H:1176:G:N2 | 2.21 | 0.73 |
| 24:14:1012:U:N3 | 24:14:1143:A:H2 | 1.86 | 0.73 |
| 24:1H:1190:G:N7 | 57:1H:3710:HOH:O | 2.21 | 0.73 |
| 1:1G:1256:A:OP2 | 3:22:26:LYS:NZ | 2.16 | 0.73 |
| 24:14:2287:A:N1 | 24:14:2346:A:H2 | 1.86 | 0.73 |
| 24:1H:2243:U:OP1 | 57:1H:3654:HOH:O | 2.06 | 0.73 |
| 25:16:40:U:H3 | 25:16:43:C:H5" | 1.53 | 0.73 |
| 44:G8:82:PRO:HG3 | 44:G8:97:ARG:HD2 | 1.71 | 0.73 |
| 27:19:37:LEU:HA | 27:19:38:LYS:HG2 | 1.68 | 0.73 |
| 28:29:24:THR:HG21 | 28:29:188:VAL:HB | 1.69 | 0.73 |
| 38:65:78:LEU:HD21 | 38:65:107:GLU:HB3 | 1.69 | 0.73 |
| 44:C5:27:VAL:HA | 44:C5:39:VAL:HG12 | 1.69 | 0.73 |
| 10:1I:26:ALA:HB1 | 10:1I:84:GLN:HG3 | 1.69 | 0.73 |
| 48:K8:17:SER:HB2 | 48:K8:20:GLU:H | 1.54 | 0.73 |
| 3:22:50:ALA:HB2 | 3:22:75:VAL:HB | 1.70 | 0.73 |
| 22:3L:85:A:O2' | 24:14:2394:C:N3 | 2.20 | 0.73 |
| 12:3I:47:LYS:HG2 | 12:3I:48:PRO:HD3 | 1.69 | 0.73 |
| 1:1G:411:A:C5 | 1:1G:413:G:H1' | 2.23 | 0.73 |
| 24:14:780:G:H21 | 24:14:783:A:H62 | 1.37 | 0.73 |
| 24:14:1084:A:N7 | 24:14:1085:A:N6 | 2.37 | 0.73 |
| 24:14:1828:G:OP2 | 57:14:3538:HOH:O | 2.05 | 0.73 |
| 31:59:10:PRO:HG2 | 31:59:50:VAL:HG13 | 1.71 | 0.73 |
| 31:59:54:ARG:NH2 | 31:59:57:ASP:OD1 | 2.21 | 0.73 |
| 1:13:1003:G:N1 | 1:13:1036:G:O6 | 2.22 | 0.73 |
| 24:1H:2836:U:H2' | 24:1H:2837:G:C8 | 2.23 | 0.73 |
| 27:11:26:LYS:O | 27:11:27:THR:OG1 | 2.07 | 0.73 |
| 42:E8:18:ARG:HD3 | 42:E8:76:VAL:HG13 | 1.70 | 0.73 |
| 8:72:12:ARG:NH1 | 8:72:25:ASP:O | 2.22 | 0.73 |
| 8:72:49:GLU:OE2 | 8:72:62:TYR:OH | 2.07 | 0.73 |
| 51:J5:16:ARG:NH1 | 51:J5:17:ASP:OD1 | 2.22 | 0.73 |
| 24:1H:620:G:H4' | 24:1H:621:A:H5" | 1.71 | 0.73 |
| 24:1H:1105:U:H2' | 24:1H:1106:G:H8 | 1.52 | 0.73 |
| 24:1H:2849:U:H4' | 24:1H:2868:A:C2 | 2.24 | 0.73 |
| 30:41:112:PRO:HB3 | 50:M8:37:SER:H | 1.54 | 0.73 |
| 45:H8:52:SER:O | 45:H8:52:SER:OG | 2.03 | 0.73 |
| 24:14:1633:G:O6 | 57:14:3534:HOH:O | 2.04 | 0.73 |
| 24:14:2785:C:O2' | 28:29:64:LYS:HE3 | 1.88 | 0.73 |
| 1:13:601:C:H2' | 1:13:602:A:H8 | 1.54 | 0.73 |
| 9:8E:13:ALA:HB2 | 9:8E:68:GLY:HA3 | 1.69 | 0.73 |
| 13:4I:59:TYR:O | 13:4I:63:THR:OG1 | 2.06 | 0.73 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 22:2K:20:C:O2' | 22:2K:21:A:OP2 | 2.06 | 0.73 |
| 24:1H:141:A:H8 | 24:1H:1595:G:H21 | 1.37 | 0.73 |
| 24:1H:2006:C:OP1 | 57:1H:3604:HOH:O | 2.06 | 0.73 |
| 19:AA:22:LEU:HB3 | 19:AA:27:GLU:HG3 | 1.70 | 0.73 |
| 24:14:674:G:O2' | 29:39:74:ARG:HG3 | 1.87 | 0.73 |
| 1:13:143:A:H2 | 1:13:220:G:H1 | 1.35 | 0.72 |
| 1:13:559:A:OP1 | 5:4E:126:ARG:NH2 | 2.22 | 0.72 |
| 5:4E:148:VAL:HG21 | 8:7E:107:LEU:HD22 | 1.72 | 0.72 |
| 24:14:1019:U:H3 | 24:14:1142(A):A:H62 | 1.35 | 0.72 |
| 24:1H:1386:C:H2' | 24:1H:1387:C:C6 | 2.23 | 0.72 |
| 30:41:144:ILE:HA | 30:41:148:MET:HE2 | 1.72 | 0.72 |
| 42:E8:45:TYR:OH | 42:E8:49:LYS:NZ | 2.21 | 0.72 |
| 24:14:654(E):C:H42 | 24:14:654(P):G:H1 | 1.38 | 0.72 |
| 24:14:2410:G:OP2 | 57:14:3540:HOH:O | 2.06 | 0.72 |
| 39:75:33:LYS:HE3 | 39:75:40:THR:HG21 | 1.69 | 0.72 |
| 5:4E:11:ILE:HD11 | 5:4E:31:LEU:HD22 | 1.71 | 0.72 |
| 8:7E:112:LEU:HB3 | 8:7E:133:LEU:HA | 1.71 | 0.72 |
| 24:1H:981:A:OP1 | 57:1H:3656:HOH:O | 2.07 | 0.72 |
| 24:1H:1281:G:N7 | 57:1H:3708:HOH:O | 2.21 | 0.72 |
| 22:2L:18:G:H4' | 22:2L:19:C:OP1 | 1.88 | 0.72 |
| 24:14:270(L):U:H3' | 24:14:270(M):U:H5" | 1.70 | 0.72 |
| 24:14:453:C:OP1 | 57:14:3542:HOH:O | 2.07 | 0.72 |
| 25:1J:80:U:H2' | 25:1J:81:G:N2 | 2.04 | 0.72 |
| 24:1H:2334:G:O6 | 46:I8:74:ARG:NH1 | 2.21 | 0.72 |
| 37:98:33:ARG:HH11 | 37:98:113:LEU:HD21 | 1.53 | 0.72 |
| 45:H8:95:PRO:HA | 45:H8:130:PRO:HD3 | 1.71 | 0.72 |
| 2:12:166:ASP:HB3 | 2:12:169:LYS:HB2 | 1.70 | 0.72 |
| 1:13:542:G:OP1 | 4:3E:10:ARG:NH2 | 2.22 | 0.72 |
| 24:1H:2298:A:H62 | 24:1H:2318:G:H8 | 1.36 | 0.72 |
| 28:21:92:THR:O | 28:21:95:ILE:HG12 | 1.88 | 0.72 |
| 32:61:110:ASP:OD2 | 32:61:113:ARG:NH1 | 2.22 | 0.72 |
| 2:12:74:LYS:NZ | 2:12:205:ASP:OD1 | 2.22 | 0.72 |
| 24:14:887:A:OP2 | 24:14:888:C:N4 | 2.22 | 0.72 |
| 24:14:2124:G:H1 | 26:79:217:THR:HA | 1.55 | 0.72 |
| 1:13:148:G:H2' | 1:13:149:A:H8 | 1.55 | 0.72 |
| 1:13:1182:G:H4' | 1:13:1183:A:H5' | 1.71 | 0.72 |
| 24:1H:761:A:OP1 | 57:1H:3603:HOH:O | 2.07 | 0.72 |
| 24:1H:972:G:O2' | 57:1H:3657:HOH:O | 2.07 | 0.72 |
| 44:G8:84:ARG:NH2 | 57:G8:301:HOH:O | 2.22 | 0.72 |
| 24:14:987:G:OP2 | 57:14:3545:HOH:O | 2.08 | 0.72 |
| 24:14:1817:G:OP1 | 27:19:88:ARG:NH2 | 2.17 | 0.72 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 45:D5:152:ALA:HA | 45:D5:171:ILE:HB | 1.70 | 0.72 |
| 1:13:266:G:H5" | 1:13:268:C:H41 | 1.54 | 0.72 |
| 13:4I:17:VAL:O | 13:4I:20:THR:OG1 | 2.05 | 0.72 |
| 24:1H:442:G:H4' | 29:31:46:ARG:HG3 | 1.71 | 0.72 |
| 35:78:45:LEU:H | 35:78:45:LEU:HD22 | 1.55 | 0.72 |
| 37:98:33:ARG:HG3 | 37:98:115:GLU:HB3 | 1.71 | 0.72 |
| 1:1G:44:G:N2 | 1:1G:398:C:O2 | 2.19 | 0.72 |
| 24:14:1058:U:O2 | 24:14:1080:A:N6 | 2.19 | 0.72 |
| 24:14:2329:G:H2' | 24:14:2330:G:C8 | 2.24 | 0.72 |
| 35:35:79:ARG:HG3 | 35:35:110:TYR:HB2 | 1.72 | 0.72 |
| 41:95:37:VAL:HG11 | 41:95:57:VAL:H | 1.55 | 0.72 |
| 1:13:411:A:C4 | 1:13:413:G:H1' | 2.24 | 0.72 |
| 24:1H:298:G:N7 | 57:1H:3713:HOH:O | 2.23 | 0.72 |
| 24:1H:1689:A:H62 | 24:1H:1698:A:H2 | 1.38 | 0.72 |
| 24:14:958:U:O2 | 25:1J:89(A):A:O2' | 2.06 | 0.72 |
| 24:14:2392:A:H2 | 24:14:2424:C:H42 | 1.35 | 0.72 |
| 32:69:1:MET:HE2 | 32:69:23:PRO:HB3 | 1.72 | 0.72 |
| 9:8E:42:ARG:NH1 | 9:8E:71:SER:OG | 2.22 | 0.72 |
| 24:1H:2126:A:O2' | 24:1H:2162:G:N2 | 2.22 | 0.72 |
| 38:A8:24:LEU:HB2 | 38:A8:85:VAL:HG12 | 1.72 | 0.72 |
| 2:12:63:MET:HG3 | 2:12:225:ALA:HB1 | 1.71 | 0.72 |
| 3:22:47:LEU:O | 3:22:50:ALA:N | 2.23 | 0.72 |
| 19:AA:40:ILE:HD11 | 19:AA:69:HIS:HB2 | 1.72 | 0.72 |
| 24:14:751:A:OP1 | 57:14:3546:HOH:O | 2.08 | 0.72 |
| 24:14:1633:G:O6 | 57:14:3537:HOH:O | 2.05 | 0.72 |
| 24:14:1652:A:OP1 | 37:55:8:ARG:NH1 | 2.23 | 0.72 |
| 24:1H:1510:A:O2' | 24:1H:1512:G:N7 | 2.22 | 0.71 |
| 1:1G:1281:U:OP2 | 1:1G:1282:C:N4 | 2.17 | 0.71 |
| 9:82:53:VAL:HG23 | 9:82:55:ALA:H | 1.53 | 0.71 |
| 20:BA:45:GLN:HA | 20:BA:91:LEU:HD22 | 1.72 | 0.71 |
| 24:14:2053:G:OP2 | 57:14:3543:HOH:O | 2.07 | 0.71 |
| 24:14:2873:A:H8 | 37:55:6:SER:H | 1.36 | 0.71 |
| 24:1H:399:G:OP2 | 57:1H:3659:HOH:O | 2.08 | 0.71 |
| 24:1H:1332:G:N2 | 24:1H:1610:A:C8 | 2.58 | 0.71 |
| 1:1G:735:C:H2' | 1:1G:736:C:H6 | 1.55 | 0.71 |
| 24:14:956:G:OP2 | 36:45:14:ARG:NH2 | 2.23 | 0.71 |
| 30:49:66:GLN:NE2 | 30:49:93:THR:O | 2.23 | 0.71 |
| 1:13:837:G:H1 | 1:13:849:C:H42 | 1.38 | 0.71 |
| 24:14:1784:A:OP1 | 57:14:3544:HOH:O | 2.07 | 0.71 |
| 24:1H:870:A:O5' | 36:88:5:ARG:NH2 | 2.22 | 0.71 |
| 24:1H:1942:C:OP2 | 24:1H:1943:U:O2' | 2.08 | 0.71 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 32:61:132:PRO:O | 32:61:133:HIS:ND1 | 2.23 | 0.71 |
| 24:14:2353:G:N7 | 57:14:3553:HOH:O | 2.21 | 0.71 |
| 43:B5:60:ARG:HH21 | 53:L5:47:ARG:HH22 | 1.38 | 0.71 |
| 46:E5:11:ARG:O | 46:E5:14:ARG:NH2 | 2.23 | 0.71 |
| 1:13:1135:U:H4' | 1:13:1136:U:H5 | 1.55 | 0.71 |
| 11:2I:86:GLY:N | 11:2I:112:THR:OG1 | 2.24 | 0.71 |
| 1:1G:1503:A:O2' | 1:1G:1504:G:O5' | 2.08 | 0.71 |
| 24:14:2577:A:OP1 | 57:14:3502:HOH:O | 2.07 | 0.71 |
| 32:61:64:GLU:HG3 | 32:61:67:ARG:HH21 | 1.55 | 0.71 |
| 47:J8:65:SER:OG | 47:J8:66:HIS:ND1 | 2.21 | 0.71 |
| 3:22:113:ALA:HB2 | 3:22:202:ILE:HG13 | 1.71 | 0.71 |
| 30:49:29:TRP:O | 30:49:33:ARG:NH1 | 2.24 | 0.71 |
| 38:65:35:ILE:HD11 | 38:65:97:ARG:HE | 1.55 | 0.71 |
| 1:13:200:G:N2 | 1:13:218:C:O2 | 2.24 | 0.71 |
| 24:1H:1434:A:H61 | 24:1H:1558:A:N6 | 1.88 | 0.71 |
| 24:1H:1798:U:H5' | 27:11:259:THR:HG22 | 1.72 | 0.71 |
| 39:B8:26:ASP:HB3 | 39:B8:92:GLY:H | 1.56 | 0.71 |
| 24:14:2720:U:H3 | 24:14:2873:A:H2 | 1.38 | 0.71 |
| 35:35:47:ASP:HB3 | 35:35:48:PRO:C | 2.16 | 0.71 |
| 39:75:108:ARG:HA | 39:75:111:ARG:HD2 | 1.73 | 0.71 |
| 47:F5:87:PRO:HA | 47:F5:90:ILE:HG22 | 1.71 | 0.71 |
| 1:13:313:A:H2' | 1:13:314:C:C6 | 2.25 | 0.71 |
| 24:1H:1187:G:OP2 | 57:1H:3664:HOH:O | 2.09 | 0.71 |
| 24:1H:1221:C:H2' | 24:1H:1222:C:H6 | 1.54 | 0.71 |
| 24:1H:1525:G:H2' | 24:1H:1526:G:C8 | 2.25 | 0.71 |
| 24:1H:1641:A:OP2 | 57:1H:3661:HOH:O | 2.09 | 0.71 |
| 24:1H:2017:U:P | 57:1H:3640:HOH:O | 2.49 | 0.71 |
| 36:88:135:ASP:HB3 | 36:88:137:TYR:H | 1.56 | 0.71 |
| 51:N8:55:ARG:HG3 | 51:N8:57:VAL:H | 1.56 | 0.71 |
| 23:4L:13:A:O2' | 23:4L:14:A:OP1 | 2.09 | 0.71 |
| 24:14:1678:G:N2 | 24:14:1989:G:H22 | 1.89 | 0.71 |
| 14:5I:24:CYS:HB2 | 14:5I:28:GLY:H | 1.55 | 0.71 |
| 24:1H:2432:A:C4 | 47:J8:33:LYS:HG2 | 2.25 | 0.71 |
| 24:1H:2701:C:H3' | 24:1H:2702:U:H5" | 1.72 | 0.71 |
| 9:82:34:ASN:HA | 9:82:37:PHE:HD2 | 1.55 | 0.71 |
| 24:14:328:U:H4' | 44:C5:68:HIS:ND1 | 2.06 | 0.71 |
| 15:6I:3:ILE:HD13 | 15:6I:34:LEU:HD23 | 1.70 | 0.71 |
| 19:AI:40:ILE:HG23 | 19:AI:41:VAL:HG13 | 1.71 | 0.71 |
| 24:14:960:A:N6 | 36:45:83:MET:HE2 | 2.06 | 0.71 |
| 38:65:93:LYS:HG2 | 38:65:95:HIS:HB2 | 1.72 | 0.71 |
| 46:I8:37:LEU:N | 46:I8:59:LEU:O | 2.21 | 0.70 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 33:15:17:ASP:OD1 | 33:15:56:ASN:ND2 | 2.24 | 0.70 |
| 24:1H:71:A:H2 | 43:F8:31:HIS:HE2 | 1.37 | 0.70 |
| 44:G8:97:ARG:NH2 | 44:G8:104:GLY:O | 2.24 | 0.70 |
| 53:P8:12:ARG:HH21 | 53:P8:44:PRO:HB3 | 1.55 | 0.70 |
| 1:1G:1151:A:H5" | 10:1A:42:THR:HG23 | 1.72 | 0.70 |
| 24:14:252:G:OP2 | 35:35:50:ARG:NH2 | 2.24 | 0.70 |
| 44:C5:48:ALA:HB3 | 44:C5:59:GLY:HA2 | 1.72 | 0.70 |
| 48:G5:68:ARG:HA | 48:G5:72:ALA:HB2 | 1.73 | 0.70 |
| 54:M5:40:GLU:H | 54:M5:43:GLN:HG3 | 1.56 | 0.70 |
| 1:13:920:U:H2' | 1:13:921:U:C6 | 2.27 | 0.70 |
| 24:1H:739:G:OP1 | 57:1H:3658:HOH:O | 2.08 | 0.70 |
| 24:1H:2392:A:H2 | 24:1H:2424:C:N4 | 1.88 | 0.70 |
| 48:K8:47:ASN:O | 48:K8:49:LYS:N | 2.24 | 0.70 |
| 4:3E:154:ASN:OD1 | 4:3E:154:ASN:N | 2.22 | 0.70 |
| 24:1H:49:A:N7 | 24:1H:120:U:C5 | 2.55 | 0.70 |
| 24:1H:273(F):C:H3' | 24:1H:274:G:H5" | 1.72 | 0.70 |
| 33:58:47:ALA:HB2 | 33:58:112:LEU:HD11 | 1.74 | 0.70 |
| 46:I8:11:ARG:O | 46:I8:14:ARG:NH2 | 2.24 | 0.70 |
| 2:12:70:PHE:O | 2:12:93:VAL:N | 2.24 | 0.70 |
| 1:13:77:C:N4 | 1:13:89:U:O4 | 2.25 | 0.70 |
| 8:7E:20:TYR:HE2 | 8:7E:75:ARG:HD2 | 1.56 | 0.70 |
| 13:4I:58:GLU:O | 13:4I:62:ASN:ND2 | 2.19 | 0.70 |
| 24:1H:607:U:N3 | 24:1H:621:A:H2 | 1.88 | 0.70 |
| 24:1H:2314:C:H2' | 24:1H:2315:G:H8 | 1.54 | 0.70 |
| 1:1G:975:A:H4' | 1:1G:976:G:H5" | 1.71 | 0.70 |
| 1:1G:1502:A:H2 | 1:1G:1505:G:N1 | 1.89 | 0.70 |
| 16:7A:40:ASP:HB3 | 16:7A:48:TRP:HB2 | 1.74 | 0.70 |
| 24:14:2776:A:OP1 | 24:14:2776:A:H3' | 1.91 | 0.70 |
| 1:13:1151:A:H2' | 1:13:1152:A:H8 | 1.54 | 0.70 |
| 24:1H:2884:U:O2 | 51:N8:52:TYR:OH | 2.10 | 0.70 |
| 29:31:28:ILE:HG12 | 29:31:119:ARG:HH21 | 1.56 | 0.70 |
| 32:61:92:VAL:HG22 | 32:61:120:ILE:HB | 1.72 | 0.70 |
| 35:78:19:VAL:HB | 35:78:27:HIS:HB2 | 1.73 | 0.70 |
| 36:88:51:ARG:HD2 | 36:88:66:ILE:HD11 | 1.73 | 0.70 |
| 24:14:1200:C:OP1 | 57:14:3551:HOH:O | 2.09 | 0.70 |
| 24:14:1756:G:OP2 | 57:14:3547:HOH:O | 2.08 | 0.70 |
| 24:14:2693:A:H2' | 24:14:2694:G:H8 | 1.56 | 0.70 |
| 41:95:38:LEU:HD13 | 41:95:55:ALA:HB1 | 1.74 | 0.70 |
| 1:13:674:G:H2' | 1:13:675:A:H8 | 1.56 | 0.70 |
| 1:13:1503:A:N1 | 57:13:1816:HOH:O | 2.25 | 0.70 |
| 9:8E:10:ARG:HG2 | 9:8E:11:LYS:HG3 | 1.73 | 0.70 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 24:1H:534:U:H5' | 40:C8:42:ALA:HB1 | 1.74 | 0.70 |
| 24:1H:682:G:N2 | 24:1H:795:C:O2 | 2.19 | 0.70 |
| 24:1H:1138:G:N2 | 33:58:106:MET:HE3 | 2.06 | 0.70 |
| 24:1H:1843:C:H5' | 27:11:253:GLN:OE1 | 1.91 | 0.70 |
| 26:71:13:LYS:NZ | 26:71:31:GLU:O | 2.24 | 0.70 |
| 28:21:47:VAL:HG11 | 28:21:86:PRO:HD2 | 1.72 | 0.70 |
| 45:H8:145:GLU:HB3 | 45:H8:148:ASP:HB2 | 1.73 | 0.70 |
| 7:62:15:ASP:OD1 | 7:62:44:TYR:OH | 2.09 | 0.70 |
| 22:2L:21:A:H8 | 22:2L:56:U:H3 | 1.37 | 0.70 |
| 24:14:2853:C:H2' | 24:14:2854:G:H8 | 1.54 | 0.70 |
| 24:1H:2056:G:OP2 | 57:1H:3667:HOH:O | 2.10 | 0.70 |
| 1:1G:631:G:H3' | 1:1G:632:A:H8 | 1.57 | 0.70 |
| 3:22:8:ILE:HG23 | 3:22:16:ARG:HD3 | 1.74 | 0.70 |
| 6:5E:38:GLU:OE1 | 6:5E:64:GLN:NE2 | 2.25 | 0.70 |
| 24:1H:1026:U:H1' | 24:1H:1027:A:O5' | 1.92 | 0.70 |
| 24:1H:1664:A:OP2 | 57:1H:3662:HOH:O | 2.09 | 0.70 |
| 24:1H:2134:A:OP2 | 24:1H:2157:G:N2 | 2.24 | 0.70 |
| 1:1G:56:U:H2' | 1:1G:57:G:C8 | 2.27 | 0.70 |
| 17:8A:53:LEU:HD21 | 17:8A:85:VAL:HG11 | 1.73 | 0.70 |
| 24:14:2371:G:O6 | 57:14:3539:HOH:O | 2.06 | 0.70 |
| 29:39:118:ALA:HB2 | 29:39:123:LEU:HD23 | 1.74 | 0.70 |
| 44:C5:40:GLU:N | 44:C5:40:GLU:OE2 | 2.25 | 0.70 |
| 1:13:1455:G:OP1 | 20:BI:35:THR:OG1 | 2.08 | 0.70 |
| 24:1H:1990:C:OP2 | 57:1H:3663:HOH:O | 2.09 | 0.70 |
| 24:1H:2584:U:H2' | 24:1H:2585:U:H2' | 1.73 | 0.70 |
| 1:1G:920:U:H2' | 1:1G:921:U:C6 | 2.27 | 0.70 |
| 1:1G:953:G:H5' | 1:1G:965:A:H61 | 1.57 | 0.70 |
| 24:14:273(F):C:H3' | 24:14:274:G:H5" | 1.74 | 0.70 |
| 1:13:177:C:OP1 | 20:BI:65:LYS:NZ | 2.23 | 0.69 |
| 24:1H:2341:G:H2' | 24:1H:2342:C:C6 | 2.27 | 0.69 |
| 47:J8:76:ARG:HB2 | 47:J8:94:LEU:HD11 | 1.74 | 0.69 |
| 1:1G:959:A:HO2' | 1:1G:984:C:HO2' | 1.35 | 0.69 |
| 1:1G:1052:U:H5" | 1:1G:1053:G:OP2 | 1.92 | 0.69 |
| 22:2L:18:G:N2 | 22:2L:66:G:H1' | 2.07 | 0.69 |
| 24:14:2357:U:O2 | 57:14:3541:HOH:O | 2.06 | 0.69 |
| 29:39:101:LEU:O | 29:39:106:ARG:NH1 | 2.25 | 0.69 |
| 39:75:93:ARG:HG3 | 39:75:117:ASP:HB3 | 1.74 | 0.69 |
| 45:D5:140:ASP:OD1 | 45:D5:140:ASP:N | 2.25 | 0.69 |
| 15:6I:32:LEU:O | 15:6I:35:ARG:N | 2.24 | 0.69 |
| 24:1H:773:U:C4' | 27:11:47:GLY:HA3 | 2.22 | 0.69 |
| 24:1H:1533:C:H2' | 24:1H:1534:G:C8 | 2.27 | 0.69 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 24:1H:2052:G:H4' | 28:21:143:ASN:O | 1.91 | 0.69 |
| 15:6A:70:LEU:HD11 | 15:6A:77:ARG:HG3 | 1.74 | 0.69 |
| 24:14:1250:G:N7 | 35:35:18:ARG:NH2 | 2.40 | 0.69 |
| 24:14:1538:G:H2' | 24:14:1539:G:H8 | 1.56 | 0.69 |
| 43:B5:8:ILE:HD12 | 43:B5:43:VAL:HG12 | 1.74 | 0.69 |
| 46:E5:27:GLU:HG3 | 46:E5:68:GLU:HA | 1.75 | 0.69 |
| 50:I5:56:VAL:HG22 | 50:I5:57:GLU:H | 1.56 | 0.69 |
| 1:13:738:C:H2' | 1:13:739:C:C6 | 2.27 | 0.69 |
| 1:13:1023:G:H3' | 1:13:1024:G:H5" | 1.73 | 0.69 |
| 24:1H:800:A:OP1 | 57:1H:3668:HOH:O | 2.10 | 0.69 |
| 26:71:59:ARG:HD2 | 26:71:164:ARG:HD2 | 1.74 | 0.69 |
| 32:61:10:GLU:O | 32:61:11:ASN:ND2 | 2.26 | 0.69 |
| 39:B8:50:ILE:HD11 | 39:B8:102:ILE:HD11 | 1.74 | 0.69 |
| 8:72:51:VAL:HG22 | 8:72:52:ASP:H | 1.57 | 0.69 |
| 24:14:751:A:P | 57:14:3546:HOH:O | 2.49 | 0.69 |
| 31:59:7:LEU:HB3 | 31:59:65:HIS:HE1 | 1.56 | 0.69 |
| 41:95:21:ARG:CZ | 41:95:91:TYR:CG | 2.76 | 0.69 |
| 44:C5:47:LYS:H | 44:C5:60:PHE:HB3 | 1.57 | 0.69 |
| 1:13:736:C:H2' | 1:13:737:A:H8 | 1.56 | 0.69 |
| 33:58:89:LYS:O | 33:58:93:THR:OG1 | 2.10 | 0.69 |
| 47:J8:85:LEU:HB3 | 47:J8:86:SER:CB | 2.22 | 0.69 |
| 1:1G:1182:G:H5' | 1:1G:1183:A:H5' | 1.73 | 0.69 |
| 1:13:975:A:H4' | 1:13:976:G:H5" | 1.74 | 0.69 |
| 9:8E:3:GLN:OE1 | 9:8E:20:ARG:NH1 | 2.25 | 0.69 |
| 24:1H:138:G:N2 | 43:F8:44:GLU:OE2 | 2.19 | 0.69 |
| 24:1H:796:C:H2' | 24:1H:797:C:C6 | 2.27 | 0.69 |
| 24:1H:958:U:OP2 | 36:88:14:ARG:NH1 | 2.25 | 0.69 |
| 33:58:134:ARG:HB3 | 33:58:134:ARG:HH11 | 1.57 | 0.69 |
| 3:22:150:LYS:HG3 | 3:22:169:ALA:HB2 | 1.74 | 0.69 |
| 38:65:3:ARG:HH21 | 38:65:4:LEU:HB2 | 1.57 | 0.69 |
| 1:13:1226:C:OP2 | 13:4I:103:THR:OG1 | 2.05 | 0.69 |
| 13:4I:31:LYS:HA | 13:4I:34:LEU:HD23 | 1.72 | 0.69 |
| 24:1H:1899:G:H22 | 24:1H:1902:C:H41 | 1.37 | 0.69 |
| 3:22:59:ARG:HE | 3:22:64:VAL:HB | 1.56 | 0.69 |
| 27:19:228:PRO:HD3 | 27:19:235:GLY:CA | 2.22 | 0.69 |
| 30:49:15:VAL:HG21 | 30:49:176:LEU:HD23 | 1.74 | 0.69 |
| 31:59:137:ASP:OD1 | 31:59:138:LYS:N | 2.26 | 0.69 |
| 32:69:130:TYR:HB3 | 32:69:136:VAL:HG13 | 1.73 | 0.69 |
| 2:1E:27:LYS:NZ | 2:1E:193:ASP:OD2 | 2.22 | 0.69 |
| 24:1H:2058:A:N6 | 57:1H:3688:HOH:O | 2.17 | 0.69 |
| 24:1H:2062:A:H2' | 24:1H:2062:A:N3 | 2.07 | 0.69 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 40:C8:34:LYS:NZ | 40:C8:37:GLU:OE1 | 2.16 | 0.69 |
| 1:1G:464:G:N2 | 1:1G:467:G:N7 | 2.41 | 0.69 |
| 1:1G:589:C:H42 | 1:1G:650:G:H1 | 1.38 | 0.69 |
| 10:1A:99:LYS:HE2 | 10:1A:100:THR:H | 1.56 | 0.69 |
| 24:14:2576:G:OP1 | 57:14:3554:HOH:O | 2.11 | 0.69 |
| 22:3K:24:G:H2' | 22:3K:25:G:C8 | 2.27 | 0.69 |
| 24:1H:142:G:H1' | 43:F8:37:THR:HG21 | 1.75 | 0.69 |
| 24:1H:456:C:H2' | 43:F8:68:ARG:HH22 | 1.57 | 0.69 |
| 31:51:4:ILE:HG13 | 31:51:6:ARG:NE | 2.07 | 0.69 |
| 47:J8:91:LYS:HA | 47:J8:91:LYS:NZ | 2.07 | 0.69 |
| 54:Q8:54:GLU:HA | 54:Q8:57:ARG:HH21 | 1.57 | 0.69 |
| 1:1G:1289:A:OP1 | 21:1B:9:ARG:NH2 | 2.25 | 0.69 |
| 4:32:29:PRO:HD2 | 4:32:30:LYS:NZ | 2.08 | 0.69 |
| 22:2L:18:G:N2 | 30:49:78:SER:OG | 2.26 | 0.69 |
| 24:14:2107:C:O2 | 24:14:2182:G:N2 | 2.24 | 0.69 |
| 32:69:101:LEU:HB3 | 32:69:105:HIS:HB2 | 1.73 | 0.69 |
| 47:F5:85:LEU:HD13 | 47:F5:87:PRO:HG2 | 1.75 | 0.69 |
| 1:13:1291:G:OP1 | 7:6E:37:ASN:ND2 | 2.23 | 0.69 |
| 24:1H:234:C:H2' | 24:1H:235:U:H6 | 1.58 | 0.69 |
| 27:11:137:PRO:O | 27:11:140:THR:HG23 | 1.93 | 0.69 |
| 24:14:1531:C:H42 | 24:14:1540:G:H1 | 1.41 | 0.69 |
| 29:39:20:LEU:HD22 | 29:39:203:GLN:HE22 | 1.56 | 0.69 |
| 24:1H:731:C:OP2 | 57:1H:3603:HOH:O | 2.09 | 0.69 |
| 1:1G:976:G:N2 | 1:1G:1362(A):C:OP2 | 2.27 | 0.69 |
| 1:1G:1086:U:H2' | 1:1G:1087:G:O4' | 1.91 | 0.69 |
| 4:32:60:GLU:OE2 | 4:32:199:ASN:N | 2.26 | 0.69 |
| 1:13:1146:A:OP2 | 57:13:1808:HOH:O | 2.10 | 0.68 |
| 7:6E:16:LEU:HD13 | 9:8E:44:VAL:HG22 | 1.76 | 0.68 |
| 24:1H:273(D):C:H2' | 24:1H:273(E):U:H6 | 1.57 | 0.68 |
| 24:1H:1509:C:H3' | 24:1H:1510:A:H5" | 1.76 | 0.68 |
| 24:1H:1643:G:N7 | 57:1H:3715:HOH:O | 2.24 | 0.68 |
| 1:1G:1191:A:OP2 | 3:22:3:ASN:ND2 | 2.27 | 0.68 |
| 22:2L:15:G:H1 | 22:2L:57:C:H5 | 1.41 | 0.68 |
| 24:14:1434:A:H61 | 24:14:1558:A:N6 | 1.90 | 0.68 |
| 24:14:2836:U:H2' | 24:14:2837:G:C8 | 2.27 | 0.68 |
| 32:69:98:ALA:HA | 32:69:109:ILE:HD11 | 1.75 | 0.68 |
| 1:13:538:G:H5" | 12:3I:114:LYS:HB2 | 1.74 | 0.68 |
| 25:16:80:U:H2' | 25:16:81:G:H21 | 1.58 | 0.68 |
| 27:11:59:LYS:HD2 | 27:11:60:ARG:N | 2.08 | 0.68 |
| 33:58:132:ALA:O | 33:58:134:ARG:NH2 | 2.26 | 0.68 |
| 17:8A:45:HIS:HB2 | 17:8A:65:ILE:HD13 | 1.75 | 0.68 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 12:3I:70:ILE:HD13 | 12:3I:77:LEU:HD12 | 1.75 | 0.68 |
| 24:1H:442:G:H1' | 29:31:48:THR:HG21 | 1.75 | 0.68 |
| 24:1H:2016:U:OP1 | 57:1H:3666:HOH:O | 2.09 | 0.68 |
| 44:G8:85:VAL:HG23 | 44:G8:96:ILE:HB | 1.76 | 0.68 |
| 24:14:811:U:H2' | 35:35:21:ARG:HA | 1.75 | 0.68 |
| 25:1J:18:G:N2 | 25:1J:65:C:N3 | 2.37 | 0.68 |
| 3:2E:72:LYS:HZ3 | 3:2E:75:VAL:HG21 | 1.58 | 0.68 |
| 27:11:38:LYS:HE2 | 27:11:39:LYS:O | 1.93 | 0.68 |
| 1:1G:503:C:OP2 | 12:3A:116:SER:OG | 2.10 | 0.68 |
| 4:32:9:CYS:HA | 4:32:12:CYS:HB2 | 1.76 | 0.68 |
| 24:14:1778:U:H2' | 24:14:1784:A:N6 | 2.08 | 0.68 |
| 24:14:2002:G:N7 | 57:14:3587:HOH:O | 2.27 | 0.68 |
| 40:85:98:LEU:HB2 | 40:85:102:GLU:HB2 | 1.75 | 0.68 |
| 1:13:1145:C:H4' | 1:13:1146:A:H8 | 1.59 | 0.68 |
| 2:1E:32:ILE:HD11 | 2:1E:40:HIS:HB3 | 1.76 | 0.68 |
| 13:4I:57:ARG:NH2 | 50:M8:32:TYR:OH | 2.26 | 0.68 |
| 21:1F:9:ARG:HH22 | 21:1F:23:PRO:HD2 | 1.58 | 0.68 |
| 50:M8:12:ALA:HA | 50:M8:29:PRO:HB3 | 1.74 | 0.68 |
| 9:82:7:THR:O | 9:82:83:ARG:NH1 | 2.25 | 0.68 |
| 24:14:993:G:OP1 | 40:85:50:ARG:NH2 | 2.26 | 0.68 |
| 24:14:2638:G:O2' | 24:14:2639:A:H8 | 1.76 | 0.68 |
| 48:G5:53:LEU:O | 48:G5:57:ILE:HG13 | 1.93 | 0.68 |
| 1:13:838:G:OP2 | 1:13:842:C:N4 | 2.26 | 0.68 |
| 24:1H:1024:G:H3' | 24:1H:1025:G:H5" | 1.76 | 0.68 |
| 24:1H:1328:G:N7 | 57:1H:3720:HOH:O | 2.26 | 0.68 |
| 24:14:1324:G:N7 | 57:14:3602:HOH:O | 2.26 | 0.68 |
| 24:14:2685:G:O6 | 57:14:3548:HOH:O | 2.08 | 0.68 |
| 36:45:20:ALA:HA | 36:45:99:PRO:HD2 | 1.76 | 0.68 |
| 1:13:1040:U:H2' | 1:13:1041:A:H8 | 1.59 | 0.68 |
| 1:13:1321:C:H3' | 1:13:1322:C:H5" | 1.76 | 0.68 |
| 6:5E:97:PHE:HB2 | 18:9I:32:ARG:HE | 1.59 | 0.68 |
| 47:J8:73:LEU:HD13 | 47:J8:90:ILE:HG22 | 1.75 | 0.68 |
| 1:1G:957:U:H1' | 1:1G:960:U:H5 | 1.56 | 0.68 |
| 1:1G:1492:A:H2' | 24:14:1913:A:C6 | 2.28 | 0.68 |
| 4:32:64:LEU:HD22 | 4:32:198:VAL:HG21 | 1.74 | 0.68 |
| 19:AA:63:THR:OG1 | 19:AA:65:ASN:OD1 | 2.12 | 0.68 |
| 53:L5:12:ARG:NH2 | 53:L5:44:PRO:HB3 | 2.09 | 0.68 |
| 2:1E:115:LEU:HD13 | 2:1E:145:LEU:HB3 | 1.76 | 0.68 |
| 24:1H:193:U:O4 | 57:1H:3660:HOH:O | 2.08 | 0.68 |
| 24:1H:2689:U:OP2 | 24:1H:2719:G:N2 | 2.26 | 0.68 |
| 36:88:66:ILE:O | 36:88:104:PHE:N | 2.26 | 0.68 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 1:1G:56:U:H2' | 1:1G:57:G:H8 | 1.59 | 0.68 |
| 13:4A:79:LYS:HA | 13:4A:82:MET:HG2 | 1.74 | 0.68 |
| 22:3L:8:4SU:HN3 | 22:3L:14:A:H62 | 1.42 | 0.68 |
| 24:1H:1853:A:H2' | 24:1H:1854:A:C8 | 2.29 | 0.68 |
| 27:11:146:GLU:HB2 | 27:11:189:CYS:HB3 | 1.76 | 0.68 |
| 31:51:4:ILE:HD13 | 31:51:4:ILE:H | 1.59 | 0.68 |
| 49:L8:18:ASP:N | 49:L8:18:ASP:OD1 | 2.22 | 0.68 |
| 31:59:7:LEU:HB3 | 31:59:65:HIS:CE1 | 2.28 | 0.68 |
| 32:69:79:ILE:HG13 | 32:69:140:LEU:HD11 | 1.75 | 0.68 |
| 7:6E:15:ASP:HB3 | 7:6E:20:ASP:H | 1.59 | 0.68 |
| 24:1H:749:C:OP2 | 57:1H:3669:HOH:O | 2.11 | 0.68 |
| 24:1H:1021:A:H8 | 24:1H:1022:G:H5" | 1.59 | 0.68 |
| 30:41:122:PRO:HB3 | 30:41:180:PHE:HD2 | 1.59 | 0.68 |
| 1:1G:1076:C:H42 | 1:1G:1081:G:H1 | 1.42 | 0.68 |
| 5:42:51:VAL:O | 5:42:55:VAL:HG23 | 1.94 | 0.68 |
| 22:3L:25:G:H2' | 22:3L:26:G:H8 | 1.57 | 0.68 |
| 24:14:2352:A:OP2 | 57:14:3553:HOH:O | 2.11 | 0.68 |
| 1:13:631:G:H2' | 1:13:632:A:C8 | 2.26 | 0.67 |
| 24:1H:1312:U:O3' | 57:1H:3674:HOH:O | 2.12 | 0.67 |
| 24:1H:1406:U:H2' | 24:1H:1407:C:C6 | 2.29 | 0.67 |
| 24:1H:1931:U:H5 | 24:1H:1969:A:N7 | 1.91 | 0.67 |
| 28:21:2:LYS:NZ | 28:21:95:ILE:O | 2.26 | 0.67 |
| 44:G8:53:PRO:HA | 44:G8:56:PRO:HG3 | 1.75 | 0.67 |
| 4:32:59:ARG:HA | 4:32:62:GLN:HB2 | 1.74 | 0.67 |
| 7:62:56:GLN:OE1 | 7:62:60:LYS:NZ | 2.27 | 0.67 |
| 10:1A:33:GLN:HB2 | 10:1A:75:ILE:HG12 | 1.76 | 0.67 |
| 24:14:2212:A:H4' | 24:14:2213:U:H5 | 1.57 | 0.67 |
| 24:14:2718:G:N7 | 57:14:3605:HOH:O | 2.27 | 0.67 |
| 25:1J:15:A:H5' | 25:1J:16:G:H8 | 1.57 | 0.67 |
| 45:D5:30:ASN:OD1 | 45:D5:31:ARG:N | 2.27 | 0.67 |
| 2:1E:87:ARG:NH1 | 2:1E:220:ASP:OD1 | 2.25 | 0.67 |
| 24:14:1342:A:H2 | 24:14:1602:U:H3 | 1.40 | 0.67 |
| 24:14:1689:A:H62 | 24:14:1698:A:H2 | 1.39 | 0.67 |
| 29:39:157:VAL:HB | 29:39:194:MET:HB3 | 1.76 | 0.67 |
| 31:59:129:THR:OG1 | 31:59:130:ARG:N | 2.26 | 0.67 |
| 34:25:68:GLU:OE2 | 34:25:78:ARG:NH1 | 2.27 | 0.67 |
| 41:95:35:LEU:O | 41:95:37:VAL:N | 2.26 | 0.67 |
| 1:13:877:C:OP1 | 8:7E:88:LYS:NZ | 2.27 | 0.67 |
| 36:88:104:PHE:HE2 | 36:88:125:LEU:HD11 | 1.58 | 0.67 |
| 46:I8:56:ASP:OD1 | 46:I8:58:THR:OG1 | 2.10 | 0.67 |
| 24:14:2611:U:C4 | 51:J5:3:LYS:HG3 | 2.29 | 0.67 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 24:1H:11:G:H2' | 24:1H:12:U:H5' | 1.75 | 0.67 |
| 44:G8:55:TYR:HB2 | 44:G8:58:GLY:HA3 | 1.76 | 0.67 |
| 45:H8:143:GLY:HA3 | 45:H8:144:LEU:HD12 | 1.77 | 0.67 |
| 47:J8:93:GLU:N | 47:J8:93:GLU:OE2 | 2.26 | 0.67 |
| 1:1G:501:C:H2' | 1:1G:502:G:H8 | 1.60 | 0.67 |
| 9:82:97:LYS:HB3 | 9:82:102:LEU:HD12 | 1.75 | 0.67 |
| 10:1A:17:ASP:OD2 | 10:1A:70:ARG:NH1 | 2.28 | 0.67 |
| 19:AA:40:ILE:HG13 | 19:AA:68:GLY:H | 1.58 | 0.67 |
| 20:BA:16:HIS:O | 20:BA:19:SER:OG | 2.13 | 0.67 |
| 24:14:1198:U:H2' | 24:14:1199:U:C6 | 2.29 | 0.67 |
| 25:1J:13:A:N1 | 25:1J:69:G:O2' | 2.25 | 0.67 |
| 1:13:659:U:H2' | 1:13:660:G:H8 | 1.57 | 0.67 |
| 1:13:1062:U:H2' | 1:13:1063:C:C6 | 2.30 | 0.67 |
| 15:6I:10:LYS:O | 15:6I:10:LYS:NZ | 2.21 | 0.67 |
| 24:1H:213:A:H2' | 24:1H:214:G:O4' | 1.95 | 0.67 |
| 24:1H:763:G:OP1 | 57:1H:3671:HOH:O | 2.12 | 0.67 |
| 24:1H:2712(A):A:OP2 | 57:1H:3647:HOH:O | 2.13 | 0.67 |
| 2:12:164:VAL:HG23 | 2:12:186:ALA:HB2 | 1.77 | 0.67 |
| 24:14:2622:C:H5' | 28:29:159:HIS:ND1 | 2.10 | 0.67 |
| 37:55:34:ILE:HG22 | 37:55:114:VAL:HB | 1.75 | 0.67 |
| 24:1H:1678:G:H21 | 24:1H:1989:G:H22 | 1.42 | 0.67 |
| 24:1H:1971:A:C4 | 27:11:241:PRO:HD3 | 2.29 | 0.67 |
| 27:11:2:ALA:HB3 | 27:11:200:ASP:OD2 | 1.93 | 0.67 |
| 28:21:34:VAL:HG22 | 28:21:48:GLN:HG2 | 1.75 | 0.67 |
| 1:1G:1305:G:H22 | 1:1G:1331:G:H2' | 1.60 | 0.67 |
| 2:12:121:LEU:HG | 2:12:126:GLU:HB2 | 1.76 | 0.67 |
| 3:22:81:GLY:HA2 | 3:22:85:ARG:HH21 | 1.60 | 0.67 |
| 24:14:739:G:OP1 | 57:14:3555:HOH:O | 2.12 | 0.67 |
| 24:14:1054:A:H3' | 24:14:1055:G:H8 | 1.60 | 0.67 |
| 1:13:407:G:O4' | 4:3E:119:GLN:NE2 | 2.28 | 0.67 |
| 24:1H:1189:A:OP2 | 57:1H:3675:HOH:O | 2.13 | 0.67 |
| 24:1H:1405:U:H2' | 24:1H:1406:U:C6 | 2.30 | 0.67 |
| 33:58:67:LEU:HA | 33:58:87:LEU:HD12 | 1.75 | 0.67 |
| 44:G8:100:ALA:HB1 | 44:G8:101:LYS:HB2 | 1.77 | 0.67 |
| 1:1G:1129:C:N4 | 1:1G:1141:C:H41 | 1.93 | 0.67 |
| 9:82:10:ARG:NH1 | 9:82:105:ASP:OD2 | 2.28 | 0.67 |
| 24:14:450:G:O6 | 57:14:3549:HOH:O | 2.09 | 0.67 |
| 24:14:646:A:H2' | 24:14:647:G:O4' | 1.94 | 0.67 |
| 24:14:1331:A:HO2' | 24:14:1332:G:H8 | 1.43 | 0.67 |
| 24:14:1636:C:OP2 | 57:14:3557:HOH:O | 2.13 | 0.67 |
| 24:14:2427:C:H5" | 24:14:2428:G:OP1 | 1.95 | 0.67 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 25:1J:45:A:O4' | 30:49:95:ARG:NH1 | 2.28 | 0.67 |
| 41:95:37:VAL:CG2 | 41:95:56:SER:HA | 2.22 | 0.67 |
| 1:13:368:U:OP1 | 32:69:91:SER:OG | 2.10 | 0.67 |
| 8:7E:11:THR:HG23 | 8:7E:14:ARG:HH12 | 1.59 | 0.67 |
| 24:1H:1607:C:H4' | 24:1H:1608:A:O5' | 1.94 | 0.67 |
| 24:1H:2286:A:H8 | 52:O8:37:ARG:HH12 | 1.39 | 0.67 |
| 24:14:761:A:N7 | 57:14:3606:HOH:O | 2.28 | 0.67 |
| 24:14:1386:C:H2' | 24:14:1387:C:H6 | 1.60 | 0.67 |
| 24:14:2873:A:H8 | 37:55:6:SER:N | 1.93 | 0.67 |
| 44:C5:81:LYS:HB2 | 44:C5:99:CYS:SG | 2.35 | 0.67 |
| 46:E5:72:ARG:HG3 | 46:E5:75:LEU:HB2 | 1.77 | 0.67 |
| 1:13:601:C:H2' | 1:13:602:A:C8 | 2.29 | 0.67 |
| 24:1H:990:A:H1' | 24:1H:1156:A:N3 | 2.10 | 0.67 |
| 24:1H:1427:A:H4' | 24:1H:1428:C:O5' | 1.93 | 0.67 |
| 25:16:8:U:O2 | 25:16:112:G:N1 | 2.18 | 0.67 |
| 1:1G:168:G:H2' | 1:1G:169:C:H5" | 1.75 | 0.67 |
| 24:14:910:A:H62 | 36:45:12:GLN:HA | 1.59 | 0.67 |
| 1:13:17:U:H2' | 1:13:18:C:C6 | 2.30 | 0.67 |
| 3:22:11:ARG:HE | 3:22:180:ALA:HB3 | 1.60 | 0.67 |
| 3:22:77:ILE:O | 3:22:79:ARG:NH2 | 2.28 | 0.67 |
| 4:32:29:PRO:HD2 | 4:32:30:LYS:HZ1 | 1.58 | 0.67 |
| 10:1A:11:PHE:HE1 | 10:1A:67:THR:HG22 | 1.60 | 0.67 |
| 22:2L:15:G:H22 | 22:2L:57:C:H41 | 1.43 | 0.67 |
| 22:3L:14:A:H3' | 22:3L:15:G:H5" | 1.76 | 0.67 |
| 24:14:529:A:H4' | 24:14:530:G:H5' | 1.77 | 0.67 |
| 24:14:2748:A:H2' | 24:14:2749:A:H8 | 1.60 | 0.67 |
| 27:19:72:LYS:HB3 | 27:19:75:ILE:HD12 | 1.77 | 0.67 |
| 29:39:132:VAL:O | 29:39:134:GLY:N | 2.28 | 0.67 |
| 39:75:107:ASP:OD2 | 39:75:109:GLU:HB2 | 1.95 | 0.67 |
| 54:M5:57:ARG:HH11 | 54:M5:57:ARG:CA | 2.07 | 0.67 |
| 1:13:980:C:O2 | 57:13:1807:HOH:O | 2.10 | 0.66 |
| 24:1H:2656:U:H3 | 24:1H:2665:A:H2 | 1.43 | 0.66 |
| 1:1G:57:G:H2' | 1:1G:58:C:C6 | 2.30 | 0.66 |
| 1:1G:1442:G:O6 | 1:1G:1446:A:N6 | 2.28 | 0.66 |
| 2:12:190:THR:O | 2:12:191:ASP:HB3 | 1.93 | 0.66 |
| 24:14:2298:A:H1' | 24:14:2321:G:N2 | 2.10 | 0.66 |
| 32:69:69:LYS:O | 32:69:72:LEU:N | 2.28 | 0.66 |
| 33:15:85:ILE:HG21 | 33:15:90:MET:HE3 | 1.77 | 0.66 |
| 35:35:138:LEU:HD21 | 35:35:144:GLU:HG3 | 1.77 | 0.66 |
| 41:95:21:ARG:CD | 41:95:91:TYR:CD1 | 2.78 | 0.66 |
| 43:B5:44:GLU:HG3 | 43:B5:51:VAL:CG2 | 2.25 | 0.66 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 46:E5:49:LYS:O | 46:E5:50:ASN:ND2 | 2.29 | 0.66 |
| 50:I5:37:SER:OG | 50:I5:38:LYS:N | 2.13 | 0.66 |
| 24:1H:1022:G:O6 | 33:58:66:LYS:NZ | 2.29 | 0.66 |
| 24:1H:2017:U:OP1 | 57:1H:3672:HOH:O | 2.12 | 0.66 |
| 24:1H:2315:G:N3 | 30:41:128:ARG:NH2 | 2.38 | 0.66 |
| 31:51:30:LYS:HE3 | 31:51:81:GLU:H | 1.59 | 0.66 |
| 1:1G:940:C:H2' | 1:1G:941:G:C8 | 2.30 | 0.66 |
| 1:1G:1492:A:H2' | 24:14:1913:A:N6 | 2.10 | 0.66 |
| 24:14:602:G:HO2' | 24:14:604:G:HO2' | 1.39 | 0.66 |
| 25:1J:5:C:N4 | 25:1J:115:G:H1 | 1.85 | 0.66 |
| 31:59:46:GLU:HB2 | 31:59:49:VAL:HG23 | 1.77 | 0.66 |
| 41:95:21:ARG:NH1 | 41:95:91:TYR:CE2 | 2.61 | 0.66 |
| 1:13:1151:A:H2' | 1:13:1152:A:C8 | 2.30 | 0.66 |
| 1:13:1508:G:OP1 | 57:13:1802:HOH:O | 2.12 | 0.66 |
| 24:1H:2010:G:N7 | 57:1H:3729:HOH:O | 2.29 | 0.66 |
| 31:51:84:SER:OG | 31:51:85:LYS:N | 2.25 | 0.66 |
| 24:14:483:A:H4' | 44:C5:49:VAL:HA | 1.76 | 0.66 |
| 42:A5:10:VAL:HG21 | 42:A5:103:ILE:HD12 | 1.77 | 0.66 |
| 24:1H:249:C:P | 57:1H:3625:HOH:O | 2.53 | 0.66 |
| 24:1H:529:A:H4' | 24:1H:530:G:H5' | 1.76 | 0.66 |
| 24:1H:860:U:H5 | 24:1H:917:A:H2 | 1.41 | 0.66 |
| 24:1H:1970:A:OP2 | 57:1H:3673:HOH:O | 2.12 | 0.66 |
| 1:1G:412:A:O2' | 1:1G:413:G:OP2 | 2.11 | 0.66 |
| 1:1G:735:C:H5" | 18:9A:71:LYS:HB3 | 1.78 | 0.66 |
| 28:29:203:LYS:NZ | 28:29:203:LYS:HB3 | 2.08 | 0.66 |
| 52:K5:18:ARG:HH11 | 52:K5:18:ARG:HA | 1.59 | 0.66 |
| 1:13:67:C:H2' | 1:13:68:G:C8 | 2.30 | 0.66 |
| 1:13:1348:U:H4' | 9:8E:120:ARG:HD2 | 1.76 | 0.66 |
| 6:5E:38:GLU:HB2 | 6:5E:64:GLN:HG2 | 1.78 | 0.66 |
| 10:1I:61:GLU:OE2 | 14:5I:45:ARG:NH1 | 2.29 | 0.66 |
| 22:2K:19:C:H3' | 22:2K:20:C:H2' | 1.77 | 0.66 |
| 24:1H:822:U:OP2 | 57:1H:3676:HOH:O | 2.13 | 0.66 |
| 31:51:17:VAL:HG21 | 31:51:50:VAL:HG11 | 1.78 | 0.66 |
| 4:32:120:LEU:HB3 | 4:32:126:ILE:HD11 | 1.77 | 0.66 |
| 24:14:603:A:H8 | 24:14:604:G:H1' | 1.61 | 0.66 |
| 24:14:2498:C:OP2 | 57:14:3556:HOH:O | 2.12 | 0.66 |
| 42:E8:51:LEU:HD23 | 42:E8:105:VAL:HG11 | 1.75 | 0.66 |
| 44:G8:20:TYR:CE2 | 44:G8:43:ASN:HA | 2.31 | 0.66 |
| 1:1G:552:U:H4' | 12:3A:86:ARG:HG2 | 1.78 | 0.66 |
| 1:1G:1410:G:N2 | 1:1G:1490:C:O2 | 2.20 | 0.66 |
| 3:22:35:GLU:HG3 | 3:22:95:THR:HG21 | 1.78 | 0.66 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 24:14:273(D):C:N4 | 24:14:363(B):G:O6 | 2.19 | 0.66 |
| 24:14:527:C:OP2 | 24:14:2779:U:H5 | 1.77 | 0.66 |
| 29:39:102:PRO:HB2 | 29:39:105:VAL:HG23 | 1.76 | 0.66 |
| 32:69:72:LEU:HD21 | 32:69:107:VAL:HG21 | 1.77 | 0.66 |
| 41:95:21:ARG:HD3 | 41:95:91:TYR:CD2 | 2.30 | 0.66 |
| 1:13:376:G:O3' | 16:7I:5:ARG:NH1 | 2.25 | 0.66 |
| 8:7E:87:SER:HA | 8:7E:93:VAL:HG23 | 1.78 | 0.66 |
| 22:2L:34:U:H5 | 22:2L:37:A:OP2 | 1.79 | 0.66 |
| 25:1J:42:C:O2' | 30:49:67:LYS:O | 2.13 | 0.66 |
| 27:19:228:PRO:O | 57:19:402:HOH:O | 2.12 | 0.66 |
| 1:13:1298:C:P | 7:6E:114:ARG:HH22 | 2.18 | 0.66 |
| 16:7I:5:ARG:HH21 | 16:7I:22:THR:HG23 | 1.60 | 0.66 |
| 17:8I:56:VAL:HG23 | 17:8I:81:ARG:HG3 | 1.77 | 0.66 |
| 24:1H:1929:G:H4' | 24:1H:1930:G:OP1 | 1.95 | 0.66 |
| 24:1H:2728:U:H5' | 34:68:70:LYS:HZ1 | 1.59 | 0.66 |
| 6:52:68:PRO:HG2 | 6:52:71:ARG:HG3 | 1.77 | 0.66 |
| 45:D5:30:ASN:HA | 45:D5:89:PHE:HE1 | 1.60 | 0.66 |
| 1:13:137:C:N4 | 1:13:226:G:O6 | 2.20 | 0.66 |
| 1:13:277:C:OP2 | 17:8I:41:LYS:NZ | 2.26 | 0.66 |
| 1:13:1292:U:P | 7:6E:41:ARG:HH22 | 2.19 | 0.66 |
| 2:1E:98:LEU:HB2 | 2:1E:101:MET:HE3 | 1.77 | 0.66 |
| 24:1H:400:G:N7 | 57:1H:3730:HOH:O | 2.29 | 0.66 |
| 24:1H:1021:A:H3' | 24:1H:1021:A:H8 | 1.61 | 0.66 |
| 44:G8:54:LYS:HA | 44:G8:56:PRO:HD3 | 1.78 | 0.66 |
| 1:1G:620:C:OP1 | 57:1G:1806:HOH:O | 2.14 | 0.66 |
| 1:1G:974:A:H5" | 14:5A:31:ARG:HD3 | 1.76 | 0.66 |
| 24:14:1062:G:OP1 | 24:14:1070:A:O2' | 2.13 | 0.66 |
| 27:19:255:LYS:H | 27:19:255:LYS:CE | 2.09 | 0.66 |
| 28:29:8:LYS:HB3 | 28:29:192:ASN:HA | 1.77 | 0.66 |
| 1:13:376:G:O3' | 16:7I:5:ARG:HD2 | 1.95 | 0.66 |
| 20:BI:14:LYS:HB2 | 20:BI:17:ARG:HH21 | 1.61 | 0.66 |
| 24:1H:2303:G:O2' | 30:41:132:ASN:HB2 | 1.96 | 0.66 |
| 24:1H:2636:U:OP1 | 28:21:79:ARG:HA | 1.95 | 0.66 |
| 1:1G:677:U:H3 | 1:1G:713:G:H22 | 1.43 | 0.66 |
| 36:45:24:GLY:HA3 | 36:45:25:ASP:HB2 | 1.78 | 0.66 |
| 39:75:6:LEU:HA | 39:75:9:LEU:HB3 | 1.77 | 0.66 |
| 47:F5:93:GLU:HA | 47:F5:97:LEU:HD22 | 1.77 | 0.66 |
| 24:1H:1359:A:H2' | 24:1H:1360:A:H5' | 1.76 | 0.65 |
| 50:M8:24:THR:OG1 | 50:M8:25:TYR:N | 2.29 | 0.65 |
| 24:14:1055:G:H21 | 24:14:1085:A:H2 | 1.44 | 0.65 |
| 24:14:2130:U:H2' | 24:14:2158:A:N1 | 2.11 | 0.65 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 27:19:70:TRP:CH2 | 27:19:150:LYS:HA | 2.31 | 0.65 |
| 39:75:13:ARG:HB3 | 39:75:13:ARG:HH11 | 1.62 | 0.65 |
| 1:13:659:U:H2' | 1:13:660:G:C8 | 2.32 | 0.65 |
| 1:13:793:U:H5' | 1:13:794:A:H5" | 1.78 | 0.65 |
| 5:4E:91:LEU:HD12 | 5:4E:120:THR:HG22 | 1.76 | 0.65 |
| 22:2K:17:OMG:HN21 | 22:2K:64:PSU:HN3 | 1.42 | 0.65 |
| 22:2K:19:C:H5" | 22:2K:20:C:H3' | 1.78 | 0.65 |
| 24:1H:1323:U:O4 | 57:1H:3670:HOH:O | 2.11 | 0.65 |
| 24:1H:2115:G:O3' | 24:1H:2165:G:N2 | 2.29 | 0.65 |
| 30:41:130:ASN:HB3 | 30:41:160:VAL:HA | 1.79 | 0.65 |
| 35:78:58:THR:HG21 | 54:Q8:54:GLU:HG3 | 1.79 | 0.65 |
| 1:1G:565:U:OP2 | 1:1G:566:G:O2' | 2.09 | 0.65 |
| 2:12:33:TYR:HB3 | 2:12:41:ILE:HG22 | 1.79 | 0.65 |
| 32:69:84:GLY:O | 32:69:87:LYS:NZ | 2.24 | 0.65 |
| 1:13:157:G:H1 | 1:13:164:U:H3 | 1.42 | 0.65 |
| 1:13:978:A:OP2 | 1:13:1362(A):C:N4 | 2.30 | 0.65 |
| 9:8E:9:ARG:HD2 | 9:8E:14:VAL:HG13 | 1.78 | 0.65 |
| 24:1H:2711:A:OP2 | 57:1H:3677:HOH:O | 2.13 | 0.65 |
| 24:1H:2712(A):A:OP2 | 57:1H:3677:HOH:O | 2.13 | 0.65 |
| 27:11:147:LEU:HD22 | 27:11:155:LEU:HD11 | 1.79 | 0.65 |
| 37:98:52:ILE:O | 37:98:55:ALA:N | 2.29 | 0.65 |
| 1:1G:1125:U:H2' | 1:1G:1126:U:C5 | 2.31 | 0.65 |
| 1:1G:1352:C:OP1 | 21:1B:3:LYS:NZ | 2.24 | 0.65 |
| 10:1A:3:LYS:HB2 | 10:1A:77:PRO:HG3 | 1.78 | 0.65 |
| 16:7A:21:VAL:HG22 | 16:7A:33:ILE:HD12 | 1.77 | 0.65 |
| 24:14:2790:A:H8 | 24:14:2790:A:OP2 | 1.79 | 0.65 |
| 29:39:110:LEU:HD21 | 29:39:181:LEU:HD13 | 1.78 | 0.65 |
| 44:C5:39:VAL:C | 44:C5:41:GLY:H | 2.04 | 0.65 |
| 45:D5:144:LEU:HB2 | 45:D5:174:VAL:HG11 | 1.77 | 0.65 |
| 1:13:390:C:O2' | 16:7I:28:ARG:NH2 | 2.29 | 0.65 |
| 6:5E:75:LEU:HD22 | 6:5E:79:LEU:HG | 1.77 | 0.65 |
| 24:1H:1926:U:H2' | 24:1H:1928:A:OP2 | 1.96 | 0.65 |
| 24:1H:2339:G:H2' | 24:1H:2340:G:C8 | 2.30 | 0.65 |
| 1:1G:1330:U:H4' | 13:4A:23:TYR:CE1 | 2.32 | 0.65 |
| 16:7A:54:GLU:OE1 | 16:7A:54:GLU:N | 2.29 | 0.65 |
| 4:3E:72:GLU:OE1 | 4:3E:207:TYR:OH | 2.14 | 0.65 |
| 24:1H:1680:U:N3 | 24:1H:1764:G:OP2 | 2.26 | 0.65 |
| 41:D8:24:LYS:HB2 | 41:D8:92:THR:HG23 | 1.79 | 0.65 |
| 1:1G:512:U:H2' | 1:1G:513:C:C6 | 2.31 | 0.65 |
| 1:1G:1095:U:P | 1:1G:1108:G:H1 | 2.20 | 0.65 |
| 10:1A:32:ALA:HA | 10:1A:76:ASN:HB2 | 1.79 | 0.65 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 24:14:451:C:H5' | 57:14:3524:HOH:O | 1.95 | 0.65 |
| 11:2I:34:ASP:OD1 | 11:2I:37:GLY:N | 2.29 | 0.65 |
| 15:6I:27:VAL:HG12 | 15:6I:31:LEU:HD22 | 1.78 | 0.65 |
| 22:2K:1:G:H2' | 22:2K:2:G:C8 | 2.30 | 0.65 |
| 24:1H:1803:A:H4' | 27:11:259:THR:HG23 | 1.79 | 0.65 |
| 40:C8:75:ASN:ND2 | 40:C8:78:THR:OG1 | 2.30 | 0.65 |
| 1:1G:142:G:H2' | 1:1G:143:A:H8 | 1.60 | 0.65 |
| 2:12:12:GLU:HG3 | 2:12:14:GLY:H | 1.60 | 0.65 |
| 14:5A:21:TYR:HE1 | 14:5A:23:ARG:HE | 1.45 | 0.65 |
| 47:F5:82:LEU:HD23 | 47:F5:82:LEU:H | 1.61 | 0.65 |
| 5:4E:110:LEU:HD13 | 5:4E:118:ILE:HG21 | 1.78 | 0.65 |
| 24:1H:1251:C:H5 | 57:1H:4060:HOH:O | 1.79 | 0.65 |
| 24:1H:1676:A:OP2 | 57:1H:3680:HOH:O | 2.15 | 0.65 |
| 37:98:67:LEU:HD13 | 37:98:76:VAL:HG21 | 1.79 | 0.65 |
| 1:1G:491:G:N7 | 57:1G:1821:HOH:O | 2.29 | 0.65 |
| 12:3A:117:ARG:HB3 | 12:3A:122:THR:HB | 1.78 | 0.65 |
| 16:7A:25:ARG:HH11 | 16:7A:25:ARG:HG3 | 1.62 | 0.65 |
| 22:3L:20:C:H5" | 22:3L:68:A:N6 | 2.08 | 0.65 |
| 27:19:3:VAL:HG13 | 27:19:17:THR:HB | 1.78 | 0.65 |
| 1:13:42:G:O2' | 1:13:622:A:N1 | 2.29 | 0.65 |
| 10:1I:49:VAL:HG23 | 14:5I:41:ARG:HB2 | 1.77 | 0.65 |
| 22:3K:38:MIA:H2' | 22:3K:39:A:C8 | 2.32 | 0.65 |
| 24:1H:1266:G:OP2 | 51:N8:19:ARG:NH1 | 2.30 | 0.65 |
| 24:1H:1980:G:O2' | 24:1H:1982:C:OP2 | 2.12 | 0.65 |
| 25:16:65:C:H41 | 25:16:108:C:H2' | 1.62 | 0.65 |
| 28:21:61:ARG:HB3 | 28:21:61:ARG:HH11 | 1.61 | 0.65 |
| 45:H8:103:ARG:HB2 | 45:H8:138:GLU:HA | 1.76 | 0.65 |
| 24:14:1388:G:O2' | 24:14:1389:G:H5' | 1.95 | 0.65 |
| 24:14:2602:A:H4' | 24:14:2603:G:O5' | 1.97 | 0.65 |
| 38:65:88:ASP:OD1 | 38:65:90:GLY:N | 2.29 | 0.65 |
| 44:C5:73:ARG:NH2 | 44:C5:81:LYS:O | 2.29 | 0.65 |
| 48:G5:4:SER:HB2 | 48:G5:6:VAL:HG23 | 1.78 | 0.65 |
| 1:13:452:A:O2' | 1:13:453:A:O4' | 2.12 | 0.65 |
| 2:1E:155:LEU:HD22 | 2:1E:159:PRO:HD3 | 1.77 | 0.65 |
| 24:1H:273(D):C:H2' | 24:1H:273(E):U:C6 | 2.32 | 0.65 |
| 24:1H:1332:G:N2 | 24:1H:1609:A:O2' | 2.29 | 0.65 |
| 24:1H:2292:C:OP1 | 38:A8:17:ARG:NH2 | 2.30 | 0.65 |
| 29:31:65:TRP:HZ3 | 29:31:73:ALA:O | 1.80 | 0.65 |
| 30:41:70:VAL:HA | 30:41:90:LEU:HD12 | 1.79 | 0.65 |
| 1:1G:731:G:OP2 | 57:1G:1807:HOH:O | 2.14 | 0.65 |
| 6:52:69:GLU:O | 6:52:72:VAL:HG12 | 1.96 | 0.65 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 8:72:12:ARG:HD3 | 8:72:26:VAL:HG12 | 1.78 | 0.65 |
| 12:3A:41:ARG:HB3 | 12:3A:41:ARG:HH11 | 1.62 | 0.65 |
| 22:3L:46:G:N2 | 22:3L:54:C:O2 | 2.29 | 0.65 |
| 24:14:593:G:O4' | 54:M5:4:MET:HE1 | 1.95 | 0.65 |
| 24:14:1126:A:H8 | 24:14:1126:A:OP1 | 1.80 | 0.65 |
| 24:14:1899:G:N2 | 24:14:1902:C:N4 | 2.37 | 0.65 |
| 1:13:186(D):C:H42 | 1:13:191(C):G:H1 | 1.43 | 0.65 |
| 1:13:673:G:O3' | 6:5E:87:ARG:NH2 | 2.30 | 0.65 |
| 1:13:1446:A:OP1 | 1:13:1446:A:H4' | 1.96 | 0.65 |
| 4:3E:25:ARG:HH12 | 4:3E:30:LYS:HZ2 | 1.42 | 0.65 |
| 29:31:192:LEU:HD21 | 29:31:194:MET:HE2 | 1.77 | 0.65 |
| 36:88:136:ALA:HB1 | 45:H8:52:SER:HB2 | 1.78 | 0.65 |
| 9:82:97:LYS:HG3 | 9:82:98:PRO:HD3 | 1.79 | 0.65 |
| 20:BA:13:LEU:H | 20:BA:13:LEU:HD12 | 1.62 | 0.65 |
| 24:14:322:A:H5' | 24:14:340:A:H1' | 1.79 | 0.65 |
| 24:14:1379:A:H4' | 24:14:1380:G:OP2 | 1.96 | 0.65 |
| 24:14:1399:C:N4 | 57:14:3609:HOH:O | 2.29 | 0.65 |
| 24:14:1514:U:H2' | 24:14:1515:C:C6 | 2.32 | 0.65 |
| 27:19:95:LEU:HD11 | 27:19:105:ILE:HD12 | 1.78 | 0.65 |
| 24:1H:2271:G:N7 | 57:1H:3733:HOH:O | 2.29 | 0.64 |
| 28:21:51:PHE:CD2 | 28:21:52:LEU:HG | 2.31 | 0.64 |
| 50:M8:56:VAL:O | 50:M8:60:GLN:NE2 | 2.29 | 0.64 |
| 1:1G:1179:A:OP2 | 9:82:93:ARG:NH2 | 2.30 | 0.64 |
| 4:32:24:GLU:OE1 | 4:32:24:GLU:N | 2.30 | 0.64 |
| 5:42:43:LEU:HD13 | 5:42:109:ILE:HD11 | 1.79 | 0.64 |
| 24:14:2420:C:P | 54:M5:34:TRP:H | 2.20 | 0.64 |
| 27:19:228:PRO:HD3 | 27:19:235:GLY:HA3 | 1.79 | 0.64 |
| 32:69:1:MET:HB3 | 32:69:21:VAL:O | 1.96 | 0.64 |
| 52:K5:12:GLU:HB2 | 52:K5:21:TYR:HB3 | 1.78 | 0.64 |
| 1:13:1104:G:OP1 | 2:1E:144:ARG:NH2 | 2.23 | 0.64 |
| 24:1H:1065:U:O2 | 24:1H:1074:G:N2 | 2.30 | 0.64 |
| 27:11:25:THR:HB | 27:11:82:ILE:H | 1.61 | 0.64 |
| 47:J8:85:LEU:HD22 | 47:J8:86:SER:HB3 | 1.79 | 0.64 |
| 1:1G:353:A:H5' | 1:1G:353:A:C8 | 2.27 | 0.64 |
| 1:1G:1291:G:OP1 | 7:62:37:ASN:ND2 | 2.30 | 0.64 |
| 22:3L:7:G:N2 | 22:3L:76:C:O2 | 2.30 | 0.64 |
| 24:14:1857:G:O2' | 24:14:1885:A:N6 | 2.31 | 0.64 |
| 36:45:54:MET:HE2 | 36:45:118:LEU:HD22 | 1.79 | 0.64 |
| 24:1H:192:C:P | 57:1H:3731:HOH:O | 2.54 | 0.64 |
| 24:1H:450:G:O6 | 57:1H:3678:HOH:O | 2.14 | 0.64 |
| 24:1H:1778:U:H2' | 24:1H:1784:A:N6 | 2.13 | 0.64 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 24:1H:2615:U:OP1 | 57:1H:3679:HOH:O | 2.14 | 0.64 |
| 25:16:95:U:H2' | 25:16:96:G:C8 | 2.32 | 0.64 |
| 32:61:8:PRO:HA | 32:61:14:ASP:HA | 1.79 | 0.64 |
| 1:1G:41:G:H2' | 1:1G:42:G:C8 | 2.33 | 0.64 |
| 7:62:24:THR:HA | 7:62:27:ILE:HD12 | 1.78 | 0.64 |
| 24:14:2175:C:H1' | 26:79:217:THR:O | 1.97 | 0.64 |
| 24:14:2588:G:OP1 | 57:14:3559:HOH:O | 2.14 | 0.64 |
| 26:79:23:ASP:OD1 | 26:79:190:ARG:NH2 | 2.30 | 0.64 |
| 39:75:105:LEU:O | 39:75:107:ASP:N | 2.31 | 0.64 |
| 50:I5:16:CYS:SG | 50:I5:36:CYS:HB2 | 2.37 | 0.64 |
| 1:13:262:A:H2' | 1:13:263:A:C8 | 2.32 | 0.64 |
| 24:1H:545:G:H2' | 24:1H:546:C:H5" | 1.79 | 0.64 |
| 24:1H:2233:U:H2' | 24:1H:2234:G:C8 | 2.32 | 0.64 |
| 24:1H:2341:G:H2' | 24:1H:2342:C:H6 | 1.62 | 0.64 |
| 25:16:15:A:H1' | 25:16:109:G:C5 | 2.33 | 0.64 |
| 25:16:95:U:H2' | 25:16:96:G:H8 | 1.62 | 0.64 |
| 31:51:83:TYR:HD1 | 31:51:84:SER:H | 1.45 | 0.64 |
| 33:58:35:ARG:HB2 | 33:58:37:LYS:HG3 | 1.78 | 0.64 |
| 1:1G:1122:U:N3 | 1:1G:1123:A:N7 | 2.45 | 0.64 |
| 1:1G:1178:G:H22 | 1:1G:1181:G:H5" | 1.62 | 0.64 |
| 4:32:18:LYS:NZ | 4:32:26:CYS:HB3 | 2.11 | 0.64 |
| 18:9A:22:VAL:HG22 | 18:9A:23:LYS:H | 1.63 | 0.64 |
| 24:14:450:G:O6 | 57:14:3558:HOH:O | 2.15 | 0.64 |
| 29:39:79:GLY:HA2 | 29:39:86:GLY:HA2 | 1.78 | 0.64 |
| 41:95:98:GLU:OE1 | 41:95:100:ARG:HD3 | 1.98 | 0.64 |
| 3:2E:53:ALA:HB2 | 3:2E:115:LEU:HD13 | 1.79 | 0.64 |
| 24:1H:1021:A:C8 | 24:1H:1022:G:H5" | 2.32 | 0.64 |
| 32:61:116:LEU:HD11 | 32:61:120:ILE:HG12 | 1.80 | 0.64 |
| 35:78:113:LYS:HG2 | 35:78:115:LEU:HD23 | 1.78 | 0.64 |
| 46:I8:17:GLN:O | 46:I8:19:LYS:HE3 | 1.98 | 0.64 |
| 22:3L:52:G:H2' | 22:3L:53:A:C8 | 2.32 | 0.64 |
| 24:14:1771:C:H1' | 24:14:1786:A:C8 | 2.32 | 0.64 |
| 27:19:253:GLN:HB3 | 27:19:255:LYS:HZ3 | 1.61 | 0.64 |
| 12:3I:97:ARG:HB2 | 12:3I:98:TYR:CE1 | 2.33 | 0.64 |
| 24:1H:2175:C:OP1 | 26:71:3:HIS:ND1 | 2.29 | 0.64 |
| 30:41:16:ARG:HH12 | 30:41:31:VAL:CG1 | 2.11 | 0.64 |
| 37:98:33:ARG:HH12 | 51:N8:55:ARG:HB3 | 1.63 | 0.64 |
| 46:I8:51:VAL:N | 46:I8:62:LEU:HD12 | 2.13 | 0.64 |
| 49:L8:43:ILE:O | 49:L8:47:VAL:HG23 | 1.98 | 0.64 |
| 1:1G:716:A:N3 | 11:2A:118:GLY:HA2 | 2.13 | 0.64 |
| 1:1G:963:G:H21 | 10:1A:55:LYS:CE | 2.11 | 0.64 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 1:1G:1162:C:H42 | 1:1G:1174:G:H1 | 1.45 | 0.64 |
| 1:1G:1194:U:H2' | 1:1G:1195:C:C6 | 2.32 | 0.64 |
| 1:1G:1322:C:O2' | 1:1G:1323:G:O5' | 2.14 | 0.64 |
| 24:14:987:G:OP2 | 57:14:3562:HOH:O | 2.15 | 0.64 |
| 24:14:1342:A:H2 | 24:14:1602:U:N3 | 1.96 | 0.64 |
| 27:19:182:LEU:H | 27:19:272:ALA:HB2 | 1.62 | 0.64 |
| 41:95:44:LYS:C | 41:95:46:VAL:H | 2.05 | 0.64 |
| 52:K5:31:PRO:HB2 | 52:K5:33:LYS:HG3 | 1.80 | 0.64 |
| 1:13:1126:U:OP2 | 1:13:1281:U:H1' | 1.97 | 0.64 |
| 4:3E:59:ARG:NH2 | 4:3E:66:ARG:HH12 | 1.96 | 0.64 |
| 4:3E:108:LEU:HB3 | 4:3E:110:PHE:CD1 | 2.33 | 0.64 |
| 24:1H:1149:G:N7 | 57:1H:3738:HOH:O | 2.30 | 0.64 |
| 37:98:70:LEU:O | 37:98:72:ASP:N | 2.31 | 0.64 |
| 52:O8:28:ARG:HD3 | 52:O8:29:ASN:H | 1.63 | 0.64 |
| 53:P8:12:ARG:NH2 | 53:P8:44:PRO:HB3 | 2.11 | 0.64 |
| 1:1G:1346:A:O5' | 9:82:120:ARG:NH1 | 2.30 | 0.64 |
| 24:14:1006:C:H1' | 33:15:106:MET:HG2 | 1.79 | 0.64 |
| 24:14:1224:G:OP2 | 41:95:66:ARG:NH2 | 2.31 | 0.64 |
| 24:14:1786:A:H2 | 24:14:2606:C:H1' | 1.62 | 0.64 |
| 27:19:65:ILE:HD11 | 27:19:67:PHE:CE1 | 2.32 | 0.64 |
| 24:1H:836:G:H5" | 24:1H:837:C:OP2 | 1.98 | 0.64 |
| 24:1H:1406:U:H2' | 24:1H:1407:C:H6 | 1.62 | 0.64 |
| 24:1H:2271:G:H5" | 46:I8:20:ARG:HH11 | 1.63 | 0.64 |
| 45:H8:16:SER:O | 45:H8:20:ARG:NH1 | 2.31 | 0.64 |
| 48:K8:32:LEU:HD11 | 48:K8:54:LYS:HG2 | 1.80 | 0.64 |
| 1:1G:1497:G:H2' | 1:1G:1498:U:H5' | 1.79 | 0.64 |
| 9:82:46:ALA:HB1 | 9:82:77:ILE:HD11 | 1.79 | 0.64 |
| 12:3A:28:LYS:HD3 | 12:3A:30:ALA:HB2 | 1.79 | 0.64 |
| 24:14:1210:A:H5" | 24:14:1211:U:H3' | 1.78 | 0.64 |
| 24:14:2370:G:H21 | 52:K5:45:LYS:NZ | 1.95 | 0.64 |
| 35:35:125:VAL:HG13 | 35:35:144:GLU:HB3 | 1.78 | 0.64 |
| 4:3E:30:LYS:C | 4:3E:32:ALA:H | 2.03 | 0.64 |
| 24:1H:1022:G:N2 | 24:1H:1142(A):A:N1 | 2.43 | 0.64 |
| 52:O8:32:ASN:OD1 | 52:O8:32:ASN:N | 2.31 | 0.64 |
| 1:1G:956:U:H1' | 1:1G:1225:A:H2 | 1.62 | 0.64 |
| 5:4E:78:HIS:CE1 | 5:4E:142:LEU:HD23 | 2.33 | 0.64 |
| 14:5I:24:CYS:SG | 14:5I:40:CYS:CB | 2.72 | 0.64 |
| 24:1H:273(C):C:H42 | 24:1H:363(C):G:H1 | 1.46 | 0.64 |
| 24:1H:1021:A:H3' | 24:1H:1021:A:C8 | 2.32 | 0.64 |
| 29:31:24:LEU:HB3 | 29:31:115:ALA:HB2 | 1.80 | 0.64 |
| 36:88:32:TYR:OH | 36:88:111:GLU:OE1 | 2.13 | 0.64 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 51:N8:33:CYS:SG | 51:N8:40:LYS:HD3 | 2.38 | 0.64 |
| 5:42:102:ALA:HB1 | 5:42:106:PRO:HG2 | 1.80 | 0.64 |
| 24:14:2143:C:H2' | 24:14:2144:U:O4' | 1.98 | 0.64 |
| 24:14:2293:C:H5" | 38:65:89:ARG:NH2 | 2.13 | 0.64 |
| 25:1J:89:G:O6 | 25:1J:89(A):A:N6 | 2.31 | 0.64 |
| 1:13:1358:U:H5" | 14:5I:33:VAL:O | 1.97 | 0.63 |
| 24:1H:1329:U:H5" | 24:1H:1330:C:H5 | 1.63 | 0.63 |
| 24:1H:1729:A:O2' | 24:1H:1730:U:H5" | 1.99 | 0.63 |
| 24:1H:2532:G:O2' | 24:1H:2657:A:N1 | 2.30 | 0.63 |
| 47:J8:87:PRO:CA | 47:J8:89:GLU:H | 2.10 | 0.63 |
| 1:1G:1015:A:H2' | 1:1G:1016:A:C8 | 2.33 | 0.63 |
| 15:6A:4:THR:OG1 | 15:6A:7:GLU:OE2 | 2.13 | 0.63 |
| 17:8A:69:LYS:C | 17:8A:70:ARG:HD2 | 2.22 | 0.63 |
| 21:1B:5:ASP:O | 21:1B:11:GLY:HA3 | 1.98 | 0.63 |
| 24:14:81:G:N7 | 57:14:3613:HOH:O | 2.30 | 0.63 |
| 26:79:42:GLU:HG3 | 26:79:215:THR:HG23 | 1.80 | 0.63 |
| 38:65:27:SER:HA | 38:65:88:ASP:HB3 | 1.80 | 0.63 |
| 41:95:21:ARG:NH2 | 41:95:65:GLY:O | 2.31 | 0.63 |
| 1:13:737:A:H2' | 1:13:738:C:C6 | 2.32 | 0.63 |
| 20:BI:10:LEU:HG | 20:BI:12:ALA:H | 1.63 | 0.63 |
| 24:1H:74:A:H5" | 24:1H:74:A:H8 | 1.63 | 0.63 |
| 24:1H:259:G:H21 | 24:1H:621:A:H8 | 1.47 | 0.63 |
| 36:88:51:ARG:HH12 | 36:88:52:VAL:HG23 | 1.63 | 0.63 |
| 54:Q8:29:LYS:HG3 | 54:Q8:30:ARG:HB3 | 1.80 | 0.63 |
| 1:1G:673:G:H2' | 1:1G:674:G:C8 | 2.34 | 0.63 |
| 1:1G:719:C:OP2 | 1:1G:720:C:N4 | 2.24 | 0.63 |
| 1:1G:940:C:H2' | 1:1G:941:G:H8 | 1.63 | 0.63 |
| 24:14:1171:G:O2' | 24:14:1173:G:O4' | 2.15 | 0.63 |
| 30:49:11:TYR:OH | 30:49:16:ARG:NH2 | 2.32 | 0.63 |
| 30:49:125:PHE:HB3 | 30:49:166:ASP:HB2 | 1.80 | 0.63 |
| 36:45:14:ARG:HG2 | 36:45:41:TRP:HH2 | 1.63 | 0.63 |
| 1:13:1305:G:N2 | 1:13:1331:G:H2' | 2.13 | 0.63 |
| 2:1E:214:ILE:HG23 | 2:1E:215:LEU:HD22 | 1.80 | 0.63 |
| 24:1H:1794:U:H2' | 24:1H:1795:C:C6 | 2.34 | 0.63 |
| 29:31:191:ARG:HB3 | 29:31:191:ARG:HH11 | 1.63 | 0.63 |
| 1:1G:235:C:H5' | 17:8A:70:ARG:HG2 | 1.81 | 0.63 |
| 7:62:12:LEU:HD11 | 7:62:28:ASN:ND2 | 2.12 | 0.63 |
| 39:75:56:GLY:O | 39:75:59:THR:HG22 | 1.99 | 0.63 |
| 41:95:1:MET:HG3 | 41:95:43:GLU:HB2 | 1.78 | 0.63 |
| 1:13:536:C:H2' | 1:13:537:G:C8 | 2.33 | 0.63 |
| 4:3E:173:TRP:CD1 | 4:3E:174:LEU:HG | 2.33 | 0.63 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 24:1H:2114:A:N1 | 24:1H:2119:A:N6 | 2.46 | 0.63 |
| 24:1H:2689:U:H4' | 24:1H:2690:C:H5' | 1.80 | 0.63 |
| 25:16:73:A:OP2 | 57:16:303:HOH:O | 2.16 | 0.63 |
| 26:71:50:ASP:N | 26:71:56:GLN:OE1 | 2.27 | 0.63 |
| 1:1G:678:U:H2' | 1:1G:679:C:C6 | 2.32 | 0.63 |
| 24:14:1525:G:H2' | 24:14:1526:G:C8 | 2.33 | 0.63 |
| 24:14:2754:U:H5" | 24:14:2754:U:H6 | 1.63 | 0.63 |
| 27:19:32:SER:O | 27:19:32:SER:OG | 2.08 | 0.63 |
| 29:39:22:ALA:C | 29:39:24:LEU:H | 2.06 | 0.63 |
| 39:75:50:ILE:HD11 | 39:75:102:ILE:CD1 | 2.29 | 0.63 |
| 46:E5:51:VAL:N | 46:E5:62:LEU:HD12 | 2.14 | 0.63 |
| 13:4I:90:LEU:HA | 13:4I:93:ARG:HG3 | 1.81 | 0.63 |
| 22:3K:18:G:H4' | 22:3K:19:C:O5' | 1.98 | 0.63 |
| 24:1H:773:U:H4' | 27:11:47:GLY:HA3 | 1.81 | 0.63 |
| 24:1H:1163:G:H2' | 24:1H:1164:G:H8 | 1.64 | 0.63 |
| 25:16:5:C:OP1 | 25:16:61:G:O2' | 2.15 | 0.63 |
| 51:N8:52:TYR:HD1 | 51:N8:53:ALA:H | 1.47 | 0.63 |
| 1:1G:542:G:P | 4:32:10:ARG:HH22 | 2.22 | 0.63 |
| 1:1G:1423:G:H2' | 1:1G:1424:C:C6 | 2.33 | 0.63 |
| 24:14:191:A:H2' | 24:14:192:C:C6 | 2.33 | 0.63 |
| 24:14:761:A:OP2 | 57:14:3563:HOH:O | 2.15 | 0.63 |
| 24:14:1639:U:O2' | 24:14:1640:C:H5' | 1.97 | 0.63 |
| 1:13:1455:G:H5' | 20:BI:32:ALA:HB2 | 1.81 | 0.63 |
| 22:3K:30:A:H2' | 22:3K:31:G:H5" | 1.79 | 0.63 |
| 24:1H:288:C:H2' | 24:1H:289:A:H8 | 1.62 | 0.63 |
| 24:1H:1054:A:H2' | 24:1H:1055:G:C8 | 2.34 | 0.63 |
| 24:1H:1062:G:N1 | 24:1H:1076:C:O2 | 2.32 | 0.63 |
| 24:1H:2291:U:O2' | 24:1H:2374:C:O2 | 2.14 | 0.63 |
| 27:11:59:LYS:HD2 | 27:11:60:ARG:H | 1.62 | 0.63 |
| 30:41:114:ILE:HG22 | 30:41:117:PHE:HB2 | 1.80 | 0.63 |
| 47:J8:91:LYS:HA | 47:J8:91:LYS:HZ2 | 1.63 | 0.63 |
| 48:K8:13:ALA:O | 48:K8:16:LEU:HB2 | 1.98 | 0.63 |
| 54:Q8:34:TRP:HA | 54:Q8:36:LYS:HB3 | 1.80 | 0.63 |
| 7:62:113:GLU:HB2 | 7:62:119:ARG:HG2 | 1.79 | 0.63 |
| 30:49:64:THR:OG1 | 30:49:66:GLN:N | 2.26 | 0.63 |
| 31:59:146:ALA:O | 31:59:150:ALA:N | 2.32 | 0.63 |
| 34:25:68:GLU:HB3 | 34:25:78:ARG:NH1 | 2.14 | 0.63 |
| 1:13:375:U:O3' | 16:7I:6:LEU:HB2 | 1.97 | 0.63 |
| 24:1H:1534:G:O2' | 24:1H:1535:U:O2 | 2.16 | 0.63 |
| 27:11:32:SER:HA | 27:11:34:VAL:HG22 | 1.81 | 0.63 |
| 27:11:213:ARG:HG3 | 27:11:213:ARG:HH11 | 1.61 | 0.63 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 30:41:43:LEU:HD22 | 30:41:53:LEU:HD12 | 1.80 | 0.63 |
| 36:88:14:ARG:HG2 | 36:88:41:TRP:CH2 | 2.28 | 0.63 |
| 38:A8:15:ARG:HD2 | 38:A8:88:ASP:OD2 | 1.98 | 0.63 |
| 46:I8:39:ARG:HD3 | 46:I8:58:THR:HG23 | 1.81 | 0.63 |
| 1:1G:690:G:H2' | 1:1G:691:G:O4' | 1.97 | 0.63 |
| 26:79:13:LYS:NZ | 26:79:31:GLU:O | 2.32 | 0.63 |
| 29:39:158:THR:HG23 | 29:39:164:ARG:HG3 | 1.81 | 0.63 |
| 53:L5:5:TRP:CD1 | 53:L5:7:PRO:HG3 | 2.34 | 0.63 |
| 14:5I:26:ARG:HH11 | 14:5I:43:CYS:HB2 | 1.64 | 0.63 |
| 16:7I:49:LEU:HD12 | 16:7I:50:LYS:H | 1.63 | 0.63 |
| 24:1H:111:A:H4' | 48:K8:69:ARG:NH2 | 2.13 | 0.63 |
| 24:1H:1534:G:O2' | 24:1H:1535:U:O4' | 2.15 | 0.63 |
| 31:51:4:ILE:HG21 | 31:51:6:ARG:NH1 | 2.13 | 0.63 |
| 1:1G:434:U:H2' | 1:1G:435:C:C6 | 2.34 | 0.63 |
| 7:62:16:LEU:HD12 | 9:82:41:VAL:O | 1.99 | 0.63 |
| 24:14:1266:G:O5' | 42:A5:15:ARG:NH2 | 2.32 | 0.63 |
| 24:14:1266:G:O2' | 24:14:2012:G:O6 | 2.15 | 0.63 |
| 24:14:2572:A:H5" | 24:14:2574:G:H4' | 1.81 | 0.63 |
| 26:79:3:HIS:O | 26:79:8:ARG:NH1 | 2.32 | 0.63 |
| 3:2E:49:SER:O | 3:2E:72:LYS:NZ | 2.32 | 0.63 |
| 19:AI:68:GLY:H | 50:M8:55:ARG:NH2 | 1.97 | 0.63 |
| 24:1H:248:G:H5" | 24:1H:386:G:N2 | 2.14 | 0.63 |
| 24:1H:1010:A:O2' | 24:1H:1152:C:O2' | 2.13 | 0.63 |
| 27:11:68:LYS:HB3 | 27:11:70:TRP:CZ3 | 2.34 | 0.63 |
| 30:41:143:GLU:OE1 | 50:M8:26:SER:OG | 2.17 | 0.63 |
| 48:K8:42:GLY:O | 48:K8:44:LEU:N | 2.31 | 0.63 |
| 1:1G:414:A:OP2 | 1:1G:428:G:N2 | 2.29 | 0.63 |
| 1:1G:1442:G:N7 | 1:1G:1446:A:C6 | 2.67 | 0.63 |
| 24:14:2853:C:H2' | 24:14:2854:G:C8 | 2.34 | 0.63 |
| 25:1J:5:C:O2' | 25:1J:27:C:O2 | 2.16 | 0.63 |
| 30:49:33:ARG:H | 30:49:162:THR:HG1 | 1.46 | 0.63 |
| 35:35:57:THR:O | 35:35:61:ARG:HG2 | 1.99 | 0.63 |
| 39:75:5:ALA:O | 39:75:6:LEU:HG | 1.99 | 0.63 |
| 1:13:321:A:C2 | 1:13:333:G:C2 | 2.87 | 0.62 |
| 3:2E:88:ARG:HB3 | 3:2E:99:VAL:HG21 | 1.80 | 0.62 |
| 22:3K:11:C:H42 | 22:3K:25:G:H1 | 1.47 | 0.62 |
| 24:1H:330:A:O2' | 24:1H:331:A:H8 | 1.82 | 0.62 |
| 27:11:8:PRO:HB3 | 27:11:14:ARG:HB2 | 1.79 | 0.62 |
| 27:11:213:ARG:NH1 | 27:11:213:ARG:HG3 | 2.14 | 0.62 |
| 44:G8:81:LYS:HB3 | 44:G8:82:PRO:HA | 1.80 | 0.62 |
| 3:22:90:GLU:HA | 3:22:93:LYS:HB2 | 1.81 | 0.62 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 24:14:540:G:H2' | 24:14:541:C:H6 | 1.64 | 0.62 |
| 24:14:2176:A:H2' | 24:14:2177:C:C6 | 2.34 | 0.62 |
| 38:65:26:LEU:HD13 | 38:65:87:PHE:HD1 | 1.63 | 0.62 |
| 45:D5:45:ASP:OD1 | 45:D5:49:ARG:NE | 2.31 | 0.62 |
| 54:M5:57:ARG:HH11 | 54:M5:57:ARG:N | 1.96 | 0.62 |
| 22:3K:18:G:H1 | 22:3K:65:C:H42 | 1.45 | 0.62 |
| 24:1H:1916:A:H2' | 24:1H:1917:U:O4' | 1.99 | 0.62 |
| 27:11:71:ASP:N | 27:11:71:ASP:OD1 | 2.29 | 0.62 |
| 28:21:53:PRO:O | 28:21:55:ASN:ND2 | 2.31 | 0.62 |
| 31:51:4:ILE:HD11 | 31:51:7:LEU:HD11 | 1.80 | 0.62 |
| 31:51:118:PRO:HG3 | 31:51:144:VAL:HG21 | 1.81 | 0.62 |
| 16:7A:6:LEU:HG | 16:7A:17:TYR:HB3 | 1.81 | 0.62 |
| 17:8A:81:ARG:HH21 | 17:8A:84:LEU:HD11 | 1.64 | 0.62 |
| 24:14:1623:G:O6 | 57:14:3561:HOH:O | 2.15 | 0.62 |
| 24:14:2273:A:O2' | 24:14:2274:A:H5' | 1.98 | 0.62 |
| 27:19:93:ALA:HB3 | 27:19:105:ILE:HG22 | 1.80 | 0.62 |
| 27:19:183:ARG:HG3 | 27:19:270:ILE:HD13 | 1.81 | 0.62 |
| 30:49:67:LYS:H | 50:I5:6:HIS:CD2 | 2.16 | 0.62 |
| 24:1H:2130:U:O2' | 24:1H:2158:A:N6 | 2.29 | 0.62 |
| 31:51:92:ILE:H | 31:51:92:ILE:HD12 | 1.64 | 0.62 |
| 35:78:82:GLY:HA2 | 35:78:113:LYS:O | 1.99 | 0.62 |
| 35:78:95:VAL:HA | 35:78:99:LEU:HD23 | 1.81 | 0.62 |
| 24:14:1093:G:H22 | 24:14:1097:U:H5" | 1.63 | 0.62 |
| 24:14:1800:C:OP2 | 27:19:183:ARG:NH2 | 2.31 | 0.62 |
| 1:13:193:C:H5' | 20:BI:57:ARG:HH21 | 1.64 | 0.62 |
| 4:3E:107:ARG:HH22 | 4:3E:194:LEU:HD23 | 1.63 | 0.62 |
| 31:51:121:ILE:HD11 | 31:51:141:VAL:HA | 1.82 | 0.62 |
| 37:98:74:LYS:C | 37:98:76:VAL:H | 2.08 | 0.62 |
| 1:1G:880:C:OP1 | 12:3A:8:ASN:ND2 | 2.32 | 0.62 |
| 24:14:1728:G:H8 | 24:14:1732:A:H62 | 1.47 | 0.62 |
| 28:29:47:VAL:HG22 | 28:29:48:GLN:H | 1.64 | 0.62 |
| 32:69:91:SER:HB3 | 32:69:121:LYS:HD2 | 1.82 | 0.62 |
| 41:95:10:LYS:NZ | 41:95:23:GLU:OE1 | 2.28 | 0.62 |
| 52:K5:16:CYS:SG | 52:K5:44:ARG:NH2 | 2.72 | 0.62 |
| 1:13:1320:C:N3 | 19:AI:36:ARG:NH1 | 2.48 | 0.62 |
| 28:21:50:GLY:HA2 | 28:21:77:ILE:HA | 1.81 | 0.62 |
| 51:N8:40:LYS:NZ | 51:N8:48:GLU:OE1 | 2.29 | 0.62 |
| 1:1G:25:C:H2' | 1:1G:26:A:C8 | 2.34 | 0.62 |
| 4:32:61:LYS:HB2 | 4:32:203:VAL:HG13 | 1.81 | 0.62 |
| 22:2L:8:4SU:H5' | 22:2L:8:4SU:C6 | 2.29 | 0.62 |
| 22:2L:19:C:O2' | 22:2L:21:A:OP1 | 2.18 | 0.62 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 50:I5:31:ILE:HG23 | 50:I5:32:TYR:HB2 | 1.80 | 0.62 |
| 1:13:67:C:H2' | 1:13:68:G:H8 | 1.63 | 0.62 |
| 1:13:1133:G:H2' | 1:13:1134:G:O4' | 1.99 | 0.62 |
| 1:13:1447:G:H1 | 1:13:1459:C:H42 | 1.46 | 0.62 |
| 2:1E:74:LYS:NZ | 2:1E:166:ASP:OD2 | 2.29 | 0.62 |
| 2:1E:212:GLN:NE2 | 2:1E:216:SER:OG | 2.32 | 0.62 |
| 24:1H:1025:G:C4 | 24:1H:1135:C:H1' | 2.35 | 0.62 |
| 24:1H:1169:G:H1 | 24:1H:1180:C:H42 | 1.48 | 0.62 |
| 24:1H:2564:A:OP1 | 24:1H:2648:C:H4' | 2.00 | 0.62 |
| 24:1H:2787:C:O3' | 28:21:61:ARG:NH1 | 2.31 | 0.62 |
| 1:1G:1178:G:H5" | 9:82:93:ARG:NH2 | 2.15 | 0.62 |
| 1:1G:1256:A:N6 | 1:1G:1277:C:H3' | 2.14 | 0.62 |
| 5:42:11:ILE:HG22 | 5:42:12:LEU:HB2 | 1.80 | 0.62 |
| 17:8A:17:LYS:HG2 | 17:8A:47:PRO:HA | 1.81 | 0.62 |
| 24:14:2720:U:N3 | 24:14:2873:A:H2 | 1.96 | 0.62 |
| 1:13:1296:C:H5' | 13:4I:14:ARG:HH11 | 1.64 | 0.62 |
| 24:1H:1266:G:O5' | 42:E8:15:ARG:NH2 | 2.33 | 0.62 |
| 25:16:111:U:H2' | 25:16:112:G:H8 | 1.63 | 0.62 |
| 29:31:107:LYS:HE2 | 29:31:206:ILE:HA | 1.82 | 0.62 |
| 1:1G:973:G:O3' | 14:5A:41:ARG:NH2 | 2.27 | 0.62 |
| 1:1G:1470:G:O6 | 57:1G:1810:HOH:O | 2.14 | 0.62 |
| 22:2L:24:G:H2' | 22:2L:25:G:H8 | 1.65 | 0.62 |
| 24:14:972:G:OP2 | 24:14:974:G:H5" | 2.00 | 0.62 |
| 30:49:59:GLU:OE1 | 30:49:138:GLN:NE2 | 2.32 | 0.62 |
| 34:25:7:TYR:CE1 | 34:25:20:MET:HE3 | 2.33 | 0.62 |
| 1:13:881:G:P | 12:3I:12:ARG:HH22 | 2.22 | 0.62 |
| 1:13:1157:A:H62 | 1:13:1178:G:N2 | 1.98 | 0.62 |
| 6:5E:100:ASN:HB2 | 18:9I:28:GLU:HA | 1.81 | 0.62 |
| 27:11:71:ASP:CG | 27:11:103:ARG:HH22 | 2.06 | 0.62 |
| 45:H8:75:ASN:O | 45:H8:84:GLU:N | 2.32 | 0.62 |
| 46:I8:50:ASN:HB2 | 46:I8:81:VAL:HG13 | 1.81 | 0.62 |
| 22:2L:59:A:N6 | 22:2L:60:A:H62 | 1.97 | 0.62 |
| 24:14:2133:G:N2 | 24:14:2157:G:N7 | 2.48 | 0.62 |
| 1:13:686:U:H1' | 11:2I:42:TRP:NE1 | 2.10 | 0.62 |
| 27:11:30:GLU:HG3 | 27:11:63:ARG:NH2 | 2.15 | 0.62 |
| 1:1G:1004:A:H1' | 1:1G:1025:U:C2 | 2.35 | 0.62 |
| 2:12:12:GLU:HA | 2:12:15:VAL:HG12 | 1.82 | 0.62 |
| 24:14:491:G:H2' | 24:14:492:A:C8 | 2.34 | 0.62 |
| 24:14:2111:C:H41 | 24:14:2147:G:H21 | 1.47 | 0.62 |
| 29:39:123:LEU:O | 29:39:124:LEU:HB3 | 1.99 | 0.62 |
| 30:49:98:ARG:NH2 | 50:I5:2:LYS:HE2 | 2.15 | 0.62 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 1:13:558:G:H5” | 1:13:559:A:OP2 | 2.00 | 0.62 |
| 1:13:974:A:OP2 | 14:5I:41:ARG:NH1 | 2.32 | 0.62 |
| 16:7I:49:LEU:HD12 | 16:7I:50:LYS:N | 2.15 | 0.62 |
| 24:1H:320:A:H2’ | 29:31:136:THR:HG21 | 1.80 | 0.62 |
| 46:I8:37:LEU:HG | 46:I8:60:PHE:HA | 1.82 | 0.62 |
| 5:42:140:ARG:O | 5:42:143:ARG:NH2 | 2.32 | 0.62 |
| 7:62:111:ARG:NH1 | 7:62:126:ASP:OD2 | 2.32 | 0.62 |
| 53:L5:9:ARG:HH12 | 53:L5:49:ARG:HD2 | 1.64 | 0.62 |
| 2:1E:178:ARG:HH21 | 8:7E:74:PRO:HB3 | 1.63 | 0.61 |
| 3:2E:148:GLY:HA3 | 3:2E:172:ARG:O | 1.99 | 0.61 |
| 4:3E:9:CYS:HB3 | 4:3E:32:ALA:HB2 | 1.82 | 0.61 |
| 16:7I:22:THR:HA | 16:7I:33:ILE:HG13 | 1.82 | 0.61 |
| 22:3K:21:A:N6 | 22:3K:56:U:O2 | 2.33 | 0.61 |
| 24:1H:816:C:H4’ | 57:1H:3953:HOH:O | 1.99 | 0.61 |
| 1:1G:1305:G:O2’ | 1:1G:1306:A:H8 | 1.82 | 0.61 |
| 24:14:320:A:N3 | 29:39:169:ASN:ND2 | 2.47 | 0.61 |
| 24:14:2134:A:N6 | 24:14:2157:G:N3 | 2.48 | 0.61 |
| 24:14:2754:U:H5’ | 24:14:2755:C:OP2 | 1.99 | 0.61 |
| 28:29:68:ALA:H | 28:29:69:LYS:C | 2.07 | 0.61 |
| 39:75:16:ARG:HH12 | 39:75:83:ILE:HB | 1.64 | 0.61 |
| 12:3I:93:LEU:O | 12:3I:96:VAL:HG12 | 1.99 | 0.61 |
| 24:1H:300:A:H2’ | 24:1H:334:C:H1’ | 1.81 | 0.61 |
| 24:1H:607:U:OP1 | 29:31:102:PRO:HA | 1.99 | 0.61 |
| 24:1H:2367:G:H2’ | 24:1H:2368:C:C6 | 2.36 | 0.61 |
| 42:E8:79:GLY:HA3 | 42:E8:100:THR:HG22 | 1.82 | 0.61 |
| 1:1G:81:G:N2 | 1:1G:88:C:N3 | 2.44 | 0.61 |
| 1:1G:279:A:OP2 | 17:8A:95:TYR:OH | 2.14 | 0.61 |
| 1:1G:1002:G:H2’ | 1:1G:1003:G:C8 | 2.35 | 0.61 |
| 4:32:187:ARG:NH2 | 4:32:193:ASP:OD2 | 2.33 | 0.61 |
| 12:3A:39:VAL:HB | 12:3A:57:LYS:HD3 | 1.79 | 0.61 |
| 24:14:2027:G:H2’ | 24:14:2028:U:O4’ | 1.98 | 0.61 |
| 24:14:2134:A:C2 | 24:14:2159:G:H1’ | 2.34 | 0.61 |
| 24:14:2469:A:OP2 | 24:14:2476:A:N6 | 2.33 | 0.61 |
| 1:13:1124:G:H2’ | 1:13:1145:C:C5 | 2.35 | 0.61 |
| 19:AI:32:LYS:HB3 | 19:AI:50:ALA:HB3 | 1.81 | 0.61 |
| 24:1H:330:A:HO2’ | 24:1H:331:A:H8 | 1.46 | 0.61 |
| 24:1H:643:A:N1 | 24:1H:2369:A:O2’ | 2.31 | 0.61 |
| 24:1H:2138:C:O2 | 24:1H:2154:G:N2 | 2.33 | 0.61 |
| 30:41:179:PRO:HB3 | 50:M8:38:LYS:HE2 | 1.82 | 0.61 |
| 46:I8:64:ASP:OD1 | 46:I8:64:ASP:N | 2.33 | 0.61 |
| 1:1G:1166:G:N2 | 1:1G:1170:A:OP2 | 2.32 | 0.61 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 9:82:125:TYR:HD1 | 9:82:126:SER:N | 1.98 | 0.61 |
| 13:4A:17:VAL:O | 13:4A:20:THR:OG1 | 2.12 | 0.61 |
| 15:6A:16:ALA:HB1 | 15:6A:21:ASP:HB3 | 1.82 | 0.61 |
| 20:BA:10:LEU:HG | 20:BA:11:SER:N | 2.16 | 0.61 |
| 24:14:2557:G:H2' | 24:14:2558:C:C6 | 2.36 | 0.61 |
| 35:35:146:VAL:HG13 | 35:35:147:LEU:HG | 1.82 | 0.61 |
| 1:13:510:A:OP2 | 57:13:1809:HOH:O | 2.16 | 0.61 |
| 1:13:1132:C:H2' | 1:13:1133:G:C8 | 2.35 | 0.61 |
| 24:1H:581:C:H2' | 24:1H:582:G:C8 | 2.35 | 0.61 |
| 24:1H:2427:C:H5" | 24:1H:2428:G:OP1 | 2.00 | 0.61 |
| 33:58:67:LEU:O | 33:58:88:GLU:HG3 | 1.99 | 0.61 |
| 39:B8:37:GLY:O | 39:B8:38:ASN:ND2 | 2.33 | 0.61 |
| 45:H8:147:GLY:HA2 | 45:H8:175:VAL:HG23 | 1.81 | 0.61 |
| 1:1G:321:A:C8 | 1:1G:328:C:H6 | 2.19 | 0.61 |
| 22:2L:35:QUO:C4 | 22:2L:35:QUO:C2 | 2.71 | 0.61 |
| 24:14:1329:U:H5" | 24:14:1330:C:H5 | 1.64 | 0.61 |
| 24:14:2683:C:OP1 | 39:75:53:ARG:NH2 | 2.30 | 0.61 |
| 30:49:47:LYS:HG2 | 30:49:48:GLU:H | 1.65 | 0.61 |
| 41:95:21:ARG:HH22 | 41:95:65:GLY:C | 2.08 | 0.61 |
| 4:3E:15:GLU:OE1 | 4:3E:66:ARG:NH1 | 2.34 | 0.61 |
| 24:1H:2682:U:O2' | 28:21:13:ARG:HG2 | 2.00 | 0.61 |
| 24:1H:2882:A:OP1 | 37:98:96:ARG:HD3 | 2.00 | 0.61 |
| 35:78:46:LYS:O | 35:78:47:ASP:HB3 | 1.99 | 0.61 |
| 36:88:110:THR:HG23 | 36:88:113:GLN:OE1 | 2.00 | 0.61 |
| 1:1G:269:C:H2' | 1:1G:270:A:C8 | 2.34 | 0.61 |
| 1:1G:382:A:H2' | 1:1G:383:A:C8 | 2.36 | 0.61 |
| 1:1G:1057:G:OP1 | 3:22:154:SER:OG | 2.19 | 0.61 |
| 13:4A:10:PRO:HB2 | 13:4A:18:ALA:HB1 | 1.82 | 0.61 |
| 24:14:910:A:N7 | 36:45:13:GLN:HG3 | 2.15 | 0.61 |
| 31:59:143:GLN:O | 31:59:147:ASN:ND2 | 2.33 | 0.61 |
| 34:25:115:VAL:HG13 | 34:25:121:VAL:HG21 | 1.82 | 0.61 |
| 35:35:30:THR:HG21 | 35:35:35:HIS:H | 1.65 | 0.61 |
| 39:75:88:ILE:HD11 | 39:75:91:ARG:CZ | 2.30 | 0.61 |
| 1:13:1145:C:H4' | 1:13:1146:A:C8 | 2.34 | 0.61 |
| 2:1E:88:ALA:HB2 | 2:1E:219:VAL:HG13 | 1.83 | 0.61 |
| 3:2E:155:GLY:O | 3:2E:157:ILE:HG13 | 2.00 | 0.61 |
| 5:4E:63:ARG:HA | 5:4E:66:MET:HE3 | 1.82 | 0.61 |
| 24:1H:1794:U:H2' | 24:1H:1795:C:H6 | 1.64 | 0.61 |
| 24:1H:1899:G:H22 | 24:1H:1902:C:N4 | 1.98 | 0.61 |
| 24:1H:2598:A:OP1 | 57:1H:3683:HOH:O | 2.16 | 0.61 |
| 45:H8:125:LEU:HG | 45:H8:164:ALA:HB3 | 1.83 | 0.61 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 1:1G:802:A:H5' | 1:1G:803:G:OP2 | 2.00 | 0.61 |
| 1:1G:1003:G:N2 | 1:1G:1038:C:N3 | 2.49 | 0.61 |
| 1:1G:1243:C:P | 21:1B:10:ARG:HH21 | 2.24 | 0.61 |
| 3:22:79:ARG:NH2 | 3:22:83:ARG:HB3 | 2.15 | 0.61 |
| 7:62:149:ARG:HD2 | 11:2A:59:TYR:CE1 | 2.36 | 0.61 |
| 24:14:2293:C:H42 | 24:14:2339:G:H1 | 1.47 | 0.61 |
| 24:14:2688:U:H1' | 24:14:2721:A:N6 | 2.15 | 0.61 |
| 32:69:76:THR:HG21 | 32:69:140:LEU:HD22 | 1.81 | 0.61 |
| 45:D5:105:VAL:O | 45:D5:108:PRO:HD2 | 2.00 | 0.61 |
| 6:5E:61:LEU:HB3 | 6:5E:63:TYR:HE1 | 1.65 | 0.61 |
| 9:8E:9:ARG:HB3 | 9:8E:14:VAL:HG13 | 1.83 | 0.61 |
| 24:1H:881:G:N1 | 24:1H:895:U:O4 | 2.33 | 0.61 |
| 24:1H:2367:G:H2' | 24:1H:2368:C:H6 | 1.65 | 0.61 |
| 1:1G:983:A:H2 | 1:1G:984:C:C6 | 2.19 | 0.61 |
| 1:1G:1272:G:H2' | 1:1G:1273:G:O4' | 2.01 | 0.61 |
| 6:52:100:ASN:ND2 | 18:9A:23:LYS:O | 2.25 | 0.61 |
| 9:82:37:PHE:CG | 9:82:43:ALA:HB2 | 2.35 | 0.61 |
| 24:14:320:A:H4' | 24:14:322:A:C8 | 2.36 | 0.61 |
| 24:14:1054:A:H3' | 24:14:1055:G:C8 | 2.36 | 0.61 |
| 24:14:1173:G:N3 | 24:14:1176:G:N2 | 2.48 | 0.61 |
| 24:14:2161:C:H2' | 24:14:2162:G:H8 | 1.65 | 0.61 |
| 28:29:79:ARG:N | 28:29:79:ARG:HD2 | 2.14 | 0.61 |
| 40:85:92:ARG:HD2 | 41:95:11:GLN:NE2 | 2.16 | 0.61 |
| 1:13:69:G:H3' | 1:13:73:G:H21 | 1.66 | 0.61 |
| 1:13:1106:G:H5" | 3:2E:172:ARG:HG2 | 1.83 | 0.61 |
| 1:13:1284:C:OP1 | 21:1F:26:LYS:NZ | 2.33 | 0.61 |
| 14:5I:15:LYS:HB3 | 14:5I:16:PHE:CD2 | 2.36 | 0.61 |
| 22:3K:75:C:H2' | 22:3K:76:C:C6 | 2.36 | 0.61 |
| 24:1H:1762:A:OP1 | 24:1H:1762:A:H4' | 2.01 | 0.61 |
| 24:1H:2439:A:H5' | 24:1H:2439:A:C8 | 2.35 | 0.61 |
| 33:58:130:HIS:O | 33:58:134:ARG:NH2 | 2.33 | 0.61 |
| 44:G8:29:GLU:HB2 | 44:G8:38:ILE:HG23 | 1.83 | 0.61 |
| 1:1G:1347:G:C8 | 9:82:107:ARG:HB3 | 2.36 | 0.61 |
| 2:12:21:ARG:O | 2:12:23:ARG:N | 2.33 | 0.61 |
| 10:1A:61:GLU:HG2 | 14:5A:58:LYS:HE3 | 1.82 | 0.61 |
| 13:4A:70:LEU:O | 13:4A:74:VAL:HG23 | 2.01 | 0.61 |
| 17:8A:87:LYS:HE2 | 17:8A:91:ARG:HH21 | 1.66 | 0.61 |
| 20:BA:26:ASN:OD1 | 20:BA:71:THR:OG1 | 2.14 | 0.61 |
| 24:14:943:U:OP2 | 35:35:36:LYS:NZ | 2.32 | 0.61 |
| 25:1J:66:A:H61 | 25:1J:107:U:H2' | 1.66 | 0.61 |
| 36:45:19:GLY:H | 36:45:98:LYS:NZ | 1.97 | 0.61 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 45:D5:146:ILE:HB | 45:D5:176:PRO:HG3 | 1.81 | 0.61 |
| 1:13:591:U:H2' | 1:13:592:G:H8 | 1.64 | 0.61 |
| 1:13:1336:C:H1' | 1:13:1337:G:N2 | 2.16 | 0.61 |
| 22:2K:72:U:H2' | 22:2K:73:U:C6 | 2.36 | 0.61 |
| 24:1H:84:A:OP2 | 44:G8:8:LYS:NZ | 2.24 | 0.61 |
| 24:1H:1971:A:C5 | 27:11:241:PRO:HD3 | 2.35 | 0.61 |
| 1:1G:1277:C:O2' | 1:1G:1279:A:H8 | 1.84 | 0.61 |
| 1:13:639:G:H2' | 1:13:640:A:H8 | 1.64 | 0.61 |
| 1:13:1454:G:OP1 | 20:BI:39:LYS:NZ | 2.28 | 0.61 |
| 24:1H:1218:C:H6 | 24:1H:1218:C:H5" | 1.66 | 0.61 |
| 25:16:66:A:H61 | 25:16:107:U:H2' | 1.66 | 0.61 |
| 1:1G:1004:A:O4' | 1:1G:1024:G:O2' | 2.19 | 0.61 |
| 2:12:173:ALA:HA | 2:12:176:GLU:HB2 | 1.83 | 0.61 |
| 10:1A:32:ALA:HB2 | 10:1A:81:THR:HG21 | 1.81 | 0.61 |
| 24:14:1332:G:C8 | 24:14:1332:G:H5' | 2.35 | 0.61 |
| 24:14:2816:C:O3' | 37:55:99:LYS:NZ | 2.27 | 0.61 |
| 30:49:36:LYS:HE2 | 30:49:160:VAL:HG21 | 1.83 | 0.61 |
| 36:45:34:LEU:HB2 | 36:45:118:LEU:HD13 | 1.82 | 0.61 |
| 38:65:14:VAL:O | 38:65:18:ILE:HG23 | 2.01 | 0.61 |
| 1:13:757:U:H2' | 1:13:758:G:O4' | 2.01 | 0.60 |
| 1:13:1095:U:H5' | 1:13:1109:C:O2 | 2.00 | 0.60 |
| 7:6E:50:ILE:HB | 7:6E:58:PRO:HG3 | 1.82 | 0.60 |
| 24:1H:1287:A:N7 | 37:98:107:ASP:HB2 | 2.17 | 0.60 |
| 24:1H:1678:G:H8 | 24:1H:1678:G:O5' | 1.84 | 0.60 |
| 24:1H:2791:C:H2' | 24:1H:2792:G:H8 | 1.66 | 0.60 |
| 28:21:97:LYS:N | 28:21:100:GLU:OE1 | 2.26 | 0.60 |
| 31:51:101:ARG:NH2 | 31:51:121:ILE:O | 2.34 | 0.60 |
| 1:1G:757:U:H2' | 1:1G:758:G:O4' | 2.01 | 0.60 |
| 10:1A:11:PHE:CE1 | 10:1A:67:THR:HG22 | 2.37 | 0.60 |
| 22:2L:35:QUO:O14 | 22:2L:38:MIA:H132 | 2.01 | 0.60 |
| 24:14:2693:A:H2' | 24:14:2694:G:C8 | 2.35 | 0.60 |
| 1:13:1241:G:O6 | 7:6E:115:ARG:NH2 | 2.34 | 0.60 |
| 1:13:1251:A:H2' | 1:13:1252:A:C8 | 2.36 | 0.60 |
| 24:1H:860:U:C5 | 24:1H:917:A:H2 | 2.18 | 0.60 |
| 24:1H:2661:G:O6 | 31:51:175:LYS:NZ | 2.34 | 0.60 |
| 29:31:12:LEU:HD13 | 29:31:124:LEU:HD11 | 1.81 | 0.60 |
| 46:I8:36:ILE:HD11 | 46:I8:39:ARG:HG2 | 1.82 | 0.60 |
| 46:I8:50:ASN:ND2 | 46:I8:81:VAL:O | 2.31 | 0.60 |
| 1:1G:1151:A:O2' | 1:1G:1152:A:O5' | 2.19 | 0.60 |
| 7:62:120:ILE:HG22 | 7:62:124:LEU:HD12 | 1.83 | 0.60 |
| 24:14:363(B):G:H2' | 24:14:363(C):G:H8 | 1.66 | 0.60 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 34:25:4:PRO:O | 34:25:5:GLN:HB2 | 2.00 | 0.60 |
| 38:65:15:ARG:HD2 | 38:65:88:ASP:OD2 | 2.01 | 0.60 |
| 1:13:535:A:H5" | 57:13:1836:HOH:O | 2.01 | 0.60 |
| 8:7E:121:ASP:HB2 | 8:7E:125:ARG:NH2 | 2.15 | 0.60 |
| 13:4I:67:GLU:CD | 13:4I:68:GLY:H | 2.07 | 0.60 |
| 29:31:6:VAL:HG11 | 29:31:119:ARG:HA | 1.84 | 0.60 |
| 47:J8:3:LYS:O | 47:J8:12:PRO:HD3 | 2.00 | 0.60 |
| 1:1G:1446:A:OP1 | 1:1G:1446:A:H4' | 2.00 | 0.60 |
| 22:3L:19:C:H2' | 22:3L:20:C:H4' | 1.82 | 0.60 |
| 22:3L:57:C:H4' | 22:3L:58:G:O5' | 2.01 | 0.60 |
| 24:14:984:A:H5" | 24:14:985:C:H5 | 1.66 | 0.60 |
| 25:1J:28:C:OP1 | 38:65:36:TYR:OH | 2.17 | 0.60 |
| 27:19:102:LYS:C | 27:19:103:ARG:HG2 | 2.25 | 0.60 |
| 27:19:182:LEU:H | 27:19:272:ALA:CB | 2.12 | 0.60 |
| 28:29:68:ALA:HB3 | 28:29:69:LYS:HB3 | 1.82 | 0.60 |
| 32:69:1:MET:N | 32:69:20:ASP:OD1 | 2.29 | 0.60 |
| 45:D5:23:LYS:NZ | 45:D5:40:ASP:HB2 | 2.16 | 0.60 |
| 1:13:910:C:OP1 | 12:3I:97:ARG:NH2 | 2.34 | 0.60 |
| 24:1H:71:A:H5' | 24:1H:73:A:C8 | 2.36 | 0.60 |
| 27:11:68:LYS:HB3 | 27:11:70:TRP:CH2 | 2.36 | 0.60 |
| 28:21:111:ARG:HD3 | 28:21:160:TYR:CE2 | 2.37 | 0.60 |
| 50:M8:17:GLY:H | 50:M8:36:CYS:HB3 | 1.67 | 0.60 |
| 2:12:80:ILE:H | 2:12:80:ILE:HD12 | 1.66 | 0.60 |
| 19:AA:48:THR:HG22 | 19:AA:61:TYR:HB2 | 1.82 | 0.60 |
| 30:49:64:THR:HB | 30:49:94:LEU:HD21 | 1.84 | 0.60 |
| 33:15:4:TYR:O | 40:85:64:ARG:NH1 | 2.34 | 0.60 |
| 46:E5:55:ARG:HH11 | 46:E5:55:ARG:HG3 | 1.66 | 0.60 |
| 1:13:1134:G:H1 | 1:13:1140:C:H42 | 1.50 | 0.60 |
| 1:13:1354:C:H2' | 1:13:1355:G:C8 | 2.37 | 0.60 |
| 1:13:1391:U:H2' | 1:13:1392:G:C8 | 2.36 | 0.60 |
| 2:1E:5:ILE:O | 2:1E:217:ARG:NH2 | 2.22 | 0.60 |
| 2:1E:14:GLY:H | 2:1E:16:HIS:CE1 | 2.19 | 0.60 |
| 3:2E:76:VAL:HA | 3:2E:83:ARG:HD3 | 1.83 | 0.60 |
| 5:4E:143:ARG:NE | 8:7E:77:GLU:OE1 | 2.31 | 0.60 |
| 19:AI:6:LYS:HG3 | 19:AI:9:VAL:HG22 | 1.82 | 0.60 |
| 29:31:158:THR:HB | 29:31:195:ASP:OD2 | 2.02 | 0.60 |
| 41:D8:44:LYS:O | 41:D8:46:VAL:N | 2.33 | 0.60 |
| 47:J8:90:ILE:O | 47:J8:94:LEU:HB2 | 2.00 | 0.60 |
| 6:52:20:ALA:HA | 6:52:23:LYS:HD3 | 1.82 | 0.60 |
| 17:8A:66:SER:OG | 17:8A:69:LYS:HB2 | 2.01 | 0.60 |
| 24:14:2074:U:P | 57:14:3504:HOH:O | 2.54 | 0.60 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 28:29:33:VAL:HG13 | 28:29:89:ASP:HA | 1.83 | 0.60 |
| 32:69:103:ARG:H | 32:69:103:ARG:HD3 | 1.67 | 0.60 |
| 2:1E:21:ARG:H | 2:1E:21:ARG:HE | 1.47 | 0.60 |
| 9:8E:70:LYS:O | 9:8E:74:ILE:HG13 | 2.02 | 0.60 |
| 24:1H:1156:A:OP2 | 57:1H:3684:HOH:O | 2.17 | 0.60 |
| 31:51:125:VAL:HG13 | 31:51:131:VAL:HB | 1.83 | 0.60 |
| 1:1G:1003:G:O6 | 1:1G:1035:A:N6 | 2.32 | 0.60 |
| 1:1G:1352:C:H2' | 1:1G:1353:G:C8 | 2.36 | 0.60 |
| 1:1G:1378:C:H5 | 1:1G:1379:G:C4 | 2.18 | 0.60 |
| 3:22:79:ARG:H | 3:22:79:ARG:NE | 1.99 | 0.60 |
| 22:2L:84:C:H2' | 22:2L:85:A:C2 | 2.36 | 0.60 |
| 22:3L:38:MIA:H121 | 22:3L:39:A:N1 | 2.17 | 0.60 |
| 24:14:956:G:H2' | 24:14:957:A:H2' | 1.83 | 0.60 |
| 24:14:2285:C:H41 | 52:K5:25:LYS:HZ1 | 1.49 | 0.60 |
| 24:14:2772:C:H2' | 24:14:2773:C:C6 | 2.36 | 0.60 |
| 1:13:451:A:N6 | 1:13:480:U:H2' | 2.17 | 0.60 |
| 1:13:1376:U:H2' | 1:13:1377:A:C8 | 2.37 | 0.60 |
| 11:2I:32:ILE:HD12 | 11:2I:72:ALA:HB2 | 1.84 | 0.60 |
| 24:1H:2295:C:OP1 | 38:A8:10:ARG:NH1 | 2.34 | 0.60 |
| 24:1H:2499:C:N3 | 57:1H:3748:HOH:O | 2.32 | 0.60 |
| 27:11:93:ALA:HB3 | 27:11:105:ILE:HG22 | 1.83 | 0.60 |
| 29:31:114:VAL:HG21 | 29:31:202:PHE:CE1 | 2.37 | 0.60 |
| 38:A8:67:ARG:NH2 | 38:A8:103:GLU:OE2 | 2.35 | 0.60 |
| 46:I8:53:MET:HG3 | 46:I8:59:LEU:HD21 | 1.82 | 0.60 |
| 52:O8:9:LEU:N | 52:O8:27:LYS:HG2 | 2.17 | 0.60 |
| 5:42:57:LYS:HG2 | 5:42:61:TYR:HE1 | 1.66 | 0.60 |
| 10:1A:9:ARG:NH1 | 10:1A:69:ASN:OD1 | 2.34 | 0.60 |
| 25:1J:6:C:H2' | 25:1J:7:G:H5" | 1.84 | 0.60 |
| 27:19:12:SER:HB2 | 27:19:208:LYS:HB3 | 1.82 | 0.60 |
| 43:B5:63:LYS:H | 43:B5:63:LYS:CE | 2.13 | 0.60 |
| 53:L5:47:ARG:HG3 | 53:L5:47:ARG:NH1 | 2.15 | 0.60 |
| 24:1H:330:A:O2' | 24:1H:331:A:C8 | 2.55 | 0.60 |
| 24:1H:581:C:H2' | 24:1H:582:G:H8 | 1.66 | 0.60 |
| 24:1H:934:G:H2' | 24:1H:935:C:C6 | 2.37 | 0.60 |
| 24:1H:1040:C:H42 | 24:1H:1115:G:H1 | 1.49 | 0.60 |
| 24:1H:1635:G:H2' | 24:1H:1636:C:C6 | 2.37 | 0.60 |
| 24:1H:2208:U:H4' | 27:11:151:LYS:HG2 | 1.83 | 0.60 |
| 24:1H:2298:A:OP1 | 30:41:74:LYS:NZ | 2.19 | 0.60 |
| 28:21:73:GLU:HG3 | 28:21:74:PRO:HD2 | 1.83 | 0.60 |
| 41:D8:44:LYS:C | 41:D8:46:VAL:H | 2.09 | 0.60 |
| 43:F8:57:LEU:N | 43:F8:57:LEU:HD23 | 2.17 | 0.60 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 45:H8:142:SER:HB2 | 45:H8:143:GLY:HA2 | 1.84 | 0.60 |
| 5:42:80:ILE:HD12 | 5:42:91:LEU:HB2 | 1.83 | 0.60 |
| 24:14:607:U:H3 | 24:14:621:A:H2 | 1.45 | 0.60 |
| 24:14:1139:G:O2' | 24:14:1143:A:N6 | 2.30 | 0.60 |
| 24:14:2396:G:H1' | 47:F5:30:VAL:HG23 | 1.84 | 0.60 |
| 34:25:119:PRO:HB2 | 39:75:68:TYR:CE2 | 2.36 | 0.60 |
| 1:13:450:G:OP1 | 16:7I:43:LYS:NZ | 2.35 | 0.60 |
| 1:13:1348:U:H2' | 1:13:1349:A:H8 | 1.67 | 0.60 |
| 1:13:1376:U:H2' | 1:13:1377:A:H8 | 1.67 | 0.60 |
| 10:1I:49:VAL:HG23 | 14:5I:41:ARG:HD2 | 1.82 | 0.60 |
| 18:9I:58:LEU:HD13 | 18:9I:62:GLU:HB3 | 1.83 | 0.60 |
| 24:1H:2329:G:H2' | 24:1H:2330:G:C8 | 2.36 | 0.60 |
| 27:11:70:TRP:HZ3 | 27:11:146:GLU:OE2 | 1.85 | 0.60 |
| 28:21:33:VAL:HG12 | 28:21:90:THR:H | 1.67 | 0.60 |
| 46:I8:68:GLU:OE2 | 46:I8:82:ARG:NH1 | 2.34 | 0.60 |
| 24:14:580:C:H2' | 24:14:581:C:C6 | 2.37 | 0.60 |
| 24:14:1535:U:C4 | 24:14:1536:A:H1' | 2.37 | 0.60 |
| 24:14:2142:C:H2' | 24:14:2143:C:C6 | 2.36 | 0.60 |
| 1:13:227:G:N2 | 16:7I:62:VAL:O | 2.35 | 0.60 |
| 17:8I:53:LEU:HD23 | 17:8I:82:MET:HE1 | 1.83 | 0.60 |
| 22:3K:37:A:H2' | 22:3K:38:MIA:O4' | 2.01 | 0.60 |
| 24:1H:2255:G:OP2 | 57:1H:3682:HOH:O | 2.16 | 0.60 |
| 27:11:6:PHE:HE1 | 27:11:18:VAL:HG23 | 1.67 | 0.60 |
| 27:11:70:TRP:CH2 | 27:11:150:LYS:HA | 2.37 | 0.60 |
| 32:61:120:ILE:HD12 | 32:61:126:TYR:CE2 | 2.36 | 0.60 |
| 36:88:20:ALA:HB3 | 45:H8:79:ARG:HH12 | 1.67 | 0.60 |
| 1:1G:603:U:H2' | 1:1G:604:G:C8 | 2.37 | 0.60 |
| 1:1G:607:A:C2 | 16:7A:31:LYS:HB2 | 2.36 | 0.60 |
| 1:1G:731:G:OP1 | 1:1G:766:A:H1' | 2.02 | 0.60 |
| 4:32:13:ARG:HD2 | 4:32:38:TYR:O | 2.02 | 0.60 |
| 12:3A:110:VAL:HG23 | 12:3A:120:TYR:HB3 | 1.83 | 0.60 |
| 24:14:527:C:H4' | 24:14:528:A:O5' | 2.01 | 0.60 |
| 24:14:1582:C:HO2' | 24:14:1586:A:H8 | 1.49 | 0.60 |
| 27:19:73:VAL:HG13 | 27:19:120:GLY:HA3 | 1.84 | 0.60 |
| 29:39:80:ALA:O | 29:39:83:PHE:HB2 | 2.02 | 0.60 |
| 45:D5:77:ASP:OD2 | 45:D5:80:ARG:NH1 | 2.34 | 0.60 |
| 50:I5:37:SER:O | 50:I5:40:HIS:N | 2.33 | 0.60 |
| 1:13:690:G:H2' | 1:13:691:G:O4' | 2.02 | 0.59 |
| 14:5I:4:LYS:O | 14:5I:7:ILE:HG12 | 2.02 | 0.59 |
| 16:7I:22:THR:HB | 16:7I:32:TYR:HA | 1.83 | 0.59 |
| 24:1H:277:C:H3' | 24:1H:278:A:O4' | 2.02 | 0.59 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 24:1H:1538:G:H2' | 24:1H:1539:G:H8 | 1.65 | 0.59 |
| 24:1H:1593:G:H2' | 24:1H:1594:G:C8 | 2.37 | 0.59 |
| 24:1H:1919:A:H5" | 24:1H:1920:C:OP2 | 2.02 | 0.59 |
| 26:71:190:ARG:O | 26:71:194:ARG:NH1 | 2.35 | 0.59 |
| 45:H8:35:ARG:HB3 | 45:H8:35:ARG:HH11 | 1.67 | 0.59 |
| 45:H8:102:LEU:HD21 | 45:H8:124:ILE:HG22 | 1.84 | 0.59 |
| 1:1G:142:G:H1 | 1:1G:221:C:H42 | 1.48 | 0.59 |
| 1:1G:728:A:H2' | 1:1G:729:A:C8 | 2.37 | 0.59 |
| 1:1G:1249:C:O2' | 9:82:73:GLN:OE1 | 2.18 | 0.59 |
| 1:1G:1286:A:H8 | 1:1G:1287:A:H4' | 1.65 | 0.59 |
| 19:AA:65:ASN:HD22 | 50:I5:55:ARG:HD2 | 1.67 | 0.59 |
| 22:3L:15:G:H4' | 22:3L:15:G:OP1 | 2.01 | 0.59 |
| 24:14:1130:U:O2 | 28:29:149:ARG:NH2 | 2.34 | 0.59 |
| 24:14:1292:U:H2' | 24:14:1293:C:C6 | 2.36 | 0.59 |
| 29:39:188:ARG:HA | 35:35:3:LEU:HD12 | 1.84 | 0.59 |
| 1:13:110:C:H2' | 1:13:111:G:O4' | 2.01 | 0.59 |
| 1:13:936:C:O2 | 1:13:1382:C:N4 | 2.30 | 0.59 |
| 3:2E:59:ARG:HH12 | 3:2E:97:LYS:HE2 | 1.67 | 0.59 |
| 5:4E:43:LEU:HD13 | 5:4E:109:ILE:HD11 | 1.84 | 0.59 |
| 24:1H:107:C:H2' | 24:1H:108:U:H6 | 1.67 | 0.59 |
| 24:1H:298:G:C5 | 57:1H:3702:HOH:O | 2.55 | 0.59 |
| 24:1H:895:U:O2' | 24:1H:897:C:OP2 | 2.16 | 0.59 |
| 24:1H:1683:C:H2' | 24:1H:1684:C:H6 | 1.67 | 0.59 |
| 24:1H:2148:G:H2' | 24:1H:2149:G:H8 | 1.67 | 0.59 |
| 39:B8:57:PHE:HA | 39:B8:79:HIS:HD2 | 1.66 | 0.59 |
| 41:D8:1:MET:SD | 41:D8:43:GLU:HG2 | 2.42 | 0.59 |
| 51:N8:38:ALA:HB3 | 51:N8:40:LYS:HZ2 | 1.66 | 0.59 |
| 1:1G:17:U:H2' | 1:1G:18:C:C6 | 2.38 | 0.59 |
| 1:1G:976:G:OP1 | 14:5A:32:SER:N | 2.28 | 0.59 |
| 8:72:69:ARG:HD3 | 8:72:75:ARG:O | 2.01 | 0.59 |
| 24:14:1001:A:H2' | 24:14:1002:G:O4' | 2.02 | 0.59 |
| 24:14:1520:U:H2' | 24:14:1521:G:O4' | 2.02 | 0.59 |
| 24:14:1992:G:N7 | 57:14:3616:HOH:O | 2.32 | 0.59 |
| 24:14:2786:U:HO2' | 28:29:63:LEU:H | 1.49 | 0.59 |
| 30:49:64:THR:HG1 | 30:49:66:GLN:H | 1.49 | 0.59 |
| 44:C5:99:CYS:SG | 44:C5:100:ALA:N | 2.74 | 0.59 |
| 45:D5:105:VAL:HG13 | 45:D5:106:GLY:H | 1.67 | 0.59 |
| 51:J5:35:GLU:OE1 | 51:J5:35:GLU:N | 2.35 | 0.59 |
| 1:13:323:U:H2' | 1:13:324:G:O4' | 2.03 | 0.59 |
| 1:13:1039:C:N4 | 1:13:1040:U:O4 | 2.35 | 0.59 |
| 24:1H:998:C:N4 | 57:1H:3759:HOH:O | 2.35 | 0.59 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 24:1H:2722:G:H2' | 24:1H:2723:C:C6 | 2.38 | 0.59 |
| 25:16:94:C:H2' | 25:16:95:U:C6 | 2.37 | 0.59 |
| 36:88:2:LEU:H | 36:88:2:LEU:HD12 | 1.68 | 0.59 |
| 42:E8:88:ARG:HB3 | 42:E8:92:ARG:HB3 | 1.84 | 0.59 |
| 43:F8:51:VAL:HG13 | 43:F8:81:VAL:HG23 | 1.85 | 0.59 |
| 45:H8:163:LEU:HD23 | 45:H8:163:LEU:H | 1.67 | 0.59 |
| 1:1G:617:G:OP2 | 57:1G:1812:HOH:O | 2.16 | 0.59 |
| 24:14:430:G:H5" | 24:14:431:U:OP2 | 2.01 | 0.59 |
| 29:39:84:VAL:O | 29:39:86:GLY:N | 2.35 | 0.59 |
| 42:A5:60:ASN:HD22 | 42:A5:60:ASN:N | 2.00 | 0.59 |
| 44:C5:37:VAL:HG23 | 44:C5:67:LEU:HB3 | 1.85 | 0.59 |
| 1:13:353:A:H8 | 1:13:353:A:H5' | 1.67 | 0.59 |
| 5:4E:101:ILE:O | 5:4E:120:THR:OG1 | 2.17 | 0.59 |
| 24:1H:861:A:N3 | 25:16:79:C:O2' | 2.35 | 0.59 |
| 24:1H:1899:G:N2 | 24:1H:1902:C:H5 | 2.00 | 0.59 |
| 24:1H:2445:G:OP1 | 29:31:74:ARG:NH2 | 2.34 | 0.59 |
| 45:H8:23:LYS:HE3 | 45:H8:40:ASP:HB2 | 1.84 | 0.59 |
| 47:J8:65:SER:HG | 47:J8:66:HIS:HD1 | 1.49 | 0.59 |
| 51:N8:40:LYS:HE2 | 51:N8:47:PRO:HG2 | 1.83 | 0.59 |
| 4:32:31:CYS:O | 4:32:33:MET:N | 2.35 | 0.59 |
| 4:32:154:ASN:OD1 | 4:32:154:ASN:N | 2.34 | 0.59 |
| 24:14:1716:U:H1' | 24:14:1746:G:N2 | 2.16 | 0.59 |
| 34:25:13:ASN:HD21 | 34:25:97:ARG:H | 1.48 | 0.59 |
| 41:95:21:ARG:CD | 41:95:91:TYR:CG | 2.85 | 0.59 |
| 45:D5:134:PRO:O | 45:D5:136:PHE:N | 2.33 | 0.59 |
| 45:D5:138:GLU:HG2 | 45:D5:156:LYS:HE2 | 1.84 | 0.59 |
| 54:M5:33:ASN:O | 54:M5:34:TRP:CE3 | 2.56 | 0.59 |
| 4:3E:150:GLU:HA | 4:3E:153:ARG:HG3 | 1.84 | 0.59 |
| 5:4E:72:GLN:O | 5:4E:75:THR:HG22 | 2.03 | 0.59 |
| 24:1H:458:G:O2' | 53:P8:39:ARG:HD3 | 2.03 | 0.59 |
| 24:1H:997:G:C2' | 24:1H:998:C:H5' | 2.33 | 0.59 |
| 24:1H:1994:C:OP1 | 57:1H:3686:HOH:O | 2.17 | 0.59 |
| 24:1H:2136:C:H2' | 24:1H:2137:C:C6 | 2.38 | 0.59 |
| 27:11:142:VAL:HG23 | 27:11:193:VAL:HA | 1.83 | 0.59 |
| 54:Q8:40:GLU:HA | 54:Q8:43:GLN:HB2 | 1.83 | 0.59 |
| 1:1G:1226:C:H4' | 19:AA:80:TYR:CZ | 2.37 | 0.59 |
| 4:32:108:LEU:HD13 | 4:32:174:LEU:HD13 | 1.83 | 0.59 |
| 9:82:17:VAL:HA | 9:82:63:ILE:HG12 | 1.83 | 0.59 |
| 17:8A:57:VAL:HA | 17:8A:77:VAL:HG23 | 1.84 | 0.59 |
| 18:9A:22:VAL:C | 18:9A:24:ALA:H | 2.11 | 0.59 |
| 24:14:2439:A:H5' | 24:14:2439:A:C8 | 2.37 | 0.59 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 27:19:253:GLN:HB3 | 27:19:255:LYS:NZ | 2.16 | 0.59 |
| 34:25:3:GLN:HB2 | 34:25:4:PRO:HD2 | 1.85 | 0.59 |
| 1:13:501:C:H2' | 1:13:502:G:C8 | 2.37 | 0.59 |
| 22:2K:72:U:O2' | 22:2K:73:U:H5' | 2.02 | 0.59 |
| 22:3K:20:C:O2' | 22:3K:22:A:O5' | 2.20 | 0.59 |
| 24:1H:450:G:N7 | 57:1H:3678:HOH:O | 2.31 | 0.59 |
| 24:1H:1045:A:H4' | 24:1H:1045:A:OP1 | 2.02 | 0.59 |
| 24:1H:1171:G:N7 | 24:1H:1174:A:N6 | 2.50 | 0.59 |
| 27:11:213:ARG:HH11 | 27:11:213:ARG:CG | 2.15 | 0.59 |
| 42:E8:57:ASN:O | 42:E8:61:ASN:HB2 | 2.03 | 0.59 |
| 45:H8:140:ASP:N | 45:H8:140:ASP:OD1 | 2.35 | 0.59 |
| 1:1G:427:U:OP1 | 4:32:13:ARG:NH2 | 2.32 | 0.59 |
| 13:4A:22:ILE:HB | 13:4A:25:ILE:HG13 | 1.85 | 0.59 |
| 13:4A:54:VAL:HA | 13:4A:57:ARG:HB3 | 1.84 | 0.59 |
| 13:4A:65:LYS:HB2 | 13:4A:69:GLU:CD | 2.27 | 0.59 |
| 27:19:232:PRO:O | 57:19:403:HOH:O | 2.17 | 0.59 |
| 39:75:134:GLU:N | 39:75:134:GLU:OE2 | 2.36 | 0.59 |
| 40:85:108:GLU:O | 40:85:111:GLU:N | 2.36 | 0.59 |
| 1:13:375:U:OP1 | 16:7I:69:THR:HG21 | 2.03 | 0.59 |
| 12:3I:62:SER:HB2 | 12:3I:64:TYR:HD1 | 1.67 | 0.59 |
| 22:2K:84:C:H3' | 22:2K:85:A:H5" | 1.84 | 0.59 |
| 24:1H:860:U:C5 | 24:1H:917:A:C2 | 2.85 | 0.59 |
| 24:1H:1140:C:OP1 | 33:58:23:LEU:HB3 | 2.03 | 0.59 |
| 24:1H:1221:C:H2' | 24:1H:1222:C:C6 | 2.36 | 0.59 |
| 24:1H:1430:C:H2' | 24:1H:1431:U:H6 | 1.66 | 0.59 |
| 24:1H:2108:C:H42 | 24:1H:2181:G:H1 | 1.51 | 0.59 |
| 25:16:30:C:OP2 | 38:A8:32:LEU:HD11 | 2.03 | 0.59 |
| 30:41:131:TYR:O | 30:41:159:VAL:HG22 | 2.02 | 0.59 |
| 31:51:113:VAL:HG11 | 31:51:151:ILE:HD13 | 1.84 | 0.59 |
| 44:G8:41:GLY:HA2 | 44:G8:64:GLU:OE1 | 2.03 | 0.59 |
| 8:72:86:ILE:HG21 | 8:72:133:LEU:HD13 | 1.85 | 0.59 |
| 9:82:9:ARG:NH1 | 9:82:9:ARG:O | 2.35 | 0.59 |
| 24:14:1709:U:H2' | 24:14:1710:C:C6 | 2.37 | 0.59 |
| 28:29:103:ASP:OD1 | 28:29:201:THR:HG23 | 2.03 | 0.59 |
| 33:15:96:GLU:HB2 | 33:15:122:VAL:HG12 | 1.85 | 0.59 |
| 45:D5:5:LEU:HD11 | 45:D5:43:GLU:HB3 | 1.82 | 0.59 |
| 1:13:1182:G:C4' | 1:13:1183:A:H5' | 2.32 | 0.59 |
| 4:3E:108:LEU:HD21 | 4:3E:183:GLY:HA3 | 1.85 | 0.59 |
| 22:2K:15:G:H21 | 22:2K:20:C:N4 | 1.98 | 0.59 |
| 31:51:4:ILE:HG21 | 31:51:6:ARG:CZ | 2.33 | 0.59 |
| 32:61:1:MET:HB3 | 32:61:21:VAL:O | 2.02 | 0.59 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 38:A8:20:ARG:NH1 | 46:I8:47:PRO:O | 2.35 | 0.59 |
| 48:K8:47:ASN:C | 48:K8:49:LYS:N | 2.61 | 0.59 |
| 24:14:1364:G:OP1 | 47:F5:3:LYS:HD3 | 2.03 | 0.59 |
| 24:14:1434:A:H61 | 24:14:1558:A:H62 | 1.51 | 0.59 |
| 24:14:1441:G:H2' | 24:14:1442:G:H8 | 1.67 | 0.59 |
| 36:45:26:TYR:OH | 36:45:141:GLN:HB2 | 2.02 | 0.59 |
| 43:B5:51:VAL:H | 43:B5:83:VAL:HG23 | 1.67 | 0.59 |
| 1:13:321:A:H62 | 1:13:328:C:H1' | 1.66 | 0.59 |
| 10:1I:34:VAL:HG12 | 10:1I:74:ILE:HG22 | 1.84 | 0.59 |
| 24:1H:593:G:O4' | 54:Q8:4:MET:HE1 | 2.03 | 0.59 |
| 24:1H:1105:U:H2' | 24:1H:1106:G:C8 | 2.36 | 0.59 |
| 24:1H:2737:G:H2' | 24:1H:2738:A:H8 | 1.68 | 0.59 |
| 30:41:66:GLN:HA | 50:M8:6:HIS:CE1 | 2.37 | 0.59 |
| 43:F8:26:TYR:HD1 | 43:F8:92:LEU:HD12 | 1.68 | 0.59 |
| 47:J8:85:LEU:H | 47:J8:86:SER:C | 2.03 | 0.59 |
| 1:1G:15:G:H2' | 1:1G:16:A:C8 | 2.38 | 0.59 |
| 1:1G:187:C:H2' | 1:1G:188:U:O4' | 2.02 | 0.59 |
| 1:1G:570:G:H2' | 1:1G:571:U:C6 | 2.37 | 0.59 |
| 1:1G:946:A:H2' | 1:1G:947:G:C8 | 2.38 | 0.59 |
| 1:1G:993:G:H1 | 1:1G:1045:C:H42 | 1.51 | 0.59 |
| 2:12:118:LEU:HD12 | 2:12:142:LEU:HB2 | 1.84 | 0.59 |
| 13:4A:92:HIS:HE1 | 13:4A:98:VAL:HG21 | 1.68 | 0.59 |
| 24:14:602:G:O2' | 24:14:655:A:N6 | 2.35 | 0.59 |
| 24:14:1140:C:H1' | 24:14:1143:A:C8 | 2.37 | 0.59 |
| 24:14:1486:A:H2' | 24:14:1487:G:H8 | 1.67 | 0.59 |
| 24:14:1496:A:H8 | 24:14:1577:C:O2' | 1.84 | 0.59 |
| 24:14:2262:U:OP1 | 24:14:2387:U:O2' | 2.20 | 0.59 |
| 24:14:2296:U:OP2 | 38:65:9:ARG:NH1 | 2.30 | 0.59 |
| 28:29:60:ASN:HB2 | 28:29:62:PRO:HD2 | 1.83 | 0.59 |
| 38:65:35:ILE:HG13 | 38:65:97:ARG:HH21 | 1.68 | 0.59 |
| 39:75:7:ILE:H | 39:75:10:VAL:HB | 1.67 | 0.59 |
| 44:C5:97:ARG:NE | 44:C5:104:GLY:O | 2.36 | 0.59 |
| 1:13:186:C:O2' | 20:BI:85:MET:SD | 2.54 | 0.59 |
| 1:13:734:G:H2' | 1:13:735:C:H6 | 1.68 | 0.59 |
| 1:13:908:A:H2' | 1:13:909:A:C8 | 2.37 | 0.59 |
| 4:3E:22:LYS:HB2 | 4:3E:26:CYS:SG | 2.43 | 0.59 |
| 24:1H:443:A:N7 | 29:31:45:ARG:HG2 | 2.17 | 0.59 |
| 24:1H:1635:G:H2' | 24:1H:1636:C:H6 | 1.68 | 0.59 |
| 31:51:56:SER:OG | 31:51:57:ASP:N | 2.34 | 0.59 |
| 1:1G:539:A:OP2 | 12:3A:115:LYS:HE2 | 2.02 | 0.59 |
| 9:82:26:VAL:HG22 | 9:82:61:ALA:HB3 | 1.84 | 0.59 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 24:14:576:U:O4 | 57:14:3560:HOH:O | 2.15 | 0.59 |
| 1:13:468:A:H4' | 16:7I:80:PHE:O | 2.03 | 0.58 |
| 4:3E:39:PRO:HD2 | 4:3E:44:GLY:HA2 | 1.85 | 0.58 |
| 12:3I:24:VAL:HB | 12:3I:27:LEU:HD12 | 1.84 | 0.58 |
| 24:1H:654(H):G:N7 | 24:1H:654(N):G:N2 | 2.50 | 0.58 |
| 24:1H:1053:C:H42 | 24:1H:1106:G:H1 | 1.51 | 0.58 |
| 1:1G:1324:A:H4' | 1:1G:1362:C:H4' | 1.83 | 0.58 |
| 4:32:59:ARG:O | 4:32:63:LYS:N | 2.30 | 0.58 |
| 9:82:10:ARG:HG3 | 9:82:105:ASP:HB3 | 1.84 | 0.58 |
| 17:8A:88:TYR:HA | 17:8A:91:ARG:HD2 | 1.85 | 0.58 |
| 20:BA:75:ASN:N | 20:BA:75:ASN:OD1 | 2.33 | 0.58 |
| 24:14:2772:C:H2' | 24:14:2773:C:H6 | 1.68 | 0.58 |
| 31:59:64:LEU:HA | 31:59:67:LEU:HD12 | 1.85 | 0.58 |
| 32:69:56:LYS:O | 32:69:60:GLU:HB2 | 2.03 | 0.58 |
| 39:75:46:GLU:H | 39:75:65:LYS:NZ | 2.00 | 0.58 |
| 1:13:52:G:H2' | 1:13:53:A:H8 | 1.67 | 0.58 |
| 1:13:171:A:H2' | 1:13:172:A:C8 | 2.38 | 0.58 |
| 1:13:735:C:H2' | 1:13:736:C:C6 | 2.38 | 0.58 |
| 28:21:21:VAL:HG13 | 28:21:185:LYS:HG3 | 1.84 | 0.58 |
| 29:31:28:ILE:HG21 | 29:31:116:ASP:HB2 | 1.85 | 0.58 |
| 29:31:157:VAL:HB | 29:31:194:MET:HB3 | 1.85 | 0.58 |
| 36:88:51:ARG:NH1 | 36:88:52:VAL:HG23 | 2.18 | 0.58 |
| 4:32:149:ALA:O | 4:32:153:ARG:HB2 | 2.02 | 0.58 |
| 19:AA:41:VAL:HG22 | 19:AA:44:MET:HE3 | 1.84 | 0.58 |
| 24:14:142:G:H2' | 24:14:143:C:C6 | 2.37 | 0.58 |
| 24:14:2130:U:O2' | 24:14:2134:A:O4' | 2.21 | 0.58 |
| 24:14:2533:A:OP2 | 57:14:3565:HOH:O | 2.17 | 0.58 |
| 25:1J:41:U:C4 | 30:49:70:VAL:HG23 | 2.38 | 0.58 |
| 27:19:10:THR:OG1 | 27:19:13:ARG:HB2 | 2.03 | 0.58 |
| 6:5E:89:MET:HE3 | 18:9I:76:LEU:HD13 | 1.85 | 0.58 |
| 24:1H:1183:G:O3' | 49:L8:29:ARG:NH1 | 2.37 | 0.58 |
| 24:1H:1435:G:O5' | 24:1H:1435:G:H8 | 1.86 | 0.58 |
| 24:1H:2776:A:H4' | 24:1H:2777:G:H5" | 1.84 | 0.58 |
| 40:C8:75:ASN:HD22 | 40:C8:75:ASN:H | 1.51 | 0.58 |
| 47:J8:80:LEU:H | 47:J8:80:LEU:HD22 | 1.67 | 0.58 |
| 1:1G:451:A:OP1 | 1:1G:481:G:N2 | 2.32 | 0.58 |
| 1:1G:1227:A:H8 | 1:1G:1227:A:H3' | 1.69 | 0.58 |
| 1:1G:1392:G:H21 | 1:1G:1502:A:H8 | 1.50 | 0.58 |
| 6:52:25:ILE:HG21 | 6:52:82:ARG:HD2 | 1.84 | 0.58 |
| 24:14:2404:C:O3' | 35:35:77:ARG:NH2 | 2.36 | 0.58 |
| 1:13:925:G:O6 | 1:13:1391:U:N3 | 2.19 | 0.58 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 14:5I:43:CYS:HA | 14:5I:46:GLU:HB2 | 1.84 | 0.58 |
| 24:1H:943:U:OP2 | 35:78:36:LYS:NZ | 2.37 | 0.58 |
| 24:1H:2023:G:H5' | 24:1H:2617:C:H4' | 1.83 | 0.58 |
| 29:31:102:PRO:HB2 | 29:31:105:VAL:HG23 | 1.85 | 0.58 |
| 32:61:63:ALA:O | 32:61:67:ARG:HB2 | 2.03 | 0.58 |
| 35:78:47:ASP:OD2 | 35:78:50:ARG:NH2 | 2.36 | 0.58 |
| 12:3A:41:ARG:HB3 | 12:3A:41:ARG:NH1 | 2.18 | 0.58 |
| 24:14:373:U:H2' | 24:14:374:A:H8 | 1.68 | 0.58 |
| 24:14:733:G:C8 | 57:14:3550:HOH:O | 2.52 | 0.58 |
| 38:65:62:LYS:HB3 | 38:65:97:ARG:HD2 | 1.83 | 0.58 |
| 1:13:280:C:H3' | 1:13:281:G:H5' | 1.85 | 0.58 |
| 1:13:674:G:H2' | 1:13:675:A:C8 | 2.38 | 0.58 |
| 1:13:1239:A:O2' | 1:13:1298:C:N4 | 2.36 | 0.58 |
| 1:13:1346:A:H5" | 9:8E:120:ARG:NH1 | 2.19 | 0.58 |
| 5:4E:139:LEU:HA | 5:4E:142:LEU:HD12 | 1.85 | 0.58 |
| 24:1H:85:G:OP2 | 44:G8:9:LYS:HB2 | 2.03 | 0.58 |
| 24:1H:2031:A:C6 | 24:1H:2498:C:H1' | 2.38 | 0.58 |
| 24:1H:2518:A:H5' | 24:1H:2518:A:C8 | 2.39 | 0.58 |
| 28:21:70:ALA:HB1 | 28:21:73:GLU:HB2 | 1.86 | 0.58 |
| 1:1G:1300:G:O2' | 1:1G:1301:U:O5' | 2.21 | 0.58 |
| 4:32:22:LYS:HG3 | 4:32:26:CYS:SG | 2.43 | 0.58 |
| 4:32:173:TRP:CD1 | 4:32:174:LEU:HG | 2.38 | 0.58 |
| 5:42:100:VAL:HA | 5:42:118:ILE:HG22 | 1.85 | 0.58 |
| 13:4A:49:THR:HG22 | 13:4A:51:ALA:H | 1.68 | 0.58 |
| 15:6A:3:ILE:H | 15:6A:3:ILE:HD13 | 1.67 | 0.58 |
| 24:14:250:G:OP1 | 35:35:60:MET:HE1 | 2.02 | 0.58 |
| 24:14:588:U:H2' | 24:14:589:C:C6 | 2.39 | 0.58 |
| 24:14:861:A:C2 | 24:14:917:A:C4 | 2.92 | 0.58 |
| 24:14:1418:G:H2' | 24:14:1579:A:N6 | 2.19 | 0.58 |
| 24:14:2270:G:OP2 | 57:14:3566:HOH:O | 2.17 | 0.58 |
| 24:14:2637:U:H5" | 28:29:82:ARG:HH21 | 1.68 | 0.58 |
| 39:75:16:ARG:HB3 | 39:75:18:ASP:OD1 | 2.03 | 0.58 |
| 39:75:118:ARG:HA | 39:75:121:ILE:HB | 1.86 | 0.58 |
| 1:13:689:C:H3' | 1:13:690:G:H21 | 1.69 | 0.58 |
| 1:13:1219:U:H2' | 1:13:1220:G:C8 | 2.39 | 0.58 |
| 1:13:1287:A:H2' | 1:13:1288:A:C8 | 2.39 | 0.58 |
| 1:13:1305:G:H21 | 1:13:1331:G:H2' | 1.66 | 0.58 |
| 24:1H:376:C:OP1 | 57:1H:3685:HOH:O | 2.17 | 0.58 |
| 24:1H:2199:A:H5' | 47:J8:50:ARG:HH21 | 1.69 | 0.58 |
| 29:31:160:ASN:OD1 | 29:31:163:VAL:HG23 | 2.02 | 0.58 |
| 33:58:134:ARG:O | 33:58:136:GLU:N | 2.37 | 0.58 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 35:78:52:GLU:CG | 35:78:57:THR:HG22 | 2.34 | 0.58 |
| 50:M8:57:GLU:O | 50:M8:61:ARG:NH1 | 2.36 | 0.58 |
| 1:1G:827:U:H5" | 1:1G:828:A:OP2 | 2.03 | 0.58 |
| 1:1G:1086:U:O5' | 1:1G:1086:U:H6 | 1.86 | 0.58 |
| 1:1G:1228:C:H2' | 1:1G:1229:A:C8 | 2.37 | 0.58 |
| 24:14:634:C:H2' | 24:14:635:C:C6 | 2.38 | 0.58 |
| 24:14:1149:G:H2' | 24:14:1150:C:C6 | 2.39 | 0.58 |
| 24:14:2319:G:N1 | 24:14:2334:G:OP2 | 2.34 | 0.58 |
| 24:14:2537:U:H2' | 24:14:2538:C:C6 | 2.39 | 0.58 |
| 28:29:101:ARG:NH1 | 28:29:169:ASN:O | 2.36 | 0.58 |
| 30:49:5:VAL:HB | 30:49:8:LYS:HB3 | 1.85 | 0.58 |
| 49:H5:8:LEU:O | 49:H5:32:GLN:N | 2.31 | 0.58 |
| 1:13:273:A:H1' | 17:8I:16:GLN:HE21 | 1.68 | 0.58 |
| 1:13:517:G:N1 | 1:13:533:A:OP2 | 2.31 | 0.58 |
| 1:13:975:A:H5" | 1:13:975:A:H8 | 1.69 | 0.58 |
| 1:13:1312:G:OP2 | 50:M8:62:ARG:NH1 | 2.37 | 0.58 |
| 24:1H:433:C:H2' | 24:1H:434:U:C6 | 2.37 | 0.58 |
| 24:1H:2275:C:H5' | 24:1H:2275:C:H6 | 1.67 | 0.58 |
| 49:L8:50:VAL:O | 49:L8:54:VAL:HG12 | 2.03 | 0.58 |
| 1:1G:197:A:C8 | 1:1G:198:G:H1' | 2.38 | 0.58 |
| 1:1G:1450:U:OP1 | 1:1G:1451:A:N6 | 2.37 | 0.58 |
| 15:6A:56:LEU:O | 15:6A:60:VAL:HG23 | 2.04 | 0.58 |
| 24:14:528:A:H2 | 24:14:2043:C:C5' | 2.16 | 0.58 |
| 24:14:739:G:P | 57:14:3555:HOH:O | 2.61 | 0.58 |
| 24:14:886:C:O2' | 24:14:887:A:O5' | 2.22 | 0.58 |
| 24:14:2134:A:H2 | 24:14:2159:G:H1' | 1.69 | 0.58 |
| 24:14:2531:A:H5' | 31:59:157:TYR:CE2 | 2.38 | 0.58 |
| 25:1J:7:G:H4' | 38:65:29:PHE:HD2 | 1.66 | 0.58 |
| 25:1J:12:C:H2' | 46:E5:73:GLY:HA3 | 1.86 | 0.58 |
| 32:69:92:VAL:HG13 | 32:69:120:ILE:HG13 | 1.85 | 0.58 |
| 36:45:78:PRO:O | 36:45:79:LEU:HB3 | 2.04 | 0.58 |
| 48:G5:38:GLN:NE2 | 48:G5:44:LEU:O | 2.32 | 0.58 |
| 1:13:235:C:H5' | 17:8I:70:ARG:HG2 | 1.86 | 0.58 |
| 1:13:667:G:H4' | 15:6I:51:HIS:CE1 | 2.39 | 0.58 |
| 1:13:735:C:H2' | 1:13:736:C:H6 | 1.66 | 0.58 |
| 1:13:1132:C:H2' | 1:13:1133:G:H8 | 1.67 | 0.58 |
| 2:1E:21:ARG:C | 2:1E:23:ARG:H | 2.12 | 0.58 |
| 2:1E:101:MET:HA | 2:1E:108:ILE:HD12 | 1.86 | 0.58 |
| 9:8E:18:PHE:HD2 | 9:8E:62:TYR:HD2 | 1.51 | 0.58 |
| 20:BI:19:SER:O | 20:BI:23:ARG:HB2 | 2.03 | 0.58 |
| 22:2K:69:U:H5" | 22:2K:70:C:H5 | 1.68 | 0.58 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 24:1H:420:C:H2' | 24:1H:421:U:C6 | 2.39 | 0.58 |
| 24:1H:1170:G:N2 | 24:1H:1180:C:O2 | 2.36 | 0.58 |
| 24:1H:2131:G:H21 | 24:1H:2158:A:H5" | 1.67 | 0.58 |
| 24:1H:2816:C:O3' | 37:98:99:LYS:NZ | 2.30 | 0.58 |
| 30:41:124:SER:HB2 | 30:41:131:TYR:CE1 | 2.38 | 0.58 |
| 2:12:7:VAL:HG13 | 2:12:8:LYS:H | 1.68 | 0.58 |
| 4:32:188:LEU:HD23 | 4:32:189:PRO:HD2 | 1.85 | 0.58 |
| 22:2L:41:C:H2' | 22:2L:42:U:H6 | 1.68 | 0.58 |
| 24:14:2123:G:O6 | 24:14:2174:C:N4 | 2.36 | 0.58 |
| 24:14:2150:U:H2' | 24:14:2151:G:H8 | 1.68 | 0.58 |
| 1:13:179:A:H2' | 1:13:180:U:H6 | 1.68 | 0.58 |
| 1:13:1213:A:O2' | 1:13:1215:G:N7 | 2.32 | 0.58 |
| 18:9I:66:LEU:O | 18:9I:70:ILE:HG13 | 2.03 | 0.58 |
| 24:1H:593:G:C1' | 54:Q8:4:MET:HE1 | 2.34 | 0.58 |
| 24:1H:2550:G:OP1 | 57:1H:3629:HOH:O | 2.17 | 0.58 |
| 28:21:15:PHE:HB3 | 39:B8:81:PRO:HG2 | 1.86 | 0.58 |
| 1:1G:908:A:H2' | 1:1G:909:A:C8 | 2.38 | 0.58 |
| 8:72:82:HIS:C | 8:72:82:HIS:CD2 | 2.82 | 0.58 |
| 13:4A:80:ARG:HB3 | 19:AA:66:MET:HE1 | 1.85 | 0.58 |
| 24:14:141:A:H8 | 24:14:1595:G:H21 | 1.51 | 0.58 |
| 24:14:2845:G:O2' | 24:14:2846:G:H5' | 2.04 | 0.58 |
| 1:13:939:G:H2' | 1:13:940:C:H6 | 1.68 | 0.58 |
| 1:13:964:A:H4' | 10:1I:55:LYS:HD2 | 1.86 | 0.58 |
| 23:4K:13:A:O2' | 23:4K:14:A:H5" | 2.04 | 0.58 |
| 24:1H:77:C:H5" | 48:K8:10:LEU:HD11 | 1.86 | 0.58 |
| 24:1H:910:A:C5 | 36:88:13:GLN:HG3 | 2.38 | 0.58 |
| 24:1H:1331:A:O2' | 24:1H:1332:G:H8 | 1.87 | 0.58 |
| 24:1H:1354:A:H2' | 24:1H:1355:G:O4' | 2.04 | 0.58 |
| 24:1H:2724:C:OP1 | 28:21:118:LYS:HE3 | 2.04 | 0.58 |
| 38:A8:93:LYS:HG2 | 38:A8:95:HIS:HB2 | 1.86 | 0.58 |
| 45:H8:23:LYS:HA | 45:H8:40:ASP:HA | 1.85 | 0.58 |
| 46:I8:49:LYS:HB2 | 46:I8:80:HIS:HB3 | 1.86 | 0.58 |
| 54:Q8:56:GLU:HG2 | 54:Q8:57:ARG:NH2 | 2.19 | 0.58 |
| 6:52:96:PRO:HB3 | 18:9A:30:ASP:CG | 2.29 | 0.58 |
| 13:4A:23:TYR:HE2 | 13:4A:71:ARG:HD3 | 1.68 | 0.58 |
| 24:14:458:G:O2' | 53:L5:39:ARG:HD3 | 2.04 | 0.58 |
| 24:14:1192:G:H2' | 24:14:1193:G:H8 | 1.67 | 0.58 |
| 24:14:2793:G:N2 | 24:14:2804:C:O2 | 2.36 | 0.58 |
| 25:1J:60:C:H2' | 25:1J:61:G:H8 | 1.68 | 0.58 |
| 28:29:52:LEU:O | 28:29:75:VAL:N | 2.31 | 0.58 |
| 29:39:84:VAL:HG12 | 29:39:85:GLY:N | 2.18 | 0.58 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 31:59:103:LEU:HD22 | 31:59:121:ILE:HG21 | 1.86 | 0.58 |
| 41:95:35:LEU:O | 41:95:37:VAL:HG22 | 2.04 | 0.58 |
| 45:D5:132:ASN:N | 45:D5:132:ASN:OD1 | 2.37 | 0.58 |
| 50:I5:21:VAL:HG22 | 50:I5:22:ILE:H | 1.68 | 0.58 |
| 1:13:1135:U:H4' | 1:13:1136:U:C5 | 2.36 | 0.57 |
| 3:2E:73:PRO:O | 3:2E:76:VAL:HG22 | 2.04 | 0.57 |
| 4:3E:190:ASP:HB3 | 4:3E:192:GLU:HG3 | 1.86 | 0.57 |
| 24:1H:459:U:H5" | 53:P8:40:TRP:CD2 | 2.39 | 0.57 |
| 24:1H:1210:A:H5' | 24:1H:1210:A:H8 | 1.69 | 0.57 |
| 24:1H:1798:U:H5' | 27:11:259:THR:CG2 | 2.34 | 0.57 |
| 24:1H:2077:A:H2' | 24:1H:2078:C:H6 | 1.69 | 0.57 |
| 24:1H:2111:C:H41 | 24:1H:2147:G:N2 | 2.01 | 0.57 |
| 24:1H:2345:G:N3 | 24:1H:2381:C:H2' | 2.19 | 0.57 |
| 24:1H:2887:U:H2' | 24:1H:2888:C:C6 | 2.39 | 0.57 |
| 1:1G:995:C:H1' | 14:5A:4:LYS:HZ2 | 1.69 | 0.57 |
| 1:1G:1152:A:OP1 | 10:1A:68:HIS:ND1 | 2.37 | 0.57 |
| 12:3A:69:TYR:HD2 | 12:3A:99:HIS:CD2 | 2.22 | 0.57 |
| 24:14:1430:C:H2' | 24:14:1431:U:C6 | 2.38 | 0.57 |
| 28:29:68:ALA:N | 28:29:69:LYS:O | 2.32 | 0.57 |
| 30:49:61:ALA:HB2 | 30:49:68:PRO:HD3 | 1.86 | 0.57 |
| 35:35:2:LYS:HG3 | 35:35:5:ASP:OD2 | 2.03 | 0.57 |
| 38:65:106:ARG:NH1 | 38:65:107:GLU:OE2 | 2.37 | 0.57 |
| 1:13:560:U:H5' | 1:13:566:G:N2 | 2.18 | 0.57 |
| 1:13:1157:A:N6 | 1:13:1178:G:N2 | 2.51 | 0.57 |
| 2:1E:185:ILE:HB | 2:1E:199:TYR:HB2 | 1.86 | 0.57 |
| 3:2E:147:LYS:HD3 | 3:2E:204:LEU:O | 2.04 | 0.57 |
| 17:8I:19:VAL:HG23 | 17:8I:44:ALA:HB3 | 1.86 | 0.57 |
| 22:2K:69:U:H5" | 22:2K:70:C:C5 | 2.38 | 0.57 |
| 24:1H:3:U:OP1 | 24:1H:2790:A:N6 | 2.37 | 0.57 |
| 24:1H:603:A:H4' | 24:1H:604:G:O5' | 2.04 | 0.57 |
| 24:1H:1009:A:OP2 | 33:58:37:LYS:NZ | 2.23 | 0.57 |
| 24:1H:1021:A:H61 | 24:1H:1142(A):A:H61 | 1.51 | 0.57 |
| 26:71:43:VAL:HG22 | 26:71:214:VAL:HG22 | 1.84 | 0.57 |
| 36:88:51:ARG:HG2 | 36:88:51:ARG:HH11 | 1.70 | 0.57 |
| 39:B8:26:ASP:OD2 | 39:B8:120:ARG:NH1 | 2.37 | 0.57 |
| 40:C8:110:VAL:O | 40:C8:113:ALA:HB3 | 2.04 | 0.57 |
| 1:1G:9:G:OP2 | 5:42:121:LYS:NZ | 2.30 | 0.57 |
| 1:1G:514:C:H2' | 1:1G:515:G:H8 | 1.67 | 0.57 |
| 1:1G:625:G:H2' | 1:1G:626:U:H6 | 1.69 | 0.57 |
| 8:72:9:MET:HG3 | 8:72:26:VAL:HG11 | 1.85 | 0.57 |
| 24:14:1098:A:H3' | 24:14:1099:G:H5' | 1.87 | 0.57 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 24:14:2365:G:H4' | 46:E5:60:PHE:CZ | 2.39 | 0.57 |
| 28:29:38:THR:HG23 | 28:29:41:LYS:HB3 | 1.87 | 0.57 |
| 28:29:201:THR:HG22 | 28:29:202:LYS:H | 1.69 | 0.57 |
| 30:49:17:PRO:HA | 30:49:20:ILE:HG22 | 1.86 | 0.57 |
| 33:15:96:GLU:H | 33:15:96:GLU:CD | 2.12 | 0.57 |
| 35:35:48:PRO:C | 35:35:50:ARG:H | 2.11 | 0.57 |
| 1:13:837:G:N2 | 1:13:850:U:O2 | 2.36 | 0.57 |
| 1:13:1238:A:N7 | 1:13:1303:C:H1' | 2.19 | 0.57 |
| 2:1E:69:LEU:HD12 | 2:1E:70:PHE:H | 1.68 | 0.57 |
| 4:3E:108:LEU:HB3 | 4:3E:110:PHE:HD1 | 1.68 | 0.57 |
| 9:8E:46:ALA:HA | 9:8E:78:LYS:HB2 | 1.86 | 0.57 |
| 22:2K:35:QUO:C4 | 22:2K:35:QUO:C2 | 2.69 | 0.57 |
| 24:1H:274:G:H2' | 24:1H:275:G:O4' | 2.03 | 0.57 |
| 24:1H:988:A:P | 49:L8:11:SER:HB2 | 2.44 | 0.57 |
| 24:1H:2404:C:OP2 | 57:1H:3687:HOH:O | 2.17 | 0.57 |
| 31:51:137:ASP:OD1 | 31:51:138:LYS:N | 2.36 | 0.57 |
| 38:A8:10:ARG:O | 38:A8:14:VAL:HG13 | 2.04 | 0.57 |
| 40:C8:25:TRP:O | 40:C8:28:ARG:HB2 | 2.04 | 0.57 |
| 1:1G:900:A:H2' | 1:1G:901:A:C8 | 2.39 | 0.57 |
| 22:2L:1:G:C2 | 22:2L:2:G:C8 | 2.91 | 0.57 |
| 24:14:863:A:H2' | 24:14:864:G:H8 | 1.67 | 0.57 |
| 24:14:2183:C:H2' | 24:14:2184:G:H8 | 1.68 | 0.57 |
| 25:1J:88:C:N3 | 25:1J:89:G:N3 | 2.52 | 0.57 |
| 30:49:2:PRO:N | 30:49:5:VAL:HG22 | 2.19 | 0.57 |
| 36:45:32:TYR:HE1 | 36:45:133:ARG:HG3 | 1.69 | 0.57 |
| 1:13:148:G:H2' | 1:13:149:A:C8 | 2.38 | 0.57 |
| 1:13:1190:G:O2' | 3:2E:3:ASN:HB3 | 2.05 | 0.57 |
| 1:13:1307:U:H2' | 1:13:1308:U:H6 | 1.68 | 0.57 |
| 5:4E:33:VAL:HG11 | 5:4E:109:ILE:HA | 1.86 | 0.57 |
| 24:1H:2093:G:H5' | 32:61:22:LYS:HD3 | 1.86 | 0.57 |
| 24:1H:2254:C:O2 | 46:I8:7:LEU:HD11 | 2.05 | 0.57 |
| 24:1H:2377:A:H2' | 24:1H:2378:A:C8 | 2.40 | 0.57 |
| 28:21:51:PHE:HD2 | 28:21:52:LEU:HG | 1.68 | 0.57 |
| 1:1G:1190:G:OP2 | 3:22:5:ILE:HD13 | 2.03 | 0.57 |
| 1:1G:1442:G:O2' | 1:1G:1443:G:OP1 | 2.18 | 0.57 |
| 6:52:7:ASN:HD21 | 18:9A:34:TYR:HE2 | 1.50 | 0.57 |
| 22:2L:55:U:O2' | 22:2L:56:U:H5" | 2.05 | 0.57 |
| 24:14:528:A:O2' | 24:14:529:A:H5' | 2.03 | 0.57 |
| 45:D5:141:VAL:HG13 | 45:D5:150:LEU:HD12 | 1.85 | 0.57 |
| 1:13:173:U:H5" | 1:13:197:A:O4' | 2.04 | 0.57 |
| 1:13:501:C:H2' | 1:13:502:G:H8 | 1.68 | 0.57 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 2:1E:82:ARG:NH1 | 2:1E:92:TYR:OH | 2.38 | 0.57 |
| 4:3E:53:ASP:HB3 | 4:3E:57:ARG:NH1 | 2.19 | 0.57 |
| 24:1H:91:A:H2' | 24:1H:92:G:H8 | 1.69 | 0.57 |
| 24:1H:142:G:H2' | 24:1H:143:C:C6 | 2.40 | 0.57 |
| 24:1H:844:C:H2' | 24:1H:845:G:O4' | 2.04 | 0.57 |
| 24:1H:1805:U:O2 | 27:11:50:THR:HB | 2.03 | 0.57 |
| 26:71:166:ASP:N | 26:71:166:ASP:OD1 | 2.36 | 0.57 |
| 43:F8:84:ALA:HB3 | 43:F8:87:GLN:OE1 | 2.03 | 0.57 |
| 1:1G:475:G:O6 | 57:1G:1814:HOH:O | 2.17 | 0.57 |
| 5:42:6:PHE:HZ | 5:42:40:ARG:HH21 | 1.51 | 0.57 |
| 24:14:79:G:O2' | 24:14:346:A:N3 | 2.34 | 0.57 |
| 24:14:389:G:H22 | 35:35:72:PRO:HD3 | 1.69 | 0.57 |
| 24:14:483:A:H5" | 44:C5:49:VAL:HG13 | 1.85 | 0.57 |
| 24:14:1118:C:H2' | 24:14:1119:C:C6 | 2.39 | 0.57 |
| 24:14:1688:U:H1' | 24:14:1701:A:C6 | 2.39 | 0.57 |
| 24:14:2065:C:H2' | 24:14:2066:C:H6 | 1.68 | 0.57 |
| 26:79:5:LYS:HA | 26:79:8:ARG:HB2 | 1.85 | 0.57 |
| 30:49:39:ILE:HD11 | 30:49:94:LEU:HD22 | 1.86 | 0.57 |
| 47:F5:25:LYS:HA | 47:F5:29:GLY:HA2 | 1.85 | 0.57 |
| 1:13:989:C:H42 | 1:13:1216:G:H1 | 1.51 | 0.57 |
| 1:13:1057:G:H4' | 3:2E:197:GLY:H | 1.68 | 0.57 |
| 1:13:1141:C:H2' | 1:13:1142:G:C8 | 2.39 | 0.57 |
| 5:4E:126:ARG:HG3 | 5:4E:126:ARG:NH1 | 2.16 | 0.57 |
| 8:7E:86:ILE:HG21 | 8:7E:133:LEU:HD22 | 1.86 | 0.57 |
| 24:1H:2287:A:C2 | 24:1H:2289:G:C8 | 2.93 | 0.57 |
| 24:1H:2855:C:H2' | 24:1H:2856:C:H6 | 1.69 | 0.57 |
| 33:58:4:TYR:CE2 | 40:C8:100:VAL:HG11 | 2.40 | 0.57 |
| 1:1G:972:C:O2 | 10:1A:55:LYS:HD3 | 2.03 | 0.57 |
| 1:1G:979:C:H3' | 1:1G:980:C:H5" | 1.85 | 0.57 |
| 1:1G:1105:A:H2' | 1:1G:1106:G:H8 | 1.69 | 0.57 |
| 1:1G:1129:C:H42 | 1:1G:1141:C:H41 | 1.50 | 0.57 |
| 1:1G:1133:G:H2' | 1:1G:1134:G:H8 | 1.69 | 0.57 |
| 20:BA:67:ALA:O | 20:BA:73:HIS:ND1 | 2.37 | 0.57 |
| 20:BA:79:ARG:HH21 | 20:BA:80:ARG:NH1 | 2.02 | 0.57 |
| 21:1B:8:THR:HG22 | 21:1B:10:ARG:H | 1.69 | 0.57 |
| 24:14:1754:C:OP1 | 39:75:96:ARG:NH1 | 2.37 | 0.57 |
| 24:14:2611:U:H2' | 51:J5:2:ALA:O | 2.04 | 0.57 |
| 25:1J:48:A:H4' | 38:65:95:HIS:HD2 | 1.69 | 0.57 |
| 26:79:41:VAL:HG22 | 26:79:216:THR:HG22 | 1.85 | 0.57 |
| 28:29:49:LEU:O | 28:29:78:LEU:HB3 | 2.05 | 0.57 |
| 32:69:86:THR:HG23 | 32:69:87:LYS:H | 1.68 | 0.57 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 40:85:92:ARG:CZ | 41:95:11:GLN:H | 2.17 | 0.57 |
| 50:I5:12:ALA:HB1 | 50:I5:29:PRO:HA | 1.86 | 0.57 |
| 54:M5:29:LYS:HB2 | 54:M5:44:LYS:CB | 2.35 | 0.57 |
| 1:13:939:G:H2' | 1:13:940:C:C6 | 2.39 | 0.57 |
| 1:13:1491[B]:G:OP1 | 12:3I:47:LYS:NZ | 2.38 | 0.57 |
| 1:13:1504:G:OP1 | 1:13:1507:A:H4' | 2.04 | 0.57 |
| 6:5E:19:LEU:HD23 | 6:5E:23:LYS:HZ2 | 1.70 | 0.57 |
| 24:1H:7:G:H1 | 24:1H:2896:C:H42 | 1.52 | 0.57 |
| 24:1H:607:U:N3 | 24:1H:621:A:C2 | 2.73 | 0.57 |
| 24:1H:674:G:O2' | 29:31:74:ARG:HD2 | 2.05 | 0.57 |
| 24:1H:1858:G:O2' | 24:1H:1884:A:N6 | 2.37 | 0.57 |
| 24:1H:2068:U:H3 | 24:1H:2430:A:H2 | 1.49 | 0.57 |
| 39:B8:54:ARG:HA | 39:B8:59:THR:OG1 | 2.05 | 0.57 |
| 43:F8:60:ARG:HH22 | 53:P8:47:ARG:NH2 | 2.03 | 0.57 |
| 47:J8:87:PRO:HA | 47:J8:89:GLU:H | 1.69 | 0.57 |
| 5:42:126:ARG:HG2 | 5:42:126:ARG:NH1 | 2.18 | 0.57 |
| 10:1A:50:ILE:HG13 | 14:5A:41:ARG:HD3 | 1.87 | 0.57 |
| 14:5A:45:ARG:O | 14:5A:49:HIS:ND1 | 2.30 | 0.57 |
| 24:14:558:G:P | 33:15:111:PRO:HD2 | 2.45 | 0.57 |
| 24:14:2129:C:H5' | 26:79:6:ARG:HH11 | 1.69 | 0.57 |
| 24:14:2619:C:OP1 | 28:29:152:LYS:HE2 | 2.04 | 0.57 |
| 30:49:173:LEU:HG | 30:49:178:PHE:CD2 | 2.39 | 0.57 |
| 32:69:125:GLU:HA | 32:69:141:LYS:HA | 1.85 | 0.57 |
| 38:65:26:LEU:HD13 | 38:65:87:PHE:CD1 | 2.39 | 0.57 |
| 46:E5:27:GLU:HB2 | 46:E5:69:PHE:HD1 | 1.68 | 0.57 |
| 51:J5:16:ARG:HH11 | 51:J5:16:ARG:HG2 | 1.70 | 0.57 |
| 1:13:49:U:C2 | 1:13:361:G:N2 | 2.73 | 0.57 |
| 1:13:730:G:C5 | 1:13:731:G:H1' | 2.40 | 0.57 |
| 2:1E:80:ILE:HD11 | 2:1E:208:ILE:HG22 | 1.86 | 0.57 |
| 3:2E:107:GLN:H | 3:2E:107:GLN:CD | 2.11 | 0.57 |
| 24:1H:795:C:H2' | 24:1H:796:C:C6 | 2.40 | 0.57 |
| 24:1H:1007:C:H5" | 33:58:35:ARG:NH1 | 2.19 | 0.57 |
| 24:1H:2829:C:H5' | 28:21:76:ARG:NH2 | 2.20 | 0.57 |
| 27:11:17:THR:HG22 | 27:11:205:VAL:N | 2.17 | 0.57 |
| 28:21:4:ILE:HG12 | 28:21:28:ALA:HB1 | 1.85 | 0.57 |
| 28:21:21:VAL:HG12 | 28:21:23:VAL:HG13 | 1.86 | 0.57 |
| 30:41:97:ASP:O | 30:41:101:ILE:HG12 | 2.05 | 0.57 |
| 32:61:75:LEU:HD21 | 32:61:105:HIS:ND1 | 2.20 | 0.57 |
| 35:78:59:LEU:O | 35:78:61:ARG:N | 2.34 | 0.57 |
| 37:98:56:LYS:NZ | 37:98:90:ARG:O | 2.38 | 0.57 |
| 40:C8:28:ARG:HD3 | 40:C8:38:THR:OG1 | 2.05 | 0.57 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 47:J8:91:LYS:O | 47:J8:95:LEU:HG | 2.05 | 0.57 |
| 1:1G:1139:G:N2 | 1:1G:1142:G:O6 | 2.38 | 0.57 |
| 1:1G:1305:G:H22 | 1:1G:1331:G:C2' | 2.17 | 0.57 |
| 2:12:189:ASP:O | 2:12:192:SER:OG | 2.12 | 0.57 |
| 7:62:26:PHE:O | 7:62:30:ILE:HG13 | 2.05 | 0.57 |
| 24:14:1028:A:H61 | 24:14:1125:G:H2' | 1.70 | 0.57 |
| 24:14:1093:G:H1 | 24:14:1097:U:P | 2.28 | 0.57 |
| 24:14:1410:G:O2' | 24:14:1411:C:H5' | 2.05 | 0.57 |
| 24:14:1450:C:H2' | 24:14:1451:C:C6 | 2.40 | 0.57 |
| 27:19:242:ARG:HG2 | 27:19:246:PRO:HG3 | 1.87 | 0.57 |
| 36:45:34:LEU:HD11 | 36:45:129:THR:HB | 1.85 | 0.57 |
| 1:13:108:G:H5" | 1:13:109:A:H5" | 1.87 | 0.57 |
| 1:13:417:C:H2' | 1:13:418:C:H6 | 1.70 | 0.57 |
| 1:13:1441:G:H4' | 1:13:1442:G:C5 | 2.40 | 0.57 |
| 2:1E:71:VAL:HG12 | 2:1E:93:VAL:HB | 1.86 | 0.57 |
| 8:7E:10:LEU:HD22 | 8:7E:83:ILE:HD11 | 1.87 | 0.57 |
| 24:1H:234:C:H2' | 24:1H:235:U:C6 | 2.39 | 0.57 |
| 24:1H:620:G:H4' | 24:1H:621:A:C5' | 2.33 | 0.57 |
| 42:E8:85:VAL:HA | 42:E8:95:ILE:HG22 | 1.85 | 0.57 |
| 47:J8:85:LEU:HB3 | 47:J8:86:SER:HB3 | 1.85 | 0.57 |
| 1:1G:827:U:H3 | 1:1G:872:A:N6 | 2.00 | 0.57 |
| 1:1G:1372:U:OP1 | 9:82:72:GLY:N | 2.37 | 0.57 |
| 7:62:26:PHE:CE2 | 7:62:30:ILE:HD11 | 2.40 | 0.57 |
| 15:6A:8:LYS:O | 15:6A:12:ILE:HG13 | 2.05 | 0.57 |
| 24:14:1175:U:O2' | 24:14:1176:G:N3 | 2.34 | 0.57 |
| 24:14:2655:G:N2 | 24:14:2665:A:OP2 | 2.34 | 0.57 |
| 30:49:47:LYS:HE2 | 30:49:81:LYS:HE3 | 1.86 | 0.57 |
| 1:13:95:G:H3' | 1:13:96:G:C8 | 2.40 | 0.57 |
| 1:13:255:G:H4' | 17:8I:17:LYS:HG2 | 1.87 | 0.57 |
| 1:13:411:A:N9 | 1:13:413:G:H1' | 2.18 | 0.57 |
| 1:13:957:U:O2' | 1:13:959:A:N7 | 2.35 | 0.57 |
| 1:13:1413:A:H2 | 1:13:1487:G:H22 | 1.50 | 0.57 |
| 22:2K:21:A:H2 | 22:2K:55:U:H3 | 1.50 | 0.57 |
| 24:1H:70:G:H21 | 24:1H:71:A:N6 | 2.02 | 0.57 |
| 24:1H:855:G:O2' | 46:I8:27:GLU:OE2 | 2.21 | 0.57 |
| 24:1H:900:A:H3' | 24:1H:901:A:H8 | 1.70 | 0.57 |
| 24:1H:1537:C:H2' | 24:1H:1538:G:C8 | 2.39 | 0.57 |
| 24:1H:2352:A:H2' | 24:1H:2353:G:O4' | 2.05 | 0.57 |
| 25:16:29:A:P | 38:A8:32:LEU:HD13 | 2.45 | 0.57 |
| 36:88:90:VAL:HG23 | 36:88:91:GLU:H | 1.70 | 0.57 |
| 1:1G:15:G:H2' | 1:1G:16:A:H8 | 1.70 | 0.57 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 2:12:88:ALA:HB2 | 2:12:219:VAL:HG23 | 1.87 | 0.57 |
| 2:12:208:ILE:HA | 2:12:211:ILE:HD12 | 1.86 | 0.57 |
| 3:22:63:ASN:HA | 3:22:98:ASN:HB3 | 1.86 | 0.57 |
| 4:32:63:LYS:HB3 | 4:32:198:VAL:HG12 | 1.86 | 0.57 |
| 10:1A:79:ARG:HA | 10:1A:82:ILE:HG22 | 1.85 | 0.57 |
| 14:5A:26:ARG:HH12 | 14:5A:47:LEU:HD21 | 1.70 | 0.57 |
| 18:9A:74:ARG:HB3 | 18:9A:81:PHE:CE1 | 2.40 | 0.57 |
| 24:14:1568:G:P | 27:19:63:ARG:HH12 | 2.28 | 0.57 |
| 24:14:2387:U:O2' | 46:E5:41:ARG:NH1 | 2.38 | 0.57 |
| 24:14:2816:C:O2 | 24:14:2883:A:O2' | 2.23 | 0.57 |
| 1:13:52:G:H2' | 1:13:53:A:C8 | 2.40 | 0.56 |
| 1:13:693:G:H2' | 1:13:694:A:C8 | 2.40 | 0.56 |
| 1:13:1244:C:H42 | 1:13:1293:G:H1 | 1.53 | 0.56 |
| 1:13:1491[A]:G:OP1 | 12:3I:47:LYS:NZ | 2.38 | 0.56 |
| 18:9I:26:LEU:HB3 | 18:9I:42:ARG:HH22 | 1.70 | 0.56 |
| 19:AI:33:THR:HG23 | 19:AI:35:SER:H | 1.70 | 0.56 |
| 24:1H:2002:G:O6 | 57:1H:3692:HOH:O | 2.18 | 0.56 |
| 24:1H:2132:U:H3 | 26:71:8:ARG:HH12 | 1.52 | 0.56 |
| 47:J8:41:ARG:HG3 | 47:J8:41:ARG:NH1 | 2.19 | 0.56 |
| 1:1G:166:G:H2' | 1:1G:167:G:H8 | 1.69 | 0.56 |
| 6:52:10:LEU:HD11 | 6:52:61:LEU:HD22 | 1.87 | 0.56 |
| 16:7A:34:GLU:OE1 | 16:7A:55:ARG:NH1 | 2.36 | 0.56 |
| 24:14:608:A:H2' | 24:14:609:A:C8 | 2.40 | 0.56 |
| 24:14:729:G:C6 | 27:19:208:LYS:HB2 | 2.40 | 0.56 |
| 24:14:1151:G:H4' | 40:85:81:HIS:CD2 | 2.40 | 0.56 |
| 24:14:1337:G:H2' | 24:14:1338:G:H8 | 1.68 | 0.56 |
| 24:14:1678:G:H22 | 24:14:1989:G:H22 | 1.53 | 0.56 |
| 24:14:2637:U:H5" | 28:29:82:ARG:NH2 | 2.20 | 0.56 |
| 25:1J:12:C:H6 | 25:1J:12:C:OP2 | 1.88 | 0.56 |
| 25:1J:87:G:N7 | 57:1J:301:HOH:O | 2.32 | 0.56 |
| 29:39:4:VAL:HG12 | 29:39:19:GLU:OE1 | 2.05 | 0.56 |
| 29:39:18:ARG:HG2 | 29:39:19:GLU:H | 1.69 | 0.56 |
| 36:45:43:THR:OG1 | 36:45:45:GLN:HG2 | 2.04 | 0.56 |
| 40:85:92:ARG:C | 40:85:94:ASN:H | 2.13 | 0.56 |
| 45:D5:103:ARG:HG2 | 45:D5:136:PHE:HB2 | 1.87 | 0.56 |
| 1:13:158:G:N1 | 1:13:163:C:O2 | 2.29 | 0.56 |
| 1:13:742:G:H5' | 15:6I:58:MET:HE3 | 1.88 | 0.56 |
| 1:13:1075:C:OP1 | 2:1E:179:LYS:NZ | 2.27 | 0.56 |
| 2:1E:80:ILE:O | 2:1E:84:GLU:HG2 | 2.05 | 0.56 |
| 2:1E:80:ILE:HD12 | 2:1E:211:ILE:HB | 1.86 | 0.56 |
| 7:6E:20:ASP:O | 7:6E:23:VAL:HG23 | 2.05 | 0.56 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 7:6E:46:ALA:HB2 | 7:6E:117:ALA:HB1 | 1.87 | 0.56 |
| 8:7E:77:GLU:HG2 | 8:7E:78:GLN:H | 1.69 | 0.56 |
| 10:1I:35:SER:HB3 | 10:1I:73:ASP:HB2 | 1.86 | 0.56 |
| 15:6I:70:LEU:HD11 | 15:6I:77:ARG:HG3 | 1.87 | 0.56 |
| 24:1H:2781:A:H5" | 24:1H:2782:G:H5' | 1.87 | 0.56 |
| 26:71:3:HIS:HB3 | 26:71:7:TYR:HB3 | 1.87 | 0.56 |
| 27:11:6:PHE:CE1 | 27:11:18:VAL:HG23 | 2.41 | 0.56 |
| 35:78:59:LEU:HD22 | 35:78:60:MET:H | 1.71 | 0.56 |
| 37:98:78:LYS:O | 37:98:83:ILE:HG13 | 2.05 | 0.56 |
| 51:N8:46:CYS:HB3 | 51:N8:50:GLY:HA3 | 1.87 | 0.56 |
| 1:1G:492:G:O6 | 57:1G:1808:HOH:O | 2.14 | 0.56 |
| 1:1G:1132:C:H2' | 1:1G:1133:G:C8 | 2.40 | 0.56 |
| 1:1G:1151:A:H5' | 10:1A:41:PRO:HA | 1.87 | 0.56 |
| 1:1G:1306:A:N6 | 1:1G:1331:G:H1' | 2.20 | 0.56 |
| 1:1G:1378:C:H5 | 1:1G:1379:G:N9 | 2.02 | 0.56 |
| 4:32:11:LEU:HD13 | 4:32:66:ARG:HG2 | 1.85 | 0.56 |
| 24:14:481:G:OP2 | 44:C5:47:LYS:HB2 | 2.05 | 0.56 |
| 24:14:1148:A:H2' | 24:14:1149:G:H8 | 1.70 | 0.56 |
| 33:15:23:LEU:HD12 | 33:15:99:LEU:HD23 | 1.87 | 0.56 |
| 43:B5:50:LYS:HG2 | 43:B5:84:ALA:HB2 | 1.87 | 0.56 |
| 1:13:193:C:H5' | 20:BI:57:ARG:NH2 | 2.20 | 0.56 |
| 1:13:431:A:H2' | 1:13:432:A:O4' | 2.05 | 0.56 |
| 1:13:438:G:OP1 | 4:3E:125:HIS:HE1 | 1.88 | 0.56 |
| 1:13:1037:C:H2' | 1:13:1038:C:C6 | 2.41 | 0.56 |
| 1:13:1412:C:H2' | 1:13:1413:A:C8 | 2.40 | 0.56 |
| 8:7E:1:MET:HE1 | 8:7E:3:THR:HG23 | 1.88 | 0.56 |
| 22:2K:4:G:H1 | 22:2K:78:C:H42 | 1.53 | 0.56 |
| 22:3K:42:U:H2' | 22:3K:43:G:C8 | 2.40 | 0.56 |
| 23:4K:9:G:O2' | 23:4K:10:G:OP1 | 2.20 | 0.56 |
| 24:1H:2870:C:H5" | 37:98:65:LEU:HD21 | 1.86 | 0.56 |
| 27:11:71:ASP:OD2 | 27:11:103:ARG:NH2 | 2.37 | 0.56 |
| 35:78:52:GLU:HG3 | 35:78:57:THR:HA | 1.86 | 0.56 |
| 35:78:96:THR:HG22 | 35:78:97:PRO:HD2 | 1.88 | 0.56 |
| 36:88:12:GLN:HG2 | 36:88:73:PRO:HD2 | 1.86 | 0.56 |
| 44:G8:93:GLY:O | 44:G8:94:LYS:HB2 | 2.05 | 0.56 |
| 45:H8:11:GLU:O | 45:H8:36:LYS:NZ | 2.28 | 0.56 |
| 49:L8:28:LEU:HA | 49:L8:33:GLN:OE1 | 2.05 | 0.56 |
| 52:O8:33:LYS:O | 52:O8:35:GLU:HG3 | 2.05 | 0.56 |
| 54:Q8:23:VAL:HG23 | 54:Q8:49:VAL:HG12 | 1.88 | 0.56 |
| 1:1G:1062:U:H2' | 1:1G:1063:C:C6 | 2.40 | 0.56 |
| 1:1G:1239:A:H4' | 1:1G:1240:U:H5" | 1.87 | 0.56 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 3:22:32:LEU:HD22 | 3:22:59:ARG:HH22 | 1.70 | 0.56 |
| 3:22:35:GLU:OE2 | 3:22:59:ARG:NH2 | 2.39 | 0.56 |
| 5:42:111:GLU:O | 5:42:114:GLY:N | 2.31 | 0.56 |
| 8:72:45:ILE:HG22 | 8:72:47:GLY:N | 2.17 | 0.56 |
| 20:BA:51:GLU:HA | 20:BA:54:LYS:HB3 | 1.88 | 0.56 |
| 24:14:234:C:H2' | 24:14:235:U:H6 | 1.69 | 0.56 |
| 24:14:1786:A:C2 | 24:14:2606:C:H1' | 2.41 | 0.56 |
| 24:14:2889:C:H3' | 24:14:2891:G:H8 | 1.70 | 0.56 |
| 28:29:34:VAL:HB | 28:29:48:GLN:HG2 | 1.87 | 0.56 |
| 29:39:167:ALA:HB1 | 29:39:173:VAL:HG11 | 1.87 | 0.56 |
| 44:C5:42:VAL:O | 44:C5:65:ALA:N | 2.27 | 0.56 |
| 54:M5:62:LEU:HB2 | 54:M5:63:PRO:CD | 2.31 | 0.56 |
| 2:1E:111:ARG:HG2 | 2:1E:111:ARG:NH1 | 2.16 | 0.56 |
| 2:1E:233:SER:HB2 | 2:1E:234:PRO:HD2 | 1.87 | 0.56 |
| 3:2E:102:ASN:OD1 | 3:2E:102:ASN:N | 2.38 | 0.56 |
| 8:7E:34:GLU:HB3 | 8:7E:118:VAL:HG21 | 1.88 | 0.56 |
| 24:1H:1864:U:H3 | 24:1H:1878:G:H1 | 1.54 | 0.56 |
| 24:1H:2495:G:H5" | 36:88:82:ARG:HB3 | 1.86 | 0.56 |
| 30:41:64:THR:HG22 | 30:41:66:GLN:H | 1.70 | 0.56 |
| 1:1G:41:G:H2' | 1:1G:42:G:H8 | 1.70 | 0.56 |
| 3:22:78:GLY:HA3 | 3:22:79:ARG:CZ | 2.36 | 0.56 |
| 4:32:76:ARG:NH2 | 4:32:80:GLU:OE1 | 2.38 | 0.56 |
| 7:62:115:ARG:HB2 | 7:62:118:VAL:HG13 | 1.88 | 0.56 |
| 16:7A:75:ARG:O | 16:7A:78:GLY:N | 2.29 | 0.56 |
| 24:14:973:A:H5' | 24:14:1188:U:H1' | 1.87 | 0.56 |
| 24:14:1047:G:N2 | 24:14:1111:A:H62 | 2.03 | 0.56 |
| 24:14:1331:A:O2' | 24:14:1332:G:H8 | 1.87 | 0.56 |
| 24:14:1408:C:C2 | 24:14:1595:G:N2 | 2.73 | 0.56 |
| 24:14:1999:C:H4' | 24:14:2723:C:O2 | 2.05 | 0.56 |
| 46:E5:53:MET:HG3 | 46:E5:59:LEU:HD23 | 1.86 | 0.56 |
| 1:13:201:C:N4 | 1:13:216:G:H1 | 1.98 | 0.56 |
| 1:13:555:C:H2' | 1:13:556:C:C6 | 2.40 | 0.56 |
| 1:13:591:U:H2' | 1:13:592:G:C8 | 2.40 | 0.56 |
| 1:13:688:G:H2' | 1:13:689:C:H6 | 1.69 | 0.56 |
| 4:3E:194:LEU:HD12 | 4:3E:195:ALA:N | 2.21 | 0.56 |
| 24:1H:730:C:H3' | 57:1H:3893:HOH:O | 2.04 | 0.56 |
| 24:1H:1449(A):G:H2' | 24:1H:1450:C:H6 | 1.69 | 0.56 |
| 26:71:226:PRO:HG2 | 26:71:227:HIS:CE1 | 2.40 | 0.56 |
| 39:B8:16:ARG:NH2 | 39:B8:83:ILE:O | 2.38 | 0.56 |
| 1:1G:625:G:H2' | 1:1G:626:U:C6 | 2.40 | 0.56 |
| 1:1G:885:G:O2' | 1:1G:914:A:N1 | 2.29 | 0.56 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 1:1G:1015:A:H2' | 1:1G:1016:A:H8 | 1.70 | 0.56 |
| 1:1G:1133:G:H2' | 1:1G:1134:G:C8 | 2.40 | 0.56 |
| 1:1G:1227:A:H3' | 1:1G:1227:A:C8 | 2.41 | 0.56 |
| 1:1G:1237:C:H3' | 1:1G:1336:C:H41 | 1.71 | 0.56 |
| 1:1G:1357:A:N7 | 1:1G:1358:U:C5 | 2.74 | 0.56 |
| 2:12:63:MET:O | 2:12:64:ARG:HB2 | 2.04 | 0.56 |
| 3:22:32:LEU:O | 3:22:36:ASP:HB2 | 2.06 | 0.56 |
| 24:14:1688:U:O2 | 24:14:1700:A:H5' | 2.05 | 0.56 |
| 28:29:112:GLY:O | 28:29:159:HIS:HA | 2.06 | 0.56 |
| 29:39:126:VAL:O | 29:39:195:ASP:HA | 2.06 | 0.56 |
| 35:35:97:PRO:C | 35:35:99:LEU:H | 2.13 | 0.56 |
| 35:35:144:GLU:CD | 35:35:144:GLU:N | 2.63 | 0.56 |
| 38:65:109:GLY:O | 38:65:111:GLU:N | 2.27 | 0.56 |
| 1:13:383:A:OP1 | 1:13:454:C:O2' | 2.19 | 0.56 |
| 1:13:403:C:OP2 | 4:3E:74:GLN:NE2 | 2.38 | 0.56 |
| 6:5E:19:LEU:O | 6:5E:23:LYS:NZ | 2.38 | 0.56 |
| 22:3K:25:G:H2' | 22:3K:26:G:C8 | 2.41 | 0.56 |
| 24:1H:1231:G:H2' | 24:1H:1232:G:C8 | 2.41 | 0.56 |
| 24:1H:2643:G:H2' | 24:1H:2644:G:O4' | 2.06 | 0.56 |
| 1:1G:693:G:H2' | 1:1G:694:A:C8 | 2.41 | 0.56 |
| 1:1G:736:C:H2' | 1:1G:737:A:C8 | 2.41 | 0.56 |
| 1:1G:1033:G:H2' | 1:1G:1034:G:H8 | 1.70 | 0.56 |
| 1:1G:1136:U:H5" | 1:1G:1137:C:H5 | 1.70 | 0.56 |
| 22:3L:9:U:H3 | 22:3L:22:A:N6 | 2.03 | 0.56 |
| 24:14:1709:U:H2' | 24:14:1710:C:H6 | 1.71 | 0.56 |
| 24:14:1728:G:N2 | 24:14:1730:U:OP2 | 2.39 | 0.56 |
| 24:14:2068:U:N3 | 24:14:2430:A:H2 | 1.99 | 0.56 |
| 29:39:22:ALA:C | 29:39:24:LEU:N | 2.61 | 0.56 |
| 31:59:91:GLY:HA3 | 31:59:94:TYR:CD2 | 2.41 | 0.56 |
| 45:D5:19:ARG:NH2 | 45:D5:84:GLU:HB3 | 2.21 | 0.56 |
| 1:13:272:C:H2' | 1:13:273:A:H8 | 1.70 | 0.56 |
| 13:4I:49:THR:HG22 | 13:4I:51:ALA:H | 1.70 | 0.56 |
| 21:1F:3:LYS:HB3 | 21:1F:14:TRP:HD1 | 1.71 | 0.56 |
| 24:1H:934:G:H2' | 24:1H:935:C:H6 | 1.69 | 0.56 |
| 24:1H:981:A:H8 | 24:1H:982:C:C5 | 2.23 | 0.56 |
| 24:1H:1385:G:O2' | 24:1H:1396:U:O2 | 2.24 | 0.56 |
| 33:58:103:VAL:HG11 | 33:58:120:LEU:HD12 | 1.88 | 0.56 |
| 44:G8:39:VAL:HB | 44:G8:42:VAL:CG1 | 2.34 | 0.56 |
| 1:1G:189:U:O4 | 17:8A:62:SER:HB2 | 2.05 | 0.56 |
| 1:1G:542:G:H5' | 4:32:41:GLY:HA3 | 1.88 | 0.56 |
| 3:22:12:LEU:HD11 | 14:5A:51:GLY:HA2 | 1.87 | 0.56 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 24:14:71:A:H5' | 24:14:71:A:C8 | 2.41 | 0.56 |
| 24:14:286:C:H2' | 24:14:287:C:C6 | 2.41 | 0.56 |
| 24:14:324:A:H2' | 24:14:325:G:O4' | 2.06 | 0.56 |
| 27:19:260:ARG:NH2 | 27:19:266:SER:OG | 2.38 | 0.56 |
| 32:69:5:LEU:O | 32:69:6:LEU:HD12 | 2.06 | 0.56 |
| 34:25:2:ILE:HD12 | 34:25:6:THR:HG21 | 1.87 | 0.56 |
| 35:35:39:LYS:HA | 35:35:45:LEU:HD13 | 1.88 | 0.56 |
| 36:45:103:MET:HE1 | 36:45:127:ILE:HD11 | 1.87 | 0.56 |
| 1:13:93:U:H2' | 1:13:95:G:O4' | 2.05 | 0.56 |
| 1:13:1124:G:N3 | 1:13:1125:U:N3 | 2.50 | 0.56 |
| 1:13:1329:A:H5" | 13:4I:26:GLY:H | 1.71 | 0.56 |
| 9:8E:93:ARG:HA | 9:8E:96:LEU:HB2 | 1.88 | 0.56 |
| 24:1H:997:G:OP1 | 40:C8:92:ARG:HB2 | 2.05 | 0.56 |
| 29:31:108:LYS:O | 29:31:112:MET:HG3 | 2.06 | 0.56 |
| 42:E8:62:HIS:HB2 | 42:E8:64:MET:HE3 | 1.87 | 0.56 |
| 43:F8:3:THR:HA | 43:F8:6:ASP:OD2 | 2.04 | 0.56 |
| 44:G8:46:LYS:HE2 | 44:G8:60:PHE:CD2 | 2.40 | 0.56 |
| 50:M8:10:VAL:HG22 | 50:M8:11:PRO:HD2 | 1.88 | 0.56 |
| 1:1G:838:G:H8 | 1:1G:838:G:O5' | 1.88 | 0.56 |
| 9:82:9:ARG:HH22 | 9:82:104:ARG:HD3 | 1.70 | 0.56 |
| 10:1A:13:HIS:HB3 | 10:1A:68:HIS:CE1 | 2.41 | 0.56 |
| 24:14:363(B):G:H2' | 24:14:363(C):G:C8 | 2.41 | 0.56 |
| 24:14:1204:A:C2 | 24:14:1241:A:N1 | 2.74 | 0.56 |
| 24:14:1651:G:H5' | 37:55:39:PRO:HG3 | 1.88 | 0.56 |
| 24:14:2002:G:OP2 | 37:55:9:LYS:NZ | 2.39 | 0.56 |
| 24:14:2137:C:N4 | 24:14:2154:G:O6 | 2.39 | 0.56 |
| 24:14:2212:A:H4' | 24:14:2213:U:C5 | 2.40 | 0.56 |
| 24:14:2543:G:H2' | 24:14:2544:G:C8 | 2.41 | 0.56 |
| 5:4E:80:ILE:HD12 | 8:7E:104:ARG:HH22 | 1.71 | 0.56 |
| 22:3K:38:MIA:H2' | 22:3K:39:A:H8 | 1.70 | 0.56 |
| 24:1H:247:G:H4' | 24:1H:386:G:C5 | 2.41 | 0.56 |
| 24:1H:998:C:OP1 | 40:C8:92:ARG:NH2 | 2.28 | 0.56 |
| 24:1H:2068:U:N3 | 24:1H:2430:A:C2 | 2.70 | 0.56 |
| 24:1H:2074:U:P | 57:1H:3651:HOH:O | 2.62 | 0.56 |
| 36:88:62:GLY:O | 36:88:63:LYS:HD2 | 2.06 | 0.56 |
| 38:A8:35:ILE:HG22 | 38:A8:97:ARG:HH21 | 1.70 | 0.56 |
| 1:1G:988:G:N2 | 1:1G:1218:C:O2 | 2.39 | 0.56 |
| 1:1G:1321:C:C4 | 1:1G:1322:C:C4 | 2.94 | 0.56 |
| 2:12:104:ASN:OD1 | 2:12:107:THR:OG1 | 2.17 | 0.56 |
| 3:22:29:TYR:OH | 14:5A:54:PRO:HD2 | 2.05 | 0.56 |
| 3:22:83:ARG:O | 3:22:86:VAL:HG22 | 2.05 | 0.56 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 4:32:62:GLN:O | 4:32:66:ARG:HB2 | 2.05 | 0.56 |
| 9:82:24:GLY:HA2 | 9:82:59:PHE:O | 2.06 | 0.56 |
| 24:14:205:G:O6 | 47:F5:39:LYS:NZ | 2.39 | 0.56 |
| 24:14:2319:G:N7 | 38:65:3:ARG:HG3 | 2.20 | 0.56 |
| 24:14:2635:C:H5" | 28:29:77:ILE:O | 2.06 | 0.56 |
| 33:15:24:GLY:O | 33:15:28:THR:HG23 | 2.06 | 0.56 |
| 38:65:103:GLU:O | 38:65:106:ARG:HG2 | 2.06 | 0.56 |
| 43:B5:50:LYS:N | 43:B5:87:GLN:OE1 | 2.31 | 0.56 |
| 45:D5:146:ILE:HD13 | 45:D5:176:PRO:HD3 | 1.88 | 0.56 |
| 54:M5:40:GLU:HA | 54:M5:43:GLN:HB2 | 1.87 | 0.56 |
| 1:13:456:C:N3 | 1:13:476:G:N2 | 2.52 | 0.56 |
| 1:13:542:G:H5' | 4:3E:41:GLY:HA3 | 1.88 | 0.56 |
| 1:13:1262:C:H2' | 1:13:1263:C:C6 | 2.41 | 0.56 |
| 1:13:1310:G:N7 | 19:AI:2:PRO:HG3 | 2.21 | 0.56 |
| 10:1I:40:LEU:HB2 | 10:1I:69:ASN:HB2 | 1.88 | 0.56 |
| 24:1H:761:A:H5" | 57:1H:3772:HOH:O | 2.06 | 0.56 |
| 24:1H:968:G:H5" | 49:L8:17:LYS:NZ | 2.21 | 0.56 |
| 24:1H:1588:C:H2' | 24:1H:1589:C:C6 | 2.41 | 0.56 |
| 32:61:29:TYR:O | 32:61:32:PRO:HD2 | 2.06 | 0.56 |
| 54:Q8:29:LYS:HB3 | 54:Q8:31:HIS:H | 1.70 | 0.56 |
| 1:1G:730:G:C5 | 1:1G:731:G:H1' | 2.41 | 0.56 |
| 1:1G:1365:G:H2' | 1:1G:1366:C:H6 | 1.71 | 0.56 |
| 2:12:47:THR:HG23 | 2:12:202:PRO:HG2 | 1.87 | 0.56 |
| 8:72:6:ILE:O | 8:72:10:LEU:HG | 2.05 | 0.56 |
| 22:3L:35:QUO:O6 | 22:3L:35:QUO:N11 | 2.39 | 0.56 |
| 24:14:1328:G:H2' | 24:14:1330:C:C5 | 2.41 | 0.56 |
| 24:14:2327:A:H2' | 24:14:2328:A:C8 | 2.41 | 0.56 |
| 24:14:2889:C:H2' | 24:14:2891:G:O4' | 2.06 | 0.56 |
| 38:65:29:PHE:HD1 | 38:65:30:ARG:N | 2.04 | 0.56 |
| 39:75:53:ARG:HG3 | 39:75:53:ARG:O | 2.05 | 0.56 |
| 1:13:540:G:H2' | 1:13:541:G:O4' | 2.07 | 0.55 |
| 2:1E:189:ASP:HB3 | 2:1E:191:ASP:HB2 | 1.89 | 0.55 |
| 16:7I:1:MET:HE2 | 16:7I:3:LYS:HE2 | 1.88 | 0.55 |
| 24:1H:74:A:H8 | 24:1H:74:A:C5' | 2.19 | 0.55 |
| 24:1H:185:U:H2' | 24:1H:186:G:H8 | 1.70 | 0.55 |
| 24:1H:528:A:N1 | 24:1H:2042:A:H2' | 2.21 | 0.55 |
| 24:1H:638:G:C5 | 24:1H:651:G:C2 | 2.94 | 0.55 |
| 24:1H:721:C:H2' | 24:1H:722:A:H8 | 1.71 | 0.55 |
| 24:1H:1213:A:H1' | 24:1H:1238:G:N3 | 2.21 | 0.55 |
| 24:1H:1997:G:H5" | 57:1H:3620:HOH:O | 2.05 | 0.55 |
| 24:1H:2829:C:H5' | 28:21:76:ARG:HH22 | 1.71 | 0.55 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 27:11:70:TRP:CD1 | 27:11:70:TRP:C | 2.84 | 0.55 |
| 31:51:5:GLY:O | 31:51:69:ARG:HG2 | 2.05 | 0.55 |
| 31:51:23:ARG:HH22 | 31:51:25:LYS:HE3 | 1.71 | 0.55 |
| 34:68:25:LEU:HD21 | 34:68:40:VAL:HG23 | 1.87 | 0.55 |
| 35:78:122:PRO:HA | 35:78:142:GLY:HA3 | 1.88 | 0.55 |
| 37:98:63:ARG:HA | 37:98:80:PHE:CZ | 2.40 | 0.55 |
| 39:B8:91:ARG:O | 39:B8:116:ALA:HA | 2.06 | 0.55 |
| 49:L8:3:ARG:HG2 | 49:L8:38:GLU:HG3 | 1.88 | 0.55 |
| 50:M8:49:PHE:HD1 | 50:M8:50:VAL:HG23 | 1.70 | 0.55 |
| 3:22:182:ILE:HG12 | 3:22:203:PHE:HB2 | 1.87 | 0.55 |
| 24:14:218:A:H2 | 24:14:235:U:H4' | 1.70 | 0.55 |
| 24:14:263:C:H2' | 24:14:264:C:O4' | 2.06 | 0.55 |
| 24:14:517:C:OP1 | 51:J5:16:ARG:NH2 | 2.38 | 0.55 |
| 32:69:76:THR:HG23 | 32:69:140:LEU:HD13 | 1.86 | 0.55 |
| 33:15:34:LEU:HD21 | 33:15:120:LEU:HB2 | 1.88 | 0.55 |
| 45:D5:39:VAL:HG21 | 45:D5:44:PHE:HB2 | 1.88 | 0.55 |
| 45:D5:132:ASN:ND2 | 45:D5:159:PRO:HB2 | 2.21 | 0.55 |
| 1:13:265:G:H5' | 17:8I:64:PRO:O | 2.07 | 0.55 |
| 1:13:606:G:O2' | 1:13:632:A:N6 | 2.38 | 0.55 |
| 1:13:918:A:H2' | 1:13:919:A:C8 | 2.41 | 0.55 |
| 2:1E:195:ASP:O | 8:7E:68:ARG:NH2 | 2.39 | 0.55 |
| 22:2K:61:G:H2' | 22:2K:62:G:O4' | 2.06 | 0.55 |
| 22:3K:9:U:H6 | 22:3K:46:G:H5" | 1.72 | 0.55 |
| 24:1H:456:C:H2' | 43:F8:68:ARG:NH2 | 2.22 | 0.55 |
| 24:1H:528:A:C2 | 24:1H:2043:C:H4' | 2.40 | 0.55 |
| 24:1H:1641:A:H2' | 24:1H:1642:G:O4' | 2.06 | 0.55 |
| 24:1H:2169:A:H2' | 24:1H:2170:A:C8 | 2.41 | 0.55 |
| 24:1H:2271:G:C5' | 46:I8:20:ARG:HH11 | 2.18 | 0.55 |
| 24:1H:2849:U:O4 | 39:B8:23:ARG:NH2 | 2.38 | 0.55 |
| 28:21:66:HIS:CG | 28:21:67:PHE:N | 2.74 | 0.55 |
| 35:78:81:GLN:OE1 | 35:78:106:LEU:HA | 2.05 | 0.55 |
| 36:88:90:VAL:O | 36:88:91:GLU:HB3 | 2.06 | 0.55 |
| 42:E8:58:ALA:O | 42:E8:64:MET:HB2 | 2.06 | 0.55 |
| 1:1G:448:A:P | 1:1G:485:G:H22 | 2.26 | 0.55 |
| 1:1G:1104:G:OP1 | 2:12:144:ARG:NH1 | 2.29 | 0.55 |
| 2:12:50:GLU:O | 2:12:54:THR:OG1 | 2.19 | 0.55 |
| 11:2A:29:ILE:HG22 | 11:2A:44:SER:HB2 | 1.86 | 0.55 |
| 14:5A:40:CYS:HB2 | 14:5A:43:CYS:H | 1.70 | 0.55 |
| 24:14:2130:U:C2 | 24:14:2158:A:H2 | 2.25 | 0.55 |
| 24:14:2261:C:O2' | 24:14:2262:U:H5' | 2.05 | 0.55 |
| 24:14:2331:G:O2' | 24:14:2336:A:N1 | 2.35 | 0.55 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 44:C5:19:LYS:CG | 44:C5:20:TYR:H | 2.17 | 0.55 |
| 44:C5:88:LYS:O | 44:C5:89:PHE:HB3 | 2.04 | 0.55 |
| 45:D5:30:ASN:HA | 45:D5:89:PHE:CE1 | 2.39 | 0.55 |
| 1:13:164:U:H2' | 1:13:165:C:C6 | 2.41 | 0.55 |
| 1:13:1316:G:N2 | 1:13:1318:A:H3' | 2.20 | 0.55 |
| 5:4E:36:ASP:OD2 | 5:4E:38:GLN:HB2 | 2.05 | 0.55 |
| 13:4I:15:VAL:HA | 13:4I:45:VAL:HG12 | 1.89 | 0.55 |
| 24:1H:270(M):U:H1' | 24:1H:270(N):G:C2 | 2.41 | 0.55 |
| 24:1H:643:A:H2' | 24:1H:644:A:C8 | 2.41 | 0.55 |
| 24:1H:795:C:H2' | 24:1H:796:C:H6 | 1.72 | 0.55 |
| 24:1H:1170:G:N2 | 24:1H:1180:C:C2 | 2.75 | 0.55 |
| 24:1H:1899:G:H22 | 24:1H:1902:C:H5 | 1.52 | 0.55 |
| 25:16:90:C:H5' | 36:88:18:LYS:HA | 1.89 | 0.55 |
| 28:21:105:THR:HG21 | 28:21:164:ARG:NH1 | 2.21 | 0.55 |
| 1:1G:173:U:O2 | 1:1G:197:A:N6 | 2.39 | 0.55 |
| 1:1G:182:U:N3 | 1:1G:183:G:H1' | 2.21 | 0.55 |
| 1:1G:1000:A:H2' | 1:1G:1001:G:H8 | 1.71 | 0.55 |
| 13:4A:77:ASN:OD1 | 13:4A:80:ARG:NH2 | 2.38 | 0.55 |
| 20:BA:29:LYS:O | 20:BA:33:ILE:HG12 | 2.05 | 0.55 |
| 21:1B:9:ARG:O | 21:1B:13:ILE:HG13 | 2.06 | 0.55 |
| 24:14:848:G:H2' | 24:14:849:A:C8 | 2.42 | 0.55 |
| 24:14:873:G:N2 | 24:14:905:U:C2 | 2.74 | 0.55 |
| 39:75:10:VAL:HG12 | 39:75:11:GLU:N | 2.21 | 0.55 |
| 40:85:92:ARG:HD2 | 41:95:11:GLN:HB2 | 1.88 | 0.55 |
| 1:13:865:A:H2 | 1:13:918:A:H4' | 1.72 | 0.55 |
| 1:13:1354:C:H2' | 1:13:1355:G:H8 | 1.71 | 0.55 |
| 2:1E:77:ALA:HB2 | 2:1E:211:ILE:HD13 | 1.86 | 0.55 |
| 20:BI:26:ASN:HD22 | 20:BI:26:ASN:H | 1.55 | 0.55 |
| 24:1H:441:U:O2 | 29:31:46:ARG:NH2 | 2.40 | 0.55 |
| 24:1H:1317:A:H2' | 24:1H:1318:C:H6 | 1.71 | 0.55 |
| 24:1H:2210:G:H5" | 24:1H:2211:G:C6 | 2.40 | 0.55 |
| 24:1H:2340:G:O2' | 24:1H:2341:G:H5' | 2.07 | 0.55 |
| 24:1H:2402:C:H3' | 24:1H:2402:C:C6 | 2.41 | 0.55 |
| 24:1H:2712:U:H1' | 24:1H:2712(A):A:C8 | 2.40 | 0.55 |
| 37:98:57:ARG:HB3 | 37:98:59:ASP:OD1 | 2.06 | 0.55 |
| 43:F8:11:PRO:HB3 | 43:F8:92:LEU:HD21 | 1.88 | 0.55 |
| 1:1G:373:A:C2 | 1:1G:374:A:C8 | 2.95 | 0.55 |
| 1:1G:501:C:H2' | 1:1G:502:G:C8 | 2.39 | 0.55 |
| 1:1G:1250:A:H4' | 9:82:68:GLY:N | 2.21 | 0.55 |
| 2:12:73:THR:HG22 | 2:12:170:GLU:OE1 | 2.06 | 0.55 |
| 24:14:2173:A:C5 | 24:14:2174:C:H4' | 2.41 | 0.55 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 24:14:2250:G:C6 | 36:45:83:MET:HB3 | 2.42 | 0.55 |
| 24:14:2530:A:C4 | 31:59:157:TYR:HE1 | 2.25 | 0.55 |
| 25:1J:8:U:H3 | 25:1J:112:G:H1 | 1.54 | 0.55 |
| 27:19:8:PRO:HB3 | 27:19:14:ARG:HB2 | 1.88 | 0.55 |
| 27:19:16:MET:HG3 | 27:19:206:LEU:O | 2.07 | 0.55 |
| 29:39:18:ARG:HG2 | 29:39:19:GLU:N | 2.22 | 0.55 |
| 37:55:52:ILE:O | 37:55:55:ALA:N | 2.34 | 0.55 |
| 38:65:15:ARG:O | 38:65:19:LYS:HD2 | 2.06 | 0.55 |
| 41:95:21:ARG:HG2 | 41:95:91:TYR:CE1 | 2.41 | 0.55 |
| 1:13:1078:U:O2' | 5:4E:130:ASN:OD1 | 2.15 | 0.55 |
| 2:1E:48:MET:HA | 2:1E:51:LEU:HD12 | 1.87 | 0.55 |
| 6:5E:74:ASP:OD1 | 6:5E:74:ASP:N | 2.37 | 0.55 |
| 22:3K:18:G:H1 | 22:3K:65:C:N4 | 2.05 | 0.55 |
| 24:1H:94:G:H2' | 24:1H:95:G:O4' | 2.06 | 0.55 |
| 24:1H:1054:A:H2' | 24:1H:1055:G:H8 | 1.70 | 0.55 |
| 24:1H:1174:A:H1' | 24:1H:1178:C:H41 | 1.72 | 0.55 |
| 24:1H:2175:C:O2' | 26:71:219:GLY:O | 2.25 | 0.55 |
| 24:1H:2345:G:H1' | 24:1H:2382:G:H5' | 1.89 | 0.55 |
| 24:1H:2728:U:H5' | 34:68:70:LYS:NZ | 2.21 | 0.55 |
| 27:11:28:GLU:OE1 | 27:11:28:GLU:N | 2.39 | 0.55 |
| 28:21:143:ASN:HD22 | 28:21:147:PRO:HD3 | 1.70 | 0.55 |
| 37:98:41:ALA:O | 37:98:44:LEU:N | 2.40 | 0.55 |
| 44:G8:17:SER:OG | 44:G8:71:LYS:HD2 | 2.06 | 0.55 |
| 22:3L:24:G:H2' | 22:3L:25:G:C8 | 2.41 | 0.55 |
| 24:14:2388:A:H2' | 24:14:2389:G:H5' | 1.87 | 0.55 |
| 30:49:60:LEU:O | 30:49:64:THR:HG23 | 2.06 | 0.55 |
| 30:49:64:THR:OG1 | 30:49:65:GLY:N | 2.38 | 0.55 |
| 35:35:14:LYS:HG2 | 35:35:15:ARG:H | 1.72 | 0.55 |
| 50:I5:56:VAL:HG13 | 50:I5:57:GLU:HG3 | 1.89 | 0.55 |
| 1:13:264:U:H4' | 17:8I:63:ARG:HD2 | 1.87 | 0.55 |
| 1:13:486:U:H2' | 1:13:487:A:C8 | 2.41 | 0.55 |
| 1:13:486:U:H2' | 1:13:487:A:H8 | 1.71 | 0.55 |
| 1:13:974:A:H1' | 14:5I:31:ARG:HE | 1.71 | 0.55 |
| 24:1H:732:C:H3' | 57:1H:3800:HOH:O | 2.06 | 0.55 |
| 24:1H:1870:C:H2' | 24:1H:1871:A:O4' | 2.06 | 0.55 |
| 24:1H:1899:G:N2 | 24:1H:1902:C:H41 | 2.05 | 0.55 |
| 24:1H:2337:G:H2' | 24:1H:2338:G:H8 | 1.72 | 0.55 |
| 24:1H:2837:G:H21 | 37:98:45:ARG:NH2 | 2.05 | 0.55 |
| 25:16:40:U:N3 | 25:16:43:C:H5" | 2.18 | 0.55 |
| 25:16:63:G:H2' | 25:16:64:C:C6 | 2.41 | 0.55 |
| 40:C8:47:TYR:CD1 | 40:C8:47:TYR:C | 2.85 | 0.55 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 1:1G:45:U:H2' | 1:1G:46:G:C8 | 2.41 | 0.55 |
| 1:1G:1179:A:H2' | 1:1G:1180:A:O4' | 2.07 | 0.55 |
| 1:1G:1226:C:H4' | 19:AA:80:TYR:OH | 2.07 | 0.55 |
| 2:12:204:ASN:HB2 | 2:12:210:SER:HB3 | 1.89 | 0.55 |
| 2:12:237:ALA:C | 2:12:239:VAL:H | 2.13 | 0.55 |
| 16:7A:71:ARG:HG2 | 16:7A:80:PHE:CE2 | 2.41 | 0.55 |
| 17:8A:59:ILE:HG22 | 17:8A:71:PHE:HD2 | 1.72 | 0.55 |
| 22:2L:69:U:H5' | 22:2L:70:C:H5 | 1.72 | 0.55 |
| 24:14:660:G:N2 | 35:35:12:ALA:HA | 2.17 | 0.55 |
| 24:14:2777:G:OP2 | 24:14:2781:A:O2' | 2.24 | 0.55 |
| 25:1J:15:A:H1' | 25:1J:109:G:C8 | 2.41 | 0.55 |
| 29:39:84:VAL:C | 29:39:86:GLY:H | 2.14 | 0.55 |
| 30:49:135:LEU:O | 30:49:154:GLY:HA3 | 2.07 | 0.55 |
| 45:D5:5:LEU:HD22 | 45:D5:47:VAL:HG21 | 1.88 | 0.55 |
| 48:G5:47:ASN:HD22 | 48:G5:47:ASN:N | 2.05 | 0.55 |
| 8:7E:121:ASP:OD1 | 8:7E:121:ASP:N | 2.40 | 0.55 |
| 11:2I:34:ASP:OD1 | 11:2I:38:ASN:N | 2.37 | 0.55 |
| 13:4I:49:THR:HB | 13:4I:52:GLU:HG3 | 1.89 | 0.55 |
| 22:2K:59:A:O2' | 22:2K:60:A:H5' | 2.06 | 0.55 |
| 22:3K:33:C:H2' | 22:3K:34:U:H5' | 1.87 | 0.55 |
| 24:1H:1021:A:O2' | 24:1H:1123:C:OP1 | 2.20 | 0.55 |
| 24:1H:2655:G:O2' | 24:1H:2664:G:O6 | 2.20 | 0.55 |
| 24:1H:2737:G:H2' | 24:1H:2738:A:C8 | 2.41 | 0.55 |
| 24:1H:2785:C:H2' | 24:1H:2786:U:O4' | 2.05 | 0.55 |
| 35:78:56:SER:HB2 | 35:78:61:ARG:HD2 | 1.89 | 0.55 |
| 40:C8:104:GLN:HG2 | 41:D8:44:LYS:HD3 | 1.89 | 0.55 |
| 1:1G:426:G:OP1 | 4:32:38:TYR:OH | 2.18 | 0.55 |
| 1:1G:509:A:C8 | 1:1G:509:A:H3' | 2.42 | 0.55 |
| 1:1G:926:G:H5" | 1:1G:927:G:O5' | 2.06 | 0.55 |
| 1:1G:1189:C:H5" | 3:22:5:ILE:HG12 | 1.89 | 0.55 |
| 1:1G:1503:A:O2' | 23:4L:13:A:N6 | 2.39 | 0.55 |
| 9:82:71:SER:HA | 9:82:74:ILE:HD12 | 1.89 | 0.55 |
| 10:1A:92:THR:HG23 | 10:1A:93:GLY:H | 1.72 | 0.55 |
| 13:4A:66:LEU:HA | 13:4A:70:LEU:HB2 | 1.88 | 0.55 |
| 24:14:443:A:H1' | 24:14:1201:C:O4' | 2.06 | 0.55 |
| 24:14:1021:A:H62 | 24:14:1141:U:H3 | 1.54 | 0.55 |
| 24:14:2250:G:N2 | 36:45:84:GLY:HA3 | 2.22 | 0.55 |
| 24:14:2849:U:H4' | 24:14:2868:A:C2 | 2.41 | 0.55 |
| 24:14:2859:G:C8 | 24:14:2859:G:H3' | 2.42 | 0.55 |
| 28:29:101:ARG:O | 28:29:201:THR:OG1 | 2.23 | 0.55 |
| 43:B5:18:TYR:HD1 | 43:B5:21:PHE:HE2 | 1.54 | 0.55 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 1:13:376:G:H1 | 1:13:387:U:H3 | 1.53 | 0.55 |
| 1:13:1074:G:H4' | 2:1E:104:ASN:HB2 | 1.89 | 0.55 |
| 24:1H:34:C:O2' | 24:1H:35:G:OP2 | 2.23 | 0.55 |
| 24:1H:250:G:H2' | 24:1H:251:A:C8 | 2.42 | 0.55 |
| 24:1H:529:A:H8 | 24:1H:530:G:C6 | 2.25 | 0.55 |
| 24:1H:931:G:O2' | 49:L8:24:LYS:HE3 | 2.06 | 0.55 |
| 24:1H:1901:A:OP2 | 27:11:255:LYS:HE2 | 2.07 | 0.55 |
| 24:1H:2150:U:H2' | 24:1H:2151:G:C8 | 2.42 | 0.55 |
| 32:61:73:GLU:OE1 | 32:61:137:PRO:HD2 | 2.06 | 0.55 |
| 39:B8:57:PHE:HA | 39:B8:79:HIS:CD2 | 2.42 | 0.55 |
| 1:1G:1288:A:H2' | 1:1G:1289:A:C8 | 2.42 | 0.55 |
| 1:1G:1359:C:H5" | 57:1G:1874:HOH:O | 2.06 | 0.55 |
| 3:22:20:SER:HB3 | 3:22:22:TRP:HE1 | 1.72 | 0.55 |
| 17:8A:59:ILE:CG2 | 17:8A:71:PHE:HB3 | 2.36 | 0.55 |
| 20:BA:50:GLU:HG3 | 20:BA:100:ILE:HG21 | 1.87 | 0.55 |
| 24:14:540:G:H2' | 24:14:541:C:C6 | 2.41 | 0.55 |
| 24:14:2096:U:H3 | 24:14:2193:G:H1 | 1.55 | 0.55 |
| 24:14:2170:A:H2' | 24:14:2171:A:H5' | 1.88 | 0.55 |
| 24:14:2402:C:H41 | 24:14:2416:C:H1' | 1.71 | 0.55 |
| 24:14:2420:C:N4 | 54:M5:31:HIS:HB3 | 2.13 | 0.55 |
| 25:1J:66:A:N6 | 25:1J:107:U:H2' | 2.22 | 0.55 |
| 28:29:97:LYS:O | 28:29:100:GLU:HG3 | 2.07 | 0.55 |
| 39:75:11:GLU:HA | 39:75:15:VAL:HG13 | 1.89 | 0.55 |
| 41:95:44:LYS:C | 41:95:46:VAL:N | 2.65 | 0.55 |
| 44:C5:17:SER:O | 44:C5:21:LYS:HB2 | 2.07 | 0.55 |
| 45:D5:10:ARG:HD2 | 45:D5:36:LYS:HE2 | 1.89 | 0.55 |
| 1:13:355:C:H5" | 1:13:389:A:OP2 | 2.07 | 0.55 |
| 1:13:618:C:H5" | 1:13:619:U:H5" | 1.89 | 0.55 |
| 1:13:814:A:N7 | 1:13:816:A:C4 | 2.75 | 0.55 |
| 2:1E:9:GLU:H | 2:1E:9:GLU:CD | 2.14 | 0.55 |
| 19:AI:65:ASN:OD1 | 19:AI:65:ASN:N | 2.39 | 0.55 |
| 24:1H:969:U:OP1 | 49:L8:17:LYS:HG3 | 2.07 | 0.55 |
| 24:1H:1640:C:H2' | 24:1H:1641:A:C8 | 2.42 | 0.55 |
| 24:1H:2305:A:H2' | 24:1H:2306:C:C6 | 2.42 | 0.55 |
| 24:1H:2348:U:H4' | 52:O8:42:TRP:HE1 | 1.70 | 0.55 |
| 24:1H:2379:G:O2' | 38:A8:17:ARG:NH1 | 2.40 | 0.55 |
| 24:1H:2636:U:H2' | 24:1H:2637:U:C6 | 2.42 | 0.55 |
| 25:16:65:C:N4 | 25:16:108:C:H2' | 2.22 | 0.55 |
| 1:1G:1075:C:H5" | 2:12:179:LYS:NZ | 2.22 | 0.55 |
| 2:12:230:VAL:HG12 | 2:12:231:GLU:H | 1.70 | 0.55 |
| 13:4A:73:GLU:O | 13:4A:77:ASN:HB2 | 2.07 | 0.55 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 13:4A:92:HIS:CE1 | 13:4A:98:VAL:HG21 | 2.42 | 0.55 |
| 24:14:242:G:O5' | 54:M5:3:LYS:HE3 | 2.07 | 0.55 |
| 24:14:2577:A:O4' | 51:J5:3:LYS:HB2 | 2.06 | 0.55 |
| 24:14:2612:C:OP2 | 51:J5:2:ALA:HA | 2.07 | 0.55 |
| 24:14:2774:C:H2' | 24:14:2775:A:O4' | 2.06 | 0.55 |
| 29:39:66:PRO:O | 29:39:67:GLN:HB3 | 2.07 | 0.55 |
| 39:75:11:GLU:HA | 39:75:15:VAL:CG1 | 2.36 | 0.55 |
| 42:A5:18:ARG:HG3 | 42:A5:76:VAL:HG13 | 1.88 | 0.55 |
| 45:D5:61:LEU:HB3 | 45:D5:62:PRO:O | 2.07 | 0.55 |
| 1:13:1218:C:H2' | 1:13:1219:U:C6 | 2.43 | 0.55 |
| 3:2E:6:HIS:CD2 | 3:2E:7:PRO:HD2 | 2.42 | 0.55 |
| 12:3I:62:SER:C | 12:3I:64:TYR:H | 2.16 | 0.55 |
| 24:1H:185:U:H4' | 24:1H:218:A:H4' | 1.88 | 0.55 |
| 24:1H:1184:G:H5' | 49:L8:29:ARG:NH1 | 2.22 | 0.55 |
| 24:1H:1857:G:O2' | 24:1H:1885:A:N6 | 2.35 | 0.55 |
| 24:1H:2502:G:H5" | 24:1H:2503:A:H5" | 1.88 | 0.55 |
| 25:16:24:G:N7 | 25:16:56:G:H2' | 2.21 | 0.55 |
| 27:11:69:ARG:NH2 | 27:11:128:GLY:O | 2.37 | 0.55 |
| 37:98:42:LYS:O | 37:98:45:ARG:HD3 | 2.06 | 0.55 |
| 1:1G:947:G:H2' | 1:1G:948:C:O4' | 2.07 | 0.55 |
| 1:1G:1208:C:H2' | 1:1G:1209:C:C6 | 2.42 | 0.55 |
| 19:AA:32:LYS:HB3 | 19:AA:57:HIS:CE1 | 2.42 | 0.55 |
| 24:14:581:C:H2' | 24:14:582:G:H8 | 1.70 | 0.55 |
| 24:14:657:U:H2' | 24:14:658:C:C6 | 2.42 | 0.55 |
| 24:14:864:G:C6 | 24:14:865:C:N4 | 2.75 | 0.55 |
| 24:14:1428:C:N4 | 24:14:1570:A:OP2 | 2.32 | 0.55 |
| 35:35:59:LEU:O | 35:35:59:LEU:HD22 | 2.06 | 0.55 |
| 39:75:102:ILE:HA | 39:75:105:LEU:HB2 | 1.87 | 0.55 |
| 43:B5:49:VAL:HB | 43:B5:83:VAL:HG21 | 1.89 | 0.55 |
| 51:J5:46:CYS:SG | 51:J5:48:GLU:HG2 | 2.47 | 0.55 |
| 52:K5:29:ASN:OD1 | 52:K5:30:THR:N | 2.40 | 0.55 |
| 1:13:1075:C:H5' | 2:1E:103:THR:HG21 | 1.88 | 0.54 |
| 1:13:1281:U:OP2 | 1:13:1282:C:N4 | 2.23 | 0.54 |
| 10:1I:47:PHE:CZ | 14:5I:37:PHE:HE1 | 2.25 | 0.54 |
| 13:4I:107:ALA:O | 13:4I:110:ARG:N | 2.40 | 0.54 |
| 15:6I:82:ILE:O | 15:6I:86:GLY:N | 2.39 | 0.54 |
| 20:BI:49:ALA:HA | 20:BI:52:ALA:HB3 | 1.88 | 0.54 |
| 24:1H:968:G:H5" | 49:L8:17:LYS:HZ3 | 1.72 | 0.54 |
| 24:1H:1668:A:OP1 | 34:68:5:GLN:HG3 | 2.07 | 0.54 |
| 24:1H:1946:U:H2' | 24:1H:1947:C:H6 | 1.72 | 0.54 |
| 24:1H:1980:G:H4' | 57:1H:3972:HOH:O | 2.06 | 0.54 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 31:51:4:ILE:HB | 31:51:6:ARG:HG3 | 1.89 | 0.54 |
| 31:51:77:LYS:HE3 | 31:51:138:LYS:NZ | 2.21 | 0.54 |
| 36:88:104:PHE:CE2 | 36:88:125:LEU:HD11 | 2.41 | 0.54 |
| 38:A8:39:ILE:HD13 | 38:A8:85:VAL:HG11 | 1.88 | 0.54 |
| 1:1G:115:G:H1' | 1:1G:116:A:N7 | 2.22 | 0.54 |
| 1:1G:537:G:H5" | 12:3A:113:ARG:NH1 | 2.23 | 0.54 |
| 1:1G:1127:G:N2 | 1:1G:1145:C:O2 | 2.40 | 0.54 |
| 2:12:12:GLU:OE1 | 2:12:16:HIS:N | 2.28 | 0.54 |
| 8:72:102:ARG:NH1 | 8:72:105:ARG:HH11 | 2.05 | 0.54 |
| 24:14:481:G:C4 | 24:14:507:A:C2 | 2.95 | 0.54 |
| 24:14:873:G:H1 | 24:14:904:C:H42 | 1.55 | 0.54 |
| 24:14:2135:A:H5" | 24:14:2136:C:H5 | 1.71 | 0.54 |
| 26:79:59:ARG:HG2 | 26:79:164:ARG:HG3 | 1.89 | 0.54 |
| 50:I5:14:ILE:HG23 | 50:I5:33:VAL:HG11 | 1.89 | 0.54 |
| 53:L5:9:ARG:NH1 | 53:L5:49:ARG:HD2 | 2.23 | 0.54 |
| 1:13:452:A:O2' | 1:13:453:A:O5' | 2.25 | 0.54 |
| 16:7I:19:ILE:HB | 16:7I:36:ILE:O | 2.07 | 0.54 |
| 24:1H:848:G:H2' | 24:1H:849:A:C8 | 2.42 | 0.54 |
| 24:1H:2035:G:P | 57:1H:3611:HOH:O | 2.60 | 0.54 |
| 27:11:125:ILE:HD12 | 27:11:137:PRO:HD3 | 1.89 | 0.54 |
| 37:98:38:VAL:HG22 | 37:98:112:ALA:HB2 | 1.89 | 0.54 |
| 40:C8:17:ILE:HG13 | 40:C8:32:PHE:HE1 | 1.72 | 0.54 |
| 40:C8:105:VAL:O | 40:C8:109:LEU:HD12 | 2.07 | 0.54 |
| 45:H8:97:GLU:HB2 | 45:H8:125:LEU:HD11 | 1.89 | 0.54 |
| 47:J8:82:LEU:HD23 | 47:J8:83:GLU:H | 1.71 | 0.54 |
| 1:1G:328:C:H4' | 1:1G:329:A:H5' | 1.88 | 0.54 |
| 1:1G:741:G:O6 | 57:1G:1811:HOH:O | 2.16 | 0.54 |
| 1:1G:920:U:H2' | 1:1G:921:U:H6 | 1.70 | 0.54 |
| 4:32:153:ARG:HG3 | 4:32:181:MET:SD | 2.47 | 0.54 |
| 20:BA:12:ALA:HA | 20:BA:15:ARG:HB2 | 1.88 | 0.54 |
| 22:2L:10:C:N4 | 22:2L:26:G:H1 | 2.04 | 0.54 |
| 24:14:1198:U:H2' | 24:14:1199:U:H6 | 1.71 | 0.54 |
| 24:14:1556:C:H2' | 24:14:1557:C:C6 | 2.43 | 0.54 |
| 24:14:2150:U:H2' | 24:14:2151:G:C8 | 2.42 | 0.54 |
| 24:14:2378:A:O2' | 38:65:21:THR:HG21 | 2.08 | 0.54 |
| 36:45:11:LYS:NZ | 36:45:88:GLY:O | 2.31 | 0.54 |
| 1:13:114:U:H2' | 1:13:115:G:C8 | 2.41 | 0.54 |
| 1:13:376:G:OP1 | 16:7I:5:ARG:HB2 | 2.07 | 0.54 |
| 1:13:536:C:H2' | 1:13:537:G:H8 | 1.70 | 0.54 |
| 1:13:657:G:H4' | 15:6I:28:GLN:HG2 | 1.90 | 0.54 |
| 6:5E:19:LEU:HD23 | 6:5E:23:LYS:NZ | 2.21 | 0.54 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 7:6E:113:GLU:HB2 | 7:6E:118:VAL:HG13 | 1.89 | 0.54 |
| 16:7I:3:LYS:O | 16:7I:21:VAL:HA | 2.08 | 0.54 |
| 20:BI:69:GLY:O | 20:BI:73:HIS:NE2 | 2.41 | 0.54 |
| 22:3K:8:4SU:O5' | 22:3K:8:4SU:H6 | 2.07 | 0.54 |
| 24:1H:508:G:H4' | 24:1H:509:C:OP2 | 2.05 | 0.54 |
| 24:1H:731:C:P | 57:1H:3603:HOH:O | 2.65 | 0.54 |
| 24:1H:1239:G:H2' | 24:1H:1240:U:O4' | 2.07 | 0.54 |
| 24:1H:1614:A:H61 | 42:E8:88:ARG:H | 1.56 | 0.54 |
| 24:1H:1826:G:H4' | 27:11:242:ARG:HH21 | 1.73 | 0.54 |
| 24:1H:2461:C:H2' | 24:1H:2462:U:C6 | 2.42 | 0.54 |
| 44:G8:28:LYS:HE3 | 44:G8:40:GLU:HB2 | 1.89 | 0.54 |
| 1:1G:986:A:N3 | 19:AA:52:TYR:OH | 2.38 | 0.54 |
| 1:1G:1072:G:H2' | 1:1G:1073:U:C6 | 2.42 | 0.54 |
| 4:32:178:VAL:C | 4:32:180:GLY:H | 2.14 | 0.54 |
| 24:14:197:A:N6 | 24:14:2430:A:H2' | 2.21 | 0.54 |
| 24:14:826:U:H4' | 35:35:55:ARG:HA | 1.89 | 0.54 |
| 24:14:1794:U:H2' | 24:14:1795:C:H6 | 1.72 | 0.54 |
| 24:14:2554:U:H2' | 24:14:2555:U:C6 | 2.41 | 0.54 |
| 28:29:120:TRP:CD1 | 28:29:155:LYS:HB3 | 2.43 | 0.54 |
| 39:75:54:ARG:HB3 | 39:75:54:ARG:HH11 | 1.70 | 0.54 |
| 45:D5:132:ASN:HD22 | 45:D5:159:PRO:HB2 | 1.73 | 0.54 |
| 48:G5:17:SER:HB2 | 48:G5:20:GLU:N | 2.19 | 0.54 |
| 1:13:264:U:O2' | 17:8I:64:PRO:O | 2.19 | 0.54 |
| 1:13:1448:C:H42 | 1:13:1455:G:H1 | 1.56 | 0.54 |
| 8:7E:20:TYR:CE2 | 8:7E:75:ARG:HD2 | 2.40 | 0.54 |
| 11:2I:58:PRO:HD3 | 11:2I:89:ALA:HB1 | 1.89 | 0.54 |
| 13:4I:82:MET:HE2 | 13:4I:92:HIS:HB3 | 1.88 | 0.54 |
| 22:3K:41:C:H2' | 22:3K:42:U:H6 | 1.73 | 0.54 |
| 24:1H:592:G:N1 | 24:1H:665:C:N3 | 2.47 | 0.54 |
| 24:1H:1680:U:H2' | 24:1H:1681:G:O4' | 2.08 | 0.54 |
| 24:1H:2667:C:H1' | 31:51:109:PHE:CD1 | 2.43 | 0.54 |
| 27:11:65:ILE:HD11 | 27:11:67:PHE:CE1 | 2.43 | 0.54 |
| 31:51:30:LYS:HE3 | 31:51:81:GLU:N | 2.22 | 0.54 |
| 31:51:30:LYS:HG3 | 31:51:81:GLU:H | 1.72 | 0.54 |
| 45:H8:171:ILE:HG23 | 45:H8:172:ALA:H | 1.71 | 0.54 |
| 1:1G:859:A:H2' | 1:1G:860:A:O4' | 2.07 | 0.54 |
| 1:1G:995:C:O2 | 14:5A:4:LYS:NZ | 2.41 | 0.54 |
| 1:1G:1131:G:H2' | 1:1G:1132:C:H6 | 1.71 | 0.54 |
| 2:12:189:ASP:OD1 | 2:12:189:ASP:N | 2.38 | 0.54 |
| 8:72:102:ARG:HD2 | 8:72:105:ARG:HA | 1.88 | 0.54 |
| 17:8A:27:PHE:CE2 | 17:8A:36:ILE:HD11 | 2.42 | 0.54 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 22:2L:20:C:H6 | 22:2L:22:A:C8 | 2.25 | 0.54 |
| 24:14:395:U:H2' | 24:14:396:G:N7 | 2.23 | 0.54 |
| 24:14:476:G:H4' | 24:14:502:A:N1 | 2.21 | 0.54 |
| 24:14:863:A:H2' | 24:14:864:G:C8 | 2.42 | 0.54 |
| 24:14:1028:A:N6 | 24:14:1125:G:H2' | 2.23 | 0.54 |
| 24:14:1057:A:N6 | 24:14:1088:A:OP2 | 2.40 | 0.54 |
| 24:14:1537:C:H2' | 24:14:1538:G:O4' | 2.07 | 0.54 |
| 24:14:2124:G:H5" | 24:14:2125:G:N7 | 2.21 | 0.54 |
| 24:14:2873:A:C8 | 37:55:5:LYS:HA | 2.41 | 0.54 |
| 29:39:148:LEU:HD21 | 29:39:191:ARG:NH1 | 2.18 | 0.54 |
| 34:25:34:THR:OG1 | 34:25:35:VAL:N | 2.38 | 0.54 |
| 35:35:52:GLU:OE1 | 35:35:55:ARG:N | 2.40 | 0.54 |
| 40:85:88:ILE:HG22 | 40:85:90:VAL:HG23 | 1.89 | 0.54 |
| 44:C5:52:SER:HA | 44:C5:55:TYR:O | 2.06 | 0.54 |
| 45:D5:18:LEU:HD12 | 45:D5:23:LYS:HB2 | 1.89 | 0.54 |
| 48:G5:42:GLY:O | 48:G5:44:LEU:N | 2.41 | 0.54 |
| 1:13:626:U:C2 | 1:13:627:G:C8 | 2.96 | 0.54 |
| 1:13:1124:G:H2' | 1:13:1145:C:C4 | 2.42 | 0.54 |
| 16:7I:23:ASP:OD1 | 16:7I:25:ARG:HD3 | 2.08 | 0.54 |
| 24:1H:92:G:H2' | 24:1H:93:C:C6 | 2.43 | 0.54 |
| 24:1H:484:C:H2' | 24:1H:485:C:C6 | 2.43 | 0.54 |
| 24:1H:601:C:O2' | 29:31:104:LYS:NZ | 2.39 | 0.54 |
| 24:1H:721:C:H2' | 24:1H:722:A:C8 | 2.42 | 0.54 |
| 24:1H:957:A:N1 | 24:1H:2458:G:H4' | 2.22 | 0.54 |
| 24:1H:998:C:P | 40:C8:92:ARG:HH22 | 2.30 | 0.54 |
| 24:1H:1164:G:H2' | 24:1H:1165:U:C6 | 2.42 | 0.54 |
| 24:1H:1568:G:H4' | 27:11:59:LYS:HB3 | 1.90 | 0.54 |
| 24:1H:2104:G:C2 | 24:1H:2186:G:C2 | 2.95 | 0.54 |
| 24:1H:2339:G:H2' | 24:1H:2340:G:H8 | 1.71 | 0.54 |
| 24:1H:2699:C:H2' | 24:1H:2700:C:O4' | 2.08 | 0.54 |
| 28:21:1:MET:N | 28:21:83:ASP:O | 2.39 | 0.54 |
| 29:31:29:ASN:HB3 | 29:31:112:MET:HE1 | 1.89 | 0.54 |
| 45:H8:4:ARG:NH1 | 45:H8:60:GLU:OE2 | 2.40 | 0.54 |
| 1:1G:198:G:H2' | 1:1G:199:G:H8 | 1.72 | 0.54 |
| 1:1G:1224:G:O2' | 13:4A:102:ARG:NH1 | 2.40 | 0.54 |
| 19:AA:33:THR:HG22 | 19:AA:35:SER:H | 1.72 | 0.54 |
| 24:14:2340:G:O2' | 24:14:2341:G:H5' | 2.07 | 0.54 |
| 40:85:66:ASN:HB2 | 40:85:76:TYR:HB2 | 1.90 | 0.54 |
| 46:E5:70:GLN:HB3 | 46:E5:80:HIS:HE2 | 1.72 | 0.54 |
| 24:1H:1113:U:OP1 | 31:51:2:SER:N | 2.41 | 0.54 |
| 47:J8:87:PRO:HA | 47:J8:89:GLU:N | 2.23 | 0.54 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 1:1G:406:G:N2 | 4:32:119:GLN:HE22 | 1.95 | 0.54 |
| 1:1G:1202:G:N2 | 14:5A:46:GLU:OE1 | 2.39 | 0.54 |
| 4:32:101:LEU:HD23 | 4:32:121:VAL:HG11 | 1.89 | 0.54 |
| 8:72:102:ARG:HH12 | 8:72:105:ARG:HH11 | 1.56 | 0.54 |
| 19:AA:36:ARG:HH12 | 19:AA:75:ALA:HB3 | 1.72 | 0.54 |
| 24:14:2563:U:O2 | 24:14:2565:A:H8 | 1.91 | 0.54 |
| 27:19:70:TRP:CD1 | 27:19:70:TRP:C | 2.86 | 0.54 |
| 30:49:47:LYS:HG2 | 30:49:48:GLU:N | 2.23 | 0.54 |
| 33:15:20:GLY:HA2 | 33:15:61:ARG:HG2 | 1.90 | 0.54 |
| 45:D5:54:HIS:NE2 | 45:D5:123:ASP:HB3 | 2.23 | 0.54 |
| 45:D5:148:ASP:OD1 | 45:D5:170:THR:OG1 | 2.12 | 0.54 |
| 1:13:576:G:OP1 | 57:13:1810:HOH:O | 2.18 | 0.54 |
| 1:13:864:A:H2' | 1:13:865:A:C8 | 2.42 | 0.54 |
| 1:13:1117:G:H5" | 9:8E:104:ARG:NH1 | 2.23 | 0.54 |
| 1:13:1179:A:H2' | 1:13:1180:A:O4' | 2.08 | 0.54 |
| 2:1E:6:THR:OG1 | 2:1E:7:VAL:N | 2.41 | 0.54 |
| 2:1E:15:VAL:HG11 | 2:1E:207:ALA:HB1 | 1.90 | 0.54 |
| 5:4E:78:HIS:HE1 | 5:4E:142:LEU:HD23 | 1.73 | 0.54 |
| 10:1I:51:ARG:HG3 | 14:5I:45:ARG:NH1 | 2.23 | 0.54 |
| 19:AI:12:ASP:H | 19:AI:38:SER:HB3 | 1.73 | 0.54 |
| 27:11:106:ILE:HD11 | 27:11:196:VAL:HG22 | 1.90 | 0.54 |
| 34:68:78:ARG:NH1 | 39:B8:73:GLU:OE1 | 2.41 | 0.54 |
| 41:D8:35:LEU:O | 41:D8:37:VAL:N | 2.37 | 0.54 |
| 53:P8:26:GLY:O | 53:P8:30:VAL:HG23 | 2.08 | 0.54 |
| 1:1G:60:A:N1 | 1:1G:107:G:O2' | 2.27 | 0.54 |
| 1:1G:1014:A:H4' | 19:AA:14:HIS:CD2 | 2.43 | 0.54 |
| 1:1G:1014:A:H2' | 1:1G:1015:A:C8 | 2.43 | 0.54 |
| 1:1G:1189:C:OP1 | 10:1A:51:ARG:NH2 | 2.39 | 0.54 |
| 1:1G:1411:C:H2' | 1:1G:1412:C:H6 | 1.73 | 0.54 |
| 5:42:81:GLU:HB3 | 5:42:90:VAL:HG13 | 1.89 | 0.54 |
| 11:2A:22:HIS:HB3 | 11:2A:29:ILE:HG12 | 1.90 | 0.54 |
| 15:6A:11:VAL:HG21 | 15:6A:34:LEU:HD13 | 1.89 | 0.54 |
| 24:14:819:A:C4 | 24:14:1189:A:C2 | 2.95 | 0.54 |
| 24:14:1053:C:N4 | 24:14:1105:U:O4 | 2.40 | 0.54 |
| 24:14:1503:U:H2' | 24:14:1504:C:H6 | 1.71 | 0.54 |
| 24:14:2378:A:H4' | 38:65:23:ARG:NH1 | 2.23 | 0.54 |
| 24:14:2733:A:C2 | 28:29:203:LYS:HA | 2.42 | 0.54 |
| 27:19:255:LYS:NZ | 27:19:255:LYS:N | 2.54 | 0.54 |
| 44:C5:17:SER:HB3 | 44:C5:71:LYS:HB3 | 1.89 | 0.54 |
| 1:13:1141:C:H2' | 1:13:1142:G:H8 | 1.72 | 0.54 |
| 4:3E:13:ARG:C | 4:3E:15:GLU:H | 2.15 | 0.54 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 7:6E:57:GLU:HB2 | 7:6E:60:LYS:HG2 | 1.90 | 0.54 |
| 22:3K:50:U:H2' | 22:3K:51:C:C6 | 2.43 | 0.54 |
| 24:1H:92:G:H2' | 24:1H:93:C:H6 | 1.72 | 0.54 |
| 24:1H:1728:G:H3' | 24:1H:1729:A:C5' | 2.34 | 0.54 |
| 24:1H:2386:C:H2' | 24:1H:2387:U:C6 | 2.43 | 0.54 |
| 24:1H:2695:C:H2' | 24:1H:2696:U:H6 | 1.72 | 0.54 |
| 25:16:89:G:H8 | 25:16:89:G:OP2 | 1.90 | 0.54 |
| 28:21:105:THR:O | 28:21:196:VAL:HG12 | 2.08 | 0.54 |
| 36:88:89:ASN:HB2 | 36:88:90:VAL:HG22 | 1.90 | 0.54 |
| 39:B8:88:ILE:HG13 | 39:B8:91:ARG:HD3 | 1.90 | 0.54 |
| 43:F8:11:PRO:HD3 | 48:K8:37:PHE:CD2 | 2.43 | 0.54 |
| 44:G8:5:MET:HE1 | 44:G8:32:PRO:HB3 | 1.89 | 0.54 |
| 46:I8:23:VAL:HG13 | 46:I8:38:VAL:HG22 | 1.90 | 0.54 |
| 1:1G:948:C:OP1 | 13:4A:109:THR:OG1 | 2.25 | 0.54 |
| 1:1G:1057:G:H2' | 1:1G:1058:G:C8 | 2.43 | 0.54 |
| 1:1G:1305:G:HO2' | 1:1G:1306:A:H8 | 1.54 | 0.54 |
| 2:12:12:GLU:OE1 | 2:12:15:VAL:N | 2.41 | 0.54 |
| 3:22:92:ALA:HB2 | 3:22:99:VAL:HG21 | 1.90 | 0.54 |
| 21:1B:6:ARG:HE | 21:1B:15:ARG:HH22 | 1.56 | 0.54 |
| 24:14:192:C:O2' | 24:14:802:A:N3 | 2.35 | 0.54 |
| 24:14:674:G:H1' | 29:39:74:ARG:HD3 | 1.90 | 0.54 |
| 24:14:862:G:OP1 | 36:45:18:LYS:HD2 | 2.07 | 0.54 |
| 24:14:1165:U:H2' | 24:14:1166:C:C6 | 2.42 | 0.54 |
| 24:14:2788:C:H5' | 28:29:61:ARG:NH1 | 2.22 | 0.54 |
| 25:1J:48:A:P | 38:65:30:ARG:HH12 | 2.31 | 0.54 |
| 29:39:152:GLU:HA | 29:39:190:GLU:OE2 | 2.08 | 0.54 |
| 32:69:4:ILE:HG21 | 32:69:47:LEU:HD13 | 1.89 | 0.54 |
| 35:35:101:VAL:HG22 | 35:35:107:LYS:O | 2.08 | 0.54 |
| 40:85:74:LEU:HD11 | 40:85:110:VAL:HG13 | 1.88 | 0.54 |
| 44:C5:17:SER:HB2 | 44:C5:71:LYS:HD2 | 1.89 | 0.54 |
| 46:E5:50:ASN:C | 46:E5:62:LEU:HD12 | 2.33 | 0.54 |
| 48:G5:13:ALA:HA | 48:G5:16:LEU:HD21 | 1.89 | 0.54 |
| 1:13:91:C:H2' | 1:13:92:G:O4' | 2.07 | 0.54 |
| 1:13:108:G:OP2 | 1:13:326:G:N1 | 2.34 | 0.54 |
| 1:13:986:A:H1' | 19:AI:55:LYS:HA | 1.90 | 0.54 |
| 11:2I:17:GLY:HA3 | 11:2I:77:MET:SD | 2.48 | 0.54 |
| 17:8I:67:LYS:O | 17:8I:69:LYS:N | 2.41 | 0.54 |
| 22:2K:18:G:N2 | 22:2K:66:G:H1' | 2.22 | 0.54 |
| 24:1H:230:U:H6 | 24:1H:230:U:OP2 | 1.91 | 0.54 |
| 24:1H:288:C:H2' | 24:1H:289:A:C8 | 2.42 | 0.54 |
| 24:1H:801:G:OP2 | 57:1H:3689:HOH:O | 2.17 | 0.54 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 24:1H:821:A:H5" | 24:1H:822:U:H6 | 1.73 | 0.54 |
| 24:1H:2788:C:OP1 | 28:21:61:ARG:NH2 | 2.41 | 0.54 |
| 30:41:173:LEU:HD22 | 30:41:178:PHE:CE1 | 2.43 | 0.54 |
| 39:B8:3:ARG:HH21 | 39:B8:6:LEU:HG | 1.72 | 0.54 |
| 47:J8:4:VAL:HG12 | 47:J8:11:ARG:HB3 | 1.89 | 0.54 |
| 1:1G:1298:C:H2' | 7:62:114:ARG:HH12 | 1.73 | 0.54 |
| 2:12:178:ARG:NH2 | 8:72:74:PRO:HG3 | 2.23 | 0.54 |
| 24:14:330:A:H2 | 24:14:1210:A:O2' | 1.88 | 0.54 |
| 24:14:2099:U:H3 | 24:14:2190:G:H1 | 1.56 | 0.54 |
| 28:29:101:ARG:HG3 | 28:29:169:ASN:ND2 | 2.23 | 0.54 |
| 28:29:134:ILE:O | 28:29:137:HIS:HB2 | 2.08 | 0.54 |
| 29:39:64:ILE:HD12 | 29:39:65:TRP:CE2 | 2.42 | 0.54 |
| 31:59:116:GLU:O | 31:59:118:PRO:HD3 | 2.08 | 0.54 |
| 41:95:44:LYS:O | 41:95:46:VAL:HG12 | 2.08 | 0.54 |
| 1:13:748:C:H6 | 1:13:748:C:O5' | 1.91 | 0.54 |
| 1:13:1432:G:OP1 | 39:B8:107:ASP:HB2 | 2.07 | 0.54 |
| 5:4E:51:VAL:O | 5:4E:55:VAL:HG23 | 2.07 | 0.54 |
| 11:2I:23:ALA:HB3 | 11:2I:86:GLY:O | 2.08 | 0.54 |
| 12:3I:93:LEU:HB2 | 12:3I:96:VAL:HG12 | 1.90 | 0.54 |
| 13:4I:34:LEU:O | 13:4I:39:ILE:N | 2.25 | 0.54 |
| 19:AI:39:THR:HG22 | 19:AI:40:ILE:H | 1.73 | 0.54 |
| 24:1H:630:G:OP2 | 54:Q8:15:LYS:NZ | 2.38 | 0.54 |
| 24:1H:994:C:O2 | 41:D8:10:LYS:HE2 | 2.07 | 0.54 |
| 24:1H:1503:U:H2' | 24:1H:1504:C:C6 | 2.43 | 0.54 |
| 24:1H:1570:A:H2' | 24:1H:1571:A:C8 | 2.43 | 0.54 |
| 25:16:78:A:H2' | 25:16:79:C:O4' | 2.08 | 0.54 |
| 33:58:73:THR:HG22 | 33:58:84:LYS:HG3 | 1.90 | 0.54 |
| 46:I8:27:GLU:HG3 | 46:I8:69:PHE:H | 1.71 | 0.54 |
| 1:1G:994:A:N7 | 1:1G:1216:G:H4' | 2.23 | 0.54 |
| 1:1G:1368:G:OP1 | 9:82:111:ARG:NH2 | 2.39 | 0.54 |
| 6:52:69:GLU:H | 6:52:69:GLU:CD | 2.16 | 0.54 |
| 9:82:83:ARG:HA | 9:82:86:VAL:HG12 | 1.88 | 0.54 |
| 24:14:30:G:H2' | 24:14:31:C:C6 | 2.42 | 0.54 |
| 24:14:93:C:H5' | 24:14:94:G:OP2 | 2.08 | 0.54 |
| 24:14:125:G:C6 | 53:L5:10:ARG:HG3 | 2.43 | 0.54 |
| 24:14:796:C:H2' | 24:14:797:C:C6 | 2.43 | 0.54 |
| 24:14:1025:G:C4 | 24:14:1135:C:H1' | 2.43 | 0.54 |
| 24:14:2554:U:H2' | 24:14:2555:U:H6 | 1.73 | 0.54 |
| 27:19:32:SER:O | 27:19:33:LEU:HB2 | 2.06 | 0.54 |
| 31:59:34:GLU:OE1 | 31:59:34:GLU:N | 2.41 | 0.54 |
| 32:69:87:LYS:O | 32:69:87:LYS:HD2 | 2.08 | 0.54 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 38:65:64:GLU:OE2 | 38:65:67:ARG:NH1 | 2.41 | 0.54 |
| 40:85:110:VAL:HG12 | 40:85:114:LYS:HE2 | 1.89 | 0.54 |
| 45:D5:7:ALA:O | 45:D5:8:TYR:CG | 2.61 | 0.54 |
| 1:13:686:U:O4 | 1:13:703:G:H1' | 2.08 | 0.53 |
| 1:13:1435:G:H2' | 1:13:1436:U:C6 | 2.43 | 0.53 |
| 21:1F:3:LYS:HB3 | 21:1F:14:TRP:CD1 | 2.43 | 0.53 |
| 24:1H:531:C:H4' | 24:1H:532:A:H5" | 1.89 | 0.53 |
| 24:1H:676:A:H8 | 24:1H:2069:G:N2 | 1.94 | 0.53 |
| 24:1H:1184:G:H5' | 49:L8:29:ARG:HH11 | 1.72 | 0.53 |
| 24:1H:1678:G:N2 | 24:1H:1989:G:N2 | 2.50 | 0.53 |
| 35:78:18:ARG:HG3 | 35:78:18:ARG:O | 2.08 | 0.53 |
| 39:B8:26:ASP:HB3 | 39:B8:92:GLY:N | 2.22 | 0.53 |
| 54:Q8:36:LYS:HG2 | 54:Q8:37:SER:H | 1.72 | 0.53 |
| 1:1G:921:U:O2' | 5:42:18:ARG:HG2 | 2.09 | 0.53 |
| 8:72:49:GLU:HG2 | 8:72:62:TYR:HE1 | 1.71 | 0.53 |
| 13:4A:48:LEU:HD11 | 13:4A:53:VAL:HG22 | 1.90 | 0.53 |
| 17:8A:45:HIS:O | 17:8A:73:VAL:HG12 | 2.08 | 0.53 |
| 20:BA:21:LYS:O | 20:BA:25:ARG:HG3 | 2.07 | 0.53 |
| 24:14:800:A:P | 57:14:3517:HOH:O | 2.65 | 0.53 |
| 24:14:1050:A:N6 | 24:14:2751:G:N7 | 2.56 | 0.53 |
| 24:14:1225:C:O2' | 41:95:85:LYS:N | 2.41 | 0.53 |
| 24:14:2136:C:H42 | 24:14:2156:G:H1 | 1.54 | 0.53 |
| 24:14:2330:G:H4' | 46:E5:44:ARG:HH12 | 1.73 | 0.53 |
| 27:19:68:LYS:HB3 | 27:19:70:TRP:CH2 | 2.43 | 0.53 |
| 31:59:26:VAL:HG21 | 31:59:76:VAL:HA | 1.90 | 0.53 |
| 45:D5:70:LEU:O | 45:D5:89:PHE:N | 2.29 | 0.53 |
| 1:13:41:G:H2' | 1:13:42:G:C8 | 2.43 | 0.53 |
| 1:13:666:G:H5' | 1:13:726:C:H1' | 1.89 | 0.53 |
| 1:13:1166:G:N2 | 1:13:1170:A:OP2 | 2.38 | 0.53 |
| 2:1E:100:GLY:O | 2:1E:104:ASN:N | 2.34 | 0.53 |
| 2:1E:112:VAL:O | 2:1E:115:LEU:HB3 | 2.09 | 0.53 |
| 3:2E:20:SER:HB3 | 3:2E:40:ARG:HH12 | 1.72 | 0.53 |
| 22:2K:21:A:C2 | 22:2K:56:U:C2 | 2.96 | 0.53 |
| 24:1H:2615:U:H2' | 24:1H:2616:C:H6 | 1.73 | 0.53 |
| 24:1H:2795:G:N2 | 24:1H:2801:A:OP2 | 2.41 | 0.53 |
| 34:68:17:ARG:HB2 | 34:68:45:GLU:HG2 | 1.91 | 0.53 |
| 40:C8:106:PHE:O | 40:C8:109:LEU:HB2 | 2.08 | 0.53 |
| 1:1G:485:G:HO2' | 1:1G:486:U:P | 2.31 | 0.53 |
| 1:1G:861:G:H2' | 1:1G:862:C:H6 | 1.73 | 0.53 |
| 1:1G:1142:G:H3' | 1:1G:1143:G:C8 | 2.43 | 0.53 |
| 1:1G:1510:U:H2' | 1:1G:1511:G:C8 | 2.43 | 0.53 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 2:12:8:LYS:H | 2:12:8:LYS:HE2 | 1.73 | 0.53 |
| 9:82:40:LEU:O | 9:82:42:ARG:N | 2.29 | 0.53 |
| 11:2A:31:THR:HG22 | 11:2A:42:TRP:HB2 | 1.89 | 0.53 |
| 13:4A:33:ALA:O | 13:4A:37:THR:OG1 | 2.15 | 0.53 |
| 24:14:1257:C:H4' | 29:39:83:PHE:CE1 | 2.43 | 0.53 |
| 24:14:2123:G:N2 | 26:79:42:GLU:OE1 | 2.36 | 0.53 |
| 24:14:2815:C:H5' | 51:J5:29:THR:HG21 | 1.89 | 0.53 |
| 32:69:93:THR:HG22 | 32:69:119:PRO:HG3 | 1.89 | 0.53 |
| 42:A5:70:TYR:H | 42:A5:70:TYR:HD1 | 1.55 | 0.53 |
| 52:K5:36:LEU:HA | 52:K5:49:HIS:O | 2.08 | 0.53 |
| 1:13:89:U:O2' | 1:13:90:C:H5" | 2.07 | 0.53 |
| 1:13:102:G:C6 | 1:13:103:C:C4 | 2.97 | 0.53 |
| 1:13:1124:G:OP2 | 1:13:1124:G:H8 | 1.91 | 0.53 |
| 1:13:1222:G:H2' | 1:13:1223:C:O4' | 2.07 | 0.53 |
| 3:2E:19:GLU:HG2 | 3:2E:54:ARG:NH1 | 2.24 | 0.53 |
| 16:7I:72:ARG:HG2 | 16:7I:73:LEU:HD23 | 1.91 | 0.53 |
| 22:3K:71:C:H2' | 22:3K:72:U:C6 | 2.43 | 0.53 |
| 24:1H:64:A:O3' | 43:F8:71:GLY:HA3 | 2.09 | 0.53 |
| 24:1H:250:G:O6 | 24:1H:386:G:N1 | 2.31 | 0.53 |
| 24:1H:376:C:P | 57:1H:3685:HOH:O | 2.66 | 0.53 |
| 24:1H:918:A:H8 | 24:1H:918:A:O5' | 1.91 | 0.53 |
| 24:1H:1047:G:H2' | 24:1H:1110:G:N1 | 2.24 | 0.53 |
| 24:1H:1056:G:H5' | 24:1H:1086:A:C8 | 2.42 | 0.53 |
| 24:1H:1590:U:H2' | 24:1H:1591:G:C8 | 2.42 | 0.53 |
| 24:1H:2137:C:H42 | 24:1H:2154:G:H1 | 1.55 | 0.53 |
| 24:1H:2531:A:H5' | 31:51:157:TYR:CZ | 2.44 | 0.53 |
| 24:1H:2887:U:H2' | 24:1H:2888:C:H6 | 1.73 | 0.53 |
| 28:21:167:VAL:HG12 | 28:21:189:PRO:HD3 | 1.89 | 0.53 |
| 29:31:116:ASP:OD2 | 35:78:1:MET:HB2 | 2.08 | 0.53 |
| 35:78:45:LEU:H | 35:78:45:LEU:CD2 | 2.19 | 0.53 |
| 45:H8:48:PHE:HE1 | 45:H8:71:VAL:HG11 | 1.72 | 0.53 |
| 46:I8:70:GLN:NE2 | 46:I8:72:ARG:HD2 | 2.23 | 0.53 |
| 1:1G:114:U:H2' | 1:1G:115:G:C8 | 2.42 | 0.53 |
| 1:1G:277:C:H5 | 17:8A:92:ARG:HH22 | 1.56 | 0.53 |
| 1:1G:591:U:OP2 | 8:72:30:ARG:HD3 | 2.09 | 0.53 |
| 1:1G:653:A:O5' | 8:72:56:LYS:HE3 | 2.08 | 0.53 |
| 1:1G:1002:G:H1 | 1:1G:1038:C:H42 | 1.55 | 0.53 |
| 1:1G:1181:G:O2' | 1:1G:1182:G:O5' | 2.25 | 0.53 |
| 1:1G:1250:A:OP1 | 9:82:67:GLY:N | 2.35 | 0.53 |
| 3:22:81:GLY:HA2 | 3:22:85:ARG:NH2 | 2.21 | 0.53 |
| 4:32:33:MET:C | 4:32:35:ARG:N | 2.65 | 0.53 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 24:14:729:G:C8 | 27:19:208:LYS:HD2 | 2.44 | 0.53 |
| 24:14:747:U:O2 | 24:14:2014:A:H1' | 2.09 | 0.53 |
| 24:14:756:C:C2' | 24:14:757:U:H5' | 2.38 | 0.53 |
| 24:14:1171:G:N2 | 24:14:1178:C:H41 | 2.07 | 0.53 |
| 28:29:119:ARG:HG2 | 28:29:160:TYR:HB2 | 1.90 | 0.53 |
| 30:49:66:GLN:HA | 50:I5:6:HIS:HD2 | 1.72 | 0.53 |
| 30:49:130:ASN:HB3 | 30:49:160:VAL:HA | 1.90 | 0.53 |
| 1:13:627:G:H2' | 1:13:628:G:H8 | 1.72 | 0.53 |
| 4:3E:88:VAL:C | 4:3E:90:GLY:H | 2.16 | 0.53 |
| 9:8E:17:VAL:HA | 9:8E:63:ILE:HG23 | 1.90 | 0.53 |
| 17:8I:86:GLU:O | 17:8I:90:ILE:HG13 | 2.07 | 0.53 |
| 24:1H:751:A:H5' | 42:E8:90:ARG:HA | 1.89 | 0.53 |
| 42:E8:39:THR:HG22 | 42:E8:44:ALA:HB2 | 1.89 | 0.53 |
| 43:F8:5:TYR:CE1 | 48:K8:30:ARG:HG3 | 2.43 | 0.53 |
| 1:1G:38:G:C2 | 1:1G:397:A:C2 | 2.97 | 0.53 |
| 1:1G:321:A:N7 | 1:1G:328:C:H6 | 2.06 | 0.53 |
| 1:1G:814:A:H2' | 1:1G:816:A:H5" | 1.89 | 0.53 |
| 1:1G:1412:C:H2' | 1:1G:1413:A:C8 | 2.44 | 0.53 |
| 1:1G:1513:A:H2' | 1:1G:1514:C:C6 | 2.43 | 0.53 |
| 5:42:16:THR:O | 5:42:16:THR:OG1 | 2.25 | 0.53 |
| 7:62:26:PHE:HB2 | 7:62:101:LEU:HD22 | 1.90 | 0.53 |
| 24:14:39:C:O2 | 29:39:46:ARG:NH2 | 2.41 | 0.53 |
| 24:14:738:G:O3' | 57:14:3555:HOH:O | 2.19 | 0.53 |
| 24:14:1041:C:H2' | 24:14:1042:G:C8 | 2.44 | 0.53 |
| 24:14:1939:U:OP1 | 24:14:2604:U:O2' | 2.20 | 0.53 |
| 24:14:2320:A:H61 | 24:14:2333:A:H2' | 1.71 | 0.53 |
| 25:1J:15:A:H1' | 25:1J:109:G:N9 | 2.23 | 0.53 |
| 31:59:158:HIS:O | 31:59:158:HIS:ND1 | 2.41 | 0.53 |
| 32:69:113:ARG:HG2 | 32:69:131:LYS:HB2 | 1.89 | 0.53 |
| 34:25:47:ILE:HG13 | 34:25:48:PRO:HD2 | 1.90 | 0.53 |
| 35:35:38:GLN:O | 35:35:41:ARG:HB2 | 2.08 | 0.53 |
| 35:35:79:ARG:O | 35:35:110:TYR:HB3 | 2.09 | 0.53 |
| 37:55:38:VAL:HG22 | 37:55:112:ALA:HB2 | 1.89 | 0.53 |
| 41:95:21:ARG:NH2 | 41:95:91:TYR:CD1 | 2.76 | 0.53 |
| 41:95:35:LEU:C | 41:95:37:VAL:N | 2.65 | 0.53 |
| 42:A5:73:ALA:HB3 | 42:A5:106:ILE:HG12 | 1.91 | 0.53 |
| 49:H5:3:ARG:HD2 | 49:H5:60:GLU:O | 2.07 | 0.53 |
| 53:L5:19:ARG:HG2 | 53:L5:19:ARG:HH11 | 1.74 | 0.53 |
| 1:13:1492[A]:A:H5' | 1:13:1493[A]:A:OP2 | 2.08 | 0.53 |
| 1:13:1525:G:OP1 | 11:2I:120:ARG:NH2 | 2.41 | 0.53 |
| 4:3E:110:PHE:HE2 | 4:3E:148:VAL:HG23 | 1.73 | 0.53 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 5:4E:98:THR:HB | 5:4E:117:ASP:HB3 | 1.90 | 0.53 |
| 15:6I:22:THR:O | 15:6I:22:THR:OG1 | 2.21 | 0.53 |
| 24:1H:1100:C:H2' | 24:1H:1101:U:C6 | 2.43 | 0.53 |
| 24:1H:2337:G:H2' | 24:1H:2338:G:C8 | 2.44 | 0.53 |
| 24:1H:2572:A:N7 | 28:21:144:ARG:HD2 | 2.23 | 0.53 |
| 34:68:19:ILE:HG22 | 34:68:43:VAL:HA | 1.90 | 0.53 |
| 38:A8:37:ALA:HB2 | 38:A8:101:LEU:HD21 | 1.90 | 0.53 |
| 40:C8:66:ASN:O | 40:C8:70:ARG:HB2 | 2.08 | 0.53 |
| 1:1G:327:A:O2' | 1:1G:329:A:H8 | 1.91 | 0.53 |
| 1:1G:476:G:O2' | 1:1G:477:G:H5' | 2.09 | 0.53 |
| 1:1G:601:C:H2' | 1:1G:602:A:C8 | 2.43 | 0.53 |
| 1:1G:861:G:HO2' | 1:1G:874:G:HO2' | 1.54 | 0.53 |
| 4:32:149:ALA:O | 4:32:153:ARG:NE | 2.42 | 0.53 |
| 12:3A:24:VAL:HG12 | 12:3A:98:TYR:CE1 | 2.44 | 0.53 |
| 22:2L:41:C:H2' | 22:2L:42:U:C6 | 2.44 | 0.53 |
| 24:14:606:U:H4' | 24:14:658:C:H4' | 1.90 | 0.53 |
| 24:14:1405:U:H2' | 24:14:1406:U:C6 | 2.43 | 0.53 |
| 24:14:1557:C:OP2 | 24:14:1558:A:O2' | 2.26 | 0.53 |
| 24:14:2648:C:H2' | 24:14:2649:U:C6 | 2.43 | 0.53 |
| 25:1J:5:C:N3 | 25:1J:115:G:N2 | 2.36 | 0.53 |
| 43:B5:60:ARG:NH2 | 53:L5:47:ARG:HH22 | 2.05 | 0.53 |
| 47:F5:57:GLU:O | 47:F5:58:ILE:HD13 | 2.09 | 0.53 |
| 1:13:431:A:OP2 | 57:13:1811:HOH:O | 2.19 | 0.53 |
| 1:13:955:U:H1' | 1:13:1227:A:N6 | 2.23 | 0.53 |
| 1:13:1202:G:O2' | 14:5I:27:CYS:HB3 | 2.08 | 0.53 |
| 1:13:1292:U:OP1 | 7:6E:41:ARG:NH2 | 2.25 | 0.53 |
| 1:13:1492[B]:A:C8 | 23:4K:20:A:O2' | 2.62 | 0.53 |
| 4:3E:153:ARG:HA | 4:3E:181:MET:HE1 | 1.90 | 0.53 |
| 9:8E:50:LEU:HD23 | 9:8E:85:LEU:HD22 | 1.91 | 0.53 |
| 17:8I:43:LEU:O | 17:8I:69:LYS:HG3 | 2.09 | 0.53 |
| 19:AI:6:LYS:HG2 | 50:M8:62:ARG:HD2 | 1.89 | 0.53 |
| 24:1H:751:A:C8 | 57:1H:3642:HOH:O | 2.54 | 0.53 |
| 24:1H:1019:U:HO2' | 24:1H:1021:A:H2 | 1.55 | 0.53 |
| 24:1H:1021:A:H62 | 24:1H:1141:U:H3 | 1.55 | 0.53 |
| 24:1H:1142:U:H5' | 24:1H:1142(A):A:H8 | 1.72 | 0.53 |
| 24:1H:2444:G:OP2 | 29:31:68:LYS:NZ | 2.37 | 0.53 |
| 39:B8:3:ARG:HB2 | 39:B8:7:ILE:HG13 | 1.91 | 0.53 |
| 42:E8:97:LYS:HE2 | 42:E8:99:ARG:NH2 | 2.23 | 0.53 |
| 43:F8:36:LYS:HG2 | 43:F8:54:VAL:HB | 1.91 | 0.53 |
| 1:1G:411:A:C6 | 1:1G:413:G:H1' | 2.43 | 0.53 |
| 1:1G:1002:G:H22 | 1:1G:1038:C:N4 | 2.07 | 0.53 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 16:7A:43:LYS:HB3 | 16:7A:48:TRP:CD1 | 2.44 | 0.53 |
| 24:14:361:G:OP1 | 57:14:3568:HOH:O | 2.19 | 0.53 |
| 24:14:907:U:O2' | 36:45:101:ARG:NH2 | 2.32 | 0.53 |
| 24:14:1048:A:H5' | 24:14:1049:C:OP2 | 2.08 | 0.53 |
| 24:14:1210:A:H5' | 24:14:1212:G:O4' | 2.09 | 0.53 |
| 24:14:1416:G:O2' | 24:14:1417:C:H6 | 1.91 | 0.53 |
| 24:14:2315:G:OP1 | 30:49:36:LYS:NZ | 2.35 | 0.53 |
| 38:65:41:ASP:OD2 | 38:65:44:LYS:HG2 | 2.09 | 0.53 |
| 39:75:3:ARG:HA | 39:75:4:GLY:O | 2.07 | 0.53 |
| 49:H5:12:PRO:O | 49:H5:15:TYR:HB2 | 2.09 | 0.53 |
| 1:13:10:A:OP2 | 5:4E:126:ARG:HD3 | 2.08 | 0.53 |
| 1:13:1060:C:H5" | 10:1I:51:ARG:HG2 | 1.89 | 0.53 |
| 2:1E:18:GLY:HA3 | 2:1E:41:ILE:HD12 | 1.91 | 0.53 |
| 16:7I:26:ARG:NH1 | 16:7I:31:LYS:O | 2.42 | 0.53 |
| 17:8I:4:LYS:HE2 | 17:8I:6:LEU:HD21 | 1.91 | 0.53 |
| 24:1H:1520:U:H2' | 24:1H:1521:G:O4' | 2.08 | 0.53 |
| 24:1H:2065:C:H2' | 24:1H:2066:C:C6 | 2.43 | 0.53 |
| 24:1H:2837:G:H21 | 37:98:45:ARG:HH21 | 1.56 | 0.53 |
| 31:51:95:ARG:HB3 | 31:51:95:ARG:NH1 | 2.24 | 0.53 |
| 33:58:73:THR:HB | 33:58:82:LEU:HD11 | 1.91 | 0.53 |
| 34:68:20:MET:HE3 | 34:68:44:LYS:HE3 | 1.91 | 0.53 |
| 34:68:104:ARG:HD3 | 39:B8:36:GLU:HG2 | 1.90 | 0.53 |
| 41:D8:69:LYS:HB2 | 41:D8:88:ARG:HG2 | 1.90 | 0.53 |
| 7:62:23:VAL:O | 7:62:27:ILE:HG13 | 2.08 | 0.53 |
| 7:62:113:GLU:O | 7:62:119:ARG:HD3 | 2.09 | 0.53 |
| 24:14:453:C:OP1 | 57:14:3549:HOH:O | 2.19 | 0.53 |
| 24:14:957:A:N6 | 24:14:2459:A:C8 | 2.77 | 0.53 |
| 24:14:1204:A:H2 | 24:14:1241:A:N1 | 2.07 | 0.53 |
| 24:14:1540:G:H2' | 24:14:1541:U:O4' | 2.09 | 0.53 |
| 24:14:1754:C:H2' | 24:14:1755:A:C8 | 2.43 | 0.53 |
| 24:14:2135:A:H62 | 24:14:2156:G:H21 | 1.56 | 0.53 |
| 24:14:2749:A:N3 | 31:59:59:ARG:NH1 | 2.56 | 0.53 |
| 27:19:43:ARG:HD2 | 27:19:43:ARG:N | 2.23 | 0.53 |
| 28:29:36:ARG:NH1 | 28:29:85:ASN:OD1 | 2.41 | 0.53 |
| 29:39:46:ARG:HG2 | 29:39:46:ARG:HH11 | 1.74 | 0.53 |
| 30:49:104:GLU:OE1 | 50:I5:23:GLU:HG2 | 2.09 | 0.53 |
| 36:45:6:ARG:O | 36:45:7:MET:HG2 | 2.09 | 0.53 |
| 1:13:1346:A:H5" | 9:8E:120:ARG:HH12 | 1.74 | 0.53 |
| 2:1E:112:VAL:HG23 | 2:1E:149:LEU:HD13 | 1.91 | 0.53 |
| 6:5E:82:ARG:HB2 | 6:5E:85:VAL:HG23 | 1.91 | 0.53 |
| 10:1I:48:THR:HG23 | 10:1I:62:HIS:CB | 2.34 | 0.53 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 24:1H:107:C:H2' | 24:1H:108:U:C6 | 2.44 | 0.53 |
| 24:1H:451:C:H5' | 57:1H:3638:HOH:O | 2.09 | 0.53 |
| 24:1H:1139:G:O2' | 24:1H:1143:A:N1 | 2.34 | 0.53 |
| 24:1H:1484:G:H2' | 24:1H:1485:G:H8 | 1.74 | 0.53 |
| 24:1H:2518:A:H5' | 24:1H:2518:A:H8 | 1.73 | 0.53 |
| 24:1H:2774:C:H2' | 24:1H:2775:A:O4' | 2.09 | 0.53 |
| 27:11:25:THR:HG21 | 27:11:81:ALA:HA | 1.90 | 0.53 |
| 32:61:131:LYS:HB3 | 32:61:132:PRO:HA | 1.91 | 0.53 |
| 35:78:15:ARG:HA | 35:78:16:ARG:HB2 | 1.91 | 0.53 |
| 37:98:22:ARG:O | 37:98:26:LYS:HG3 | 2.07 | 0.53 |
| 52:O8:15:GLU:HG3 | 52:O8:16:CYS:H | 1.73 | 0.53 |
| 1:1G:186(D):C:H2' | 1:1G:186(E):C:C6 | 2.43 | 0.53 |
| 1:1G:1400:C:N4 | 22:2L:35:QUO:H1' | 2.24 | 0.53 |
| 4:32:5:ILE:O | 4:32:5:ILE:HG22 | 2.09 | 0.53 |
| 24:14:589:C:H2' | 24:14:590:A:C8 | 2.43 | 0.53 |
| 24:14:676:A:H8 | 24:14:2069:G:N2 | 1.92 | 0.53 |
| 24:14:863:A:H2 | 24:14:914:C:H41 | 1.56 | 0.53 |
| 24:14:868:U:N3 | 24:14:869:G:N7 | 2.57 | 0.53 |
| 24:14:1386:C:H2' | 24:14:1387:C:C6 | 2.42 | 0.53 |
| 24:14:1470:G:H5" | 24:14:1471:A:OP1 | 2.09 | 0.53 |
| 24:14:2109:U:H3 | 24:14:2180:U:H3 | 1.57 | 0.53 |
| 24:14:2320:A:H1' | 24:14:2321:G:C6 | 2.43 | 0.53 |
| 25:1J:12:C:O2 | 46:E5:74:ARG:NH1 | 2.41 | 0.53 |
| 27:19:11:PRO:C | 27:19:13:ARG:H | 2.16 | 0.53 |
| 28:29:102:VAL:HB | 28:29:199:ARG:O | 2.08 | 0.53 |
| 1:13:1510:U:H2' | 1:13:1511:G:C8 | 2.44 | 0.53 |
| 2:1E:91:PRO:HB3 | 2:1E:154:LEU:HB2 | 1.91 | 0.53 |
| 14:5I:4:LYS:HD2 | 14:5I:7:ILE:HD11 | 1.89 | 0.53 |
| 24:1H:456:C:C2' | 43:F8:68:ARG:HH22 | 2.22 | 0.53 |
| 24:1H:2131:G:N2 | 24:1H:2158:A:H5" | 2.24 | 0.53 |
| 24:1H:2263:C:H2' | 24:1H:2264:C:C6 | 2.44 | 0.53 |
| 24:1H:2629:A:OP1 | 24:1H:2629:A:H4' | 2.08 | 0.53 |
| 34:68:25:LEU:HD12 | 34:68:38:VAL:HG13 | 1.90 | 0.53 |
| 36:88:30:GLY:CA | 36:88:107:ALA:HB2 | 2.39 | 0.53 |
| 1:1G:1096:C:H2' | 1:1G:1097:C:H6 | 1.73 | 0.53 |
| 1:1G:1142:G:H3' | 1:1G:1143:G:H8 | 1.74 | 0.53 |
| 2:12:126:GLU:O | 2:12:130:ARG:HG3 | 2.09 | 0.53 |
| 5:42:100:VAL:O | 5:42:107:ARG:NH2 | 2.38 | 0.53 |
| 24:14:429:A:H2' | 24:14:430:G:C8 | 2.44 | 0.53 |
| 24:14:2638:G:H1' | 24:14:2778:A:H61 | 1.74 | 0.53 |
| 24:14:2698:U:H2' | 24:14:2699:C:C6 | 2.44 | 0.53 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 35:35:105:LEU:O | 35:35:106:LEU:HB3 | 2.08 | 0.53 |
| 42:A5:82:LEU:HB2 | 42:A5:98:LYS:HB2 | 1.91 | 0.53 |
| 49:H5:28:LEU:HA | 49:H5:33:GLN:OE1 | 2.09 | 0.53 |
| 1:13:79:G:N2 | 1:13:89:U:O2 | 2.41 | 0.53 |
| 1:13:651:C:H2' | 1:13:652:U:C6 | 2.44 | 0.53 |
| 1:13:1315:U:H2' | 1:13:1316:G:O4' | 2.08 | 0.53 |
| 6:5E:100:ASN:O | 18:9I:28:GLU:HB2 | 2.08 | 0.53 |
| 12:3I:53:ARG:HG3 | 12:3I:53:ARG:HH11 | 1.74 | 0.53 |
| 18:9I:53:ARG:HH21 | 18:9I:59:SER:HA | 1.74 | 0.53 |
| 24:1H:559:G:H22 | 40:C8:49:HIS:CE1 | 2.26 | 0.53 |
| 24:1H:1541:U:H2' | 24:1H:1542:G:O4' | 2.09 | 0.53 |
| 26:71:39:GLU:OE2 | 26:71:216:THR:OG1 | 2.24 | 0.53 |
| 33:58:97:ARG:HA | 33:58:100:GLU:HB2 | 1.90 | 0.53 |
| 35:78:30:THR:HG21 | 35:78:35:HIS:H | 1.73 | 0.53 |
| 36:88:77:LYS:HD2 | 36:88:78:PRO:HD2 | 1.91 | 0.53 |
| 39:B8:5:ALA:HA | 39:B8:8:LYS:HG2 | 1.91 | 0.53 |
| 42:E8:20:VAL:HG22 | 42:E8:47:VAL:HG21 | 1.91 | 0.53 |
| 49:L8:50:VAL:HB | 49:L8:53:LEU:HD12 | 1.91 | 0.53 |
| 1:1G:828:A:H5" | 1:1G:859:A:C2 | 2.44 | 0.53 |
| 1:1G:1058:G:H1 | 1:1G:1199:U:H3 | 1.57 | 0.53 |
| 3:22:159:GLY:HA2 | 3:22:193:TYR:CE1 | 2.44 | 0.53 |
| 24:14:150:C:H2' | 24:14:151:C:C6 | 2.44 | 0.53 |
| 24:14:581:C:H2' | 24:14:582:G:C8 | 2.44 | 0.53 |
| 24:14:815:C:H2' | 24:14:816:C:H6 | 1.74 | 0.53 |
| 24:14:916:G:C2' | 24:14:917:A:H5" | 2.39 | 0.53 |
| 24:14:925:C:H2' | 24:14:926:A:H8 | 1.74 | 0.53 |
| 24:14:1022:G:C6 | 24:14:1140:C:C4 | 2.97 | 0.53 |
| 24:14:1858:G:H8 | 24:14:1858:G:OP2 | 1.91 | 0.53 |
| 24:14:2335:A:C8 | 24:14:2337:G:C5 | 2.97 | 0.53 |
| 34:25:24:VAL:HB | 34:25:33:ALA:HB2 | 1.90 | 0.53 |
| 42:A5:65:LEU:HB3 | 42:A5:68:ARG:HD2 | 1.91 | 0.53 |
| 50:I5:14:ILE:HG22 | 50:I5:20:ASN:HB3 | 1.91 | 0.53 |
| 1:13:108:G:P | 1:13:326:G:H22 | 2.32 | 0.52 |
| 2:1E:118:LEU:HB3 | 2:1E:142:LEU:HD12 | 1.91 | 0.52 |
| 3:2E:43:LEU:O | 3:2E:47:LEU:HB2 | 2.09 | 0.52 |
| 4:3E:59:ARG:HH22 | 4:3E:66:ARG:HH12 | 1.57 | 0.52 |
| 9:8E:89:ASN:O | 9:8E:92:TYR:HB2 | 2.08 | 0.52 |
| 24:1H:18:C:O3' | 40:C8:23:GLY:HA2 | 2.08 | 0.52 |
| 24:1H:250:G:OP2 | 54:Q8:13:ARG:NH2 | 2.42 | 0.52 |
| 24:1H:850:C:O3' | 49:L8:49:LYS:HE2 | 2.08 | 0.52 |
| 24:1H:1379:A:H4' | 24:1H:1380:G:OP2 | 2.08 | 0.52 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 24:1H:1486:A:H2' | 24:1H:1487:G:H8 | 1.74 | 0.52 |
| 24:1H:2153:G:H2' | 24:1H:2154:G:O4' | 2.09 | 0.52 |
| 24:1H:2286:A:H4' | 24:1H:2287:A:O4' | 2.09 | 0.52 |
| 24:1H:2348:U:H4' | 52:O8:42:TRP:NE1 | 2.23 | 0.52 |
| 24:1H:2549:G:H5" | 24:1H:2549:G:H8 | 1.74 | 0.52 |
| 24:1H:2698:U:H2' | 24:1H:2699:C:C6 | 2.43 | 0.52 |
| 27:11:171:ASP:OD1 | 27:11:171:ASP:N | 2.37 | 0.52 |
| 29:31:185:ASP:HA | 29:31:188:ARG:NH1 | 2.23 | 0.52 |
| 35:78:134:ALA:O | 35:78:138:LEU:HB2 | 2.09 | 0.52 |
| 45:H8:108:PRO:HD2 | 45:H8:113:ALA:H | 1.74 | 0.52 |
| 52:O8:37:ARG:HG2 | 52:O8:38:LYS:H | 1.73 | 0.52 |
| 1:1G:1147:C:H4' | 1:1G:1147:C:OP1 | 2.09 | 0.52 |
| 19:AA:48:THR:HA | 19:AA:61:TYR:HA | 1.91 | 0.52 |
| 22:3L:85:A:H61 | 24:14:2422:A:H5" | 1.74 | 0.52 |
| 24:14:958:U:OP2 | 36:45:14:ARG:HD3 | 2.09 | 0.52 |
| 24:14:1785:A:H4' | 24:14:1982:C:O2' | 2.09 | 0.52 |
| 26:79:214:VAL:HG23 | 26:79:224:ILE:HG12 | 1.92 | 0.52 |
| 30:49:141:PHE:HD1 | 30:49:142:PRO:HD2 | 1.74 | 0.52 |
| 39:75:27:THR:HG23 | 39:75:90:GLN:HB3 | 1.90 | 0.52 |
| 41:95:21:ARG:CG | 41:95:91:TYR:CE1 | 2.92 | 0.52 |
| 49:H5:40:THR:HG23 | 49:H5:43:ILE:HG12 | 1.91 | 0.52 |
| 1:13:371:G:O2' | 1:13:373:A:N7 | 2.42 | 0.52 |
| 1:13:974:A:OP2 | 14:5I:29:ARG:NH2 | 2.42 | 0.52 |
| 1:13:1422:G:O3' | 34:68:49:ARG:NH1 | 2.42 | 0.52 |
| 22:2K:19:C:C3' | 22:2K:20:C:H2' | 2.39 | 0.52 |
| 24:1H:125:G:H5' | 24:1H:125:G:C8 | 2.44 | 0.52 |
| 24:1H:1503:U:H2' | 24:1H:1504:C:H6 | 1.73 | 0.52 |
| 24:1H:1952:A:C6 | 34:68:22:ILE:HD12 | 2.45 | 0.52 |
| 24:1H:1983:C:O2' | 24:1H:1984:G:H5' | 2.09 | 0.52 |
| 24:1H:2243:U:H2' | 24:1H:2244:U:C6 | 2.44 | 0.52 |
| 24:1H:2270:G:H2' | 24:1H:2271:G:O4' | 2.09 | 0.52 |
| 24:1H:2292:C:P | 38:A8:17:ARG:HH22 | 2.32 | 0.52 |
| 24:1H:2564:A:C2 | 24:1H:2647:U:H4' | 2.43 | 0.52 |
| 27:11:69:ARG:HD3 | 27:11:105:ILE:HD11 | 1.90 | 0.52 |
| 27:11:97:TYR:CE1 | 27:11:103:ARG:HG3 | 2.45 | 0.52 |
| 30:41:112:PRO:HB3 | 50:M8:37:SER:N | 2.23 | 0.52 |
| 44:G8:68:HIS:ND1 | 44:G8:70:SER:HB3 | 2.24 | 0.52 |
| 1:1G:57:G:H2' | 1:1G:58:C:H6 | 1.74 | 0.52 |
| 14:5A:8:GLU:OE2 | 14:5A:11:LYS:NZ | 2.34 | 0.52 |
| 24:14:1678:G:N2 | 24:14:1989:G:N2 | 2.57 | 0.52 |
| 24:14:1889:A:N1 | 24:14:2234:G:H1' | 2.25 | 0.52 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 29:39:66:PRO:O | 29:39:68:LYS:N | 2.42 | 0.52 |
| 29:39:143:ALA:O | 29:39:148:LEU:N | 2.30 | 0.52 |
| 37:55:57:ARG:NE | 37:55:59:ASP:OD1 | 2.37 | 0.52 |
| 38:65:24:LEU:HD12 | 38:65:41:ASP:HB2 | 1.91 | 0.52 |
| 41:95:21:ARG:NH2 | 41:95:91:TYR:CG | 2.77 | 0.52 |
| 42:A5:87:PRO:HA | 42:A5:93:ALA:HA | 1.90 | 0.52 |
| 43:B5:39:ILE:HD13 | 43:B5:79:ALA:HB2 | 1.92 | 0.52 |
| 45:D5:163:LEU:HD23 | 45:D5:163:LEU:H | 1.73 | 0.52 |
| 1:13:6:G:O2' | 1:13:7:G:O5' | 2.26 | 0.52 |
| 1:13:510:A:P | 57:13:1809:HOH:O | 2.67 | 0.52 |
| 1:13:703:G:H4' | 1:13:704:A:O5' | 2.10 | 0.52 |
| 24:1H:270:A:H1' | 24:1H:370:G:C2 | 2.45 | 0.52 |
| 24:1H:944:G:H5" | 24:1H:945:A:H5' | 1.92 | 0.52 |
| 24:1H:1316:U:H2' | 24:1H:1317:A:C8 | 2.44 | 0.52 |
| 24:1H:2053:G:OP1 | 57:1H:3698:HOH:O | 2.19 | 0.52 |
| 24:1H:2306:C:H3' | 24:1H:2307:G:H5' | 1.92 | 0.52 |
| 24:1H:2472:G:N2 | 24:1H:2477:C:O2' | 2.42 | 0.52 |
| 25:16:112:G:H2' | 25:16:113:C:C6 | 2.45 | 0.52 |
| 30:41:67:LYS:H | 50:M8:6:HIS:CE1 | 2.28 | 0.52 |
| 30:41:113:ARG:HD2 | 50:M8:33:VAL:HG13 | 1.91 | 0.52 |
| 35:78:120:ALA:HB1 | 35:78:138:LEU:HD23 | 1.92 | 0.52 |
| 37:98:12:ARG:HG2 | 37:98:16:HIS:CG | 2.45 | 0.52 |
| 1:1G:974:A:P | 14:5A:41:ARG:HH22 | 2.32 | 0.52 |
| 4:32:30:LYS:HB2 | 4:32:35:ARG:HB2 | 1.91 | 0.52 |
| 24:14:1915:U:H2' | 24:14:1916:A:O4' | 2.09 | 0.52 |
| 24:14:2272:U:H5" | 24:14:2273:A:OP1 | 2.08 | 0.52 |
| 24:14:2741:A:H2' | 24:14:2742:C:O4' | 2.09 | 0.52 |
| 28:29:37:ARG:O | 28:29:45:THR:HA | 2.09 | 0.52 |
| 39:75:106:SER:HA | 39:75:110:ILE:CD1 | 2.39 | 0.52 |
| 1:13:22:G:C6 | 1:13:23:C:C4 | 2.97 | 0.52 |
| 1:13:963:G:H5' | 57:13:1815:HOH:O | 2.09 | 0.52 |
| 1:13:1352:C:H2' | 1:13:1353:G:C8 | 2.44 | 0.52 |
| 5:4E:72:GLN:HE22 | 5:4E:144:THR:HG23 | 1.74 | 0.52 |
| 16:7I:4:ILE:HA | 16:7I:20:VAL:O | 2.08 | 0.52 |
| 24:1H:551:G:OP1 | 41:D8:68:LYS:NZ | 2.41 | 0.52 |
| 24:1H:587:C:N3 | 35:78:33:ARG:NH1 | 2.58 | 0.52 |
| 24:1H:654(G):C:H2' | 24:1H:654(H):G:H8 | 1.73 | 0.52 |
| 24:1H:1751:C:H2' | 24:1H:1752:C:C6 | 2.44 | 0.52 |
| 24:1H:2331:G:O3' | 46:I8:43:THR:HG22 | 2.09 | 0.52 |
| 24:1H:2850:A:H2' | 24:1H:2851:A:C8 | 2.44 | 0.52 |
| 28:21:119:ARG:HB3 | 28:21:120:TRP:CD1 | 2.45 | 0.52 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 29:31:185:ASP:HA | 29:31:188:ARG:HH12 | 1.73 | 0.52 |
| 30:41:49:ASP:OD2 | 30:41:51:ARG:NH2 | 2.40 | 0.52 |
| 32:61:57:ARG:HA | 32:61:60:GLU:HB2 | 1.90 | 0.52 |
| 37:98:15:SER:HB3 | 57:98:301:HOH:O | 2.09 | 0.52 |
| 45:H8:75:ASN:HB2 | 45:H8:85:HIS:HB3 | 1.90 | 0.52 |
| 47:J8:2:SER:O | 47:J8:2:SER:OG | 2.23 | 0.52 |
| 1:1G:1326:C:H2' | 1:1G:1327:C:C6 | 2.44 | 0.52 |
| 4:32:177:ASP:HB3 | 4:32:182:LYS:HG3 | 1.92 | 0.52 |
| 6:52:89:MET:HG2 | 6:52:91:VAL:HG23 | 1.92 | 0.52 |
| 9:82:97:LYS:HG3 | 9:82:98:PRO:CD | 2.39 | 0.52 |
| 24:14:639:U:H2' | 24:14:640:C:C6 | 2.45 | 0.52 |
| 24:14:795:C:H2' | 24:14:796:C:H6 | 1.75 | 0.52 |
| 24:14:1641:A:H5" | 24:14:1642:G:OP2 | 2.09 | 0.52 |
| 24:14:2823:A:OP1 | 28:29:159:HIS:NE2 | 2.32 | 0.52 |
| 42:A5:59:VAL:HG12 | 42:A5:60:ASN:ND2 | 2.23 | 0.52 |
| 45:D5:30:ASN:N | 45:D5:33:LEU:O | 2.40 | 0.52 |
| 53:L5:8:ASN:OD1 | 53:L5:11:LYS:HB2 | 2.10 | 0.52 |
| 1:13:586:C:O2' | 1:13:878:G:H4' | 2.10 | 0.52 |
| 1:13:955:U:H1' | 1:13:1227:A:H61 | 1.75 | 0.52 |
| 1:13:1055:A:H2' | 3:2E:156:ARG:HD2 | 1.91 | 0.52 |
| 1:13:1336:C:H1' | 1:13:1337:G:C2 | 2.45 | 0.52 |
| 1:13:1373:G:O3' | 7:6E:36:LYS:NZ | 2.42 | 0.52 |
| 3:2E:7:PRO:O | 3:2E:11:ARG:HG2 | 2.09 | 0.52 |
| 24:1H:845:G:H21 | 24:1H:933:A:N6 | 2.07 | 0.52 |
| 24:1H:1472:A:H2' | 24:1H:1473:G:O4' | 2.09 | 0.52 |
| 24:1H:1619:G:N7 | 57:1H:3754:HOH:O | 2.34 | 0.52 |
| 24:1H:1935:G:H1' | 24:1H:1964:G:N2 | 2.24 | 0.52 |
| 24:1H:2317:C:H2' | 24:1H:2318:G:O4' | 2.09 | 0.52 |
| 24:1H:2393:A:H2' | 24:1H:2394:C:H6 | 1.74 | 0.52 |
| 28:21:53:PRO:HA | 28:21:74:PRO:HA | 1.91 | 0.52 |
| 1:1G:1028:C:H42 | 1:1G:1033:G:H1 | 1.58 | 0.52 |
| 1:1G:1208:C:H2' | 1:1G:1209:C:H6 | 1.74 | 0.52 |
| 4:32:101:LEU:HD23 | 4:32:121:VAL:CG1 | 2.40 | 0.52 |
| 8:72:123:GLU:HA | 8:72:126:LYS:HB2 | 1.90 | 0.52 |
| 9:82:73:GLN:O | 9:82:76:ALA:HB3 | 2.09 | 0.52 |
| 12:3A:70:ILE:HG12 | 12:3A:100:ILE:HD12 | 1.91 | 0.52 |
| 22:3L:24:G:H2' | 22:3L:25:G:H8 | 1.73 | 0.52 |
| 27:19:181:GLU:HG3 | 27:19:272:ALA:CB | 2.40 | 0.52 |
| 27:19:246:PRO:HB2 | 27:19:255:LYS:HE3 | 1.92 | 0.52 |
| 31:59:6:ARG:O | 31:59:69:ARG:HG2 | 2.10 | 0.52 |
| 38:65:18:ILE:O | 38:65:21:THR:HG22 | 2.10 | 0.52 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 39:75:105:LEU:HB3 | 39:75:110:ILE:HG12 | 1.90 | 0.52 |
| 42:A5:17:VAL:HG23 | 42:A5:76:VAL:HG11 | 1.91 | 0.52 |
| 53:L5:5:TRP:NE1 | 53:L5:7:PRO:HG3 | 2.24 | 0.52 |
| 1:13:300:A:H1' | 1:13:565:U:O2 | 2.09 | 0.52 |
| 1:13:321:A:N6 | 1:13:328:C:H1' | 2.25 | 0.52 |
| 1:13:1123:A:H4' | 10:1I:36:GLY:HA3 | 1.92 | 0.52 |
| 1:13:1317:C:H5" | 1:13:1318:A:OP2 | 2.09 | 0.52 |
| 1:13:1363:A:H1' | 1:13:1365:G:N7 | 2.25 | 0.52 |
| 1:13:1497:G:H2' | 1:13:1498:U:H5' | 1.92 | 0.52 |
| 1:13:1508:G:H2' | 1:13:1509:C:C6 | 2.45 | 0.52 |
| 4:3E:108:LEU:HD13 | 4:3E:174:LEU:HD13 | 1.91 | 0.52 |
| 5:4E:8:GLU:HB2 | 5:4E:34:VAL:HG22 | 1.92 | 0.52 |
| 24:1H:375:C:H2' | 24:1H:376:C:C6 | 2.45 | 0.52 |
| 24:1H:818:G:O2' | 24:1H:838:C:O2' | 2.26 | 0.52 |
| 24:1H:991:C:H2' | 24:1H:992:C:H6 | 1.74 | 0.52 |
| 24:1H:1329:U:H5" | 24:1H:1330:C:C5 | 2.45 | 0.52 |
| 24:1H:1784:A:H4' | 24:1H:1785:A:O5' | 2.10 | 0.52 |
| 24:1H:2403:C:H2' | 24:1H:2404:C:H6 | 1.75 | 0.52 |
| 31:51:83:TYR:CB | 31:51:134:SER:HA | 2.40 | 0.52 |
| 32:61:110:ASP:HB3 | 32:61:113:ARG:H | 1.75 | 0.52 |
| 35:78:115:LEU:HA | 35:78:134:ALA:HB2 | 1.90 | 0.52 |
| 41:D8:79:VAL:HG13 | 41:D8:81:TYR:HB3 | 1.91 | 0.52 |
| 43:F8:72:LYS:HE2 | 43:F8:73:ARG:O | 2.10 | 0.52 |
| 44:G8:17:SER:HA | 44:G8:21:LYS:HB2 | 1.91 | 0.52 |
| 50:M8:14:ILE:HG13 | 50:M8:24:THR:HG22 | 1.91 | 0.52 |
| 50:M8:52:THR:OG1 | 50:M8:53:GLU:N | 2.41 | 0.52 |
| 1:1G:143:A:O3' | 1:1G:144:G:H8 | 1.92 | 0.52 |
| 1:1G:418:C:H42 | 1:1G:425:G:H1 | 1.58 | 0.52 |
| 1:1G:1281:U:H3' | 1:1G:1282:C:H5 | 1.74 | 0.52 |
| 8:72:11:THR:HG22 | 8:72:15:ASN:ND2 | 2.24 | 0.52 |
| 13:4A:15:VAL:HG13 | 13:4A:43:THR:O | 2.09 | 0.52 |
| 22:2L:21:A:C8 | 22:2L:56:U:N3 | 2.74 | 0.52 |
| 24:14:185:U:H4' | 24:14:218:A:H4' | 1.92 | 0.52 |
| 24:14:304:G:H2' | 24:14:305:U:C6 | 2.45 | 0.52 |
| 24:14:621:A:H3' | 24:14:622:G:H8 | 1.74 | 0.52 |
| 24:14:1777:U:O2' | 24:14:1778:U:H5' | 2.08 | 0.52 |
| 28:29:87:GLU:CD | 28:29:87:GLU:H | 2.17 | 0.52 |
| 38:65:105:ALA:C | 38:65:106:ARG:HG3 | 2.34 | 0.52 |
| 1:13:19:C:OP1 | 5:4E:125:SER:OG | 2.18 | 0.52 |
| 1:13:671:G:C2 | 1:13:672:U:C2 | 2.98 | 0.52 |
| 1:13:1032(A):G:H2' | 1:13:1032(B):G:H8 | 1.75 | 0.52 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 1:13:1401:G:C2 | 1:13:1402:C:H1' | 2.45 | 0.52 |
| 24:1H:557:U:H2' | 24:1H:558:G:H8 | 1.75 | 0.52 |
| 24:1H:906:G:OP1 | 36:88:26:TYR:OH | 2.19 | 0.52 |
| 24:1H:919:G:H4' | 25:16:81:G:H4' | 1.91 | 0.52 |
| 24:1H:1263:U:O4' | 51:N8:10:LYS:HD2 | 2.10 | 0.52 |
| 24:1H:2147:G:H2' | 24:1H:2148:G:O4' | 2.09 | 0.52 |
| 24:1H:2244:U:O2' | 24:1H:2245:U:H5' | 2.09 | 0.52 |
| 24:1H:2695:C:H2' | 24:1H:2696:U:C6 | 2.44 | 0.52 |
| 25:16:31:C:H4' | 30:41:29:TRP:CH2 | 2.44 | 0.52 |
| 26:71:6:ARG:NH2 | 26:71:34:THR:OG1 | 2.41 | 0.52 |
| 27:11:148:GLU:HB2 | 27:11:151:LYS:HD2 | 1.92 | 0.52 |
| 32:61:31:LEU:HD21 | 32:61:38:LEU:HG | 1.91 | 0.52 |
| 39:B8:27:THR:HG23 | 39:B8:90:GLN:HB3 | 1.90 | 0.52 |
| 45:H8:76:LEU:HD23 | 45:H8:76:LEU:H | 1.74 | 0.52 |
| 1:1G:857:C:H2' | 1:1G:858:G:O4' | 2.10 | 0.52 |
| 1:1G:1279:A:O2' | 1:1G:1281:U:OP2 | 2.28 | 0.52 |
| 1:1G:1316:G:H4' | 14:5A:18:VAL:HG11 | 1.91 | 0.52 |
| 3:22:134:ILE:HG23 | 3:22:151:VAL:HB | 1.92 | 0.52 |
| 22:2L:73:U:H2' | 22:2L:74:C:C6 | 2.44 | 0.52 |
| 24:14:1050:A:C2 | 24:14:1051:G:H1' | 2.45 | 0.52 |
| 24:14:1110:G:H2' | 24:14:1111:A:H8 | 1.75 | 0.52 |
| 24:14:1257:C:H4' | 29:39:83:PHE:CD1 | 2.45 | 0.52 |
| 24:14:1486:A:H2' | 24:14:1487:G:C8 | 2.44 | 0.52 |
| 24:14:1732:A:H2' | 24:14:1733:G:O4' | 2.09 | 0.52 |
| 24:14:2264:C:N4 | 46:E5:15:ASP:OD2 | 2.42 | 0.52 |
| 29:39:63:LYS:HE2 | 29:39:67:GLN:HB2 | 1.92 | 0.52 |
| 29:39:132:VAL:C | 29:39:134:GLY:H | 2.17 | 0.52 |
| 51:J5:16:ARG:HH11 | 51:J5:16:ARG:CG | 2.22 | 0.52 |
| 1:13:323:U:O3' | 20:BI:22:ARG:HD3 | 2.09 | 0.52 |
| 1:13:419:C:H5' | 1:13:420:U:OP2 | 2.10 | 0.52 |
| 8:7E:4:ASP:CG | 8:7E:85:ARG:HH11 | 2.18 | 0.52 |
| 22:3K:41:C:H2' | 22:3K:42:U:C6 | 2.45 | 0.52 |
| 24:1H:978:G:OP2 | 57:1H:3695:HOH:O | 2.18 | 0.52 |
| 24:1H:1557:C:OP2 | 24:1H:1558:A:O2' | 2.27 | 0.52 |
| 24:1H:1657:C:H2' | 24:1H:1658:C:C6 | 2.44 | 0.52 |
| 24:1H:2018:G:H21 | 40:C8:34:LYS:HZ1 | 1.58 | 0.52 |
| 35:78:52:GLU:OE1 | 35:78:55:ARG:NH1 | 2.35 | 0.52 |
| 42:E8:29:LEU:O | 42:E8:33:ARG:HG3 | 2.09 | 0.52 |
| 46:I8:50:ASN:C | 46:I8:62:LEU:HD12 | 2.35 | 0.52 |
| 53:P8:45:ALA:O | 53:P8:46:VAL:HB | 2.10 | 0.52 |
| 1:1G:992:U:O2' | 1:1G:993:G:OP2 | 2.24 | 0.52 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 1:1G:1060:C:C5 | 3:22:2:GLY:HA3 | 2.45 | 0.52 |
| 1:1G:1279:A:O2' | 1:1G:1282:C:N4 | 2.43 | 0.52 |
| 2:12:71:VAL:HG13 | 2:12:93:VAL:HB | 1.91 | 0.52 |
| 5:42:6:PHE:HB3 | 5:42:34:VAL:HG13 | 1.92 | 0.52 |
| 5:42:101:ILE:HG12 | 5:42:118:ILE:O | 2.09 | 0.52 |
| 6:52:83:ASP:OD1 | 6:52:83:ASP:N | 2.43 | 0.52 |
| 15:6A:63:ARG:NH1 | 15:6A:87:ILE:HD13 | 2.25 | 0.52 |
| 24:14:616:A:C5 | 29:39:180:GLY:HA3 | 2.45 | 0.52 |
| 24:14:996:A:N6 | 24:14:1160:G:C6 | 2.78 | 0.52 |
| 24:14:1110:G:O2' | 24:14:1111:A:O4' | 2.18 | 0.52 |
| 24:14:1861:G:H5' | 26:79:205:LYS:NZ | 2.19 | 0.52 |
| 24:14:2704:C:H2' | 24:14:2705:A:O4' | 2.09 | 0.52 |
| 25:1J:103:U:O2' | 45:D5:72:ARG:HG3 | 2.09 | 0.52 |
| 30:49:39:ILE:HG23 | 30:49:157:ILE:HG12 | 1.92 | 0.52 |
| 41:95:49:THR:O | 41:95:51:VAL:N | 2.43 | 0.52 |
| 45:D5:9:TYR:CZ | 45:D5:35:ARG:HD3 | 2.44 | 0.52 |
| 1:13:502:G:OP1 | 12:3I:118:SER:HB3 | 2.09 | 0.52 |
| 1:13:1271:G:H2' | 1:13:1272:G:H5" | 1.91 | 0.52 |
| 1:13:1443:G:O2' | 39:B8:122:ASP:OD2 | 2.27 | 0.52 |
| 1:13:1497:G:C2' | 1:13:1498:U:H5' | 2.40 | 0.52 |
| 2:1E:83:MET:HG3 | 2:1E:234:PRO:HG2 | 1.91 | 0.52 |
| 14:5I:29:ARG:HH11 | 14:5I:42:ILE:HG12 | 1.74 | 0.52 |
| 22:2K:64:PSU:P | 22:2K:64:PSU:H2' | 2.50 | 0.52 |
| 24:1H:588:U:H1' | 29:31:90:PHE:HB3 | 1.92 | 0.52 |
| 24:1H:1141:U:C2' | 33:58:63:THR:HG21 | 2.40 | 0.52 |
| 24:1H:1171:G:C5 | 24:1H:1174:A:C6 | 2.98 | 0.52 |
| 24:1H:1502:C:O2' | 24:1H:1503:U:H5' | 2.10 | 0.52 |
| 24:1H:2184:G:C6 | 24:1H:2185:C:C4 | 2.98 | 0.52 |
| 24:1H:2598:A:P | 57:1H:3653:HOH:O | 2.67 | 0.52 |
| 36:88:39:PRO:HA | 36:88:97:VAL:O | 2.10 | 0.52 |
| 51:N8:48:GLU:OE1 | 51:N8:48:GLU:N | 2.43 | 0.52 |
| 1:1G:660:G:H2' | 1:1G:661:G:O4' | 2.09 | 0.52 |
| 1:1G:719:C:O2' | 18:9A:49:LYS:HB3 | 2.10 | 0.52 |
| 1:1G:987:G:H5' | 19:AA:55:LYS:NZ | 2.25 | 0.52 |
| 1:1G:1291:G:P | 7:62:37:ASN:HD22 | 2.33 | 0.52 |
| 4:32:67:ILE:HD13 | 4:32:196:LEU:HD22 | 1.92 | 0.52 |
| 17:8A:31:LEU:HD23 | 17:8A:32:TYR:CZ | 2.45 | 0.52 |
| 24:14:328:U:H4' | 44:C5:68:HIS:CE1 | 2.45 | 0.52 |
| 24:14:1012:U:P | 40:85:70:ARG:HH22 | 2.33 | 0.52 |
| 24:14:1794:U:H2' | 24:14:1795:C:C6 | 2.45 | 0.52 |
| 24:14:2328:A:H2' | 24:14:2329:G:O4' | 2.09 | 0.52 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 24:14:2794:C:N4 | 24:14:2795:G:O6 | 2.43 | 0.52 |
| 29:39:63:LYS:HA | 29:39:76:GLY:O | 2.10 | 0.52 |
| 37:55:104:ARG:HD2 | 37:55:109:ALA:HB3 | 1.91 | 0.52 |
| 39:75:91:ARG:O | 39:75:116:ALA:HA | 2.10 | 0.52 |
| 1:13:1195:C:H5" | 1:13:1196:U:H5" | 1.90 | 0.52 |
| 2:1E:61:LEU:HD23 | 2:1E:68:ILE:HD11 | 1.90 | 0.52 |
| 6:5E:21:LEU:O | 6:5E:25:ILE:HG13 | 2.10 | 0.52 |
| 12:3I:93:LEU:HD12 | 12:3I:96:VAL:HG11 | 1.91 | 0.52 |
| 20:BI:14:LYS:O | 20:BI:18:GLN:HG3 | 2.10 | 0.52 |
| 20:BI:89:ARG:HB2 | 20:BI:104:LEU:HD21 | 1.92 | 0.52 |
| 24:1H:1830:C:O2' | 24:1H:1831:G:H5' | 2.08 | 0.52 |
| 24:1H:2579:C:H2' | 24:1H:2580:U:O4' | 2.09 | 0.52 |
| 28:21:111:ARG:HD3 | 28:21:160:TYR:CD2 | 2.45 | 0.52 |
| 31:51:4:ILE:O | 31:51:4:ILE:HG12 | 2.09 | 0.52 |
| 31:51:7:LEU:HD23 | 31:51:65:HIS:CE1 | 2.45 | 0.52 |
| 35:78:49:ARG:HD2 | 54:Q8:59:LYS:HB3 | 1.90 | 0.52 |
| 43:F8:60:ARG:NH2 | 53:P8:47:ARG:HH12 | 2.07 | 0.52 |
| 2:12:12:GLU:OE2 | 2:12:16:HIS:ND1 | 2.43 | 0.52 |
| 2:12:45:GLN:O | 2:12:48:MET:HB3 | 2.09 | 0.52 |
| 17:8A:45:HIS:NE2 | 17:8A:47:PRO:HG3 | 2.24 | 0.52 |
| 24:14:1059:G:H3' | 24:14:1060:U:H2' | 1.92 | 0.52 |
| 24:14:1271:G:O3' | 24:14:1272:A:H4' | 2.09 | 0.52 |
| 24:14:1533:C:H3' | 24:14:1534:G:O4' | 2.09 | 0.52 |
| 24:14:2064:C:H2' | 24:14:2065:C:C6 | 2.45 | 0.52 |
| 24:14:2458:G:H21 | 24:14:2459:A:H61 | 1.56 | 0.52 |
| 27:19:43:ARG:HG2 | 27:19:43:ARG:HH11 | 1.74 | 0.52 |
| 1:13:310:G:H5" | 16:7I:31:LYS:HB2 | 1.90 | 0.51 |
| 1:13:581:G:N2 | 1:13:582:U:C4 | 2.78 | 0.51 |
| 1:13:707:C:H2' | 1:13:708:C:H6 | 1.74 | 0.51 |
| 1:13:742:G:P | 15:6I:35:ARG:HH22 | 2.33 | 0.51 |
| 1:13:801:U:H2' | 1:13:802:A:C8 | 2.45 | 0.51 |
| 1:13:1071:C:H2' | 1:13:1072:G:H8 | 1.75 | 0.51 |
| 1:13:1127:G:N2 | 1:13:1145:C:H1' | 2.25 | 0.51 |
| 2:1E:42:ILE:HD13 | 2:1E:202:PRO:HB2 | 1.92 | 0.51 |
| 20:BI:29:LYS:O | 20:BI:33:ILE:HG12 | 2.10 | 0.51 |
| 22:3K:21:A:H1' | 22:3K:22:A:H5" | 1.91 | 0.51 |
| 24:1H:62:C:H42 | 24:1H:92:G:H1 | 1.56 | 0.51 |
| 24:1H:444:C:H4' | 29:31:49:ALA:HB2 | 1.91 | 0.51 |
| 24:1H:456:C:H3' | 43:F8:68:ARG:HH22 | 1.75 | 0.51 |
| 24:1H:654(K):C:H3' | 24:1H:654(L):G:H5" | 1.92 | 0.51 |
| 24:1H:800:A:OP1 | 24:1H:800:A:H8 | 1.93 | 0.51 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 24:1H:2294:C:OP1 | 38:A8:89:ARG:NH2 | 2.42 | 0.51 |
| 24:1H:2864:G:OP1 | 39:B8:119:LYS:HD2 | 2.09 | 0.51 |
| 28:21:75:VAL:C | 28:21:76:ARG:HD2 | 2.36 | 0.51 |
| 39:B8:26:ASP:O | 39:B8:49:VAL:HG22 | 2.09 | 0.51 |
| 45:H8:56:VAL:HA | 45:H8:70:LEU:HD23 | 1.91 | 0.51 |
| 54:Q8:22:VAL:HG13 | 54:Q8:50:LEU:HB2 | 1.90 | 0.51 |
| 1:1G:396:G:O2' | 1:1G:398:C:OP1 | 2.15 | 0.51 |
| 1:1G:1092:A:H5" | 7:62:4:ARG:NH2 | 2.25 | 0.51 |
| 1:1G:1342:C:H5" | 9:82:125:TYR:HB3 | 1.92 | 0.51 |
| 24:14:1019:U:O2' | 24:14:1021:A:H2 | 1.92 | 0.51 |
| 24:14:1043:C:H42 | 24:14:1112:G:H1 | 1.58 | 0.51 |
| 24:14:1406:U:H2' | 24:14:1407:C:C6 | 2.44 | 0.51 |
| 24:14:2050:C:H1' | 28:29:156:MET:CE | 2.39 | 0.51 |
| 24:14:2505:G:O6 | 24:14:2576:G:H2' | 2.10 | 0.51 |
| 27:19:75:ILE:HG21 | 27:19:99:ASP:OD2 | 2.10 | 0.51 |
| 30:49:107:LEU:HA | 30:49:111:LEU:HD12 | 1.91 | 0.51 |
| 38:65:78:LEU:HD11 | 38:65:107:GLU:HG2 | 1.91 | 0.51 |
| 39:75:21:GLU:N | 39:75:21:GLU:OE2 | 2.43 | 0.51 |
| 42:A5:88:ARG:H | 42:A5:93:ALA:H | 1.58 | 0.51 |
| 53:L5:10:ARG:O | 53:L5:14:LYS:HG2 | 2.10 | 0.51 |
| 1:13:272:C:H2' | 1:13:273:A:C8 | 2.45 | 0.51 |
| 1:13:612:C:O2 | 1:13:629:G:N2 | 2.44 | 0.51 |
| 1:13:636:U:H2' | 1:13:637:G:C8 | 2.45 | 0.51 |
| 1:13:865:A:C2 | 1:13:918:A:H4' | 2.45 | 0.51 |
| 1:13:1178:G:N2 | 1:13:1181:G:C8 | 2.73 | 0.51 |
| 1:13:1276:G:N3 | 1:13:1282:C:O2' | 2.37 | 0.51 |
| 4:3E:79:PHE:HE2 | 4:3E:204:ILE:HD12 | 1.75 | 0.51 |
| 21:1F:9:ARG:NH1 | 21:1F:22:ARG:HG3 | 2.25 | 0.51 |
| 24:1H:380:U:H5' | 47:J8:18:ILE:HD12 | 1.92 | 0.51 |
| 24:1H:950:G:H2' | 24:1H:951:C:C6 | 2.45 | 0.51 |
| 24:1H:969:U:OP2 | 49:L8:17:LYS:NZ | 2.44 | 0.51 |
| 24:1H:1914:C:H2' | 24:1H:1915:U:H6 | 1.74 | 0.51 |
| 24:1H:2400:G:H3' | 24:1H:2401:U:C6 | 2.45 | 0.51 |
| 24:1H:2766:G:H5" | 24:1H:2767:C:OP2 | 2.09 | 0.51 |
| 25:16:14:U:H5' | 25:16:70:C:O2 | 2.10 | 0.51 |
| 31:51:6:ARG:HA | 31:51:66:GLY:HA2 | 1.91 | 0.51 |
| 31:51:95:ARG:HB3 | 31:51:95:ARG:HH11 | 1.75 | 0.51 |
| 33:58:55:VAL:HB | 33:58:126:PRO:HA | 1.93 | 0.51 |
| 36:88:20:ALA:HB1 | 36:88:99:PRO:HD2 | 1.92 | 0.51 |
| 44:G8:94:LYS:HA | 44:G8:94:LYS:NZ | 2.21 | 0.51 |
| 46:I8:23:VAL:HA | 46:I8:38:VAL:HG22 | 1.92 | 0.51 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 51:N8:33:CYS:HB2 | 51:N8:38:ALA:O | 2.09 | 0.51 |
| 1:1G:1118:C:H5' | 9:82:104:ARG:HG2 | 1.93 | 0.51 |
| 1:1G:1162:C:N4 | 1:1G:1174:G:H1 | 2.08 | 0.51 |
| 4:32:14:ARG:HB2 | 4:32:40:PRO:HD2 | 1.93 | 0.51 |
| 24:14:180:G:OP2 | 53:L5:32:LYS:HE2 | 2.10 | 0.51 |
| 24:14:249:C:OP1 | 57:14:3571:HOH:O | 2.19 | 0.51 |
| 24:14:676:A:H2 | 24:14:802:A:H61 | 1.58 | 0.51 |
| 24:14:857:C:H4' | 46:E5:23:VAL:HG21 | 1.93 | 0.51 |
| 24:14:1465:G:H5' | 24:14:1528:A:O2' | 2.09 | 0.51 |
| 24:14:2534:A:N7 | 57:14:3625:HOH:O | 2.34 | 0.51 |
| 26:79:202:GLU:CD | 26:79:202:GLU:H | 2.19 | 0.51 |
| 30:49:47:LYS:HG2 | 30:49:48:GLU:HG3 | 1.92 | 0.51 |
| 36:45:21:THR:C | 36:45:23:GLY:N | 2.66 | 0.51 |
| 45:D5:1:MET:HG3 | 45:D5:2:GLU:N | 2.25 | 0.51 |
| 46:E5:49:LYS:HB3 | 46:E5:80:HIS:HB3 | 1.92 | 0.51 |
| 1:13:940:C:H2' | 1:13:941:G:H8 | 1.75 | 0.51 |
| 1:13:1023:G:H3' | 1:13:1024:G:C5' | 2.41 | 0.51 |
| 1:13:1240:U:H5" | 1:13:1241:G:C8 | 2.45 | 0.51 |
| 1:13:1317:C:O2 | 19:AI:37:ARG:NH2 | 2.41 | 0.51 |
| 7:6E:80:VAL:HB | 7:6E:85:TYR:HE2 | 1.75 | 0.51 |
| 24:1H:192:C:OP2 | 57:1H:3697:HOH:O | 2.19 | 0.51 |
| 24:1H:1408:C:C2 | 24:1H:1595:G:N2 | 2.79 | 0.51 |
| 24:1H:1435:G:H1 | 24:1H:1557:C:H42 | 1.58 | 0.51 |
| 24:1H:2400:G:N2 | 24:1H:2417:C:C2 | 2.78 | 0.51 |
| 24:1H:2661:G:H2' | 24:1H:2662:A:C8 | 2.45 | 0.51 |
| 31:51:83:TYR:HB3 | 31:51:134:SER:HA | 1.92 | 0.51 |
| 37:98:86:ARG:HG2 | 37:98:118:GLU:OE1 | 2.10 | 0.51 |
| 42:E8:84:ARG:HB2 | 42:E8:96:ILE:CD1 | 2.41 | 0.51 |
| 43:F8:63:LYS:O | 43:F8:64:LYS:HG2 | 2.09 | 0.51 |
| 44:G8:81:LYS:HB3 | 44:G8:82:PRO:CA | 2.40 | 0.51 |
| 1:1G:168:G:C2' | 1:1G:169:C:H5" | 2.40 | 0.51 |
| 1:1G:186(B):C:O4' | 20:BA:89:ARG:NH2 | 2.43 | 0.51 |
| 1:1G:1060:C:N4 | 3:22:2:GLY:HA3 | 2.26 | 0.51 |
| 1:1G:1176:A:H2' | 1:1G:1177:G:O4' | 2.10 | 0.51 |
| 2:12:69:LEU:HD11 | 2:12:152:PHE:CE1 | 2.45 | 0.51 |
| 24:14:528:A:C2 | 24:14:2042:A:H2' | 2.45 | 0.51 |
| 24:14:908:C:C2' | 24:14:909:A:H5' | 2.40 | 0.51 |
| 26:79:10:LEU:HB3 | 26:79:220:PRO:HG3 | 1.92 | 0.51 |
| 27:19:255:LYS:H | 27:19:255:LYS:HZ1 | 1.56 | 0.51 |
| 30:49:41:GLN:NE2 | 30:49:154:GLY:O | 2.43 | 0.51 |
| 30:49:121:ASN:HA | 30:49:181:ARG:HH12 | 1.76 | 0.51 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 40:85:99:ALA:HB2 | 40:85:106:PHE:CD1 | 2.46 | 0.51 |
| 1:13:1101:A:H61 | 2:1E:103:THR:HG21 | 1.74 | 0.51 |
| 1:13:1502:A:H2 | 1:13:1505:G:N1 | 1.93 | 0.51 |
| 3:2E:79:ARG:NH1 | 18:9A:87:ARG:HH12 | 2.09 | 0.51 |
| 4:3E:179:GLU:CD | 4:3E:179:GLU:H | 2.19 | 0.51 |
| 5:4E:64:ARG:N | 5:4E:64:ARG:HH11 | 2.07 | 0.51 |
| 7:6E:107:ALA:O | 7:6E:110:GLN:HB2 | 2.10 | 0.51 |
| 8:7E:49:GLU:O | 8:7E:51:VAL:HG13 | 2.09 | 0.51 |
| 17:8I:48:GLU:O | 17:8I:50:LYS:HG2 | 2.10 | 0.51 |
| 24:1H:723:G:H2' | 24:1H:724:U:O4' | 2.10 | 0.51 |
| 24:1H:1058:U:H2' | 24:1H:1059:G:H8 | 1.75 | 0.51 |
| 24:1H:1065:U:H3 | 24:1H:1069:A:H3' | 1.75 | 0.51 |
| 24:1H:1292:U:H2' | 24:1H:1293:C:C6 | 2.45 | 0.51 |
| 24:1H:2271:G:H5' | 46:I8:20:ARG:HD3 | 1.91 | 0.51 |
| 24:1H:2848:G:C8 | 39:B8:97:ALA:HB2 | 2.45 | 0.51 |
| 38:A8:111:GLU:HG3 | 38:A8:112:PHE:CD2 | 2.46 | 0.51 |
| 54:Q8:61:LEU:C | 54:Q8:62:LEU:HG | 2.33 | 0.51 |
| 1:1G:422:C:O2' | 1:1G:423:G:N2 | 2.43 | 0.51 |
| 1:1G:758:G:H5' | 1:1G:880:C:H1' | 1.92 | 0.51 |
| 3:22:130:VAL:O | 3:22:134:ILE:HG12 | 2.10 | 0.51 |
| 16:7A:70:ALA:O | 16:7A:74:LEU:HB2 | 2.09 | 0.51 |
| 22:2L:10:C:H41 | 22:2L:26:G:H1 | 1.58 | 0.51 |
| 24:14:350:U:H2' | 24:14:351:G:O4' | 2.11 | 0.51 |
| 24:14:883:G:N2 | 24:14:893:C:N3 | 2.56 | 0.51 |
| 24:14:924:C:H2' | 24:14:925:C:C6 | 2.45 | 0.51 |
| 24:14:2212:A:O2' | 24:14:2213:U:O5' | 2.27 | 0.51 |
| 27:19:215:LEU:HB2 | 27:19:217:ARG:HG3 | 1.91 | 0.51 |
| 28:29:69:LYS:HG3 | 28:29:70:ALA:H | 1.76 | 0.51 |
| 28:29:137:HIS:HB3 | 28:29:138:PRO:HD2 | 1.93 | 0.51 |
| 36:45:30:GLY:H | 36:45:105:GLU:HG3 | 1.76 | 0.51 |
| 45:D5:118:GLN:NE2 | 45:D5:118:GLN:H | 2.08 | 0.51 |
| 1:13:881:G:H2' | 1:13:882:C:O4' | 2.09 | 0.51 |
| 1:13:940:C:H2' | 1:13:941:G:C8 | 2.45 | 0.51 |
| 1:13:1370:G:O6 | 9:8E:118:LYS:NZ | 2.43 | 0.51 |
| 24:1H:150:C:H2' | 24:1H:151:C:C6 | 2.45 | 0.51 |
| 24:1H:593:G:H4' | 54:Q8:62:LEU:HD22 | 1.92 | 0.51 |
| 24:1H:692:C:O2' | 27:11:38:LYS:HE3 | 2.11 | 0.51 |
| 24:1H:725:G:C6 | 24:1H:726:G:N1 | 2.79 | 0.51 |
| 24:1H:886:C:H3' | 24:1H:887:A:H4' | 1.92 | 0.51 |
| 24:1H:1778:U:P | 57:1H:3863:HOH:O | 2.68 | 0.51 |
| 24:1H:2164:C:OP2 | 24:1H:2166:G:N2 | 2.43 | 0.51 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 24:1H:2166:G:O6 | 24:1H:2168:G:N1 | 2.43 | 0.51 |
| 30:41:64:THR:HG23 | 30:41:94:LEU:HD21 | 1.93 | 0.51 |
| 31:51:102:ALA:HA | 31:51:117:PRO:HD3 | 1.93 | 0.51 |
| 32:61:110:ASP:N | 32:61:130:TYR:OH | 2.44 | 0.51 |
| 33:58:96:GLU:CG | 33:58:97:ARG:H | 2.15 | 0.51 |
| 36:88:66:ILE:O | 36:88:67:ARG:HB2 | 2.11 | 0.51 |
| 53:P8:8:ASN:OD1 | 53:P8:8:ASN:C | 2.53 | 0.51 |
| 1:1G:67:C:H2' | 1:1G:68:G:C8 | 2.45 | 0.51 |
| 1:1G:685:G:C2 | 1:1G:686:U:C4 | 2.99 | 0.51 |
| 1:1G:975:A:H4' | 1:1G:976:G:C5' | 2.39 | 0.51 |
| 1:1G:1037:C:H2' | 1:1G:1038:C:C6 | 2.46 | 0.51 |
| 1:1G:1478:C:H2' | 1:1G:1479:C:H6 | 1.75 | 0.51 |
| 1:1G:1493:A:H3' | 1:1G:1494:G:H5' | 1.93 | 0.51 |
| 8:72:1:MET:SD | 8:72:1:MET:N | 2.77 | 0.51 |
| 24:14:78:A:H2' | 24:14:79:G:C8 | 2.44 | 0.51 |
| 24:14:673:C:H4' | 29:39:82:ILE:HG12 | 1.93 | 0.51 |
| 24:14:1314:C:H6 | 24:14:1314:C:H5' | 1.74 | 0.51 |
| 24:14:1416:G:HO2' | 24:14:1417:C:P | 2.30 | 0.51 |
| 24:14:1676:A:P | 57:14:3614:HOH:O | 2.68 | 0.51 |
| 24:14:2293:C:O3' | 38:65:89:ARG:NH2 | 2.44 | 0.51 |
| 27:19:40:THR:OG1 | 27:19:41:GLY:N | 2.43 | 0.51 |
| 36:45:66:ILE:O | 36:45:67:ARG:HB2 | 2.10 | 0.51 |
| 39:75:77:PRO:HB2 | 39:75:80:SER:HB2 | 1.93 | 0.51 |
| 41:95:69:LYS:HD2 | 41:95:86:GLY:HA3 | 1.92 | 0.51 |
| 43:B5:30:VAL:HG21 | 43:B5:39:ILE:HD11 | 1.91 | 0.51 |
| 47:F5:18:ILE:HG12 | 47:F5:37:ILE:HD12 | 1.93 | 0.51 |
| 1:13:674:G:H21 | 11:2I:116:HIS:HB2 | 1.74 | 0.51 |
| 1:13:908:A:H2' | 1:13:909:A:H8 | 1.75 | 0.51 |
| 3:2E:123:GLN:O | 3:2E:128:PHE:HB2 | 2.11 | 0.51 |
| 5:4E:31:LEU:HG | 5:4E:45:PHE:HB2 | 1.93 | 0.51 |
| 7:6E:122:HIS:O | 7:6E:125:MET:N | 2.43 | 0.51 |
| 12:3I:53:ARG:HB3 | 12:3I:69:TYR:HE1 | 1.76 | 0.51 |
| 20:BI:54:LYS:O | 20:BI:57:ARG:HB2 | 2.10 | 0.51 |
| 22:2K:7:G:H8 | 22:2K:7:G:OP2 | 1.92 | 0.51 |
| 24:1H:462:C:H42 | 24:1H:467:G:H1 | 1.59 | 0.51 |
| 24:1H:1032:A:H2 | 24:1H:1122:G:H22 | 1.59 | 0.51 |
| 24:1H:1786:A:C2 | 24:1H:2606:C:H1' | 2.46 | 0.51 |
| 24:1H:2706:G:H5" | 24:1H:2851:A:H5' | 1.91 | 0.51 |
| 27:11:133:LEU:HA | 27:11:136:ILE:HG13 | 1.92 | 0.51 |
| 28:21:2:LYS:HA | 28:21:84:PHE:CD1 | 2.46 | 0.51 |
| 32:61:29:TYR:C | 32:61:32:PRO:HD2 | 2.36 | 0.51 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 41:D8:58:VAL:O | 41:D8:97:LYS:HB2 | 2.11 | 0.51 |
| 1:1G:142:G:H2' | 1:1G:143:A:C8 | 2.44 | 0.51 |
| 1:1G:1181:G:HO2' | 1:1G:1182:G:P | 2.33 | 0.51 |
| 3:22:44:GLU:HA | 3:22:52:LEU:HD11 | 1.93 | 0.51 |
| 13:4A:97:PRO:N | 13:4A:110:ARG:HG2 | 2.26 | 0.51 |
| 22:2L:42:U:H2' | 22:2L:43:G:H8 | 1.75 | 0.51 |
| 24:14:579:G:H2' | 24:14:580:C:C6 | 2.44 | 0.51 |
| 24:14:863:A:H2 | 24:14:914:C:N4 | 2.08 | 0.51 |
| 24:14:1022:G:N2 | 24:14:1142(A):A:C2 | 2.73 | 0.51 |
| 24:14:1799:G:O6 | 27:19:179:SER:HB3 | 2.11 | 0.51 |
| 25:1J:101:A:N7 | 57:1J:302:HOH:O | 2.34 | 0.51 |
| 32:69:144:VAL:HG22 | 32:69:145:VAL:H | 1.76 | 0.51 |
| 45:D5:25:PRO:O | 45:D5:85:HIS:HA | 2.11 | 0.51 |
| 1:13:417:C:H2' | 1:13:418:C:C6 | 2.46 | 0.51 |
| 1:13:631:G:N2 | 57:13:1831:HOH:O | 2.43 | 0.51 |
| 1:13:1219:U:H2' | 1:13:1220:G:H8 | 1.75 | 0.51 |
| 1:13:1329:A:H5" | 13:4I:26:GLY:N | 2.26 | 0.51 |
| 4:3E:110:PHE:CE2 | 4:3E:148:VAL:HG23 | 2.46 | 0.51 |
| 8:7E:9:MET:O | 8:7E:12:ARG:N | 2.43 | 0.51 |
| 18:9I:25:THR:HB | 18:9I:42:ARG:HH12 | 1.75 | 0.51 |
| 23:4K:11:U:O2' | 23:4K:12:A:OP2 | 2.28 | 0.51 |
| 24:1H:654(F):C:H42 | 24:1H:654(O):G:H1 | 1.59 | 0.51 |
| 24:1H:1102:C:H2' | 24:1H:1103:A:C8 | 2.45 | 0.51 |
| 24:1H:1425:G:O2' | 24:1H:1426:G:H5' | 2.11 | 0.51 |
| 28:21:145:LYS:O | 28:21:148:GLY:N | 2.44 | 0.51 |
| 29:31:116:ASP:CG | 35:78:1:MET:HB2 | 2.35 | 0.51 |
| 37:98:35:THR:HG22 | 37:98:113:LEU:HD12 | 1.93 | 0.51 |
| 38:A8:7:TYR:CE1 | 38:A8:91:PRO:HG3 | 2.45 | 0.51 |
| 39:B8:25:GLY:H | 39:B8:49:VAL:HG23 | 1.75 | 0.51 |
| 47:J8:6:GLU:HG3 | 47:J8:61:ARG:O | 2.11 | 0.51 |
| 54:Q8:29:LYS:HB3 | 54:Q8:30:ARG:C | 2.36 | 0.51 |
| 1:1G:438:G:H4' | 4:32:123:HIS:ND1 | 2.26 | 0.51 |
| 3:22:6:HIS:CD2 | 3:22:7:PRO:HD2 | 2.46 | 0.51 |
| 12:3A:110:VAL:CG2 | 12:3A:120:TYR:HB3 | 2.40 | 0.51 |
| 20:BA:11:SER:HA | 20:BA:13:LEU:HD12 | 1.93 | 0.51 |
| 24:14:981:A:N1 | 24:14:2027:G:O2' | 2.44 | 0.51 |
| 24:14:1356:G:H2' | 24:14:1357:U:O4' | 2.11 | 0.51 |
| 24:14:1771:C:C1' | 24:14:1786:A:C8 | 2.93 | 0.51 |
| 24:14:2850:A:C2 | 24:14:2851:A:C4 | 2.99 | 0.51 |
| 26:79:14:VAL:HG22 | 26:79:222:VAL:HG22 | 1.92 | 0.51 |
| 29:39:3:GLU:HA | 29:39:24:LEU:HG | 1.93 | 0.51 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 33:15:137:LYS:HA | 33:15:137:LYS:NZ | 2.26 | 0.51 |
| 37:55:37:THR:CG2 | 37:55:39:PRO:HD2 | 2.39 | 0.51 |
| 43:B5:18:TYR:HA | 43:B5:21:PHE:CD2 | 2.45 | 0.51 |
| 44:C5:27:VAL:HA | 44:C5:39:VAL:CG1 | 2.40 | 0.51 |
| 3:2E:155:GLY:HA3 | 3:2E:196:LEU:HB3 | 1.93 | 0.51 |
| 24:1H:588:U:H2' | 24:1H:589:C:C6 | 2.46 | 0.51 |
| 24:1H:631:A:OP1 | 35:78:65:ARG:NH1 | 2.43 | 0.51 |
| 24:1H:792:G:O2' | 24:1H:2440:C:N3 | 2.41 | 0.51 |
| 24:1H:924:C:H2' | 24:1H:925:C:C6 | 2.46 | 0.51 |
| 24:1H:2096:U:H2' | 24:1H:2097:C:C6 | 2.46 | 0.51 |
| 29:31:6:VAL:HG12 | 29:31:7:TYR:H | 1.75 | 0.51 |
| 32:61:110:ASP:HB2 | 32:61:113:ARG:HB2 | 1.93 | 0.51 |
| 35:78:19:VAL:CB | 35:78:27:HIS:HB2 | 2.40 | 0.51 |
| 35:78:19:VAL:HG13 | 35:78:21:ARG:HB2 | 1.93 | 0.51 |
| 38:A8:59:LYS:HG2 | 38:A8:60:GLY:H | 1.74 | 0.51 |
| 1:1G:1129:C:C2 | 1:1G:1139:G:C6 | 2.98 | 0.51 |
| 1:1G:1151:A:O2' | 1:1G:1152:A:O4' | 2.24 | 0.51 |
| 1:1G:1192:C:OP2 | 3:22:4:LYS:NZ | 2.44 | 0.51 |
| 1:1G:1312:G:H1 | 1:1G:1325:C:H42 | 1.57 | 0.51 |
| 3:22:6:HIS:HD2 | 3:22:7:PRO:HD2 | 1.74 | 0.51 |
| 4:32:104:VAL:HG21 | 4:32:140:VAL:HG21 | 1.92 | 0.51 |
| 10:1A:13:HIS:O | 10:1A:17:ASP:HB2 | 2.11 | 0.51 |
| 22:3L:57:C:H5" | 22:3L:59:A:OP2 | 2.10 | 0.51 |
| 24:14:396:G:O2' | 47:F5:43:TYR:O | 2.27 | 0.51 |
| 24:14:746:A:C6 | 24:14:2611:U:H5" | 2.46 | 0.51 |
| 24:14:1164:G:H2' | 24:14:1165:U:C6 | 2.45 | 0.51 |
| 24:14:1448:G:H1' | 24:14:1528:A:H62 | 1.76 | 0.51 |
| 24:14:2081:C:H2' | 24:14:2082:A:C8 | 2.45 | 0.51 |
| 24:14:2122:U:H2' | 24:14:2123:G:O4' | 2.11 | 0.51 |
| 24:14:2177:C:H5" | 26:79:213:TYR:CD2 | 2.45 | 0.51 |
| 24:14:2334:G:O6 | 46:E5:74:ARG:NH2 | 2.43 | 0.51 |
| 24:14:2469:A:H2' | 24:14:2470:G:O4' | 2.11 | 0.51 |
| 24:14:2747:G:O6 | 24:14:2754:U:H3' | 2.10 | 0.51 |
| 25:1J:84:C:OP1 | 49:H5:15:TYR:OH | 2.26 | 0.51 |
| 27:19:71:ASP:CG | 27:19:103:ARG:HH22 | 2.18 | 0.51 |
| 29:39:53:THR:HG23 | 29:39:55:GLY:N | 2.20 | 0.51 |
| 31:59:56:SER:OG | 31:59:57:ASP:N | 2.41 | 0.51 |
| 32:69:71:ILE:HG23 | 32:69:72:LEU:HD23 | 1.93 | 0.51 |
| 34:25:31:LYS:HB3 | 34:25:32:TYR:CE1 | 2.46 | 0.51 |
| 35:35:22:GLY:HA3 | 35:35:25:SER:HB3 | 1.92 | 0.51 |
| 1:13:490:G:H2' | 1:13:491:G:C8 | 2.46 | 0.51 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 1:13:833:U:H2' | 1:13:834:C:H6 | 1.76 | 0.51 |
| 11:2I:31:THR:HA | 11:2I:42:TRP:HA | 1.93 | 0.51 |
| 15:6I:25:THR:HG21 | 15:6I:70:LEU:HB2 | 1.92 | 0.51 |
| 24:1H:1257:C:H4' | 29:31:83:PHE:CD1 | 2.46 | 0.51 |
| 24:1H:1449(A):G:H2' | 24:1H:1450:C:C6 | 2.45 | 0.51 |
| 24:1H:1820:U:C2 | 27:11:202:LYS:HB3 | 2.45 | 0.51 |
| 24:1H:2146:C:H4' | 24:1H:2147:G:C4 | 2.46 | 0.51 |
| 24:1H:2611:U:H6 | 24:1H:2611:U:H5' | 1.75 | 0.51 |
| 24:1H:2679:A:H4' | 28:21:165:VAL:HG11 | 1.93 | 0.51 |
| 29:31:123:LEU:HD12 | 29:31:124:LEU:H | 1.76 | 0.51 |
| 34:68:112:MET:O | 34:68:115:VAL:HG23 | 2.11 | 0.51 |
| 42:E8:29:LEU:HD21 | 42:E8:33:ARG:NH2 | 2.25 | 0.51 |
| 50:M8:11:PRO:HA | 50:M8:25:TYR:HA | 1.93 | 0.51 |
| 1:1G:589:C:N4 | 1:1G:650:G:H1 | 2.08 | 0.51 |
| 1:1G:738:C:H5" | 6:52:69:GLU:HB2 | 1.93 | 0.51 |
| 1:1G:986:A:H1' | 19:AA:54:GLY:O | 2.09 | 0.51 |
| 1:1G:1171:G:H2' | 1:1G:1172:C:C6 | 2.46 | 0.51 |
| 1:1G:1288:A:H2' | 1:1G:1289:A:H8 | 1.75 | 0.51 |
| 1:1G:1387:G:H2' | 1:1G:1388:C:C6 | 2.46 | 0.51 |
| 3:22:195:VAL:C | 3:22:196:LEU:HD23 | 2.36 | 0.51 |
| 4:32:105:VAL:O | 4:32:108:LEU:N | 2.42 | 0.51 |
| 5:42:81:GLU:HB2 | 5:42:88:LYS:HE3 | 1.93 | 0.51 |
| 11:2A:86:GLY:H | 11:2A:112:THR:HG1 | 1.58 | 0.51 |
| 13:4A:88:ARG:HG2 | 13:4A:98:VAL:HG13 | 1.93 | 0.51 |
| 17:8A:31:LEU:HD23 | 17:8A:32:TYR:CE1 | 2.46 | 0.51 |
| 22:2L:12:C:H5 | 22:2L:24:G:N1 | 2.07 | 0.51 |
| 24:14:528:A:OP2 | 33:15:114:ARG:NH1 | 2.44 | 0.51 |
| 24:14:745:G:H5" | 24:14:746:A:OP2 | 2.10 | 0.51 |
| 24:14:795:C:H2' | 24:14:796:C:C6 | 2.46 | 0.51 |
| 24:14:2210:G:H5' | 24:14:2211:G:C6 | 2.46 | 0.51 |
| 24:14:2520:C:H41 | 24:14:2542:A:H62 | 1.59 | 0.51 |
| 25:1J:43:C:OP1 | 50:I5:2:LYS:HB3 | 2.11 | 0.51 |
| 29:39:21:ALA:O | 29:39:23:ASP:N | 2.44 | 0.51 |
| 32:69:87:LYS:H | 32:69:87:LYS:HE3 | 1.75 | 0.51 |
| 34:25:90:GLN:O | 34:25:91:LEU:HB2 | 2.09 | 0.51 |
| 35:35:82:GLY:HA2 | 35:35:113:LYS:O | 2.11 | 0.51 |
| 35:35:131:SER:HB3 | 35:35:134:ALA:HB2 | 1.91 | 0.51 |
| 39:75:91:ARG:NH1 | 39:75:124:ASP:OD2 | 2.36 | 0.51 |
| 45:D5:96:VAL:N | 45:D5:128:VAL:O | 2.26 | 0.51 |
| 46:E5:47:PRO:HG3 | 46:E5:53:MET:HB2 | 1.93 | 0.51 |
| 50:I5:9:LEU:HD22 | 50:I5:9:LEU:H | 1.76 | 0.51 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 50:I5:31:ILE:HD13 | 50:I5:32:TYR:H | 1.75 | 0.51 |
| 1:13:576:G:OP1 | 57:13:1813:HOH:O | 2.19 | 0.51 |
| 1:13:639:G:H2' | 1:13:640:A:C8 | 2.46 | 0.51 |
| 1:13:1525:G:P | 11:2I:120:ARG:HH22 | 2.33 | 0.51 |
| 22:2K:84:C:H2' | 22:2K:85:A:C8 | 2.46 | 0.51 |
| 24:1H:2019:A:O4' | 40:C8:34:LYS:HD2 | 2.11 | 0.51 |
| 24:1H:2173:A:H3' | 24:1H:2174:C:C6 | 2.46 | 0.51 |
| 35:78:13:ASN:CG | 35:78:15:ARG:HD2 | 2.35 | 0.51 |
| 36:88:36:ALA:O | 36:88:99:PRO:HA | 2.11 | 0.51 |
| 37:98:97:VAL:HA | 37:98:113:LEU:O | 2.10 | 0.51 |
| 45:H8:105:VAL:HG13 | 45:H8:106:GLY:H | 1.76 | 0.51 |
| 49:L8:31:LEU:O | 49:L8:32:GLN:HB2 | 2.11 | 0.51 |
| 51:N8:49:CYS:C | 51:N8:56:LYS:HB2 | 2.36 | 0.51 |
| 1:1G:501:C:OP1 | 12:3A:117:ARG:NH2 | 2.26 | 0.51 |
| 1:1G:947:G:H5" | 13:4A:109:THR:HG23 | 1.93 | 0.51 |
| 1:1G:960:U:N3 | 1:1G:1225:A:C4 | 2.77 | 0.51 |
| 1:1G:975:A:H5' | 1:1G:975:A:H8 | 1.75 | 0.51 |
| 1:1G:1326:C:H2' | 1:1G:1327:C:H6 | 1.76 | 0.51 |
| 2:12:84:GLU:OE1 | 2:12:216:SER:HA | 2.11 | 0.51 |
| 3:22:113:ALA:HA | 3:22:202:ILE:HD11 | 1.93 | 0.51 |
| 10:1A:40:LEU:HD13 | 10:1A:71:LEU:HB2 | 1.92 | 0.51 |
| 13:4A:49:THR:N | 13:4A:52:GLU:OE1 | 2.35 | 0.51 |
| 20:BA:66:ALA:HB1 | 20:BA:71:THR:HG21 | 1.93 | 0.51 |
| 22:2L:21:A:C8 | 22:2L:46:G:N7 | 2.79 | 0.51 |
| 24:14:439:G:H2' | 24:14:440:G:H8 | 1.74 | 0.51 |
| 24:14:468:G:N7 | 53:L5:39:ARG:NH2 | 2.59 | 0.51 |
| 24:14:874:G:N2 | 24:14:904:C:C2 | 2.79 | 0.51 |
| 24:14:1148:A:H2' | 24:14:1149:G:C8 | 2.45 | 0.51 |
| 24:14:2393:A:OP1 | 54:M5:30:ARG:HB3 | 2.11 | 0.51 |
| 24:14:2788:C:O2' | 24:14:2809:A:N3 | 2.42 | 0.51 |
| 24:14:2849:U:O4 | 39:75:23:ARG:NH2 | 2.43 | 0.51 |
| 28:29:8:LYS:CB | 28:29:192:ASN:HA | 2.40 | 0.51 |
| 31:59:4:ILE:HB | 31:59:6:ARG:HG2 | 1.92 | 0.51 |
| 54:M5:28:GLY:O | 54:M5:34:TRP:HH2 | 1.94 | 0.51 |
| 1:13:143:A:H5" | 1:13:144:G:O5' | 2.10 | 0.50 |
| 1:13:236:G:H5" | 17:8I:42:TYR:OH | 2.11 | 0.50 |
| 1:13:565:U:OP2 | 1:13:566:G:O2' | 2.27 | 0.50 |
| 1:13:605:U:H2' | 1:13:606:G:O4' | 2.11 | 0.50 |
| 2:1E:167:PRO:HG2 | 2:1E:192:SER:HB3 | 1.93 | 0.50 |
| 4:3E:53:ASP:HB3 | 4:3E:57:ARG:HH12 | 1.76 | 0.50 |
| 5:4E:35:GLY:HA3 | 5:4E:112:LEU:HB3 | 1.93 | 0.50 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 5:4E:53:LEU:O | 5:4E:57:LYS:HG3 | 2.11 | 0.50 |
| 14:5I:3:ARG:HA | 14:5I:3:ARG:HH11 | 1.77 | 0.50 |
| 17:8I:75:ARG:HH12 | 17:8I:77:VAL:HG13 | 1.75 | 0.50 |
| 24:1H:575:A:OP2 | 24:1H:2055:C:N4 | 2.40 | 0.50 |
| 24:1H:671:C:OP1 | 35:78:42:SER:O | 2.29 | 0.50 |
| 24:1H:969:U:O3' | 49:L8:14:GLY:HA2 | 2.12 | 0.50 |
| 24:1H:1826:G:H4' | 27:11:242:ARG:NH2 | 2.25 | 0.50 |
| 24:1H:1972:A:H2' | 24:1H:1973:G:H8 | 1.75 | 0.50 |
| 24:1H:2488:A:H2' | 24:1H:2489:G:O4' | 2.10 | 0.50 |
| 25:16:29:A:OP2 | 38:A8:31:SER:HB2 | 2.12 | 0.50 |
| 25:16:102:G:O2' | 45:H8:73:GLN:NE2 | 2.43 | 0.50 |
| 28:21:105:THR:HG1 | 28:21:199:ARG:HH21 | 1.58 | 0.50 |
| 29:31:122:LYS:HD2 | 29:31:191:ARG:HG2 | 1.93 | 0.50 |
| 33:58:13:TRP:O | 33:58:135:PRO:HD2 | 2.11 | 0.50 |
| 35:78:19:VAL:HG13 | 35:78:21:ARG:CB | 2.40 | 0.50 |
| 1:1G:321:A:C2 | 1:1G:333:G:C2 | 2.99 | 0.50 |
| 1:1G:626:U:H4' | 16:7A:38:TYR:CZ | 2.46 | 0.50 |
| 1:1G:1167:A:H2' | 1:1G:1169:A:O4' | 2.11 | 0.50 |
| 4:32:72:GLU:OE1 | 4:32:207:TYR:OH | 2.29 | 0.50 |
| 7:62:91:VAL:HG12 | 7:62:95:ARG:HB3 | 1.93 | 0.50 |
| 22:2L:24:G:H2' | 22:2L:25:G:C8 | 2.45 | 0.50 |
| 22:2L:61:G:N3 | 22:2L:62:G:H1' | 2.25 | 0.50 |
| 24:14:830:G:H4' | 24:14:831:G:OP2 | 2.11 | 0.50 |
| 24:14:1181:C:H2' | 24:14:1182:A:C8 | 2.46 | 0.50 |
| 24:14:1187:G:H8 | 24:14:1187:G:O5' | 1.94 | 0.50 |
| 24:14:1378:A:O2' | 24:14:1380:G:N7 | 2.34 | 0.50 |
| 24:14:2124:G:H2' | 24:14:2124:G:N3 | 2.25 | 0.50 |
| 24:14:2749:A:O4' | 31:59:63:SER:HA | 2.12 | 0.50 |
| 24:14:2845:G:H2' | 24:14:2846:G:C8 | 2.45 | 0.50 |
| 29:39:29:ASN:HB3 | 29:39:112:MET:HE1 | 1.93 | 0.50 |
| 30:49:180:PHE:O | 50:I5:43:TYR:OH | 2.29 | 0.50 |
| 44:C5:20:TYR:CE2 | 44:C5:42:VAL:HA | 2.46 | 0.50 |
| 1:13:186(F):C:H2' | 1:13:187:C:O4' | 2.11 | 0.50 |
| 1:13:322:C:H5 | 1:13:328:C:H5 | 1.58 | 0.50 |
| 1:13:801:U:H2' | 1:13:802:A:H8 | 1.77 | 0.50 |
| 1:13:1032(A):G:H2' | 1:13:1032(B):G:C8 | 2.46 | 0.50 |
| 1:13:1303:C:C4 | 1:13:1304:G:C5 | 3.00 | 0.50 |
| 1:13:1414:U:H2' | 1:13:1415:G:H8 | 1.77 | 0.50 |
| 19:AI:5:LEU:HD11 | 19:AI:10:PHE:HD1 | 1.76 | 0.50 |
| 24:1H:443:A:H1' | 24:1H:1201:C:O4' | 2.09 | 0.50 |
| 24:1H:593:G:H1' | 54:Q8:4:MET:HE1 | 1.94 | 0.50 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 24:1H:602:G:O2' | 24:1H:655:A:N6 | 2.44 | 0.50 |
| 24:1H:897:C:H2' | 24:1H:898:C:H6 | 1.76 | 0.50 |
| 24:1H:945:A:OP2 | 24:1H:945:A:H4' | 2.11 | 0.50 |
| 24:1H:1931:U:C5 | 24:1H:1969:A:N7 | 2.77 | 0.50 |
| 28:21:119:ARG:HG3 | 28:21:119:ARG:NH1 | 2.20 | 0.50 |
| 29:31:8:GLN:OE1 | 29:31:8:GLN:N | 2.37 | 0.50 |
| 30:41:28:VAL:HG22 | 30:41:29:TRP:CD1 | 2.46 | 0.50 |
| 35:78:125:VAL:O | 35:78:144:GLU:HB2 | 2.10 | 0.50 |
| 37:98:70:LEU:C | 37:98:72:ASP:H | 2.19 | 0.50 |
| 44:G8:39:VAL:O | 44:G8:42:VAL:HG13 | 2.11 | 0.50 |
| 45:H8:52:SER:C | 45:H8:54:HIS:H | 2.19 | 0.50 |
| 47:J8:91:LYS:HZ2 | 47:J8:91:LYS:CA | 2.24 | 0.50 |
| 1:1G:1441:G:O5' | 1:1G:1441:G:H8 | 1.95 | 0.50 |
| 2:12:16:HIS:CD2 | 2:12:209:ARG:HB3 | 2.46 | 0.50 |
| 2:12:84:GLU:HB3 | 2:12:219:VAL:HG11 | 1.93 | 0.50 |
| 5:42:57:LYS:HG2 | 5:42:61:TYR:CE1 | 2.44 | 0.50 |
| 9:82:24:GLY:HA3 | 9:82:57:GLY:HA2 | 1.93 | 0.50 |
| 11:2A:18:ARG:HB3 | 11:2A:33:THR:OG1 | 2.10 | 0.50 |
| 11:2A:79:SER:OG | 11:2A:106:LYS:HG3 | 2.11 | 0.50 |
| 24:14:341:G:C6 | 24:14:342:G:C5 | 3.00 | 0.50 |
| 24:14:569:U:C4 | 24:14:570:G:C6 | 3.00 | 0.50 |
| 24:14:699:A:H2' | 24:14:700:G:O4' | 2.11 | 0.50 |
| 24:14:873:G:N2 | 24:14:905:U:O2 | 2.44 | 0.50 |
| 24:14:1581:G:H5" | 24:14:1581:G:H8 | 1.75 | 0.50 |
| 24:14:1826:G:H2' | 24:14:1827:C:O4' | 2.11 | 0.50 |
| 24:14:2157:G:H2' | 24:14:2158:A:C8 | 2.35 | 0.50 |
| 24:14:2370:G:H2' | 24:14:2371:G:C8 | 2.46 | 0.50 |
| 24:14:2588:G:OP1 | 57:14:3572:HOH:O | 2.19 | 0.50 |
| 24:14:2722:G:H5" | 24:14:2820:A:N7 | 2.26 | 0.50 |
| 25:1J:11:C:H3' | 25:1J:12:C:H6 | 1.77 | 0.50 |
| 27:19:92:ILE:HD12 | 27:19:104:TYR:CD1 | 2.46 | 0.50 |
| 28:29:113:PHE:N | 28:29:159:HIS:HD2 | 2.08 | 0.50 |
| 50:I5:20:ASN:CG | 50:I5:21:VAL:H | 2.18 | 0.50 |
| 54:M5:57:ARG:HB2 | 54:M5:57:ARG:NH1 | 2.26 | 0.50 |
| 1:13:227:G:H2' | 1:13:228:A:O4' | 2.12 | 0.50 |
| 1:13:257:G:C4 | 1:13:258:G:C8 | 2.99 | 0.50 |
| 1:13:313:A:H2' | 1:13:314:C:H6 | 1.75 | 0.50 |
| 1:13:858:G:N1 | 1:13:870:U:OP2 | 2.39 | 0.50 |
| 9:8E:22:GLY:N | 9:8E:58:HIS:O | 2.34 | 0.50 |
| 9:8E:110:GLU:OE2 | 9:8E:113:LYS:NZ | 2.42 | 0.50 |
| 17:8I:76:LEU:HD21 | 17:8I:79:SER:OG | 2.11 | 0.50 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 22:2K:47:U:O2' | 22:2K:48:C:O4' | 2.26 | 0.50 |
| 22:2K:59:A:C2' | 22:2K:60:A:H5' | 2.42 | 0.50 |
| 24:1H:38:A:N3 | 29:31:48:THR:OG1 | 2.44 | 0.50 |
| 24:1H:817:C:H4' | 24:1H:932:G:C5 | 2.47 | 0.50 |
| 24:1H:896:A:H5" | 45:H8:116:VAL:HG11 | 1.93 | 0.50 |
| 24:1H:1005:C:O2' | 33:58:28:THR:HG21 | 2.11 | 0.50 |
| 24:1H:1290:C:H2' | 24:1H:1291:C:C6 | 2.46 | 0.50 |
| 24:1H:1371:G:H2' | 24:1H:1372:U:H5 | 1.75 | 0.50 |
| 27:11:85:ASP:OD2 | 27:11:88:ARG:HD2 | 2.12 | 0.50 |
| 28:21:103:ASP:OD1 | 28:21:201:THR:HA | 2.11 | 0.50 |
| 34:68:2:ILE:HG13 | 34:68:8:LEU:HD11 | 1.94 | 0.50 |
| 1:1G:603:U:H2' | 1:1G:604:G:H8 | 1.74 | 0.50 |
| 1:1G:622:A:C8 | 1:1G:623:C:C6 | 2.99 | 0.50 |
| 1:1G:690:G:H22 | 11:2A:55:LYS:HZ2 | 1.59 | 0.50 |
| 1:1G:976:G:H5' | 1:1G:1358:U:O2' | 2.12 | 0.50 |
| 1:1G:1000:A:H2' | 1:1G:1001:G:C8 | 2.46 | 0.50 |
| 1:1G:1274:G:H2' | 1:1G:1275:A:C8 | 2.46 | 0.50 |
| 1:1G:1292:U:H2' | 1:1G:1293:G:C8 | 2.46 | 0.50 |
| 2:12:19:HIS:CE1 | 2:12:204:ASN:HB3 | 2.46 | 0.50 |
| 3:22:3:ASN:OD1 | 3:22:3:ASN:N | 2.45 | 0.50 |
| 3:22:61:ALA:N | 3:22:63:ASN:OD1 | 2.44 | 0.50 |
| 4:32:22:LYS:O | 4:32:113:SER:HB3 | 2.11 | 0.50 |
| 16:7A:71:ARG:HG2 | 16:7A:80:PHE:HE2 | 1.76 | 0.50 |
| 22:2L:38:MIA:H113 | 22:2L:39:A:H1' | 1.93 | 0.50 |
| 24:14:445:C:OP1 | 40:85:2:PRO:HA | 2.11 | 0.50 |
| 24:14:829:A:N7 | 24:14:2248:C:H5' | 2.25 | 0.50 |
| 24:14:1973:G:H2' | 24:14:1974:C:C6 | 2.46 | 0.50 |
| 25:1J:38:C:O4' | 38:65:95:HIS:NE2 | 2.44 | 0.50 |
| 27:19:64:ILE:HG13 | 27:19:64:ILE:O | 2.10 | 0.50 |
| 27:19:201:HIS:O | 27:19:204:ILE:HG13 | 2.10 | 0.50 |
| 31:59:12:PRO:HG3 | 31:59:49:VAL:HA | 1.94 | 0.50 |
| 31:59:122:THR:O | 31:59:131:VAL:HG13 | 2.12 | 0.50 |
| 33:15:91:LEU:HA | 33:15:95:PRO:HB3 | 1.92 | 0.50 |
| 35:35:81:GLN:OE1 | 35:35:107:LYS:HG2 | 2.10 | 0.50 |
| 37:55:54:LEU:HD23 | 37:55:66:VAL:HG23 | 1.92 | 0.50 |
| 44:C5:19:LYS:HG3 | 44:C5:20:TYR:HD2 | 1.77 | 0.50 |
| 48:G5:42:GLY:C | 48:G5:44:LEU:H | 2.19 | 0.50 |
| 1:13:57:G:H2' | 1:13:58:C:C6 | 2.47 | 0.50 |
| 1:13:1392:G:H21 | 1:13:1502:A:H8 | 1.60 | 0.50 |
| 2:1E:67:THR:HA | 2:1E:90:MET:HE1 | 1.93 | 0.50 |
| 14:5I:3:ARG:C | 14:5I:3:ARG:HD3 | 2.36 | 0.50 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 16:7I:5:ARG:O | 16:7I:20:VAL:HG12 | 2.10 | 0.50 |
| 20:BI:26:ASN:O | 20:BI:30:LYS:HB2 | 2.10 | 0.50 |
| 22:3K:52:G:H2' | 22:3K:53:A:C8 | 2.46 | 0.50 |
| 24:1H:458:G:C8 | 53:P8:37:LYS:HG2 | 2.46 | 0.50 |
| 24:1H:1914:C:H2' | 24:1H:1915:U:O4' | 2.12 | 0.50 |
| 24:1H:2148:G:H2' | 24:1H:2149:G:C8 | 2.45 | 0.50 |
| 24:1H:2682:U:HO2' | 28:21:13:ARG:HG2 | 1.75 | 0.50 |
| 25:16:7:G:H1 | 25:16:113:C:H42 | 1.59 | 0.50 |
| 30:41:110:ALA:HA | 30:41:140:ILE:O | 2.11 | 0.50 |
| 34:68:7:TYR:CZ | 34:68:44:LYS:HG3 | 2.46 | 0.50 |
| 35:78:114:ILE:HD13 | 35:78:125:VAL:HG11 | 1.94 | 0.50 |
| 37:98:37:THR:HA | 37:98:111:LEU:HD23 | 1.93 | 0.50 |
| 37:98:44:LEU:HD22 | 37:98:48:VAL:HG23 | 1.92 | 0.50 |
| 45:H8:4:ARG:HA | 45:H8:58:VAL:HB | 1.94 | 0.50 |
| 1:1G:458:C:H2' | 1:1G:464:G:H8 | 1.76 | 0.50 |
| 4:32:49:ARG:HA | 4:32:49:ARG:NE | 2.26 | 0.50 |
| 5:42:78:HIS:HE1 | 5:42:142:LEU:HD23 | 1.76 | 0.50 |
| 8:72:13:ILE:O | 8:72:17:THR:HG23 | 2.11 | 0.50 |
| 12:3A:60:LEU:HB3 | 12:3A:62:SER:H | 1.76 | 0.50 |
| 24:14:13:A:N1 | 24:14:525:U:H2' | 2.26 | 0.50 |
| 24:14:1278:A:O2' | 37:55:34:ILE:HD11 | 2.12 | 0.50 |
| 24:14:1288:U:C2 | 24:14:1327:C:O2 | 2.65 | 0.50 |
| 25:1J:29:A:OP2 | 38:65:31:SER:HB2 | 2.11 | 0.50 |
| 36:45:37:LEU:HD21 | 36:45:130:LYS:HB2 | 1.94 | 0.50 |
| 37:55:76:VAL:O | 37:55:80:PHE:N | 2.39 | 0.50 |
| 39:75:2:ASN:O | 39:75:4:GLY:HA3 | 2.12 | 0.50 |
| 49:H5:18:ASP:OD1 | 49:H5:18:ASP:N | 2.39 | 0.50 |
| 1:13:310:G:OP2 | 16:7I:27:LYS:NZ | 2.19 | 0.50 |
| 1:13:989:C:N4 | 1:13:1216:G:H1 | 2.10 | 0.50 |
| 24:1H:301:G:C4 | 24:1H:302:C:C5 | 2.99 | 0.50 |
| 24:1H:307:G:N2 | 24:1H:310:A:O5' | 2.43 | 0.50 |
| 24:1H:325:G:O2' | 24:1H:326:G:H5' | 2.11 | 0.50 |
| 24:1H:573:G:OP2 | 41:D8:78:LYS:NZ | 2.42 | 0.50 |
| 24:1H:1100:C:H2' | 24:1H:1101:U:H6 | 1.76 | 0.50 |
| 24:1H:1339:G:N2 | 24:1H:1603:A:H1' | 2.26 | 0.50 |
| 24:1H:1885:A:H2' | 24:1H:1886:C:O4' | 2.11 | 0.50 |
| 24:1H:2176:A:OP1 | 26:71:7:TYR:OH | 2.12 | 0.50 |
| 31:51:4:ILE:HG13 | 31:51:6:ARG:HB2 | 1.94 | 0.50 |
| 34:68:47:ILE:HG13 | 34:68:48:PRO:HD2 | 1.93 | 0.50 |
| 37:98:10:LEU:O | 37:98:12:ARG:NH1 | 2.44 | 0.50 |
| 1:1G:976:G:OP1 | 14:5A:31:ARG:HB2 | 2.12 | 0.50 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 1:1G:1326:C:OP1 | 21:1B:17:THR:OG1 | 2.19 | 0.50 |
| 1:1G:1422:G:H5" | 34:25:48:PRO:HB3 | 1.94 | 0.50 |
| 2:12:15:VAL:HG13 | 2:12:16:HIS:CD2 | 2.46 | 0.50 |
| 2:12:69:LEU:HD11 | 2:12:152:PHE:HE1 | 1.77 | 0.50 |
| 11:2A:16:SER:OG | 11:2A:106:LYS:NZ | 2.44 | 0.50 |
| 20:BA:89:ARG:NH1 | 20:BA:105:SER:O | 2.45 | 0.50 |
| 22:2L:69:U:H5' | 22:2L:70:C:C5 | 2.47 | 0.50 |
| 24:14:142:G:H2' | 24:14:143:C:H6 | 1.76 | 0.50 |
| 24:14:1209:G:H21 | 24:14:1210:A:H62 | 1.60 | 0.50 |
| 24:14:1328:G:H8 | 24:14:1328:G:O5' | 1.95 | 0.50 |
| 24:14:2317:C:H2' | 24:14:2318:G:O4' | 2.11 | 0.50 |
| 24:14:2820:A:C5 | 37:55:4:LEU:HD11 | 2.47 | 0.50 |
| 27:19:4:LYS:HB3 | 27:19:18:VAL:HG23 | 1.92 | 0.50 |
| 37:55:88:ARG:HB3 | 37:55:88:ARG:CZ | 2.41 | 0.50 |
| 38:65:97:ARG:O | 38:65:101:LEU:N | 2.38 | 0.50 |
| 39:75:26:ASP:OD1 | 39:75:120:ARG:NH2 | 2.43 | 0.50 |
| 45:D5:106:GLY:HA3 | 45:D5:140:ASP:HA | 1.94 | 0.50 |
| 1:13:640:A:N3 | 8:7E:115:SER:OG | 2.40 | 0.50 |
| 1:13:944:G:O6 | 1:13:1337:G:H8 | 1.95 | 0.50 |
| 1:13:1210:C:O2 | 1:13:1214:C:O2' | 2.28 | 0.50 |
| 15:6I:74:ASP:HB3 | 15:6I:77:ARG:HG2 | 1.93 | 0.50 |
| 22:2K:19:C:H3' | 22:2K:20:C:C2' | 2.41 | 0.50 |
| 24:1H:524:U:H4' | 24:1H:554:U:H4' | 1.94 | 0.50 |
| 24:1H:1423:G:H2' | 24:1H:1424:G:H8 | 1.76 | 0.50 |
| 24:1H:2853:C:O2' | 24:1H:2854:G:H5' | 2.12 | 0.50 |
| 25:16:10:C:H2' | 25:16:11:C:H6 | 1.76 | 0.50 |
| 30:41:16:ARG:HH12 | 30:41:31:VAL:HG13 | 1.76 | 0.50 |
| 32:61:144:VAL:HG23 | 32:61:145:VAL:HG23 | 1.93 | 0.50 |
| 35:78:36:LYS:HB2 | 35:78:40:SER:HB3 | 1.93 | 0.50 |
| 46:I8:23:VAL:HB | 46:I8:26:TYR:HE1 | 1.76 | 0.50 |
| 49:L8:23:LEU:H | 49:L8:23:LEU:HD12 | 1.76 | 0.50 |
| 51:N8:40:LYS:HE2 | 51:N8:47:PRO:HD2 | 1.94 | 0.50 |
| 1:1G:345:C:H1' | 1:1G:346:G:N1 | 2.26 | 0.50 |
| 1:1G:405:U:H5" | 1:1G:406:G:O4' | 2.12 | 0.50 |
| 1:1G:509:A:C6 | 1:1G:510:A:N1 | 2.80 | 0.50 |
| 2:12:112:VAL:O | 2:12:115:LEU:HB3 | 2.12 | 0.50 |
| 10:1A:30:SER:HB3 | 10:1A:81:THR:HG22 | 1.93 | 0.50 |
| 15:6A:41:GLU:HA | 15:6A:44:LYS:HG3 | 1.94 | 0.50 |
| 22:3L:12:C:H2' | 22:3L:13:G:O4' | 2.12 | 0.50 |
| 24:14:996:A:OP2 | 40:85:92:ARG:NH2 | 2.45 | 0.50 |
| 24:14:1105:U:H2' | 24:14:1106:G:C8 | 2.38 | 0.50 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 24:14:1751:C:H2' | 24:14:1752:C:C6 | 2.46 | 0.50 |
| 24:14:2350:C:H2' | 24:14:2351:G:O4' | 2.11 | 0.50 |
| 24:14:2392:A:H2 | 24:14:2424:C:N4 | 2.07 | 0.50 |
| 25:1J:28:C:N4 | 25:1J:56:G:H1 | 2.07 | 0.50 |
| 31:59:144:VAL:O | 31:59:148:ILE:HG12 | 2.11 | 0.50 |
| 33:15:62:VAL:HG22 | 33:15:66:LYS:HD2 | 1.92 | 0.50 |
| 35:35:123:LEU:H | 35:35:123:LEU:HD23 | 1.75 | 0.50 |
| 38:65:35:ILE:CD1 | 38:65:97:ARG:HE | 2.24 | 0.50 |
| 39:75:29:ARG:HB3 | 39:75:87:ASP:HB2 | 1.92 | 0.50 |
| 44:C5:42:VAL:HG13 | 44:C5:65:ALA:HB3 | 1.92 | 0.50 |
| 46:E5:51:VAL:HG23 | 46:E5:81:VAL:HG23 | 1.94 | 0.50 |
| 1:13:1128:C:O2' | 1:13:1130:A:H5' | 2.11 | 0.50 |
| 9:8E:17:VAL:HG11 | 9:8E:81:ILE:HG12 | 1.94 | 0.50 |
| 11:2I:41:THR:HG22 | 11:2I:42:TRP:N | 2.27 | 0.50 |
| 19:AI:6:LYS:HE3 | 19:AI:9:VAL:HG22 | 1.93 | 0.50 |
| 20:BI:26:ASN:HB2 | 20:BI:71:THR:OG1 | 2.12 | 0.50 |
| 21:1F:12:LYS:HB3 | 21:1F:17:THR:O | 2.12 | 0.50 |
| 24:1H:1322:A:N7 | 57:1H:3670:HOH:O | 2.35 | 0.50 |
| 24:1H:2688:U:H5 | 24:1H:2720:U:OP2 | 1.95 | 0.50 |
| 37:98:2:ARG:HA | 37:98:5:LYS:HG3 | 1.93 | 0.50 |
| 37:98:117:VAL:HG22 | 37:98:118:GLU:H | 1.77 | 0.50 |
| 54:Q8:34:TRP:HA | 54:Q8:36:LYS:CB | 2.41 | 0.50 |
| 1:1G:792:A:H1' | 1:1G:794:A:N7 | 2.27 | 0.50 |
| 1:1G:1117:G:H2' | 9:82:104:ARG:NH1 | 2.27 | 0.50 |
| 1:1G:1191:A:H5" | 3:22:4:LYS:NZ | 2.26 | 0.50 |
| 1:1G:1266:G:N2 | 1:1G:1269:A:OP2 | 2.44 | 0.50 |
| 3:22:11:ARG:NE | 3:22:180:ALA:HB3 | 2.27 | 0.50 |
| 5:42:55:VAL:O | 5:42:58:ALA:HB3 | 2.11 | 0.50 |
| 6:52:8:ILE:HD12 | 6:52:26:ILE:HD13 | 1.94 | 0.50 |
| 12:3A:31:PRO:HB2 | 12:3A:32:PHE:CD2 | 2.45 | 0.50 |
| 17:8A:59:ILE:HG22 | 17:8A:71:PHE:CD2 | 2.47 | 0.50 |
| 24:14:53:A:OP2 | 57:14:3569:HOH:O | 2.19 | 0.50 |
| 24:14:192:C:P | 57:14:3523:HOH:O | 2.66 | 0.50 |
| 24:14:912:C:OP1 | 36:45:8:LYS:NZ | 2.41 | 0.50 |
| 24:14:1047:G:H2' | 24:14:1109:C:H42 | 1.77 | 0.50 |
| 24:14:1506:C:H2' | 24:14:1507:A:H8 | 1.77 | 0.50 |
| 24:14:1531:C:N4 | 24:14:1540:G:H1 | 2.09 | 0.50 |
| 24:14:2239:G:OP2 | 27:19:244:ARG:NH2 | 2.23 | 0.50 |
| 24:14:2392:A:C8 | 35:35:61:ARG:HB3 | 2.41 | 0.50 |
| 24:14:2784:C:H1' | 28:29:37:ARG:HH12 | 1.76 | 0.50 |
| 29:39:178:PRO:HG2 | 29:39:179:GLU:OE1 | 2.12 | 0.50 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 36:45:54:MET:HE3 | 36:45:121:ALA:HB2 | 1.94 | 0.50 |
| 41:95:35:LEU:HB2 | 41:95:37:VAL:HG13 | 1.94 | 0.50 |
| 43:B5:63:LYS:HA | 43:B5:72:LYS:HA | 1.94 | 0.50 |
| 45:D5:19:ARG:HH21 | 45:D5:84:GLU:HB3 | 1.74 | 0.50 |
| 54:M5:29:LYS:HB2 | 54:M5:44:LYS:HB2 | 1.93 | 0.50 |
| 1:13:163:C:H2' | 1:13:164:U:C6 | 2.47 | 0.50 |
| 1:13:322:C:H5 | 1:13:328:C:C5 | 2.30 | 0.50 |
| 1:13:576:G:N2 | 1:13:759:A:OP1 | 2.45 | 0.50 |
| 1:13:953:G:H2' | 1:13:954:G:O4' | 2.11 | 0.50 |
| 1:13:1044:A:C5 | 1:13:1045:C:H1' | 2.47 | 0.50 |
| 1:13:1157:A:N6 | 1:13:1180:A:C5 | 2.79 | 0.50 |
| 1:13:1296:C:H5' | 13:4I:14:ARG:NH1 | 2.27 | 0.50 |
| 2:1E:104:ASN:OD1 | 2:1E:107:THR:OG1 | 2.27 | 0.50 |
| 2:1E:208:ILE:HD12 | 2:1E:209:ARG:H | 1.76 | 0.50 |
| 3:2E:77:ILE:HA | 3:2E:84:ILE:HB | 1.93 | 0.50 |
| 7:6E:23:VAL:HG12 | 7:6E:43:PHE:CE2 | 2.47 | 0.50 |
| 12:3I:86:ARG:HG3 | 12:3I:101:VAL:HG22 | 1.94 | 0.50 |
| 24:1H:871:U:OP2 | 36:88:5:ARG:NE | 2.45 | 0.50 |
| 24:1H:1198:U:H2' | 24:1H:1199:U:C6 | 2.46 | 0.50 |
| 24:1H:2022:U:O2' | 24:1H:2617:C:H5' | 2.12 | 0.50 |
| 24:1H:2784:C:O2 | 28:21:37:ARG:NH2 | 2.44 | 0.50 |
| 30:41:37:VAL:O | 30:41:94:LEU:HB2 | 2.11 | 0.50 |
| 31:51:154:PRO:HB3 | 31:51:163:TYR:CE2 | 2.46 | 0.50 |
| 1:1G:984:C:H42 | 1:1G:1221:G:H1 | 1.60 | 0.50 |
| 4:32:175:SER:HB3 | 4:32:186:LEU:HD21 | 1.92 | 0.50 |
| 6:52:101:ALA:C | 18:9A:28:GLU:HB2 | 2.37 | 0.50 |
| 15:6A:4:THR:N | 15:6A:7:GLU:OE2 | 2.45 | 0.50 |
| 24:14:1310:G:OP2 | 53:L5:9:ARG:NE | 2.44 | 0.50 |
| 24:14:2031:A:C6 | 24:14:2498:C:H1' | 2.47 | 0.50 |
| 24:14:2130:U:H2' | 24:14:2158:A:C2 | 2.47 | 0.50 |
| 24:14:2608:G:H5" | 24:14:2609:U:OP1 | 2.12 | 0.50 |
| 24:14:2688:U:H5 | 24:14:2720:U:OP2 | 1.95 | 0.50 |
| 24:14:2858:C:C2' | 24:14:2859:G:H5' | 2.42 | 0.50 |
| 36:45:21:THR:O | 36:45:21:THR:HG23 | 2.11 | 0.50 |
| 37:55:33:ARG:HD2 | 37:55:33:ARG:C | 2.37 | 0.50 |
| 38:65:52:SER:O | 38:65:56:LEU:HB2 | 2.11 | 0.50 |
| 40:85:110:VAL:O | 40:85:114:LYS:HG3 | 2.12 | 0.50 |
| 45:D5:144:LEU:HB2 | 45:D5:174:VAL:CG1 | 2.40 | 0.50 |
| 1:13:191(C):G:H2' | 1:13:191(D):U:O4' | 2.12 | 0.50 |
| 1:13:833:U:H2' | 1:13:834:C:C6 | 2.47 | 0.50 |
| 1:13:1256:A:H4' | 1:13:1258:G:C4 | 2.47 | 0.50 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 1:13:1309:G:C6 | 1:13:1329:A:N1 | 2.80 | 0.50 |
| 5:4E:87:SER:HB3 | 5:4E:125:SER:O | 2.12 | 0.50 |
| 24:1H:780:G:H21 | 24:1H:783:A:H62 | 1.58 | 0.50 |
| 24:1H:1355:G:OP1 | 27:11:38:LYS:NZ | 2.45 | 0.50 |
| 25:16:82:G:C4 | 25:16:83:G:C8 | 3.00 | 0.50 |
| 43:F8:11:PRO:HG2 | 43:F8:13:LEU:HD21 | 1.93 | 0.50 |
| 1:1G:1392:G:H8 | 1:1G:1392:G:O5' | 1.93 | 0.50 |
| 7:62:60:LYS:O | 7:62:63:LYS:NZ | 2.45 | 0.50 |
| 24:14:527:C:C4 | 24:14:2779:U:H2' | 2.47 | 0.50 |
| 24:14:1110:G:H2' | 24:14:1111:A:C8 | 2.47 | 0.50 |
| 24:14:1142:U:H5" | 24:14:1142(A):A:C5' | 2.41 | 0.50 |
| 24:14:1427:A:H4' | 24:14:1428:C:O5' | 2.11 | 0.50 |
| 24:14:2662:A:C4 | 24:14:2663:G:H1' | 2.46 | 0.50 |
| 25:1J:51:G:N7 | 38:65:62:LYS:NZ | 2.59 | 0.50 |
| 28:29:165:VAL:HG12 | 28:29:189:PRO:HG3 | 1.94 | 0.50 |
| 44:C5:37:VAL:O | 44:C5:67:LEU:N | 2.43 | 0.50 |
| 44:C5:87:LYS:H | 44:C5:94:LYS:HB3 | 1.76 | 0.50 |
| 1:13:232:G:H1' | 1:13:262:A:N1 | 2.27 | 0.49 |
| 1:13:872:A:C5 | 1:13:874:G:C8 | 3.00 | 0.49 |
| 24:1H:189:G:H2' | 24:1H:205:G:N2 | 2.26 | 0.49 |
| 24:1H:897:C:H2' | 24:1H:898:C:C6 | 2.47 | 0.49 |
| 24:1H:969:U:P | 49:L8:17:LYS:HZ3 | 2.34 | 0.49 |
| 24:1H:1505:C:H2' | 24:1H:1506:C:H6 | 1.77 | 0.49 |
| 25:16:80:U:H2' | 25:16:81:G:N2 | 2.26 | 0.49 |
| 27:11:134:ARG:HG3 | 27:11:135:PHE:CE1 | 2.47 | 0.49 |
| 27:11:182:LEU:H | 27:11:272:ALA:CB | 2.19 | 0.49 |
| 54:Q8:28:GLY:HA3 | 54:Q8:44:LYS:HD3 | 1.95 | 0.49 |
| 1:1G:33:A:N3 | 12:3A:32:PHE:HE2 | 2.09 | 0.49 |
| 1:1G:922:G:N3 | 1:1G:1398:A:H2 | 2.10 | 0.49 |
| 1:1G:1376:U:OP1 | 7:62:98:SER:HB3 | 2.11 | 0.49 |
| 5:42:7:GLU:O | 5:42:34:VAL:HA | 2.12 | 0.49 |
| 10:1A:39:PRO:HA | 10:1A:70:ARG:HE | 1.76 | 0.49 |
| 24:14:38:A:H2' | 24:14:39:C:C6 | 2.47 | 0.49 |
| 24:14:248:G:OP1 | 57:14:3570:HOH:O | 2.19 | 0.49 |
| 24:14:661:C:O2' | 35:35:13:ASN:O | 2.27 | 0.49 |
| 24:14:740:U:O4' | 24:14:1981:A:C4 | 2.65 | 0.49 |
| 24:14:1536:A:H5" | 24:14:1537:C:C6 | 2.47 | 0.49 |
| 24:14:1885:A:H2' | 24:14:1886:C:O4' | 2.12 | 0.49 |
| 24:14:1967:C:H2' | 24:14:1968:G:O4' | 2.11 | 0.49 |
| 24:14:2050:C:H1' | 28:29:156:MET:HE1 | 1.93 | 0.49 |
| 24:14:2341:G:H2' | 24:14:2342:C:C6 | 2.47 | 0.49 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 24:14:2698:U:C4 | 57:14:3520:HOH:O | 2.64 | 0.49 |
| 25:1J:13:A:H2' | 25:1J:70:C:O2' | 2.12 | 0.49 |
| 25:1J:14:U:H5' | 25:1J:71:C:H1' | 1.93 | 0.49 |
| 27:19:37:LEU:HA | 27:19:38:LYS:CG | 2.38 | 0.49 |
| 27:19:49:ILE:HD11 | 27:19:52:ARG:HA | 1.92 | 0.49 |
| 29:39:20:LEU:HD13 | 29:39:199:TRP:HH2 | 1.77 | 0.49 |
| 34:25:120:GLU:CD | 34:25:122:LEU:HD21 | 2.37 | 0.49 |
| 36:45:75:THR:HA | 36:45:90:VAL:H | 1.76 | 0.49 |
| 38:65:105:ALA:HB3 | 38:65:112:PHE:HE1 | 1.77 | 0.49 |
| 39:75:91:ARG:HD2 | 39:75:124:ASP:OD2 | 2.12 | 0.49 |
| 45:D5:17:ALA:HA | 45:D5:20:ARG:HD2 | 1.93 | 0.49 |
| 47:F5:85:LEU:HD12 | 47:F5:88:LYS:HG3 | 1.94 | 0.49 |
| 54:M5:61:LEU:C | 54:M5:62:LEU:HG | 2.37 | 0.49 |
| 1:13:355:C:O4' | 1:13:388:G:O2' | 2.26 | 0.49 |
| 1:13:649:G:H2' | 1:13:650:G:H8 | 1.76 | 0.49 |
| 1:13:1255:G:O6 | 10:1I:43:ARG:NH2 | 2.34 | 0.49 |
| 5:4E:78:HIS:CD2 | 8:7E:104:ARG:HD3 | 2.47 | 0.49 |
| 7:6E:50:ILE:HG21 | 7:6E:58:PRO:HA | 1.94 | 0.49 |
| 8:7E:129:VAL:HG23 | 8:7E:130:GLY:H | 1.77 | 0.49 |
| 16:7I:48:TRP:CD1 | 16:7I:48:TRP:H | 2.30 | 0.49 |
| 22:3K:83:C:H4' | 47:J8:23:LYS:HE2 | 1.94 | 0.49 |
| 24:1H:302:C:H2' | 24:1H:303:U:H6 | 1.76 | 0.49 |
| 24:1H:448:U:O4 | 24:1H:583:G:H1' | 2.12 | 0.49 |
| 24:1H:699:A:H2' | 24:1H:700:G:O4' | 2.12 | 0.49 |
| 24:1H:1064:C:O2 | 24:1H:1076:C:O2' | 2.29 | 0.49 |
| 24:1H:2057:A:P | 57:1H:3628:HOH:O | 2.66 | 0.49 |
| 24:1H:2260:C:C2' | 24:1H:2261:C:H5' | 2.43 | 0.49 |
| 25:16:40:U:O4 | 50:M8:1:MET:N | 2.41 | 0.49 |
| 29:31:12:LEU:O | 29:31:127:GLU:N | 2.45 | 0.49 |
| 29:31:152:GLU:OE1 | 29:31:191:ARG:HD2 | 2.13 | 0.49 |
| 30:41:165:THR:OG1 | 30:41:168:GLU:HG3 | 2.13 | 0.49 |
| 34:68:10:VAL:HG11 | 34:68:16:ALA:HB3 | 1.94 | 0.49 |
| 38:A8:24:LEU:HD12 | 38:A8:41:ASP:HB2 | 1.94 | 0.49 |
| 39:B8:52:ILE:HG23 | 39:B8:61:PHE:HB3 | 1.93 | 0.49 |
| 1:1G:1243:C:OP1 | 21:1B:8:THR:HG21 | 2.12 | 0.49 |
| 1:1G:1410:G:H2' | 1:1G:1411:C:C6 | 2.47 | 0.49 |
| 4:32:134:ASP:OD1 | 4:32:134:ASP:N | 2.44 | 0.49 |
| 9:82:73:GLN:O | 9:82:77:ILE:HG23 | 2.12 | 0.49 |
| 20:BA:67:ALA:HA | 20:BA:73:HIS:H | 1.75 | 0.49 |
| 24:14:221:A:N6 | 24:14:265:A:C8 | 2.80 | 0.49 |
| 24:14:522:G:H2' | 24:14:523:C:C6 | 2.48 | 0.49 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 24:14:654(J):A:OP2 | 24:14:654(M):C:N4 | 2.45 | 0.49 |
| 24:14:1607:C:H4' | 24:14:1608:A:O5' | 2.11 | 0.49 |
| 24:14:2053:G:H5' | 28:29:144:ARG:O | 2.12 | 0.49 |
| 24:14:2079:U:OP1 | 47:F5:21:ARG:NH1 | 2.36 | 0.49 |
| 24:14:2262:U:H4' | 24:14:2328:A:C2 | 2.46 | 0.49 |
| 24:14:2445:G:OP1 | 29:39:74:ARG:NH2 | 2.40 | 0.49 |
| 24:14:2562:U:H1' | 34:25:23:ARG:NH1 | 2.27 | 0.49 |
| 25:1J:44:G:H1' | 25:1J:47:C:N4 | 2.26 | 0.49 |
| 27:19:181:GLU:HA | 27:19:272:ALA:HB1 | 1.94 | 0.49 |
| 28:29:96:PHE:HD2 | 28:29:182:LEU:HD21 | 1.77 | 0.49 |
| 29:39:21:ALA:C | 29:39:23:ASP:H | 2.20 | 0.49 |
| 22:3K:33:C:N4 | 22:3K:34:U:O4 | 2.44 | 0.49 |
| 24:1H:302:C:H2' | 24:1H:303:U:C6 | 2.48 | 0.49 |
| 24:1H:415:A:H2' | 24:1H:416:C:C6 | 2.47 | 0.49 |
| 24:1H:637:A:H2' | 35:78:117:GLU:OE1 | 2.13 | 0.49 |
| 24:1H:1357:U:OP2 | 57:1H:3700:HOH:O | 2.19 | 0.49 |
| 24:1H:2005:A:H5" | 24:1H:2006:C:OP2 | 2.12 | 0.49 |
| 24:1H:2137:C:N4 | 24:1H:2154:G:H1 | 2.09 | 0.49 |
| 24:1H:2352:A:C4 | 24:1H:2366:A:C2 | 3.00 | 0.49 |
| 27:11:18:VAL:HG12 | 27:11:19:ALA:N | 2.26 | 0.49 |
| 29:31:50:SER:OG | 29:31:51:THR:N | 2.43 | 0.49 |
| 31:51:4:ILE:HD12 | 31:51:6:ARG:NH2 | 2.27 | 0.49 |
| 45:H8:30:ASN:HA | 45:H8:89:PHE:HE1 | 1.78 | 0.49 |
| 45:H8:44:PHE:O | 45:H8:47:VAL:HG13 | 2.12 | 0.49 |
| 48:K8:33:MET:HG2 | 48:K8:37:PHE:CD1 | 2.47 | 0.49 |
| 1:1G:380:G:C2 | 1:1G:384:G:C6 | 3.00 | 0.49 |
| 1:1G:782:A:H2' | 1:1G:783:C:O4' | 2.12 | 0.49 |
| 1:1G:792:A:H4' | 1:1G:793:U:O5' | 2.12 | 0.49 |
| 1:1G:868:C:H2' | 1:1G:869:G:O4' | 2.12 | 0.49 |
| 2:12:83:MET:HG3 | 2:12:234:PRO:O | 2.12 | 0.49 |
| 2:12:87:ARG:NH1 | 2:12:220:ASP:OD1 | 2.39 | 0.49 |
| 2:12:178:ARG:HH12 | 2:12:196:LEU:C | 2.17 | 0.49 |
| 4:32:75:PHE:CE1 | 4:32:93:PHE:HZ | 2.30 | 0.49 |
| 5:42:80:ILE:HD13 | 5:42:138:ALA:HB1 | 1.93 | 0.49 |
| 22:2L:71:C:O2' | 22:2L:72:U:P | 2.70 | 0.49 |
| 22:3L:18:G:H4' | 22:3L:19:C:O5' | 2.12 | 0.49 |
| 24:14:71:A:H2 | 43:B5:31:HIS:HE2 | 1.57 | 0.49 |
| 24:14:655:A:H5' | 24:14:656:G:OP2 | 2.12 | 0.49 |
| 24:14:1146:C:H2' | 24:14:1147:C:H6 | 1.75 | 0.49 |
| 24:14:1298:C:H5" | 24:14:1299:G:OP2 | 2.12 | 0.49 |
| 24:14:2098:U:H2' | 24:14:2099:U:C6 | 2.48 | 0.49 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 24:14:2462:U:H2' | 24:14:2463:C:C6 | 2.48 | 0.49 |
| 24:14:2784:C:H1' | 28:29:37:ARG:NH1 | 2.26 | 0.49 |
| 30:49:75:LYS:HA | 30:49:84:LYS:HE2 | 1.94 | 0.49 |
| 32:69:77:LEU:HD12 | 32:69:78:THR:H | 1.77 | 0.49 |
| 48:G5:5:GLU:CD | 48:G5:5:GLU:H | 2.20 | 0.49 |
| 1:13:129(A):G:C2 | 1:13:188:U:O2' | 2.65 | 0.49 |
| 1:13:826:C:H4' | 8:7E:12:ARG:HG3 | 1.94 | 0.49 |
| 1:13:1387:G:H2' | 1:13:1388:C:H6 | 1.77 | 0.49 |
| 3:2E:77:ILE:HG12 | 3:2E:84:ILE:HD12 | 1.94 | 0.49 |
| 19:AI:53:ASN:O | 19:AI:77:THR:HG22 | 2.12 | 0.49 |
| 22:2K:64:PSU:H2' | 22:2K:64:PSU:OP2 | 2.12 | 0.49 |
| 24:1H:270(T):G:C6 | 24:1H:270(U):C:C4 | 3.00 | 0.49 |
| 24:1H:997:G:H2' | 24:1H:998:C:H5' | 1.94 | 0.49 |
| 24:1H:1021:A:C8 | 24:1H:1021:A:C3' | 2.95 | 0.49 |
| 24:1H:1141:U:OP2 | 33:58:63:THR:OG1 | 2.31 | 0.49 |
| 24:1H:1291:C:H2' | 24:1H:1292:U:C6 | 2.47 | 0.49 |
| 24:1H:2133:G:O2' | 24:1H:2158:A:N6 | 2.45 | 0.49 |
| 24:1H:2173:A:H3' | 24:1H:2174:C:H6 | 1.77 | 0.49 |
| 24:1H:2259:G:H1' | 24:1H:2427:C:C2 | 2.47 | 0.49 |
| 27:11:25:THR:O | 27:11:26:LYS:O | 2.30 | 0.49 |
| 39:B8:16:ARG:HE | 39:B8:19:LEU:HD21 | 1.77 | 0.49 |
| 39:B8:23:ARG:HG3 | 39:B8:120:ARG:NH1 | 2.27 | 0.49 |
| 45:H8:126:VAL:HG12 | 45:H8:163:LEU:HA | 1.93 | 0.49 |
| 1:1G:321:A:C8 | 1:1G:328:C:C6 | 2.99 | 0.49 |
| 1:1G:1036:G:H3' | 1:1G:1037:C:C6 | 2.48 | 0.49 |
| 1:1G:1301:U:O2 | 1:1G:1301:U:H2' | 2.11 | 0.49 |
| 22:2L:62:G:H2' | 22:2L:63:5MU:OP1 | 2.12 | 0.49 |
| 24:14:218:A:C2 | 24:14:235:U:H4' | 2.47 | 0.49 |
| 24:14:270(L):U:O2' | 24:14:270(M):U:OP1 | 2.28 | 0.49 |
| 24:14:2065:C:H2' | 24:14:2066:C:C6 | 2.47 | 0.49 |
| 24:14:2745:C:H4' | 31:59:142:GLY:O | 2.11 | 0.49 |
| 30:49:97:ASP:HA | 30:49:100:TRP:HD1 | 1.76 | 0.49 |
| 40:85:29:SER:C | 40:85:30:LYS:HD3 | 2.38 | 0.49 |
| 43:B5:55:ASN:HB2 | 43:B5:80:ILE:HG23 | 1.93 | 0.49 |
| 50:I5:58:ARG:NH2 | 50:I5:61:ARG:HB3 | 2.27 | 0.49 |
| 1:13:22:G:H2' | 1:13:23:C:C6 | 2.48 | 0.49 |
| 1:13:448:A:P | 1:13:485:G:H22 | 2.36 | 0.49 |
| 1:13:828:A:H2' | 1:13:829:G:O4' | 2.12 | 0.49 |
| 3:2E:130:VAL:O | 3:2E:134:ILE:HG12 | 2.13 | 0.49 |
| 7:6E:26:PHE:CE2 | 7:6E:30:ILE:HD11 | 2.46 | 0.49 |
| 7:6E:130:GLY:O | 7:6E:135:VAL:HG11 | 2.13 | 0.49 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 8:7E:116:LYS:HG3 | 8:7E:127:LEU:HD22 | 1.95 | 0.49 |
| 13:4I:32:GLU:OE1 | 13:4I:36:LYS:HG3 | 2.13 | 0.49 |
| 24:1H:252:G:P | 35:78:50:ARG:HH12 | 2.35 | 0.49 |
| 24:1H:314:A:C2' | 24:1H:315:G:H5' | 2.43 | 0.49 |
| 24:1H:1417:C:H2' | 24:1H:1418:G:O4' | 2.13 | 0.49 |
| 24:1H:2171:A:H2' | 24:1H:2172:U:O4' | 2.12 | 0.49 |
| 24:1H:2286:A:H2' | 52:O8:31:PRO:HD3 | 1.95 | 0.49 |
| 24:1H:2507:C:H5' | 24:1H:2573:C:N4 | 2.28 | 0.49 |
| 24:1H:2666:C:H3' | 24:1H:2667:C:H6 | 1.77 | 0.49 |
| 28:21:14:ILE:CG2 | 28:21:21:VAL:HB | 2.42 | 0.49 |
| 29:31:29:ASN:H | 29:31:112:MET:CE | 2.25 | 0.49 |
| 32:61:125:GLU:OE2 | 32:61:141:LYS:HB3 | 2.12 | 0.49 |
| 36:88:54:MET:HE3 | 36:88:64:ILE:HD13 | 1.94 | 0.49 |
| 46:I8:50:ASN:HB3 | 46:I8:63:VAL:HG22 | 1.94 | 0.49 |
| 1:1G:522:C:OP2 | 12:3A:69:TYR:OH | 2.22 | 0.49 |
| 1:1G:938:A:C6 | 1:1G:939:G:C5 | 3.01 | 0.49 |
| 17:8A:62:SER:OG | 17:8A:72:ARG:HG3 | 2.12 | 0.49 |
| 24:14:195:A:H61 | 24:14:198:C:H3' | 1.77 | 0.49 |
| 24:14:240:G:H1' | 24:14:257:A:N6 | 2.28 | 0.49 |
| 24:14:815:C:H2' | 24:14:816:C:C6 | 2.48 | 0.49 |
| 24:14:1454:U:O2 | 37:55:60:LEU:HD11 | 2.13 | 0.49 |
| 24:14:1489:U:O3' | 24:14:1490:A:H8 | 1.95 | 0.49 |
| 24:14:2615:U:C2 | 51:J5:7:PRO:HA | 2.47 | 0.49 |
| 35:35:101:VAL:HG23 | 35:35:106:LEU:HD23 | 1.93 | 0.49 |
| 38:65:106:ARG:HA | 38:65:110:LEU:HD11 | 1.94 | 0.49 |
| 46:E5:12:ASN:HA | 46:E5:14:ARG:NH2 | 2.27 | 0.49 |
| 1:13:522:C:H2' | 1:13:523:A:C8 | 2.48 | 0.49 |
| 1:13:1307:U:H2' | 1:13:1308:U:C6 | 2.47 | 0.49 |
| 1:13:1374:A:C5 | 1:13:1375:A:C8 | 3.00 | 0.49 |
| 1:13:1394:A:C5 | 1:13:1501:C:H4' | 2.48 | 0.49 |
| 8:7E:21:LYS:O | 8:7E:65:TYR:OH | 2.29 | 0.49 |
| 10:1I:4:ILE:O | 10:1I:74:ILE:HG12 | 2.12 | 0.49 |
| 24:1H:705:A:C8 | 24:1H:727:A:C2 | 3.01 | 0.49 |
| 24:1H:1889:A:H2' | 24:1H:1890:A:C8 | 2.47 | 0.49 |
| 24:1H:2102:U:H2' | 24:1H:2103:C:C6 | 2.47 | 0.49 |
| 24:1H:2263:C:H2' | 24:1H:2264:C:H6 | 1.76 | 0.49 |
| 24:1H:2306:C:H3' | 24:1H:2307:G:C5' | 2.43 | 0.49 |
| 24:1H:2438:U:O3' | 24:1H:2439:A:H3' | 2.13 | 0.49 |
| 31:51:4:ILE:C | 31:51:6:ARG:H | 2.20 | 0.49 |
| 37:98:25:ALA:O | 37:98:26:LYS:C | 2.55 | 0.49 |
| 39:B8:1:MET:O | 39:B8:3:ARG:N | 2.46 | 0.49 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 1:1G:116:A:H61 | 1:1G:313:A:H1' | 1.77 | 0.49 |
| 1:1G:337:C:H2' | 1:1G:338:A:C8 | 2.47 | 0.49 |
| 1:1G:539:A:H2' | 1:1G:540:G:C8 | 2.47 | 0.49 |
| 1:1G:791:G:C5 | 1:1G:792:A:N7 | 2.81 | 0.49 |
| 1:1G:896:C:H5' | 17:8A:100:LYS:HG2 | 1.95 | 0.49 |
| 1:1G:933:G:O6 | 7:62:3:ARG:NH2 | 2.46 | 0.49 |
| 3:22:120:VAL:O | 3:22:123:GLN:N | 2.45 | 0.49 |
| 5:42:137:GLU:HG2 | 5:42:140:ARG:HH11 | 1.78 | 0.49 |
| 8:72:86:ILE:HG13 | 8:72:133:LEU:HD22 | 1.94 | 0.49 |
| 16:7A:5:ARG:NH1 | 16:7A:22:THR:HG21 | 2.26 | 0.49 |
| 20:BA:54:LYS:HA | 20:BA:57:ARG:NH2 | 2.27 | 0.49 |
| 21:1B:2:GLY:O | 21:1B:4:GLY:N | 2.46 | 0.49 |
| 24:14:265:A:C8 | 24:14:266:G:H1' | 2.48 | 0.49 |
| 24:14:337:C:H2' | 24:14:338:G:O4' | 2.12 | 0.49 |
| 24:14:2183:C:H2' | 24:14:2184:G:C8 | 2.47 | 0.49 |
| 24:14:2250:G:C5 | 36:45:83:MET:HB3 | 2.48 | 0.49 |
| 24:14:2646:C:H2' | 24:14:2647:U:O4' | 2.13 | 0.49 |
| 24:14:2659:G:O2' | 24:14:2661:G:N7 | 2.35 | 0.49 |
| 24:14:2757:A:C2 | 31:59:67:LEU:HD11 | 2.47 | 0.49 |
| 27:19:210:GLY:O | 27:19:213:ARG:HB2 | 2.12 | 0.49 |
| 28:29:178:GLU:OE1 | 28:29:178:GLU:N | 2.39 | 0.49 |
| 31:59:52:VAL:HG12 | 31:59:69:ARG:HB2 | 1.94 | 0.49 |
| 35:35:100:LEU:HD12 | 35:35:112:LEU:HD11 | 1.94 | 0.49 |
| 40:85:17:ILE:HG23 | 40:85:39:LEU:HD12 | 1.94 | 0.49 |
| 1:13:427:U:H3' | 1:13:428:G:H2' | 1.94 | 0.49 |
| 1:13:613:C:O3' | 4:3E:86:LYS:NZ | 2.45 | 0.49 |
| 1:13:713:G:H2' | 1:13:714:G:C8 | 2.48 | 0.49 |
| 2:1E:14:GLY:H | 2:1E:16:HIS:HE1 | 1.58 | 0.49 |
| 4:3E:107:ARG:HH22 | 4:3E:194:LEU:CD2 | 2.26 | 0.49 |
| 7:6E:111:ARG:HB3 | 7:6E:113:GLU:OE2 | 2.13 | 0.49 |
| 8:7E:6:ILE:O | 8:7E:10:LEU:HG | 2.12 | 0.49 |
| 9:8E:16:ARG:HB2 | 9:8E:64:THR:HG23 | 1.94 | 0.49 |
| 17:8I:29:HIS:O | 17:8I:33:GLY:N | 2.36 | 0.49 |
| 20:BI:26:ASN:HB2 | 20:BI:71:THR:HG23 | 1.95 | 0.49 |
| 24:1H:272:G:H2' | 24:1H:273:G:C8 | 2.48 | 0.49 |
| 24:1H:710:G:H2' | 24:1H:711:G:H8 | 1.78 | 0.49 |
| 24:1H:910:A:N6 | 36:88:12:GLN:HA | 2.23 | 0.49 |
| 24:1H:1204:A:C2 | 24:1H:1241:A:N1 | 2.81 | 0.49 |
| 24:1H:1681:G:H21 | 24:1H:1762:A:H3' | 1.76 | 0.49 |
| 24:1H:1972:A:H2' | 24:1H:1973:G:C8 | 2.47 | 0.49 |
| 24:1H:2277:G:C6 | 24:1H:2278:A:N7 | 2.80 | 0.49 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 24:1H:2572:A:N7 | 28:21:145:LYS:HB2 | 2.28 | 0.49 |
| 36:88:43:THR:HB | 36:88:45:GLN:HG2 | 1.95 | 0.49 |
| 42:E8:29:LEU:O | 42:E8:29:LEU:HG | 2.11 | 0.49 |
| 43:F8:53:LYS:HG2 | 43:F8:82:GLN:HB2 | 1.94 | 0.49 |
| 1:1G:328:C:H4' | 1:1G:329:A:C5' | 2.43 | 0.49 |
| 1:1G:427:U:H3' | 1:1G:428:G:H2' | 1.93 | 0.49 |
| 1:1G:1014:A:P | 1:1G:1014:A:H8 | 2.36 | 0.49 |
| 7:62:91:VAL:HB | 7:62:96:GLN:HG2 | 1.94 | 0.49 |
| 10:1A:35:SER:OG | 10:1A:73:ASP:HB2 | 2.13 | 0.49 |
| 13:4A:29:ARG:HD3 | 13:4A:64:TRP:CZ2 | 2.47 | 0.49 |
| 19:AA:80:TYR:CZ | 19:AA:82:GLY:HA2 | 2.47 | 0.49 |
| 20:BA:56:MET:HE2 | 20:BA:88:VAL:HG11 | 1.95 | 0.49 |
| 24:14:67:U:N3 | 24:14:74:A:H2 | 2.02 | 0.49 |
| 24:14:71:A:H4' | 24:14:72:U:H5" | 1.93 | 0.49 |
| 24:14:126:A:O5' | 53:L5:19:ARG:HG3 | 2.13 | 0.49 |
| 24:14:1112:G:H5' | 31:59:3:ARG:HD3 | 1.95 | 0.49 |
| 24:14:1149:G:H2' | 24:14:1150:C:H6 | 1.75 | 0.49 |
| 24:14:1181:C:H2' | 24:14:1182:A:H8 | 1.77 | 0.49 |
| 24:14:1464:C:O2' | 24:14:1528:A:H8 | 1.94 | 0.49 |
| 24:14:1531:C:N3 | 24:14:1540:G:N2 | 2.48 | 0.49 |
| 24:14:1945:G:H2' | 24:14:1946:U:C6 | 2.48 | 0.49 |
| 24:14:2744:G:N2 | 31:59:143:GLN:OE1 | 2.46 | 0.49 |
| 25:1J:40:U:H1' | 25:1J:46:A:N1 | 2.28 | 0.49 |
| 25:1J:89:G:C6 | 25:1J:89(A):A:C6 | 3.01 | 0.49 |
| 26:79:13:LYS:HD2 | 26:79:32:LEU:HD23 | 1.95 | 0.49 |
| 28:29:77:ILE:C | 28:29:78:LEU:HG | 2.38 | 0.49 |
| 28:29:81:ILE:O | 28:29:81:ILE:HG22 | 2.12 | 0.49 |
| 31:59:125:VAL:HG12 | 31:59:127:GLU:H | 1.77 | 0.49 |
| 33:15:42:TRP:CD1 | 33:15:42:TRP:C | 2.91 | 0.49 |
| 34:25:8:LEU:HD13 | 34:25:82:ASN:HB2 | 1.95 | 0.49 |
| 1:13:1003:G:H2' | 1:13:1004:A:O3' | 2.13 | 0.49 |
| 1:13:1074:G:O2' | 1:13:1101:A:N1 | 2.38 | 0.49 |
| 1:13:1513:A:H2' | 1:13:1514:C:C6 | 2.48 | 0.49 |
| 4:3E:134:ASP:O | 4:3E:136:PRO:HD3 | 2.12 | 0.49 |
| 22:2K:17:OMG:H1' | 22:2K:66:G:N2 | 2.28 | 0.49 |
| 24:1H:1434:A:H61 | 24:1H:1558:A:H62 | 1.58 | 0.49 |
| 24:1H:1545(A):A:H2' | 24:1H:1546:C:O4' | 2.12 | 0.49 |
| 24:1H:2123:G:H3' | 24:1H:2124:G:H8 | 1.77 | 0.49 |
| 24:1H:2327:A:H2' | 24:1H:2328:A:H8 | 1.71 | 0.49 |
| 24:1H:2485:G:H5" | 36:88:46:GLN:NE2 | 2.24 | 0.49 |
| 29:31:65:TRP:CZ3 | 29:31:73:ALA:O | 2.63 | 0.49 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 30:41:63:ILE:HB | 30:41:141:PHE:CD2 | 2.47 | 0.49 |
| 30:41:109:VAL:O | 30:41:113:ARG:HG3 | 2.13 | 0.49 |
| 36:88:74:TYR:O | 36:88:90:VAL:O | 2.31 | 0.49 |
| 42:E8:88:ARG:HD3 | 42:E8:94:ASP:OD2 | 2.13 | 0.49 |
| 1:1G:814:A:N7 | 1:1G:816:A:C4 | 2.80 | 0.49 |
| 1:1G:843:U:C5 | 1:1G:848:C:H1' | 2.48 | 0.49 |
| 1:1G:1128:C:H4' | 9:82:16:ARG:NH1 | 2.28 | 0.49 |
| 15:6A:15:PHE:CZ | 15:6A:84:LYS:HG2 | 2.48 | 0.49 |
| 16:7A:20:VAL:HG21 | 16:7A:32:TYR:CD2 | 2.48 | 0.49 |
| 22:2L:8:4SU:H6 | 22:2L:8:4SU:C5' | 2.38 | 0.49 |
| 22:2L:63:5MU:H2' | 22:2L:64:PSU:H5" | 1.93 | 0.49 |
| 24:14:75:G:H4' | 48:G5:55:ARG:NH2 | 2.28 | 0.49 |
| 24:14:673:C:H5" | 29:39:81:PRO:HD2 | 1.94 | 0.49 |
| 24:14:868:U:C2 | 24:14:869:G:C8 | 3.01 | 0.49 |
| 24:14:1331:A:O2' | 24:14:1332:G:C8 | 2.65 | 0.49 |
| 24:14:1505:C:H2' | 24:14:1506:C:C6 | 2.47 | 0.49 |
| 24:14:2458:G:O2' | 24:14:2460:U:O4 | 2.29 | 0.49 |
| 24:14:2831:G:OP1 | 28:29:58:ARG:NH1 | 2.42 | 0.49 |
| 25:1J:102:G:N2 | 45:D5:73:GLN:OE1 | 2.37 | 0.49 |
| 28:29:46:ALA:HB1 | 28:29:82:ARG:H | 1.78 | 0.49 |
| 35:35:52:GLU:HB2 | 35:35:55:ARG:HD2 | 1.95 | 0.49 |
| 39:75:9:LEU:C | 39:75:9:LEU:HD13 | 2.38 | 0.49 |
| 43:B5:60:ARG:HH21 | 53:L5:47:ARG:NH2 | 2.07 | 0.49 |
| 44:C5:8:LYS:HG2 | 44:C5:9:LYS:H | 1.77 | 0.49 |
| 45:D5:99:TYR:HA | 45:D5:124:ILE:O | 2.13 | 0.49 |
| 47:F5:83:GLU:OE1 | 47:F5:85:LEU:HB2 | 2.13 | 0.49 |
| 1:13:328:C:H4' | 1:13:329:A:H5' | 1.94 | 0.49 |
| 1:13:509:A:H3' | 57:13:1817:HOH:O | 2.12 | 0.49 |
| 1:13:587:G:C2 | 1:13:755:G:C5 | 3.01 | 0.49 |
| 1:13:960:U:C4 | 1:13:1225:A:H1' | 2.46 | 0.49 |
| 1:13:964:A:N3 | 1:13:969:A:O2' | 2.42 | 0.49 |
| 1:13:1339:A:H2' | 1:13:1340:A:O4' | 2.12 | 0.49 |
| 2:1E:220:ASP:HA | 2:1E:223:ILE:HD12 | 1.94 | 0.49 |
| 6:5E:5:GLU:HG3 | 6:5E:93:SER:OG | 2.13 | 0.49 |
| 9:8E:25:LYS:N | 9:8E:60:ASP:OD1 | 2.45 | 0.49 |
| 19:AI:24:ALA:C | 19:AI:26:GLY:H | 2.21 | 0.49 |
| 24:1H:185:U:H2' | 24:1H:186:G:C8 | 2.47 | 0.49 |
| 24:1H:500:G:N1 | 24:1H:503:A:OP2 | 2.45 | 0.49 |
| 24:1H:619:G:H3' | 24:1H:620:G:N2 | 2.27 | 0.49 |
| 24:1H:937:U:H2' | 24:1H:938:G:O4' | 2.13 | 0.49 |
| 24:1H:1124:C:H2' | 24:1H:1125:G:O4' | 2.13 | 0.49 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 24:1H:1359:A:N1 | 24:1H:1372:U:C4 | 2.80 | 0.49 |
| 24:1H:2032:G:C8 | 57:1H:3652:HOH:O | 2.60 | 0.49 |
| 24:1H:2126:A:N6 | 24:1H:2172:U:OP1 | 2.46 | 0.49 |
| 24:1H:2175:C:H1' | 26:71:217:THR:O | 2.13 | 0.49 |
| 25:16:94:C:H2' | 25:16:95:U:H6 | 1.78 | 0.49 |
| 27:11:10:THR:OG1 | 27:11:13:ARG:HB2 | 2.13 | 0.49 |
| 31:51:153:LYS:H | 31:51:153:LYS:HD2 | 1.78 | 0.49 |
| 46:I8:53:MET:HG3 | 46:I8:59:LEU:CD2 | 2.43 | 0.49 |
| 54:Q8:54:GLU:OE1 | 54:Q8:54:GLU:N | 2.45 | 0.49 |
| 1:1G:300:A:H2' | 1:1G:301:G:O4' | 2.13 | 0.49 |
| 1:1G:491:G:H2' | 1:1G:492:G:O4' | 2.13 | 0.49 |
| 1:1G:582:U:H5" | 15:6A:64:ARG:NH2 | 2.28 | 0.49 |
| 2:12:77:ALA:O | 2:12:81:VAL:HG23 | 2.13 | 0.49 |
| 9:82:77:ILE:O | 9:82:81:ILE:HG23 | 2.12 | 0.49 |
| 24:14:558:G:OP2 | 33:15:111:PRO:HD2 | 2.13 | 0.49 |
| 24:14:2113:U:C5 | 24:14:2114:A:H1' | 2.48 | 0.49 |
| 24:14:2132:U:H3 | 26:79:8:ARG:HH21 | 1.60 | 0.49 |
| 30:49:138:GLN:OE1 | 30:49:153:ARG:N | 2.39 | 0.49 |
| 45:D5:17:ALA:O | 45:D5:20:ARG:HB2 | 2.13 | 0.49 |
| 1:13:475:G:H2' | 1:13:476:G:O4' | 2.13 | 0.49 |
| 1:13:562:C:H1' | 12:3I:15:ARG:HB3 | 1.94 | 0.49 |
| 1:13:572:A:N3 | 1:13:917:G:H1' | 2.28 | 0.49 |
| 1:13:890:G:O2' | 1:13:906:G:O6 | 2.29 | 0.49 |
| 2:1E:24:TRP:CZ3 | 2:1E:26:PRO:HA | 2.47 | 0.49 |
| 2:1E:237:ALA:O | 2:1E:239:VAL:N | 2.45 | 0.49 |
| 7:6E:26:PHE:O | 7:6E:30:ILE:HG13 | 2.12 | 0.49 |
| 12:3I:10:LEU:HD22 | 17:8I:32:TYR:CE1 | 2.48 | 0.49 |
| 13:4I:15:VAL:O | 13:4I:19:LEU:HD13 | 2.13 | 0.49 |
| 24:1H:845:G:H21 | 24:1H:933:A:H62 | 1.60 | 0.49 |
| 24:1H:981:A:N1 | 24:1H:2027:G:O2' | 2.43 | 0.49 |
| 24:1H:1899:G:O2' | 24:1H:1900:A:P | 2.71 | 0.49 |
| 25:16:73:A:H2' | 25:16:74:U:O4' | 2.13 | 0.49 |
| 27:11:94:LEU:HD22 | 27:11:95:LEU:N | 2.27 | 0.49 |
| 27:11:232:PRO:HB3 | 27:11:244:ARG:CZ | 2.43 | 0.49 |
| 34:68:85:VAL:HG11 | 34:68:114:ILE:HD13 | 1.95 | 0.49 |
| 1:1G:433:C:H2' | 1:1G:434:U:H6 | 1.78 | 0.49 |
| 1:1G:1075:C:O3' | 2:12:175:ARG:NH1 | 2.39 | 0.49 |
| 1:1G:1374:A:H2' | 1:1G:1375:A:H5' | 1.95 | 0.49 |
| 1:1G:1508:G:H2' | 1:1G:1509:C:O4' | 2.13 | 0.49 |
| 2:12:5:ILE:HD12 | 2:12:56:ARG:HH22 | 1.78 | 0.49 |
| 4:32:26:CYS:HA | 4:32:31:CYS:HB3 | 1.95 | 0.49 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 22:3L:13:G:H2' | 22:3L:14:A:H8 | 1.78 | 0.49 |
| 24:14:414:C:O2' | 24:14:415:A:H5' | 2.12 | 0.49 |
| 24:14:849:A:H5" | 24:14:850:C:OP2 | 2.12 | 0.49 |
| 24:14:1050:A:O2' | 24:14:2752:C:H1' | 2.13 | 0.49 |
| 24:14:1106:G:H3' | 24:14:1107:G:H8 | 1.78 | 0.49 |
| 24:14:1542:G:O5' | 24:14:1543:A:H5" | 2.13 | 0.49 |
| 24:14:2503:A:H4' | 24:14:2504:U:OP1 | 2.12 | 0.49 |
| 25:1J:20:C:H42 | 25:1J:63:G:H1 | 1.60 | 0.49 |
| 32:69:38:LEU:HB3 | 32:69:40:THR:HG22 | 1.95 | 0.49 |
| 35:35:30:THR:CG2 | 35:35:35:HIS:H | 2.26 | 0.49 |
| 40:85:28:ARG:HD3 | 40:85:38:THR:OG1 | 2.12 | 0.49 |
| 45:D5:14:LYS:HA | 45:D5:15:PRO:HD3 | 1.69 | 0.49 |
| 50:I5:58:ARG:HH12 | 50:I5:62:ARG:HB2 | 1.78 | 0.49 |
| 1:13:160:A:H1' | 1:13:344:A:C5 | 2.48 | 0.48 |
| 1:13:373:A:C2 | 1:13:374:A:C8 | 3.00 | 0.48 |
| 1:13:448:A:H2' | 1:13:449:C:O2 | 2.13 | 0.48 |
| 1:13:703:G:H8 | 1:13:703:G:O5' | 1.96 | 0.48 |
| 1:13:1349:A:H2' | 1:13:1350:A:C8 | 2.48 | 0.48 |
| 2:1E:15:VAL:HG22 | 2:1E:209:ARG:HB2 | 1.95 | 0.48 |
| 3:2E:57:ILE:HG12 | 3:2E:66:VAL:HG13 | 1.94 | 0.48 |
| 12:3I:28:LYS:HB2 | 12:3I:33:ARG:HH11 | 1.78 | 0.48 |
| 22:3K:17:OMG:H2' | 22:3K:66:G:N2 | 2.27 | 0.48 |
| 24:1H:654(G):C:N4 | 24:1H:654(L):G:OP2 | 2.45 | 0.48 |
| 24:1H:1224:G:OP2 | 41:D8:66:ARG:NH2 | 2.46 | 0.48 |
| 24:1H:1429:G:H2' | 24:1H:1430:C:C6 | 2.48 | 0.48 |
| 24:1H:2791:C:H2' | 24:1H:2792:G:C8 | 2.45 | 0.48 |
| 24:1H:2850:A:C2 | 24:1H:2851:A:C4 | 3.01 | 0.48 |
| 27:11:69:ARG:HH11 | 27:11:69:ARG:HG3 | 1.77 | 0.48 |
| 35:78:49:ARG:HG3 | 35:78:49:ARG:HH11 | 1.77 | 0.48 |
| 35:78:52:GLU:HG2 | 35:78:57:THR:HG22 | 1.94 | 0.48 |
| 48:K8:48:HIS:O | 48:K8:52:ASP:HB2 | 2.13 | 0.48 |
| 1:1G:438:G:OP1 | 4:32:125:HIS:HE1 | 1.96 | 0.48 |
| 1:1G:1505:G:H1' | 23:4L:13:A:C2 | 2.48 | 0.48 |
| 4:32:139:ARG:HH11 | 4:32:139:ARG:CG | 2.24 | 0.48 |
| 22:3L:80:C:H2' | 22:3L:81:C:H6 | 1.77 | 0.48 |
| 24:14:1416:G:O2' | 24:14:1417:C:C6 | 2.66 | 0.48 |
| 24:14:1614:A:H62 | 42:A5:93:ALA:HB2 | 1.78 | 0.48 |
| 24:14:1728:G:O6 | 24:14:1730:U:H5' | 2.13 | 0.48 |
| 24:14:1848:A:H2' | 24:14:1849:G:C8 | 2.48 | 0.48 |
| 24:14:2112:G:H2' | 24:14:2113:U:H5 | 1.77 | 0.48 |
| 24:14:2720:U:N3 | 24:14:2873:A:C2 | 2.69 | 0.48 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 47:F5:84:GLY:O | 47:F5:87:PRO:HD2 | 2.13 | 0.48 |
| 49:H5:26:LEU:HD21 | 49:H5:46:ASN:HB2 | 1.94 | 0.48 |
| 1:13:134:A:H1' | 1:13:325:A:C5 | 2.48 | 0.48 |
| 1:13:256:U:H2' | 1:13:257:G:C8 | 2.48 | 0.48 |
| 1:13:877:C:H5" | 8:7E:88:LYS:HD3 | 1.95 | 0.48 |
| 1:13:1118:C:H1' | 1:13:1179:A:C4 | 2.48 | 0.48 |
| 1:13:1284:C:H3' | 1:13:1285:A:C8 | 2.47 | 0.48 |
| 4:3E:33:MET:HG3 | 4:3E:37:PRO:HA | 1.95 | 0.48 |
| 4:3E:108:LEU:CD1 | 4:3E:174:LEU:HD13 | 2.43 | 0.48 |
| 6:5E:89:MET:HG2 | 6:5E:91:VAL:HG23 | 1.96 | 0.48 |
| 11:2I:46:GLY:HA2 | 11:2I:50:TYR:O | 2.13 | 0.48 |
| 14:5I:24:CYS:SG | 14:5I:27:CYS:HB2 | 2.52 | 0.48 |
| 22:3K:51:C:C5 | 22:3K:52:G:H1' | 2.48 | 0.48 |
| 24:1H:557:U:C2 | 24:1H:558:G:C8 | 3.00 | 0.48 |
| 24:1H:718:A:H3' | 24:1H:719:C:H6 | 1.77 | 0.48 |
| 24:1H:1278:A:OP1 | 37:98:36:THR:HG22 | 2.12 | 0.48 |
| 24:1H:2370:G:N3 | 52:O8:45:LYS:NZ | 2.61 | 0.48 |
| 33:58:14:VAL:HG13 | 33:58:137:LYS:HG2 | 1.95 | 0.48 |
| 34:68:7:TYR:CE1 | 34:68:20:MET:HB2 | 2.48 | 0.48 |
| 37:98:101:ALA:HA | 51:N8:44:THR:HG21 | 1.95 | 0.48 |
| 40:C8:5:LYS:HB2 | 40:C8:5:LYS:NZ | 2.28 | 0.48 |
| 44:G8:55:TYR:CE2 | 44:G8:61:ILE:HD11 | 2.49 | 0.48 |
| 44:G8:78:ALA:HB3 | 44:G8:79:CYS:SG | 2.53 | 0.48 |
| 44:G8:89:PHE:HD1 | 44:G8:90:LEU:N | 2.12 | 0.48 |
| 45:H8:137:ILE:HG21 | 45:H8:155:LEU:HD13 | 1.94 | 0.48 |
| 49:L8:6:VAL:HB | 49:L8:54:VAL:HG21 | 1.94 | 0.48 |
| 1:1G:392:G:H2' | 1:1G:393:A:C8 | 2.48 | 0.48 |
| 1:1G:1349:A:H2' | 1:1G:1350:A:O4' | 2.13 | 0.48 |
| 3:22:9:GLY:HA3 | 14:5A:49:HIS:HA | 1.95 | 0.48 |
| 5:42:152:ARG:HB3 | 8:72:43:GLY:HA3 | 1.95 | 0.48 |
| 9:82:26:VAL:HG13 | 9:82:61:ALA:HB3 | 1.95 | 0.48 |
| 9:82:27:THR:OG1 | 9:82:32:ASP:HA | 2.13 | 0.48 |
| 11:2A:84:VAL:HG21 | 11:2A:95:ILE:HD11 | 1.95 | 0.48 |
| 12:3A:109:GLY:HA3 | 12:3A:121:GLY:O | 2.14 | 0.48 |
| 24:14:832:G:H5' | 35:35:45:LEU:HD11 | 1.94 | 0.48 |
| 24:14:972:G:H3' | 24:14:973:A:H2' | 1.95 | 0.48 |
| 24:14:1230:C:H2' | 24:14:1231:G:C8 | 2.48 | 0.48 |
| 24:14:1459:G:H5" | 24:14:1460:A:OP2 | 2.13 | 0.48 |
| 24:14:1778:U:P | 57:14:3595:HOH:O | 2.70 | 0.48 |
| 24:14:2075:U:C4 | 24:14:2238:G:C6 | 3.01 | 0.48 |
| 30:49:143:GLU:HA | 50:I5:28:LYS:HD2 | 1.94 | 0.48 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 32:69:90:GLY:O | 32:69:121:LYS:HD2 | 2.13 | 0.48 |
| 41:95:2:PHE:H | 41:95:42:GLY:HA3 | 1.78 | 0.48 |
| 45:D5:152:ALA:HB2 | 45:D5:169:GLU:O | 2.13 | 0.48 |
| 46:E5:27:GLU:HB2 | 46:E5:69:PHE:CD1 | 2.47 | 0.48 |
| 1:13:191:G:H1' | 20:BI:105:SER:HA | 1.94 | 0.48 |
| 1:13:411:A:C6 | 1:13:429:U:C4 | 3.01 | 0.48 |
| 1:13:928:G:C2 | 1:13:1390:U:O2 | 2.67 | 0.48 |
| 1:13:1253:G:H1 | 1:13:1284:C:H42 | 1.60 | 0.48 |
| 15:6I:11:VAL:HG21 | 15:6I:34:LEU:HD13 | 1.95 | 0.48 |
| 24:1H:275:G:N7 | 24:1H:363:G:C2 | 2.81 | 0.48 |
| 24:1H:399:G:OP2 | 57:1H:3699:HOH:O | 2.19 | 0.48 |
| 24:1H:556:G:H2' | 24:1H:557:U:C6 | 2.48 | 0.48 |
| 24:1H:768:G:C6 | 24:1H:769:G:C5 | 3.01 | 0.48 |
| 24:1H:1222:C:H2' | 24:1H:1223:C:H6 | 1.78 | 0.48 |
| 24:1H:2473:U:O2' | 24:1H:2474:C:O4' | 2.19 | 0.48 |
| 24:1H:2864:G:H2' | 24:1H:2865:U:C6 | 2.48 | 0.48 |
| 44:G8:28:LYS:CE | 44:G8:40:GLU:HB2 | 2.43 | 0.48 |
| 45:H8:27:VAL:HG22 | 45:H8:29:TYR:HD1 | 1.77 | 0.48 |
| 1:1G:197:A:C6 | 1:1G:221:C:H4' | 2.48 | 0.48 |
| 1:1G:1223:C:P | 19:AA:78:ARG:HH22 | 2.35 | 0.48 |
| 3:22:25:GLY:H | 3:22:28:GLN:NE2 | 2.11 | 0.48 |
| 4:32:119:GLN:HG2 | 4:32:123:HIS:CD2 | 2.47 | 0.48 |
| 20:BA:42:GLN:O | 20:BA:46:GLU:HG3 | 2.12 | 0.48 |
| 24:14:973:A:H5' | 24:14:1188:U:C1' | 2.43 | 0.48 |
| 24:14:1491:G:O2' | 27:19:101:GLU:HB2 | 2.13 | 0.48 |
| 24:14:2377:A:O3' | 38:65:111:GLU:HG2 | 2.14 | 0.48 |
| 24:14:2861:G:H2' | 24:14:2862:G:H8 | 1.77 | 0.48 |
| 25:1J:91:C:OP1 | 45:D5:79:ARG:NH2 | 2.47 | 0.48 |
| 28:29:105:THR:HG1 | 28:29:199:ARG:HH22 | 1.59 | 0.48 |
| 33:15:42:TRP:HA | 33:15:48:MET:SD | 2.54 | 0.48 |
| 36:45:136:ALA:HB1 | 45:D5:48:PHE:CE1 | 2.49 | 0.48 |
| 41:95:56:SER:O | 41:95:100:ARG:N | 2.46 | 0.48 |
| 50:I5:23:GLU:C | 50:I5:24:THR:HG1 | 2.16 | 0.48 |
| 52:K5:14:THR:HG21 | 52:K5:20:ASN:N | 2.28 | 0.48 |
| 1:13:130:A:OP2 | 17:8I:63:ARG:NE | 2.36 | 0.48 |
| 1:13:300:A:C5 | 1:13:301:G:H1' | 2.48 | 0.48 |
| 1:13:686:U:HO2' | 1:13:687:A:P | 2.35 | 0.48 |
| 1:13:962:C:O2' | 57:13:1815:HOH:O | 2.20 | 0.48 |
| 1:13:1082:G:H2' | 1:13:1083:U:O4' | 2.13 | 0.48 |
| 1:13:1192:C:OP2 | 3:2E:4:LYS:NZ | 2.43 | 0.48 |
| 7:6E:15:ASP:OD1 | 7:6E:44:TYR:OH | 2.30 | 0.48 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 20:BI:83:ARG:HA | 20:BI:86:ARG:HB3 | 1.94 | 0.48 |
| 22:3K:79:A:H2' | 22:3K:80:C:C6 | 2.48 | 0.48 |
| 24:1H:50:U:H3' | 24:1H:51:G:H5' | 1.95 | 0.48 |
| 24:1H:234:C:C2 | 24:1H:235:U:C5 | 3.02 | 0.48 |
| 24:1H:270(X):G:C6 | 24:1H:270(Y):G:C2 | 3.01 | 0.48 |
| 24:1H:286:C:H2' | 24:1H:287:C:H6 | 1.79 | 0.48 |
| 24:1H:478:A:C6 | 24:1H:480:A:C6 | 3.01 | 0.48 |
| 24:1H:1359:A:C2 | 24:1H:1372:U:O4 | 2.67 | 0.48 |
| 24:1H:2115:G:C6 | 24:1H:2117:A:H3' | 2.48 | 0.48 |
| 24:1H:2290:G:C2 | 24:1H:2291:U:C2 | 3.01 | 0.48 |
| 24:1H:2371:G:O2' | 52:O8:46:HIS:ND1 | 2.30 | 0.48 |
| 29:31:6:VAL:HG12 | 29:31:7:TYR:N | 2.29 | 0.48 |
| 29:31:150:GLY:HA2 | 29:31:172:TRP:CE3 | 2.49 | 0.48 |
| 32:61:3:VAL:HG12 | 32:61:37:VAL:O | 2.13 | 0.48 |
| 38:A8:83:LYS:NZ | 38:A8:110:LEU:HB2 | 2.28 | 0.48 |
| 40:C8:84:LYS:HD2 | 40:C8:84:LYS:C | 2.38 | 0.48 |
| 44:G8:99:CYS:SG | 44:G8:100:ALA:N | 2.85 | 0.48 |
| 47:J8:78:LYS:HD2 | 47:J8:79:GLY:N | 2.28 | 0.48 |
| 1:1G:36:C:O2' | 12:3A:117:ARG:NH2 | 2.45 | 0.48 |
| 1:1G:165:C:H2' | 1:1G:166:G:H8 | 1.78 | 0.48 |
| 1:1G:526:C:C5 | 1:1G:527:G:H1' | 2.48 | 0.48 |
| 1:1G:1095:U:H5" | 1:1G:1109:C:O2 | 2.13 | 0.48 |
| 4:32:70:ILE:HD11 | 4:32:75:PHE:HD1 | 1.78 | 0.48 |
| 24:14:403:U:H4' | 24:14:404:C:H5' | 1.95 | 0.48 |
| 24:14:603:A:C8 | 24:14:604:G:H1' | 2.47 | 0.48 |
| 24:14:631:A:H2' | 24:14:632:A:O4' | 2.13 | 0.48 |
| 24:14:1056:G:H5" | 24:14:1057:A:H5' | 1.95 | 0.48 |
| 24:14:1160:G:C6 | 24:14:1161:C:C4 | 3.02 | 0.48 |
| 24:14:1197:G:H2' | 24:14:1198:U:H6 | 1.77 | 0.48 |
| 24:14:1448:G:O2' | 24:14:1529:A:N1 | 2.39 | 0.48 |
| 24:14:1500:G:O2' | 27:19:100:GLY:O | 2.27 | 0.48 |
| 24:14:2224:G:H4' | 24:14:2226:C:C2 | 2.48 | 0.48 |
| 24:14:2704:C:H2' | 24:14:2705:A:C8 | 2.49 | 0.48 |
| 28:29:201:THR:HG22 | 28:29:202:LYS:N | 2.27 | 0.48 |
| 29:39:111:ALA:HB2 | 29:39:206:ILE:HG21 | 1.94 | 0.48 |
| 30:49:41:GLN:O | 30:49:43:LEU:HD22 | 2.14 | 0.48 |
| 38:65:24:LEU:HB2 | 38:65:85:VAL:HG12 | 1.96 | 0.48 |
| 43:B5:59:VAL:N | 43:B5:76:ARG:O | 2.45 | 0.48 |
| 1:13:625:G:C4 | 1:13:626:U:C5 | 3.02 | 0.48 |
| 1:13:742:G:OP2 | 15:6I:35:ARG:NH2 | 2.45 | 0.48 |
| 1:13:983:A:H2 | 1:13:984:C:C6 | 2.31 | 0.48 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 2:1E:167:PRO:HG2 | 2:1E:192:SER:CB | 2.43 | 0.48 |
| 9:8E:83:ARG:O | 9:8E:86:VAL:HG12 | 2.13 | 0.48 |
| 22:2K:23:A:H2' | 22:2K:24:G:O4' | 2.12 | 0.48 |
| 22:2K:24:G:H2' | 22:2K:25:G:H5" | 1.95 | 0.48 |
| 24:1H:638:G:H2' | 24:1H:639:U:O4' | 2.13 | 0.48 |
| 24:1H:1210:A:H5' | 24:1H:1210:A:C8 | 2.47 | 0.48 |
| 24:1H:1473:G:H2' | 24:1H:1474:C:O4' | 2.14 | 0.48 |
| 24:1H:1517:G:H2' | 24:1H:1518:C:C6 | 2.49 | 0.48 |
| 24:1H:1547:C:H2' | 24:1H:1548:C:C6 | 2.49 | 0.48 |
| 24:1H:1833:U:O2' | 24:1H:1969:A:N1 | 2.39 | 0.48 |
| 24:1H:2298:A:H2' | 24:1H:2299:G:O4' | 2.14 | 0.48 |
| 24:1H:2441:C:OP2 | 24:1H:2586:C:O2' | 2.26 | 0.48 |
| 25:16:2:C:H2' | 25:16:3:C:C6 | 2.48 | 0.48 |
| 27:11:66:ASP:HB3 | 27:11:105:ILE:CD1 | 2.42 | 0.48 |
| 27:11:182:LEU:N | 27:11:272:ALA:HB3 | 2.17 | 0.48 |
| 30:41:12:TYR:HA | 30:41:16:ARG:HG3 | 1.95 | 0.48 |
| 31:51:129:THR:O | 31:51:129:THR:OG1 | 2.28 | 0.48 |
| 32:61:88:ILE:HG22 | 32:61:90:GLY:H | 1.78 | 0.48 |
| 40:C8:17:ILE:HG23 | 40:C8:39:LEU:HD12 | 1.96 | 0.48 |
| 1:1G:661:G:C2 | 1:1G:662:G:C8 | 3.01 | 0.48 |
| 1:1G:1025:U:H2' | 1:1G:1026:G:C8 | 2.49 | 0.48 |
| 1:1G:1267:C:O2 | 1:1G:1267:C:H2' | 2.13 | 0.48 |
| 1:1G:1321:C:H3' | 1:1G:1322:C:H5" | 1.96 | 0.48 |
| 4:32:18:LYS:HZ3 | 4:32:26:CYS:HB3 | 1.78 | 0.48 |
| 11:2A:85:ARG:HE | 11:2A:111:ASP:HB3 | 1.78 | 0.48 |
| 22:2L:15:G:N2 | 22:2L:57:C:H41 | 2.09 | 0.48 |
| 22:2L:71:C:H1' | 22:2L:72:U:OP2 | 2.13 | 0.48 |
| 24:14:869:G:N2 | 24:14:870:A:H1' | 2.29 | 0.48 |
| 24:14:948:G:C2 | 24:14:970:C:O2 | 2.67 | 0.48 |
| 24:14:1742:C:H5' | 24:14:1743:G:OP2 | 2.14 | 0.48 |
| 24:14:2893:G:H4' | 24:14:2894:G:O5' | 2.14 | 0.48 |
| 25:1J:8:U:O3' | 38:65:25:ARG:NH2 | 2.46 | 0.48 |
| 36:45:20:ALA:HB2 | 45:D5:79:ARG:CZ | 2.43 | 0.48 |
| 36:45:75:THR:HA | 36:45:90:VAL:HA | 1.95 | 0.48 |
| 39:75:74:ARG:HG2 | 39:75:74:ARG:HH11 | 1.78 | 0.48 |
| 39:75:102:ILE:C | 39:75:105:LEU:HB2 | 2.39 | 0.48 |
| 54:M5:40:GLU:N | 54:M5:43:GLN:HG3 | 2.27 | 0.48 |
| 1:13:958:A:OP1 | 19:AI:79:THR:HG21 | 2.14 | 0.48 |
| 1:13:1128:C:HO2' | 1:13:1130:A:H8 | 1.60 | 0.48 |
| 1:13:1169:A:C6 | 1:13:1170:A:N1 | 2.82 | 0.48 |
| 1:13:1180:A:OP1 | 9:8E:103:THR:OG1 | 2.27 | 0.48 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 3:2E:149:ALA:HA | 3:2E:201:TYR:O | 2.13 | 0.48 |
| 5:4E:153:LYS:HD2 | 5:4E:154:GLY:N | 2.28 | 0.48 |
| 6:5E:16:GLN:HA | 6:5E:19:LEU:HB3 | 1.94 | 0.48 |
| 6:5E:60:PHE:C | 6:5E:61:LEU:HD12 | 2.38 | 0.48 |
| 15:6I:56:LEU:O | 15:6I:60:VAL:HG23 | 2.12 | 0.48 |
| 20:BI:18:GLN:O | 20:BI:22:ARG:HB2 | 2.14 | 0.48 |
| 22:2K:1:G:O2' | 46:I8:6:GLY:HA2 | 2.12 | 0.48 |
| 24:1H:276:A:H2' | 24:1H:277:C:H5" | 1.96 | 0.48 |
| 24:1H:664:C:H4' | 24:1H:941:A:OP1 | 2.13 | 0.48 |
| 24:1H:1464:C:O2' | 24:1H:1528:A:H8 | 1.97 | 0.48 |
| 31:51:97:ARG:HG2 | 31:51:98:LEU:H | 1.77 | 0.48 |
| 35:78:52:GLU:HG3 | 35:78:57:THR:HG22 | 1.95 | 0.48 |
| 42:E8:18:ARG:NH1 | 42:E8:76:VAL:O | 2.47 | 0.48 |
| 48:K8:15:LYS:H | 48:K8:67:LYS:NZ | 2.12 | 0.48 |
| 1:1G:765:G:H5" | 1:1G:766:A:OP1 | 2.13 | 0.48 |
| 1:1G:791:G:C6 | 1:1G:792:A:N7 | 2.81 | 0.48 |
| 1:1G:1122:U:C2 | 1:1G:1123:A:C8 | 3.02 | 0.48 |
| 1:1G:1264:C:H2' | 1:1G:1265:G:C8 | 2.48 | 0.48 |
| 1:1G:1411:C:H2' | 1:1G:1412:C:C6 | 2.48 | 0.48 |
| 3:22:7:PRO:O | 3:22:11:ARG:NH1 | 2.47 | 0.48 |
| 22:2L:57:C:C5 | 22:2L:68:A:H1' | 2.49 | 0.48 |
| 24:14:270(H):C:O2' | 47:F5:78:LYS:NZ | 2.47 | 0.48 |
| 24:14:284:U:H2' | 24:14:285:C:C6 | 2.49 | 0.48 |
| 24:14:566:U:H5" | 35:35:29:LYS:HE3 | 1.96 | 0.48 |
| 24:14:1153:C:H2' | 24:14:1154:G:O4' | 2.13 | 0.48 |
| 24:14:1184:G:OP2 | 49:H5:30:ARG:NH2 | 2.46 | 0.48 |
| 24:14:1418:G:OP1 | 24:14:1588:C:O2' | 2.31 | 0.48 |
| 24:14:1431:U:H2' | 24:14:1432:C:C6 | 2.49 | 0.48 |
| 24:14:1952:A:H8 | 24:14:1952:A:O5' | 1.97 | 0.48 |
| 24:14:2626:C:H2' | 24:14:2627:G:O4' | 2.14 | 0.48 |
| 24:14:2729:G:H2' | 24:14:2730:C:C6 | 2.48 | 0.48 |
| 25:1J:40:U:O4 | 50:I5:2:LYS:HA | 2.13 | 0.48 |
| 25:1J:60:C:H2' | 25:1J:61:G:C8 | 2.48 | 0.48 |
| 29:39:41:LEU:H | 29:39:41:LEU:HG | 1.47 | 0.48 |
| 29:39:122:LYS:HD2 | 29:39:191:ARG:HB3 | 1.96 | 0.48 |
| 41:95:35:LEU:HB2 | 41:95:37:VAL:CG1 | 2.44 | 0.48 |
| 46:E5:23:VAL:HA | 46:E5:38:VAL:HG22 | 1.95 | 0.48 |
| 50:I5:58:ARG:HH21 | 50:I5:61:ARG:HB3 | 1.78 | 0.48 |
| 1:13:77:C:H2' | 1:13:78:G:C8 | 2.49 | 0.48 |
| 1:13:428:G:C8 | 1:13:430:A:C4 | 3.02 | 0.48 |
| 1:13:619:U:C2 | 4:3E:135:LEU:HD21 | 2.48 | 0.48 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 1:13:692:U:O2' | 1:13:694:A:N7 | 2.26 | 0.48 |
| 1:13:859:A:H2' | 1:13:860:A:O4' | 2.13 | 0.48 |
| 1:13:1157:A:H2' | 1:13:1157:A:N3 | 2.29 | 0.48 |
| 12:3I:44:THR:HG22 | 12:3I:52:LEU:HD23 | 1.96 | 0.48 |
| 19:AI:50:ALA:HA | 19:AI:58:VAL:O | 2.14 | 0.48 |
| 24:1H:142:G:H2' | 24:1H:143:C:H6 | 1.79 | 0.48 |
| 24:1H:757:U:H2' | 24:1H:758:C:O4' | 2.13 | 0.48 |
| 24:1H:1036:G:H2' | 24:1H:1037:G:O4' | 2.14 | 0.48 |
| 24:1H:1141:U:H4' | 24:1H:1142(A):A:N9 | 2.28 | 0.48 |
| 24:1H:1184:G:N2 | 57:1H:3814:HOH:O | 2.46 | 0.48 |
| 24:1H:2402:C:H2' | 24:1H:2403:C:C6 | 2.48 | 0.48 |
| 24:1H:2591:C:P | 27:11:239:ARG:HG3 | 2.53 | 0.48 |
| 24:1H:2679:A:H2' | 24:1H:2680:C:H6 | 1.77 | 0.48 |
| 24:1H:2751:G:C2 | 31:51:3:ARG:HB3 | 2.48 | 0.48 |
| 24:1H:2799:A:O3' | 24:1H:2895:U:H4' | 2.14 | 0.48 |
| 25:16:30:C:H2' | 25:16:31:C:H5' | 1.95 | 0.48 |
| 31:51:20:ALA:HB1 | 31:51:21:PRO:HD2 | 1.95 | 0.48 |
| 32:61:84:GLY:N | 32:61:89:TYR:HE1 | 2.12 | 0.48 |
| 33:58:42:TRP:HA | 33:58:48:MET:HE1 | 1.95 | 0.48 |
| 36:88:135:ASP:N | 36:88:138:ASP:OD2 | 2.46 | 0.48 |
| 43:F8:15:GLU:H | 43:F8:15:GLU:CD | 2.20 | 0.48 |
| 45:H8:132:ASN:OD1 | 45:H8:132:ASN:N | 2.46 | 0.48 |
| 1:1G:804:U:H5" | 1:1G:805:C:OP2 | 2.13 | 0.48 |
| 1:1G:993:G:H2' | 1:1G:995:C:H41 | 1.78 | 0.48 |
| 1:1G:1192:C:C5 | 1:1G:1193:G:C8 | 3.02 | 0.48 |
| 1:1G:1245:A:H2' | 1:1G:1246:C:O4' | 2.13 | 0.48 |
| 4:32:141:ARG:HB3 | 4:32:141:ARG:NH1 | 2.29 | 0.48 |
| 5:42:147:ASP:OD1 | 5:42:147:ASP:N | 2.38 | 0.48 |
| 9:82:48:GLU:HB3 | 9:82:101:PHE:HE2 | 1.77 | 0.48 |
| 10:1A:49:VAL:O | 10:1A:60:ARG:HB3 | 2.14 | 0.48 |
| 12:3A:49:ASN:ND2 | 12:3A:92:ASP:OD2 | 2.34 | 0.48 |
| 22:2L:42:U:H2' | 22:2L:43:G:C8 | 2.48 | 0.48 |
| 24:14:2081:C:H2' | 24:14:2082:A:H8 | 1.77 | 0.48 |
| 24:14:2324:C:H5" | 24:14:2325:G:C5' | 2.44 | 0.48 |
| 24:14:2364:C:H4' | 46:E5:56:ASP:OD1 | 2.13 | 0.48 |
| 24:14:2493:U:H2' | 24:14:2494:G:O4' | 2.14 | 0.48 |
| 25:1J:87:G:H2' | 25:1J:88:C:H5" | 1.96 | 0.48 |
| 29:39:20:LEU:HD23 | 29:39:21:ALA:H | 1.78 | 0.48 |
| 29:39:21:ALA:C | 29:39:23:ASP:N | 2.72 | 0.48 |
| 29:39:131:GLY:HA2 | 29:39:138:GLU:HB3 | 1.96 | 0.48 |
| 39:75:26:ASP:O | 39:75:49:VAL:HG13 | 2.14 | 0.48 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 45:D5:23:LYS:HZ3 | 45:D5:40:ASP:HB2 | 1.78 | 0.48 |
| 1:13:265:G:O2' | 17:8I:66:SER:O | 2.30 | 0.48 |
| 1:13:434:U:H2' | 1:13:435:C:C6 | 2.49 | 0.48 |
| 1:13:1165:C:H2' | 1:13:1166:G:O4' | 2.13 | 0.48 |
| 1:13:1298:C:OP2 | 7:6E:114:ARG:NH2 | 2.41 | 0.48 |
| 2:1E:145:LEU:HD12 | 2:1E:149:LEU:HD12 | 1.95 | 0.48 |
| 2:1E:237:ALA:C | 2:1E:239:VAL:N | 2.69 | 0.48 |
| 6:5E:18:GLN:O | 6:5E:21:LEU:HB2 | 2.14 | 0.48 |
| 13:4I:90:LEU:HA | 13:4I:93:ARG:CG | 2.44 | 0.48 |
| 17:8I:6:LEU:HD13 | 17:8I:23:VAL:HG11 | 1.95 | 0.48 |
| 20:BI:25:ARG:HH11 | 20:BI:25:ARG:HG3 | 1.78 | 0.48 |
| 24:1H:1012:U:O4 | 33:58:25:ARG:HA | 2.14 | 0.48 |
| 24:1H:1479:G:H5' | 24:1H:1558:A:H2 | 1.78 | 0.48 |
| 24:1H:1571:A:O5' | 24:1H:1571:A:H8 | 1.96 | 0.48 |
| 24:1H:1677:A:H2' | 24:1H:1678:G:C8 | 2.49 | 0.48 |
| 24:1H:1983:C:C2' | 24:1H:1984:G:H5' | 2.43 | 0.48 |
| 24:1H:2262:U:O2' | 24:1H:2263:C:H5' | 2.13 | 0.48 |
| 24:1H:2275:C:O2 | 36:88:85:LYS:HG3 | 2.13 | 0.48 |
| 36:88:135:ASP:HB3 | 36:88:137:TYR:N | 2.26 | 0.48 |
| 37:98:96:ARG:CZ | 37:98:117:VAL:HG23 | 2.44 | 0.48 |
| 41:D8:2:PHE:C | 41:D8:2:PHE:CD1 | 2.92 | 0.48 |
| 42:E8:78:GLU:OE1 | 42:E8:99:ARG:HG2 | 2.14 | 0.48 |
| 45:H8:54:HIS:HD2 | 45:H8:99:TYR:O | 1.97 | 0.48 |
| 1:1G:1002:G:H22 | 1:1G:1038:C:H42 | 1.62 | 0.48 |
| 1:1G:1105:A:H2' | 1:1G:1106:G:C8 | 2.48 | 0.48 |
| 1:1G:1297:C:OP2 | 1:1G:1297:C:H6 | 1.97 | 0.48 |
| 24:14:263:C:O2' | 24:14:429:A:N3 | 2.44 | 0.48 |
| 24:14:1226:G:C4' | 41:95:84:LYS:HA | 2.43 | 0.48 |
| 24:14:2017:U:O2 | 51:J5:10:LYS:HB2 | 2.13 | 0.48 |
| 24:14:2306:C:C3' | 24:14:2307:G:H5" | 2.39 | 0.48 |
| 29:39:51:THR:HB | 29:39:88:VAL:HG11 | 1.96 | 0.48 |
| 30:49:36:LYS:CE | 30:49:160:VAL:HG21 | 2.44 | 0.48 |
| 30:49:95:ARG:O | 30:49:99:MET:HG2 | 2.13 | 0.48 |
| 32:69:110:ASP:H | 32:69:130:TYR:HH | 1.59 | 0.48 |
| 38:65:83:LYS:HB3 | 38:65:109:GLY:H | 1.78 | 0.48 |
| 52:K5:41:PRO:HG2 | 52:K5:43:CYS:O | 2.14 | 0.48 |
| 1:13:1285:A:H3' | 21:1F:26:LYS:HD3 | 1.96 | 0.48 |
| 6:5E:22:GLU:O | 6:5E:26:ILE:HG13 | 2.14 | 0.48 |
| 6:5E:55:ASP:HA | 6:5E:56:PRO:HD2 | 1.73 | 0.48 |
| 16:7I:20:VAL:HG21 | 16:7I:32:TYR:CD2 | 2.48 | 0.48 |
| 22:2K:17:OMG:C2 | 22:2K:67:A:C5 | 3.02 | 0.48 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 22:3K:7:G:N2 | 22:3K:75:C:O2 | 2.40 | 0.48 |
| 24:1H:813:U:H2' | 24:1H:814:C:C6 | 2.48 | 0.48 |
| 24:1H:1132:A:H2' | 24:1H:1133:U:C6 | 2.48 | 0.48 |
| 24:1H:1512:G:H2' | 24:1H:1513:C:C6 | 2.49 | 0.48 |
| 25:16:15:A:H1' | 25:16:109:G:C4 | 2.49 | 0.48 |
| 27:11:8:PRO:CB | 27:11:14:ARG:HB2 | 2.42 | 0.48 |
| 27:11:25:THR:C | 27:11:26:LYS:O | 2.55 | 0.48 |
| 28:21:101:ARG:CZ | 28:21:171:GLU:HB2 | 2.43 | 0.48 |
| 33:58:5:VAL:HG22 | 33:58:6:PRO:HD2 | 1.95 | 0.48 |
| 37:98:33:ARG:NH2 | 51:N8:55:ARG:HG2 | 2.25 | 0.48 |
| 45:H8:144:LEU:HD23 | 45:H8:148:ASP:HB3 | 1.96 | 0.48 |
| 49:L8:41:PRO:HA | 49:L8:44:ARG:HG2 | 1.95 | 0.48 |
| 1:1G:986:A:O2' | 19:AA:55:LYS:NZ | 2.29 | 0.48 |
| 1:1G:1134:G:C2 | 1:1G:1135:U:H1' | 2.49 | 0.48 |
| 2:12:215:LEU:O | 2:12:219:VAL:HG12 | 2.14 | 0.48 |
| 10:1A:63:PHE:HD1 | 14:5A:58:LYS:HA | 1.78 | 0.48 |
| 16:7A:39:TYR:HB2 | 16:7A:49:LEU:HD13 | 1.94 | 0.48 |
| 19:AA:65:ASN:HB2 | 50:I5:55:ARG:HB2 | 1.95 | 0.48 |
| 24:14:75:G:N2 | 24:14:112:U:O2 | 2.42 | 0.48 |
| 24:14:142:G:H1' | 43:B5:37:THR:HG21 | 1.96 | 0.48 |
| 24:14:2536:G:C6 | 24:14:2537:U:C4 | 3.01 | 0.48 |
| 24:14:2684:U:H1' | 34:25:70:LYS:HD3 | 1.96 | 0.48 |
| 24:14:2773:C:H5" | 28:29:164:ARG:HG2 | 1.96 | 0.48 |
| 24:14:2820:A:C6 | 37:55:4:LEU:HD11 | 2.49 | 0.48 |
| 32:69:120:ILE:HG22 | 32:69:122:GLU:H | 1.79 | 0.48 |
| 32:69:144:VAL:HG22 | 32:69:145:VAL:HG22 | 1.96 | 0.48 |
| 40:85:98:LEU:O | 40:85:99:ALA:HB3 | 2.14 | 0.48 |
| 44:C5:43:ASN:HB3 | 44:C5:64:GLU:HA | 1.96 | 0.48 |
| 46:E5:68:GLU:HG3 | 46:E5:82:ARG:HH11 | 1.79 | 0.48 |
| 1:13:178:C:H2' | 1:13:179:A:O4' | 2.13 | 0.48 |
| 1:13:952:U:H4' | 1:13:964:A:N1 | 2.29 | 0.48 |
| 1:13:1295:G:O3' | 13:4I:14:ARG:NH1 | 2.47 | 0.48 |
| 24:1H:30:G:H2' | 24:1H:31:C:C6 | 2.49 | 0.48 |
| 24:1H:184:C:H2' | 24:1H:185:U:C6 | 2.48 | 0.48 |
| 24:1H:485:C:H2' | 24:1H:486:C:H6 | 1.79 | 0.48 |
| 24:1H:1424:G:H2' | 24:1H:1425:G:O4' | 2.14 | 0.48 |
| 24:1H:1657:C:H2' | 24:1H:1658:C:H6 | 1.79 | 0.48 |
| 24:1H:2502:G:H5" | 24:1H:2503:A:C5' | 2.43 | 0.48 |
| 27:11:121:PRO:HB3 | 27:11:135:PHE:CE2 | 2.49 | 0.48 |
| 29:31:114:VAL:HG21 | 29:31:202:PHE:CZ | 2.49 | 0.48 |
| 32:61:110:ASP:HB3 | 32:61:111:PRO:C | 2.39 | 0.48 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 35:78:59:LEU:HA | 35:78:62:LEU:HD22 | 1.96 | 0.48 |
| 42:E8:79:GLY:CA | 42:E8:100:THR:HG22 | 2.43 | 0.48 |
| 1:1G:571:U:O2 | 1:1G:918:A:H5' | 2.14 | 0.48 |
| 1:1G:583:A:H2' | 1:1G:584:G:O4' | 2.14 | 0.48 |
| 1:1G:922:G:H2' | 1:1G:923:A:C8 | 2.49 | 0.48 |
| 1:1G:1387:G:H2' | 1:1G:1388:C:H6 | 1.79 | 0.48 |
| 5:42:90:VAL:HG23 | 5:42:121:LYS:O | 2.14 | 0.48 |
| 11:2A:17:GLY:HA3 | 11:2A:77:MET:SD | 2.53 | 0.48 |
| 13:4A:39:ILE:HG12 | 13:4A:55:ARG:NH2 | 2.29 | 0.48 |
| 15:6A:25:THR:HG21 | 15:6A:70:LEU:HB2 | 1.94 | 0.48 |
| 22:2L:21:A:N3 | 22:2L:21:A:H2' | 2.27 | 0.48 |
| 24:14:251:A:C5 | 24:14:252:G:H1' | 2.49 | 0.48 |
| 24:14:1342:A:C2 | 24:14:1397:U:C2 | 3.02 | 0.48 |
| 24:14:1771:C:C1' | 24:14:1786:A:H8 | 2.25 | 0.48 |
| 24:14:2052:G:O4' | 28:29:142:GLY:HA3 | 2.14 | 0.48 |
| 24:14:2175:C:O2' | 26:79:219:GLY:O | 2.30 | 0.48 |
| 28:29:120:TRP:CG | 28:29:155:LYS:HB3 | 2.48 | 0.48 |
| 30:49:114:ILE:HG12 | 30:49:140:ILE:HD13 | 1.96 | 0.48 |
| 36:45:6:ARG:C | 36:45:7:MET:HG2 | 2.38 | 0.48 |
| 39:75:113:LYS:O | 39:75:114:LEU:HD23 | 2.14 | 0.48 |
| 45:D5:80:ARG:HD3 | 45:D5:82:ARG:NH1 | 2.29 | 0.48 |
| 1:13:56:U:H2' | 1:13:57:G:C8 | 2.49 | 0.47 |
| 1:13:155:C:H2' | 1:13:156:G:C8 | 2.48 | 0.47 |
| 1:13:1418:A:C2 | 1:13:1483:A:C2 | 3.02 | 0.47 |
| 2:1E:87:ARG:NE | 2:1E:233:SER:OG | 2.44 | 0.47 |
| 8:7E:106:GLY:HA2 | 8:7E:122:ARG:HH12 | 1.78 | 0.47 |
| 9:8E:23:ASN:HD21 | 9:8E:25:LYS:HE3 | 1.77 | 0.47 |
| 15:6I:26:GLU:OE2 | 15:6I:77:ARG:HD2 | 2.14 | 0.47 |
| 20:BI:75:ASN:N | 20:BI:75:ASN:OD1 | 2.45 | 0.47 |
| 22:2K:20:C:C5 | 22:2K:22:A:H1' | 2.49 | 0.47 |
| 22:3K:25:G:H2' | 22:3K:26:G:H8 | 1.79 | 0.47 |
| 24:1H:140:A:C8 | 24:1H:1408:C:O2' | 2.67 | 0.47 |
| 24:1H:298:G:H5" | 24:1H:299:A:OP1 | 2.13 | 0.47 |
| 24:1H:429:A:H2' | 24:1H:430:G:C8 | 2.49 | 0.47 |
| 24:1H:739:G:P | 57:1H:3658:HOH:O | 2.72 | 0.47 |
| 24:1H:1592:C:H2' | 24:1H:1593:G:C8 | 2.49 | 0.47 |
| 24:1H:1946:U:H2' | 24:1H:1947:C:C6 | 2.49 | 0.47 |
| 24:1H:2626:C:H2' | 24:1H:2627:G:O4' | 2.14 | 0.47 |
| 30:41:142:PRO:HB2 | 50:M8:31:ILE:HG21 | 1.96 | 0.47 |
| 31:51:8:PRO:O | 31:51:9:ILE:HG13 | 2.13 | 0.47 |
| 32:61:40:THR:O | 32:61:44:LEU:N | 2.46 | 0.47 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 37:98:74:LYS:O | 37:98:75:LEU:HB3 | 2.13 | 0.47 |
| 1:1G:1095:U:OP1 | 1:1G:1108:G:N2 | 2.46 | 0.47 |
| 1:1G:1145:C:H5" | 1:1G:1146:A:OP1 | 2.14 | 0.47 |
| 2:12:101:MET:HA | 2:12:108:ILE:HG13 | 1.95 | 0.47 |
| 5:42:131:ILE:O | 5:42:134:ALA:HB3 | 2.14 | 0.47 |
| 12:3A:84:LEU:HD23 | 12:3A:105:TYR:HE2 | 1.79 | 0.47 |
| 13:4A:5:ALA:HB2 | 13:4A:61:GLU:CD | 2.39 | 0.47 |
| 20:BA:95:ALA:C | 20:BA:97:ALA:H | 2.21 | 0.47 |
| 22:3L:17:OMG:HN21 | 22:3L:64:PSU:HN3 | 1.62 | 0.47 |
| 24:14:396:G:H8 | 24:14:396:G:O5' | 1.96 | 0.47 |
| 24:14:654(E):C:N4 | 24:14:654(P):G:H1 | 2.09 | 0.47 |
| 24:14:1337:G:H2' | 24:14:1338:G:C8 | 2.47 | 0.47 |
| 24:14:2112:G:H8 | 24:14:2112:G:OP1 | 1.97 | 0.47 |
| 24:14:2578:G:N7 | 28:29:140:SER:HB2 | 2.29 | 0.47 |
| 24:14:2747:G:O2' | 31:59:67:LEU:HD23 | 2.14 | 0.47 |
| 24:14:2773:C:OP1 | 28:29:166:THR:OG1 | 2.32 | 0.47 |
| 27:19:254:THR:N | 27:19:255:LYS:HZ1 | 2.12 | 0.47 |
| 28:29:24:THR:HB | 28:29:184:VAL:HG23 | 1.95 | 0.47 |
| 29:39:185:ASP:CG | 29:39:188:ARG:HH21 | 2.22 | 0.47 |
| 30:49:61:ALA:HB2 | 30:49:67:LYS:HA | 1.97 | 0.47 |
| 30:49:70:VAL:HA | 30:49:90:LEU:HD12 | 1.94 | 0.47 |
| 36:45:57:HIS:HD2 | 36:45:117:ALA:HB2 | 1.78 | 0.47 |
| 37:55:56:LYS:HE3 | 37:55:87:TYR:O | 2.14 | 0.47 |
| 38:65:87:PHE:CZ | 38:65:102:ALA:HB2 | 2.49 | 0.47 |
| 39:75:22:PHE:HA | 39:75:91:ARG:HH21 | 1.79 | 0.47 |
| 1:13:186(D):C:N4 | 1:13:191(C):G:H1 | 2.10 | 0.47 |
| 1:13:735:C:C2 | 1:13:736:C:C5 | 3.02 | 0.47 |
| 1:13:807:A:H2' | 1:13:808:C:C6 | 2.49 | 0.47 |
| 1:13:1006:C:H2' | 1:13:1007:C:C6 | 2.49 | 0.47 |
| 1:13:1319:A:O2' | 1:13:1323:G:N7 | 2.34 | 0.47 |
| 1:13:1378:C:C5 | 1:13:1379:G:C8 | 3.02 | 0.47 |
| 3:2E:3:ASN:N | 3:2E:3:ASN:OD1 | 2.47 | 0.47 |
| 7:6E:22:LEU:HG | 7:6E:62:PHE:HE1 | 1.79 | 0.47 |
| 8:7E:7:ALA:HB2 | 8:7E:85:ARG:HD2 | 1.96 | 0.47 |
| 24:1H:563:G:OP2 | 57:1H:3693:HOH:O | 2.18 | 0.47 |
| 24:1H:1141:U:H4' | 24:1H:1142(A):A:O4' | 2.14 | 0.47 |
| 24:1H:2086:U:H2' | 24:1H:2087:G:C8 | 2.49 | 0.47 |
| 24:1H:2533:A:OP1 | 24:1H:2665:A:H1' | 2.14 | 0.47 |
| 25:16:37:C:C2' | 25:16:38:C:H5' | 2.44 | 0.47 |
| 26:71:45:ALA:HB2 | 26:71:212:VAL:HG22 | 1.96 | 0.47 |
| 37:98:100:LEU:HD11 | 37:98:113:LEU:HD13 | 1.95 | 0.47 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 39:B8:74:ARG:HB3 | 39:B8:74:ARG:HH11 | 1.78 | 0.47 |
| 44:G8:54:LYS:HE2 | 44:G8:54:LYS:O | 2.13 | 0.47 |
| 45:H8:75:ASN:HB3 | 45:H8:84:GLU:HG3 | 1.96 | 0.47 |
| 54:Q8:54:GLU:CA | 54:Q8:57:ARG:HH21 | 2.26 | 0.47 |
| 1:1G:1011:G:H22 | 1:1G:1018:C:H42 | 1.62 | 0.47 |
| 1:1G:1057:G:H2' | 1:1G:1058:G:O4' | 2.15 | 0.47 |
| 5:42:13:ILE:HG22 | 5:42:30:ALA:HB2 | 1.96 | 0.47 |
| 8:72:106:GLY:HA2 | 8:72:122:ARG:HH22 | 1.78 | 0.47 |
| 24:14:330:A:C2 | 24:14:1210:A:O2' | 2.63 | 0.47 |
| 24:14:442:G:C4 | 24:14:444:C:C5 | 3.02 | 0.47 |
| 24:14:760:G:H2' | 24:14:761:A:O4' | 2.14 | 0.47 |
| 24:14:1063:G:H2' | 24:14:1063:G:N3 | 2.29 | 0.47 |
| 24:14:1860:G:O3' | 26:79:205:LYS:NZ | 2.47 | 0.47 |
| 24:14:2029:G:H2' | 24:14:2031:A:OP1 | 2.14 | 0.47 |
| 24:14:2286:A:H4' | 24:14:2287:A:O4' | 2.14 | 0.47 |
| 29:39:7:TYR:HE1 | 29:39:16:GLY:HA3 | 1.79 | 0.47 |
| 31:59:4:ILE:HG21 | 31:59:6:ARG:NE | 2.28 | 0.47 |
| 31:59:89:ILE:HG13 | 31:59:90:LYS:N | 2.29 | 0.47 |
| 35:35:63:PRO:HD3 | 54:M5:27:THR:HG22 | 1.95 | 0.47 |
| 36:45:77:LYS:O | 36:45:79:LEU:N | 2.47 | 0.47 |
| 45:D5:72:ARG:N | 45:D5:87:ASP:O | 2.34 | 0.47 |
| 1:13:1192:C:C5 | 1:13:1193:G:C8 | 3.02 | 0.47 |
| 1:13:1292:U:H5' | 9:8E:38:GLN:OE1 | 2.13 | 0.47 |
| 2:1E:21:ARG:HH21 | 2:1E:23:ARG:HG3 | 1.79 | 0.47 |
| 2:1E:141:GLU:HG2 | 2:1E:145:LEU:HD23 | 1.96 | 0.47 |
| 5:4E:148:VAL:O | 5:4E:151:LEU:HB2 | 2.14 | 0.47 |
| 6:5E:28:ARG:O | 6:5E:31:GLU:HB3 | 2.14 | 0.47 |
| 8:7E:88:LYS:HB3 | 8:7E:89:PRO:HD2 | 1.96 | 0.47 |
| 10:1I:7:LYS:HB2 | 10:1I:97:GLU:HB2 | 1.96 | 0.47 |
| 18:9I:47:THR:O | 18:9I:83:GLU:N | 2.47 | 0.47 |
| 24:1H:533:G:H5' | 40:C8:24:TYR:CE1 | 2.49 | 0.47 |
| 24:1H:675:A:N3 | 24:1H:2443:C:O2' | 2.46 | 0.47 |
| 24:1H:2361:A:H5' | 54:Q8:27:THR:OG1 | 2.14 | 0.47 |
| 25:16:7:G:N2 | 25:16:113:C:N3 | 2.56 | 0.47 |
| 25:16:44:G:OP2 | 50:M8:1:MET:N | 2.47 | 0.47 |
| 34:68:106:LEU:O | 34:68:110:GLY:N | 2.48 | 0.47 |
| 36:88:33:GLY:HA2 | 36:88:105:GLU:HA | 1.95 | 0.47 |
| 40:C8:8:VAL:HG23 | 40:C8:11:ARG:HH21 | 1.79 | 0.47 |
| 40:C8:70:ARG:HA | 40:C8:74:LEU:O | 2.14 | 0.47 |
| 41:D8:15:GLU:HG2 | 41:D8:16:PRO:HD2 | 1.96 | 0.47 |
| 1:1G:201:C:N4 | 1:1G:216:G:H1 | 2.11 | 0.47 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 1:1G:373:A:N3 | 1:1G:374:A:C8 | 2.82 | 0.47 |
| 1:1G:895:G:H1 | 1:1G:904:C:N4 | 2.08 | 0.47 |
| 1:1G:1097:C:H2' | 1:1G:1098:C:C6 | 2.49 | 0.47 |
| 1:1G:1259:C:N4 | 1:1G:1260:C:O2 | 2.46 | 0.47 |
| 2:12:103:THR:HG23 | 2:12:176:GLU:OE1 | 2.15 | 0.47 |
| 4:32:102:ASP:HA | 4:32:121:VAL:HG21 | 1.96 | 0.47 |
| 4:32:148:VAL:HG11 | 4:32:158:ILE:HD12 | 1.96 | 0.47 |
| 11:2A:24:SER:OG | 11:2A:26:ASN:N | 2.47 | 0.47 |
| 17:8A:86:GLU:O | 17:8A:90:ILE:HG12 | 2.13 | 0.47 |
| 20:BA:14:LYS:HG2 | 20:BA:18:GLN:OE1 | 2.14 | 0.47 |
| 24:14:1359:A:N7 | 24:14:1372:U:C4 | 2.82 | 0.47 |
| 24:14:1676:A:H2' | 24:14:1677:A:O4' | 2.13 | 0.47 |
| 24:14:2114:A:H2' | 24:14:2168:G:O2' | 2.14 | 0.47 |
| 28:29:1:MET:HA | 28:29:83:ASP:O | 2.15 | 0.47 |
| 29:39:84:VAL:C | 29:39:86:GLY:N | 2.72 | 0.47 |
| 32:69:86:THR:HG23 | 32:69:87:LYS:HE3 | 1.96 | 0.47 |
| 33:15:131:GLN:NE2 | 33:15:132:ALA:HB2 | 2.29 | 0.47 |
| 36:45:24:GLY:HA3 | 36:45:25:ASP:CB | 2.43 | 0.47 |
| 44:C5:14:LEU:HG | 44:C5:15:VAL:N | 2.26 | 0.47 |
| 44:C5:75:ILE:O | 44:C5:80:GLY:N | 2.47 | 0.47 |
| 45:D5:76:LEU:H | 45:D5:76:LEU:HD23 | 1.79 | 0.47 |
| 1:13:467:G:H3' | 1:13:467:G:OP2 | 2.14 | 0.47 |
| 1:13:725:G:O2' | 1:13:726:C:H5' | 2.14 | 0.47 |
| 1:13:1030:C:H2' | 1:13:1031:G:O4' | 2.14 | 0.47 |
| 1:13:1117:G:H5" | 9:8E:104:ARG:CZ | 2.44 | 0.47 |
| 4:3E:109:GLY:HA3 | 4:3E:165:MET:HE2 | 1.97 | 0.47 |
| 7:6E:46:ALA:HA | 7:6E:49:ILE:HG12 | 1.96 | 0.47 |
| 24:1H:284:U:H2' | 24:1H:285:C:C6 | 2.49 | 0.47 |
| 24:1H:821:A:H5" | 24:1H:822:U:C6 | 2.49 | 0.47 |
| 24:1H:982:C:O5' | 24:1H:982:C:H6 | 1.97 | 0.47 |
| 24:1H:1270:C:O2' | 24:1H:1648:C:OP2 | 2.27 | 0.47 |
| 24:1H:1786:A:P | 57:1H:3717:HOH:O | 2.72 | 0.47 |
| 24:1H:2324:C:H5" | 24:1H:2325:G:H5' | 1.95 | 0.47 |
| 25:16:42:C:O2 | 30:41:92:VAL:HG23 | 2.13 | 0.47 |
| 27:11:97:TYR:HE1 | 27:11:103:ARG:HG3 | 1.78 | 0.47 |
| 28:21:14:ILE:HG22 | 28:21:21:VAL:HB | 1.96 | 0.47 |
| 36:88:64:ILE:HG12 | 36:88:106:VAL:HG12 | 1.96 | 0.47 |
| 37:98:18:LEU:HD11 | 37:98:22:ARG:HH21 | 1.79 | 0.47 |
| 37:98:74:LYS:H | 37:98:74:LYS:HD2 | 1.80 | 0.47 |
| 39:B8:80:SER:HB3 | 39:B8:83:ILE:HG13 | 1.96 | 0.47 |
| 46:I8:24:LYS:O | 46:I8:25:ARG:NH1 | 2.44 | 0.47 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 47:J8:20:ARG:HG2 | 47:J8:20:ARG:HH11 | 1.79 | 0.47 |
| 47:J8:71:TYR:O | 47:J8:75:GLU:HG2 | 2.15 | 0.47 |
| 48:K8:51:ARG:O | 48:K8:54:LYS:HB2 | 2.15 | 0.47 |
| 1:1G:119:A:H5" | 1:1G:120:A:H5' | 1.95 | 0.47 |
| 1:1G:562:C:H4' | 1:1G:563:A:O5' | 2.14 | 0.47 |
| 1:1G:833:U:H2' | 1:1G:834:C:H6 | 1.79 | 0.47 |
| 1:1G:1010:G:H2' | 1:1G:1011:G:O4' | 2.14 | 0.47 |
| 7:62:16:LEU:HD11 | 9:82:45:ALA:HB2 | 1.96 | 0.47 |
| 24:14:554:U:O2' | 24:14:556:G:N7 | 2.42 | 0.47 |
| 24:14:610:C:H2' | 24:14:611:C:C6 | 2.50 | 0.47 |
| 24:14:616:A:C4 | 29:39:180:GLY:HA3 | 2.49 | 0.47 |
| 24:14:901:A:H2' | 24:14:901:A:N3 | 2.29 | 0.47 |
| 24:14:2101:G:H2' | 24:14:2102:U:O4' | 2.14 | 0.47 |
| 24:14:2377:A:H2' | 24:14:2378:A:C8 | 2.49 | 0.47 |
| 24:14:2388:A:C2' | 24:14:2389:G:H5' | 2.45 | 0.47 |
| 24:14:2849:U:H1' | 24:14:2866:U:O2 | 2.15 | 0.47 |
| 24:14:2869:G:H2' | 24:14:2870:C:O4' | 2.14 | 0.47 |
| 24:14:2889:C:H3' | 24:14:2891:G:C8 | 2.49 | 0.47 |
| 25:1J:11:C:H3' | 25:1J:12:C:C6 | 2.49 | 0.47 |
| 36:45:136:ALA:O | 36:45:139:GLU:HG2 | 2.14 | 0.47 |
| 37:55:38:VAL:HG12 | 37:55:42:LYS:HE3 | 1.97 | 0.47 |
| 54:M5:57:ARG:HD3 | 54:M5:57:ARG:HA | 1.43 | 0.47 |
| 1:13:129(A):G:H21 | 1:13:190:G:H5' | 1.80 | 0.47 |
| 1:13:191:G:C4 | 20:BI:105:SER:HB2 | 2.50 | 0.47 |
| 1:13:380:G:N2 | 1:13:384:G:C5 | 2.82 | 0.47 |
| 1:13:827:U:C5 | 1:13:870:U:C4 | 3.02 | 0.47 |
| 1:13:939:G:C4 | 1:13:940:C:C5 | 3.01 | 0.47 |
| 8:7E:44:PHE:HA | 8:7E:79:VAL:CG1 | 2.45 | 0.47 |
| 14:5I:6:LEU:HA | 14:5I:6:LEU:HD23 | 1.74 | 0.47 |
| 22:3K:47:U:H2' | 22:3K:48:C:C6 | 2.50 | 0.47 |
| 24:1H:139:G:N3 | 24:1H:141:A:N1 | 2.62 | 0.47 |
| 24:1H:253:C:H2' | 24:1H:254:G:O4' | 2.13 | 0.47 |
| 24:1H:710:G:H2' | 24:1H:711:G:C8 | 2.49 | 0.47 |
| 24:1H:753:C:OP2 | 24:1H:753:C:H6 | 1.97 | 0.47 |
| 31:51:41:MET:HE3 | 31:51:41:MET:HB2 | 1.71 | 0.47 |
| 44:G8:104:GLY:H | 44:G8:105:ALA:HB3 | 1.78 | 0.47 |
| 45:H8:25:PRO:HB2 | 45:H8:85:HIS:HD2 | 1.79 | 0.47 |
| 54:Q8:61:LEU:O | 54:Q8:62:LEU:HD12 | 2.14 | 0.47 |
| 1:1G:200:G:O2' | 1:1G:201:C:H5' | 2.15 | 0.47 |
| 1:1G:280:C:H3' | 1:1G:281:G:H5' | 1.95 | 0.47 |
| 1:1G:313:A:H2' | 1:1G:314:C:C6 | 2.50 | 0.47 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 1:1G:352:C:O2' | 1:1G:354:G:OP1 | 2.28 | 0.47 |
| 1:1G:674:G:H2' | 1:1G:675:A:C8 | 2.50 | 0.47 |
| 1:1G:1431:C:O3' | 39:75:107:ASP:HB3 | 2.15 | 0.47 |
| 3:22:39:ILE:HG21 | 3:22:57:ILE:HD11 | 1.96 | 0.47 |
| 24:14:198:C:H5' | 24:14:2244:U:OP1 | 2.15 | 0.47 |
| 24:14:304:G:H2' | 24:14:305:U:H6 | 1.80 | 0.47 |
| 24:14:458:G:C8 | 53:L5:37:LYS:HG2 | 2.50 | 0.47 |
| 24:14:781:A:H2 | 24:14:1776:G:N3 | 2.12 | 0.47 |
| 24:14:1210:A:H5' | 24:14:1212:G:C5' | 2.45 | 0.47 |
| 24:14:1591:G:H2' | 24:14:1592:C:C6 | 2.49 | 0.47 |
| 24:14:2053:G:P | 57:14:3543:HOH:O | 2.70 | 0.47 |
| 24:14:2880:C:H1' | 37:55:92:GLY:HA3 | 1.95 | 0.47 |
| 27:19:43:ARG:HH11 | 27:19:43:ARG:CG | 2.28 | 0.47 |
| 40:85:91:ASP:O | 40:85:92:ARG:HG2 | 2.15 | 0.47 |
| 41:95:20:LEU:HA | 41:95:20:LEU:HD12 | 1.65 | 0.47 |
| 42:A5:29:LEU:HG | 42:A5:33:ARG:HD2 | 1.97 | 0.47 |
| 44:C5:36:ALA:HB1 | 44:C5:66:PRO:HB3 | 1.96 | 0.47 |
| 45:D5:145:GLU:O | 45:D5:174:VAL:HB | 2.14 | 0.47 |
| 1:13:1223:C:P | 1:13:1224:G:H2' | 2.55 | 0.47 |
| 1:13:1386:G:O2' | 1:13:1387:G:H5' | 2.14 | 0.47 |
| 5:4E:102:ALA:HB3 | 5:4E:107:ARG:HB2 | 1.95 | 0.47 |
| 8:7E:4:ASP:OD2 | 8:7E:85:ARG:NH1 | 2.47 | 0.47 |
| 12:3I:93:LEU:HB2 | 12:3I:96:VAL:CG1 | 2.45 | 0.47 |
| 22:2K:4:G:C2 | 22:2K:79:A:C2 | 3.03 | 0.47 |
| 24:1H:64:A:C5 | 43:F8:66:LEU:HD23 | 2.49 | 0.47 |
| 24:1H:1243:G:O2' | 35:78:7:ARG:NH2 | 2.43 | 0.47 |
| 24:1H:2409:G:H8 | 24:1H:2409:G:O5' | 1.98 | 0.47 |
| 25:16:39:A:H5' | 25:16:40:U:OP2 | 2.15 | 0.47 |
| 34:68:110:GLY:HA2 | 34:68:112:MET:HE2 | 1.96 | 0.47 |
| 35:78:35:HIS:HA | 57:78:202:HOH:O | 2.14 | 0.47 |
| 36:88:86:GLY:HA3 | 36:88:87:LYS:CG | 2.39 | 0.47 |
| 40:C8:31:SER:O | 40:C8:32:PHE:C | 2.57 | 0.47 |
| 50:M8:14:ILE:O | 50:M8:20:ASN:ND2 | 2.47 | 0.47 |
| 1:1G:130:A:H1' | 1:1G:263:A:O2' | 2.13 | 0.47 |
| 1:1G:818:G:O2' | 1:1G:819:A:H5' | 2.13 | 0.47 |
| 1:1G:901:A:C5 | 1:1G:902:G:H1' | 2.50 | 0.47 |
| 1:1G:1237:C:H5" | 1:1G:1238:A:O4' | 2.15 | 0.47 |
| 1:1G:1301:U:O3' | 13:4A:21:TYR:OH | 2.29 | 0.47 |
| 3:22:73:PRO:HG3 | 3:22:105:GLU:HG3 | 1.96 | 0.47 |
| 4:32:105:VAL:HG12 | 4:32:106:TYR:N | 2.29 | 0.47 |
| 13:4A:7:VAL:HG11 | 30:49:115:ARG:HE | 1.80 | 0.47 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 22:2L:17:OMG:C2 | 22:2L:67:A:C5 | 3.02 | 0.47 |
| 24:14:84:A:N6 | 24:14:102:G:H1' | 2.29 | 0.47 |
| 24:14:1728:G:H8 | 24:14:1732:A:N6 | 2.11 | 0.47 |
| 24:14:2572:A:H62 | 28:29:145:LYS:HD2 | 1.78 | 0.47 |
| 27:19:71:ASP:N | 27:19:71:ASP:OD1 | 2.47 | 0.47 |
| 30:49:28:VAL:HG13 | 30:49:31:VAL:HG11 | 1.95 | 0.47 |
| 41:95:7:THR:HG23 | 41:95:22:VAL:HG21 | 1.96 | 0.47 |
| 43:B5:18:TYR:HA | 43:B5:21:PHE:CE2 | 2.49 | 0.47 |
| 45:D5:43:GLU:O | 45:D5:47:VAL:HG23 | 2.14 | 0.47 |
| 1:13:474:G:H5" | 16:7I:81:ARG:CZ | 2.45 | 0.47 |
| 1:13:585:G:H8 | 1:13:585:G:O5' | 1.97 | 0.47 |
| 1:13:762:C:H2' | 1:13:763:G:H8 | 1.80 | 0.47 |
| 1:13:1078:U:C5 | 1:13:1079:G:C5 | 3.03 | 0.47 |
| 1:13:1081:G:OP2 | 5:4E:27:ARG:HD2 | 2.15 | 0.47 |
| 1:13:1196:U:C4 | 23:4K:23:A:C8 | 3.03 | 0.47 |
| 1:13:1202:G:H1' | 14:5I:29:ARG:HD2 | 1.97 | 0.47 |
| 1:13:1255:G:C2 | 1:13:1283:G:C2 | 3.03 | 0.47 |
| 2:1E:8:LYS:HD3 | 2:1E:8:LYS:H | 1.79 | 0.47 |
| 2:1E:111:ARG:HH11 | 2:1E:111:ARG:CG | 2.24 | 0.47 |
| 3:2E:19:GLU:O | 3:2E:56:ASP:HA | 2.14 | 0.47 |
| 3:2E:67:THR:HG23 | 3:2E:102:ASN:HB2 | 1.97 | 0.47 |
| 8:7E:49:GLU:HG2 | 8:7E:62:TYR:HE2 | 1.80 | 0.47 |
| 11:2I:67:ASP:O | 11:2I:71:LYS:HG2 | 2.14 | 0.47 |
| 14:5I:39:LEU:HD11 | 14:5I:47:LEU:HD12 | 1.96 | 0.47 |
| 17:8I:45:HIS:O | 17:8I:73:VAL:HG23 | 2.15 | 0.47 |
| 18:9I:26:LEU:HD13 | 18:9I:42:ARG:NH2 | 2.30 | 0.47 |
| 24:1H:38:A:H2' | 24:1H:39:C:C6 | 2.49 | 0.47 |
| 24:1H:155:C:H42 | 24:1H:171:G:H1 | 1.61 | 0.47 |
| 24:1H:300:A:N3 | 24:1H:319:C:H1' | 2.29 | 0.47 |
| 24:1H:320:A:OP2 | 29:31:137:LYS:HE3 | 2.15 | 0.47 |
| 24:1H:455:C:N3 | 24:1H:472:A:H2' | 2.29 | 0.47 |
| 24:1H:546:C:H6 | 24:1H:546:C:OP1 | 1.97 | 0.47 |
| 24:1H:643:A:H2' | 24:1H:644:A:H8 | 1.79 | 0.47 |
| 24:1H:729:G:O2' | 24:1H:763:G:H4' | 2.15 | 0.47 |
| 24:1H:954:G:N3 | 24:1H:2274:A:C2 | 2.83 | 0.47 |
| 24:1H:988:A:O5' | 49:L8:11:SER:HB2 | 2.14 | 0.47 |
| 24:1H:1176:G:H5" | 24:1H:1177:A:C5 | 2.49 | 0.47 |
| 24:1H:1188:U:H4' | 41:D8:79:VAL:HG22 | 1.96 | 0.47 |
| 24:1H:1313:U:H4' | 24:1H:1332:G:H4' | 1.95 | 0.47 |
| 24:1H:1449:A:H5' | 24:1H:1449(A):G:OP2 | 2.15 | 0.47 |
| 24:1H:1903:G:OP1 | 27:11:241:PRO:HB2 | 2.15 | 0.47 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 24:1H:1970:A:P | 57:1H:3673:HOH:O | 2.71 | 0.47 |
| 24:1H:2210:G:H3' | 24:1H:2211:G:N7 | 2.28 | 0.47 |
| 24:1H:2308:G:H2' | 24:1H:2308:G:N3 | 2.30 | 0.47 |
| 24:1H:2519:U:C6 | 24:1H:2542:A:N6 | 2.83 | 0.47 |
| 27:11:109:ASP:HB2 | 27:11:197:GLY:HA3 | 1.96 | 0.47 |
| 30:41:135:LEU:O | 30:41:154:GLY:HA3 | 2.15 | 0.47 |
| 31:51:6:ARG:NE | 31:51:54:ARG:HH12 | 2.12 | 0.47 |
| 32:61:59:ALA:O | 32:61:63:ALA:HB2 | 2.14 | 0.47 |
| 34:68:2:ILE:HB | 34:68:33:ALA:HB3 | 1.96 | 0.47 |
| 38:A8:15:ARG:O | 38:A8:19:LYS:HD3 | 2.15 | 0.47 |
| 38:A8:83:LYS:HG2 | 38:A8:109:GLY:HA2 | 1.97 | 0.47 |
| 44:G8:55:TYR:N | 44:G8:56:PRO:HD3 | 2.29 | 0.47 |
| 45:H8:53:ILE:HG22 | 45:H8:71:VAL:HG13 | 1.97 | 0.47 |
| 45:H8:155:LEU:HD22 | 45:H8:156:LYS:H | 1.79 | 0.47 |
| 46:I8:70:GLN:HB2 | 46:I8:80:HIS:HE2 | 1.80 | 0.47 |
| 49:L8:8:LEU:HB2 | 49:L8:28:LEU:HD23 | 1.97 | 0.47 |
| 1:1G:198:G:H2' | 1:1G:199:G:C8 | 2.50 | 0.47 |
| 1:1G:345:C:H1' | 1:1G:346:G:C2 | 2.50 | 0.47 |
| 1:1G:500:G:N2 | 1:1G:546:G:H1' | 2.30 | 0.47 |
| 1:1G:523:A:H61 | 12:3A:53:ARG:NH1 | 2.12 | 0.47 |
| 1:1G:570:G:H2' | 1:1G:571:U:H6 | 1.77 | 0.47 |
| 1:1G:580:U:H2' | 1:1G:581:G:O4' | 2.15 | 0.47 |
| 1:1G:861:G:H2' | 1:1G:862:C:C6 | 2.49 | 0.47 |
| 1:1G:992:U:H3 | 1:1G:1044:A:N6 | 2.13 | 0.47 |
| 1:1G:1065:U:C5 | 1:1G:1190:G:H1' | 2.49 | 0.47 |
| 1:1G:1207:G:C6 | 1:1G:1208:C:C4 | 3.03 | 0.47 |
| 1:1G:1327:C:H2' | 1:1G:1328:C:C6 | 2.50 | 0.47 |
| 2:12:5:ILE:HG12 | 2:12:6:THR:O | 2.15 | 0.47 |
| 3:22:59:ARG:HG3 | 3:22:63:ASN:O | 2.14 | 0.47 |
| 3:22:148:GLY:HA3 | 3:22:172:ARG:O | 2.14 | 0.47 |
| 4:32:153:ARG:HH12 | 4:32:181:MET:HB2 | 1.80 | 0.47 |
| 5:42:76:ILE:HG23 | 5:42:77:PRO:HD2 | 1.95 | 0.47 |
| 6:52:44:GLY:HA2 | 6:52:59:TYR:CE2 | 2.49 | 0.47 |
| 7:62:93:PRO:HD2 | 7:62:94:ARG:HG3 | 1.95 | 0.47 |
| 8:72:121:ASP:OD2 | 8:72:125:ARG:NH2 | 2.47 | 0.47 |
| 9:82:9:ARG:HB2 | 9:82:14:VAL:HG22 | 1.97 | 0.47 |
| 11:2A:51:LYS:HA | 11:2A:55:LYS:HD3 | 1.97 | 0.47 |
| 12:3A:27:LEU:C | 12:3A:29:GLY:H | 2.23 | 0.47 |
| 13:4A:39:ILE:HD12 | 13:4A:56:LEU:HG | 1.95 | 0.47 |
| 20:BA:74:LYS:HB3 | 20:BA:75:ASN:H | 1.37 | 0.47 |
| 24:14:686:G:H5" | 53:L5:11:LYS:NZ | 2.29 | 0.47 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 24:14:724:U:H2' | 24:14:725:G:O4' | 2.15 | 0.47 |
| 24:14:780:G:H21 | 24:14:783:A:N6 | 2.10 | 0.47 |
| 24:14:782:A:H5' | 24:14:783:A:C2 | 2.49 | 0.47 |
| 24:14:881:G:N3 | 24:14:882:G:H1' | 2.30 | 0.47 |
| 24:14:999:U:C5 | 24:14:1154:G:C5 | 3.02 | 0.47 |
| 24:14:1197:G:H2' | 24:14:1198:U:C6 | 2.50 | 0.47 |
| 24:14:1690:A:H5" | 24:14:1691:C:OP2 | 2.14 | 0.47 |
| 24:14:2257:U:H2' | 24:14:2258:C:C6 | 2.50 | 0.47 |
| 24:14:2402:C:O2' | 24:14:2403:C:OP1 | 2.26 | 0.47 |
| 25:1J:5:C:OP1 | 25:1J:62:C:H5' | 2.14 | 0.47 |
| 28:29:54:GLN:O | 28:29:55:ASN:CG | 2.58 | 0.47 |
| 28:29:122:PHE:HZ | 28:29:155:LYS:HB2 | 1.80 | 0.47 |
| 30:49:11:TYR:O | 30:49:16:ARG:HB3 | 2.14 | 0.47 |
| 34:25:102:VAL:HB | 34:25:106:LEU:HD12 | 1.96 | 0.47 |
| 35:35:65:ARG:HH22 | 54:M5:15:LYS:HB2 | 1.80 | 0.47 |
| 35:35:147:LEU:HD13 | 35:35:148:LEU:H | 1.79 | 0.47 |
| 37:55:97:VAL:HA | 37:55:113:LEU:O | 2.15 | 0.47 |
| 37:55:116:LEU:HD23 | 37:55:116:LEU:HA | 1.75 | 0.47 |
| 38:65:83:LYS:O | 38:65:110:LEU:HB3 | 2.15 | 0.47 |
| 52:K5:23:THR:OG1 | 52:K5:24:GLU:N | 2.48 | 0.47 |
| 54:M5:9:GLY:O | 54:M5:13:ARG:HD2 | 2.14 | 0.47 |
| 1:13:322:C:O3' | 20:BI:23:ARG:HG3 | 2.14 | 0.47 |
| 1:13:728:A:C5 | 15:6I:54:ARG:HD2 | 2.50 | 0.47 |
| 1:13:1226:C:H2' | 13:4I:103:THR:HB | 1.96 | 0.47 |
| 1:13:1431:C:H2' | 1:13:1432:G:O4' | 2.14 | 0.47 |
| 4:3E:156:GLU:O | 4:3E:160:GLN:HG3 | 2.15 | 0.47 |
| 8:7E:86:ILE:HG22 | 8:7E:93:VAL:HG21 | 1.96 | 0.47 |
| 9:8E:10:ARG:HD2 | 9:8E:105:ASP:HB2 | 1.95 | 0.47 |
| 11:2I:78:GLN:O | 11:2I:103:LEU:HA | 2.15 | 0.47 |
| 12:3I:82:VAL:HG23 | 12:3I:106:ASP:OD2 | 2.15 | 0.47 |
| 24:1H:270(D):C:H2' | 24:1H:270(E):G:C8 | 2.50 | 0.47 |
| 24:1H:550:G:O2' | 24:1H:1220:A:N3 | 2.42 | 0.47 |
| 24:1H:590:A:OP1 | 29:31:95:ARG:NH1 | 2.48 | 0.47 |
| 24:1H:654(J):A:N1 | 24:1H:654(M):C:N4 | 2.62 | 0.47 |
| 24:1H:764:A:H5' | 27:11:210:GLY:CA | 2.43 | 0.47 |
| 24:1H:1050:A:H1' | 24:1H:2751:G:C8 | 2.50 | 0.47 |
| 24:1H:1802:A:H2' | 24:1H:1803:A:C8 | 2.49 | 0.47 |
| 24:1H:1996:C:OP1 | 34:68:31:LYS:HE3 | 2.15 | 0.47 |
| 24:1H:2212:A:O2' | 24:1H:2213:U:P | 2.72 | 0.47 |
| 24:1H:2400:G:N2 | 24:1H:2417:C:O2 | 2.48 | 0.47 |
| 24:1H:2495:G:OP1 | 36:88:82:ARG:HD2 | 2.14 | 0.47 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 25:16:103:U:O2' | 45:H8:72:ARG:HG2 | 2.15 | 0.47 |
| 27:11:44:ASN:O | 27:11:46:GLN:O | 2.33 | 0.47 |
| 28:21:101:ARG:HD2 | 28:21:171:GLU:HA | 1.97 | 0.47 |
| 32:61:82:ARG:O | 32:61:89:TYR:HD1 | 1.97 | 0.47 |
| 33:58:53:VAL:HG11 | 33:58:128:HIS:HD2 | 1.80 | 0.47 |
| 39:B8:76:PHE:HA | 39:B8:77:PRO:HD3 | 1.59 | 0.47 |
| 46:I8:38:VAL:CG1 | 46:I8:40:GLN:HG2 | 2.38 | 0.47 |
| 1:1G:261:U:OP2 | 20:BA:79:ARG:NH2 | 2.48 | 0.47 |
| 1:1G:644:G:H4' | 8:72:92:ARG:NH1 | 2.29 | 0.47 |
| 1:1G:1141:C:H2' | 1:1G:1142:G:H8 | 1.80 | 0.47 |
| 1:1G:1143:G:H2' | 1:1G:1144:G:C8 | 2.50 | 0.47 |
| 1:1G:1274:G:H2' | 1:1G:1275:A:H8 | 1.79 | 0.47 |
| 1:1G:1342:C:H1' | 9:82:124:GLN:OE1 | 2.14 | 0.47 |
| 2:12:5:ILE:HG13 | 2:12:221:LEU:HD22 | 1.97 | 0.47 |
| 3:22:18:TRP:CD1 | 14:5A:54:PRO:HA | 2.50 | 0.47 |
| 5:42:50:GLU:OE2 | 5:42:51:VAL:HG23 | 2.15 | 0.47 |
| 6:52:76:ALA:O | 6:52:80:ARG:HG3 | 2.15 | 0.47 |
| 10:1A:68:HIS:CD2 | 10:1A:68:HIS:N | 2.83 | 0.47 |
| 13:4A:96:LEU:C | 13:4A:110:ARG:HG2 | 2.39 | 0.47 |
| 13:4A:98:VAL:C | 13:4A:100:GLY:H | 2.22 | 0.47 |
| 18:9A:43:PHE:C | 18:9A:51:LEU:HD12 | 2.40 | 0.47 |
| 22:3L:83:C:H4' | 47:F5:23:LYS:HB2 | 1.97 | 0.47 |
| 24:14:189:G:H2' | 24:14:205:G:N2 | 2.29 | 0.47 |
| 24:14:231:C:C5 | 24:14:232:G:C6 | 3.02 | 0.47 |
| 24:14:439:G:H2' | 24:14:440:G:C8 | 2.49 | 0.47 |
| 24:14:1011:G:C2 | 24:14:1151:G:C2 | 3.03 | 0.47 |
| 24:14:1060:U:C2 | 24:14:1062:G:H4' | 2.50 | 0.47 |
| 24:14:1832:C:N4 | 24:14:1833:U:C4 | 2.83 | 0.47 |
| 24:14:2116:G:H2' | 24:14:2117:A:O4' | 2.15 | 0.47 |
| 24:14:2140:C:H1' | 24:14:2152:G:N2 | 2.29 | 0.47 |
| 28:29:9:VAL:HB | 28:29:25:VAL:O | 2.14 | 0.47 |
| 30:49:35:GLU:O | 30:49:36:LYS:HG2 | 2.14 | 0.47 |
| 39:75:65:LYS:HB3 | 39:75:65:LYS:HE2 | 1.74 | 0.47 |
| 39:75:80:SER:HB3 | 39:75:83:ILE:HG13 | 1.96 | 0.47 |
| 42:A5:57:ASN:O | 42:A5:61:ASN:HB2 | 2.15 | 0.47 |
| 1:13:197:A:C6 | 1:13:221:C:H4' | 2.50 | 0.47 |
| 1:13:784:C:H2' | 1:13:785:G:O4' | 2.15 | 0.47 |
| 1:13:1127:G:H22 | 1:13:1145:C:H1' | 1.79 | 0.47 |
| 1:13:1194:U:H2' | 1:13:1195:C:C6 | 2.50 | 0.47 |
| 4:3E:155:LEU:O | 4:3E:158:ILE:N | 2.46 | 0.47 |
| 6:5E:67:MET:SD | 6:5E:75:LEU:HD12 | 2.55 | 0.47 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 7:6E:81:GLY:C | 7:6E:83:ALA:H | 2.23 | 0.47 |
| 13:4I:15:VAL:HG23 | 13:4I:43:THR:O | 2.14 | 0.47 |
| 17:8I:76:LEU:HD11 | 17:8I:78:GLU:O | 2.15 | 0.47 |
| 18:9I:36:ASN:ND2 | 18:9I:39:VAL:HG21 | 2.30 | 0.47 |
| 24:1H:142:G:O3' | 43:F8:35:THR:HG21 | 2.14 | 0.47 |
| 24:1H:624:C:O2' | 24:1H:657:U:OP1 | 2.28 | 0.47 |
| 24:1H:997:G:H5" | 40:C8:92:ARG:HH21 | 1.79 | 0.47 |
| 24:1H:1371:G:H2' | 24:1H:1372:U:C5 | 2.50 | 0.47 |
| 24:1H:1416:G:H2' | 24:1H:1417:C:C6 | 2.50 | 0.47 |
| 24:1H:1471:A:C2 | 24:1H:1472:A:C4 | 3.03 | 0.47 |
| 24:1H:1914:C:H2' | 24:1H:1915:U:C6 | 2.49 | 0.47 |
| 24:1H:2138:C:C2 | 24:1H:2154:G:N2 | 2.83 | 0.47 |
| 24:1H:2860:A:C8 | 24:1H:2861:G:H1' | 2.50 | 0.47 |
| 25:16:73:A:C4 | 25:16:104:A:C2 | 3.02 | 0.47 |
| 27:11:3:VAL:HG13 | 27:11:17:THR:HG23 | 1.97 | 0.47 |
| 29:31:64:ILE:HG23 | 29:31:65:TRP:CD1 | 2.49 | 0.47 |
| 38:A8:61:ASN:OD1 | 38:A8:64:GLU:HG3 | 2.15 | 0.47 |
| 48:K8:16:LEU:HD13 | 48:K8:16:LEU:HA | 1.78 | 0.47 |
| 48:K8:16:LEU:HB3 | 48:K8:21:LEU:HG | 1.97 | 0.47 |
| 1:1G:28:G:H21 | 1:1G:296:U:H4' | 1.80 | 0.47 |
| 1:1G:1158:C:O3' | 1:1G:1159:U:H4' | 2.14 | 0.47 |
| 1:1G:1186:G:O3' | 9:82:113:LYS:NZ | 2.42 | 0.47 |
| 1:1G:1260:C:H4' | 1:1G:1283:G:O2' | 2.15 | 0.47 |
| 2:12:6:THR:OG1 | 2:12:7:VAL:N | 2.48 | 0.47 |
| 8:72:51:VAL:HG21 | 8:72:60:ARG:NH1 | 2.30 | 0.47 |
| 24:14:331:A:N6 | 24:14:1210:A:OP2 | 2.35 | 0.47 |
| 24:14:882:G:OP2 | 24:14:882:G:H8 | 1.98 | 0.47 |
| 24:14:1192:G:H2' | 24:14:1193:G:C8 | 2.49 | 0.47 |
| 24:14:1519:G:H2' | 24:14:1520:U:O4' | 2.15 | 0.47 |
| 24:14:2231:C:OP1 | 47:F5:42:GLN:HA | 2.14 | 0.47 |
| 24:14:2279:G:N7 | 46:E5:14:ARG:NH1 | 2.63 | 0.47 |
| 24:14:2346:A:N6 | 52:K5:28:ARG:HH21 | 2.12 | 0.47 |
| 24:14:2762:G:H5' | 24:14:2763:G:OP2 | 2.15 | 0.47 |
| 27:19:24:ILE:HG23 | 27:19:83:GLU:HA | 1.97 | 0.47 |
| 28:29:144:ARG:HB3 | 28:29:145:LYS:H | 1.59 | 0.47 |
| 30:49:142:PRO:HG2 | 30:49:143:GLU:OE2 | 2.15 | 0.47 |
| 33:15:41:ASP:O | 40:85:64:ARG:NH2 | 2.48 | 0.47 |
| 1:13:936:C:O2' | 1:13:1382:C:N3 | 2.41 | 0.47 |
| 1:13:1284:C:H3' | 1:13:1285:A:H8 | 1.80 | 0.47 |
| 8:7E:11:THR:HG23 | 8:7E:14:ARG:NH1 | 2.29 | 0.47 |
| 11:2I:18:ARG:HB3 | 11:2I:33:THR:OG1 | 2.14 | 0.47 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 17:8I:15:MET:HE3 | 17:8I:15:MET:HB2 | 1.79 | 0.47 |
| 20:BI:83:ARG:O | 20:BI:87:LYS:HB2 | 2.15 | 0.47 |
| 22:2K:2:G:H2' | 22:2K:2:G:N3 | 2.28 | 0.47 |
| 24:1H:249:C:O2' | 35:78:64:LYS:HE2 | 2.14 | 0.47 |
| 24:1H:370:G:H4' | 24:1H:371:A:OP2 | 2.15 | 0.47 |
| 24:1H:574:C:P | 57:1H:3617:HOH:O | 2.67 | 0.47 |
| 24:1H:674:G:H1' | 29:31:74:ARG:NH1 | 2.30 | 0.47 |
| 24:1H:985:C:C2' | 24:1H:986:C:H5' | 2.45 | 0.47 |
| 24:1H:994:C:O2' | 24:1H:996:A:OP1 | 2.28 | 0.47 |
| 24:1H:1419:A:C8 | 24:1H:1421:G:C6 | 3.03 | 0.47 |
| 24:1H:1432:C:H2' | 24:1H:1433:U:O4' | 2.14 | 0.47 |
| 24:1H:2018:G:H21 | 40:C8:34:LYS:NZ | 2.11 | 0.47 |
| 24:1H:2378:A:H4' | 38:A8:23:ARG:CZ | 2.45 | 0.47 |
| 24:1H:2646:C:OP2 | 24:1H:2732:G:O2' | 2.28 | 0.47 |
| 24:1H:2830:G:H5" | 24:1H:2830:G:H8 | 1.80 | 0.47 |
| 31:51:46:GLU:OE1 | 31:51:51:ARG:NH2 | 2.48 | 0.47 |
| 32:61:79:ILE:HD13 | 32:61:79:ILE:HA | 1.83 | 0.47 |
| 32:61:104:GLN:HG2 | 32:61:105:HIS:CD2 | 2.50 | 0.47 |
| 33:58:133:GLN:O | 33:58:134:ARG:NH1 | 2.48 | 0.47 |
| 47:J8:78:LYS:HD2 | 47:J8:79:GLY:H | 1.79 | 0.47 |
| 52:O8:36:LEU:HD13 | 52:O8:50:ARG:NH2 | 2.30 | 0.47 |
| 1:1G:690:G:H22 | 11:2A:55:LYS:NZ | 2.12 | 0.47 |
| 1:1G:1351:U:O4 | 9:82:118:LYS:NZ | 2.46 | 0.47 |
| 1:1G:1391:U:H2' | 1:1G:1392:G:C8 | 2.50 | 0.47 |
| 3:22:21:ARG:HB3 | 3:22:21:ARG:HH11 | 1.79 | 0.47 |
| 13:4A:23:TYR:CE2 | 13:4A:71:ARG:HD3 | 2.48 | 0.47 |
| 16:7A:21:VAL:CG1 | 16:7A:34:GLU:HB3 | 2.44 | 0.47 |
| 16:7A:23:ASP:OD1 | 16:7A:25:ARG:HG3 | 2.14 | 0.47 |
| 22:2L:62:G:H2' | 22:2L:62:G:N3 | 2.29 | 0.47 |
| 24:14:783:A:H8 | 24:14:784:A:H4' | 1.79 | 0.47 |
| 24:14:1079:C:N4 | 24:14:1088:A:OP1 | 2.48 | 0.47 |
| 24:14:1113:U:H2' | 24:14:1114:G:O4' | 2.15 | 0.47 |
| 24:14:1651:G:OP1 | 37:55:40:LYS:HE3 | 2.15 | 0.47 |
| 24:14:1871:A:H2' | 24:14:1872:A:C8 | 2.50 | 0.47 |
| 24:14:2063:C:O2 | 24:14:2450:A:N1 | 2.48 | 0.47 |
| 24:14:2151:G:H2' | 24:14:2152:G:H8 | 1.80 | 0.47 |
| 24:14:2360:A:H8 | 24:14:2360:A:O5' | 1.97 | 0.47 |
| 25:1J:93:C:H2' | 25:1J:94:C:H6 | 1.79 | 0.47 |
| 25:1J:113:C:O2' | 38:65:46:VAL:HG13 | 2.15 | 0.47 |
| 30:49:56:ALA:HA | 30:49:153:ARG:HH21 | 1.80 | 0.47 |
| 40:85:90:VAL:HA | 41:95:39:LEU:HD22 | 1.97 | 0.47 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 41:95:72:VAL:HB | 41:95:85:LYS:HB3 | 1.97 | 0.47 |
| 42:A5:1:MET:HE3 | 42:A5:62:HIS:HB3 | 1.97 | 0.47 |
| 43:B5:15:GLU:CD | 43:B5:15:GLU:H | 2.23 | 0.47 |
| 44:C5:62:GLU:H | 44:C5:62:GLU:HG3 | 1.54 | 0.47 |
| 45:D5:73:GLN:H | 45:D5:87:ASP:HB2 | 1.80 | 0.47 |
| 1:13:37:U:O2' | 1:13:500:G:H4' | 2.16 | 0.46 |
| 1:13:328:C:H4' | 1:13:329:A:C5' | 2.44 | 0.46 |
| 1:13:658:G:O2' | 1:13:659:U:H5' | 2.15 | 0.46 |
| 1:13:1269:A:N1 | 1:13:1312:G:O2' | 2.42 | 0.46 |
| 4:3E:15:GLU:HG3 | 4:3E:63:LYS:HG3 | 1.97 | 0.46 |
| 6:5E:62:TRP:C | 6:5E:63:TYR:CD1 | 2.93 | 0.46 |
| 13:4I:67:GLU:CG | 13:4I:68:GLY:H | 2.29 | 0.46 |
| 17:8I:18:THR:HG23 | 17:8I:69:LYS:HD2 | 1.96 | 0.46 |
| 19:AI:52:TYR:HA | 19:AI:56:GLN:O | 2.14 | 0.46 |
| 22:2K:20:C:H5 | 22:2K:57:C:H41 | 1.62 | 0.46 |
| 24:1H:363(B):G:H2' | 24:1H:363(C):G:C8 | 2.51 | 0.46 |
| 24:1H:375:C:H2' | 24:1H:376:C:H6 | 1.80 | 0.46 |
| 24:1H:479:A:N3 | 24:1H:481:G:H5" | 2.30 | 0.46 |
| 24:1H:606:U:H4' | 24:1H:658:C:H4' | 1.96 | 0.46 |
| 24:1H:817:C:O2' | 24:1H:839:U:H5" | 2.15 | 0.46 |
| 24:1H:1021:A:H61 | 24:1H:1142(A):A:N6 | 2.13 | 0.46 |
| 24:1H:1022:G:N2 | 24:1H:1023:U:O4 | 2.42 | 0.46 |
| 24:1H:1026:U:O2 | 24:1H:1027:A:H3' | 2.15 | 0.46 |
| 24:1H:1027:A:C2 | 24:1H:2488:A:H5' | 2.50 | 0.46 |
| 24:1H:1057:A:N6 | 24:1H:1087:G:OP2 | 2.48 | 0.46 |
| 24:1H:1178:C:HO2' | 24:1H:1179:C:H6 | 1.63 | 0.46 |
| 24:1H:1614:A:N6 | 42:E8:88:ARG:H | 2.12 | 0.46 |
| 24:1H:2154:G:H2' | 24:1H:2155:G:C8 | 2.38 | 0.46 |
| 24:1H:2287:A:C2 | 24:1H:2346:A:N1 | 2.83 | 0.46 |
| 24:1H:2291:U:H5" | 24:1H:2380:C:O2' | 2.15 | 0.46 |
| 24:1H:2334:G:O6 | 46:I8:74:ARG:NH2 | 2.48 | 0.46 |
| 24:1H:2388:A:N7 | 24:1H:2389:G:C6 | 2.83 | 0.46 |
| 28:21:66:HIS:ND1 | 28:21:66:HIS:C | 2.71 | 0.46 |
| 29:31:134:GLY:H | 29:31:162:LEU:HB3 | 1.80 | 0.46 |
| 32:61:68:LEU:HA | 32:61:71:ILE:HG23 | 1.96 | 0.46 |
| 37:98:12:ARG:HG2 | 37:98:16:HIS:ND1 | 2.30 | 0.46 |
| 50:M8:12:ALA:HB3 | 50:M8:24:THR:HB | 1.96 | 0.46 |
| 1:1G:265:G:H5' | 17:8A:64:PRO:O | 2.15 | 0.46 |
| 1:1G:505:G:C6 | 1:1G:535:A:C2 | 3.03 | 0.46 |
| 1:1G:1128:C:N3 | 1:1G:1139:G:C6 | 2.83 | 0.46 |
| 1:1G:1410:G:N1 | 1:1G:1490:C:N3 | 2.54 | 0.46 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 1:1G:1423:G:H2' | 1:1G:1424:C:H6 | 1.78 | 0.46 |
| 2:12:31:TYR:O | 2:12:42:ILE:HG13 | 2.15 | 0.46 |
| 3:22:182:ILE:HA | 3:22:202:ILE:O | 2.15 | 0.46 |
| 4:32:9:CYS:SG | 4:32:22:LYS:NZ | 2.88 | 0.46 |
| 7:62:111:ARG:NH2 | 7:62:122:HIS:HB3 | 2.30 | 0.46 |
| 13:4A:14:ARG:HG3 | 13:4A:41:PRO:O | 2.14 | 0.46 |
| 15:6A:67:LEU:HD23 | 15:6A:67:LEU:HA | 1.68 | 0.46 |
| 24:14:162:U:H4' | 24:14:171:G:C8 | 2.50 | 0.46 |
| 24:14:2643:G:H2' | 24:14:2644:G:O4' | 2.14 | 0.46 |
| 26:79:15:ASP:HB3 | 26:79:18:LYS:HB3 | 1.97 | 0.46 |
| 32:69:139:GLN:H | 32:69:139:GLN:HG2 | 1.57 | 0.46 |
| 33:15:91:LEU:HA | 33:15:91:LEU:HD23 | 1.56 | 0.46 |
| 42:A5:65:LEU:HD13 | 42:A5:68:ARG:HD2 | 1.97 | 0.46 |
| 50:I5:21:VAL:HG22 | 50:I5:22:ILE:HG13 | 1.96 | 0.46 |
| 1:13:260:G:H2' | 1:13:261:U:C6 | 2.50 | 0.46 |
| 1:13:409:G:H1 | 1:13:433:C:H42 | 1.63 | 0.46 |
| 1:13:530:G:O2' | 1:13:531:U:OP1 | 2.28 | 0.46 |
| 1:13:974:A:P | 14:5I:41:ARG:HH12 | 2.38 | 0.46 |
| 1:13:1048:G:OP1 | 14:5I:3:ARG:HB3 | 2.15 | 0.46 |
| 1:13:1349:A:H2' | 1:13:1350:A:H8 | 1.78 | 0.46 |
| 2:1E:115:LEU:HD23 | 2:1E:153:ARG:HD3 | 1.97 | 0.46 |
| 2:1E:164:VAL:HB | 2:1E:186:ALA:CB | 2.45 | 0.46 |
| 12:3I:52:LEU:O | 12:3I:54:LYS:NZ | 2.29 | 0.46 |
| 17:8I:12:SER:HB3 | 17:8I:20:THR:HB | 1.97 | 0.46 |
| 17:8I:81:ARG:O | 17:8I:84:LEU:N | 2.44 | 0.46 |
| 24:1H:270(U):C:H2' | 24:1H:270(V):G:H8 | 1.80 | 0.46 |
| 24:1H:2094:G:C2 | 24:1H:2196:C:C2 | 3.04 | 0.46 |
| 24:1H:2432:A:C5 | 47:J8:33:LYS:HG2 | 2.50 | 0.46 |
| 24:1H:2608:G:N7 | 57:1H:3761:HOH:O | 2.35 | 0.46 |
| 24:1H:2784:C:H2' | 24:1H:2785:C:H6 | 1.80 | 0.46 |
| 25:16:19:G:H1 | 25:16:64:C:N4 | 2.03 | 0.46 |
| 25:16:40:U:C2' | 25:16:45:A:H61 | 2.28 | 0.46 |
| 28:21:14:ILE:HD12 | 28:21:14:ILE:HA | 1.54 | 0.46 |
| 44:G8:87:LYS:O | 44:G8:94:LYS:HB2 | 2.15 | 0.46 |
| 1:1G:595:G:H1 | 1:1G:641:U:HO2' | 1.63 | 0.46 |
| 1:1G:957:U:H2' | 1:1G:959:A:OP2 | 2.15 | 0.46 |
| 1:1G:1442:G:N7 | 1:1G:1446:A:N1 | 2.64 | 0.46 |
| 5:42:57:LYS:O | 5:42:60:TYR:HB3 | 2.15 | 0.46 |
| 13:4A:15:VAL:HG12 | 13:4A:45:VAL:HG22 | 1.98 | 0.46 |
| 24:14:108:U:H2' | 24:14:109:G:C8 | 2.50 | 0.46 |
| 24:14:459:U:H5" | 53:L5:40:TRP:CD2 | 2.50 | 0.46 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 24:14:654(R):C:N4 | 24:14:654(S):G:O6 | 2.48 | 0.46 |
| 24:14:706:A:H2' | 24:14:707:G:O4' | 2.15 | 0.46 |
| 24:14:756:C:H2' | 24:14:757:U:H5' | 1.98 | 0.46 |
| 24:14:1140:C:O3' | 33:15:25:ARG:NH1 | 2.48 | 0.46 |
| 24:14:1580:A:H8 | 24:14:1580:A:OP2 | 1.98 | 0.46 |
| 24:14:2394:C:H5" | 35:35:64:LYS:CD | 2.44 | 0.46 |
| 24:14:2649:U:H2' | 24:14:2650:U:C6 | 2.50 | 0.46 |
| 24:14:2688:U:C5 | 24:14:2720:U:OP2 | 2.69 | 0.46 |
| 29:39:113:ALA:HB1 | 29:39:186:ILE:HG21 | 1.97 | 0.46 |
| 29:39:117:ARG:HA | 29:39:117:ARG:HD3 | 1.59 | 0.46 |
| 33:15:56:ASN:H | 33:15:125:GLY:HA3 | 1.80 | 0.46 |
| 37:55:82:GLU:C | 37:55:85:PRO:HD2 | 2.40 | 0.46 |
| 38:65:3:ARG:HA | 38:65:3:ARG:HD2 | 1.59 | 0.46 |
| 38:65:100:ALA:HA | 38:65:103:GLU:HB2 | 1.97 | 0.46 |
| 40:85:91:ASP:OD1 | 40:85:96:ALA:N | 2.48 | 0.46 |
| 42:A5:83:LYS:O | 42:A5:84:ARG:HD3 | 2.15 | 0.46 |
| 45:D5:53:ILE:HG22 | 45:D5:71:VAL:HG13 | 1.96 | 0.46 |
| 53:L5:8:ASN:OD1 | 53:L5:8:ASN:C | 2.58 | 0.46 |
| 1:13:683:G:C6 | 1:13:684:A:C6 | 3.04 | 0.46 |
| 1:13:828:A:N6 | 1:13:858:G:O2' | 2.47 | 0.46 |
| 1:13:1489:G:H2' | 1:13:1490[B]:C:O4' | 2.15 | 0.46 |
| 2:1E:185:ILE:HA | 2:1E:199:TYR:O | 2.15 | 0.46 |
| 3:2E:14:ILE:HG13 | 3:2E:15:THR:OG1 | 2.15 | 0.46 |
| 24:1H:329:G:N7 | 44:G8:71:LYS:NZ | 2.63 | 0.46 |
| 24:1H:624:C:O2' | 24:1H:657:U:H5" | 2.16 | 0.46 |
| 24:1H:662:G:O2' | 24:1H:663:G:H5' | 2.15 | 0.46 |
| 24:1H:1168:G:C2 | 24:1H:1182:A:C2 | 3.03 | 0.46 |
| 24:1H:2019:A:H2' | 24:1H:2020:A:O5' | 2.15 | 0.46 |
| 24:1H:2344:U:OP1 | 52:O8:38:LYS:HD3 | 2.15 | 0.46 |
| 25:16:28:C:H2' | 25:16:29:A:O4' | 2.16 | 0.46 |
| 32:61:78:THR:HG1 | 32:61:141:LYS:HZ2 | 1.56 | 0.46 |
| 41:D8:7:THR:HG23 | 41:D8:12:TYR:CE1 | 2.51 | 0.46 |
| 41:D8:65:GLY:HA3 | 41:D8:91:TYR:CE1 | 2.51 | 0.46 |
| 44:G8:87:LYS:HG2 | 44:G8:88:LYS:H | 1.81 | 0.46 |
| 49:L8:37:LEU:HD12 | 49:L8:37:LEU:H | 1.80 | 0.46 |
| 1:1G:32:A:C2 | 1:1G:33:A:C4 | 3.02 | 0.46 |
| 1:1G:279:A:H5" | 1:1G:281:G:O4' | 2.15 | 0.46 |
| 1:1G:1060:C:H41 | 3:22:2:GLY:HA3 | 1.81 | 0.46 |
| 1:1G:1126:U:C4 | 1:1G:1281:U:C6 | 3.04 | 0.46 |
| 1:1G:1154:G:H2' | 1:1G:1155:G:H8 | 1.80 | 0.46 |
| 1:1G:1186:G:N2 | 14:5A:61:TRP:O | 2.34 | 0.46 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 1:1G:1247:U:H1' | 1:1G:1291:G:N2 | 2.30 | 0.46 |
| 4:32:191:ARG:NH1 | 4:32:200:GLU:OE1 | 2.49 | 0.46 |
| 9:82:35:GLU:O | 9:82:38:GLN:HG2 | 2.16 | 0.46 |
| 10:1A:38:ILE:HB | 10:1A:71:LEU:O | 2.15 | 0.46 |
| 21:1B:9:ARG:HG3 | 21:1B:10:ARG:N | 2.29 | 0.46 |
| 24:14:314:A:H2' | 24:14:315:G:C8 | 2.50 | 0.46 |
| 24:14:571:A:H5' | 24:14:2030:A:N7 | 2.31 | 0.46 |
| 24:14:654(I):C:H2' | 24:14:654(M):C:H42 | 1.81 | 0.46 |
| 24:14:1556:C:H2' | 24:14:1557:C:H6 | 1.79 | 0.46 |
| 24:14:1912:A:N6 | 24:14:1918:A:H1' | 2.30 | 0.46 |
| 24:14:2563:U:O2 | 24:14:2565:A:C8 | 2.68 | 0.46 |
| 26:79:215:THR:OG1 | 26:79:216:THR:N | 2.49 | 0.46 |
| 32:69:109:ILE:HB | 32:69:130:TYR:CZ | 2.50 | 0.46 |
| 34:25:31:LYS:HB3 | 34:25:32:TYR:CD1 | 2.51 | 0.46 |
| 35:35:19:VAL:HG12 | 35:35:27:HIS:HB3 | 1.97 | 0.46 |
| 36:45:17:LEU:HB3 | 36:45:39:PRO:HB2 | 1.96 | 0.46 |
| 40:85:88:ILE:HG22 | 40:85:90:VAL:CG2 | 2.45 | 0.46 |
| 45:D5:144:LEU:C | 45:D5:174:VAL:HG11 | 2.40 | 0.46 |
| 48:G5:17:SER:CB | 48:G5:20:GLU:H | 2.26 | 0.46 |
| 50:I5:60:GLN:N | 50:I5:60:GLN:OE1 | 2.49 | 0.46 |
| 1:13:79:G:H2' | 1:13:79:G:N3 | 2.29 | 0.46 |
| 1:13:189:U:O2 | 17:8I:63:ARG:NH2 | 2.48 | 0.46 |
| 1:13:1163:C:H2' | 1:13:1164:G:C8 | 2.50 | 0.46 |
| 1:13:1191:A:H5" | 1:13:1192:C:OP2 | 2.15 | 0.46 |
| 1:13:1427:U:H2' | 1:13:1428:A:C8 | 2.50 | 0.46 |
| 7:6E:118:VAL:O | 7:6E:121:ALA:HB3 | 2.15 | 0.46 |
| 11:2I:59:TYR:CZ | 11:2I:63:LEU:HD21 | 2.51 | 0.46 |
| 12:3I:90:VAL:HG12 | 12:3I:92:ASP:H | 1.81 | 0.46 |
| 22:2K:61:G:C4 | 22:2K:62:G:C8 | 3.03 | 0.46 |
| 22:3K:7:G:N2 | 22:3K:76:C:O2 | 2.48 | 0.46 |
| 24:1H:661:C:O2' | 35:78:14:LYS:N | 2.43 | 0.46 |
| 24:1H:729:G:C6 | 27:11:208:LYS:HB2 | 2.50 | 0.46 |
| 24:1H:828:U:H2' | 24:1H:829:A:C8 | 2.50 | 0.46 |
| 24:1H:1198:U:H2' | 24:1H:1199:U:H6 | 1.80 | 0.46 |
| 24:1H:1339:G:H5" | 43:F8:16:LYS:HD3 | 1.96 | 0.46 |
| 24:1H:1497:U:H5" | 24:1H:1498:C:H5 | 1.80 | 0.46 |
| 24:1H:1678:G:H21 | 24:1H:1989:G:N2 | 2.11 | 0.46 |
| 24:1H:2822:G:H2' | 24:1H:2823:A:H5" | 1.97 | 0.46 |
| 33:58:96:GLU:O | 33:58:99:LEU:N | 2.44 | 0.46 |
| 36:88:104:PHE:O | 36:88:105:GLU:HB3 | 2.15 | 0.46 |
| 40:C8:97:ASP:OD1 | 40:C8:101:ARG:NH1 | 2.48 | 0.46 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 51:N8:46:CYS:HA | 51:N8:47:PRO:HD2 | 1.81 | 0.46 |
| 1:1G:127:G:C2 | 1:1G:128:G:C8 | 3.03 | 0.46 |
| 1:1G:735:C:H2' | 1:1G:736:C:C6 | 2.45 | 0.46 |
| 1:1G:790:A:OP1 | 22:2L:39:A:O2' | 2.30 | 0.46 |
| 1:1G:1077:G:N2 | 1:1G:1080:A:OP2 | 2.48 | 0.46 |
| 1:1G:1269:A:N1 | 1:1G:1312:G:O2' | 2.30 | 0.46 |
| 3:22:32:LEU:HD22 | 3:22:59:ARG:HH12 | 1.80 | 0.46 |
| 3:22:125:GLU:HG2 | 3:22:190:ARG:O | 2.16 | 0.46 |
| 7:62:28:ASN:OD1 | 7:62:36:LYS:NZ | 2.44 | 0.46 |
| 17:8A:60:ILE:HB | 17:8A:74:LEU:HD12 | 1.97 | 0.46 |
| 17:8A:63:ARG:HG2 | 17:8A:64:PRO:HD2 | 1.98 | 0.46 |
| 19:AA:66:MET:N | 19:AA:67:VAL:HB | 2.31 | 0.46 |
| 22:3L:14:A:H1' | 22:3L:23:A:C6 | 2.50 | 0.46 |
| 24:14:26:G:C6 | 24:14:27:G:N1 | 2.83 | 0.46 |
| 24:14:997:G:O2' | 24:14:998:C:H5' | 2.15 | 0.46 |
| 24:14:1018:C:H2' | 24:14:1019:U:H6 | 1.81 | 0.46 |
| 24:14:1180:C:O2' | 24:14:1181:C:H5' | 2.16 | 0.46 |
| 24:14:1280:G:OP1 | 37:55:33:ARG:NH2 | 2.48 | 0.46 |
| 24:14:1479:G:O2' | 24:14:1558:A:H5' | 2.15 | 0.46 |
| 24:14:1848:A:H2' | 24:14:1849:G:H8 | 1.79 | 0.46 |
| 24:14:1932:A:H2' | 24:14:1933:G:O4' | 2.15 | 0.46 |
| 24:14:2032:G:H21 | 28:29:146:THR:HG23 | 1.79 | 0.46 |
| 24:14:2335:A:C8 | 24:14:2337:G:N7 | 2.83 | 0.46 |
| 24:14:2531:A:H5' | 31:59:157:TYR:CZ | 2.50 | 0.46 |
| 24:14:2724:C:OP1 | 28:29:118:LYS:HE3 | 2.14 | 0.46 |
| 32:69:77:LEU:HD21 | 32:69:141:LYS:HD3 | 1.98 | 0.46 |
| 33:15:39:ARG:C | 33:15:41:ASP:H | 2.23 | 0.46 |
| 35:35:97:PRO:HG3 | 35:35:112:LEU:HD12 | 1.97 | 0.46 |
| 42:A5:40:ASN:O | 42:A5:41:LYS:HG2 | 2.15 | 0.46 |
| 49:H5:5:LYS:HE3 | 49:H5:5:LYS:HB3 | 1.72 | 0.46 |
| 50:I5:36:CYS:HB3 | 50:I5:39:CYS:CB | 2.45 | 0.46 |
| 1:13:853:G:O6 | 57:13:1814:HOH:O | 2.20 | 0.46 |
| 1:13:1103:C:H2' | 1:13:1104:G:O4' | 2.15 | 0.46 |
| 1:13:1327:C:OP1 | 21:1F:21:TYR:HD1 | 1.98 | 0.46 |
| 7:6E:91:VAL:HG12 | 7:6E:95:ARG:HB3 | 1.96 | 0.46 |
| 9:8E:93:ARG:O | 9:8E:97:LYS:N | 2.45 | 0.46 |
| 17:8I:41:LYS:HD3 | 17:8I:88:TYR:OH | 2.15 | 0.46 |
| 19:AI:41:VAL:O | 50:M8:63:TYR:OH | 2.28 | 0.46 |
| 20:BI:40:ALA:HB2 | 20:BI:55:ILE:HG22 | 1.98 | 0.46 |
| 22:2K:19:C:OP1 | 22:2K:19:C:H4' | 2.13 | 0.46 |
| 24:1H:932:G:H4' | 24:1H:933:A:O5' | 2.16 | 0.46 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 24:1H:1800:C:OP2 | 27:11:183:ARG:NH2 | 2.29 | 0.46 |
| 24:1H:2067:G:H4' | 24:1H:2068:U:OP2 | 2.15 | 0.46 |
| 24:1H:2348:U:H4' | 52:O8:42:TRP:CD1 | 2.51 | 0.46 |
| 24:1H:2582:G:C2 | 24:1H:2583:G:C8 | 3.04 | 0.46 |
| 24:1H:2608:G:H8 | 24:1H:2608:G:O5' | 1.99 | 0.46 |
| 24:1H:2745:C:C4 | 24:1H:2746:U:C4 | 3.03 | 0.46 |
| 27:11:85:ASP:OD1 | 27:11:86:PRO:HD2 | 2.16 | 0.46 |
| 29:31:101:LEU:O | 29:31:106:ARG:NH1 | 2.48 | 0.46 |
| 31:51:26:VAL:HG22 | 31:51:33:LEU:O | 2.16 | 0.46 |
| 44:G8:12:THR:O | 44:G8:75:ILE:HB | 2.16 | 0.46 |
| 44:G8:97:ARG:NH2 | 44:G8:104:GLY:HA3 | 2.31 | 0.46 |
| 46:I8:40:GLN:NE2 | 46:I8:57:PHE:HB3 | 2.30 | 0.46 |
| 48:K8:53:LEU:O | 48:K8:57:ILE:HG13 | 2.14 | 0.46 |
| 1:1G:247:G:OP2 | 17:8A:100:LYS:HB2 | 2.16 | 0.46 |
| 1:1G:646:U:H2' | 1:1G:647:C:H6 | 1.81 | 0.46 |
| 1:1G:1277:C:O2' | 1:1G:1279:A:C8 | 2.66 | 0.46 |
| 1:1G:1492:A:C4 | 24:14:1913:A:N6 | 2.83 | 0.46 |
| 2:12:30:ARG:NH2 | 2:12:194:PRO:HB2 | 2.30 | 0.46 |
| 5:42:131:ILE:HD13 | 5:42:131:ILE:HA | 1.81 | 0.46 |
| 8:72:20:TYR:HA | 8:72:65:TYR:CZ | 2.50 | 0.46 |
| 9:82:13:ALA:HB2 | 9:82:68:GLY:HA3 | 1.96 | 0.46 |
| 24:14:14:A:H3' | 24:14:15:G:H5" | 1.98 | 0.46 |
| 24:14:547:A:H3' | 24:14:548:A:C8 | 2.50 | 0.46 |
| 24:14:1663:C:H2' | 57:14:3501:HOH:O | 2.15 | 0.46 |
| 24:14:2251:G:OP1 | 36:45:82:ARG:NH1 | 2.49 | 0.46 |
| 24:14:2840:C:H4' | 37:55:53:HIS:CE1 | 2.51 | 0.46 |
| 25:1J:118:G:H3' | 25:1J:119:A:H8 | 1.79 | 0.46 |
| 29:39:122:LYS:HD2 | 29:39:191:ARG:HE | 1.80 | 0.46 |
| 29:39:183:VAL:O | 29:39:187:VAL:HG23 | 2.15 | 0.46 |
| 40:85:39:LEU:HD23 | 40:85:39:LEU:HA | 1.67 | 0.46 |
| 43:B5:5:TYR:CE1 | 48:G5:30:ARG:HG3 | 2.51 | 0.46 |
| 45:D5:4:ARG:CZ | 45:D5:58:VAL:HG11 | 2.45 | 0.46 |
| 45:D5:100:VAL:N | 45:D5:124:ILE:O | 2.42 | 0.46 |
| 1:13:109:A:C6 | 1:13:326:G:C6 | 3.03 | 0.46 |
| 1:13:405:U:O4 | 4:3E:2:GLY:N | 2.49 | 0.46 |
| 1:13:1148:U:O4' | 9:8E:16:ARG:HD3 | 2.16 | 0.46 |
| 1:13:1157:A:N1 | 1:13:1180:A:H2' | 2.30 | 0.46 |
| 2:1E:215:LEU:O | 2:1E:219:VAL:HG23 | 2.16 | 0.46 |
| 9:8E:37:PHE:CZ | 9:8E:74:ILE:HG12 | 2.50 | 0.46 |
| 9:8E:46:ALA:O | 9:8E:49:PRO:HD2 | 2.16 | 0.46 |
| 14:5I:12:ARG:HG3 | 14:5I:12:ARG:O | 2.14 | 0.46 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 16:7I:67:THR:N | 16:7I:70:ALA:HB3 | 2.30 | 0.46 |
| 20:BI:10:LEU:HD11 | 20:BI:12:ALA:HB3 | 1.98 | 0.46 |
| 24:1H:598:G:H1' | 35:78:12:ALA:HB2 | 1.96 | 0.46 |
| 24:1H:1007:C:OP2 | 24:1H:1008:C:O2' | 2.14 | 0.46 |
| 24:1H:1906:G:C8 | 24:1H:1929:G:H2' | 2.50 | 0.46 |
| 24:1H:2092:U:H5" | 32:61:24:GLY:HA2 | 1.98 | 0.46 |
| 24:1H:2210:G:H2' | 24:1H:2211:G:N7 | 2.29 | 0.46 |
| 24:1H:2311:A:N3 | 30:41:88:ILE:HD13 | 2.30 | 0.46 |
| 26:71:200:LYS:HE3 | 26:71:204:ALA:HB3 | 1.97 | 0.46 |
| 30:41:16:ARG:HH12 | 30:41:31:VAL:HG11 | 1.78 | 0.46 |
| 33:58:39:ARG:HA | 33:58:40:PRO:HD3 | 1.86 | 0.46 |
| 37:98:63:ARG:HA | 37:98:80:PHE:HZ | 1.79 | 0.46 |
| 43:F8:31:HIS:HA | 43:F8:32:PRO:HD3 | 1.71 | 0.46 |
| 43:F8:54:VAL:C | 43:F8:55:ASN:HD22 | 2.24 | 0.46 |
| 1:1G:369:C:O2' | 1:1G:370:C:H5' | 2.16 | 0.46 |
| 1:1G:457:C:H2' | 1:1G:458:C:C6 | 2.50 | 0.46 |
| 1:1G:542:G:OP1 | 4:32:10:ARG:NH2 | 2.48 | 0.46 |
| 1:1G:674:G:H2' | 1:1G:675:A:H8 | 1.80 | 0.46 |
| 1:1G:1255:G:OP1 | 10:1A:45:ARG:NH2 | 2.42 | 0.46 |
| 4:32:30:LYS:HD2 | 4:32:30:LYS:O | 2.15 | 0.46 |
| 4:32:106:TYR:HE1 | 4:32:112:VAL:O | 1.99 | 0.46 |
| 9:82:70:LYS:O | 9:82:74:ILE:HG13 | 2.14 | 0.46 |
| 18:9A:68:LYS:O | 18:9A:72:ARG:HG3 | 2.15 | 0.46 |
| 22:3L:14:A:H3' | 22:3L:15:G:C5' | 2.43 | 0.46 |
| 24:14:654(S):G:H1' | 24:14:654(T):A:OP1 | 2.15 | 0.46 |
| 24:14:1685:C:H2' | 24:14:1686:C:C6 | 2.51 | 0.46 |
| 24:14:1716:U:O2' | 24:14:1717:G:H5' | 2.16 | 0.46 |
| 24:14:2515:C:H1' | 24:14:2570:G:N2 | 2.30 | 0.46 |
| 24:14:2688:U:O2 | 24:14:2688:U:H3' | 2.15 | 0.46 |
| 24:14:2897:U:H5' | 24:14:2898:U:OP2 | 2.16 | 0.46 |
| 30:49:145:THR:O | 30:49:146:TYR:HB3 | 2.16 | 0.46 |
| 36:45:21:THR:H | 36:45:98:LYS:CB | 2.29 | 0.46 |
| 37:55:51:LEU:HD23 | 37:55:51:LEU:HA | 1.78 | 0.46 |
| 39:75:12:SER:HA | 39:75:13:ARG:HA | 1.49 | 0.46 |
| 46:E5:53:MET:HA | 46:E5:58:THR:O | 2.15 | 0.46 |
| 1:13:664:G:OP1 | 18:9I:64:ARG:NE | 2.33 | 0.46 |
| 1:13:740:U:H4' | 15:6I:39:LEU:HD23 | 1.98 | 0.46 |
| 1:13:838:G:H2' | 1:13:841:U:H5" | 1.97 | 0.46 |
| 1:13:992:U:H4' | 1:13:993:G:H5" | 1.98 | 0.46 |
| 1:13:1152:A:H2' | 1:13:1153:C:C6 | 2.50 | 0.46 |
| 1:13:1177:G:C6 | 1:13:1178:G:C2 | 3.04 | 0.46 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 1:13:1409:C:H2' | 1:13:1410:G:H8 | 1.80 | 0.46 |
| 4:3E:59:ARG:NH2 | 4:3E:66:ARG:NH1 | 2.64 | 0.46 |
| 13:4I:3:ARG:HE | 13:4I:7:VAL:HG13 | 1.80 | 0.46 |
| 14:5I:53:LEU:HA | 14:5I:53:LEU:HD23 | 1.47 | 0.46 |
| 16:7I:9:PHE:HB2 | 16:7I:16:HIS:O | 2.16 | 0.46 |
| 20:BI:30:LYS:NZ | 20:BI:80:ARG:HH12 | 2.14 | 0.46 |
| 22:2K:18:G:H5" | 22:2K:19:C:H1' | 1.97 | 0.46 |
| 22:2K:19:C:H3' | 22:2K:20:C:C3' | 2.46 | 0.46 |
| 22:3K:13:G:H2' | 22:3K:14:A:C8 | 2.51 | 0.46 |
| 24:1H:244:A:C2 | 24:1H:255:A:C4 | 3.04 | 0.46 |
| 24:1H:485:C:H2' | 24:1H:486:C:C6 | 2.51 | 0.46 |
| 24:1H:566:U:P | 35:78:29:LYS:HZ3 | 2.39 | 0.46 |
| 24:1H:579:G:H2' | 24:1H:580:C:C6 | 2.50 | 0.46 |
| 24:1H:1742:C:H5' | 24:1H:1743:G:OP2 | 2.16 | 0.46 |
| 24:1H:2081:C:H2' | 24:1H:2082:A:C8 | 2.50 | 0.46 |
| 24:1H:2110:G:C6 | 24:1H:2120:G:C8 | 3.04 | 0.46 |
| 24:1H:2262:U:H4' | 24:1H:2328:A:C2 | 2.51 | 0.46 |
| 24:1H:2345:G:OP2 | 52:O8:39:TYR:HA | 2.15 | 0.46 |
| 24:1H:2476:A:N1 | 24:1H:2477:C:N4 | 2.63 | 0.46 |
| 24:1H:2875:C:H4' | 39:B8:5:ALA:HB2 | 1.98 | 0.46 |
| 31:51:8:PRO:O | 31:51:9:ILE:HG23 | 2.15 | 0.46 |
| 31:51:46:GLU:HB2 | 31:51:49:VAL:HG22 | 1.96 | 0.46 |
| 37:98:15:SER:CB | 57:98:301:HOH:O | 2.64 | 0.46 |
| 1:1G:310:G:OP2 | 16:7A:27:LYS:NZ | 2.38 | 0.46 |
| 1:1G:952:U:H4' | 1:1G:964:A:N1 | 2.31 | 0.46 |
| 1:1G:961:U:OP2 | 1:1G:1223:C:O2' | 2.14 | 0.46 |
| 1:1G:1253:G:H2' | 1:1G:1254:C:C6 | 2.50 | 0.46 |
| 4:32:174:LEU:HD23 | 4:32:174:LEU:HA | 1.67 | 0.46 |
| 14:5A:37:PHE:HB3 | 14:5A:39:LEU:HG | 1.98 | 0.46 |
| 22:3L:3:U:H2' | 22:3L:4:G:C8 | 2.51 | 0.46 |
| 24:14:288:C:O2 | 24:14:288:C:H2' | 2.16 | 0.46 |
| 24:14:653:A:H5" | 24:14:654:A:C8 | 2.51 | 0.46 |
| 24:14:2394:C:H5" | 35:35:64:LYS:HD2 | 1.98 | 0.46 |
| 27:19:204:ILE:HD12 | 27:19:204:ILE:O | 2.16 | 0.46 |
| 41:95:67:GLY:O | 41:95:88:ARG:HD2 | 2.15 | 0.46 |
| 1:13:283:C:C2 | 1:13:284:G:C8 | 3.04 | 0.46 |
| 1:13:297:G:H4' | 1:13:557:G:H4' | 1.98 | 0.46 |
| 1:13:567:G:H2' | 1:13:568:G:O4' | 2.15 | 0.46 |
| 1:13:585:G:H2' | 1:13:586:C:O4' | 2.16 | 0.46 |
| 3:2E:104:GLN:OE1 | 3:2E:105:GLU:N | 2.48 | 0.46 |
| 4:3E:23:GLY:HA2 | 4:3E:112:VAL:HG22 | 1.98 | 0.46 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 9:8E:9:ARG:HB3 | 9:8E:14:VAL:HA | 1.98 | 0.46 |
| 12:3I:89:ARG:CB | 12:3I:97:ARG:HA | 2.46 | 0.46 |
| 20:BI:30:LYS:HA | 20:BI:30:LYS:HD2 | 1.48 | 0.46 |
| 22:2K:20:C:O2' | 22:2K:21:A:P | 2.74 | 0.46 |
| 24:1H:314:A:O2' | 24:1H:315:G:H5' | 2.15 | 0.46 |
| 24:1H:547:A:H2' | 24:1H:548:A:C8 | 2.51 | 0.46 |
| 24:1H:596:G:H2' | 24:1H:597:U:O4' | 2.16 | 0.46 |
| 24:1H:826:U:H2' | 24:1H:828:U:O4' | 2.16 | 0.46 |
| 24:1H:1087:G:C5 | 24:1H:1089:G:H1' | 2.51 | 0.46 |
| 24:1H:1268:A:H5' | 57:1H:4132:HOH:O | 2.16 | 0.46 |
| 24:1H:1312:U:OP1 | 43:F8:63:LYS:HE2 | 2.15 | 0.46 |
| 24:1H:1454:U:H5 | 37:98:73:VAL:HG13 | 1.80 | 0.46 |
| 24:1H:1771:C:H1' | 24:1H:1786:A:C8 | 2.51 | 0.46 |
| 25:16:7:G:H1 | 25:16:113:C:N4 | 2.13 | 0.46 |
| 28:21:6:GLY:HA2 | 28:21:51:PHE:CZ | 2.51 | 0.46 |
| 28:21:60:ASN:OD1 | 28:21:62:PRO:HD2 | 2.16 | 0.46 |
| 30:41:145:THR:O | 30:41:146:TYR:HB3 | 2.16 | 0.46 |
| 45:H8:95:PRO:HB3 | 45:H8:129:SER:HA | 1.98 | 0.46 |
| 46:I8:75:LEU:HD23 | 46:I8:75:LEU:HA | 1.64 | 0.46 |
| 1:1G:620:C:H2' | 1:1G:621:A:O4' | 2.16 | 0.46 |
| 1:1G:678:U:H2' | 1:1G:679:C:H6 | 1.77 | 0.46 |
| 5:42:79:GLU:OE1 | 8:72:104:ARG:HA | 2.15 | 0.46 |
| 10:1A:13:HIS:HB3 | 10:1A:68:HIS:ND1 | 2.31 | 0.46 |
| 24:14:27:G:N2 | 24:14:512:G:O2' | 2.34 | 0.46 |
| 24:14:1384:A:N3 | 24:14:1405:U:H1' | 2.31 | 0.46 |
| 24:14:1399:C:O2' | 24:14:1400:G:H5' | 2.16 | 0.46 |
| 24:14:1538:G:H2' | 24:14:1539:G:C8 | 2.45 | 0.46 |
| 24:14:2774:C:H2' | 24:14:2775:A:C8 | 2.51 | 0.46 |
| 27:19:127:VAL:HA | 27:19:193:VAL:O | 2.16 | 0.46 |
| 28:29:111:ARG:HD2 | 28:29:160:TYR:CD2 | 2.51 | 0.46 |
| 30:49:145:THR:C | 30:49:147:ASP:H | 2.24 | 0.46 |
| 33:15:73:THR:HB | 33:15:82:LEU:HD11 | 1.98 | 0.46 |
| 34:25:111:PHE:O | 34:25:115:VAL:HG23 | 2.16 | 0.46 |
| 35:35:71:VAL:HG12 | 35:35:72:PRO:HD3 | 1.97 | 0.46 |
| 44:C5:13:VAL:HG21 | 44:C5:39:VAL:HG11 | 1.97 | 0.46 |
| 1:13:186:C:H2' | 1:13:186(A):C:H6 | 1.81 | 0.46 |
| 1:13:247:G:OP2 | 17:8I:101:ARG:HG2 | 2.16 | 0.46 |
| 1:13:439:A:C5 | 1:13:440:A:H1' | 2.50 | 0.46 |
| 1:13:707:C:C2 | 1:13:708:C:C5 | 3.04 | 0.46 |
| 1:13:892:A:H61 | 1:13:906:G:H1' | 1.79 | 0.46 |
| 1:13:1268:A:N3 | 1:13:1326:C:O2' | 2.46 | 0.46 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 1:13:1291:G:H2' | 1:13:1292:U:C6 | 2.51 | 0.46 |
| 1:13:1429:C:H2' | 1:13:1430:C:C6 | 2.51 | 0.46 |
| 4:3E:148:VAL:HG12 | 4:3E:149:ALA:O | 2.16 | 0.46 |
| 13:4I:3:ARG:O | 13:4I:57:ARG:NH1 | 2.49 | 0.46 |
| 16:7I:51:VAL:HG12 | 16:7I:52:ASP:C | 2.41 | 0.46 |
| 20:BI:26:ASN:HB2 | 20:BI:71:THR:CG2 | 2.46 | 0.46 |
| 22:2K:71:C:H2' | 22:2K:72:U:C6 | 2.51 | 0.46 |
| 24:1H:760:G:H2' | 24:1H:761:A:O4' | 2.15 | 0.46 |
| 24:1H:871:U:P | 36:88:5:ARG:HE | 2.39 | 0.46 |
| 24:1H:978:G:H2' | 24:1H:979:G:O4' | 2.15 | 0.46 |
| 24:1H:2208:U:O2' | 24:1H:2209:C:H5' | 2.16 | 0.46 |
| 24:1H:2280:G:C2 | 24:1H:2281:C:C6 | 3.04 | 0.46 |
| 24:1H:2572:A:C8 | 28:21:144:ARG:HD2 | 2.51 | 0.46 |
| 25:16:6:C:H2' | 25:16:7:G:H5" | 1.97 | 0.46 |
| 29:31:140:LEU:O | 29:31:143:ALA:HB3 | 2.15 | 0.46 |
| 35:78:47:ASP:OD1 | 35:78:49:ARG:HG3 | 2.16 | 0.46 |
| 35:78:94:GLU:OE2 | 35:78:124:LYS:HD3 | 2.15 | 0.46 |
| 37:98:74:LYS:O | 37:98:76:VAL:N | 2.47 | 0.46 |
| 39:B8:21:GLU:H | 39:B8:21:GLU:HG3 | 1.53 | 0.46 |
| 49:L8:3:ARG:HG2 | 49:L8:38:GLU:CD | 2.41 | 0.46 |
| 51:N8:6:VAL:HA | 51:N8:7:PRO:HD3 | 1.85 | 0.46 |
| 1:1G:69:G:C2 | 1:1G:73:G:C8 | 3.04 | 0.46 |
| 1:1G:714:G:H2' | 1:1G:715:A:C8 | 2.51 | 0.46 |
| 1:1G:918:A:H2' | 1:1G:919:A:O4' | 2.16 | 0.46 |
| 4:32:13:ARG:O | 4:32:16:GLY:N | 2.42 | 0.46 |
| 4:32:33:MET:C | 4:32:35:ARG:H | 2.24 | 0.46 |
| 5:42:107:ARG:O | 5:42:111:GLU:HB2 | 2.16 | 0.46 |
| 13:4A:7:VAL:HG21 | 30:49:115:ARG:HE | 1.81 | 0.46 |
| 22:2L:62:G:C5 | 22:2L:63:5MU:H71 | 2.51 | 0.46 |
| 22:3L:76:C:H2' | 22:3L:77:C:H6 | 1.80 | 0.46 |
| 24:14:864:G:O2' | 24:14:865:C:H5' | 2.15 | 0.46 |
| 24:14:1021:A:H2' | 24:14:1023:U:H5' | 1.97 | 0.46 |
| 24:14:1188:U:H4' | 41:95:79:VAL:HG12 | 1.98 | 0.46 |
| 24:14:1217:C:P | 40:85:15:LYS:HE2 | 2.56 | 0.46 |
| 24:14:1441:G:H2' | 24:14:1442:G:C8 | 2.49 | 0.46 |
| 24:14:1972:A:OP2 | 57:14:3573:HOH:O | 2.20 | 0.46 |
| 24:14:2685:G:O2' | 24:14:2726:U:H5 | 1.98 | 0.46 |
| 24:14:2768:C:H2' | 24:14:2769:C:O4' | 2.16 | 0.46 |
| 40:85:61:TRP:O | 40:85:65:ILE:HG13 | 2.16 | 0.46 |
| 44:C5:19:LYS:HG3 | 44:C5:20:TYR:CD2 | 2.51 | 0.46 |
| 47:F5:87:PRO:O | 47:F5:91:LYS:HB2 | 2.16 | 0.46 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 48:G5:17:SER:HB3 | 48:G5:20:GLU:HB2 | 1.98 | 0.46 |
| 1:13:943:U:H2' | 1:13:944:G:H5' | 1.98 | 0.46 |
| 1:13:1014:A:H4' | 19:AI:14:HIS:CD2 | 2.51 | 0.46 |
| 1:13:1024:G:H4' | 1:13:1024:G:OP1 | 2.15 | 0.46 |
| 1:13:1238:A:C8 | 1:13:1303:C:H1' | 2.51 | 0.46 |
| 1:13:1330:U:H5" | 1:13:1331:G:OP2 | 2.16 | 0.46 |
| 2:1E:178:ARG:HG3 | 8:7E:72:PRO:HA | 1.98 | 0.46 |
| 2:1E:211:ILE:H | 2:1E:211:ILE:HG13 | 1.53 | 0.46 |
| 6:5E:69:GLU:H | 6:5E:69:GLU:CD | 2.24 | 0.46 |
| 7:6E:38:LEU:O | 7:6E:42:ILE:HB | 2.16 | 0.46 |
| 8:7E:100:ILE:HA | 8:7E:101:PRO:HD3 | 1.64 | 0.46 |
| 19:AI:5:LEU:HD11 | 19:AI:10:PHE:CD1 | 2.50 | 0.46 |
| 24:1H:272:G:H2' | 24:1H:273:G:H8 | 1.80 | 0.46 |
| 24:1H:285:C:H2' | 24:1H:286:C:C6 | 2.51 | 0.46 |
| 24:1H:773:U:H4' | 27:11:47:GLY:CA | 2.46 | 0.46 |
| 24:1H:986:C:O2' | 24:1H:987:G:H5' | 2.16 | 0.46 |
| 24:1H:1045:A:OP1 | 24:1H:1046:A:H5' | 2.16 | 0.46 |
| 24:1H:1189:A:P | 57:1H:3675:HOH:O | 2.73 | 0.46 |
| 24:1H:1340:U:H4' | 24:1H:1341:U:OP2 | 2.15 | 0.46 |
| 24:1H:1448:G:H2' | 24:1H:1449:A:C8 | 2.51 | 0.46 |
| 24:1H:1530:G:C5 | 24:1H:1531:C:C4 | 3.04 | 0.46 |
| 24:1H:1587:A:H2' | 24:1H:1588:C:C6 | 2.51 | 0.46 |
| 24:1H:2705:A:O2' | 24:1H:2852:G:OP1 | 2.17 | 0.46 |
| 27:11:70:TRP:CE2 | 27:11:150:LYS:HD3 | 2.51 | 0.46 |
| 27:11:205:VAL:O | 27:11:205:VAL:HG12 | 2.16 | 0.46 |
| 30:41:16:ARG:O | 30:41:20:ILE:HG13 | 2.15 | 0.46 |
| 31:51:12:PRO:HD2 | 31:51:49:VAL:HA | 1.97 | 0.46 |
| 31:51:26:VAL:HG23 | 31:51:27:LYS:H | 1.81 | 0.46 |
| 35:78:36:LYS:HB3 | 35:78:37:GLY:H | 1.33 | 0.46 |
| 36:88:20:ALA:HB3 | 45:H8:79:ARG:NH1 | 2.30 | 0.46 |
| 42:E8:58:ALA:HB1 | 42:E8:64:MET:SD | 2.56 | 0.46 |
| 43:F8:3:THR:O | 43:F8:6:ASP:HB2 | 2.16 | 0.46 |
| 44:G8:21:LYS:HB3 | 44:G8:21:LYS:HE2 | 1.47 | 0.46 |
| 46:I8:42:GLY:O | 46:I8:57:PHE:HD2 | 1.98 | 0.46 |
| 1:1G:57:G:C2 | 1:1G:58:C:C2 | 3.04 | 0.46 |
| 1:1G:391:G:C6 | 1:1G:392:G:C5 | 3.04 | 0.46 |
| 1:1G:540:G:C4 | 1:1G:541:G:C8 | 3.05 | 0.46 |
| 1:1G:1152:A:H5' | 10:1A:13:HIS:CD2 | 2.50 | 0.46 |
| 1:1G:1300:G:HO2' | 1:1G:1301:U:P | 2.39 | 0.46 |
| 1:1G:1413:A:H2' | 1:1G:1414:U:O4' | 2.16 | 0.46 |
| 4:32:50:ARG:HH22 | 5:42:10:MET:HE3 | 1.81 | 0.46 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 4:32:152:SER:HA | 4:32:155:LEU:HD12 | 1.98 | 0.46 |
| 6:52:46:ARG:HE | 6:52:46:ARG:HB3 | 1.54 | 0.46 |
| 9:82:34:ASN:HA | 9:82:37:PHE:CD2 | 2.45 | 0.46 |
| 17:8A:43:LEU:HD12 | 17:8A:68:ARG:HG2 | 1.98 | 0.46 |
| 24:14:57:C:H2' | 24:14:58:G:O4' | 2.16 | 0.46 |
| 24:14:489:G:N7 | 42:A5:49:LYS:NZ | 2.63 | 0.46 |
| 24:14:806:C:OP2 | 35:35:41:ARG:HD3 | 2.15 | 0.46 |
| 24:14:2170:A:H2' | 24:14:2170:A:N3 | 2.31 | 0.46 |
| 24:14:2716:U:O2' | 24:14:2717:G:H5' | 2.15 | 0.46 |
| 27:19:70:TRP:HZ3 | 27:19:146:GLU:OE2 | 1.99 | 0.46 |
| 30:49:138:GLN:C | 30:49:140:ILE:H | 2.24 | 0.46 |
| 34:25:4:PRO:HA | 34:25:21:CYS:O | 2.15 | 0.46 |
| 41:95:76:LYS:HD2 | 41:95:80:GLN:O | 2.16 | 0.46 |
| 49:H5:59:VAL:HG22 | 49:H5:60:GLU:H | 1.79 | 0.46 |
| 1:13:78:G:C6 | 1:13:90:C:N4 | 2.85 | 0.45 |
| 1:13:377:G:OP1 | 16:7I:3:LYS:HD2 | 2.15 | 0.45 |
| 1:13:569:C:H5" | 1:13:570:G:OP1 | 2.16 | 0.45 |
| 1:13:1260:C:O5' | 1:13:1284:C:H4' | 2.16 | 0.45 |
| 3:2E:70:VAL:N | 3:2E:106:VAL:HG23 | 2.30 | 0.45 |
| 11:2I:24:SER:HB3 | 11:2I:27:ASN:O | 2.16 | 0.45 |
| 12:3I:25:PRO:HD2 | 12:3I:98:TYR:OH | 2.16 | 0.45 |
| 24:1H:270(R):G:N7 | 57:1H:3764:HOH:O | 2.36 | 0.45 |
| 24:1H:302:C:O2' | 24:1H:303:U:H5' | 2.16 | 0.45 |
| 24:1H:329:G:H4' | 24:1H:330:A:OP2 | 2.15 | 0.45 |
| 24:1H:811:U:C4 | 35:78:21:ARG:NH2 | 2.84 | 0.45 |
| 24:1H:1181:C:H2' | 24:1H:1182:A:C8 | 2.52 | 0.45 |
| 24:1H:2333:A:N3 | 24:1H:2335:A:N6 | 2.64 | 0.45 |
| 24:1H:2376:A:H2' | 24:1H:2377:A:O4' | 2.16 | 0.45 |
| 24:1H:2393:A:H4' | 35:78:62:LEU:O | 2.16 | 0.45 |
| 26:71:22:ILE:HG23 | 26:71:189:ILE:HD12 | 1.97 | 0.45 |
| 27:11:148:GLU:CB | 27:11:151:LYS:HD2 | 2.45 | 0.45 |
| 30:41:131:TYR:HE2 | 30:41:133:LEU:HD23 | 1.80 | 0.45 |
| 36:88:72:LYS:HA | 36:88:73:PRO:HD3 | 1.74 | 0.45 |
| 45:H8:3:TYR:OH | 45:H8:50:GLN:HB3 | 2.15 | 0.45 |
| 45:H8:11:GLU:HA | 45:H8:36:LYS:HD2 | 1.97 | 0.45 |
| 46:I8:70:GLN:CD | 46:I8:72:ARG:HD2 | 2.42 | 0.45 |
| 50:M8:13:ARG:HB2 | 50:M8:30:GLU:HA | 1.97 | 0.45 |
| 1:1G:235:C:C5' | 17:8A:70:ARG:HG2 | 2.46 | 0.45 |
| 1:1G:254:G:OP1 | 17:8A:68:ARG:HB3 | 2.15 | 0.45 |
| 1:1G:779:C:H2' | 1:1G:780:A:O4' | 2.17 | 0.45 |
| 1:1G:1100:C:O2' | 1:1G:1102:A:OP1 | 2.35 | 0.45 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 1:1G:1103:C:H5” | 2:12:98:LEU:HD13 | 1.98 | 0.45 |
| 1:1G:1118:C:O5’ | 1:1G:1118:C:H6 | 1.99 | 0.45 |
| 3:22:180:ALA:HB1 | 3:22:182:ILE:HG13 | 1.98 | 0.45 |
| 8:72:21:LYS:HG2 | 8:72:23:SER:O | 2.16 | 0.45 |
| 9:82:5:TYR:HE1 | 9:82:16:ARG:HG2 | 1.81 | 0.45 |
| 11:2A:32:ILE:HD12 | 11:2A:68:ALA:HB1 | 1.98 | 0.45 |
| 11:2A:109:VAL:HG12 | 18:9A:86:VAL:HA | 1.97 | 0.45 |
| 18:9A:40:LEU:HA | 18:9A:40:LEU:HD23 | 1.74 | 0.45 |
| 22:3L:73:U:H2’ | 22:3L:74:C:O4’ | 2.17 | 0.45 |
| 24:14:659:C:H4’ | 29:39:100:THR:O | 2.16 | 0.45 |
| 24:14:971:C:H2’ | 24:14:972:G:C5’ | 2.46 | 0.45 |
| 24:14:1582:C:O2’ | 24:14:1586:A:C8 | 2.66 | 0.45 |
| 24:14:1946:U:H2’ | 24:14:1947:C:C6 | 2.51 | 0.45 |
| 24:14:2023:G:OP2 | 24:14:2617:C:H4’ | 2.16 | 0.45 |
| 24:14:2127:G:H21 | 24:14:2173:A:H5” | 1.80 | 0.45 |
| 24:14:2575:C:H2’ | 24:14:2578:G:O6 | 2.16 | 0.45 |
| 25:1J:118:G:H3’ | 25:1J:119:A:C8 | 2.51 | 0.45 |
| 27:19:76:PRO:HB2 | 27:19:116:GLN:HE21 | 1.81 | 0.45 |
| 28:29:6:GLY:HA2 | 28:29:28:ALA:HA | 1.98 | 0.45 |
| 39:75:6:LEU:CA | 39:75:9:LEU:HB3 | 2.46 | 0.45 |
| 46:E5:44:ARG:HH11 | 46:E5:44:ARG:CG | 2.29 | 0.45 |
| 46:E5:68:GLU:HG3 | 46:E5:82:ARG:NH1 | 2.31 | 0.45 |
| 1:13:909:A:H2’ | 1:13:910:C:O4’ | 2.15 | 0.45 |
| 2:1E:178:ARG:NH1 | 2:1E:196:LEU:O | 2.26 | 0.45 |
| 5:4E:121:LYS:HE3 | 5:4E:122:GLU:O | 2.17 | 0.45 |
| 6:5E:4:TYR:HD1 | 6:5E:92:LYS:HA | 1.81 | 0.45 |
| 14:5I:23:ARG:NH1 | 14:5I:28:GLY:O | 2.49 | 0.45 |
| 15:6I:18:PHE:CD1 | 15:6I:18:PHE:C | 2.94 | 0.45 |
| 18:9I:38:GLU:CD | 18:9I:41:LYS:HD3 | 2.41 | 0.45 |
| 22:2K:38:MIA:H152 | 22:2K:38:MIA:HN6 | 1.81 | 0.45 |
| 24:1H:68:G:H2’ | 24:1H:69:C:C6 | 2.51 | 0.45 |
| 24:1H:263:C:H2’ | 24:1H:264:C:O4’ | 2.17 | 0.45 |
| 24:1H:460:A:P | 53:P8:41:ARG:HH22 | 2.39 | 0.45 |
| 24:1H:534:U:H5’ | 40:C8:42:ALA:CB | 2.45 | 0.45 |
| 24:1H:552:G:H2’ | 24:1H:553:U:O4’ | 2.16 | 0.45 |
| 24:1H:806:C:OP2 | 35:78:41:ARG:HD3 | 2.17 | 0.45 |
| 24:1H:919:G:N2 | 24:1H:2269:A:OP2 | 2.49 | 0.45 |
| 24:1H:1288:U:H4’ | 24:1H:1289:C:OP2 | 2.16 | 0.45 |
| 24:1H:2053:G:P | 57:1H:3698:HOH:O | 2.74 | 0.45 |
| 24:1H:2768:C:C4 | 24:1H:2769:C:C5 | 3.04 | 0.45 |
| 25:16:24:G:C2 | 25:16:56:G:C2 | 3.04 | 0.45 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 28:21:167:VAL:CG1 | 28:21:189:PRO:HD3 | 2.46 | 0.45 |
| 30:41:17:PRO:HA | 30:41:20:ILE:HD12 | 1.98 | 0.45 |
| 30:41:76:SER:OG | 30:41:84:LYS:N | 2.50 | 0.45 |
| 35:78:13:ASN:OD1 | 35:78:15:ARG:HD2 | 2.16 | 0.45 |
| 49:L8:3:ARG:HG2 | 49:L8:38:GLU:CG | 2.46 | 0.45 |
| 49:L8:23:LEU:HB3 | 49:L8:28:LEU:HB2 | 1.98 | 0.45 |
| 52:O8:41:PRO:HD2 | 52:O8:46:HIS:HA | 1.97 | 0.45 |
| 52:O8:45:LYS:HD3 | 52:O8:45:LYS:HA | 1.80 | 0.45 |
| 1:1G:382:A:H2' | 1:1G:383:A:H8 | 1.80 | 0.45 |
| 1:1G:458:C:H2' | 1:1G:464:G:C8 | 2.50 | 0.45 |
| 1:1G:567:G:H2' | 1:1G:568:G:O4' | 2.16 | 0.45 |
| 1:1G:632:A:H1' | 1:1G:633:G:OP2 | 2.16 | 0.45 |
| 1:1G:689:C:P | 11:2A:46:GLY:HA3 | 2.56 | 0.45 |
| 1:1G:803:G:C5 | 1:1G:804:U:C4 | 3.04 | 0.45 |
| 1:1G:1286:A:OP1 | 21:1B:25:LYS:NZ | 2.48 | 0.45 |
| 2:12:47:THR:O | 2:12:51:LEU:HB2 | 2.16 | 0.45 |
| 4:32:58:LEU:HD22 | 4:32:62:GLN:HG2 | 1.97 | 0.45 |
| 4:32:112:VAL:HG12 | 4:32:116:GLN:OE1 | 2.17 | 0.45 |
| 6:52:33:TYR:OH | 6:52:78:GLU:HG3 | 2.15 | 0.45 |
| 6:52:70:ASP:OD1 | 6:52:70:ASP:N | 2.37 | 0.45 |
| 9:82:48:GLU:HB3 | 9:82:101:PHE:CE2 | 2.50 | 0.45 |
| 12:3A:6:THR:H | 12:3A:9:GLN:HB2 | 1.81 | 0.45 |
| 16:7A:14:ASN:OD1 | 16:7A:16:HIS:NE2 | 2.48 | 0.45 |
| 22:2L:62:G:C6 | 22:2L:63:5MU:H71 | 2.51 | 0.45 |
| 24:14:307:G:H21 | 24:14:330:A:H62 | 1.64 | 0.45 |
| 24:14:455:C:N3 | 24:14:472:A:H2' | 2.30 | 0.45 |
| 24:14:513:A:C2 | 24:14:514:A:C4 | 3.04 | 0.45 |
| 24:14:580:C:H2' | 24:14:581:C:H6 | 1.77 | 0.45 |
| 24:14:814:C:H5" | 41:95:84:LYS:HB3 | 1.97 | 0.45 |
| 24:14:952:G:C6 | 24:14:953:A:N7 | 2.85 | 0.45 |
| 24:14:1364:G:N7 | 47:F5:2:SER:HB2 | 2.31 | 0.45 |
| 24:14:1535:U:C5 | 24:14:1536:A:H1' | 2.51 | 0.45 |
| 24:14:2392:A:O4' | 24:14:2392:A:N3 | 2.48 | 0.45 |
| 27:19:37:LEU:HA | 27:19:38:LYS:CB | 2.46 | 0.45 |
| 29:39:129:PHE:HA | 29:39:142:TRP:CD1 | 2.50 | 0.45 |
| 31:59:6:ARG:HH12 | 31:59:7:LEU:HD23 | 1.81 | 0.45 |
| 39:75:3:ARG:HA | 39:75:4:GLY:C | 2.42 | 0.45 |
| 44:C5:47:LYS:N | 44:C5:60:PHE:HB3 | 2.28 | 0.45 |
| 1:13:160:A:H1' | 1:13:344:A:N7 | 2.31 | 0.45 |
| 1:13:186:C:H2' | 1:13:186(A):C:C6 | 2.51 | 0.45 |
| 1:13:195:A:OP1 | 20:BI:65:LYS:HE3 | 2.17 | 0.45 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 1:13:224:C:H2' | 1:13:225:C:C6 | 2.50 | 0.45 |
| 1:13:445:G:H1 | 1:13:489:C:H42 | 1.63 | 0.45 |
| 1:13:691:G:O6 | 11:2I:52:GLY:HA2 | 2.15 | 0.45 |
| 1:13:877:C:O2 | 8:7E:3:THR:OG1 | 2.34 | 0.45 |
| 1:13:973:G:OP1 | 10:1I:57:LYS:NZ | 2.31 | 0.45 |
| 1:13:1129:C:H5" | 1:13:1139:G:N7 | 2.32 | 0.45 |
| 1:13:1237:C:H4' | 1:13:1334:G:N2 | 2.30 | 0.45 |
| 2:1E:41:ILE:HD12 | 2:1E:41:ILE:HA | 1.69 | 0.45 |
| 24:1H:14:A:O5' | 24:1H:14:A:H8 | 1.99 | 0.45 |
| 24:1H:221:A:O4' | 24:1H:233:A:H1' | 2.17 | 0.45 |
| 24:1H:1070:A:OP2 | 24:1H:1074:G:N1 | 2.35 | 0.45 |
| 24:1H:1211:U:OP2 | 57:1H:3705:HOH:O | 2.21 | 0.45 |
| 24:1H:1952:A:C5 | 34:68:22:ILE:HD12 | 2.52 | 0.45 |
| 26:71:192:PHE:CZ | 26:71:196:LEU:HD11 | 2.52 | 0.45 |
| 27:11:158:ALA:O | 27:11:159:ALA:C | 2.59 | 0.45 |
| 32:61:11:ASN:CG | 32:61:12:LEU:H | 2.24 | 0.45 |
| 44:G8:13:VAL:HG12 | 44:G8:74:PRO:HA | 1.99 | 0.45 |
| 45:H8:107:THR:O | 45:H8:109:ALA:N | 2.40 | 0.45 |
| 1:1G:131:C:H2' | 1:1G:132:C:C6 | 2.52 | 0.45 |
| 1:1G:201:C:H42 | 1:1G:216:G:H1 | 1.62 | 0.45 |
| 1:1G:626:U:C2 | 1:1G:627:G:C8 | 3.04 | 0.45 |
| 1:1G:1262:C:H2' | 1:1G:1263:C:C6 | 2.51 | 0.45 |
| 3:22:6:HIS:HB3 | 14:5A:49:HIS:HD2 | 1.80 | 0.45 |
| 11:2A:17:GLY:N | 11:2A:79:SER:O | 2.40 | 0.45 |
| 15:6A:67:LEU:HD22 | 15:6A:78:TYR:CE2 | 2.52 | 0.45 |
| 19:AA:42:PRO:C | 19:AA:44:MET:H | 2.24 | 0.45 |
| 22:3L:47:U:H2' | 22:3L:48:C:C6 | 2.50 | 0.45 |
| 24:14:531:C:H4' | 24:14:532:A:H5" | 1.98 | 0.45 |
| 24:14:1062:G:H2' | 24:14:1063:G:N7 | 2.31 | 0.45 |
| 24:14:1641:A:N6 | 24:14:1642:G:C2 | 2.84 | 0.45 |
| 24:14:1657:C:H2' | 24:14:1658:C:C6 | 2.52 | 0.45 |
| 28:29:16:ARG:NH2 | 28:29:171:GLU:OE1 | 2.48 | 0.45 |
| 29:39:130:ALA:H | 29:39:142:TRP:CD1 | 2.34 | 0.45 |
| 32:69:76:THR:CG2 | 32:69:140:LEU:HD13 | 2.47 | 0.45 |
| 34:25:101:PRO:HG3 | 39:75:67:SER:OG | 2.15 | 0.45 |
| 36:45:37:LEU:HD12 | 36:45:128:LYS:HB3 | 1.98 | 0.45 |
| 39:75:105:LEU:O | 39:75:107:ASP:CG | 2.60 | 0.45 |
| 42:A5:13:SER:O | 42:A5:14:PRO:C | 2.60 | 0.45 |
| 45:D5:120:ILE:HD12 | 45:D5:173:ALA:HB2 | 1.99 | 0.45 |
| 54:M5:19:SER:OG | 54:M5:21:LYS:HD2 | 2.17 | 0.45 |
| 54:M5:50:LEU:HD12 | 54:M5:50:LEU:HA | 1.83 | 0.45 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 1:13:344:A:H8 | 1:13:346:G:N7 | 2.15 | 0.45 |
| 1:13:813:U:OP2 | 1:13:813:U:H6 | 2.00 | 0.45 |
| 1:13:1053:G:N7 | 1:13:1200:C:H5' | 2.31 | 0.45 |
| 1:13:1336:C:O2' | 1:13:1337:G:O5' | 2.35 | 0.45 |
| 2:1E:55:PHE:CD1 | 2:1E:58:ILE:HD12 | 2.51 | 0.45 |
| 4:3E:55:ALA:O | 4:3E:59:ARG:HG2 | 2.16 | 0.45 |
| 4:3E:173:TRP:HA | 4:3E:187:ARG:CG | 2.47 | 0.45 |
| 22:3K:57:C:C2 | 22:3K:68:A:H1' | 2.50 | 0.45 |
| 24:1H:74:A:H4' | 24:1H:75:G:O5' | 2.17 | 0.45 |
| 24:1H:466:A:N3 | 24:1H:683:C:H1' | 2.31 | 0.45 |
| 24:1H:654:A:H3' | 24:1H:654:A:N3 | 2.32 | 0.45 |
| 24:1H:827:U:H5' | 24:1H:828:U:O5' | 2.16 | 0.45 |
| 24:1H:910:A:N7 | 36:88:13:GLN:HG3 | 2.31 | 0.45 |
| 24:1H:1169:G:N2 | 24:1H:1181:C:C2 | 2.85 | 0.45 |
| 24:1H:2028:U:H2' | 24:1H:2029:G:O4' | 2.15 | 0.45 |
| 24:1H:2147:G:C5 | 24:1H:2148:G:H1' | 2.51 | 0.45 |
| 24:1H:2355:C:H1' | 46:I8:39:ARG:HH21 | 1.82 | 0.45 |
| 24:1H:2402:C:HO2' | 24:1H:2403:C:P | 2.40 | 0.45 |
| 24:1H:2404:C:H1' | 35:78:67:MET:HE1 | 1.98 | 0.45 |
| 24:1H:2552:U:C2 | 24:1H:2554:U:H5' | 2.52 | 0.45 |
| 24:1H:2689:U:P | 24:1H:2719:G:H22 | 2.39 | 0.45 |
| 30:41:15:VAL:HG13 | 30:41:175:LEU:HB2 | 1.97 | 0.45 |
| 31:51:69:ARG:NH1 | 31:51:73:ALA:HB2 | 2.31 | 0.45 |
| 32:61:95:LYS:O | 32:61:99:GLU:HG3 | 2.16 | 0.45 |
| 37:98:18:LEU:HD22 | 37:98:22:ARG:HG3 | 1.98 | 0.45 |
| 37:98:38:VAL:HB | 37:98:39:PRO:HD3 | 1.98 | 0.45 |
| 40:C8:59:ARG:O | 40:C8:63:VAL:HG23 | 2.16 | 0.45 |
| 41:D8:35:LEU:C | 41:D8:37:VAL:H | 2.18 | 0.45 |
| 44:G8:6:HIS:HE1 | 44:G8:69:ALA:O | 1.99 | 0.45 |
| 46:I8:36:ILE:CD1 | 46:I8:39:ARG:HG2 | 2.44 | 0.45 |
| 51:N8:39:MET:O | 51:N8:40:LYS:HE3 | 2.17 | 0.45 |
| 1:1G:189:U:O2' | 17:8A:63:ARG:NH2 | 2.49 | 0.45 |
| 1:1G:498:A:H4' | 1:1G:500:G:H5' | 1.98 | 0.45 |
| 1:1G:547:A:OP2 | 4:32:2:GLY:HA2 | 2.16 | 0.45 |
| 1:1G:837:G:C2 | 1:1G:850:U:O2 | 2.70 | 0.45 |
| 1:1G:994:A:C5 | 1:1G:1216:G:H4' | 2.51 | 0.45 |
| 1:1G:1346:A:O4' | 1:1G:1348:U:C6 | 2.70 | 0.45 |
| 2:12:62:ALA:O | 2:12:65:GLY:N | 2.46 | 0.45 |
| 3:22:149:ALA:HA | 3:22:201:TYR:O | 2.17 | 0.45 |
| 9:82:125:TYR:CD1 | 9:82:126:SER:N | 2.83 | 0.45 |
| 13:4A:97:PRO:HB2 | 13:4A:101:GLN:NE2 | 2.21 | 0.45 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 18:9A:22:VAL:HG22 | 18:9A:23:LYS:N | 2.31 | 0.45 |
| 21:1B:6:ARG:CZ | 21:1B:15:ARG:HH12 | 2.29 | 0.45 |
| 24:14:27:G:O2' | 24:14:28:A:OP2 | 2.32 | 0.45 |
| 24:14:270(M):U:H1' | 24:14:270(N):G:C6 | 2.50 | 0.45 |
| 24:14:397:G:O2' | 24:14:2231:C:H1' | 2.17 | 0.45 |
| 24:14:1314:C:H5' | 24:14:1314:C:C6 | 2.51 | 0.45 |
| 24:14:1582:C:O2' | 24:14:1586:A:H8 | 1.98 | 0.45 |
| 24:14:1614:A:OP1 | 57:14:3574:HOH:O | 2.21 | 0.45 |
| 24:14:1929:G:H4' | 24:14:1930:G:OP1 | 2.15 | 0.45 |
| 24:14:2448:A:P | 57:14:3505:HOH:O | 2.67 | 0.45 |
| 24:14:2870:C:C2' | 24:14:2871:C:H5' | 2.47 | 0.45 |
| 25:1J:78:A:C2 | 25:1J:99:A:C4 | 3.04 | 0.45 |
| 27:19:33:LEU:C | 27:19:64:ILE:HG23 | 2.41 | 0.45 |
| 34:25:63:VAL:HG12 | 34:25:106:LEU:HD11 | 1.99 | 0.45 |
| 34:25:87:ILE:HG23 | 34:25:91:LEU:HA | 1.98 | 0.45 |
| 39:75:54:ARG:HA | 39:75:59:THR:HB | 1.97 | 0.45 |
| 41:95:67:GLY:O | 41:95:88:ARG:NH1 | 2.42 | 0.45 |
| 1:13:627:G:H2' | 1:13:628:G:C8 | 2.50 | 0.45 |
| 1:13:686:U:O2' | 1:13:687:A:P | 2.75 | 0.45 |
| 1:13:1086:U:H2' | 1:13:1087:G:O4' | 2.17 | 0.45 |
| 1:13:1288:A:N3 | 1:13:1352:C:O2' | 2.45 | 0.45 |
| 1:13:1365:G:H2' | 1:13:1366:C:H6 | 1.81 | 0.45 |
| 6:5E:19:LEU:HD21 | 6:5E:59:TYR:CE1 | 2.52 | 0.45 |
| 7:6E:150:ALA:HB2 | 11:2I:50:TYR:OH | 2.16 | 0.45 |
| 19:AI:18:LYS:NZ | 19:AI:22:LEU:HD21 | 2.31 | 0.45 |
| 19:AI:42:PRO:HD3 | 50:M8:63:TYR:CE1 | 2.52 | 0.45 |
| 22:3K:35:QUO:H162 | 23:4K:14:A:H8 | 1.82 | 0.45 |
| 24:1H:768:G:O2' | 24:1H:1379:A:N6 | 2.47 | 0.45 |
| 24:1H:1387:C:H5' | 24:1H:1469:A:H4' | 1.99 | 0.45 |
| 24:1H:1686:C:H2' | 24:1H:1687:G:O4' | 2.16 | 0.45 |
| 24:1H:1690:A:H3' | 24:1H:1691:C:H6 | 1.81 | 0.45 |
| 24:1H:1783:A:H5' | 24:1H:2608:G:H4' | 1.98 | 0.45 |
| 24:1H:2209:C:O2 | 24:1H:2216:G:C2 | 2.69 | 0.45 |
| 24:1H:2397:G:N2 | 24:1H:2420:C:H1' | 2.31 | 0.45 |
| 24:1H:2410:G:C2 | 24:1H:2411:A:H1' | 2.51 | 0.45 |
| 24:1H:2712:U:O2 | 24:1H:2712:U:H2' | 2.17 | 0.45 |
| 24:1H:2799:A:H2' | 24:1H:2801:A:H8 | 1.80 | 0.45 |
| 27:11:232:PRO:HB3 | 27:11:244:ARG:NH1 | 2.31 | 0.45 |
| 29:31:164:ARG:HG2 | 29:31:175:THR:OG1 | 2.16 | 0.45 |
| 30:41:125:PHE:HA | 30:41:130:ASN:O | 2.17 | 0.45 |
| 36:88:133:ARG:O | 36:88:134:ARG:HB2 | 2.17 | 0.45 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 39:B8:20:PRO:HD2 | 39:B8:86:ILE:HG12 | 1.97 | 0.45 |
| 41:D8:8:GLY:O | 41:D8:10:LYS:HE3 | 2.17 | 0.45 |
| 41:D8:64:HIS:CG | 41:D8:92:THR:HG22 | 2.51 | 0.45 |
| 43:F8:14:SER:O | 43:F8:15:GLU:C | 2.60 | 0.45 |
| 45:H8:89:PHE:HE2 | 45:H8:96:VAL:HG21 | 1.80 | 0.45 |
| 48:K8:24:LEU:HD23 | 48:K8:24:LEU:HA | 1.74 | 0.45 |
| 1:1G:553:A:H2' | 1:1G:554:C:H6 | 1.81 | 0.45 |
| 1:1G:833:U:O2' | 1:1G:834:C:H5' | 2.16 | 0.45 |
| 1:1G:1190:G:OP2 | 1:1G:1190:G:H8 | 2.00 | 0.45 |
| 1:1G:1347:G:N2 | 1:1G:1373:G:H2' | 2.32 | 0.45 |
| 17:8A:83:ASP:N | 17:8A:83:ASP:OD1 | 2.50 | 0.45 |
| 22:2L:1:G:N3 | 22:2L:2:G:C8 | 2.84 | 0.45 |
| 22:3L:36:U:H2' | 22:3L:37:A:O4' | 2.17 | 0.45 |
| 24:14:99:U:O2 | 24:14:102:G:N1 | 2.50 | 0.45 |
| 24:14:286:C:H2' | 24:14:287:C:H6 | 1.82 | 0.45 |
| 24:14:315:G:H2' | 24:14:316:C:C6 | 2.51 | 0.45 |
| 24:14:910:A:N1 | 24:14:2277:G:H1' | 2.31 | 0.45 |
| 24:14:1092:C:N4 | 24:14:1099:G:H1 | 2.15 | 0.45 |
| 24:14:1141:U:H2' | 33:15:63:THR:HG21 | 1.99 | 0.45 |
| 24:14:1274:A:N3 | 24:14:1297:C:H1' | 2.31 | 0.45 |
| 24:14:2262:U:H5 | 46:E5:16:SER:OG | 1.99 | 0.45 |
| 24:14:2636:U:OP1 | 28:29:80:GLU:N | 2.45 | 0.45 |
| 30:49:6:ALA:O | 30:49:9:ARG:HB3 | 2.16 | 0.45 |
| 31:59:149:ARG:HG2 | 31:59:154:PRO:HB3 | 1.99 | 0.45 |
| 39:75:125:ARG:HD3 | 39:75:125:ARG:HA | 1.78 | 0.45 |
| 43:B5:57:LEU:N | 43:B5:57:LEU:HD23 | 2.32 | 0.45 |
| 1:13:707:C:H2' | 1:13:708:C:C6 | 2.52 | 0.45 |
| 1:13:954:G:O6 | 13:4I:104:ARG:NH1 | 2.50 | 0.45 |
| 2:1E:184:VAL:O | 2:1E:198:ASP:HB2 | 2.17 | 0.45 |
| 3:2E:15:THR:HG21 | 3:2E:181:ASN:HA | 1.99 | 0.45 |
| 3:2E:46:GLU:HB2 | 3:2E:83:ARG:HH21 | 1.80 | 0.45 |
| 9:8E:128:ARG:NH2 | 22:2K:34:U:H3' | 2.31 | 0.45 |
| 10:1I:40:LEU:HB3 | 10:1I:41:PRO:HD2 | 1.99 | 0.45 |
| 17:8I:58:GLU:OE2 | 17:8I:75:ARG:NH2 | 2.49 | 0.45 |
| 18:9I:74:ARG:HG2 | 18:9I:79:LEU:HB2 | 1.99 | 0.45 |
| 20:BI:13:LEU:HD12 | 20:BI:14:LYS:N | 2.31 | 0.45 |
| 20:BI:63:ILE:HD12 | 20:BI:81:LYS:HG2 | 1.99 | 0.45 |
| 22:2K:79:A:H2' | 22:2K:80:C:O4' | 2.16 | 0.45 |
| 24:1H:739:G:H8 | 24:1H:739:G:O5' | 1.99 | 0.45 |
| 24:1H:1359:A:H2' | 24:1H:1360:A:C5' | 2.46 | 0.45 |
| 24:1H:1470:G:N2 | 24:1H:1522:G:OP2 | 2.47 | 0.45 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 24:1H:1486:A:H2' | 24:1H:1487:G:C8 | 2.51 | 0.45 |
| 24:1H:2146:C:H4' | 24:1H:2147:G:C5 | 2.51 | 0.45 |
| 24:1H:2314:C:O3' | 30:41:36:LYS:NZ | 2.49 | 0.45 |
| 24:1H:2602:A:H4' | 24:1H:2603:G:O5' | 2.17 | 0.45 |
| 24:1H:2653:U:OP2 | 24:1H:2654:A:O2' | 2.30 | 0.45 |
| 25:16:9:G:C6 | 25:16:10:C:C4 | 3.05 | 0.45 |
| 31:51:80:SER:C | 31:51:81:GLU:HG3 | 2.42 | 0.45 |
| 33:58:95:PRO:O | 33:58:97:ARG:N | 2.49 | 0.45 |
| 44:G8:9:LYS:HA | 44:G8:27:VAL:HG22 | 1.97 | 0.45 |
| 45:H8:151:HIS:N | 45:H8:154:ASP:OD2 | 2.50 | 0.45 |
| 52:O8:15:GLU:HG3 | 52:O8:16:CYS:N | 2.31 | 0.45 |
| 1:1G:191(F):U:H2' | 1:1G:191:G:H8 | 1.82 | 0.45 |
| 1:1G:403:C:OP1 | 4:32:137:SER:OG | 2.30 | 0.45 |
| 1:1G:1365:G:H2' | 1:1G:1366:C:C6 | 2.50 | 0.45 |
| 3:22:79:ARG:H | 3:22:79:ARG:CZ | 2.30 | 0.45 |
| 3:22:92:ALA:HB2 | 3:22:99:VAL:CG2 | 2.47 | 0.45 |
| 4:32:117:ALA:O | 4:32:121:VAL:HG23 | 2.16 | 0.45 |
| 20:BA:97:ALA:O | 20:BA:99:LEU:HG | 2.17 | 0.45 |
| 24:14:1114:G:H2' | 24:14:1115:G:C8 | 2.51 | 0.45 |
| 24:14:1810:A:H2' | 24:14:1811:G:O4' | 2.16 | 0.45 |
| 24:14:2009:G:H1' | 37:55:107:ASP:O | 2.17 | 0.45 |
| 24:14:2016:U:H1' | 51:J5:6:VAL:HG13 | 1.98 | 0.45 |
| 24:14:2287:A:N1 | 24:14:2346:A:C2 | 2.76 | 0.45 |
| 24:14:2790:A:H5' | 24:14:2791:C:H5' | 1.97 | 0.45 |
| 27:19:228:PRO:HD3 | 27:19:235:GLY:N | 2.31 | 0.45 |
| 28:29:27:LEU:HA | 28:29:180:ASN:O | 2.16 | 0.45 |
| 30:49:55:LYS:HA | 30:49:55:LYS:HD2 | 1.80 | 0.45 |
| 32:69:85:GLU:OE1 | 32:69:86:THR:HG22 | 2.16 | 0.45 |
| 44:C5:15:VAL:HG12 | 44:C5:21:LYS:HA | 1.99 | 0.45 |
| 1:13:775:G:O2' | 1:13:776:G:H5' | 2.16 | 0.45 |
| 1:13:1264:C:H1' | 1:13:1272:G:N2 | 2.32 | 0.45 |
| 1:13:1502:A:H5' | 1:13:1504:G:N7 | 2.32 | 0.45 |
| 4:3E:50:ARG:HA | 4:3E:51:PRO:HD3 | 1.83 | 0.45 |
| 5:4E:12:LEU:O | 5:4E:30:ALA:HA | 2.17 | 0.45 |
| 9:8E:17:VAL:HG21 | 9:8E:80:GLY:HA3 | 1.99 | 0.45 |
| 13:4I:107:ALA:HB3 | 13:4I:111:LYS:HE2 | 1.99 | 0.45 |
| 13:4I:107:ALA:HB3 | 13:4I:111:LYS:HG2 | 1.99 | 0.45 |
| 20:BI:33:ILE:HD11 | 20:BI:62:LEU:HD22 | 1.98 | 0.45 |
| 24:1H:33:U:H4' | 24:1H:34:C:OP1 | 2.16 | 0.45 |
| 24:1H:483:A:O2' | 44:G8:49:VAL:O | 2.23 | 0.45 |
| 24:1H:528:A:N1 | 24:1H:2043:C:O5' | 2.50 | 0.45 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 24:1H:639:U:H2' | 24:1H:640:C:C6 | 2.52 | 0.45 |
| 24:1H:1510:A:OP1 | 24:1H:1511:A:H5' | 2.17 | 0.45 |
| 24:1H:1533:C:H2' | 24:1H:1534:G:H8 | 1.79 | 0.45 |
| 24:1H:1590:U:H2' | 24:1H:1591:G:H8 | 1.80 | 0.45 |
| 24:1H:2343:C:HO2' | 24:1H:2373:G:HO2' | 1.60 | 0.45 |
| 24:1H:2822:G:OP1 | 28:21:159:HIS:NE2 | 2.49 | 0.45 |
| 24:1H:2854:G:C6 | 24:1H:2855:C:C4 | 3.05 | 0.45 |
| 26:71:5:LYS:HA | 26:71:8:ARG:HB2 | 1.99 | 0.45 |
| 36:88:75:THR:HG22 | 36:88:90:VAL:H | 1.82 | 0.45 |
| 40:C8:70:ARG:NH2 | 40:C8:75:ASN:HB2 | 2.32 | 0.45 |
| 49:L8:7:LYS:HG3 | 49:L8:34:GLU:HG3 | 1.99 | 0.45 |
| 1:1G:359:U:H2' | 1:1G:360:A:C8 | 2.52 | 0.45 |
| 1:1G:518:C:H5 | 1:1G:530:G:OP2 | 2.00 | 0.45 |
| 1:1G:545:C:H5' | 4:32:72:GLU:HB2 | 1.98 | 0.45 |
| 1:1G:988:G:C6 | 1:1G:989:C:C2 | 3.04 | 0.45 |
| 1:1G:1251:A:H4' | 9:82:12:GLU:CD | 2.42 | 0.45 |
| 1:1G:1256:A:C8 | 1:1G:1278:U:O4' | 2.70 | 0.45 |
| 6:52:78:GLU:O | 6:52:81:ILE:HG13 | 2.16 | 0.45 |
| 12:3A:97:ARG:HB2 | 12:3A:98:TYR:CE2 | 2.52 | 0.45 |
| 19:AA:20:LEU:O | 19:AA:23:ASN:HB2 | 2.17 | 0.45 |
| 22:2L:15:G:H22 | 22:2L:57:C:N4 | 2.13 | 0.45 |
| 22:2L:29:C:H2' | 22:2L:30:A:C8 | 2.51 | 0.45 |
| 24:14:71:A:H5" | 24:14:73:A:C8 | 2.52 | 0.45 |
| 24:14:78:A:H2' | 24:14:79:G:H8 | 1.81 | 0.45 |
| 24:14:249:C:P | 57:14:3510:HOH:O | 2.70 | 0.45 |
| 24:14:1045:A:N3 | 24:14:1045:A:H2' | 2.32 | 0.45 |
| 24:14:1568:G:OP2 | 27:19:63:ARG:NH2 | 2.47 | 0.45 |
| 24:14:1680:U:H2' | 24:14:1681:G:O4' | 2.17 | 0.45 |
| 24:14:2123:G:N2 | 26:79:44:HIS:HE1 | 2.14 | 0.45 |
| 24:14:2418:A:P | 54:M5:29:LYS:HZ1 | 2.39 | 0.45 |
| 24:14:2748:A:H2' | 24:14:2749:A:C8 | 2.47 | 0.45 |
| 27:19:58:HIS:CD2 | 27:19:59:LYS:N | 2.85 | 0.45 |
| 28:29:112:GLY:C | 28:29:159:HIS:HD2 | 2.25 | 0.45 |
| 30:49:44:GLY:O | 30:49:47:LYS:HD2 | 2.16 | 0.45 |
| 30:49:93:THR:HG21 | 30:49:95:ARG:HH21 | 1.81 | 0.45 |
| 30:49:110:ALA:HA | 30:49:140:ILE:O | 2.17 | 0.45 |
| 31:59:10:PRO:HD2 | 31:59:50:VAL:O | 2.17 | 0.45 |
| 34:25:113:LYS:HE3 | 34:25:117:LEU:HD11 | 1.98 | 0.45 |
| 39:75:16:ARG:NH2 | 39:75:19:LEU:HD21 | 2.32 | 0.45 |
| 47:F5:80:LEU:HD12 | 47:F5:82:LEU:HD21 | 1.98 | 0.45 |
| 47:F5:82:LEU:H | 47:F5:82:LEU:CD2 | 2.29 | 0.45 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 47:F5:90:ILE:HA | 47:F5:94:LEU:HD12 | 1.98 | 0.45 |
| 54:M5:28:GLY:O | 54:M5:34:TRP:CH2 | 2.70 | 0.45 |
| 1:13:105:G:H2' | 1:13:106:C:C6 | 2.52 | 0.45 |
| 1:13:585:G:O3' | 17:8I:34:LYS:NZ | 2.45 | 0.45 |
| 1:13:591:U:C2 | 1:13:592:G:C8 | 3.05 | 0.45 |
| 1:13:643:C:H5' | 8:7E:31:PHE:CD1 | 2.52 | 0.45 |
| 1:13:1117:G:O3' | 9:8E:104:ARG:HD3 | 2.15 | 0.45 |
| 1:13:1277:C:O2' | 1:13:1279:A:H1' | 2.17 | 0.45 |
| 3:2E:40:ARG:O | 3:2E:44:GLU:HG2 | 2.16 | 0.45 |
| 3:2E:152:ILE:HB | 3:2E:199:LYS:HB2 | 1.99 | 0.45 |
| 16:7I:26:ARG:CZ | 16:7I:31:LYS:HB3 | 2.47 | 0.45 |
| 22:3K:72:U:H2' | 22:3K:73:U:O4' | 2.17 | 0.45 |
| 24:1H:420:C:H2' | 24:1H:421:U:H6 | 1.82 | 0.45 |
| 24:1H:482:A:O2' | 24:1H:497:A:N1 | 2.41 | 0.45 |
| 24:1H:569:U:C4 | 24:1H:570:G:C6 | 3.05 | 0.45 |
| 24:1H:603:A:C8 | 24:1H:655:A:C6 | 3.04 | 0.45 |
| 24:1H:636:G:H4' | 24:1H:638:G:O3' | 2.16 | 0.45 |
| 24:1H:649:G:C5 | 24:1H:650:C:C4 | 3.05 | 0.45 |
| 24:1H:1006:C:H1' | 33:58:106:MET:HG2 | 1.98 | 0.45 |
| 24:1H:1709:U:H2' | 24:1H:1710:C:C6 | 2.51 | 0.45 |
| 24:1H:1853:A:H2' | 24:1H:1854:A:H8 | 1.80 | 0.45 |
| 24:1H:2470:G:H5' | 36:88:56:ARG:HH21 | 1.82 | 0.45 |
| 24:1H:2543:G:H2' | 24:1H:2544:G:O4' | 2.17 | 0.45 |
| 24:1H:2824:C:H2' | 24:1H:2825:C:O4' | 2.17 | 0.45 |
| 30:41:56:ALA:HB2 | 30:41:153:ARG:CZ | 2.47 | 0.45 |
| 31:51:41:MET:HE2 | 31:51:54:ARG:CB | 2.46 | 0.45 |
| 31:51:71:LEU:HD12 | 31:51:71:LEU:HA | 1.83 | 0.45 |
| 32:61:11:ASN:CG | 32:61:12:LEU:N | 2.74 | 0.45 |
| 35:78:49:ARG:O | 54:Q8:56:GLU:HG3 | 2.16 | 0.45 |
| 36:88:28:ALA:HB3 | 36:88:29:PHE:CD1 | 2.52 | 0.45 |
| 37:98:51:LEU:HD13 | 37:98:70:LEU:HD11 | 1.98 | 0.45 |
| 39:B8:16:ARG:HD3 | 39:B8:79:HIS:HA | 1.99 | 0.45 |
| 41:D8:1:MET:HE1 | 41:D8:43:GLU:HB2 | 1.97 | 0.45 |
| 46:I8:60:PHE:CD1 | 46:I8:60:PHE:N | 2.84 | 0.45 |
| 1:1G:20:U:H2' | 1:1G:21:G:O4' | 2.16 | 0.45 |
| 1:1G:148:G:N2 | 1:1G:149:A:C2 | 2.85 | 0.45 |
| 1:1G:1088:G:C5 | 1:1G:1089:G:N7 | 2.85 | 0.45 |
| 1:1G:1251:A:H2' | 1:1G:1252:A:C8 | 2.51 | 0.45 |
| 5:42:72:GLN:N | 5:42:72:GLN:OE1 | 2.49 | 0.45 |
| 6:52:17:SER:O | 6:52:21:LEU:HB2 | 2.17 | 0.45 |
| 6:52:67:MET:HE3 | 6:52:67:MET:HB2 | 1.83 | 0.45 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 6:52:97:PHE:N | 18:9A:30:ASP:OD1 | 2.46 | 0.45 |
| 8:72:11:THR:HG23 | 8:72:14:ARG:HH12 | 1.81 | 0.45 |
| 8:72:51:VAL:HG22 | 8:72:52:ASP:N | 2.28 | 0.45 |
| 12:3A:70:ILE:HG21 | 12:3A:75:HIS:CD2 | 2.51 | 0.45 |
| 18:9A:52:PRO:O | 18:9A:56:THR:HG23 | 2.16 | 0.45 |
| 19:AA:16:LEU:HG | 19:AA:20:LEU:HD23 | 1.98 | 0.45 |
| 19:AA:62:ILE:HD11 | 19:AA:71:LEU:HD21 | 1.98 | 0.45 |
| 22:3L:80:C:H2' | 22:3L:81:C:C6 | 2.52 | 0.45 |
| 24:14:34:C:H2' | 24:14:35:G:H5' | 1.98 | 0.45 |
| 24:14:35:G:H2' | 24:14:36:G:O4' | 2.17 | 0.45 |
| 24:14:240:G:H1' | 24:14:257:A:H61 | 1.82 | 0.45 |
| 24:14:643:A:N1 | 24:14:2369:A:O2' | 2.44 | 0.45 |
| 24:14:1132:A:N1 | 24:14:2039:C:O2' | 2.46 | 0.45 |
| 24:14:1926:U:H2' | 24:14:1928:A:OP2 | 2.16 | 0.45 |
| 24:14:1971:A:C5 | 27:19:241:PRO:HD3 | 2.52 | 0.45 |
| 27:19:26:LYS:HB3 | 27:19:83:GLU:HG2 | 1.98 | 0.45 |
| 28:29:27:LEU:HB2 | 28:29:181:LEU:HD12 | 1.98 | 0.45 |
| 28:29:182:LEU:O | 28:29:183:LEU:HD12 | 2.17 | 0.45 |
| 35:35:36:LYS:HB3 | 35:35:37:GLY:H | 1.44 | 0.45 |
| 36:45:98:LYS:HB3 | 36:45:99:PRO:HD2 | 1.98 | 0.45 |
| 48:G5:47:ASN:O | 48:G5:49:LYS:N | 2.50 | 0.45 |
| 1:13:690:G:N3 | 1:13:690:G:O4' | 2.48 | 0.45 |
| 2:1E:149:LEU:HD23 | 2:1E:149:LEU:HA | 1.52 | 0.45 |
| 3:2E:23:TYR:CD2 | 3:2E:24:ALA:N | 2.85 | 0.45 |
| 4:3E:96:LEU:HD11 | 4:3E:139:ARG:NH1 | 2.32 | 0.45 |
| 6:5E:67:MET:HE1 | 6:5E:75:LEU:HD12 | 1.98 | 0.45 |
| 7:6E:73:MET:HB2 | 7:6E:73:MET:HE2 | 1.50 | 0.45 |
| 7:6E:138:LYS:HD3 | 7:6E:142:GLU:HG3 | 1.99 | 0.45 |
| 9:8E:111:ARG:HE | 9:8E:111:ARG:HB2 | 1.62 | 0.45 |
| 11:2I:58:PRO:HB2 | 11:2I:93:GLN:HG3 | 1.99 | 0.45 |
| 16:7I:28:ARG:HG3 | 16:7I:29:ASP:N | 2.32 | 0.45 |
| 22:2K:1:G:C2 | 22:2K:2:G:N7 | 2.85 | 0.45 |
| 22:3K:83:C:H2' | 22:3K:84:C:C6 | 2.51 | 0.45 |
| 24:1H:483:A:N7 | 24:1H:497:A:H2 | 2.15 | 0.45 |
| 24:1H:706:A:OP1 | 27:11:7:LYS:HE3 | 2.17 | 0.45 |
| 24:1H:994:C:OP1 | 40:C8:53:ARG:NH2 | 2.49 | 0.45 |
| 24:1H:1060:U:H1' | 24:1H:1061:U:OP2 | 2.15 | 0.45 |
| 24:1H:2131:G:O2' | 24:1H:2133:G:N3 | 2.48 | 0.45 |
| 24:1H:2716:U:O2' | 24:1H:2717:G:H5' | 2.17 | 0.45 |
| 24:1H:2881:C:C2 | 24:1H:2882:A:C8 | 3.05 | 0.45 |
| 24:1H:2888:C:H2' | 24:1H:2889:C:H6 | 1.82 | 0.45 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 25:16:44:G:C2 | 25:16:48:A:C2 | 3.05 | 0.45 |
| 27:11:149:PRO:O | 27:11:150:LYS:HB2 | 2.17 | 0.45 |
| 31:51:40:GLU:O | 31:51:41:MET:HB3 | 2.17 | 0.45 |
| 32:61:76:THR:HG21 | 32:61:141:LYS:HE3 | 1.99 | 0.45 |
| 35:78:47:ASP:HA | 35:78:48:PRO:HD3 | 1.68 | 0.45 |
| 37:98:111:LEU:HD23 | 37:98:111:LEU:HA | 1.71 | 0.45 |
| 38:A8:34:HIS:HB2 | 38:A8:36:TYR:CE1 | 2.52 | 0.45 |
| 39:B8:23:ARG:O | 39:B8:49:VAL:HG21 | 2.17 | 0.45 |
| 39:B8:102:ILE:HA | 39:B8:105:LEU:HD22 | 1.99 | 0.45 |
| 42:E8:84:ARG:HB2 | 42:E8:96:ILE:HD11 | 1.99 | 0.45 |
| 45:H8:144:LEU:HB3 | 45:H8:148:ASP:HB3 | 1.99 | 0.45 |
| 48:K8:42:GLY:C | 48:K8:44:LEU:N | 2.72 | 0.45 |
| 49:L8:24:LYS:O | 49:L8:27:GLY:N | 2.44 | 0.45 |
| 49:L8:44:ARG:HA | 49:L8:47:VAL:HB | 1.98 | 0.45 |
| 1:1G:32:A:H2' | 1:1G:33:A:C8 | 2.52 | 0.45 |
| 1:1G:197:A:H1' | 1:1G:198:G:O4' | 2.17 | 0.45 |
| 1:1G:545:C:OP1 | 4:32:61:LYS:NZ | 2.50 | 0.45 |
| 1:1G:749:C:H2' | 1:1G:750:G:H8 | 1.81 | 0.45 |
| 1:1G:862:C:H2' | 1:1G:863:U:C6 | 2.52 | 0.45 |
| 1:1G:1141:C:H2' | 1:1G:1142:G:C8 | 2.51 | 0.45 |
| 1:1G:1386:G:H2' | 1:1G:1387:G:H8 | 1.81 | 0.45 |
| 2:12:36:ARG:HB3 | 2:12:41:ILE:HD13 | 1.98 | 0.45 |
| 5:42:15:ARG:HG3 | 5:42:26:PHE:HB3 | 1.99 | 0.45 |
| 7:62:115:ARG:O | 7:62:118:VAL:HG22 | 2.17 | 0.45 |
| 15:6A:55:GLY:O | 15:6A:59:MET:HG3 | 2.17 | 0.45 |
| 24:14:247:G:H4' | 24:14:386:G:C5 | 2.52 | 0.45 |
| 24:14:270(D):C:H2' | 24:14:270(E):G:O4' | 2.16 | 0.45 |
| 24:14:685:A:OP1 | 53:L5:11:LYS:NZ | 2.49 | 0.45 |
| 24:14:686:G:H5" | 53:L5:11:LYS:HZ2 | 1.81 | 0.45 |
| 24:14:729:G:C5 | 27:19:208:LYS:HB2 | 2.52 | 0.45 |
| 24:14:863:A:O2' | 24:14:864:G:H5' | 2.16 | 0.45 |
| 24:14:1466:G:H5' | 24:14:1467:C:OP1 | 2.16 | 0.45 |
| 24:14:1478:G:H2' | 24:14:1479:G:H8 | 1.82 | 0.45 |
| 24:14:1485:G:O2' | 24:14:1486:A:H5' | 2.16 | 0.45 |
| 24:14:1503:U:H2' | 24:14:1504:C:C6 | 2.50 | 0.45 |
| 24:14:2114:A:N6 | 24:14:2119:A:N7 | 2.65 | 0.45 |
| 24:14:2129:C:H2' | 24:14:2130:U:O4' | 2.17 | 0.45 |
| 29:39:20:LEU:HD13 | 29:39:199:TRP:CH2 | 2.52 | 0.45 |
| 29:39:29:ASN:O | 29:39:33:LEU:HD22 | 2.17 | 0.45 |
| 33:15:68:GLU:H | 33:15:68:GLU:HG3 | 1.61 | 0.45 |
| 38:65:88:ASP:OD1 | 38:65:88:ASP:C | 2.59 | 0.45 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 42:A5:90:ARG:NH1 | 42:A5:90:ARG:HG3 | 2.32 | 0.45 |
| 54:M5:54:GLU:OE1 | 54:M5:54:GLU:N | 2.50 | 0.45 |
| 1:13:165:C:H2' | 1:13:166:G:C8 | 2.52 | 0.45 |
| 1:13:478:A:H2' | 1:13:479:C:C6 | 2.52 | 0.45 |
| 1:13:582:U:H2' | 1:13:583:A:C8 | 2.52 | 0.45 |
| 1:13:792:A:H1' | 1:13:794:A:N7 | 2.32 | 0.45 |
| 1:13:951:G:HO2' | 1:13:972:C:H5 | 1.63 | 0.45 |
| 1:13:997:U:H2' | 1:13:998:G:O4' | 2.17 | 0.45 |
| 1:13:1014:A:H2' | 1:13:1015:A:C8 | 2.52 | 0.45 |
| 1:13:1128:C:H1' | 1:13:1146:A:H61 | 1.82 | 0.45 |
| 1:13:1291:G:O2' | 9:8E:38:GLN:OE1 | 2.25 | 0.45 |
| 2:1E:67:THR:O | 2:1E:68:ILE:HD12 | 2.17 | 0.45 |
| 3:2E:10:PHE:HD1 | 14:5I:58:LYS:NZ | 2.15 | 0.45 |
| 9:8E:53:VAL:HB | 9:8E:95:LYS:NZ | 2.32 | 0.45 |
| 13:4I:67:GLU:OE2 | 13:4I:68:GLY:N | 2.42 | 0.45 |
| 24:1H:105:C:H2' | 24:1H:106:C:H6 | 1.82 | 0.45 |
| 24:1H:323:G:HO2' | 24:1H:1205:U:H3 | 1.61 | 0.45 |
| 24:1H:956:G:N2 | 24:1H:959:A:H3' | 2.32 | 0.45 |
| 24:1H:1543:A:C2 | 24:1H:1545:A:C4 | 3.05 | 0.45 |
| 24:1H:1561:G:H2' | 24:1H:1562:A:H8 | 1.82 | 0.45 |
| 24:1H:1827:C:H5' | 24:1H:1971:A:H5' | 1.98 | 0.45 |
| 24:1H:1932:A:H2' | 24:1H:1933:G:O4' | 2.17 | 0.45 |
| 24:1H:2215:G:O2' | 24:1H:2216:G:H5' | 2.17 | 0.45 |
| 24:1H:2336:A:H61 | 46:I8:43:THR:HB | 1.81 | 0.45 |
| 24:1H:2356:C:H2' | 24:1H:2357:U:O4' | 2.16 | 0.45 |
| 24:1H:2888:C:H2' | 24:1H:2889:C:C6 | 2.52 | 0.45 |
| 30:41:27:ASN:HB3 | 30:41:30:GLU:HB2 | 1.98 | 0.45 |
| 30:41:161:THR:HG21 | 30:41:172:LEU:HD22 | 2.00 | 0.45 |
| 37:98:2:ARG:HA | 37:98:5:LYS:HE2 | 1.99 | 0.45 |
| 44:G8:75:ILE:HG23 | 44:G8:76:CYS:O | 2.17 | 0.45 |
| 50:M8:37:SER:HB3 | 50:M8:42:PHE:HB3 | 1.98 | 0.45 |
| 52:O8:13:CYS:HA | 52:O8:51:GLU:HA | 1.98 | 0.45 |
| 53:P8:31:LEU:HD22 | 53:P8:42:LEU:HD13 | 1.99 | 0.45 |
| 4:32:31:CYS:C | 4:32:33:MET:N | 2.54 | 0.45 |
| 9:82:18:PHE:HB2 | 9:82:62:TYR:O | 2.17 | 0.45 |
| 13:4A:56:LEU:O | 13:4A:60:VAL:HG23 | 2.17 | 0.45 |
| 24:14:142:G:OP1 | 24:14:1598:C:H1' | 2.17 | 0.45 |
| 24:14:881:G:C2 | 24:14:882:G:H1' | 2.52 | 0.45 |
| 24:14:1012:U:OP1 | 40:85:75:ASN:ND2 | 2.38 | 0.45 |
| 24:14:1496:A:C8 | 24:14:1577:C:O2' | 2.69 | 0.45 |
| 24:14:1769:G:H2' | 24:14:1770:G:H5' | 1.99 | 0.45 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 24:14:1796:U:H2' | 24:14:1797:C:C6 | 2.52 | 0.45 |
| 25:1J:12:C:OP2 | 25:1J:12:C:C6 | 2.70 | 0.45 |
| 25:1J:89(A):A:C8 | 25:1J:90:C:H1' | 2.52 | 0.45 |
| 26:79:10:LEU:HB3 | 26:79:220:PRO:HD3 | 1.98 | 0.45 |
| 27:19:137:PRO:O | 27:19:140:THR:HG23 | 2.16 | 0.45 |
| 27:19:146:GLU:HB2 | 27:19:189:CYS:HB3 | 1.99 | 0.45 |
| 27:19:242:ARG:N | 27:19:242:ARG:HD3 | 2.31 | 0.45 |
| 33:15:137:LYS:HA | 33:15:137:LYS:HZ2 | 1.82 | 0.45 |
| 36:45:118:LEU:HD12 | 36:45:131:ILE:HG23 | 1.99 | 0.45 |
| 40:85:95:LEU:O | 40:85:98:LEU:HG | 2.17 | 0.45 |
| 41:95:77:ALA:O | 41:95:79:VAL:HG22 | 2.17 | 0.45 |
| 43:B5:25:LYS:HA | 43:B5:81:VAL:O | 2.17 | 0.45 |
| 50:I5:11:PRO:HA | 50:I5:25:TYR:CD1 | 2.51 | 0.45 |
| 50:I5:32:TYR:HB3 | 50:I5:33:VAL:H | 1.43 | 0.45 |
| 1:13:406:G:H5' | 4:3E:5:ILE:HD13 | 1.99 | 0.44 |
| 1:13:808:C:H2' | 1:13:809:G:O4' | 2.16 | 0.44 |
| 1:13:1323:G:H4' | 1:13:1362(A):C:N3 | 2.33 | 0.44 |
| 1:13:1371:G:C5 | 1:13:1372:U:C5 | 3.04 | 0.44 |
| 2:1E:212:GLN:O | 2:1E:216:SER:HB2 | 2.17 | 0.44 |
| 4:3E:84:LYS:HA | 4:3E:84:LYS:HD2 | 1.49 | 0.44 |
| 4:3E:117:ALA:O | 4:3E:121:VAL:HG23 | 2.16 | 0.44 |
| 5:4E:153:LYS:O | 8:7E:64:LYS:NZ | 2.42 | 0.44 |
| 7:6E:16:LEU:HD11 | 9:8E:45:ALA:HB2 | 1.99 | 0.44 |
| 7:6E:116:ALA:C | 7:6E:118:VAL:H | 2.25 | 0.44 |
| 10:1I:38:ILE:HA | 10:1I:39:PRO:HD3 | 1.72 | 0.44 |
| 16:7I:67:THR:H | 16:7I:70:ALA:HB3 | 1.81 | 0.44 |
| 18:9I:44:LEU:HD11 | 18:9I:70:ILE:HG21 | 1.99 | 0.44 |
| 22:3K:37:A:N6 | 22:3K:38:MIA:H122 | 2.32 | 0.44 |
| 24:1H:74:A:C5' | 24:1H:74:A:C8 | 2.98 | 0.44 |
| 24:1H:270(X):G:O6 | 24:1H:270(Y):G:N1 | 2.50 | 0.44 |
| 24:1H:482:A:H5" | 24:1H:483:A:OP1 | 2.17 | 0.44 |
| 24:1H:577:G:OP1 | 24:1H:2502:G:O2' | 2.28 | 0.44 |
| 24:1H:1403:C:H5" | 24:1H:1471:A:C1' | 2.42 | 0.44 |
| 24:1H:1709:U:H1' | 24:1H:2860:A:N3 | 2.31 | 0.44 |
| 24:1H:2641:G:OP1 | 33:58:74:ARG:NE | 2.40 | 0.44 |
| 24:1H:2666:C:H3' | 24:1H:2667:C:C6 | 2.52 | 0.44 |
| 28:21:108:SER:OG | 28:21:163:GLU:HG2 | 2.17 | 0.44 |
| 29:31:192:LEU:CD2 | 29:31:194:MET:HE2 | 2.44 | 0.44 |
| 38:A8:99:LYS:HE2 | 38:A8:103:GLU:OE1 | 2.18 | 0.44 |
| 44:G8:54:LYS:O | 44:G8:55:TYR:CG | 2.70 | 0.44 |
| 44:G8:104:GLY:N | 44:G8:105:ALA:HB3 | 2.31 | 0.44 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 45:H8:23:LYS:HG2 | 45:H8:38:TYR:CE1 | 2.51 | 0.44 |
| 47:J8:19:GLN:O | 47:J8:35:THR:N | 2.45 | 0.44 |
| 1:1G:166:G:H2' | 1:1G:167:G:C8 | 2.51 | 0.44 |
| 1:1G:391:G:C5 | 1:1G:392:G:C8 | 3.06 | 0.44 |
| 1:1G:403:C:O2' | 1:1G:404:U:H5' | 2.17 | 0.44 |
| 1:1G:445:G:H2' | 1:1G:446:G:O4' | 2.17 | 0.44 |
| 1:1G:748:C:H6 | 1:1G:748:C:O5' | 2.00 | 0.44 |
| 1:1G:1112:C:N3 | 3:22:178:LEU:HB2 | 2.32 | 0.44 |
| 1:1G:1118:C:H1' | 1:1G:1179:A:C4 | 2.52 | 0.44 |
| 1:1G:1144:G:N2 | 1:1G:1146:A:H62 | 2.16 | 0.44 |
| 1:1G:1151:A:C5 | 1:1G:1152:A:N7 | 2.85 | 0.44 |
| 5:42:30:ALA:O | 5:42:45:PHE:HD1 | 2.00 | 0.44 |
| 10:1A:54:PHE:CE1 | 10:1A:55:LYS:HE3 | 2.52 | 0.44 |
| 19:AA:66:MET:HA | 19:AA:67:VAL:O | 2.17 | 0.44 |
| 20:BA:20:LEU:HA | 20:BA:20:LEU:HD23 | 1.69 | 0.44 |
| 22:3L:20:C:O2' | 22:3L:22:A:O5' | 2.32 | 0.44 |
| 24:14:533:G:H5' | 40:85:24:TYR:CE1 | 2.53 | 0.44 |
| 24:14:537:C:O2 | 33:15:45:ASN:ND2 | 2.50 | 0.44 |
| 24:14:696:G:H2' | 24:14:697:C:H6 | 1.82 | 0.44 |
| 24:14:912:C:C2 | 24:14:913:U:C5 | 3.06 | 0.44 |
| 24:14:996:A:H4' | 40:85:92:ARG:NE | 2.33 | 0.44 |
| 24:14:1000:A:C6 | 24:14:1001:A:N1 | 2.85 | 0.44 |
| 24:14:1259:G:H2' | 24:14:1260:G:C8 | 2.52 | 0.44 |
| 24:14:1697:G:OP2 | 24:14:1698:A:O2' | 2.26 | 0.44 |
| 24:14:1790:C:H2' | 24:14:1791:A:C5 | 2.52 | 0.44 |
| 24:14:2273:A:H2' | 24:14:2274:A:C8 | 2.52 | 0.44 |
| 24:14:2286:A:O5' | 52:K5:28:ARG:HD2 | 2.17 | 0.44 |
| 24:14:2543:G:H21 | 24:14:2646:C:H5" | 1.81 | 0.44 |
| 25:1J:29:A:C2 | 25:1J:56:G:C2 | 3.05 | 0.44 |
| 29:39:192:LEU:HD22 | 29:39:194:MET:HE2 | 1.99 | 0.44 |
| 30:49:40:ASN:HB2 | 30:49:91:ARG:HG3 | 1.99 | 0.44 |
| 32:69:75:LEU:HD12 | 32:69:76:THR:H | 1.81 | 0.44 |
| 34:25:7:TYR:CE1 | 34:25:44:LYS:HG3 | 2.52 | 0.44 |
| 34:25:9:GLU:O | 34:25:83:ALA:HA | 2.18 | 0.44 |
| 38:65:107:GLU:H | 38:65:110:LEU:CD2 | 2.19 | 0.44 |
| 41:95:62:LEU:HD11 | 41:95:95:LEU:HB2 | 1.98 | 0.44 |
| 44:C5:20:TYR:CZ | 44:C5:42:VAL:HA | 2.52 | 0.44 |
| 1:13:89:U:C2 | 1:13:90:C:C5 | 3.05 | 0.44 |
| 1:13:304:U:H2' | 1:13:305:G:C8 | 2.53 | 0.44 |
| 1:13:666:G:H8 | 1:13:666:G:OP1 | 2.00 | 0.44 |
| 1:13:1122:U:O4 | 1:13:1123:A:N6 | 2.50 | 0.44 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 1:13:1434:A:H2' | 1:13:1435:G:O4' | 2.17 | 0.44 |
| 4:3E:96:LEU:HA | 4:3E:96:LEU:HD13 | 1.64 | 0.44 |
| 14:5I:26:ARG:HD3 | 14:5I:43:CYS:HB2 | 2.00 | 0.44 |
| 20:BI:73:HIS:O | 20:BI:76:ALA:HB3 | 2.17 | 0.44 |
| 22:2K:84:C:H5' | 57:1H:3757:HOH:O | 2.16 | 0.44 |
| 22:3K:21:A:C5 | 22:3K:46:G:C8 | 3.05 | 0.44 |
| 24:1H:1838:C:C2 | 24:1H:1898:U:C4 | 3.05 | 0.44 |
| 24:1H:1864:U:OP1 | 24:1H:2410:G:O2' | 2.21 | 0.44 |
| 24:1H:2014:A:H2' | 24:1H:2015:A:C8 | 2.52 | 0.44 |
| 24:1H:2212:A:H1' | 24:1H:2215:G:C5 | 2.52 | 0.44 |
| 24:1H:2744:G:O2' | 24:1H:2745:C:H5' | 2.16 | 0.44 |
| 24:1H:2821:A:H2' | 24:1H:2822:G:O4' | 2.17 | 0.44 |
| 28:21:134:ILE:C | 28:21:134:ILE:HD12 | 2.43 | 0.44 |
| 29:31:134:GLY:CA | 29:31:166:ALA:HB2 | 2.47 | 0.44 |
| 31:51:8:PRO:HG2 | 31:51:69:ARG:NH2 | 2.18 | 0.44 |
| 42:E8:73:ALA:HB3 | 42:E8:106:ILE:HG12 | 1.99 | 0.44 |
| 52:O8:10:LEU:HD23 | 54:Q8:35:GLN:NE2 | 2.33 | 0.44 |
| 1:1G:118:U:H3' | 1:1G:288:A:H61 | 1.82 | 0.44 |
| 1:1G:191(F):U:H2' | 1:1G:191:G:C8 | 2.53 | 0.44 |
| 1:1G:262:A:C6 | 1:1G:263:A:C6 | 3.04 | 0.44 |
| 1:1G:614:A:C2 | 1:1G:627:G:C2 | 3.05 | 0.44 |
| 1:1G:828:A:H5" | 1:1G:859:A:N1 | 2.31 | 0.44 |
| 1:1G:908:A:H2' | 1:1G:909:A:H8 | 1.79 | 0.44 |
| 1:1G:1200:C:O2' | 1:1G:1205:U:O4 | 2.26 | 0.44 |
| 2:12:10:LEU:HD12 | 2:12:13:ALA:HB2 | 1.99 | 0.44 |
| 15:6A:82:ILE:HB | 15:6A:87:ILE:HB | 1.99 | 0.44 |
| 22:3L:26:G:H2' | 22:3L:27:A:O4' | 2.17 | 0.44 |
| 24:14:494:G:OP1 | 42:A5:8:ARG:NH1 | 2.50 | 0.44 |
| 24:14:883:G:H2' | 24:14:884:C:C6 | 2.53 | 0.44 |
| 24:14:1032:A:H2 | 24:14:1122:G:H1 | 1.65 | 0.44 |
| 24:14:1728:G:C6 | 24:14:1730:U:H5' | 2.53 | 0.44 |
| 24:14:1729:A:O2' | 24:14:1730:U:H5" | 2.16 | 0.44 |
| 24:14:2625:G:H2' | 24:14:2626:C:O4' | 2.17 | 0.44 |
| 28:29:4:ILE:C | 28:29:5:LEU:HD23 | 2.43 | 0.44 |
| 28:29:9:VAL:HA | 39:75:3:ARG:HD3 | 1.99 | 0.44 |
| 32:69:40:THR:O | 32:69:44:LEU:N | 2.46 | 0.44 |
| 35:35:147:LEU:CD1 | 35:35:148:LEU:H | 2.29 | 0.44 |
| 45:D5:5:LEU:HD12 | 45:D5:5:LEU:HA | 1.79 | 0.44 |
| 45:D5:113:ALA:HB1 | 45:D5:178:GLU:HA | 1.99 | 0.44 |
| 45:D5:134:PRO:C | 45:D5:136:PHE:H | 2.25 | 0.44 |
| 52:K5:18:ARG:HA | 52:K5:18:ARG:NH1 | 2.27 | 0.44 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 1:13:64:G:H4' | 1:13:65:U:H5' | 1.99 | 0.44 |
| 1:13:555:C:H2' | 1:13:556:C:H6 | 1.80 | 0.44 |
| 1:13:718:G:H5' | 11:2I:117:ASN:ND2 | 2.32 | 0.44 |
| 1:13:875:C:C4 | 1:13:876:G:N7 | 2.85 | 0.44 |
| 1:13:1133:G:C4 | 1:13:1134:G:C8 | 3.05 | 0.44 |
| 1:13:1366:C:O2' | 10:1I:60:ARG:NH2 | 2.49 | 0.44 |
| 2:1E:21:ARG:O | 2:1E:23:ARG:N | 2.50 | 0.44 |
| 2:1E:102:LEU:HD23 | 2:1E:182:ILE:HD12 | 1.98 | 0.44 |
| 11:2I:44:SER:OG | 11:2I:47:VAL:HG23 | 2.17 | 0.44 |
| 12:3I:62:SER:HB2 | 12:3I:64:TYR:CD1 | 2.51 | 0.44 |
| 13:4I:45:VAL:O | 13:4I:48:LEU:HD22 | 2.17 | 0.44 |
| 20:BI:35:THR:O | 20:BI:38:LYS:HB3 | 2.17 | 0.44 |
| 22:3K:14:A:H3' | 22:3K:15:G:H5" | 1.98 | 0.44 |
| 22:3K:63:5MU:C4 | 22:3K:64:PSU:C2 | 3.05 | 0.44 |
| 24:1H:191:A:H2' | 24:1H:192:C:C6 | 2.52 | 0.44 |
| 24:1H:265:A:C8 | 24:1H:266:G:H1' | 2.53 | 0.44 |
| 24:1H:270(X):G:C6 | 24:1H:270(Y):G:N1 | 2.86 | 0.44 |
| 24:1H:562:U:O4 | 24:1H:2036:C:H1' | 2.18 | 0.44 |
| 24:1H:778:G:OP2 | 57:1H:3709:HOH:O | 2.21 | 0.44 |
| 24:1H:998:C:P | 40:C8:92:ARG:NH2 | 2.89 | 0.44 |
| 24:1H:1038:C:H2' | 24:1H:1039:G:O4' | 2.17 | 0.44 |
| 24:1H:1055:G:N3 | 24:1H:1055:G:H2' | 2.32 | 0.44 |
| 24:1H:1832:C:N4 | 24:1H:1833:U:C4 | 2.86 | 0.44 |
| 24:1H:2378:A:H4' | 38:A8:23:ARG:NH1 | 2.32 | 0.44 |
| 24:1H:2450:A:C2 | 24:1H:2451:A:C4 | 3.05 | 0.44 |
| 24:1H:2662:A:C4 | 24:1H:2663:G:H1' | 2.52 | 0.44 |
| 25:16:108:C:H5' | 25:16:109:G:O5' | 2.17 | 0.44 |
| 27:11:223:GLY:HA3 | 27:11:231:HIS:CE1 | 2.51 | 0.44 |
| 27:11:245:PRO:HG2 | 27:11:253:GLN:HE21 | 1.82 | 0.44 |
| 39:B8:26:ASP:HB2 | 39:B8:90:GLN:O | 2.16 | 0.44 |
| 40:C8:76:TYR:OH | 40:C8:92:ARG:NH1 | 2.47 | 0.44 |
| 49:L8:4:LEU:HD23 | 49:L8:4:LEU:HA | 1.70 | 0.44 |
| 1:1G:42:G:H2' | 1:1G:43:C:C6 | 2.52 | 0.44 |
| 1:1G:1056:U:O3' | 3:22:155:GLY:HA2 | 2.17 | 0.44 |
| 1:1G:1298:C:H4' | 1:1G:1299:A:N9 | 2.33 | 0.44 |
| 5:42:31:LEU:CD1 | 5:42:45:PHE:HB2 | 2.39 | 0.44 |
| 9:82:116:LYS:HB3 | 9:82:121:ARG:O | 2.17 | 0.44 |
| 10:1A:48:THR:OG1 | 10:1A:62:HIS:HB3 | 2.17 | 0.44 |
| 13:4A:16:ASP:OD1 | 13:4A:17:VAL:N | 2.50 | 0.44 |
| 18:9A:22:VAL:CG1 | 18:9A:56:THR:HA | 2.47 | 0.44 |
| 18:9A:53:ARG:HA | 18:9A:56:THR:OG1 | 2.17 | 0.44 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 19:AA:29:ARG:HD2 | 19:AA:48:THR:O | 2.18 | 0.44 |
| 22:2L:17:OMG:HM23 | 22:2L:66:G:H1 | 1.83 | 0.44 |
| 24:14:586:A:P | 57:14:3652:HOH:O | 2.75 | 0.44 |
| 24:14:795:C:O2' | 24:14:796:C:H5' | 2.17 | 0.44 |
| 24:14:1026:U:H6 | 24:14:1026:U:H5" | 1.81 | 0.44 |
| 24:14:1030:G:OP2 | 36:45:128:LYS:NZ | 2.33 | 0.44 |
| 24:14:1301:A:O2' | 24:14:1302:A:H3' | 2.17 | 0.44 |
| 24:14:1845:G:OP1 | 27:19:258:LYS:NZ | 2.45 | 0.44 |
| 24:14:2887:U:O2' | 24:14:2888:C:H5' | 2.17 | 0.44 |
| 25:1J:32:C:C2 | 25:1J:51:G:N2 | 2.85 | 0.44 |
| 28:29:26:ILE:HD13 | 28:29:196:VAL:HG21 | 1.99 | 0.44 |
| 32:69:26:ALA:HA | 32:69:30:LEU:HB2 | 1.98 | 0.44 |
| 33:15:17:ASP:O | 33:15:56:ASN:HB2 | 2.17 | 0.44 |
| 35:35:47:ASP:OD1 | 35:35:49:ARG:HB2 | 2.17 | 0.44 |
| 35:35:52:GLU:OE1 | 35:35:56:SER:N | 2.50 | 0.44 |
| 39:75:36:GLU:OE2 | 39:75:41:ARG:HD3 | 2.17 | 0.44 |
| 41:95:51:VAL:HG12 | 41:95:52:VAL:O | 2.17 | 0.44 |
| 1:13:342:C:H2' | 1:13:343:U:O4' | 2.18 | 0.44 |
| 1:13:582:U:OP1 | 15:6I:64:ARG:NH1 | 2.50 | 0.44 |
| 1:13:619:U:C4 | 4:3E:135:LEU:HD11 | 2.52 | 0.44 |
| 2:1E:144:ARG:O | 2:1E:147:LYS:HB3 | 2.18 | 0.44 |
| 4:3E:133:VAL:HG11 | 4:3E:138:TYR:CD2 | 2.52 | 0.44 |
| 11:2I:125:PHE:N | 11:2I:125:PHE:CD1 | 2.84 | 0.44 |
| 16:7I:58:TYR:C | 16:7I:58:TYR:CD1 | 2.95 | 0.44 |
| 22:2K:4:G:H1 | 22:2K:78:C:N4 | 2.15 | 0.44 |
| 22:2K:85:A:O3' | 24:1H:2602:A:C6 | 2.65 | 0.44 |
| 24:1H:491:G:H2' | 24:1H:492:A:C8 | 2.53 | 0.44 |
| 24:1H:515:A:H2 | 24:1H:1260:G:N3 | 2.15 | 0.44 |
| 24:1H:821:A:O2' | 24:1H:946:G:H5" | 2.18 | 0.44 |
| 24:1H:1024:G:C3' | 24:1H:1025:G:H5" | 2.47 | 0.44 |
| 24:1H:1332:G:N2 | 24:1H:1610:A:H8 | 2.12 | 0.44 |
| 24:1H:1810:A:H2' | 24:1H:1811:G:O4' | 2.18 | 0.44 |
| 24:1H:2115:G:C2 | 24:1H:2117:A:C8 | 3.04 | 0.44 |
| 24:1H:2320:A:H1' | 24:1H:2321:G:C6 | 2.52 | 0.44 |
| 24:1H:2636:U:H4' | 28:21:80:GLU:OE2 | 2.17 | 0.44 |
| 24:1H:2680:C:OP2 | 28:21:111:ARG:NH2 | 2.51 | 0.44 |
| 24:1H:2784:C:H2' | 24:1H:2785:C:C6 | 2.52 | 0.44 |
| 24:1H:2836:U:H2' | 24:1H:2837:G:H8 | 1.77 | 0.44 |
| 25:16:80:U:O2' | 25:16:81:G:H5' | 2.17 | 0.44 |
| 25:16:89:G:C6 | 25:16:89(A):A:C6 | 3.06 | 0.44 |
| 28:21:2:LYS:HB2 | 28:21:95:ILE:HG21 | 2.00 | 0.44 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 29:31:68:LYS:C | 29:31:70:THR:H | 2.24 | 0.44 |
| 36:88:4:PRO:HD3 | 36:88:70:PRO:O | 2.18 | 0.44 |
| 36:88:35:VAL:HG12 | 36:88:130:LYS:O | 2.18 | 0.44 |
| 39:B8:42:ILE:HG12 | 39:B8:84:GLN:NE2 | 2.33 | 0.44 |
| 47:J8:82:LEU:CD2 | 47:J8:83:GLU:H | 2.30 | 0.44 |
| 49:L8:5:LYS:HB2 | 49:L8:36:VAL:HG12 | 1.98 | 0.44 |
| 1:1G:642:A:N3 | 8:72:113:SER:OG | 2.45 | 0.44 |
| 1:1G:1021:G:H2' | 1:1G:1022:G:C8 | 2.52 | 0.44 |
| 1:1G:1235:U:O2' | 1:1G:1305:G:O5' | 2.35 | 0.44 |
| 9:82:37:PHE:O | 9:82:40:LEU:HG | 2.17 | 0.44 |
| 10:1A:78:ASN:H | 10:1A:78:ASN:ND2 | 2.15 | 0.44 |
| 13:4A:69:GLU:O | 13:4A:73:GLU:N | 2.50 | 0.44 |
| 13:4A:88:ARG:O | 13:4A:92:HIS:ND1 | 2.50 | 0.44 |
| 16:7A:14:ASN:N | 16:7A:15:PRO:HD3 | 2.33 | 0.44 |
| 24:14:85:G:N3 | 24:14:103:A:C2 | 2.86 | 0.44 |
| 24:14:226:G:H21 | 24:14:228:A:H62 | 1.64 | 0.44 |
| 24:14:391:G:H1' | 24:14:411:G:O4' | 2.17 | 0.44 |
| 24:14:547:A:C5 | 24:14:548:A:C6 | 3.05 | 0.44 |
| 24:14:871:U:H5' | 36:45:69:PHE:CE2 | 2.52 | 0.44 |
| 24:14:1140:C:H5' | 33:15:24:GLY:HA3 | 1.99 | 0.44 |
| 24:14:1341:U:OP1 | 24:14:1397:U:N3 | 2.42 | 0.44 |
| 24:14:1423:G:H2' | 24:14:1424:G:H8 | 1.81 | 0.44 |
| 24:14:2402:C:H2' | 24:14:2403:C:H5' | 2.00 | 0.44 |
| 24:14:2480:C:H2' | 24:14:2481:G:H5' | 2.00 | 0.44 |
| 24:14:2557:G:H2' | 24:14:2558:C:H6 | 1.80 | 0.44 |
| 26:79:37:PHE:HZ | 26:79:217:THR:HG21 | 1.81 | 0.44 |
| 27:19:141:VAL:HG23 | 27:19:162:SER:HB2 | 2.00 | 0.44 |
| 29:39:42:ALA:O | 29:39:45:ARG:HG2 | 2.18 | 0.44 |
| 31:59:103:LEU:N | 31:59:103:LEU:HD23 | 2.33 | 0.44 |
| 31:59:109:PHE:CZ | 31:59:152:ARG:HB2 | 2.52 | 0.44 |
| 33:15:12:ARG:HG2 | 33:15:50:ASP:CB | 2.47 | 0.44 |
| 35:35:48:PRO:O | 35:35:50:ARG:N | 2.24 | 0.44 |
| 36:45:73:PRO:HA | 36:45:93:TYR:CD2 | 2.52 | 0.44 |
| 37:55:103:ARG:NH1 | 37:55:108:GLY:O | 2.51 | 0.44 |
| 38:65:36:TYR:CD1 | 38:65:36:TYR:N | 2.85 | 0.44 |
| 39:75:9:LEU:C | 39:75:10:VAL:O | 2.59 | 0.44 |
| 40:85:92:ARG:O | 40:85:94:ASN:N | 2.51 | 0.44 |
| 1:13:222:U:H2' | 1:13:223:U:C6 | 2.52 | 0.44 |
| 1:13:360:A:H2' | 1:13:361:G:C8 | 2.53 | 0.44 |
| 1:13:581:G:N2 | 1:13:582:U:O4 | 2.50 | 0.44 |
| 1:13:664:G:H22 | 1:13:741:G:H1 | 1.63 | 0.44 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 1:13:767:A:H2' | 1:13:768:A:O4' | 2.18 | 0.44 |
| 1:13:1330:U:H3' | 1:13:1331:G:O4' | 2.16 | 0.44 |
| 2:1E:71:VAL:HG23 | 2:1E:164:VAL:HG22 | 1.99 | 0.44 |
| 4:3E:207:TYR:HD1 | 4:3E:207:TYR:HA | 1.63 | 0.44 |
| 6:5E:64:GLN:HG3 | 6:5E:65:VAL:N | 2.32 | 0.44 |
| 13:4I:56:LEU:HD12 | 13:4I:56:LEU:HA | 1.78 | 0.44 |
| 24:1H:35:G:H2' | 24:1H:36:G:O4' | 2.17 | 0.44 |
| 24:1H:576:U:H2' | 24:1H:577:G:C8 | 2.53 | 0.44 |
| 24:1H:662:G:OP1 | 35:78:15:ARG:CZ | 2.65 | 0.44 |
| 24:1H:704:G:N2 | 24:1H:726:G:C4 | 2.86 | 0.44 |
| 24:1H:724:U:H2' | 24:1H:725:G:O4' | 2.17 | 0.44 |
| 24:1H:933:A:C4 | 24:1H:934:G:C8 | 3.06 | 0.44 |
| 24:1H:1277:G:H2' | 24:1H:1278:A:O4' | 2.17 | 0.44 |
| 24:1H:1588:C:H2' | 24:1H:1589:C:H6 | 1.80 | 0.44 |
| 24:1H:1678:G:H22 | 24:1H:1989:G:H22 | 1.62 | 0.44 |
| 24:1H:1809:A:C6 | 24:1H:1810:A:C6 | 3.06 | 0.44 |
| 24:1H:2002:G:C6 | 57:1H:3692:HOH:O | 2.71 | 0.44 |
| 24:1H:2238:G:H2' | 24:1H:2238:G:N3 | 2.33 | 0.44 |
| 24:1H:2593:U:O2' | 24:1H:2594:C:H5' | 2.17 | 0.44 |
| 25:16:104:A:OP1 | 45:H8:72:ARG:NH1 | 2.50 | 0.44 |
| 27:11:2:ALA:O | 27:11:3:VAL:HB | 2.18 | 0.44 |
| 31:51:133:VAL:HG21 | 31:51:145:ALA:HB2 | 2.00 | 0.44 |
| 31:51:164:TYR:O | 31:51:167:GLU:HB3 | 2.18 | 0.44 |
| 41:D8:62:LEU:HD12 | 41:D8:62:LEU:HA | 1.65 | 0.44 |
| 43:F8:60:ARG:HH22 | 53:P8:47:ARG:HH12 | 1.64 | 0.44 |
| 44:G8:57:GLN:H | 44:G8:57:GLN:HG3 | 1.59 | 0.44 |
| 47:J8:64:ALA:HA | 47:J8:67:ILE:HG13 | 1.99 | 0.44 |
| 47:J8:88:LYS:HD2 | 47:J8:91:LYS:HD3 | 1.99 | 0.44 |
| 1:1G:125:U:H2' | 1:1G:126:G:C8 | 2.52 | 0.44 |
| 1:1G:587:G:N1 | 1:1G:754:C:OP2 | 2.50 | 0.44 |
| 1:1G:797:C:O2' | 1:1G:798:G:H5' | 2.17 | 0.44 |
| 1:1G:1272:G:C6 | 1:1G:1273:G:C5 | 3.05 | 0.44 |
| 1:1G:1324:A:C4' | 1:1G:1362:C:H4' | 2.45 | 0.44 |
| 1:1G:1329:A:H2' | 1:1G:1330:U:O4' | 2.18 | 0.44 |
| 4:32:12:CYS:SG | 4:32:19:LEU:O | 2.76 | 0.44 |
| 22:2L:22:A:C6 | 22:2L:57:C:C4 | 3.05 | 0.44 |
| 22:2L:72:U:P | 22:2L:72:U:H2' | 2.57 | 0.44 |
| 22:3L:30:A:C6 | 22:3L:43:G:C6 | 3.06 | 0.44 |
| 24:14:945:A:C4 | 24:14:2448:A:C2 | 3.05 | 0.44 |
| 24:14:1019:U:OP1 | 24:14:1035:U:O2' | 2.12 | 0.44 |
| 24:14:1068:G:H1' | 24:14:1095:A:H4' | 1.99 | 0.44 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 24:14:1464:C:C2 | 24:14:1465:G:C8 | 3.06 | 0.44 |
| 24:14:2212:A:H1' | 24:14:2215:G:C4 | 2.52 | 0.44 |
| 24:14:2354:G:O2' | 46:E5:36:ILE:HG23 | 2.18 | 0.44 |
| 24:14:2540:C:H2' | 24:14:2541:A:O4' | 2.17 | 0.44 |
| 25:1J:89(A):A:H5' | 25:1J:90:C:OP2 | 2.18 | 0.44 |
| 26:79:29:VAL:HA | 26:79:32:LEU:HD12 | 1.99 | 0.44 |
| 28:29:48:GLN:HE21 | 28:29:48:GLN:HB2 | 1.57 | 0.44 |
| 29:39:24:LEU:HB3 | 29:39:25:PRO:HD2 | 1.99 | 0.44 |
| 38:65:3:ARG:NH2 | 38:65:4:LEU:HB2 | 2.31 | 0.44 |
| 40:85:92:ARG:O | 40:85:92:ARG:HG3 | 2.18 | 0.44 |
| 45:D5:102:LEU:O | 45:D5:104:PHE:HB2 | 2.17 | 0.44 |
| 1:13:90:C:H5' | 1:13:91:C:OP1 | 2.18 | 0.44 |
| 1:13:666:G:H5" | 1:13:732:C:O2 | 2.18 | 0.44 |
| 1:13:872:A:C4 | 1:13:874:G:N7 | 2.85 | 0.44 |
| 1:13:1200:C:H4' | 1:13:1201:A:H5" | 2.00 | 0.44 |
| 2:1E:9:GLU:HA | 2:1E:12:GLU:OE2 | 2.18 | 0.44 |
| 2:1E:33:TYR:HB2 | 2:1E:43:ASP:HB2 | 1.99 | 0.44 |
| 3:2E:6:HIS:HD2 | 3:2E:8:ILE:H | 1.64 | 0.44 |
| 4:3E:14:ARG:HA | 4:3E:39:PRO:HB3 | 1.99 | 0.44 |
| 5:4E:26:PHE:CD1 | 5:4E:26:PHE:N | 2.85 | 0.44 |
| 13:4I:12:ASN:HA | 13:4I:46:LYS:HB2 | 1.98 | 0.44 |
| 14:5I:24:CYS:SG | 14:5I:29:ARG:HG2 | 2.56 | 0.44 |
| 22:2K:81:C:C2' | 22:2K:82:A:H5' | 2.48 | 0.44 |
| 24:1H:270(M):U:O2' | 24:1H:270(N):G:O5' | 2.35 | 0.44 |
| 24:1H:578:A:OP1 | 24:1H:1255:U:O2' | 2.31 | 0.44 |
| 24:1H:696:G:O2' | 24:1H:697:C:H5' | 2.17 | 0.44 |
| 24:1H:975:G:H1' | 24:1H:990:A:C2 | 2.53 | 0.44 |
| 24:1H:1028:A:N3 | 24:1H:2486:G:O2' | 2.43 | 0.44 |
| 24:1H:1174:A:H62 | 24:1H:1175:U:H5 | 1.65 | 0.44 |
| 24:1H:1491:G:O2' | 24:1H:1492:G:H5' | 2.18 | 0.44 |
| 24:1H:2314:C:H2' | 24:1H:2315:G:C8 | 2.43 | 0.44 |
| 24:1H:2328:A:H2' | 24:1H:2329:G:C8 | 2.52 | 0.44 |
| 24:1H:2467:C:C2' | 24:1H:2468:G:H5' | 2.48 | 0.44 |
| 24:1H:2670:A:C2 | 24:1H:2671:A:C4 | 3.06 | 0.44 |
| 24:1H:2723:C:OP1 | 28:21:109:LYS:HD3 | 2.18 | 0.44 |
| 24:1H:2780:G:OP2 | 33:58:118:LYS:NZ | 2.38 | 0.44 |
| 27:11:25:THR:CG2 | 27:11:26:LYS:N | 2.80 | 0.44 |
| 29:31:106:ARG:H | 29:31:106:ARG:HG2 | 1.67 | 0.44 |
| 31:51:101:ARG:NH2 | 31:51:122:THR:HA | 2.33 | 0.44 |
| 32:61:11:ASN:OD1 | 32:61:12:LEU:N | 2.45 | 0.44 |
| 42:E8:73:ALA:HB3 | 42:E8:106:ILE:CG1 | 2.48 | 0.44 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 44:G8:51:VAL:O | 44:G8:56:PRO:HA | 2.18 | 0.44 |
| 44:G8:97:ARG:HH21 | 44:G8:104:GLY:HA3 | 1.82 | 0.44 |
| 45:H8:61:LEU:HA | 45:H8:62:PRO:HD3 | 1.84 | 0.44 |
| 48:K8:33:MET:O | 48:K8:37:PHE:HD1 | 2.01 | 0.44 |
| 48:K8:42:GLY:C | 48:K8:44:LEU:H | 2.26 | 0.44 |
| 49:L8:11:SER:HA | 49:L8:12:PRO:HD3 | 1.70 | 0.44 |
| 54:Q8:4:MET:HE2 | 54:Q8:4:MET:HB2 | 1.72 | 0.44 |
| 1:1G:538:G:H5" | 12:3A:114:LYS:HB2 | 2.00 | 0.44 |
| 1:1G:589:C:N3 | 1:1G:650:G:N2 | 2.47 | 0.44 |
| 1:1G:1033:G:H2' | 1:1G:1034:G:C8 | 2.51 | 0.44 |
| 1:1G:1106:G:H2' | 1:1G:1107:C:H6 | 1.82 | 0.44 |
| 1:1G:1147:C:O2 | 9:82:16:ARG:NE | 2.50 | 0.44 |
| 1:1G:1452:C:H4' | 1:1G:1453:G:H5' | 1.98 | 0.44 |
| 2:12:21:ARG:C | 2:12:23:ARG:H | 2.26 | 0.44 |
| 3:22:40:ARG:O | 3:22:44:GLU:HB2 | 2.16 | 0.44 |
| 4:32:24:GLU:HG2 | 4:32:25:ARG:H | 1.82 | 0.44 |
| 6:52:3:ARG:O | 6:52:93:SER:HB2 | 2.17 | 0.44 |
| 17:8A:59:ILE:HG22 | 17:8A:71:PHE:HB3 | 1.99 | 0.44 |
| 18:9A:44:LEU:HD21 | 18:9A:79:LEU:HD22 | 1.99 | 0.44 |
| 24:14:620:G:H4' | 24:14:621:A:O5' | 2.17 | 0.44 |
| 24:14:706:A:OP1 | 27:19:7:LYS:HE3 | 2.18 | 0.44 |
| 24:14:925:C:H2' | 24:14:926:A:C8 | 2.52 | 0.44 |
| 24:14:1210:A:H5' | 24:14:1212:G:H5' | 1.99 | 0.44 |
| 24:14:1410:G:H2' | 24:14:1411:C:C6 | 2.52 | 0.44 |
| 24:14:2845:G:H2' | 24:14:2846:G:H8 | 1.83 | 0.44 |
| 24:14:2849:U:OP1 | 39:75:95:ARG:NH1 | 2.51 | 0.44 |
| 24:14:2872:G:C4 | 24:14:2873:A:C2 | 3.06 | 0.44 |
| 25:1J:110:G:H2' | 25:1J:111:U:O4' | 2.18 | 0.44 |
| 28:29:26:ILE:O | 28:29:27:LEU:HB3 | 2.17 | 0.44 |
| 29:39:2:LYS:NZ | 29:39:25:PRO:HG2 | 2.32 | 0.44 |
| 29:39:2:LYS:O | 29:39:24:LEU:HG | 2.17 | 0.44 |
| 30:49:25:TYR:HB3 | 30:49:30:GLU:OE1 | 2.18 | 0.44 |
| 47:F5:46:LEU:C | 47:F5:47:GLN:HG2 | 2.42 | 0.44 |
| 1:13:28:G:C6 | 1:13:29:G:C5 | 3.06 | 0.44 |
| 1:13:95:G:H3' | 1:13:96:G:H8 | 1.80 | 0.44 |
| 1:13:380:G:C2 | 1:13:384:G:C6 | 3.06 | 0.44 |
| 1:13:503:C:OP2 | 12:3I:116:SER:HB3 | 2.18 | 0.44 |
| 1:13:625:G:H2' | 1:13:626:U:H6 | 1.83 | 0.44 |
| 1:13:734:G:H2' | 1:13:735:C:C6 | 2.50 | 0.44 |
| 1:13:1005:A:H1' | 1:13:1036:G:H22 | 1.82 | 0.44 |
| 1:13:1053:G:N7 | 1:13:1199:U:H3' | 2.32 | 0.44 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 1:13:1508:G:H2' | 1:13:1509:C:H6 | 1.82 | 0.44 |
| 2:1E:208:ILE:HD12 | 2:1E:209:ARG:N | 2.32 | 0.44 |
| 3:2E:172:ARG:NH2 | 3:2E:174:PRO:HG2 | 2.33 | 0.44 |
| 4:3E:112:VAL:HG12 | 4:3E:116:GLN:OE1 | 2.17 | 0.44 |
| 8:7E:14:ARG:O | 8:7E:18:ARG:HD3 | 2.17 | 0.44 |
| 9:8E:96:LEU:HD23 | 9:8E:96:LEU:HA | 1.77 | 0.44 |
| 13:4I:3:ARG:NH2 | 13:4I:7:VAL:HG22 | 2.32 | 0.44 |
| 16:7I:5:ARG:HH21 | 16:7I:22:THR:CG2 | 2.30 | 0.44 |
| 24:1H:211:A:H2' | 24:1H:212:G:O4' | 2.18 | 0.44 |
| 24:1H:320:A:H4' | 24:1H:322:A:N7 | 2.33 | 0.44 |
| 24:1H:618:G:H2' | 24:1H:618(A):C:O4' | 2.17 | 0.44 |
| 24:1H:751:A:C6 | 24:1H:789:A:C5 | 3.06 | 0.44 |
| 24:1H:952:G:C6 | 24:1H:953:A:N7 | 2.85 | 0.44 |
| 24:1H:1211:U:H4' | 24:1H:1212:G:OP2 | 2.18 | 0.44 |
| 24:1H:1219:G:OP2 | 40:C8:19:LYS:HE3 | 2.17 | 0.44 |
| 24:1H:1329:U:H3' | 24:1H:1330:C:H6 | 1.83 | 0.44 |
| 24:1H:1344:G:H4' | 24:1H:1384:A:C5 | 2.53 | 0.44 |
| 24:1H:1561:G:H2' | 24:1H:1562:A:C8 | 2.53 | 0.44 |
| 24:1H:2512:C:H4' | 28:21:122:PHE:CE2 | 2.53 | 0.44 |
| 28:21:176:ILE:HD12 | 28:21:181:LEU:HD23 | 1.99 | 0.44 |
| 29:31:116:ASP:OD1 | 29:31:119:ARG:NH2 | 2.42 | 0.44 |
| 30:41:111:LEU:HD22 | 30:41:179:PRO:HG2 | 1.98 | 0.44 |
| 35:78:21:ARG:HB3 | 35:78:22:GLY:H | 1.59 | 0.44 |
| 38:A8:51:ALA:HB3 | 38:A8:73:LEU:HG | 1.99 | 0.44 |
| 41:D8:62:LEU:HD22 | 41:D8:95:LEU:HB2 | 1.99 | 0.44 |
| 43:F8:77:LYS:HG2 | 43:F8:78:LYS:N | 2.32 | 0.44 |
| 44:G8:80:GLY:C | 44:G8:81:LYS:O | 2.60 | 0.44 |
| 44:G8:89:PHE:CD1 | 44:G8:90:LEU:N | 2.86 | 0.44 |
| 47:J8:18:ILE:HG22 | 47:J8:20:ARG:HG3 | 1.99 | 0.44 |
| 54:Q8:57:ARG:HE | 54:Q8:57:ARG:HB2 | 1.54 | 0.44 |
| 1:1G:573:A:H2' | 1:1G:574:A:C8 | 2.53 | 0.44 |
| 1:1G:1220:G:H5' | 19:AA:34:TRP:O | 2.18 | 0.44 |
| 5:42:75:THR:HG23 | 5:42:76:ILE:N | 2.32 | 0.44 |
| 5:42:101:ILE:HD11 | 5:42:119:LEU:CD2 | 2.41 | 0.44 |
| 8:72:5:PRO:O | 8:72:8:ASP:HB3 | 2.18 | 0.44 |
| 8:72:35:ILE:O | 8:72:39:LEU:HB2 | 2.18 | 0.44 |
| 9:82:6:GLY:HA3 | 9:82:83:ARG:HB2 | 2.00 | 0.44 |
| 9:82:97:LYS:C | 9:82:100:GLY:H | 2.26 | 0.44 |
| 10:1A:33:GLN:O | 10:1A:75:ILE:HG23 | 2.18 | 0.44 |
| 17:8A:81:ARG:NH2 | 17:8A:84:LEU:HD21 | 2.33 | 0.44 |
| 22:3L:16:C:N4 | 22:3L:68:A:C8 | 2.85 | 0.44 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 22:3L:22:A:H2' | 22:3L:22:A:N3 | 2.33 | 0.44 |
| 24:14:162:U:H4' | 24:14:171:G:C5 | 2.52 | 0.44 |
| 24:14:260:G:O4' | 24:14:621:A:H1' | 2.18 | 0.44 |
| 24:14:892:G:O6 | 24:14:893:C:N4 | 2.51 | 0.44 |
| 24:14:1115:G:H2' | 24:14:1116:C:C6 | 2.53 | 0.44 |
| 24:14:1285:G:C5 | 24:14:1329:U:C4 | 3.05 | 0.44 |
| 24:14:1336:A:H2' | 24:14:1337:G:C8 | 2.52 | 0.44 |
| 24:14:1612:C:H5" | 53:L5:7:PRO:HG2 | 1.99 | 0.44 |
| 24:14:2050:C:H2' | 24:14:2051:A:C8 | 2.53 | 0.44 |
| 26:79:213:TYR:CD1 | 26:79:221:SER:HB2 | 2.53 | 0.44 |
| 28:29:71:GLY:C | 28:29:73:GLU:H | 2.26 | 0.44 |
| 29:39:34:TRP:CZ3 | 35:35:8:PRO:HB3 | 2.53 | 0.44 |
| 43:B5:26:TYR:O | 43:B5:81:VAL:HG22 | 2.18 | 0.44 |
| 46:E5:53:MET:HG3 | 46:E5:59:LEU:CD2 | 2.47 | 0.44 |
| 54:M5:55:ALA:O | 54:M5:59:LYS:HE3 | 2.17 | 0.44 |
| 1:13:41:G:H2' | 1:13:42:G:H8 | 1.82 | 0.44 |
| 1:13:375:U:O2' | 16:7I:6:LEU:O | 2.34 | 0.44 |
| 1:13:1239:A:H4' | 1:13:1240:U:H5" | 2.00 | 0.44 |
| 1:13:1251:A:H5" | 9:8E:12:GLU:OE1 | 2.18 | 0.44 |
| 2:1E:51:LEU:HD23 | 2:1E:201:ILE:HD12 | 2.00 | 0.44 |
| 2:1E:116:GLU:OE2 | 2:1E:156:LYS:NZ | 2.46 | 0.44 |
| 3:2E:129:ALA:HB3 | 3:2E:132:ARG:HE | 1.83 | 0.44 |
| 11:2I:52:GLY:H | 11:2I:55:LYS:NZ | 2.15 | 0.44 |
| 15:6I:33:THR:HG21 | 15:6I:85:LEU:HD22 | 2.00 | 0.44 |
| 17:8I:40:LYS:HD3 | 17:8I:42:TYR:CE1 | 2.53 | 0.44 |
| 24:1H:192:C:O2' | 24:1H:802:A:N3 | 2.48 | 0.44 |
| 24:1H:203:C:O5' | 24:1H:203:C:H6 | 2.00 | 0.44 |
| 24:1H:260:G:O2' | 24:1H:608:A:N1 | 2.42 | 0.44 |
| 24:1H:657:U:H2' | 24:1H:658:C:C6 | 2.53 | 0.44 |
| 24:1H:674:G:H1' | 29:31:74:ARG:HH11 | 1.82 | 0.44 |
| 24:1H:729:G:C5 | 27:11:208:LYS:HB2 | 2.52 | 0.44 |
| 24:1H:1127:A:N3 | 24:1H:2518:A:H5" | 2.33 | 0.44 |
| 24:1H:1525:G:C4 | 24:1H:1526:G:C8 | 3.06 | 0.44 |
| 24:1H:2314:C:H5" | 30:41:38:VAL:HG21 | 1.99 | 0.44 |
| 26:71:59:ARG:HB2 | 26:71:164:ARG:HG3 | 1.99 | 0.44 |
| 30:41:96:ARG:O | 30:41:98:ARG:N | 2.41 | 0.44 |
| 31:51:69:ARG:HH11 | 31:51:73:ALA:HB2 | 1.83 | 0.44 |
| 31:51:124:GLU:C | 31:51:126:PRO:HD3 | 2.43 | 0.44 |
| 40:C8:72:HIS:HB2 | 40:C8:110:VAL:HG11 | 2.00 | 0.44 |
| 41:D8:3:ALA:HB1 | 41:D8:38:LEU:HD11 | 1.99 | 0.44 |
| 43:F8:53:LYS:HB2 | 43:F8:53:LYS:HE3 | 1.70 | 0.44 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 46:I8:48:GLY:HA3 | 46:I8:80:HIS:ND1 | 2.31 | 0.44 |
| 47:J8:93:GLU:H | 47:J8:93:GLU:CD | 2.22 | 0.44 |
| 48:K8:4:SER:N | 48:K8:7:ARG:H | 2.16 | 0.44 |
| 48:K8:28:LYS:HD3 | 48:K8:53:LEU:HD21 | 1.99 | 0.44 |
| 48:K8:66:GLU:HG2 | 48:K8:67:LYS:N | 2.33 | 0.44 |
| 1:1G:490:G:OP2 | 4:32:132:ARG:NH2 | 2.51 | 0.44 |
| 4:32:196:LEU:HD23 | 4:32:197:PRO:HD2 | 2.00 | 0.44 |
| 5:42:30:ALA:C | 5:42:45:PHE:HD1 | 2.26 | 0.44 |
| 5:42:60:TYR:HE1 | 5:42:64:ARG:NH2 | 2.15 | 0.44 |
| 6:52:55:ASP:HA | 6:52:56:PRO:HD3 | 1.82 | 0.44 |
| 11:2A:96:ARG:HA | 11:2A:99:GLN:HB2 | 2.00 | 0.44 |
| 12:3A:28:LYS:HB3 | 12:3A:33:ARG:NE | 2.32 | 0.44 |
| 13:4A:34:LEU:HA | 13:4A:34:LEU:HD23 | 1.80 | 0.44 |
| 20:BA:73:HIS:HB3 | 20:BA:74:LYS:H | 1.56 | 0.44 |
| 24:14:273(F):C:H3' | 24:14:274:G:C5' | 2.45 | 0.44 |
| 24:14:1198:U:C2 | 24:14:1199:U:C5 | 3.05 | 0.44 |
| 24:14:1372:U:H2' | 24:14:1373:A:C8 | 2.53 | 0.44 |
| 24:14:1692:U:O2' | 24:14:1693:U:H2' | 2.17 | 0.44 |
| 24:14:1902:C:H5' | 27:19:246:PRO:HD3 | 1.99 | 0.44 |
| 24:14:2115:G:N3 | 24:14:2171:A:H2 | 2.16 | 0.44 |
| 24:14:2255:G:H21 | 46:E5:9:SER:HB2 | 1.83 | 0.44 |
| 24:14:2473:U:H2' | 24:14:2474:C:H5' | 1.99 | 0.44 |
| 24:14:2537:U:H2' | 24:14:2538:C:H6 | 1.82 | 0.44 |
| 24:14:2788:C:H5' | 28:29:61:ARG:HH12 | 1.82 | 0.44 |
| 26:79:200:LYS:HE3 | 26:79:208:PHE:HB2 | 1.99 | 0.44 |
| 28:29:87:GLU:CD | 28:29:87:GLU:N | 2.75 | 0.44 |
| 32:69:144:VAL:HG13 | 32:69:145:VAL:N | 2.33 | 0.44 |
| 33:15:71:ILE:HA | 33:15:86:PRO:HA | 2.00 | 0.44 |
| 38:65:26:LEU:O | 38:65:88:ASP:HB3 | 2.18 | 0.44 |
| 45:D5:23:LYS:HZ2 | 45:D5:40:ASP:HB2 | 1.82 | 0.44 |
| 1:13:196:A:O2' | 1:13:221:C:O2' | 2.32 | 0.44 |
| 1:13:977:A:C8 | 1:13:1223:C:N3 | 2.86 | 0.44 |
| 1:13:1097:C:H1' | 1:13:1170:A:H1' | 2.00 | 0.44 |
| 1:13:1103:C:C4 | 1:13:1104:G:N7 | 2.85 | 0.44 |
| 1:13:1347:G:N2 | 1:13:1373:G:H2' | 2.32 | 0.44 |
| 1:13:1492[A]:A:H2' | 24:1H:1913:A:C2 | 2.52 | 0.44 |
| 2:1E:196:LEU:HA | 8:7E:74:PRO:HG3 | 2.00 | 0.44 |
| 2:1E:214:ILE:HG23 | 2:1E:215:LEU:N | 2.32 | 0.44 |
| 6:5E:4:TYR:CD1 | 6:5E:92:LYS:HA | 2.53 | 0.44 |
| 9:8E:93:ARG:HG3 | 9:8E:94:ALA:N | 2.32 | 0.44 |
| 9:8E:112:LYS:HD3 | 9:8E:113:LYS:N | 2.32 | 0.44 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 16:7I:21:VAL:HG23 | 16:7I:33:ILE:HB | 2.00 | 0.44 |
| 22:3K:22:A:N3 | 22:3K:22:A:H2' | 2.32 | 0.44 |
| 24:1H:34:C:HO2' | 24:1H:35:G:P | 2.41 | 0.44 |
| 24:1H:221:A:N6 | 24:1H:265:A:C8 | 2.86 | 0.44 |
| 24:1H:278:A:H3' | 24:1H:279:C:C6 | 2.52 | 0.44 |
| 24:1H:489:G:C5 | 24:1H:1284:A:C2 | 3.06 | 0.44 |
| 24:1H:636:G:H5' | 24:1H:639:U:OP1 | 2.18 | 0.44 |
| 24:1H:752:A:H3' | 53:P8:1:MET:SD | 2.58 | 0.44 |
| 24:1H:918:A:O2' | 25:16:96:G:N2 | 2.43 | 0.44 |
| 24:1H:1044:G:H4' | 24:1H:1048:A:H1' | 2.00 | 0.44 |
| 24:1H:1271:G:N2 | 24:1H:1617:C:O4' | 2.51 | 0.44 |
| 24:1H:1433:U:O2 | 24:1H:1561:G:C2 | 2.71 | 0.44 |
| 24:1H:1680:U:O2 | 24:1H:1763:G:H3' | 2.16 | 0.44 |
| 24:1H:1728:G:C2 | 24:1H:1730:U:OP2 | 2.71 | 0.44 |
| 24:1H:2375:G:N7 | 57:1H:3714:HOH:O | 2.35 | 0.44 |
| 24:1H:2408:U:H2' | 24:1H:2409:G:C8 | 2.53 | 0.44 |
| 24:1H:2787:C:H1' | 28:21:62:PRO:HG3 | 2.00 | 0.44 |
| 24:1H:2820:A:O2' | 24:1H:2821:A:OP1 | 2.35 | 0.44 |
| 25:16:11:C:H3' | 25:16:12:C:H6 | 1.82 | 0.44 |
| 27:11:147:LEU:HD11 | 27:11:183:ARG:NH2 | 2.33 | 0.44 |
| 30:41:23:PHE:HB2 | 30:41:25:TYR:CE2 | 2.53 | 0.44 |
| 30:41:138:GLN:NE2 | 30:41:151:ALA:O | 2.50 | 0.44 |
| 31:51:154:PRO:HB3 | 31:51:163:TYR:CZ | 2.53 | 0.44 |
| 32:61:130:TYR:HB3 | 32:61:136:VAL:HG13 | 2.00 | 0.44 |
| 33:58:90:MET:HG3 | 33:58:94:HIS:O | 2.18 | 0.44 |
| 42:E8:45:TYR:CD1 | 42:E8:45:TYR:C | 2.94 | 0.44 |
| 44:G8:90:LEU:HA | 44:G8:91:GLU:HA | 1.64 | 0.44 |
| 45:H8:28:MET:O | 45:H8:34:ASN:HA | 2.18 | 0.44 |
| 45:H8:142:SER:CB | 45:H8:143:GLY:HA2 | 2.48 | 0.44 |
| 45:H8:145:GLU:HG2 | 45:H8:146:ILE:H | 1.83 | 0.44 |
| 54:Q8:59:LYS:HE2 | 54:Q8:59:LYS:HB2 | 1.51 | 0.44 |
| 1:1G:188:U:O2' | 1:1G:189:U:H5' | 2.18 | 0.44 |
| 1:1G:438:G:O2' | 1:1G:494:U:O4 | 2.28 | 0.44 |
| 1:1G:878:G:H5' | 8:72:89:PRO:HG2 | 2.00 | 0.44 |
| 1:1G:1117:G:N2 | 1:1G:1180:A:H1' | 2.32 | 0.44 |
| 1:1G:1122:U:C2 | 1:1G:1123:A:N7 | 2.86 | 0.44 |
| 1:1G:1202:G:H22 | 14:5A:46:GLU:CD | 2.24 | 0.44 |
| 9:82:77:ILE:HG13 | 9:82:78:LYS:N | 2.32 | 0.44 |
| 24:14:262:A:H2' | 24:14:263:C:C6 | 2.53 | 0.44 |
| 24:14:479:A:H4' | 24:14:480:A:OP1 | 2.17 | 0.44 |
| 24:14:535:C:C2' | 24:14:536:A:H5' | 2.47 | 0.44 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 24:14:1729:A:C2' | 24:14:1731:G:H22 | 2.30 | 0.44 |
| 24:14:1784:A:H4' | 24:14:1785:A:O5' | 2.18 | 0.44 |
| 24:14:2574:G:O2' | 28:29:143:ASN:HB3 | 2.18 | 0.44 |
| 24:14:2654:A:N3 | 24:14:2656:U:C4 | 2.86 | 0.44 |
| 24:14:2745:C:H2' | 24:14:2746:U:O4' | 2.17 | 0.44 |
| 27:19:175:LEU:HD12 | 27:19:185:VAL:HG21 | 2.00 | 0.44 |
| 28:29:8:LYS:HB3 | 28:29:193:GLY:H | 1.82 | 0.44 |
| 29:39:53:THR:HG22 | 29:39:56:GLU:CG | 2.42 | 0.44 |
| 38:65:67:ARG:NH1 | 38:65:67:ARG:HB2 | 2.33 | 0.44 |
| 49:H5:51:ALA:HA | 49:H5:54:VAL:HG12 | 2.00 | 0.44 |
| 1:13:124:G:H2' | 1:13:125:U:O4' | 2.18 | 0.43 |
| 1:13:153:C:N4 | 1:13:168:G:H1 | 2.16 | 0.43 |
| 1:13:358:U:H4' | 32:69:87:LYS:HD3 | 2.00 | 0.43 |
| 1:13:913:A:OP1 | 12:3I:46:LYS:NZ | 2.50 | 0.43 |
| 1:13:947:G:H2' | 1:13:948:C:C6 | 2.53 | 0.43 |
| 1:13:1358:U:H5" | 14:5I:34:TYR:HA | 2.00 | 0.43 |
| 1:13:1521:G:H2' | 1:13:1522:U:C6 | 2.53 | 0.43 |
| 10:1I:24:VAL:O | 10:1I:28:ARG:HB3 | 2.18 | 0.43 |
| 12:3I:39:VAL:HG22 | 12:3I:57:LYS:HB2 | 1.99 | 0.43 |
| 17:8I:57:VAL:HG21 | 17:8I:73:VAL:HG13 | 2.00 | 0.43 |
| 22:3K:33:C:C2' | 22:3K:34:U:H5' | 2.48 | 0.43 |
| 22:3K:33:C:C4 | 22:3K:34:U:C5 | 3.05 | 0.43 |
| 22:3K:85:A:H5" | 47:J8:30:VAL:HG11 | 1.99 | 0.43 |
| 24:1H:125:G:H5' | 24:1H:125:G:H8 | 1.82 | 0.43 |
| 24:1H:270(G):C:H2' | 24:1H:270(H):C:C6 | 2.53 | 0.43 |
| 24:1H:511:U:C5 | 24:1H:512:G:C5 | 3.05 | 0.43 |
| 24:1H:1952:A:C2 | 34:68:22:ILE:HG23 | 2.53 | 0.43 |
| 24:1H:2275:C:H5' | 24:1H:2275:C:C6 | 2.51 | 0.43 |
| 24:1H:2361:A:OP1 | 54:Q8:27:THR:OG1 | 2.31 | 0.43 |
| 25:16:22:U:H3 | 25:16:61:G:H1 | 1.66 | 0.43 |
| 32:61:91:SER:HB3 | 32:61:121:LYS:HD2 | 2.00 | 0.43 |
| 34:68:17:ARG:HD2 | 34:68:17:ARG:HA | 1.62 | 0.43 |
| 36:88:17:LEU:HD13 | 36:88:39:PRO:HB2 | 2.00 | 0.43 |
| 36:88:20:ALA:HB1 | 36:88:99:PRO:CD | 2.48 | 0.43 |
| 39:B8:55:ASN:H | 39:B8:59:THR:HA | 1.81 | 0.43 |
| 40:C8:90:VAL:HG22 | 40:C8:95:LEU:HD22 | 1.99 | 0.43 |
| 41:D8:5:VAL:HG21 | 41:D8:35:LEU:HD23 | 1.99 | 0.43 |
| 43:F8:89:ILE:HG22 | 43:F8:92:LEU:HB2 | 2.00 | 0.43 |
| 45:H8:69:THR:HG22 | 45:H8:90:VAL:HG22 | 2.00 | 0.43 |
| 1:1G:232:G:H2' | 1:1G:233:C:O4' | 2.18 | 0.43 |
| 1:1G:604:G:C5 | 1:1G:605:U:C5 | 3.06 | 0.43 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 2:12:56:ARG:HA | 2:12:56:ARG:HD3 | 1.75 | 0.43 |
| 3:22:35:GLU:O | 3:22:39:ILE:HD13 | 2.18 | 0.43 |
| 5:42:71:LEU:HD21 | 5:42:115:VAL:HG12 | 2.00 | 0.43 |
| 19:AA:66:MET:HE2 | 50:I5:55:ARG:HB3 | 1.98 | 0.43 |
| 24:14:9:U:H2' | 24:14:10:G:C8 | 2.53 | 0.43 |
| 24:14:65:C:H2' | 24:14:66:C:H6 | 1.83 | 0.43 |
| 24:14:259:G:N2 | 24:14:621:A:C8 | 2.73 | 0.43 |
| 24:14:488:G:O2' | 24:14:491:G:N7 | 2.49 | 0.43 |
| 24:14:565:C:H4' | 24:14:1253:A:N6 | 2.33 | 0.43 |
| 24:14:1050:A:H2' | 24:14:1051:G:O4' | 2.17 | 0.43 |
| 24:14:1788:C:H2' | 24:14:1789:A:O4' | 2.18 | 0.43 |
| 24:14:2092:U:H5 | 24:14:2226:C:OP2 | 2.01 | 0.43 |
| 24:14:2791:C:H2' | 24:14:2792:G:C8 | 2.52 | 0.43 |
| 24:14:2845:G:H5" | 39:75:54:ARG:O | 2.18 | 0.43 |
| 24:14:2865:U:C4 | 24:14:2866:U:C4 | 3.06 | 0.43 |
| 28:29:120:TRP:CE3 | 28:29:155:LYS:HD3 | 2.53 | 0.43 |
| 28:29:175:VAL:HG23 | 28:29:177:PRO:HD3 | 2.00 | 0.43 |
| 30:49:138:GLN:CD | 30:49:153:ARG:H | 2.23 | 0.43 |
| 32:69:123:LEU:HD22 | 32:69:143:SER:HA | 2.00 | 0.43 |
| 36:45:64:ILE:H | 36:45:64:ILE:HD13 | 1.83 | 0.43 |
| 40:85:98:LEU:C | 40:85:100:VAL:H | 2.25 | 0.43 |
| 44:C5:89:PHE:O | 44:C5:89:PHE:CG | 2.70 | 0.43 |
| 45:D5:54:HIS:CE1 | 45:D5:123:ASP:HB3 | 2.53 | 0.43 |
| 1:13:238:G:P | 17:8I:25:ARG:HH22 | 2.41 | 0.43 |
| 1:13:644:G:H2' | 1:13:645:C:O4' | 2.18 | 0.43 |
| 1:13:869:G:H8 | 1:13:869:G:O5' | 2.01 | 0.43 |
| 1:13:1327:C:H2' | 1:13:1328:C:C6 | 2.53 | 0.43 |
| 2:1E:164:VAL:HG11 | 2:1E:167:PRO:HA | 2.00 | 0.43 |
| 3:2E:23:TYR:CG | 3:2E:24:ALA:N | 2.86 | 0.43 |
| 3:2E:119:ARG:O | 3:2E:123:GLN:HG3 | 2.19 | 0.43 |
| 4:3E:188:LEU:HD22 | 4:3E:188:LEU:HA | 1.79 | 0.43 |
| 7:6E:22:LEU:HD21 | 7:6E:66:VAL:HG11 | 2.00 | 0.43 |
| 9:8E:42:ARG:HE | 9:8E:42:ARG:HB2 | 1.38 | 0.43 |
| 10:1I:38:ILE:HG23 | 10:1I:71:LEU:HB3 | 2.00 | 0.43 |
| 13:4I:3:ARG:HG3 | 13:4I:9:ILE:HD11 | 2.00 | 0.43 |
| 22:2K:12:C:H2' | 22:2K:13:G:O4' | 2.18 | 0.43 |
| 22:3K:61:G:C4 | 22:3K:62:G:C8 | 3.06 | 0.43 |
| 24:1H:207:A:H2' | 24:1H:208:C:O4' | 2.18 | 0.43 |
| 24:1H:270:A:H1' | 24:1H:370:G:N2 | 2.32 | 0.43 |
| 24:1H:280:C:C2 | 24:1H:361:G:N2 | 2.87 | 0.43 |
| 24:1H:540:G:H2' | 24:1H:541:C:C6 | 2.53 | 0.43 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 24:1H:753:C:OP2 | 24:1H:753:C:C6 | 2.70 | 0.43 |
| 24:1H:958:U:OP2 | 36:88:14:ARG:HD3 | 2.17 | 0.43 |
| 24:1H:1255:U:O5' | 24:1H:1256:G:H5" | 2.18 | 0.43 |
| 24:1H:2683:C:OP1 | 39:B8:53:ARG:NH2 | 2.48 | 0.43 |
| 28:21:81:ILE:O | 28:21:81:ILE:HG22 | 2.18 | 0.43 |
| 29:31:67:GLN:O | 29:31:67:GLN:HG3 | 2.18 | 0.43 |
| 29:31:123:LEU:HD12 | 29:31:124:LEU:N | 2.33 | 0.43 |
| 36:88:17:LEU:HB3 | 36:88:39:PRO:HB2 | 2.00 | 0.43 |
| 36:88:90:VAL:HG23 | 36:88:91:GLU:N | 2.33 | 0.43 |
| 42:E8:86:LEU:HD12 | 42:E8:87:PRO:HD2 | 2.00 | 0.43 |
| 46:I8:70:GLN:CB | 46:I8:80:HIS:HE2 | 2.31 | 0.43 |
| 51:N8:38:ALA:HB3 | 51:N8:40:LYS:NZ | 2.32 | 0.43 |
| 54:Q8:41:ILE:HD13 | 54:Q8:41:ILE:HA | 1.78 | 0.43 |
| 1:1G:22:G:O2' | 1:1G:913:A:N1 | 2.46 | 0.43 |
| 1:1G:629:G:H2' | 1:1G:630:G:O4' | 2.17 | 0.43 |
| 1:1G:980:C:H3' | 1:1G:981:U:C6 | 2.53 | 0.43 |
| 1:1G:1104:G:H4' | 2:12:111:ARG:NH1 | 2.33 | 0.43 |
| 2:12:174:VAL:HG13 | 2:12:184:VAL:HG21 | 2.00 | 0.43 |
| 2:12:223:ILE:HG22 | 2:12:227:GLY:O | 2.18 | 0.43 |
| 4:32:141:ARG:HB3 | 4:32:141:ARG:HH11 | 1.82 | 0.43 |
| 11:2A:17:GLY:O | 11:2A:80:VAL:HA | 2.18 | 0.43 |
| 13:4A:13:LYS:O | 13:4A:45:VAL:HG23 | 2.18 | 0.43 |
| 13:4A:106:ASN:OD1 | 13:4A:106:ASN:N | 2.50 | 0.43 |
| 15:6A:4:THR:O | 15:6A:7:GLU:N | 2.52 | 0.43 |
| 22:2L:72:U:O2' | 22:2L:73:U:P | 2.77 | 0.43 |
| 22:3L:22:A:N7 | 22:3L:57:C:N4 | 2.65 | 0.43 |
| 24:14:185:U:H2' | 24:14:186:G:H8 | 1.83 | 0.43 |
| 24:14:450:G:C6 | 57:14:3558:HOH:O | 2.71 | 0.43 |
| 24:14:1022:G:N2 | 24:14:1142(A):A:H2 | 1.98 | 0.43 |
| 24:14:1093:G:H1' | 24:14:1099:G:N1 | 2.33 | 0.43 |
| 24:14:1142:U:H5" | 24:14:1142(A):A:H5" | 2.00 | 0.43 |
| 24:14:1630(A):C:H2' | 57:14:3651:HOH:O | 2.19 | 0.43 |
| 24:14:1827:C:O2' | 24:14:1970:A:N3 | 2.38 | 0.43 |
| 24:14:2136:C:OP1 | 24:14:2160:G:H4' | 2.18 | 0.43 |
| 25:1J:15:A:H1' | 25:1J:109:G:C4 | 2.53 | 0.43 |
| 31:59:151:ILE:HG22 | 31:59:152:ARG:H | 1.83 | 0.43 |
| 36:45:70:PRO:HA | 36:45:94:VAL:C | 2.42 | 0.43 |
| 39:75:85:LYS:HE3 | 39:75:87:ASP:CG | 2.43 | 0.43 |
| 39:75:133:GLU:C | 39:75:136:GLN:HG2 | 2.43 | 0.43 |
| 40:85:98:LEU:HD12 | 40:85:99:ALA:N | 2.33 | 0.43 |
| 45:D5:161:VAL:HB | 45:D5:162:GLU:H | 1.55 | 0.43 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 52:K5:14:THR:HA | 52:K5:49:HIS:ND1 | 2.33 | 0.43 |
| 1:13:66:G:O4' | 1:13:173:U:C4 | 2.71 | 0.43 |
| 1:13:1189:C:P | 10:1I:51:ARG:HH22 | 2.41 | 0.43 |
| 1:13:1309:G:C4 | 1:13:1329:A:C2 | 3.06 | 0.43 |
| 3:2E:138:VAL:HG23 | 3:2E:151:VAL:HG23 | 2.00 | 0.43 |
| 5:4E:144:THR:O | 5:4E:147:ASP:N | 2.51 | 0.43 |
| 8:7E:17:THR:HB | 8:7E:78:GLN:OE1 | 2.19 | 0.43 |
| 12:3I:117:ARG:HB3 | 12:3I:122:THR:HB | 1.99 | 0.43 |
| 13:4I:50:GLU:O | 13:4I:54:VAL:HG23 | 2.18 | 0.43 |
| 13:4I:98:VAL:HG23 | 13:4I:99:ARG:HG3 | 1.99 | 0.43 |
| 14:5I:26:ARG:NH1 | 14:5I:43:CYS:HB2 | 2.30 | 0.43 |
| 16:7I:12:LYS:HG2 | 16:7I:13:HIS:CD2 | 2.53 | 0.43 |
| 19:AI:16:LEU:HD12 | 19:AI:19:VAL:HB | 1.99 | 0.43 |
| 24:1H:86:C:H4' | 24:1H:104:U:H1' | 1.99 | 0.43 |
| 24:1H:498:G:C6 | 24:1H:499:U:C4 | 3.05 | 0.43 |
| 24:1H:533:G:H5' | 40:C8:24:TYR:CD1 | 2.53 | 0.43 |
| 24:1H:946:G:OP2 | 57:1H:3676:HOH:O | 2.21 | 0.43 |
| 24:1H:1230:C:H2' | 24:1H:1231:G:C8 | 2.53 | 0.43 |
| 24:1H:1271:G:O3' | 24:1H:1272:A:H4' | 2.19 | 0.43 |
| 24:1H:1649:G:C6 | 24:1H:2009:G:C6 | 3.05 | 0.43 |
| 24:1H:1683:C:H2' | 24:1H:1684:C:C6 | 2.51 | 0.43 |
| 24:1H:2010:G:H5" | 42:E8:42:ARG:HB2 | 2.00 | 0.43 |
| 24:1H:2467:C:N4 | 24:1H:2468:G:C6 | 2.86 | 0.43 |
| 24:1H:2517:C:C5 | 24:1H:2542:A:C5 | 3.05 | 0.43 |
| 24:1H:2599:G:N7 | 27:11:237:GLU:HG2 | 2.33 | 0.43 |
| 24:1H:2845:G:H8 | 24:1H:2845:G:O5' | 2.00 | 0.43 |
| 24:1H:2870:C:H2' | 24:1H:2871:C:O4' | 2.17 | 0.43 |
| 27:11:108:PRO:HB3 | 27:11:143:HIS:CE1 | 2.53 | 0.43 |
| 27:11:147:LEU:HD13 | 27:11:155:LEU:HD21 | 1.99 | 0.43 |
| 28:21:165:VAL:O | 28:21:189:PRO:HG2 | 2.18 | 0.43 |
| 30:41:66:GLN:OE1 | 30:41:98:ARG:NH1 | 2.51 | 0.43 |
| 34:68:25:LEU:HD21 | 34:68:40:VAL:CG2 | 2.48 | 0.43 |
| 36:88:78:PRO:C | 36:88:79:LEU:HG | 2.44 | 0.43 |
| 38:A8:30:ARG:HG3 | 38:A8:30:ARG:O | 2.18 | 0.43 |
| 45:H8:24:LEU:HA | 45:H8:25:PRO:HD3 | 1.65 | 0.43 |
| 45:H8:127:LYS:O | 45:H8:161:VAL:HB | 2.17 | 0.43 |
| 54:Q8:54:GLU:CB | 54:Q8:57:ARG:HH21 | 2.31 | 0.43 |
| 1:1G:109:A:H5' | 1:1G:110:C:C5 | 2.52 | 0.43 |
| 1:1G:1111:A:H2' | 1:1G:1112:C:C6 | 2.52 | 0.43 |
| 1:1G:1151:A:C4 | 1:1G:1152:A:C8 | 3.06 | 0.43 |
| 1:1G:1250:A:H2' | 1:1G:1251:A:C8 | 2.53 | 0.43 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 2:12:24:TRP:CD1 | 2:12:24:TRP:C | 2.96 | 0.43 |
| 2:12:144:ARG:O | 2:12:147:LYS:HB3 | 2.18 | 0.43 |
| 14:5A:9:LYS:HA | 14:5A:12:ARG:HD3 | 2.00 | 0.43 |
| 16:7A:54:GLU:HA | 16:7A:57:ARG:HB2 | 1.99 | 0.43 |
| 17:8A:70:ARG:HD2 | 17:8A:70:ARG:N | 2.33 | 0.43 |
| 17:8A:81:ARG:HD2 | 17:8A:81:ARG:HA | 1.74 | 0.43 |
| 24:14:11:G:N2 | 24:14:2627:G:O3' | 2.51 | 0.43 |
| 24:14:621:A:H3' | 24:14:622:G:C8 | 2.53 | 0.43 |
| 24:14:657:U:H2' | 24:14:658:C:H6 | 1.82 | 0.43 |
| 24:14:748:G:C8 | 42:A5:89:ALA:HB1 | 2.53 | 0.43 |
| 24:14:864:G:H4' | 25:1J:101:A:H4' | 2.00 | 0.43 |
| 24:14:1127:A:N1 | 24:14:2463:C:O2' | 2.49 | 0.43 |
| 24:14:1138:G:C4 | 24:14:1139:G:H1' | 2.53 | 0.43 |
| 24:14:1568:G:OP1 | 27:19:63:ARG:NH1 | 2.30 | 0.43 |
| 24:14:1818:U:O2' | 27:19:154:LYS:O | 2.28 | 0.43 |
| 24:14:1889:A:H2' | 24:14:1890:A:C8 | 2.54 | 0.43 |
| 24:14:2124:G:N2 | 26:79:217:THR:OG1 | 2.51 | 0.43 |
| 24:14:2271:G:C6 | 24:14:2272:U:C4 | 3.05 | 0.43 |
| 24:14:2621:A:HO2' | 28:29:159:HIS:H | 1.64 | 0.43 |
| 26:79:167:LYS:H | 26:79:167:LYS:HG3 | 1.61 | 0.43 |
| 28:29:197:ILE:HD13 | 28:29:197:ILE:HG21 | 1.65 | 0.43 |
| 30:49:14:GLU:O | 30:49:17:PRO:HG2 | 2.17 | 0.43 |
| 36:45:111:GLU:O | 36:45:115:MET:HG2 | 2.18 | 0.43 |
| 41:95:2:PHE:HB3 | 41:95:15:GLU:HG2 | 2.01 | 0.43 |
| 41:95:37:VAL:HG21 | 41:95:56:SER:CA | 2.29 | 0.43 |
| 45:D5:171:ILE:HD12 | 45:D5:171:ILE:HA | 1.83 | 0.43 |
| 1:13:238:G:OP1 | 17:8I:25:ARG:NH2 | 2.38 | 0.43 |
| 1:13:408:A:OP1 | 4:3E:113:SER:OG | 2.30 | 0.43 |
| 1:13:889:A:H4' | 1:13:890:G:OP1 | 2.19 | 0.43 |
| 1:13:1285:A:H8 | 1:13:1285:A:O5' | 2.00 | 0.43 |
| 1:13:1329:A:H4' | 13:4I:24:GLY:C | 2.43 | 0.43 |
| 1:13:1360:A:H2' | 1:13:1361:G:O4' | 2.18 | 0.43 |
| 1:13:1364:U:O2' | 1:13:1365:G:H5' | 2.18 | 0.43 |
| 2:1E:164:VAL:HB | 2:1E:186:ALA:HB2 | 1.99 | 0.43 |
| 5:4E:42:GLY:HA3 | 5:4E:66:MET:HE2 | 2.00 | 0.43 |
| 16:7I:58:TYR:O | 16:7I:61:SER:N | 2.48 | 0.43 |
| 19:AI:40:ILE:HD11 | 19:AI:62:ILE:HD12 | 2.00 | 0.43 |
| 24:1H:142:G:H1' | 43:F8:37:THR:CG2 | 2.44 | 0.43 |
| 24:1H:196:A:H2' | 24:1H:196:A:N3 | 2.33 | 0.43 |
| 24:1H:484:C:OP1 | 44:G8:51:VAL:HG22 | 2.18 | 0.43 |
| 24:1H:1152:C:H4' | 40:C8:77:SER:HA | 2.00 | 0.43 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 24:1H:1205:U:H4' | 24:1H:1206:G:OP2 | 2.18 | 0.43 |
| 24:1H:1509:C:H2' | 24:1H:1511:A:C8 | 2.53 | 0.43 |
| 24:1H:1542:G:OP2 | 24:1H:1543:A:O2' | 2.33 | 0.43 |
| 24:1H:1936:A:H3' | 24:1H:1937:A:H5' | 2.00 | 0.43 |
| 24:1H:2269:A:N3 | 24:1H:2269:A:H2' | 2.34 | 0.43 |
| 24:1H:2313:C:H2' | 24:1H:2314:C:C6 | 2.53 | 0.43 |
| 24:1H:2393:A:H5' | 35:78:61:ARG:O | 2.19 | 0.43 |
| 24:1H:2496:C:OP1 | 36:88:82:ARG:HB2 | 2.18 | 0.43 |
| 25:16:78:A:C2 | 25:16:99:A:C4 | 3.05 | 0.43 |
| 29:31:126:VAL:HG23 | 29:31:195:ASP:HA | 2.01 | 0.43 |
| 31:51:144:VAL:HA | 31:51:147:ASN:ND2 | 2.34 | 0.43 |
| 32:61:6:LEU:HD13 | 32:61:36:ALA:HA | 1.99 | 0.43 |
| 35:78:52:GLU:HB2 | 35:78:55:ARG:HG2 | 2.00 | 0.43 |
| 37:98:74:LYS:C | 37:98:76:VAL:N | 2.71 | 0.43 |
| 38:A8:30:ARG:HB3 | 38:A8:35:ILE:HD12 | 2.00 | 0.43 |
| 38:A8:110:LEU:O | 38:A8:111:GLU:HG2 | 2.18 | 0.43 |
| 45:H8:4:ARG:NH1 | 45:H8:58:VAL:HG11 | 2.33 | 0.43 |
| 46:I8:23:VAL:HG13 | 46:I8:38:VAL:CG2 | 2.48 | 0.43 |
| 1:1G:444:C:H2' | 1:1G:445:G:H8 | 1.83 | 0.43 |
| 1:1G:503:C:O2' | 1:1G:504:C:H5' | 2.18 | 0.43 |
| 1:1G:523:A:H61 | 12:3A:92:ASP:HB2 | 1.83 | 0.43 |
| 1:1G:1127:G:H1' | 1:1G:1147:C:N4 | 2.33 | 0.43 |
| 1:1G:1281:U:H3' | 1:1G:1282:C:C5 | 2.53 | 0.43 |
| 1:1G:1375:A:H2' | 1:1G:1376:U:H6 | 1.83 | 0.43 |
| 2:12:21:ARG:C | 2:12:23:ARG:N | 2.73 | 0.43 |
| 4:32:50:ARG:HH22 | 5:42:10:MET:CE | 2.31 | 0.43 |
| 8:72:103:VAL:HG11 | 8:72:109:ILE:O | 2.18 | 0.43 |
| 9:82:9:ARG:HB3 | 9:82:14:VAL:HG13 | 2.00 | 0.43 |
| 10:1A:87:THR:HB | 10:1A:88:LEU:HD12 | 2.00 | 0.43 |
| 12:3A:24:VAL:N | 12:3A:25:PRO:HD3 | 2.32 | 0.43 |
| 22:3L:13:G:H2' | 22:3L:14:A:C8 | 2.52 | 0.43 |
| 24:14:877:U:HO2' | 24:14:878:A:P | 2.41 | 0.43 |
| 24:14:1006:C:C2 | 24:14:1138:G:N2 | 2.86 | 0.43 |
| 24:14:1043:C:N4 | 24:14:1112:G:H1 | 2.17 | 0.43 |
| 24:14:1070:A:C8 | 24:14:1096:A:H1' | 2.54 | 0.43 |
| 24:14:1268:A:H2' | 24:14:1269:A:O4' | 2.18 | 0.43 |
| 24:14:1523:U:C2 | 24:14:1524:G:C8 | 3.06 | 0.43 |
| 24:14:2591:C:OP1 | 27:19:239:ARG:HG3 | 2.18 | 0.43 |
| 25:1J:66:A:H61 | 25:1J:108:C:H5" | 1.82 | 0.43 |
| 25:1J:89:G:C5 | 25:1J:89(A):A:C6 | 3.06 | 0.43 |
| 28:29:21:VAL:HG13 | 28:29:185:LYS:HE2 | 2.00 | 0.43 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 29:39:134:GLY:HA2 | 29:39:166:ALA:HB2 | 2.01 | 0.43 |
| 29:39:155:LEU:HD22 | 29:39:185:ASP:O | 2.18 | 0.43 |
| 31:59:90:LYS:HA | 31:59:90:LYS:HD2 | 1.89 | 0.43 |
| 32:69:74:ASN:O | 32:69:75:LEU:HB2 | 2.19 | 0.43 |
| 35:35:97:PRO:C | 35:35:99:LEU:N | 2.76 | 0.43 |
| 35:35:125:VAL:O | 35:35:144:GLU:HB3 | 2.18 | 0.43 |
| 42:A5:68:ARG:HB2 | 42:A5:109:GLU:HG2 | 2.01 | 0.43 |
| 43:B5:18:TYR:HD1 | 43:B5:21:PHE:CE2 | 2.34 | 0.43 |
| 52:K5:16:CYS:O | 52:K5:18:ARG:HB2 | 2.18 | 0.43 |
| 54:M5:29:LYS:HB2 | 54:M5:44:LYS:HB3 | 2.01 | 0.43 |
| 1:13:352:C:H4' | 1:13:354:G:OP1 | 2.19 | 0.43 |
| 1:13:727:G:N2 | 1:13:730:G:OP2 | 2.43 | 0.43 |
| 1:13:1330:U:H4' | 13:4I:23:TYR:CE1 | 2.53 | 0.43 |
| 2:1E:95:GLN:O | 2:1E:96:ARG:HD2 | 2.18 | 0.43 |
| 2:1E:145:LEU:O | 2:1E:149:LEU:HB2 | 2.18 | 0.43 |
| 3:2E:131:ARG:HD3 | 5:4E:50:GLU:HG2 | 2.00 | 0.43 |
| 6:5E:24:GLU:HB3 | 6:5E:28:ARG:CZ | 2.48 | 0.43 |
| 7:6E:139:GLU:H | 7:6E:139:GLU:HG3 | 1.63 | 0.43 |
| 15:6I:26:GLU:H | 15:6I:26:GLU:HG2 | 1.50 | 0.43 |
| 16:7I:28:ARG:HD2 | 16:7I:29:ASP:OD1 | 2.19 | 0.43 |
| 19:AI:67:VAL:HG13 | 50:M8:55:ARG:CZ | 2.48 | 0.43 |
| 20:BI:56:MET:HA | 20:BI:59:ALA:HB3 | 1.99 | 0.43 |
| 24:1H:384:U:O2' | 24:1H:385:C:H5' | 2.18 | 0.43 |
| 24:1H:529:A:C8 | 24:1H:530:G:C6 | 3.05 | 0.43 |
| 24:1H:1274:A:N3 | 24:1H:1297:C:H1' | 2.33 | 0.43 |
| 24:1H:1464:C:O2' | 24:1H:1528:A:C8 | 2.72 | 0.43 |
| 24:1H:1726:G:H2' | 24:1H:1727:U:O4' | 2.18 | 0.43 |
| 24:1H:2119:A:N1 | 24:1H:2170:A:N6 | 2.66 | 0.43 |
| 24:1H:2593:U:H2' | 24:1H:2594:C:C6 | 2.52 | 0.43 |
| 24:1H:2749:A:H5" | 31:51:6:ARG:HH11 | 1.82 | 0.43 |
| 26:71:201:PRO:HD2 | 26:71:208:PHE:HE1 | 1.84 | 0.43 |
| 27:11:72:LYS:NZ | 27:11:99:ASP:OD2 | 2.52 | 0.43 |
| 30:41:131:TYR:CE2 | 30:41:133:LEU:HD23 | 2.53 | 0.43 |
| 33:58:1:MET:HE3 | 33:58:1:MET:HB3 | 1.76 | 0.43 |
| 38:A8:69:VAL:HA | 38:A8:72:ALA:HB3 | 2.01 | 0.43 |
| 39:B8:78:LEU:HD12 | 39:B8:79:HIS:CE1 | 2.54 | 0.43 |
| 39:B8:124:ASP:O | 39:B8:128:GLU:N | 2.51 | 0.43 |
| 40:C8:114:LYS:H | 40:C8:114:LYS:HG2 | 1.53 | 0.43 |
| 1:1G:1459:C:H2' | 1:1G:1460:A:O4' | 2.19 | 0.43 |
| 1:1G:1464:G:OP1 | 39:75:108:ARG:NH1 | 2.51 | 0.43 |
| 3:22:47:LEU:HB3 | 3:22:52:LEU:HD22 | 2.00 | 0.43 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 13:4A:19:LEU:HD12 | 13:4A:25:ILE:HD12 | 2.00 | 0.43 |
| 22:3L:16:C:C4 | 22:3L:69:U:C2 | 3.06 | 0.43 |
| 24:14:289:A:H3' | 24:14:290:G:H8 | 1.83 | 0.43 |
| 24:14:396:G:H1' | 47:F5:42:GLN:HB2 | 2.00 | 0.43 |
| 24:14:483:A:H5' | 44:C5:49:VAL:HG22 | 2.00 | 0.43 |
| 24:14:1489:U:O3' | 24:14:1490:A:C8 | 2.72 | 0.43 |
| 24:14:1508:A:O2' | 24:14:1509:C:H5' | 2.18 | 0.43 |
| 24:14:2689:U:H5" | 24:14:2713:A:C2 | 2.53 | 0.43 |
| 29:39:1:MET:HE3 | 29:39:26:ALA:HB2 | 2.00 | 0.43 |
| 29:39:89:VAL:HG12 | 29:39:90:PHE:N | 2.32 | 0.43 |
| 30:49:121:ASN:HA | 30:49:181:ARG:NH1 | 2.33 | 0.43 |
| 31:59:166:GLY:O | 31:59:167:GLU:HB3 | 2.19 | 0.43 |
| 35:35:135:LEU:HD22 | 35:35:139:LYS:HD3 | 1.99 | 0.43 |
| 36:45:2:LEU:HD13 | 36:45:69:PHE:CE1 | 2.54 | 0.43 |
| 39:75:26:ASP:CG | 39:75:120:ARG:HH22 | 2.26 | 0.43 |
| 41:95:68:LYS:HD3 | 41:95:69:LYS:H | 1.82 | 0.43 |
| 45:D5:70:LEU:HD23 | 45:D5:70:LEU:HA | 1.66 | 0.43 |
| 54:M5:41:ILE:HD13 | 54:M5:41:ILE:HA | 1.88 | 0.43 |
| 1:13:188:U:H2' | 1:13:189:U:H5" | 1.99 | 0.43 |
| 1:13:222:U:C2 | 1:13:223:U:C5 | 3.06 | 0.43 |
| 1:13:718:G:H5' | 11:2I:117:ASN:CG | 2.44 | 0.43 |
| 1:13:977:A:C8 | 1:13:1223:C:C4 | 3.06 | 0.43 |
| 1:13:977:A:O2' | 1:13:979:C:OP2 | 2.33 | 0.43 |
| 1:13:1152:A:H2' | 1:13:1153:C:H6 | 1.84 | 0.43 |
| 1:13:1398:A:C6 | 5:4E:19:MET:HE1 | 2.53 | 0.43 |
| 3:2E:133:ALA:O | 3:2E:136:GLN:HG2 | 2.19 | 0.43 |
| 6:5E:24:GLU:HB3 | 6:5E:28:ARG:NH1 | 2.34 | 0.43 |
| 8:7E:7:ALA:HA | 8:7E:85:ARG:HG3 | 1.99 | 0.43 |
| 8:7E:19:VAL:HG23 | 8:7E:21:LYS:HG2 | 1.99 | 0.43 |
| 8:7E:86:ILE:O | 8:7E:88:LYS:HG3 | 2.19 | 0.43 |
| 24:1H:91:A:C4 | 24:1H:92:G:C8 | 3.07 | 0.43 |
| 24:1H:152:G:H2' | 24:1H:153:C:C6 | 2.54 | 0.43 |
| 24:1H:728:G:H4' | 27:11:13:ARG:HD3 | 2.00 | 0.43 |
| 24:1H:1519:G:C2' | 24:1H:1520:U:H5' | 2.49 | 0.43 |
| 24:1H:1530:G:H2' | 24:1H:1531:C:C6 | 2.53 | 0.43 |
| 24:1H:2799:A:O2' | 24:1H:2801:A:H5' | 2.18 | 0.43 |
| 25:16:19:G:N2 | 25:16:65:C:C2 | 2.87 | 0.43 |
| 25:16:73:A:C2' | 25:16:74:U:H5' | 2.48 | 0.43 |
| 28:21:146:THR:HA | 28:21:147:PRO:HA | 1.66 | 0.43 |
| 30:41:122:PRO:HB3 | 30:41:180:PHE:CD2 | 2.47 | 0.43 |
| 32:61:81:VAL:HG22 | 32:61:143:SER:O | 2.18 | 0.43 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 35:78:59:LEU:C | 35:78:61:ARG:H | 2.26 | 0.43 |
| 35:78:60:MET:H | 54:Q8:13:ARG:HD2 | 1.84 | 0.43 |
| 35:78:113:LYS:HE2 | 35:78:115:LEU:HD23 | 2.01 | 0.43 |
| 47:J8:84:GLY:HA3 | 47:J8:85:LEU:HA | 1.85 | 0.43 |
| 50:M8:43:TYR:HA | 50:M8:46:GLN:HG3 | 2.00 | 0.43 |
| 52:O8:9:LEU:N | 52:O8:27:LYS:HA | 2.33 | 0.43 |
| 1:1G:15:G:C4 | 1:1G:16:A:C8 | 3.07 | 0.43 |
| 1:1G:514:C:H2' | 1:1G:515:G:C8 | 2.51 | 0.43 |
| 1:1G:530:G:O2' | 1:1G:531:U:OP1 | 2.35 | 0.43 |
| 1:1G:540:G:H2' | 1:1G:541:G:O4' | 2.19 | 0.43 |
| 1:1G:806:C:O2' | 1:1G:807:A:H5' | 2.19 | 0.43 |
| 1:1G:1132:C:H2' | 1:1G:1133:G:H8 | 1.82 | 0.43 |
| 1:1G:1517:G:C6 | 1:1G:1518:A:C5 | 3.06 | 0.43 |
| 2:12:222:ILE:HG22 | 2:12:226:ARG:HD2 | 2.00 | 0.43 |
| 4:32:203:VAL:O | 4:32:206:PHE:HB3 | 2.18 | 0.43 |
| 5:42:30:ALA:O | 5:42:45:PHE:HA | 2.18 | 0.43 |
| 17:8A:51:TYR:HE1 | 17:8A:76:LEU:HB2 | 1.83 | 0.43 |
| 19:AA:60:VAL:HG21 | 19:AA:74:PHE:CD2 | 2.54 | 0.43 |
| 20:BA:69:GLY:O | 20:BA:73:HIS:NE2 | 2.52 | 0.43 |
| 20:BA:81:LYS:O | 20:BA:85:MET:HG2 | 2.17 | 0.43 |
| 22:2L:59:A:H61 | 22:2L:60:A:H62 | 1.65 | 0.43 |
| 24:14:528:A:C2 | 24:14:2043:C:H4' | 2.54 | 0.43 |
| 24:14:642:G:H21 | 24:14:646:A:H2 | 1.65 | 0.43 |
| 24:14:1048:A:H2 | 24:14:1112:G:H21 | 1.64 | 0.43 |
| 24:14:1161:C:O2' | 41:95:23:GLU:HG2 | 2.19 | 0.43 |
| 24:14:1451:C:H42 | 24:14:1459:G:H1 | 1.66 | 0.43 |
| 24:14:1459:G:H2' | 24:14:1461:G:OP2 | 2.18 | 0.43 |
| 24:14:1543:A:OP1 | 24:14:1543:A:C4' | 2.66 | 0.43 |
| 24:14:1668:A:C8 | 24:14:1674:G:C6 | 3.07 | 0.43 |
| 24:14:2355:C:H1' | 46:E5:39:ARG:HH21 | 1.83 | 0.43 |
| 24:14:2846:G:H2' | 24:14:2847:U:C6 | 2.54 | 0.43 |
| 25:1J:30:C:N4 | 25:1J:31:C:O2 | 2.51 | 0.43 |
| 27:19:130:ALA:HB1 | 27:19:190:TYR:HD2 | 1.83 | 0.43 |
| 27:19:132:PRO:HD3 | 27:19:190:TYR:CZ | 2.53 | 0.43 |
| 30:49:7:LEU:HB2 | 30:49:104:GLU:OE1 | 2.18 | 0.43 |
| 32:69:111:PRO:O | 32:69:114:LEU:HB2 | 2.18 | 0.43 |
| 43:B5:40:LYS:O | 43:B5:41:ASN:C | 2.60 | 0.43 |
| 44:C5:23:ARG:CZ | 44:C5:23:ARG:HB2 | 2.48 | 0.43 |
| 44:C5:61:ILE:HG22 | 44:C5:62:GLU:HG3 | 2.01 | 0.43 |
| 47:F5:10:LYS:NZ | 47:F5:65:SER:OG | 2.51 | 0.43 |
| 1:13:1225:A:H2' | 1:13:1225:A:N3 | 2.34 | 0.43 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 4:3E:108:LEU:HD23 | 4:3E:110:PHE:CE1 | 2.53 | 0.43 |
| 5:4E:45:PHE:CE2 | 5:4E:47:LYS:HD2 | 2.54 | 0.43 |
| 7:6E:44:TYR:HA | 7:6E:47:CYS:HB2 | 1.99 | 0.43 |
| 8:7E:118:VAL:O | 8:7E:119:LEU:HD23 | 2.19 | 0.43 |
| 20:BI:64:ASP:OD2 | 20:BI:81:LYS:NZ | 2.45 | 0.43 |
| 22:3K:18:G:H1' | 22:3K:19:C:OP2 | 2.19 | 0.43 |
| 24:1H:442:G:C4' | 29:31:46:ARG:HG3 | 2.46 | 0.43 |
| 24:1H:720:C:H2' | 24:1H:721:C:C6 | 2.53 | 0.43 |
| 24:1H:870:A:OP1 | 36:88:6:ARG:NE | 2.48 | 0.43 |
| 24:1H:944:G:H2' | 57:1H:3606:HOH:O | 2.18 | 0.43 |
| 24:1H:1062:G:C2 | 24:1H:1063:G:N1 | 2.87 | 0.43 |
| 24:1H:1103:A:H3' | 24:1H:1104:C:C6 | 2.54 | 0.43 |
| 24:1H:1315:C:C2 | 24:1H:1338:G:N2 | 2.86 | 0.43 |
| 24:1H:1323:U:H2' | 24:1H:1324:G:H5' | 1.99 | 0.43 |
| 24:1H:1392:A:N6 | 24:1H:1393:A:N6 | 2.67 | 0.43 |
| 24:1H:1655:A:H3' | 24:1H:1656:C:H6 | 1.83 | 0.43 |
| 24:1H:1816:G:N7 | 27:11:35:LYS:NZ | 2.66 | 0.43 |
| 24:1H:2384:G:O2' | 24:1H:2386:C:OP2 | 2.36 | 0.43 |
| 24:1H:2679:A:H2' | 24:1H:2680:C:C6 | 2.54 | 0.43 |
| 26:71:46:LYS:NZ | 26:71:210:ARG:HH21 | 2.16 | 0.43 |
| 29:31:23:ASP:OD1 | 29:31:23:ASP:N | 2.47 | 0.43 |
| 29:31:80:ALA:HA | 29:31:81:PRO:HD3 | 1.88 | 0.43 |
| 35:78:19:VAL:HB | 35:78:27:HIS:CB | 2.45 | 0.43 |
| 43:F8:66:LEU:C | 43:F8:67:GLY:O | 2.61 | 0.43 |
| 45:H8:130:PRO:HA | 45:H8:133:ILE:HD11 | 2.00 | 0.43 |
| 1:1G:256:U:H2' | 1:1G:257:G:C8 | 2.53 | 0.43 |
| 1:1G:512:U:C2 | 1:1G:513:C:C5 | 3.07 | 0.43 |
| 1:1G:709:G:H2' | 1:1G:710:G:H8 | 1.84 | 0.43 |
| 1:1G:1121:U:C4 | 1:1G:1122:U:C4 | 3.07 | 0.43 |
| 1:1G:1128:C:C4 | 1:1G:1139:G:C5 | 3.06 | 0.43 |
| 1:1G:1178:G:H5" | 9:82:93:ARG:HH22 | 1.83 | 0.43 |
| 1:1G:1251:A:H4' | 9:82:12:GLU:OE2 | 2.19 | 0.43 |
| 2:12:77:ALA:HB2 | 2:12:211:ILE:HD13 | 2.01 | 0.43 |
| 2:12:198:ASP:OD1 | 8:72:68:ARG:NH1 | 2.50 | 0.43 |
| 3:22:36:ASP:CG | 3:22:57:ILE:HD12 | 2.44 | 0.43 |
| 4:32:162:LEU:HA | 4:32:162:LEU:HD23 | 1.81 | 0.43 |
| 6:52:77:ARG:HH12 | 6:52:78:GLU:HG2 | 1.83 | 0.43 |
| 7:62:90:GLU:H | 7:62:90:GLU:HG2 | 1.43 | 0.43 |
| 10:1A:92:THR:HG23 | 10:1A:93:GLY:N | 2.34 | 0.43 |
| 15:6A:9:GLN:O | 15:6A:13:GLN:HG2 | 2.19 | 0.43 |
| 24:14:326:G:H2' | 24:14:327:G:O4' | 2.18 | 0.43 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 24:14:444:C:H4' | 29:39:49:ALA:HB2 | 1.99 | 0.43 |
| 24:14:1068:G:H21 | 24:14:1094:U:H2' | 1.83 | 0.43 |
| 24:14:1184:G:C6 | 24:14:1185:C:C4 | 3.07 | 0.43 |
| 24:14:2110:G:C6 | 24:14:2120:G:C8 | 3.06 | 0.43 |
| 24:14:2287:A:C2 | 24:14:2346:A:C2 | 3.07 | 0.43 |
| 24:14:2324:C:H5" | 24:14:2325:G:H5' | 2.00 | 0.43 |
| 24:14:2335:A:O2' | 24:14:2336:A:OP2 | 2.27 | 0.43 |
| 24:14:2611:U:OP2 | 24:14:2611:U:H6 | 2.02 | 0.43 |
| 25:1J:76:G:H2' | 25:1J:77:U:O4' | 2.19 | 0.43 |
| 27:19:255:LYS:HZ2 | 27:19:255:LYS:C | 2.27 | 0.43 |
| 30:49:47:LYS:HE2 | 30:49:81:LYS:HB2 | 1.99 | 0.43 |
| 30:49:119:GLY:O | 30:49:181:ARG:HB2 | 2.19 | 0.43 |
| 31:59:59:ARG:O | 31:59:63:SER:OG | 2.29 | 0.43 |
| 32:69:25:TYR:CE1 | 32:69:29:TYR:CD2 | 3.07 | 0.43 |
| 32:69:128:LEU:HD12 | 32:69:128:LEU:HA | 1.68 | 0.43 |
| 38:65:64:GLU:O | 38:65:68:GLN:HG3 | 2.19 | 0.43 |
| 39:75:19:LEU:HD22 | 39:75:86:ILE:HG23 | 2.00 | 0.43 |
| 52:K5:15:GLU:HB3 | 52:K5:16:CYS:H | 1.45 | 0.43 |
| 1:13:6:G:H4' | 1:13:298:A:H4' | 2.01 | 0.43 |
| 1:13:153:C:H42 | 1:13:168:G:H1 | 1.65 | 0.43 |
| 1:13:267:C:OP1 | 17:8I:67:LYS:HD2 | 2.19 | 0.43 |
| 1:13:724:G:C2 | 1:13:725:G:C8 | 3.07 | 0.43 |
| 3:2E:40:ARG:NH2 | 3:2E:55:VAL:O | 2.41 | 0.43 |
| 3:2E:79:ARG:HH11 | 18:9A:87:ARG:NH1 | 2.17 | 0.43 |
| 4:3E:142:PRO:HA | 4:3E:185:PHE:HD2 | 1.84 | 0.43 |
| 15:6I:71:GLN:O | 15:6I:71:GLN:HG2 | 2.18 | 0.43 |
| 24:1H:71:A:H2 | 43:F8:31:HIS:NE2 | 2.08 | 0.43 |
| 24:1H:392:C:OP1 | 57:1H:3612:HOH:O | 2.20 | 0.43 |
| 24:1H:814:C:H2' | 24:1H:815:C:C6 | 2.53 | 0.43 |
| 24:1H:1060:U:H5' | 24:1H:1061:U:H5 | 1.84 | 0.43 |
| 24:1H:1206:G:C6 | 24:1H:1207:C:C4 | 3.06 | 0.43 |
| 24:1H:1222:C:C2 | 24:1H:1223:C:C5 | 3.06 | 0.43 |
| 24:1H:2027:G:C5 | 24:1H:2028:U:C5 | 3.07 | 0.43 |
| 24:1H:2331:G:H4' | 46:I8:43:THR:N | 2.26 | 0.43 |
| 25:16:83:G:C6 | 25:16:84:C:C5 | 3.07 | 0.43 |
| 27:11:143:HIS:HD2 | 27:11:144:ALA:HB2 | 1.83 | 0.43 |
| 36:88:90:VAL:C | 36:88:92:GLY:H | 2.27 | 0.43 |
| 36:88:105:GLU:O | 36:88:105:GLU:HG2 | 2.19 | 0.43 |
| 43:F8:53:LYS:HE2 | 43:F8:55:ASN:HD21 | 1.83 | 0.43 |
| 44:G8:64:GLU:H | 44:G8:64:GLU:HG2 | 1.56 | 0.43 |
| 45:H8:1:MET:HG2 | 45:H8:135:GLU:OE1 | 2.19 | 0.43 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 47:J8:57:GLU:C | 47:J8:58:ILE:HD12 | 2.43 | 0.43 |
| 1:1G:57:G:C6 | 1:1G:58:C:C4 | 3.07 | 0.43 |
| 1:1G:79:G:H8 | 1:1G:79:G:OP2 | 2.02 | 0.43 |
| 1:1G:152:A:N6 | 1:1G:170:U:C2 | 2.87 | 0.43 |
| 1:1G:176:C:H2' | 1:1G:177:C:H6 | 1.84 | 0.43 |
| 1:1G:298:A:H3' | 1:1G:299:G:C8 | 2.54 | 0.43 |
| 1:1G:376:G:H5" | 16:7A:5:ARG:HD3 | 1.99 | 0.43 |
| 1:1G:408:A:H2' | 1:1G:409:G:O4' | 2.19 | 0.43 |
| 1:1G:464:G:H1' | 1:1G:468:A:H61 | 1.84 | 0.43 |
| 1:1G:949:A:C2 | 1:1G:1233:G:N3 | 2.87 | 0.43 |
| 1:1G:1206:G:C4 | 1:1G:1207:G:C8 | 3.07 | 0.43 |
| 1:1G:1236:A:OP1 | 21:1B:3:LYS:HG3 | 2.18 | 0.43 |
| 1:1G:1375:A:H4' | 7:62:29:LYS:NZ | 2.34 | 0.43 |
| 8:72:11:THR:HG23 | 8:72:14:ARG:NH1 | 2.33 | 0.43 |
| 8:72:97:VAL:HG13 | 8:72:129:VAL:O | 2.19 | 0.43 |
| 9:82:46:ALA:HB2 | 9:82:74:ILE:HG23 | 1.99 | 0.43 |
| 24:14:55:G:O2' | 24:14:127:A:N1 | 2.43 | 0.43 |
| 24:14:558:G:OP1 | 33:15:111:PRO:HD2 | 2.19 | 0.43 |
| 24:14:875:G:N2 | 24:14:903:C:C2 | 2.87 | 0.43 |
| 24:14:918:A:C2 | 25:1J:80:U:H4' | 2.53 | 0.43 |
| 24:14:931:G:O2' | 49:H5:24:LYS:HE3 | 2.19 | 0.43 |
| 24:14:1138:G:H2' | 33:15:106:MET:HE3 | 2.01 | 0.43 |
| 24:14:2634:G:O3' | 28:29:77:ILE:HG12 | 2.19 | 0.43 |
| 24:14:2685:G:P | 39:75:51:ARG:HH22 | 2.40 | 0.43 |
| 29:39:10:PRO:HA | 29:39:127:GLU:HB3 | 2.00 | 0.43 |
| 30:49:19:LEU:HG | 30:49:175:LEU:HD12 | 2.01 | 0.43 |
| 34:25:44:LYS:HA | 34:25:44:LYS:HD3 | 1.68 | 0.43 |
| 38:65:42:ASP:OD1 | 38:65:42:ASP:N | 2.50 | 0.43 |
| 40:85:25:TRP:CD1 | 40:85:25:TRP:C | 2.96 | 0.43 |
| 40:85:83:LEU:CD2 | 40:85:88:ILE:HB | 2.49 | 0.43 |
| 44:C5:50:ARG:HG2 | 44:C5:53:PRO:HB3 | 2.00 | 0.43 |
| 45:D5:62:PRO:O | 45:D5:63:ASP:HB3 | 2.19 | 0.43 |
| 50:I5:14:ILE:O | 50:I5:20:ASN:HB3 | 2.18 | 0.43 |
| 50:I5:36:CYS:HB3 | 50:I5:39:CYS:HB2 | 1.99 | 0.43 |
| 1:13:99:C:N3 | 1:13:101:A:N6 | 2.66 | 0.43 |
| 1:13:200:G:N2 | 1:13:218:C:C2 | 2.86 | 0.43 |
| 1:13:1298:C:N4 | 7:6E:114:ARG:HB3 | 2.34 | 0.43 |
| 1:13:1374:A:H2' | 1:13:1375:A:H5' | 2.01 | 0.43 |
| 1:13:1459:C:H5' | 20:BI:27:LYS:HE3 | 1.99 | 0.43 |
| 2:1E:103:THR:HB | 2:1E:176:GLU:OE1 | 2.19 | 0.43 |
| 2:1E:126:GLU:HA | 2:1E:129:GLU:HB2 | 2.01 | 0.43 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 2:1E:154:LEU:O | 2:1E:155:LEU:HD12 | 2.19 | 0.43 |
| 3:2E:20:SER:HB3 | 3:2E:40:ARG:HH22 | 1.84 | 0.43 |
| 7:6E:57:GLU:H | 7:6E:57:GLU:CD | 2.26 | 0.43 |
| 9:8E:42:ARG:NH2 | 9:8E:75:ASP:OD2 | 2.40 | 0.43 |
| 11:2I:45:GLY:O | 11:2I:50:TYR:HB2 | 2.18 | 0.43 |
| 24:1H:64:A:C4 | 43:F8:66:LEU:HD23 | 2.54 | 0.43 |
| 24:1H:273(C):C:C2 | 24:1H:363(D):G:N2 | 2.86 | 0.43 |
| 24:1H:654(G):C:H2' | 24:1H:654(H):G:C8 | 2.52 | 0.43 |
| 24:1H:1287:A:N7 | 37:98:107:ASP:CB | 2.82 | 0.43 |
| 24:1H:1386:C:C2 | 24:1H:1387:C:C5 | 3.07 | 0.43 |
| 24:1H:2027:G:H2' | 24:1H:2028:U:H6 | 1.83 | 0.43 |
| 24:1H:2271:G:H5" | 46:I8:20:ARG:NH1 | 2.33 | 0.43 |
| 24:1H:2330:G:H2' | 24:1H:2331:G:O4' | 2.18 | 0.43 |
| 24:1H:2391:G:O6 | 24:1H:2425:A:H8 | 2.02 | 0.43 |
| 24:1H:2663:G:C2 | 24:1H:2664:G:H1' | 2.53 | 0.43 |
| 26:71:66:HIS:HD2 | 26:71:184:LYS:O | 2.02 | 0.43 |
| 31:51:94:TYR:CE1 | 31:51:107:VAL:O | 2.72 | 0.43 |
| 31:51:144:VAL:O | 31:51:148:ILE:HG12 | 2.19 | 0.43 |
| 32:61:133:HIS:O | 32:61:134:PRO:C | 2.62 | 0.43 |
| 39:B8:56:GLY:O | 39:B8:59:THR:HG22 | 2.19 | 0.43 |
| 39:B8:74:ARG:HD3 | 39:B8:76:PHE:CZ | 2.53 | 0.43 |
| 45:H8:27:VAL:HG13 | 45:H8:87:ASP:HB2 | 1.99 | 0.43 |
| 45:H8:28:MET:N | 45:H8:35:ARG:O | 2.40 | 0.43 |
| 47:J8:67:ILE:N | 47:J8:68:PRO:HD2 | 2.33 | 0.43 |
| 1:1G:465:A:N6 | 1:1G:467:G:C2 | 2.87 | 0.43 |
| 1:1G:685:G:N1 | 1:1G:686:U:O4 | 2.52 | 0.43 |
| 1:1G:691:G:H3' | 11:2A:26:ASN:HD21 | 1.84 | 0.43 |
| 1:1G:1004:A:O2' | 1:1G:1036:G:N1 | 2.43 | 0.43 |
| 1:1G:1032(B):G:C6 | 1:1G:1033:G:C2 | 3.07 | 0.43 |
| 1:1G:1206:G:O4' | 3:22:194:GLY:HA2 | 2.18 | 0.43 |
| 2:12:152:PHE:CE1 | 2:12:155:LEU:HD12 | 2.53 | 0.43 |
| 4:32:122:ARG:NH2 | 4:32:134:ASP:HB2 | 2.33 | 0.43 |
| 5:42:6:PHE:HB2 | 5:42:63:ARG:NH1 | 2.34 | 0.43 |
| 5:42:146:ALA:O | 5:42:149:GLU:N | 2.52 | 0.43 |
| 15:6A:10:LYS:O | 15:6A:10:LYS:HE3 | 2.17 | 0.43 |
| 15:6A:32:LEU:HA | 15:6A:32:LEU:HD23 | 1.82 | 0.43 |
| 16:7A:23:ASP:OD2 | 16:7A:25:ARG:NH1 | 2.52 | 0.43 |
| 20:BA:37:SER:HB3 | 20:BA:84:LEU:HG | 2.01 | 0.43 |
| 24:14:142:G:O3' | 43:B5:35:THR:HG21 | 2.18 | 0.43 |
| 24:14:185:U:H2' | 24:14:186:G:C8 | 2.54 | 0.43 |
| 24:14:389:G:N2 | 35:35:72:PRO:HD3 | 2.33 | 0.43 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 24:14:565:C:H4' | 24:14:1253:A:C6 | 2.54 | 0.43 |
| 24:14:607:U:OP1 | 29:39:102:PRO:HA | 2.19 | 0.43 |
| 24:14:661:C:H2' | 24:14:662:G:C8 | 2.54 | 0.43 |
| 24:14:693:C:H2' | 24:14:694:U:C6 | 2.53 | 0.43 |
| 24:14:935:C:H2' | 24:14:936:C:H6 | 1.84 | 0.43 |
| 24:14:996:A:N3 | 24:14:997:G:C8 | 2.87 | 0.43 |
| 24:14:1015:G:O2' | 24:14:1016:G:H5' | 2.19 | 0.43 |
| 24:14:1106:G:H3' | 24:14:1107:G:C8 | 2.53 | 0.43 |
| 24:14:1327:C:C5 | 24:14:1328:G:C6 | 3.07 | 0.43 |
| 24:14:1543:A:OP1 | 24:14:1543:A:H4' | 2.17 | 0.43 |
| 24:14:2161:C:H2' | 24:14:2162:G:C8 | 2.50 | 0.43 |
| 24:14:2218:G:O2' | 27:19:148:GLU:HG2 | 2.19 | 0.43 |
| 24:14:2228:G:O6 | 57:14:3575:HOH:O | 2.21 | 0.43 |
| 24:14:2291:U:H5" | 24:14:2380:C:O2' | 2.18 | 0.43 |
| 24:14:2408:U:H2' | 24:14:2409:G:H8 | 1.84 | 0.43 |
| 24:14:2584:U:H5" | 24:14:2585:U:OP2 | 2.19 | 0.43 |
| 24:14:2615:U:H2' | 24:14:2616:C:H6 | 1.84 | 0.43 |
| 24:14:2870:C:H2' | 24:14:2871:C:H5' | 2.01 | 0.43 |
| 25:1J:26:A:OP2 | 25:1J:26:A:H8 | 2.02 | 0.43 |
| 27:19:106:ILE:O | 27:19:108:PRO:HD3 | 2.18 | 0.43 |
| 29:39:114:VAL:HG13 | 29:39:192:LEU:CD1 | 2.48 | 0.43 |
| 29:39:132:VAL:HG13 | 29:39:133:ASN:HB2 | 1.99 | 0.43 |
| 32:69:31:LEU:HD21 | 32:69:38:LEU:HD12 | 1.99 | 0.43 |
| 37:55:33:ARG:HD3 | 51:J5:55:ARG:HH22 | 1.84 | 0.43 |
| 44:C5:17:SER:OG | 44:C5:18:GLY:O | 2.35 | 0.43 |
| 46:E5:50:ASN:O | 46:E5:62:LEU:HB2 | 2.18 | 0.43 |
| 52:K5:9:LEU:HD21 | 52:K5:11:LEU:HD22 | 2.00 | 0.43 |
| 1:13:560:U:HO2' | 1:13:561:U:P | 2.35 | 0.43 |
| 1:13:892:A:O2' | 1:13:1415:G:H4' | 2.19 | 0.43 |
| 1:13:940:C:C2 | 1:13:941:G:C8 | 3.06 | 0.43 |
| 1:13:1167:A:H8 | 1:13:1167:A:OP1 | 2.02 | 0.43 |
| 1:13:1262:C:H2' | 1:13:1263:C:H6 | 1.84 | 0.43 |
| 1:13:1300:G:C5 | 1:13:1334:G:C6 | 3.06 | 0.43 |
| 1:13:1402:C:H2' | 1:13:1403:C:O4' | 2.19 | 0.43 |
| 7:6E:54:THR:C | 7:6E:56:GLN:H | 2.26 | 0.43 |
| 17:8I:92:ARG:HA | 17:8I:92:ARG:HD3 | 1.87 | 0.43 |
| 24:1H:176:G:O2' | 24:1H:177:G:H5' | 2.19 | 0.43 |
| 24:1H:270:A:OP2 | 24:1H:270(Y):G:N2 | 2.44 | 0.43 |
| 24:1H:286:C:H2' | 24:1H:287:C:C6 | 2.54 | 0.43 |
| 24:1H:322:A:OP2 | 29:31:169:ASN:HB2 | 2.19 | 0.43 |
| 24:1H:570:G:H2' | 24:1H:2030:A:C5 | 2.54 | 0.43 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 24:1H:686:G:H4' | 24:1H:687:C:OP2 | 2.18 | 0.43 |
| 24:1H:929:G:H8 | 24:1H:929:G:O5' | 2.02 | 0.43 |
| 24:1H:1176:G:O2' | 24:1H:1178:C:N4 | 2.52 | 0.43 |
| 24:1H:1749:A:H2' | 24:1H:1750:G:O4' | 2.19 | 0.43 |
| 24:1H:2098:U:H2' | 24:1H:2099:U:O4' | 2.19 | 0.43 |
| 24:1H:2132:U:N3 | 26:71:5:LYS:HB3 | 2.34 | 0.43 |
| 24:1H:2285:C:P | 52:O8:28:ARG:HG3 | 2.59 | 0.43 |
| 24:1H:2431:U:O2 | 24:1H:2433:A:C8 | 2.72 | 0.43 |
| 24:1H:2592:G:C5 | 24:1H:2593:U:C5 | 3.07 | 0.43 |
| 24:1H:2740:A:H2' | 24:1H:2741:A:C8 | 2.54 | 0.43 |
| 25:16:31:C:O2' | 25:16:53:A:N1 | 2.44 | 0.43 |
| 27:11:108:PRO:HG3 | 27:11:143:HIS:CE1 | 2.54 | 0.43 |
| 30:41:12:TYR:O | 30:41:16:ARG:HB2 | 2.19 | 0.43 |
| 30:41:96:ARG:C | 30:41:98:ARG:H | 2.26 | 0.43 |
| 32:61:116:LEU:HD22 | 32:61:116:LEU:HA | 1.75 | 0.43 |
| 35:78:37:GLY:HA2 | 35:78:41:ARG:NH2 | 2.34 | 0.43 |
| 35:78:106:LEU:O | 35:78:106:LEU:HD22 | 2.19 | 0.43 |
| 39:B8:26:ASP:CB | 39:B8:91:ARG:HA | 2.49 | 0.43 |
| 50:M8:17:GLY:N | 50:M8:36:CYS:H | 2.17 | 0.43 |
| 51:N8:40:LYS:HE2 | 51:N8:47:PRO:CG | 2.46 | 0.43 |
| 1:1G:683:G:H2' | 1:1G:684:A:C8 | 2.53 | 0.43 |
| 1:1G:843:U:H3' | 1:1G:848:C:O4' | 2.19 | 0.43 |
| 1:1G:996:A:H2' | 1:1G:997:U:O4' | 2.19 | 0.43 |
| 1:1G:1004:A:H1' | 1:1G:1025:U:N3 | 2.34 | 0.43 |
| 1:1G:1191:A:H5" | 3:22:4:LYS:HZ2 | 1.84 | 0.43 |
| 1:1G:1329:A:P | 13:4A:28:ALA:HB3 | 2.59 | 0.43 |
| 1:1G:1371:G:O2' | 1:1G:1372:U:H5' | 2.19 | 0.43 |
| 4:32:92:VAL:O | 4:32:96:LEU:HG | 2.19 | 0.43 |
| 5:42:9:LYS:HB2 | 5:42:112:LEU:HD11 | 2.01 | 0.43 |
| 12:3A:76:ASN:ND2 | 12:3A:106:ASP:O | 2.51 | 0.43 |
| 20:BA:95:ALA:O | 20:BA:97:ALA:N | 2.51 | 0.43 |
| 24:14:586:A:H5' | 29:39:89:VAL:HG21 | 2.00 | 0.43 |
| 24:14:1021:A:O2' | 24:14:1123:C:OP1 | 2.34 | 0.43 |
| 24:14:1385:G:O2' | 24:14:1396:U:H6 | 2.02 | 0.43 |
| 24:14:1685:C:H2' | 24:14:1686:C:H6 | 1.83 | 0.43 |
| 24:14:2215:G:H8 | 24:14:2215:G:O5' | 2.01 | 0.43 |
| 24:14:2400:G:H2' | 24:14:2401:U:C6 | 2.53 | 0.43 |
| 24:14:2648:C:H2' | 24:14:2649:U:H6 | 1.83 | 0.43 |
| 25:1J:69:G:H2' | 25:1J:70:C:O4' | 2.19 | 0.43 |
| 27:19:206:LEU:HA | 27:19:206:LEU:HD23 | 1.56 | 0.43 |
| 28:29:93:VAL:HG21 | 28:29:180:ASN:C | 2.43 | 0.43 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 29:39:179:GLU:O | 29:39:205:ARG:NH2 | 2.52 | 0.43 |
| 30:49:106:LEU:HA | 30:49:110:ALA:HB3 | 2.01 | 0.43 |
| 32:69:15:VAL:C | 32:69:17:GLN:H | 2.27 | 0.43 |
| 32:69:128:LEU:O | 32:69:137:PRO:HA | 2.19 | 0.43 |
| 45:D5:72:ARG:HD3 | 45:D5:72:ARG:HA | 1.53 | 0.43 |
| 50:I5:18:CYS:N | 50:I5:19:GLY:HA2 | 2.34 | 0.43 |
| 54:M5:34:TRP:CZ3 | 54:M5:36:LYS:HG3 | 2.53 | 0.43 |
| 1:13:234:C:H2' | 1:13:235:C:H6 | 1.83 | 0.42 |
| 1:13:314:C:O2' | 1:13:315:A:H5' | 2.19 | 0.42 |
| 1:13:875:C:O2' | 8:7E:14:ARG:NH1 | 2.52 | 0.42 |
| 1:13:965:A:C2 | 1:13:969:A:C2 | 3.07 | 0.42 |
| 1:13:1002:G:H2' | 1:13:1003:G:O4' | 2.19 | 0.42 |
| 1:13:1021:G:H2' | 1:13:1022:G:O4' | 2.19 | 0.42 |
| 1:13:1131:G:OP1 | 9:8E:20:ARG:NH2 | 2.52 | 0.42 |
| 1:13:1250:A:H4' | 9:8E:68:GLY:N | 2.34 | 0.42 |
| 1:13:1392:G:N2 | 1:13:1502:A:H8 | 2.16 | 0.42 |
| 1:13:1417:G:N2 | 1:13:1482:G:H2' | 2.33 | 0.42 |
| 2:1E:7:VAL:HB | 2:1E:217:ARG:NH1 | 2.34 | 0.42 |
| 2:1E:187:LEU:HD23 | 2:1E:201:ILE:O | 2.19 | 0.42 |
| 3:2E:79:ARG:HH11 | 18:9A:87:ARG:HH12 | 1.64 | 0.42 |
| 4:3E:166:LYS:H | 4:3E:166:LYS:HE2 | 1.83 | 0.42 |
| 7:6E:113:GLU:CG | 7:6E:119:ARG:HG2 | 2.49 | 0.42 |
| 10:1I:9:ARG:HG2 | 10:1I:69:ASN:OD1 | 2.19 | 0.42 |
| 11:2I:33:THR:HA | 11:2I:39:PRO:HA | 2.00 | 0.42 |
| 19:AI:42:PRO:HD3 | 50:M8:63:TYR:CZ | 2.54 | 0.42 |
| 24:1H:3:U:O5' | 24:1H:3:U:H6 | 2.02 | 0.42 |
| 24:1H:186:G:H2' | 24:1H:187:G:H8 | 1.83 | 0.42 |
| 24:1H:285:C:H2' | 24:1H:286:C:H6 | 1.83 | 0.42 |
| 24:1H:345:A:O2' | 57:1H:3706:HOH:O | 2.21 | 0.42 |
| 24:1H:444:C:C4' | 29:31:49:ALA:HB2 | 2.49 | 0.42 |
| 24:1H:565:C:H4' | 24:1H:1253:A:N6 | 2.34 | 0.42 |
| 24:1H:581:C:OP1 | 40:C8:33:ARG:HG3 | 2.19 | 0.42 |
| 24:1H:823:G:H2' | 24:1H:824:A:C8 | 2.54 | 0.42 |
| 24:1H:908:C:O2' | 24:1H:909:A:H5' | 2.19 | 0.42 |
| 24:1H:1063:G:C5 | 24:1H:1064:C:C4 | 3.07 | 0.42 |
| 24:1H:1268:A:C2 | 24:1H:2013:A:C4 | 3.07 | 0.42 |
| 24:1H:1639:U:O2' | 24:1H:1640:C:H5' | 2.19 | 0.42 |
| 24:1H:2283:C:C4 | 24:1H:2389:G:C4 | 3.07 | 0.42 |
| 24:1H:2523:G:O5' | 24:1H:2523:G:H8 | 2.03 | 0.42 |
| 25:16:29:A:H2' | 25:16:30:C:O4' | 2.19 | 0.42 |
| 30:41:82:LEU:HA | 30:41:86:MET:HE1 | 2.00 | 0.42 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 34:68:115:VAL:HG12 | 34:68:121:VAL:HG21 | 2.01 | 0.42 |
| 35:78:18:ARG:O | 35:78:19:VAL:HG22 | 2.19 | 0.42 |
| 38:A8:92:TYR:CB | 38:A8:98:VAL:HG21 | 2.48 | 0.42 |
| 39:B8:26:ASP:HB2 | 39:B8:91:ARG:HA | 2.01 | 0.42 |
| 45:H8:146:ILE:HA | 45:H8:174:VAL:HG11 | 2.01 | 0.42 |
| 1:1G:332:G:H2' | 1:1G:333:G:H8 | 1.83 | 0.42 |
| 1:1G:877:C:H5" | 8:72:88:LYS:HD2 | 2.00 | 0.42 |
| 1:1G:1161:C:H42 | 1:1G:1175:G:H1 | 1.67 | 0.42 |
| 2:12:82:ARG:HG3 | 2:12:92:TYR:CZ | 2.54 | 0.42 |
| 3:22:23:TYR:HA | 10:1A:11:PHE:CE2 | 2.54 | 0.42 |
| 4:32:153:ARG:NH1 | 4:32:181:MET:HB2 | 2.34 | 0.42 |
| 6:52:80:ARG:HH11 | 6:52:80:ARG:HD3 | 1.70 | 0.42 |
| 8:72:9:MET:SD | 8:72:32:LYS:HB3 | 2.59 | 0.42 |
| 8:72:20:TYR:HE2 | 8:72:75:ARG:HD2 | 1.84 | 0.42 |
| 12:3A:32:PHE:HB3 | 12:3A:84:LEU:HD11 | 2.01 | 0.42 |
| 19:AA:83:HIS:H | 19:AA:83:HIS:CD2 | 2.37 | 0.42 |
| 20:BA:76:ALA:O | 20:BA:80:ARG:HB2 | 2.19 | 0.42 |
| 22:3L:23:A:H2' | 22:3L:24:G:O4' | 2.19 | 0.42 |
| 24:14:69:C:H2' | 24:14:70:G:C8 | 2.54 | 0.42 |
| 24:14:902:C:H2' | 24:14:903:C:C6 | 2.53 | 0.42 |
| 24:14:911:A:H2' | 36:45:9:TYR:OH | 2.19 | 0.42 |
| 24:14:1019:U:H3 | 24:14:1142(A):A:N6 | 2.11 | 0.42 |
| 24:14:1138:G:C5 | 24:14:1139:G:H1' | 2.53 | 0.42 |
| 24:14:1394:U:H2' | 24:14:1395:A:O4' | 2.19 | 0.42 |
| 24:14:1670:C:C5 | 24:14:1671:U:C4 | 3.07 | 0.42 |
| 24:14:1851:U:H2' | 24:14:1852:C:O4' | 2.19 | 0.42 |
| 24:14:2320:A:N6 | 24:14:2333:A:H2' | 2.34 | 0.42 |
| 24:14:2342:C:O2' | 24:14:2374:C:H5" | 2.19 | 0.42 |
| 24:14:2578:G:OP2 | 24:14:2578:G:H4' | 2.18 | 0.42 |
| 28:29:67:PHE:HA | 28:29:68:ALA:HA | 1.71 | 0.42 |
| 33:15:136:GLU:HG3 | 33:15:137:LYS:N | 2.34 | 0.42 |
| 35:35:124:LYS:HA | 35:35:143:GLY:O | 2.18 | 0.42 |
| 36:45:33:GLY:HA2 | 36:45:105:GLU:HA | 2.00 | 0.42 |
| 38:65:24:LEU:CD1 | 38:65:41:ASP:HB2 | 2.49 | 0.42 |
| 38:65:65:VAL:O | 38:65:69:VAL:HG12 | 2.19 | 0.42 |
| 41:95:16:PRO:HA | 41:95:96:ILE:HB | 2.00 | 0.42 |
| 43:B5:5:TYR:HB3 | 48:G5:33:MET:HB2 | 2.01 | 0.42 |
| 45:D5:1:MET:N | 45:D5:135:GLU:OE2 | 2.51 | 0.42 |
| 47:F5:21:ARG:HD3 | 47:F5:35:THR:HG21 | 2.01 | 0.42 |
| 48:G5:32:LEU:HD22 | 48:G5:53:LEU:HB3 | 2.01 | 0.42 |
| 1:13:17:U:H2' | 1:13:18:C:H6 | 1.81 | 0.42 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 1:13:255:G:C5 | 1:13:256:U:C5 | 3.07 | 0.42 |
| 1:13:474:G:H2' | 1:13:475:G:C8 | 2.54 | 0.42 |
| 1:13:894:G:C6 | 1:13:895:G:C5 | 3.07 | 0.42 |
| 1:13:945:G:N1 | 1:13:1337:G:C2 | 2.87 | 0.42 |
| 1:13:1091:U:H2' | 1:13:1093:A:OP2 | 2.18 | 0.42 |
| 1:13:1100:C:O2' | 1:13:1102:A:OP1 | 2.36 | 0.42 |
| 1:13:1336:C:O2 | 1:13:1336:C:H2' | 2.19 | 0.42 |
| 4:3E:78:LEU:HD23 | 4:3E:78:LEU:HA | 1.92 | 0.42 |
| 9:8E:114:TYR:HD2 | 10:1I:60:ARG:HB2 | 1.83 | 0.42 |
| 14:5I:41:ARG:HG3 | 14:5I:42:ILE:N | 2.33 | 0.42 |
| 15:6I:30:ALA:HB2 | 15:6I:85:LEU:HD11 | 2.02 | 0.42 |
| 22:3K:25:G:C2 | 22:3K:26:G:C4 | 3.07 | 0.42 |
| 24:1H:182:A:H2' | 24:1H:183:C:C6 | 2.55 | 0.42 |
| 24:1H:495:G:H1' | 42:E8:57:ASN:OD1 | 2.19 | 0.42 |
| 24:1H:660:G:H21 | 35:78:12:ALA:HA | 1.84 | 0.42 |
| 24:1H:759:G:O4' | 24:1H:1981:A:C2 | 2.72 | 0.42 |
| 24:1H:1022:G:H4' | 24:1H:1023:U:O5' | 2.19 | 0.42 |
| 24:1H:1257:C:H4' | 29:31:83:PHE:CE1 | 2.54 | 0.42 |
| 24:1H:1930:G:O2' | 24:1H:1968:G:O6 | 2.18 | 0.42 |
| 24:1H:2178:C:H5' | 26:71:46:LYS:HD3 | 2.01 | 0.42 |
| 24:1H:2238:G:H4' | 24:1H:2239:G:OP1 | 2.19 | 0.42 |
| 25:16:63:G:C2 | 25:16:64:C:C2 | 3.08 | 0.42 |
| 26:71:6:ARG:NH1 | 26:71:7:TYR:HB2 | 2.33 | 0.42 |
| 31:51:8:PRO:CD | 31:51:69:ARG:HE | 2.28 | 0.42 |
| 32:61:104:GLN:HG2 | 32:61:105:HIS:NE2 | 2.34 | 0.42 |
| 32:61:126:TYR:HB2 | 32:61:140:LEU:O | 2.19 | 0.42 |
| 33:58:28:THR:N | 33:58:106:MET:HE2 | 2.35 | 0.42 |
| 33:58:62:VAL:HG22 | 33:58:63:THR:N | 2.34 | 0.42 |
| 35:78:43:GLY:HA3 | 57:78:203:HOH:O | 2.19 | 0.42 |
| 36:88:2:LEU:HB3 | 36:88:69:PHE:CE1 | 2.54 | 0.42 |
| 1:1G:197:A:H8 | 1:1G:198:G:H1' | 1.81 | 0.42 |
| 1:1G:553:A:C5 | 1:1G:554:C:C5 | 3.06 | 0.42 |
| 1:1G:568:G:N3 | 1:1G:574:A:H2 | 2.17 | 0.42 |
| 1:1G:720:C:O5' | 1:1G:720:C:H6 | 2.02 | 0.42 |
| 1:1G:820:U:H4' | 1:1G:821:G:OP2 | 2.19 | 0.42 |
| 1:1G:976:G:P | 14:5A:32:SER:H | 2.40 | 0.42 |
| 1:1G:1118:C:OP1 | 9:82:9:ARG:NE | 2.52 | 0.42 |
| 1:1G:1401:G:C2 | 1:1G:1402:C:H1' | 2.54 | 0.42 |
| 4:32:18:LYS:NZ | 4:32:19:LEU:O | 2.46 | 0.42 |
| 7:62:138:LYS:HE2 | 7:62:142:GLU:OE2 | 2.18 | 0.42 |
| 9:82:16:ARG:O | 9:82:63:ILE:HG23 | 2.19 | 0.42 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 9:82:25:LYS:HD3 | 9:82:25:LYS:HA | 1.80 | 0.42 |
| 13:4A:25:ILE:HG22 | 13:4A:26:GLY:O | 2.19 | 0.42 |
| 24:14:511:U:H5" | 24:14:512:G:OP2 | 2.17 | 0.42 |
| 24:14:513:A:C2 | 24:14:514:A:C5 | 3.07 | 0.42 |
| 24:14:1111:A:O3' | 24:14:1112:G:H4' | 2.19 | 0.42 |
| 24:14:1155:A:O2' | 24:14:1156:A:H2' | 2.19 | 0.42 |
| 24:14:1291:C:H2' | 24:14:1292:U:C6 | 2.54 | 0.42 |
| 24:14:1728:G:C2 | 24:14:1730:U:OP2 | 2.72 | 0.42 |
| 24:14:1995:U:H3' | 24:14:1996:C:H2' | 2.00 | 0.42 |
| 24:14:2286:A:H8 | 24:14:2287:A:N6 | 2.17 | 0.42 |
| 24:14:2786:U:HO2' | 28:29:63:LEU:N | 2.09 | 0.42 |
| 24:14:2805:G:H2' | 24:14:2807:G:C8 | 2.55 | 0.42 |
| 24:14:2886:G:C6 | 24:14:2887:U:C4 | 3.07 | 0.42 |
| 32:69:120:ILE:CG2 | 32:69:126:TYR:HE2 | 2.32 | 0.42 |
| 39:75:102:ILE:CA | 39:75:105:LEU:HB2 | 2.49 | 0.42 |
| 42:A5:83:LYS:C | 42:A5:84:ARG:HD3 | 2.44 | 0.42 |
| 44:C5:50:ARG:HB3 | 44:C5:53:PRO:HD3 | 2.00 | 0.42 |
| 48:G5:32:LEU:HD21 | 48:G5:54:LYS:HG2 | 2.01 | 0.42 |
| 1:13:598:U:H4' | 8:7E:94:TYR:CG | 2.54 | 0.42 |
| 1:13:947:G:OP1 | 13:4I:108:ARG:HB3 | 2.20 | 0.42 |
| 1:13:1110:A:N6 | 1:13:1111:A:N1 | 2.68 | 0.42 |
| 1:13:1198:G:O2' | 10:1I:55:LYS:HD3 | 2.19 | 0.42 |
| 1:13:1406:U:O2 | 1:13:1517:G:N2 | 2.48 | 0.42 |
| 1:13:1429:C:H2' | 1:13:1430:C:H6 | 1.84 | 0.42 |
| 3:2E:175:LEU:HD21 | 3:2E:201:TYR:CE2 | 2.54 | 0.42 |
| 6:5E:78:GLU:O | 6:5E:81:ILE:HG13 | 2.19 | 0.42 |
| 10:1I:26:ALA:HA | 10:1I:29:ARG:HH21 | 1.84 | 0.42 |
| 10:1I:35:SER:N | 10:1I:73:ASP:O | 2.43 | 0.42 |
| 14:5I:6:LEU:HB3 | 14:5I:23:ARG:HH22 | 1.83 | 0.42 |
| 15:6I:43:LEU:HD23 | 15:6I:43:LEU:HA | 1.77 | 0.42 |
| 15:6I:87:ILE:HG22 | 15:6I:88:ARG:N | 2.25 | 0.42 |
| 22:2K:17:OMG:C4 | 22:2K:67:A:C2 | 3.07 | 0.42 |
| 24:1H:7:G:H2' | 24:1H:8:A:C8 | 2.54 | 0.42 |
| 24:1H:194:G:H2' | 24:1H:195:A:O4' | 2.19 | 0.42 |
| 24:1H:270(Y):G:C2 | 24:1H:270(Z):U:O4 | 2.72 | 0.42 |
| 24:1H:456:C:C3' | 43:F8:68:ARG:HH22 | 2.31 | 0.42 |
| 24:1H:612:G:O2' | 24:1H:616:A:N1 | 2.43 | 0.42 |
| 24:1H:787:U:H5" | 24:1H:788:A:H5' | 2.00 | 0.42 |
| 24:1H:997:G:C2 | 24:1H:1159:U:C2 | 3.07 | 0.42 |
| 24:1H:1019:U:N3 | 24:1H:1020:A:N7 | 2.67 | 0.42 |
| 24:1H:1019:U:H3 | 24:1H:1142(A):A:H62 | 1.66 | 0.42 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 24:1H:1300:U:H4' | 24:1H:1301:A:H5' | 2.00 | 0.42 |
| 24:1H:1341:U:OP1 | 24:1H:1397:U:N3 | 2.31 | 0.42 |
| 24:1H:1516:U:C2 | 24:1H:1517:G:C8 | 3.08 | 0.42 |
| 24:1H:1816:G:H8 | 27:11:62:TYR:CZ | 2.37 | 0.42 |
| 24:1H:2726:U:O4' | 34:68:1:MET:HE1 | 2.19 | 0.42 |
| 25:16:10:C:H2' | 25:16:11:C:C6 | 2.53 | 0.42 |
| 26:71:165:ASN:ND2 | 26:71:166:ASP:O | 2.53 | 0.42 |
| 28:21:37:ARG:HD2 | 28:21:80:GLU:OE2 | 2.19 | 0.42 |
| 29:31:101:LEU:HB3 | 29:31:106:ARG:HD3 | 2.00 | 0.42 |
| 32:61:101:LEU:HD23 | 32:61:101:LEU:HA | 1.77 | 0.42 |
| 37:98:34:ILE:HD13 | 37:98:34:ILE:HA | 1.74 | 0.42 |
| 38:A8:74:ALA:HB3 | 38:A8:107:GLU:HG3 | 2.01 | 0.42 |
| 41:D8:27:ALA:CB | 41:D8:61:VAL:HG21 | 2.49 | 0.42 |
| 41:D8:76:LYS:O | 41:D8:79:VAL:HG12 | 2.19 | 0.42 |
| 43:F8:60:ARG:NH2 | 53:P8:47:ARG:HH22 | 2.10 | 0.42 |
| 45:H8:6:LYS:O | 45:H8:59:LEU:HD22 | 2.19 | 0.42 |
| 48:K8:15:LYS:H | 48:K8:67:LYS:HZ3 | 1.67 | 0.42 |
| 1:1G:4:U:H4' | 1:1G:5:U:OP1 | 2.19 | 0.42 |
| 1:1G:89:U:O2' | 1:1G:90:C:O5' | 2.27 | 0.42 |
| 1:1G:111:G:O6 | 1:1G:330:C:N4 | 2.51 | 0.42 |
| 1:1G:324:G:OP2 | 57:1G:1816:HOH:O | 2.21 | 0.42 |
| 1:1G:428:G:H4' | 1:1G:429:U:O5' | 2.18 | 0.42 |
| 1:1G:735:C:H5" | 18:9A:71:LYS:CB | 2.48 | 0.42 |
| 3:22:128:PHE:CG | 3:22:129:ALA:N | 2.87 | 0.42 |
| 4:32:15:GLU:HG3 | 4:32:63:LYS:HG3 | 2.00 | 0.42 |
| 4:32:107:ARG:HD2 | 4:32:173:TRP:HZ2 | 1.84 | 0.42 |
| 5:42:79:GLU:HG2 | 5:42:92:LYS:HG2 | 2.00 | 0.42 |
| 5:42:81:GLU:HA | 5:42:89:ILE:O | 2.18 | 0.42 |
| 8:72:32:LYS:HA | 8:72:35:ILE:HD12 | 2.00 | 0.42 |
| 8:72:36:LEU:HD23 | 8:72:36:LEU:HA | 1.84 | 0.42 |
| 13:4A:8:GLU:HG3 | 13:4A:22:ILE:HG23 | 2.00 | 0.42 |
| 13:4A:29:ARG:HD3 | 13:4A:64:TRP:CH2 | 2.54 | 0.42 |
| 18:9A:73:ALA:HB3 | 18:9A:79:LEU:HD12 | 2.01 | 0.42 |
| 20:BA:90:GLN:HA | 20:BA:93:GLU:HG2 | 2.01 | 0.42 |
| 22:3L:76:C:H2' | 22:3L:77:C:C6 | 2.53 | 0.42 |
| 24:14:195:A:H2' | 24:14:198:C:N4 | 2.34 | 0.42 |
| 24:14:573:G:O2' | 24:14:574:C:H3' | 2.20 | 0.42 |
| 24:14:588:U:C2 | 29:39:90:PHE:CE1 | 3.08 | 0.42 |
| 24:14:972:G:O2' | 57:14:3577:HOH:O | 2.22 | 0.42 |
| 24:14:1328:G:H2' | 24:14:1330:C:C4 | 2.55 | 0.42 |
| 24:14:1612:C:H5" | 53:L5:7:PRO:CG | 2.49 | 0.42 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 24:14:1769:G:C2' | 24:14:1770:G:H5' | 2.49 | 0.42 |
| 24:14:2188:C:H2' | 24:14:2189:U:O4' | 2.19 | 0.42 |
| 24:14:2837:G:H2' | 24:14:2838:G:H8 | 1.83 | 0.42 |
| 30:49:141:PHE:CD1 | 30:49:142:PRO:HD2 | 2.54 | 0.42 |
| 35:35:134:ALA:O | 35:35:138:LEU:HD12 | 2.19 | 0.42 |
| 43:B5:11:PRO:HD3 | 48:G5:37:PHE:CD2 | 2.54 | 0.42 |
| 53:L5:14:LYS:HG2 | 53:L5:14:LYS:H | 1.56 | 0.42 |
| 54:M5:4:MET:HB2 | 54:M5:4:MET:HE3 | 1.57 | 0.42 |
| 54:M5:23:VAL:HG22 | 54:M5:47:LYS:HB3 | 2.00 | 0.42 |
| 1:13:254:G:H8 | 1:13:254:G:O5' | 2.02 | 0.42 |
| 1:13:498:A:C6 | 1:13:547:A:C8 | 3.08 | 0.42 |
| 1:13:864:A:H5' | 5:4E:86:ALA:HB2 | 2.00 | 0.42 |
| 1:13:1031:G:H2' | 1:13:1032:A:H8 | 1.85 | 0.42 |
| 1:13:1226:C:H5" | 13:4I:96:LEU:HD11 | 2.02 | 0.42 |
| 6:5E:62:TRP:C | 6:5E:63:TYR:HD1 | 2.27 | 0.42 |
| 7:6E:99:LEU:HD22 | 7:6E:103:TRP:CZ2 | 2.54 | 0.42 |
| 8:7E:85:ARG:O | 8:7E:86:ILE:HD13 | 2.20 | 0.42 |
| 10:1I:79:ARG:HA | 10:1I:79:ARG:HD3 | 1.66 | 0.42 |
| 11:2I:22:HIS:HB3 | 11:2I:29:ILE:HG23 | 2.01 | 0.42 |
| 12:3I:8:ASN:O | 12:3I:11:VAL:HG23 | 2.19 | 0.42 |
| 13:4I:87:TYR:HA | 13:4I:90:LEU:HG | 1.99 | 0.42 |
| 16:7I:57:ARG:HH21 | 16:7I:79:VAL:HA | 1.85 | 0.42 |
| 19:AI:40:ILE:O | 19:AI:41:VAL:HG22 | 2.19 | 0.42 |
| 20:BI:25:ARG:O | 20:BI:29:LYS:HG3 | 2.18 | 0.42 |
| 21:1F:5:ASP:O | 21:1F:11:GLY:HA3 | 2.19 | 0.42 |
| 24:1H:309:G:H4' | 44:G8:18:GLY:HA2 | 2.00 | 0.42 |
| 24:1H:448:U:C4 | 24:1H:583:G:H1' | 2.54 | 0.42 |
| 24:1H:1019:U:O2' | 24:1H:1021:A:H2 | 2.02 | 0.42 |
| 24:1H:1290:C:H2' | 24:1H:1291:C:H6 | 1.84 | 0.42 |
| 24:1H:1638:C:H5" | 24:1H:2710:C:O2' | 2.19 | 0.42 |
| 24:1H:1826:G:C2' | 24:1H:1827:C:O5' | 2.67 | 0.42 |
| 24:1H:2020:A:OP1 | 40:C8:27:LEU:HB2 | 2.19 | 0.42 |
| 24:1H:2037:G:H2' | 24:1H:2038:G:C8 | 2.54 | 0.42 |
| 24:1H:2140:C:O2 | 24:1H:2151:G:N1 | 2.47 | 0.42 |
| 24:1H:2344:U:C6 | 52:O8:37:ARG:HD3 | 2.55 | 0.42 |
| 24:1H:2850:A:H2' | 24:1H:2851:A:H8 | 1.83 | 0.42 |
| 25:16:37:C:H2' | 25:16:38:C:H5' | 2.02 | 0.42 |
| 25:16:73:A:O2' | 25:16:74:U:H5' | 2.20 | 0.42 |
| 27:11:30:GLU:HG3 | 27:11:63:ARG:CZ | 2.48 | 0.42 |
| 27:11:145:VAL:HG12 | 27:11:146:GLU:O | 2.19 | 0.42 |
| 27:11:177:LEU:HD11 | 27:11:183:ARG:HB2 | 2.01 | 0.42 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 29:31:53:THR:O | 29:31:54:ARG:C | 2.62 | 0.42 |
| 31:51:26:VAL:HG21 | 31:51:75:ALA:HB1 | 2.00 | 0.42 |
| 31:51:42:ARG:HB3 | 31:51:42:ARG:HH11 | 1.84 | 0.42 |
| 35:78:59:LEU:CD2 | 54:Q8:13:ARG:HD2 | 2.50 | 0.42 |
| 41:D8:79:VAL:CG1 | 41:D8:81:TYR:HB3 | 2.49 | 0.42 |
| 44:G8:75:ILE:O | 44:G8:76:CYS:HB3 | 2.19 | 0.42 |
| 45:H8:48:PHE:CE1 | 45:H8:71:VAL:HG11 | 2.53 | 0.42 |
| 47:J8:8:SER:HB3 | 47:J8:66:HIS:CD2 | 2.54 | 0.42 |
| 50:M8:17:GLY:HA3 | 50:M8:35:VAL:HG13 | 2.00 | 0.42 |
| 1:1G:15:G:H1' | 5:42:19:MET:CE | 2.50 | 0.42 |
| 1:1G:1085:U:H5' | 1:1G:1094:G:N2 | 2.34 | 0.42 |
| 1:1G:1205:U:H4' | 3:22:195:VAL:CG1 | 2.45 | 0.42 |
| 1:1G:1206:G:O2' | 3:22:193:TYR:HA | 2.19 | 0.42 |
| 2:12:223:ILE:HA | 2:12:226:ARG:HB2 | 2.00 | 0.42 |
| 4:32:175:SER:HB3 | 4:32:186:LEU:HD11 | 2.02 | 0.42 |
| 10:1A:8:LEU:HD23 | 10:1A:96:ILE:HD11 | 2.01 | 0.42 |
| 11:2A:124:LYS:HB3 | 11:2A:125:PHE:HD1 | 1.84 | 0.42 |
| 14:5A:4:LYS:HE2 | 14:5A:4:LYS:HB3 | 1.69 | 0.42 |
| 15:6A:48:LYS:HE3 | 15:6A:48:LYS:HB2 | 1.90 | 0.42 |
| 20:BA:69:GLY:O | 20:BA:73:HIS:CE1 | 2.73 | 0.42 |
| 21:1B:6:ARG:NE | 21:1B:15:ARG:HH12 | 2.16 | 0.42 |
| 24:14:547:A:N7 | 24:14:548:A:N6 | 2.68 | 0.42 |
| 24:14:588:U:H2' | 24:14:589:C:H6 | 1.84 | 0.42 |
| 24:14:901:A:H5' | 24:14:902:C:OP2 | 2.20 | 0.42 |
| 24:14:1517:G:H2' | 24:14:1518:C:C6 | 2.54 | 0.42 |
| 24:14:1848:A:C4 | 24:14:1849:G:C8 | 3.07 | 0.42 |
| 24:14:1931:U:H2' | 24:14:1932:A:C8 | 2.55 | 0.42 |
| 24:14:2002:G:C6 | 57:14:3587:HOH:O | 2.72 | 0.42 |
| 24:14:2135:A:H3' | 24:14:2136:C:C6 | 2.55 | 0.42 |
| 24:14:2151:G:H2' | 24:14:2152:G:C8 | 2.55 | 0.42 |
| 27:19:123:ALA:HA | 27:19:124:PRO:HD2 | 1.74 | 0.42 |
| 29:39:103:LYS:HA | 29:39:106:ARG:HG3 | 2.01 | 0.42 |
| 29:39:110:LEU:HD23 | 29:39:110:LEU:HA | 1.89 | 0.42 |
| 31:59:6:ARG:C | 31:59:8:PRO:HD2 | 2.43 | 0.42 |
| 31:59:26:VAL:HG13 | 31:59:27:LYS:H | 1.84 | 0.42 |
| 34:25:10:VAL:HG13 | 34:25:17:ARG:C | 2.45 | 0.42 |
| 34:25:71:ARG:HH12 | 34:25:122:LEU:C | 2.28 | 0.42 |
| 36:45:41:TRP:HB3 | 36:45:94:VAL:HG11 | 2.01 | 0.42 |
| 36:45:43:THR:O | 36:45:46:GLN:HB2 | 2.20 | 0.42 |
| 37:55:35:THR:HG23 | 37:55:112:ALA:O | 2.19 | 0.42 |
| 40:85:92:ARG:CD | 41:95:11:GLN:HB2 | 2.50 | 0.42 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 42:A5:6:ILE:HG12 | 42:A5:104:THR:OG1 | 2.20 | 0.42 |
| 42:A5:90:ARG:HG3 | 42:A5:90:ARG:HH11 | 1.84 | 0.42 |
| 47:F5:86:SER:N | 47:F5:87:PRO:HD2 | 2.34 | 0.42 |
| 51:J5:33:CYS:SG | 51:J5:46:CYS:SG | 3.13 | 0.42 |
| 1:13:448:A:OP2 | 1:13:485:G:N2 | 2.48 | 0.42 |
| 1:13:498:A:H4' | 1:13:500:G:OP1 | 2.20 | 0.42 |
| 1:13:590:C:H42 | 1:13:649:G:H1 | 1.66 | 0.42 |
| 1:13:632:A:N3 | 1:13:632:A:H2' | 2.33 | 0.42 |
| 1:13:765:G:H5" | 1:13:766:A:OP1 | 2.20 | 0.42 |
| 2:1E:114:ARG:HA | 2:1E:117:GLU:HB3 | 2.01 | 0.42 |
| 2:1E:145:LEU:HD13 | 2:1E:145:LEU:HA | 1.83 | 0.42 |
| 3:2E:33:LEU:HD21 | 14:5I:53:LEU:HD21 | 2.00 | 0.42 |
| 4:3E:13:ARG:O | 4:3E:14:ARG:HB3 | 2.19 | 0.42 |
| 15:6I:18:PHE:HD1 | 15:6I:19:PRO:O | 2.02 | 0.42 |
| 22:2K:64:PSU:O4 | 22:2K:66:G:C8 | 2.73 | 0.42 |
| 24:1H:363(B):G:H2' | 24:1H:363(C):G:H8 | 1.85 | 0.42 |
| 24:1H:467:G:OP2 | 53:P8:34:ARG:NH1 | 2.53 | 0.42 |
| 24:1H:496:G:C6 | 24:1H:497:A:C4 | 3.08 | 0.42 |
| 24:1H:574:C:H4' | 24:1H:575:A:O5' | 2.19 | 0.42 |
| 24:1H:775:G:O5' | 24:1H:777:A:H1' | 2.20 | 0.42 |
| 24:1H:849:A:H61 | 24:1H:929:G:H1' | 1.85 | 0.42 |
| 24:1H:1024:G:O5' | 24:1H:1024:G:H8 | 2.02 | 0.42 |
| 24:1H:1045:A:H4' | 24:1H:1046:A:H5' | 2.01 | 0.42 |
| 24:1H:1056:G:H5' | 24:1H:1086:A:H8 | 1.84 | 0.42 |
| 24:1H:1178:C:H1' | 24:1H:1179:C:O5' | 2.20 | 0.42 |
| 24:1H:1288:U:C2 | 24:1H:1327:C:O2 | 2.72 | 0.42 |
| 24:1H:2251:G:N7 | 36:88:82:ARG:NH1 | 2.67 | 0.42 |
| 24:1H:2281:C:O2' | 24:1H:2282:G:H5' | 2.19 | 0.42 |
| 24:1H:2292:C:P | 38:A8:17:ARG:NH2 | 2.92 | 0.42 |
| 24:1H:2393:A:H2' | 24:1H:2394:C:C6 | 2.53 | 0.42 |
| 24:1H:2636:U:H2' | 24:1H:2637:U:H6 | 1.82 | 0.42 |
| 24:1H:2653:U:H2' | 24:1H:2654:A:C8 | 2.54 | 0.42 |
| 27:11:125:ILE:CD1 | 27:11:137:PRO:HD3 | 2.49 | 0.42 |
| 27:11:248:SER:HB3 | 27:11:252:TRP:CH2 | 2.54 | 0.42 |
| 28:21:8:LYS:HD2 | 28:21:188:VAL:HG22 | 2.01 | 0.42 |
| 28:21:117:MET:HA | 28:21:122:PHE:N | 2.34 | 0.42 |
| 31:51:137:ASP:HB3 | 31:51:140:LYS:HB3 | 2.01 | 0.42 |
| 32:61:75:LEU:HD21 | 32:61:105:HIS:HD1 | 1.84 | 0.42 |
| 40:C8:39:LEU:HD23 | 40:C8:39:LEU:HA | 1.82 | 0.42 |
| 43:F8:66:LEU:O | 43:F8:66:LEU:HG | 2.17 | 0.42 |
| 44:G8:65:ALA:HA | 44:G8:66:PRO:HD3 | 1.93 | 0.42 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 1:1G:145:G:H2' | 1:1G:146:G:O4' | 2.19 | 0.42 |
| 1:1G:582:U:C2 | 1:1G:760:G:C6 | 3.08 | 0.42 |
| 1:1G:1141:C:C2 | 1:1G:1142:G:C8 | 3.08 | 0.42 |
| 1:1G:1387:G:C4 | 1:1G:1388:C:C5 | 3.07 | 0.42 |
| 1:1G:1478:C:H2' | 1:1G:1479:C:C6 | 2.53 | 0.42 |
| 3:22:112:SER:O | 3:22:116:VAL:HG23 | 2.20 | 0.42 |
| 7:62:151:TYR:C | 7:62:153:HIS:N | 2.78 | 0.42 |
| 11:2A:67:ASP:OD1 | 11:2A:71:LYS:HE3 | 2.19 | 0.42 |
| 13:4A:59:TYR:O | 13:4A:63:THR:OG1 | 2.31 | 0.42 |
| 17:8A:57:VAL:HG13 | 17:8A:76:LEU:HA | 2.01 | 0.42 |
| 17:8A:81:ARG:NE | 17:8A:84:LEU:HD21 | 2.34 | 0.42 |
| 24:14:51:G:N3 | 24:14:119:A:C2 | 2.88 | 0.42 |
| 24:14:500:G:N1 | 24:14:503:A:OP2 | 2.53 | 0.42 |
| 24:14:784:A:C8 | 24:14:792:G:C5 | 3.08 | 0.42 |
| 24:14:918:A:O2' | 25:1J:96:G:N2 | 2.45 | 0.42 |
| 24:14:1825:A:OP1 | 27:19:249:PRO:HD3 | 2.19 | 0.42 |
| 24:14:2104:G:C2 | 24:14:2186:G:C2 | 3.07 | 0.42 |
| 24:14:2287:A:C2 | 24:14:2346:A:H2 | 2.35 | 0.42 |
| 24:14:2338:G:H2' | 24:14:2339:G:C8 | 2.55 | 0.42 |
| 24:14:2638:G:P | 28:29:82:ARG:HH22 | 2.43 | 0.42 |
| 27:19:80:ALA:HB3 | 27:19:94:LEU:HB3 | 2.01 | 0.42 |
| 30:49:138:GLN:C | 30:49:140:ILE:N | 2.78 | 0.42 |
| 35:35:59:LEU:HD21 | 54:M5:10:ALA:HA | 2.01 | 0.42 |
| 35:35:99:LEU:HD12 | 35:35:99:LEU:HA | 1.90 | 0.42 |
| 36:45:21:THR:H | 36:45:98:LYS:HB2 | 1.84 | 0.42 |
| 37:55:77:ARG:O | 37:55:80:PHE:N | 2.52 | 0.42 |
| 47:F5:85:LEU:HD13 | 47:F5:85:LEU:HA | 1.62 | 0.42 |
| 1:13:223:U:H2' | 1:13:224:C:O4' | 2.19 | 0.42 |
| 1:13:234:C:H2' | 1:13:235:C:C6 | 2.53 | 0.42 |
| 1:13:299:G:H2' | 1:13:300:A:C8 | 2.55 | 0.42 |
| 1:13:428:G:H5" | 4:3E:7:PRO:HB3 | 2.02 | 0.42 |
| 1:13:482:A:H2' | 1:13:483:C:O4' | 2.20 | 0.42 |
| 1:13:976:G:C8 | 1:13:1358:U:O2 | 2.73 | 0.42 |
| 1:13:1155:G:H2' | 1:13:1156:G:O4' | 2.19 | 0.42 |
| 1:13:1157:A:C6 | 1:13:1180:A:C4 | 3.07 | 0.42 |
| 1:13:1196:U:N3 | 23:4K:23:A:H8 | 2.17 | 0.42 |
| 1:13:1269:A:H2 | 1:13:1312:G:N3 | 2.17 | 0.42 |
| 2:1E:223:ILE:H | 2:1E:223:ILE:HG13 | 1.48 | 0.42 |
| 11:2I:15:ALA:O | 11:2I:78:GLN:N | 2.47 | 0.42 |
| 12:3I:58:VAL:O | 12:3I:65:GLU:HA | 2.19 | 0.42 |
| 17:8I:70:ARG:C | 17:8I:71:PHE:HD1 | 2.27 | 0.42 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 24:1H:174:C:H2' | 24:1H:175:G:O4' | 2.20 | 0.42 |
| 24:1H:320:A:H4' | 24:1H:322:A:C8 | 2.55 | 0.42 |
| 24:1H:869:G:H2' | 24:1H:870:A:O4' | 2.19 | 0.42 |
| 24:1H:1538:G:H2' | 24:1H:1539:G:C8 | 2.51 | 0.42 |
| 24:1H:1959:G:H2' | 24:1H:1960:A:O4' | 2.18 | 0.42 |
| 24:1H:2082:A:H2' | 24:1H:2083:G:O4' | 2.19 | 0.42 |
| 24:1H:2404:C:H3' | 24:1H:2405:G:H8 | 1.85 | 0.42 |
| 24:1H:2467:C:H4' | 36:88:123:HIS:CG | 2.53 | 0.42 |
| 24:1H:2637:U:C4 | 24:1H:2638:G:C6 | 3.08 | 0.42 |
| 24:1H:2766:G:H2' | 24:1H:2766:G:N3 | 2.35 | 0.42 |
| 24:1H:2789:C:H4' | 24:1H:2789:C:OP1 | 2.19 | 0.42 |
| 28:21:144:ARG:HB3 | 28:21:145:LYS:H | 1.32 | 0.42 |
| 32:61:118:LYS:HA | 32:61:119:PRO:HD3 | 1.85 | 0.42 |
| 33:58:94:HIS:C | 33:58:95:PRO:O | 2.62 | 0.42 |
| 38:A8:41:ASP:OD1 | 38:A8:44:LYS:HB2 | 2.19 | 0.42 |
| 46:I8:5:LYS:HG3 | 46:I8:6:GLY:N | 2.35 | 0.42 |
| 48:K8:17:SER:HB2 | 48:K8:20:GLU:HG3 | 2.00 | 0.42 |
| 51:N8:40:LYS:HG3 | 51:N8:47:PRO:HD2 | 2.01 | 0.42 |
| 54:Q8:36:LYS:HG2 | 54:Q8:37:SER:N | 2.33 | 0.42 |
| 1:1G:500:G:H2' | 1:1G:501:C:C6 | 2.55 | 0.42 |
| 1:1G:690:G:O4' | 1:1G:690:G:N3 | 2.53 | 0.42 |
| 1:1G:803:G:C6 | 1:1G:804:U:N3 | 2.88 | 0.42 |
| 1:1G:1068:G:N3 | 1:1G:1191:A:C2 | 2.88 | 0.42 |
| 1:1G:1193:G:H2' | 1:1G:1194:U:H5' | 2.02 | 0.42 |
| 4:32:38:TYR:CE2 | 4:32:45:GLN:HB3 | 2.54 | 0.42 |
| 5:42:126:ARG:HH11 | 5:42:126:ARG:CG | 2.23 | 0.42 |
| 9:82:46:ALA:HB1 | 9:82:77:ILE:CD1 | 2.47 | 0.42 |
| 16:7A:19:ILE:H | 16:7A:19:ILE:HG13 | 1.69 | 0.42 |
| 19:AA:40:ILE:HG13 | 19:AA:68:GLY:N | 2.30 | 0.42 |
| 24:14:128:C:H2' | 24:14:129:C:O4' | 2.19 | 0.42 |
| 24:14:250:G:H2' | 24:14:251:A:C8 | 2.55 | 0.42 |
| 24:14:513:A:N1 | 24:14:514:A:C5 | 2.88 | 0.42 |
| 24:14:566:U:H2' | 24:14:567:A:O4' | 2.20 | 0.42 |
| 24:14:572:A:OP2 | 41:95:78:LYS:HE2 | 2.20 | 0.42 |
| 24:14:768:G:H5' | 24:14:1622:G:H4' | 2.02 | 0.42 |
| 24:14:774:A:H2 | 24:14:787:U:O2' | 2.02 | 0.42 |
| 24:14:975:G:H1' | 24:14:990:A:C2 | 2.55 | 0.42 |
| 24:14:2162:G:H2' | 24:14:2163:C:C6 | 2.54 | 0.42 |
| 24:14:2271:G:H5" | 46:E5:20:ARG:NE | 2.34 | 0.42 |
| 24:14:2370:G:H21 | 52:K5:45:LYS:HZ2 | 1.66 | 0.42 |
| 24:14:2371:G:H1' | 52:K5:45:LYS:HG2 | 2.02 | 0.42 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 24:14:2572:A:C8 | 28:29:144:ARG:HD2 | 2.54 | 0.42 |
| 25:1J:70:C:H2' | 25:1J:71:C:H6 | 1.85 | 0.42 |
| 27:19:72:LYS:HG3 | 27:19:103:ARG:NH2 | 2.35 | 0.42 |
| 27:19:146:GLU:HA | 27:19:153:ALA:HA | 2.02 | 0.42 |
| 28:29:62:PRO:O | 28:29:63:LEU:HD12 | 2.20 | 0.42 |
| 30:49:8:LYS:O | 30:49:12:TYR:HD1 | 2.03 | 0.42 |
| 30:49:82:LEU:HD21 | 30:49:88:ILE:HG21 | 2.01 | 0.42 |
| 33:15:73:THR:HG22 | 33:15:84:LYS:HG2 | 2.01 | 0.42 |
| 34:25:13:ASN:HD21 | 34:25:96:THR:HB | 1.83 | 0.42 |
| 37:55:104:ARG:NH1 | 37:55:107:ASP:OD2 | 2.45 | 0.42 |
| 38:65:6:ALA:HA | 38:65:9:ARG:NH1 | 2.35 | 0.42 |
| 39:75:128:GLU:O | 39:75:132:LYS:HD3 | 2.19 | 0.42 |
| 42:A5:41:LYS:HD2 | 51:J5:25:LEU:HD21 | 2.01 | 0.42 |
| 45:D5:100:VAL:O | 45:D5:124:ILE:HG22 | 2.18 | 0.42 |
| 45:D5:178:GLU:H | 45:D5:178:GLU:HG2 | 1.52 | 0.42 |
| 48:G5:15:LYS:HD2 | 48:G5:67:LYS:NZ | 2.34 | 0.42 |
| 50:I5:14:ILE:HG22 | 50:I5:20:ASN:CB | 2.50 | 0.42 |
| 1:13:127:G:O2' | 17:8I:2:PRO:O | 2.38 | 0.42 |
| 1:13:439:A:H2' | 1:13:440:A:O4' | 2.20 | 0.42 |
| 1:13:628:G:O2' | 1:13:629:G:H5' | 2.20 | 0.42 |
| 1:13:1127:G:H21 | 1:13:1147:C:N4 | 2.18 | 0.42 |
| 1:13:1218:C:OP1 | 14:5I:9:LYS:HE2 | 2.19 | 0.42 |
| 2:1E:188:ALA:O | 2:1E:203:GLY:N | 2.53 | 0.42 |
| 3:2E:91:LEU:HD12 | 3:2E:91:LEU:H | 1.84 | 0.42 |
| 5:4E:121:LYS:HA | 5:4E:121:LYS:HD2 | 1.67 | 0.42 |
| 9:8E:53:VAL:HB | 9:8E:95:LYS:HD3 | 2.01 | 0.42 |
| 13:4I:16:ASP:OD1 | 13:4I:16:ASP:N | 2.49 | 0.42 |
| 19:AI:38:SER:OG | 19:AI:71:LEU:HD13 | 2.19 | 0.42 |
| 22:2K:81:C:C4 | 22:2K:82:A:N7 | 2.88 | 0.42 |
| 24:1H:251:A:C5 | 24:1H:252:G:H1' | 2.55 | 0.42 |
| 24:1H:270(M):U:HO2' | 24:1H:270(N):G:P | 2.42 | 0.42 |
| 24:1H:373:U:H2' | 24:1H:374:A:H8 | 1.84 | 0.42 |
| 24:1H:475:U:C4 | 24:1H:481:G:O6 | 2.73 | 0.42 |
| 24:1H:654(A):A:C2 | 24:1H:654(T):A:N1 | 2.87 | 0.42 |
| 24:1H:654(N):G:C2 | 24:1H:654(O):G:C5 | 3.07 | 0.42 |
| 24:1H:1062:G:P | 24:1H:1062:G:H8 | 2.43 | 0.42 |
| 24:1H:1299:G:H3' | 24:1H:1639:U:O4 | 2.20 | 0.42 |
| 24:1H:1692:U:H2' | 24:1H:1694:C:C5 | 2.55 | 0.42 |
| 24:1H:1858:G:H1' | 24:1H:1884:A:N6 | 2.35 | 0.42 |
| 24:1H:1899:G:HO2' | 24:1H:1900:A:P | 2.40 | 0.42 |
| 24:1H:2119:A:C6 | 24:1H:2170:A:N6 | 2.87 | 0.42 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 24:1H:2749:A:H5" | 31:51:6:ARG:HD3 | 2.00 | 0.42 |
| 35:78:107:LYS:HD2 | 35:78:107:LYS:HA | 1.86 | 0.42 |
| 36:88:30:GLY:HA2 | 36:88:107:ALA:HB2 | 2.00 | 0.42 |
| 45:H8:67:LEU:O | 45:H8:69:THR:HG23 | 2.20 | 0.42 |
| 50:M8:38:LYS:HA | 50:M8:38:LYS:HD2 | 1.72 | 0.42 |
| 54:Q8:9:GLY:O | 54:Q8:13:ARG:HB2 | 2.19 | 0.42 |
| 54:Q8:28:GLY:O | 54:Q8:29:LYS:C | 2.62 | 0.42 |
| 1:1G:599:C:H4' | 8:72:130:GLY:C | 2.44 | 0.42 |
| 1:1G:1257:U:H6 | 1:1G:1257:U:OP1 | 2.01 | 0.42 |
| 1:1G:1318:A:H1' | 19:AA:37:ARG:HH21 | 1.85 | 0.42 |
| 5:42:63:ARG:HA | 5:42:66:MET:CE | 2.50 | 0.42 |
| 8:72:10:LEU:HD22 | 8:72:83:ILE:HD11 | 2.01 | 0.42 |
| 10:1A:4:ILE:HD13 | 10:1A:4:ILE:HA | 1.85 | 0.42 |
| 16:7A:25:ARG:HG3 | 16:7A:25:ARG:NH1 | 2.32 | 0.42 |
| 24:14:270(R):G:OP1 | 32:69:42:SER:OG | 2.36 | 0.42 |
| 24:14:373:U:H2' | 24:14:374:A:C8 | 2.51 | 0.42 |
| 24:14:450:G:P | 57:14:3589:HOH:O | 2.77 | 0.42 |
| 24:14:765:G:H2' | 24:14:766:C:C6 | 2.54 | 0.42 |
| 24:14:1349:A:N6 | 24:14:1598:C:H42 | 2.17 | 0.42 |
| 24:14:1786:A:H1' | 24:14:1938:A:N6 | 2.34 | 0.42 |
| 24:14:2130:U:C2 | 24:14:2158:A:C2 | 3.08 | 0.42 |
| 27:19:41:GLY:C | 27:19:43:ARG:H | 2.28 | 0.42 |
| 28:29:11:MET:HE2 | 28:29:24:THR:OG1 | 2.20 | 0.42 |
| 30:49:43:LEU:O | 30:49:88:ILE:HG13 | 2.19 | 0.42 |
| 31:59:9:ILE:H | 31:59:9:ILE:HG12 | 1.59 | 0.42 |
| 40:85:92:ARG:C | 40:85:94:ASN:N | 2.78 | 0.42 |
| 42:A5:24:ILE:O | 42:A5:71:VAL:HG21 | 2.20 | 0.42 |
| 52:K5:9:LEU:N | 52:K5:27:LYS:HG3 | 2.33 | 0.42 |
| 1:13:712:A:O2' | 1:13:713:G:H5' | 2.20 | 0.42 |
| 1:13:721:G:H4' | 1:13:722:A:O5' | 2.20 | 0.42 |
| 1:13:1005:A:N1 | 1:13:1024:G:O2' | 2.44 | 0.42 |
| 1:13:1118:C:P | 9:8E:104:ARG:HH11 | 2.43 | 0.42 |
| 2:1E:21:ARG:HG3 | 2:1E:38:GLY:O | 2.20 | 0.42 |
| 2:1E:68:ILE:HG22 | 2:1E:70:PHE:CE1 | 2.55 | 0.42 |
| 8:7E:120:THR:OG1 | 8:7E:123:GLU:HG3 | 2.20 | 0.42 |
| 13:4I:50:GLU:OE2 | 13:4I:50:GLU:N | 2.35 | 0.42 |
| 16:7I:21:VAL:O | 16:7I:33:ILE:N | 2.41 | 0.42 |
| 20:BI:39:LYS:HB2 | 20:BI:55:ILE:HG21 | 2.02 | 0.42 |
| 24:1H:1266:G:OP2 | 51:N8:20:ARG:NE | 2.37 | 0.42 |
| 24:1H:1796:U:H2' | 24:1H:1797:C:C6 | 2.55 | 0.42 |
| 24:1H:1933:G:N2 | 24:1H:1968:G:H1' | 2.35 | 0.42 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 24:1H:2286:A:O2' | 52:O8:31:PRO:HG3 | 2.20 | 0.42 |
| 24:1H:2601:C:H2' | 24:1H:2603:G:C8 | 2.55 | 0.42 |
| 27:11:206:LEU:O | 27:11:211:ARG:HD3 | 2.20 | 0.42 |
| 28:21:117:MET:HB2 | 28:21:122:PHE:O | 2.19 | 0.42 |
| 35:78:91:PHE:HE2 | 35:78:99:LEU:HD11 | 1.85 | 0.42 |
| 36:88:20:ALA:CB | 36:88:99:PRO:HD2 | 2.49 | 0.42 |
| 38:A8:34:HIS:HB2 | 38:A8:36:TYR:HE1 | 1.84 | 0.42 |
| 42:E8:20:VAL:HG21 | 42:E8:44:ALA:HA | 2.02 | 0.42 |
| 42:E8:41:LYS:HE3 | 51:N8:25:LEU:HD21 | 2.02 | 0.42 |
| 45:H8:14:LYS:C | 45:H8:16:SER:N | 2.77 | 0.42 |
| 46:I8:19:LYS:C | 46:I8:20:ARG:HG2 | 2.43 | 0.42 |
| 1:1G:524:G:H2' | 1:1G:525:C:C6 | 2.54 | 0.42 |
| 1:1G:590:C:C4 | 1:1G:591:U:C5 | 3.08 | 0.42 |
| 1:1G:612:C:O2 | 1:1G:629:G:N2 | 2.52 | 0.42 |
| 1:1G:613:C:C2 | 1:1G:628:G:N2 | 2.87 | 0.42 |
| 1:1G:969:A:H2' | 1:1G:970:C:O4' | 2.20 | 0.42 |
| 1:1G:1126:U:O4 | 1:1G:1281:U:C6 | 2.73 | 0.42 |
| 2:12:119:GLU:HG3 | 2:12:142:LEU:HD11 | 2.01 | 0.42 |
| 2:12:185:ILE:HA | 2:12:199:TYR:O | 2.20 | 0.42 |
| 2:12:231:GLU:CD | 2:12:232:PRO:HD2 | 2.45 | 0.42 |
| 24:14:76:C:O3' | 48:G5:59:ARG:HG3 | 2.19 | 0.42 |
| 24:14:270(E):G:H2' | 24:14:270(F):U:O4' | 2.20 | 0.42 |
| 24:14:470:A:H2' | 24:14:471:A:O4' | 2.18 | 0.42 |
| 24:14:759:G:O2' | 24:14:760:G:H5' | 2.20 | 0.42 |
| 24:14:835:A:C2' | 24:14:836:G:H5' | 2.49 | 0.42 |
| 24:14:921:G:C6 | 24:14:922:U:C4 | 3.07 | 0.42 |
| 24:14:1005:C:H2' | 24:14:1006:C:C6 | 2.54 | 0.42 |
| 24:14:1156:A:N7 | 40:85:51:LYS:HG2 | 2.35 | 0.42 |
| 24:14:1508:A:H4' | 24:14:1510:A:C2 | 2.55 | 0.42 |
| 24:14:1665:A:H4' | 34:25:67:LYS:HB2 | 2.01 | 0.42 |
| 24:14:2213:U:H4' | 47:F5:52:ARG:CZ | 2.50 | 0.42 |
| 24:14:2238:G:H2' | 24:14:2238:G:N3 | 2.34 | 0.42 |
| 24:14:2337:G:H5" | 24:14:2338:G:OP2 | 2.20 | 0.42 |
| 24:14:2726:U:H4' | 34:25:1:MET:HE1 | 2.02 | 0.42 |
| 24:14:2885:C:N3 | 24:14:2886:G:H1' | 2.34 | 0.42 |
| 27:19:55:GLY:O | 27:19:216:GLY:HA2 | 2.18 | 0.42 |
| 27:19:177:LEU:HB3 | 27:19:178:PRO:HD2 | 2.01 | 0.42 |
| 29:39:13:SER:HA | 29:39:14:PRO:HD3 | 1.72 | 0.42 |
| 29:39:130:ALA:H | 29:39:142:TRP:HD1 | 1.68 | 0.42 |
| 32:69:61:ARG:O | 32:69:64:GLU:N | 2.52 | 0.42 |
| 36:45:14:ARG:HG2 | 36:45:41:TRP:CH2 | 2.50 | 0.42 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 37:55:60:LEU:O | 37:55:64:ARG:HG3 | 2.20 | 0.42 |
| 38:65:93:LYS:HE3 | 38:65:93:LYS:HB2 | 1.88 | 0.42 |
| 42:A5:68:ARG:O | 42:A5:110:LYS:N | 2.52 | 0.42 |
| 43:B5:18:TYR:C | 43:B5:20:GLY:N | 2.77 | 0.42 |
| 50:I5:14:ILE:HD13 | 50:I5:14:ILE:HA | 1.87 | 0.42 |
| 1:13:590:C:H2' | 1:13:591:U:H6 | 1.85 | 0.42 |
| 1:13:631:G:O2' | 1:13:632:A:O4' | 2.25 | 0.42 |
| 1:13:891:U:H2' | 1:13:892:A:H8 | 1.84 | 0.42 |
| 1:13:1393:U:H5' | 1:13:1502:A:OP1 | 2.20 | 0.42 |
| 5:4E:6:PHE:HZ | 5:4E:40:ARG:HH12 | 1.68 | 0.42 |
| 13:4I:46:LYS:HE3 | 13:4I:47:ASP:OD2 | 2.20 | 0.42 |
| 15:6I:11:VAL:O | 15:6I:15:PHE:HD2 | 2.03 | 0.42 |
| 17:8I:75:ARG:NH1 | 17:8I:77:VAL:HG22 | 2.35 | 0.42 |
| 22:2K:32:A:C5 | 22:2K:33:C:C5 | 3.08 | 0.42 |
| 22:3K:37:A:H61 | 22:3K:38:MIA:H162 | 1.85 | 0.42 |
| 24:1H:401:A:H2' | 24:1H:402:A:O4' | 2.20 | 0.42 |
| 24:1H:559:G:N2 | 40:C8:49:HIS:CE1 | 2.88 | 0.42 |
| 24:1H:796:C:H2' | 24:1H:797:C:H6 | 1.82 | 0.42 |
| 24:1H:1313:U:H2' | 24:1H:1610:A:C2 | 2.54 | 0.42 |
| 24:1H:1444:G:N2 | 24:1H:1548:C:C2 | 2.88 | 0.42 |
| 24:1H:1592:C:H2' | 24:1H:1593:G:H8 | 1.82 | 0.42 |
| 24:1H:1697:G:O2' | 24:1H:1978:A:OP1 | 2.27 | 0.42 |
| 24:1H:1792:G:H2' | 24:1H:1793:C:C6 | 2.55 | 0.42 |
| 24:1H:2068:U:N3 | 24:1H:2430:A:H2 | 2.11 | 0.42 |
| 24:1H:2437:U:H2' | 24:1H:2438:U:C6 | 2.55 | 0.42 |
| 24:1H:2861:G:H2' | 24:1H:2862:G:H8 | 1.85 | 0.42 |
| 27:11:98:VAL:C | 27:11:100:GLY:H | 2.27 | 0.42 |
| 30:41:138:GLN:O | 30:41:144:ILE:HG13 | 2.20 | 0.42 |
| 40:C8:85:LYS:NZ | 40:C8:117:GLN:HB2 | 2.34 | 0.42 |
| 42:E8:82:LEU:HD23 | 42:E8:84:ARG:NH2 | 2.35 | 0.42 |
| 50:M8:55:ARG:HD2 | 50:M8:55:ARG:HA | 1.59 | 0.42 |
| 53:P8:35:ARG:HG3 | 53:P8:42:LEU:HD11 | 2.02 | 0.42 |
| 1:1G:8:A:N6 | 4:32:209:ARG:HB2 | 2.35 | 0.42 |
| 1:1G:99:C:H2' | 1:1G:101:A:C8 | 2.54 | 0.42 |
| 1:1G:322:C:O3' | 20:BA:23:ARG:HG3 | 2.20 | 0.42 |
| 1:1G:449:C:O2 | 1:1G:449:C:O4' | 2.38 | 0.42 |
| 1:1G:540:G:C6 | 1:1G:541:G:C5 | 3.08 | 0.42 |
| 1:1G:1137:C:H5" | 1:1G:1138:G:OP1 | 2.20 | 0.42 |
| 1:1G:1349:A:C4 | 1:1G:1350:A:C8 | 3.08 | 0.42 |
| 2:12:44:LEU:H | 2:12:44:LEU:HG | 1.64 | 0.42 |
| 3:22:6:HIS:HD2 | 3:22:8:ILE:H | 1.67 | 0.42 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 4:32:165:MET:SD | 4:32:168:ARG:NH2 | 2.93 | 0.42 |
| 7:62:146:GLU:OE2 | 7:62:149:ARG:NH1 | 2.53 | 0.42 |
| 15:6A:21:ASP:OD2 | 15:6A:24:SER:OG | 2.35 | 0.42 |
| 19:AA:45:VAL:HA | 19:AA:62:ILE:HG22 | 2.01 | 0.42 |
| 24:14:270(E):G:C6 | 24:14:270(F):U:C4 | 3.07 | 0.42 |
| 24:14:971:C:H3' | 24:14:971:C:C6 | 2.55 | 0.42 |
| 24:14:996:A:C2 | 24:14:997:G:C8 | 3.08 | 0.42 |
| 24:14:1692:U:H2' | 24:14:1694:C:C5 | 2.55 | 0.42 |
| 24:14:2124:G:H5" | 24:14:2125:G:C8 | 2.55 | 0.42 |
| 24:14:2348:U:HO2' | 52:K5:42:TRP:CD1 | 2.38 | 0.42 |
| 24:14:2401:U:H2' | 24:14:2402:C:O4' | 2.19 | 0.42 |
| 24:14:2443:C:O2' | 24:14:2444:G:H5' | 2.20 | 0.42 |
| 24:14:2839:G:H5' | 37:55:46:GLY:HA2 | 2.00 | 0.42 |
| 25:1J:18:G:H2' | 25:1J:19:G:C8 | 2.54 | 0.42 |
| 28:29:29:GLY:HA2 | 28:29:180:ASN:ND2 | 2.34 | 0.42 |
| 29:39:7:TYR:CE1 | 29:39:16:GLY:HA3 | 2.55 | 0.42 |
| 32:69:123:LEU:HD23 | 32:69:123:LEU:HA | 1.89 | 0.42 |
| 33:15:58:ASP:OD1 | 33:15:58:ASP:N | 2.52 | 0.42 |
| 35:35:110:TYR:HB3 | 35:35:111:ARG:H | 1.66 | 0.42 |
| 39:75:133:GLU:O | 39:75:136:GLN:HG2 | 2.20 | 0.42 |
| 40:85:83:LEU:HD23 | 40:85:88:ILE:HB | 2.02 | 0.42 |
| 41:95:84:LYS:O | 41:95:85:LYS:C | 2.63 | 0.42 |
| 43:B5:44:GLU:HG2 | 43:B5:49:VAL:O | 2.20 | 0.42 |
| 44:C5:97:ARG:HD2 | 44:C5:104:GLY:H | 1.85 | 0.42 |
| 45:D5:133:ILE:O | 45:D5:135:GLU:N | 2.53 | 0.42 |
| 48:G5:16:LEU:HD12 | 48:G5:17:SER:HB3 | 2.00 | 0.42 |
| 1:13:375:U:C2 | 1:13:376:G:C8 | 3.07 | 0.42 |
| 1:13:878:G:H5' | 8:7E:89:PRO:HG2 | 2.02 | 0.42 |
| 1:13:926:G:H5" | 1:13:927:G:O5' | 2.18 | 0.42 |
| 1:13:954:G:C2 | 1:13:955:U:C2 | 3.08 | 0.42 |
| 1:13:1122:U:C4 | 1:13:1123:A:N7 | 2.88 | 0.42 |
| 1:13:1147:C:O2' | 9:8E:16:ARG:HD2 | 2.20 | 0.42 |
| 1:13:1230:C:H2' | 1:13:1231:G:C8 | 2.54 | 0.42 |
| 1:13:1327:C:P | 21:1F:12:LYS:HZ1 | 2.43 | 0.42 |
| 2:1E:69:LEU:HD12 | 2:1E:70:PHE:N | 2.32 | 0.42 |
| 3:2E:12:LEU:O | 3:2E:14:ILE:N | 2.53 | 0.42 |
| 5:4E:19:MET:HB3 | 5:4E:19:MET:HE2 | 1.50 | 0.42 |
| 10:1I:49:VAL:CG2 | 14:5I:41:ARG:HB2 | 2.48 | 0.42 |
| 11:2I:73:MET:SD | 11:2I:102:GLY:HA3 | 2.60 | 0.42 |
| 12:3I:20:LYS:HE2 | 12:3I:20:LYS:HB3 | 1.78 | 0.42 |
| 12:3I:84:LEU:HD23 | 12:3I:101:VAL:HG21 | 2.01 | 0.42 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 20:BI:76:ALA:O | 20:BI:80:ARG:HG2 | 2.20 | 0.42 |
| 22:2K:81:C:N3 | 22:2K:82:A:N7 | 2.68 | 0.42 |
| 22:3K:7:G:OP2 | 22:3K:7:G:H8 | 2.03 | 0.42 |
| 24:1H:7:G:H2' | 24:1H:8:A:O4' | 2.20 | 0.42 |
| 24:1H:818:G:H4' | 24:1H:838:C:O3' | 2.20 | 0.42 |
| 24:1H:926:A:N3 | 24:1H:926:A:H2' | 2.34 | 0.42 |
| 24:1H:1174:A:N6 | 24:1H:1175:U:H5 | 2.18 | 0.42 |
| 24:1H:1299:G:H5" | 24:1H:1300:U:OP1 | 2.20 | 0.42 |
| 24:1H:1418:G:H2' | 24:1H:1579:A:N6 | 2.34 | 0.42 |
| 24:1H:1453:A:O2' | 24:1H:1454:U:H2' | 2.19 | 0.42 |
| 24:1H:1568:G:P | 27:11:63:ARG:HH12 | 2.43 | 0.42 |
| 24:1H:1997:G:P | 57:1H:3620:HOH:O | 2.68 | 0.42 |
| 24:1H:2064:C:H2' | 24:1H:2065:C:C6 | 2.54 | 0.42 |
| 24:1H:2788:C:H5' | 28:21:61:ARG:HH22 | 1.85 | 0.42 |
| 27:11:70:TRP:CZ3 | 27:11:146:GLU:OE2 | 2.68 | 0.42 |
| 27:11:108:PRO:HD2 | 27:11:111:LEU:HG | 2.01 | 0.42 |
| 27:11:240:ALA:HA | 27:11:241:PRO:HD2 | 1.67 | 0.42 |
| 30:41:10:LYS:O | 30:41:15:VAL:HG23 | 2.20 | 0.42 |
| 30:41:138:GLN:OE1 | 30:41:153:ARG:N | 2.32 | 0.42 |
| 31:51:8:PRO:HD2 | 31:51:69:ARG:NE | 2.28 | 0.42 |
| 31:51:126:PRO:HB2 | 31:51:130:ARG:HH12 | 1.84 | 0.42 |
| 37:98:20:LEU:HD21 | 37:98:40:LYS:CD | 2.50 | 0.42 |
| 44:G8:88:LYS:HA | 44:G8:88:LYS:HD3 | 1.84 | 0.42 |
| 48:K8:18:PRO:O | 48:K8:21:LEU:HB2 | 2.20 | 0.42 |
| 50:M8:21:VAL:HG12 | 50:M8:23:GLU:H | 1.85 | 0.42 |
| 1:1G:522:C:H2' | 1:1G:523:A:O4' | 2.20 | 0.42 |
| 1:1G:553:A:H2' | 1:1G:554:C:C6 | 2.55 | 0.42 |
| 1:1G:1216:G:H5" | 14:5A:5:ALA:CB | 2.49 | 0.42 |
| 2:12:97:TRP:HZ2 | 2:12:102:LEU:HD13 | 1.83 | 0.42 |
| 17:8A:59:ILE:HD13 | 17:8A:73:VAL:HA | 2.02 | 0.42 |
| 24:14:85:G:C5 | 24:14:98:G:C2 | 3.08 | 0.42 |
| 24:14:601:C:O2' | 24:14:605:C:H5" | 2.20 | 0.42 |
| 24:14:720:C:H2' | 24:14:721:C:C6 | 2.55 | 0.42 |
| 24:14:1003:G:N2 | 24:14:1153:C:C2 | 2.88 | 0.42 |
| 24:14:1444:G:C2 | 24:14:1548:C:C2 | 3.07 | 0.42 |
| 24:14:1794:U:H1' | 24:14:1900:A:N3 | 2.34 | 0.42 |
| 24:14:2319:G:C2 | 24:14:2320:A:N1 | 2.88 | 0.42 |
| 24:14:2332:U:H5' | 24:14:2336:A:N6 | 2.35 | 0.42 |
| 24:14:2332:U:O2' | 24:14:2335:A:N3 | 2.46 | 0.42 |
| 24:14:2409:G:C6 | 24:14:2410:G:C5 | 3.08 | 0.42 |
| 24:14:2591:C:P | 27:19:239:ARG:HG3 | 2.59 | 0.42 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 24:14:2846:G:OP1 | 39:75:54:ARG:HG3 | 2.20 | 0.42 |
| 25:1J:21:G:H2' | 25:1J:22:U:O4' | 2.19 | 0.42 |
| 31:59:67:LEU:O | 31:59:71:LEU:N | 2.53 | 0.42 |
| 38:65:29:PHE:CD1 | 38:65:30:ARG:N | 2.87 | 0.42 |
| 43:B5:48:LYS:HE2 | 43:B5:48:LYS:HB2 | 1.88 | 0.42 |
| 44:C5:28:LYS:HE3 | 44:C5:64:GLU:OE2 | 2.19 | 0.42 |
| 53:L5:12:ARG:HH21 | 53:L5:44:PRO:HB3 | 1.80 | 0.42 |
| 1:13:186(C):G:C6 | 1:13:186(D):C:C4 | 3.08 | 0.41 |
| 1:13:942:G:C2 | 1:13:1342:C:C2 | 3.09 | 0.41 |
| 1:13:984:C:H42 | 1:13:1221:G:H1 | 1.67 | 0.41 |
| 1:13:1240:U:OP2 | 7:6E:116:ALA:N | 2.34 | 0.41 |
| 1:13:1357:A:C5 | 1:13:1358:U:C5 | 3.08 | 0.41 |
| 2:1E:30:ARG:HB2 | 2:1E:46:LYS:NZ | 2.34 | 0.41 |
| 2:1E:208:ILE:HA | 2:1E:211:ILE:HD12 | 2.02 | 0.41 |
| 3:2E:5:ILE:HG13 | 3:2E:6:HIS:N | 2.35 | 0.41 |
| 3:2E:13:GLY:HA2 | 14:5I:57:ARG:HH21 | 1.85 | 0.41 |
| 3:2E:121:ALA:O | 3:2E:125:GLU:HG3 | 2.20 | 0.41 |
| 3:2E:173:VAL:O | 3:2E:175:LEU:HD12 | 2.20 | 0.41 |
| 6:5E:97:PHE:N | 18:9I:30:ASP:OD1 | 2.47 | 0.41 |
| 7:6E:44:TYR:O | 7:6E:48:LYS:HG3 | 2.20 | 0.41 |
| 17:8I:90:ILE:HG13 | 17:8I:90:ILE:H | 1.64 | 0.41 |
| 19:AI:64:GLU:H | 19:AI:64:GLU:HG3 | 1.62 | 0.41 |
| 24:1H:27:G:O2' | 24:1H:28:A:OP2 | 2.35 | 0.41 |
| 24:1H:289:A:H2' | 24:1H:290:G:O4' | 2.20 | 0.41 |
| 24:1H:483:A:O4' | 44:G8:48:ALA:HB1 | 2.20 | 0.41 |
| 24:1H:598:G:C1' | 35:78:12:ALA:HB2 | 2.50 | 0.41 |
| 24:1H:832:G:N7 | 57:1H:3768:HOH:O | 2.37 | 0.41 |
| 24:1H:1263:U:O2' | 24:1H:1264:G:H5' | 2.19 | 0.41 |
| 24:1H:1591:G:H2' | 24:1H:1592:C:C6 | 2.54 | 0.41 |
| 24:1H:1999:C:OP1 | 24:1H:2723:C:O2' | 2.34 | 0.41 |
| 24:1H:2123:G:H3' | 24:1H:2124:G:C8 | 2.55 | 0.41 |
| 24:1H:2356:C:C5 | 24:1H:2357:U:C4 | 3.08 | 0.41 |
| 24:1H:2693:A:H2' | 24:1H:2694:G:H8 | 1.85 | 0.41 |
| 25:16:60:C:H6 | 25:16:60:C:O5' | 2.03 | 0.41 |
| 28:21:101:ARG:NH1 | 28:21:171:GLU:HB2 | 2.35 | 0.41 |
| 30:41:37:VAL:HG13 | 30:41:158:ALA:O | 2.20 | 0.41 |
| 31:51:56:SER:HB3 | 31:51:61:HIS:ND1 | 2.34 | 0.41 |
| 33:58:47:ALA:HB2 | 33:58:112:LEU:CD1 | 2.48 | 0.41 |
| 35:78:19:VAL:HA | 35:78:20:GLY:HA3 | 1.83 | 0.41 |
| 35:78:144:GLU:N | 35:78:144:GLU:CD | 2.78 | 0.41 |
| 37:98:9:LYS:HA | 37:98:17:ARG:CD | 2.50 | 0.41 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 42:E8:80:PRO:O | 42:E8:100:THR:HB | 2.19 | 0.41 |
| 51:N8:31:VAL:HG13 | 51:N8:42:PRO:HG3 | 2.01 | 0.41 |
| 1:1G:160:A:N6 | 1:1G:347:G:H1' | 2.35 | 0.41 |
| 1:1G:246:A:OP1 | 17:8A:100:LYS:NZ | 2.53 | 0.41 |
| 1:1G:692:U:H2' | 1:1G:693:G:H3' | 2.02 | 0.41 |
| 1:1G:1004:A:N3 | 1:1G:1024:G:H1' | 2.35 | 0.41 |
| 1:1G:1106:G:H2' | 1:1G:1107:C:C6 | 2.55 | 0.41 |
| 1:1G:1368:G:N2 | 1:1G:1369:C:H1' | 2.35 | 0.41 |
| 2:12:237:ALA:C | 2:12:239:VAL:N | 2.77 | 0.41 |
| 3:22:94:LEU:H | 3:22:94:LEU:HD12 | 1.85 | 0.41 |
| 4:32:173:TRP:NE1 | 4:32:174:LEU:HG | 2.34 | 0.41 |
| 5:42:63:ARG:HA | 5:42:66:MET:HE1 | 2.01 | 0.41 |
| 9:82:117:HIS:NE2 | 9:82:123:PRO:HB3 | 2.35 | 0.41 |
| 10:1A:38:ILE:HA | 10:1A:39:PRO:HD3 | 1.87 | 0.41 |
| 19:AA:40:ILE:H | 19:AA:40:ILE:HG12 | 1.63 | 0.41 |
| 19:AA:66:MET:HA | 19:AA:67:VAL:C | 2.45 | 0.41 |
| 24:14:460:A:H2' | 24:14:461:C:O4' | 2.19 | 0.41 |
| 24:14:859:G:H5' | 24:14:2268:A:O2' | 2.19 | 0.41 |
| 24:14:999:U:H5 | 24:14:1154:G:N7 | 2.18 | 0.41 |
| 24:14:1126:A:H4' | 24:14:1127:A:O5' | 2.20 | 0.41 |
| 24:14:1175:U:OP2 | 24:14:1175:U:H4' | 2.20 | 0.41 |
| 24:14:1324:G:H4' | 24:14:1616:A:C2 | 2.55 | 0.41 |
| 24:14:1420:U:O2' | 24:14:1421:G:OP1 | 2.33 | 0.41 |
| 24:14:1728:G:H5' | 24:14:1729:A:OP2 | 2.20 | 0.41 |
| 24:14:2150:U:O5' | 24:14:2150:U:H6 | 2.03 | 0.41 |
| 24:14:2628:C:H1' | 24:14:2781:A:H2' | 2.01 | 0.41 |
| 24:14:2660:A:H2' | 24:14:2661:G:O4' | 2.20 | 0.41 |
| 24:14:2811:G:N2 | 24:14:2891:G:H1' | 2.35 | 0.41 |
| 25:1J:93:C:H2' | 25:1J:94:C:C6 | 2.55 | 0.41 |
| 27:19:70:TRP:O | 27:19:73:VAL:HG23 | 2.20 | 0.41 |
| 29:39:63:LYS:HG3 | 29:39:65:TRP:O | 2.19 | 0.41 |
| 30:49:29:TRP:HE3 | 30:49:33:ARG:CZ | 2.33 | 0.41 |
| 31:59:35:VAL:HB | 31:59:71:LEU:HD21 | 2.02 | 0.41 |
| 31:59:153:LYS:O | 31:59:161:GLY:HA3 | 2.20 | 0.41 |
| 35:35:80:TYR:CD2 | 35:35:111:ARG:HB3 | 2.55 | 0.41 |
| 36:45:77:LYS:HA | 36:45:78:PRO:HD3 | 1.90 | 0.41 |
| 41:95:72:VAL:HB | 41:95:85:LYS:CB | 2.49 | 0.41 |
| 47:F5:52:ARG:HH11 | 47:F5:57:GLU:HG3 | 1.85 | 0.41 |
| 52:K5:18:ARG:HB3 | 52:K5:19:ARG:H | 1.47 | 0.41 |
| 1:13:221:C:H2' | 1:13:222:U:C6 | 2.55 | 0.41 |
| 1:13:596:C:H2' | 1:13:597:G:H8 | 1.84 | 0.41 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 1:13:622:A:N7 | 1:13:623:C:C2 | 2.88 | 0.41 |
| 1:13:703:G:O5' | 1:13:703:G:C8 | 2.73 | 0.41 |
| 1:13:1251:A:H5' | 9:8E:12:GLU:HB3 | 2.01 | 0.41 |
| 1:13:1321:C:C3' | 1:13:1322:C:H5" | 2.47 | 0.41 |
| 1:13:1324:A:O4' | 1:13:1362:C:H4' | 2.20 | 0.41 |
| 1:13:1405:G:O4' | 1:13:1519:A:H4' | 2.21 | 0.41 |
| 3:2E:90:GLU:HA | 3:2E:93:LYS:HG3 | 2.02 | 0.41 |
| 4:3E:57:ARG:HB3 | 4:3E:206:PHE:HB2 | 2.01 | 0.41 |
| 7:6E:26:PHE:CD2 | 7:6E:30:ILE:HD11 | 2.55 | 0.41 |
| 8:7E:20:TYR:HD1 | 8:7E:65:TYR:CD2 | 2.38 | 0.41 |
| 8:7E:25:ASP:OD2 | 8:7E:60:ARG:HG3 | 2.20 | 0.41 |
| 9:8E:28:VAL:HG22 | 9:8E:63:ILE:HB | 2.01 | 0.41 |
| 10:1I:48:THR:HG23 | 10:1I:62:HIS:CD2 | 2.55 | 0.41 |
| 10:1I:78:ASN:OD1 | 10:1I:78:ASN:N | 2.51 | 0.41 |
| 11:2I:99:GLN:H | 11:2I:99:GLN:HG2 | 1.52 | 0.41 |
| 12:3I:113:ARG:HH11 | 12:3I:113:ARG:HD2 | 1.74 | 0.41 |
| 14:5I:21:TYR:HE2 | 14:5I:23:ARG:NE | 2.18 | 0.41 |
| 18:9I:25:THR:HB | 18:9I:42:ARG:NH1 | 2.35 | 0.41 |
| 18:9I:54:ARG:HG2 | 18:9I:55:ARG:N | 2.35 | 0.41 |
| 22:3K:85:A:O2' | 24:1H:2394:C:O2 | 2.38 | 0.41 |
| 24:1H:270(G):C:N4 | 57:1H:3849:HOH:O | 2.52 | 0.41 |
| 24:1H:661:C:H4' | 35:78:13:ASN:OD1 | 2.20 | 0.41 |
| 24:1H:825:C:H4' | 24:1H:2428:G:C5 | 2.55 | 0.41 |
| 24:1H:1062:G:H8 | 24:1H:1062:G:OP1 | 2.03 | 0.41 |
| 24:1H:1814:G:H4' | 27:11:51:VAL:HG21 | 2.01 | 0.41 |
| 24:1H:2019:A:C2' | 24:1H:2020:A:O5' | 2.68 | 0.41 |
| 24:1H:2199:A:H3' | 24:1H:2205:C:H6 | 1.84 | 0.41 |
| 24:1H:2402:C:C6 | 24:1H:2402:C:C3' | 3.02 | 0.41 |
| 24:1H:2807:G:H3' | 24:1H:2808:U:H5" | 2.02 | 0.41 |
| 24:1H:2825:C:O5' | 24:1H:2825:C:H6 | 2.03 | 0.41 |
| 28:21:78:LEU:HD21 | 28:21:79:ARG:HD2 | 2.02 | 0.41 |
| 29:31:101:LEU:HD12 | 29:31:101:LEU:HA | 1.54 | 0.41 |
| 32:61:29:TYR:CE1 | 32:61:33:ARG:CZ | 3.02 | 0.41 |
| 32:61:87:LYS:HB2 | 32:61:87:LYS:HE3 | 1.81 | 0.41 |
| 32:61:129:THR:HA | 32:61:137:PRO:HA | 2.02 | 0.41 |
| 33:58:90:MET:O | 33:58:94:HIS:N | 2.53 | 0.41 |
| 37:98:52:ILE:HB | 37:98:94:TYR:HD2 | 1.85 | 0.41 |
| 45:H8:45:ASP:O | 45:H8:49:ARG:HG2 | 2.20 | 0.41 |
| 1:1G:137:C:O2' | 1:1G:138:G:H5' | 2.20 | 0.41 |
| 1:1G:555:C:H2' | 1:1G:556:C:C6 | 2.55 | 0.41 |
| 1:1G:811:C:H2' | 1:1G:812:C:H5' | 2.02 | 0.41 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 1:1G:981:U:O5' | 1:1G:981:U:H6 | 2.03 | 0.41 |
| 1:1G:1052:U:N3 | 1:1G:1200:C:N3 | 2.68 | 0.41 |
| 1:1G:1128:C:H5' | 9:82:16:ARG:HH22 | 1.85 | 0.41 |
| 1:1G:1190:G:OP1 | 3:22:5:ILE:HB | 2.21 | 0.41 |
| 1:1G:1329:A:H5' | 13:4A:29:ARG:HE | 1.85 | 0.41 |
| 3:22:18:TRP:NE1 | 14:5A:55:GLY:H | 2.18 | 0.41 |
| 4:32:68:TYR:OH | 4:32:98:GLU:OE1 | 2.33 | 0.41 |
| 4:32:88:VAL:O | 4:32:92:VAL:HG23 | 2.20 | 0.41 |
| 6:52:43:LEU:HD12 | 6:52:43:LEU:N | 2.35 | 0.41 |
| 7:62:69:VAL:HG11 | 7:62:134:ALA:HB1 | 2.02 | 0.41 |
| 13:4A:65:LYS:NZ | 13:4A:73:GLU:HG3 | 2.34 | 0.41 |
| 22:3L:57:C:H5" | 22:3L:59:A:P | 2.60 | 0.41 |
| 24:14:1336:A:C2 | 24:14:1337:G:C5 | 3.08 | 0.41 |
| 24:14:1386:C:C2 | 24:14:1387:C:C5 | 3.08 | 0.41 |
| 24:14:1572:A:H2' | 24:14:1573:G:O4' | 2.19 | 0.41 |
| 24:14:2598:A:OP1 | 57:14:3576:HOH:O | 2.21 | 0.41 |
| 24:14:2887:U:H2' | 24:14:2888:C:C6 | 2.55 | 0.41 |
| 29:39:170:LEU:HD13 | 29:39:172:TRP:CZ2 | 2.55 | 0.41 |
| 33:15:37:LYS:HG3 | 33:15:42:TRP:CZ3 | 2.55 | 0.41 |
| 34:25:34:THR:O | 34:25:37:ASP:HB2 | 2.20 | 0.41 |
| 35:35:15:ARG:HD3 | 35:35:15:ARG:HA | 1.52 | 0.41 |
| 38:65:107:GLU:O | 38:65:110:LEU:HG | 2.20 | 0.41 |
| 39:75:39:ARG:NH1 | 39:75:41:ARG:HD2 | 2.35 | 0.41 |
| 40:85:81:HIS:HE1 | 40:85:85:LYS:HE2 | 1.85 | 0.41 |
| 41:95:35:LEU:O | 41:95:37:VAL:HG13 | 2.21 | 0.41 |
| 48:G5:30:ARG:O | 48:G5:34:GLU:HG3 | 2.19 | 0.41 |
| 1:13:28:G:C6 | 1:13:29:G:N7 | 2.88 | 0.41 |
| 1:13:177:C:P | 20:BI:65:LYS:NZ | 2.93 | 0.41 |
| 1:13:621:A:H2' | 1:13:622:A:O4' | 2.19 | 0.41 |
| 1:13:691:G:C6 | 11:2I:52:GLY:HA2 | 2.55 | 0.41 |
| 1:13:1079:G:H2' | 1:13:1080:A:C8 | 2.55 | 0.41 |
| 1:13:1451:A:H3' | 1:13:1452:C:H5" | 2.01 | 0.41 |
| 3:2E:12:LEU:HD23 | 3:2E:12:LEU:HA | 1.78 | 0.41 |
| 3:2E:45:LYS:HB2 | 3:2E:45:LYS:NZ | 2.35 | 0.41 |
| 4:3E:19:LEU:HB3 | 4:3E:21:LEU:HD21 | 2.01 | 0.41 |
| 4:3E:126:ILE:HG22 | 4:3E:127:THR:N | 2.36 | 0.41 |
| 5:4E:130:ASN:O | 5:4E:134:ALA:HB2 | 2.20 | 0.41 |
| 9:8E:10:ARG:NH1 | 9:8E:105:ASP:OD2 | 2.53 | 0.41 |
| 13:4I:14:ARG:HG2 | 13:4I:16:ASP:OD1 | 2.20 | 0.41 |
| 24:1H:155:C:N4 | 24:1H:171:G:H1 | 2.19 | 0.41 |
| 24:1H:333:G:C8 | 24:1H:333:G:O5' | 2.74 | 0.41 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 24:1H:642:G:C8 | 24:1H:642:G:H3' | 2.55 | 0.41 |
| 24:1H:906:G:H5" | 36:88:26:TYR:HE1 | 1.83 | 0.41 |
| 24:1H:931:G:C4 | 24:1H:933:A:C8 | 3.08 | 0.41 |
| 24:1H:1153:C:C4 | 24:1H:1154:G:C5 | 3.08 | 0.41 |
| 24:1H:1281:G:H2' | 24:1H:1282:U:O4' | 2.20 | 0.41 |
| 24:1H:1448:G:O2' | 24:1H:1529:A:N1 | 2.38 | 0.41 |
| 24:1H:1530:G:C6 | 24:1H:1531:C:C4 | 3.08 | 0.41 |
| 24:1H:1565:C:O2' | 24:1H:1567:A:N7 | 2.35 | 0.41 |
| 24:1H:1894:C:O2' | 24:1H:1895:C:H5' | 2.20 | 0.41 |
| 24:1H:2019:A:C4' | 40:C8:34:LYS:HD2 | 2.50 | 0.41 |
| 24:1H:2335:A:C8 | 24:1H:2337:G:C5 | 3.08 | 0.41 |
| 24:1H:2371:G:C6 | 24:1H:2372:G:N7 | 2.89 | 0.41 |
| 24:1H:2615:U:C2 | 51:N8:7:PRO:HA | 2.55 | 0.41 |
| 24:1H:2629:A:O2' | 24:1H:2630:G:H5" | 2.20 | 0.41 |
| 24:1H:2877:G:O2' | 24:1H:2878:U:H5' | 2.20 | 0.41 |
| 29:31:120:GLU:HG3 | 29:31:122:LYS:HG2 | 2.02 | 0.41 |
| 30:41:64:THR:CG2 | 30:41:94:LEU:HD21 | 2.50 | 0.41 |
| 36:88:43:THR:O | 36:88:46:GLN:N | 2.51 | 0.41 |
| 41:D8:44:LYS:O | 41:D8:46:VAL:HG12 | 2.20 | 0.41 |
| 44:G8:5:MET:HE2 | 44:G8:5:MET:HB2 | 1.67 | 0.41 |
| 44:G8:33:LYS:HE2 | 44:G8:33:LYS:HB2 | 1.95 | 0.41 |
| 45:H8:92:SER:O | 45:H8:130:PRO:HG2 | 2.19 | 0.41 |
| 45:H8:108:PRO:C | 45:H8:110:GLY:H | 2.28 | 0.41 |
| 45:H8:149:SER:HA | 45:H8:172:ALA:O | 2.20 | 0.41 |
| 45:H8:154:ASP:OD1 | 45:H8:154:ASP:N | 2.46 | 0.41 |
| 49:L8:7:LYS:CG | 49:L8:34:GLU:HG3 | 2.49 | 0.41 |
| 1:1G:197:A:H8 | 1:1G:198:G:C1' | 2.33 | 0.41 |
| 1:1G:327:A:C5 | 1:1G:329:A:C5 | 3.07 | 0.41 |
| 1:1G:411:A:N7 | 1:1G:413:G:N3 | 2.69 | 0.41 |
| 1:1G:536:C:H2' | 1:1G:537:G:C8 | 2.55 | 0.41 |
| 1:1G:670:G:C6 | 1:1G:671:G:C5 | 3.08 | 0.41 |
| 1:1G:951:G:O2' | 1:1G:970:C:O2' | 2.33 | 0.41 |
| 1:1G:968:A:H8 | 1:1G:968:A:O5' | 2.03 | 0.41 |
| 1:1G:1194:U:H2' | 1:1G:1195:C:H6 | 1.82 | 0.41 |
| 1:1G:1227:A:C8 | 1:1G:1227:A:C3' | 3.00 | 0.41 |
| 1:1G:1271:G:H5' | 1:1G:1314:C:H5' | 2.01 | 0.41 |
| 1:1G:1378:C:C5 | 1:1G:1379:G:N9 | 2.86 | 0.41 |
| 2:12:20:GLU:HG3 | 2:12:190:THR:O | 2.21 | 0.41 |
| 2:12:82:ARG:HB2 | 2:12:94:ASN:ND2 | 2.35 | 0.41 |
| 7:62:20:ASP:HB3 | 7:62:23:VAL:HG23 | 2.00 | 0.41 |
| 8:72:73:ASP:OD1 | 8:72:75:ARG:HB2 | 2.20 | 0.41 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 9:82:46:ALA:HB1 | 9:82:77:ILE:CG1 | 2.50 | 0.41 |
| 18:9A:22:VAL:C | 18:9A:24:ALA:N | 2.78 | 0.41 |
| 24:14:26:G:H1' | 24:14:515:A:H61 | 1.85 | 0.41 |
| 24:14:1638:C:H1' | 24:14:2698:U:O2' | 2.21 | 0.41 |
| 24:14:1638:C:H4' | 24:14:2710:C:O2 | 2.21 | 0.41 |
| 24:14:1828:G:OP1 | 57:14:3573:HOH:O | 2.20 | 0.41 |
| 24:14:2165:G:O2' | 24:14:2166:G:H5' | 2.21 | 0.41 |
| 25:1J:78:A:H2' | 25:1J:79:C:O4' | 2.20 | 0.41 |
| 28:29:4:ILE:HD12 | 28:29:28:ALA:HB3 | 2.03 | 0.41 |
| 28:29:82:ARG:HA | 28:29:82:ARG:HD3 | 1.85 | 0.41 |
| 29:39:2:LYS:HD3 | 29:39:2:LYS:N | 2.35 | 0.41 |
| 30:49:11:TYR:HA | 30:49:15:VAL:HB | 2.02 | 0.41 |
| 32:69:64:GLU:HA | 32:69:67:ARG:HD2 | 2.03 | 0.41 |
| 36:45:52:VAL:O | 36:45:56:ARG:HB2 | 2.20 | 0.41 |
| 37:55:29:LEU:HD12 | 37:55:29:LEU:HA | 1.72 | 0.41 |
| 40:85:61:TRP:HB3 | 40:85:93:LYS:O | 2.20 | 0.41 |
| 49:H5:43:ILE:O | 49:H5:47:VAL:HG23 | 2.19 | 0.41 |
| 50:I5:39:CYS:C | 50:I5:41:PRO:HD3 | 2.45 | 0.41 |
| 52:K5:9:LEU:O | 52:K5:27:LYS:HB2 | 2.21 | 0.41 |
| 1:13:129(A):G:N3 | 1:13:190:G:H5" | 2.36 | 0.41 |
| 1:13:229:U:H2' | 1:13:230:G:O4' | 2.20 | 0.41 |
| 1:13:538:G:H2' | 1:13:539:A:C8 | 2.56 | 0.41 |
| 1:13:858:G:O6 | 1:13:869:G:H3' | 2.20 | 0.41 |
| 1:13:1151:A:OP1 | 10:1I:41:PRO:HA | 2.19 | 0.41 |
| 1:13:1239:A:H62 | 1:13:1299:A:H62 | 1.69 | 0.41 |
| 1:13:1305:G:H8 | 1:13:1305:G:OP2 | 2.04 | 0.41 |
| 1:13:1368:G:OP1 | 9:8E:111:ARG:NH2 | 2.53 | 0.41 |
| 1:13:1399:C:H4' | 1:13:1400:C:H5" | 2.03 | 0.41 |
| 6:5E:45:LEU:HD11 | 6:5E:57:GLN:HB2 | 2.02 | 0.41 |
| 6:5E:95:GLU:HA | 6:5E:96:PRO:HD3 | 1.86 | 0.41 |
| 7:6E:23:VAL:HG12 | 7:6E:43:PHE:CZ | 2.56 | 0.41 |
| 7:6E:27:ILE:HD11 | 7:6E:43:PHE:HD2 | 1.86 | 0.41 |
| 7:6E:75:VAL:HA | 7:6E:87:VAL:O | 2.20 | 0.41 |
| 7:6E:100:ALA:O | 7:6E:104:LEU:HB2 | 2.21 | 0.41 |
| 8:7E:108:GLY:HA3 | 8:7E:138:TRP:HB3 | 2.02 | 0.41 |
| 13:4I:11:ARG:HG2 | 13:4I:12:ASN:H | 1.86 | 0.41 |
| 15:6I:54:ARG:O | 15:6I:58:MET:HG2 | 2.21 | 0.41 |
| 17:8I:84:LEU:O | 17:8I:87:LYS:HB2 | 2.20 | 0.41 |
| 24:1H:189:G:O5' | 24:1H:189:G:H8 | 2.03 | 0.41 |
| 24:1H:528:A:O2' | 24:1H:529:A:H5" | 2.20 | 0.41 |
| 24:1H:805:G:H4' | 24:1H:806:C:OP2 | 2.21 | 0.41 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 24:1H:918:A:N3 | 25:16:80:U:O2' | 2.48 | 0.41 |
| 24:1H:1252:G:N3 | 40:C8:33:ARG:HD2 | 2.34 | 0.41 |
| 24:1H:1400:G:C6 | 24:1H:1401:G:C6 | 3.09 | 0.41 |
| 24:1H:1951:U:O2 | 24:1H:1953:A:H8 | 2.03 | 0.41 |
| 25:16:90:C:OP1 | 36:88:16:ARG:HD2 | 2.20 | 0.41 |
| 27:11:105:ILE:HA | 27:11:105:ILE:HD12 | 1.57 | 0.41 |
| 28:21:50:GLY:HA3 | 28:21:74:PRO:HG3 | 2.02 | 0.41 |
| 39:B8:3:ARG:HB3 | 39:B8:6:LEU:HB3 | 2.02 | 0.41 |
| 40:C8:45:TYR:O | 40:C8:49:HIS:N | 2.44 | 0.41 |
| 47:J8:11:ARG:HH11 | 47:J8:11:ARG:HD2 | 1.67 | 0.41 |
| 48:K8:6:VAL:H | 48:K8:6:VAL:HG23 | 1.57 | 0.41 |
| 48:K8:28:LYS:HD3 | 48:K8:53:LEU:CD2 | 2.50 | 0.41 |
| 53:P8:5:TRP:NE1 | 53:P8:7:PRO:HB3 | 2.35 | 0.41 |
| 1:1G:222:U:H2' | 1:1G:223:U:C6 | 2.55 | 0.41 |
| 1:1G:518:C:C6 | 1:1G:530:G:H5' | 2.55 | 0.41 |
| 1:1G:938:A:N6 | 1:1G:939:G:C5 | 2.89 | 0.41 |
| 1:1G:980:C:H5' | 1:1G:981:U:C5 | 2.55 | 0.41 |
| 1:1G:1349:A:OP1 | 9:82:118:LYS:HE2 | 2.21 | 0.41 |
| 2:12:8:LYS:HB3 | 2:12:9:GLU:H | 1.59 | 0.41 |
| 2:12:97:TRP:HH2 | 2:12:176:GLU:CD | 2.29 | 0.41 |
| 3:22:156:ARG:HB3 | 3:22:160:ALA:O | 2.20 | 0.41 |
| 6:52:67:MET:HB2 | 6:52:68:PRO:HD2 | 2.02 | 0.41 |
| 11:2A:31:THR:HG22 | 11:2A:42:TRP:CB | 2.51 | 0.41 |
| 16:7A:27:LYS:HB3 | 16:7A:27:LYS:HE3 | 1.84 | 0.41 |
| 16:7A:75:ARG:HG3 | 16:7A:80:PHE:HD2 | 1.86 | 0.41 |
| 19:AA:27:GLU:HG2 | 19:AA:47:HIS:NE2 | 2.36 | 0.41 |
| 24:14:90:U:H6 | 24:14:90:U:OP1 | 2.03 | 0.41 |
| 24:14:271(B):G:N7 | 24:14:421:U:H2' | 2.35 | 0.41 |
| 24:14:271:G:H2' | 24:14:272:G:C8 | 2.55 | 0.41 |
| 24:14:443:A:N6 | 29:39:41:LEU:O | 2.53 | 0.41 |
| 24:14:569:U:H5" | 57:14:3749:HOH:O | 2.20 | 0.41 |
| 24:14:684:G:OP1 | 53:L5:16:HIS:ND1 | 2.51 | 0.41 |
| 24:14:740:U:H2' | 24:14:741:G:C8 | 2.55 | 0.41 |
| 24:14:2111:C:N4 | 24:14:2147:G:H21 | 2.15 | 0.41 |
| 24:14:2286:A:C8 | 24:14:2287:A:N6 | 2.89 | 0.41 |
| 24:14:2401:U:O2 | 24:14:2402:C:C6 | 2.73 | 0.41 |
| 24:14:2467:C:H2' | 24:14:2468:G:H1' | 2.01 | 0.41 |
| 24:14:2530:A:C5 | 31:59:157:TYR:HE1 | 2.38 | 0.41 |
| 25:1J:53:A:H2' | 25:1J:54:G:O4' | 2.20 | 0.41 |
| 27:19:133:LEU:HD13 | 27:19:173:VAL:HG22 | 2.02 | 0.41 |
| 28:29:31:CYS:HB3 | 28:29:50:GLY:H | 1.85 | 0.41 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 28:29:114:ALA:O | 28:29:157:ALA:HB1 | 2.20 | 0.41 |
| 29:39:148:LEU:HD11 | 29:39:193:VAL:HG21 | 2.02 | 0.41 |
| 32:69:58:LEU:HD12 | 32:69:58:LEU:HA | 1.81 | 0.41 |
| 34:25:23:ARG:HG3 | 34:25:24:VAL:N | 2.34 | 0.41 |
| 34:25:113:LYS:O | 34:25:117:LEU:HD13 | 2.20 | 0.41 |
| 42:A5:11:ARG:CZ | 42:A5:98:LYS:HB3 | 2.51 | 0.41 |
| 44:C5:52:SER:CB | 44:C5:56:PRO:HA | 2.50 | 0.41 |
| 45:D5:112:ARG:HA | 45:D5:112:ARG:HD2 | 1.73 | 0.41 |
| 47:F5:83:GLU:H | 47:F5:83:GLU:HG3 | 1.51 | 0.41 |
| 1:13:102:G:C2 | 1:13:103:C:C2 | 3.09 | 0.41 |
| 1:13:117:G:H2' | 1:13:118:U:H6 | 1.85 | 0.41 |
| 1:13:155:C:H1' | 1:13:167:G:N2 | 2.35 | 0.41 |
| 1:13:353:A:H5' | 1:13:353:A:C8 | 2.50 | 0.41 |
| 1:13:373:A:C2 | 1:13:482:A:C6 | 3.08 | 0.41 |
| 1:13:433:C:O2' | 1:13:434:U:H5' | 2.21 | 0.41 |
| 1:13:456:C:O2 | 1:13:477:G:N2 | 2.53 | 0.41 |
| 1:13:902:G:H2' | 1:13:903:G:H8 | 1.86 | 0.41 |
| 1:13:980:C:C5 | 1:13:981:U:C2 | 3.08 | 0.41 |
| 1:13:991:U:OP2 | 1:13:991:U:H6 | 2.03 | 0.41 |
| 1:13:1071:C:H2' | 1:13:1072:G:C8 | 2.54 | 0.41 |
| 1:13:1166:G:H2' | 1:13:1169:A:OP2 | 2.20 | 0.41 |
| 1:13:1240:U:O2' | 7:6E:38:LEU:HG | 2.21 | 0.41 |
| 1:13:1315:U:C4 | 1:13:1316:G:C5 | 3.08 | 0.41 |
| 1:13:1399:C:H4' | 1:13:1400:C:C5' | 2.51 | 0.41 |
| 1:13:1510:U:H1' | 1:13:1526:G:N2 | 2.35 | 0.41 |
| 4:3E:20:TYR:CZ | 6:52:15:ASP:HB3 | 2.55 | 0.41 |
| 6:5E:33:TYR:CE2 | 6:5E:75:LEU:HA | 2.56 | 0.41 |
| 7:6E:38:LEU:HA | 7:6E:38:LEU:HD13 | 1.74 | 0.41 |
| 8:7E:20:TYR:HA | 8:7E:65:TYR:CE2 | 2.55 | 0.41 |
| 8:7E:25:ASP:HA | 8:7E:59:LEU:O | 2.21 | 0.41 |
| 10:1I:6:ILE:HG22 | 10:1I:98:ILE:HG12 | 2.02 | 0.41 |
| 10:1I:84:GLN:H | 10:1I:84:GLN:HG2 | 1.49 | 0.41 |
| 12:3I:39:VAL:HG23 | 12:3I:41:ARG:HG2 | 2.03 | 0.41 |
| 13:4I:11:ARG:HG2 | 13:4I:12:ASN:N | 2.35 | 0.41 |
| 16:7I:14:ASN:N | 16:7I:15:PRO:HD3 | 2.35 | 0.41 |
| 19:AI:18:LYS:HE3 | 19:AI:22:LEU:HD11 | 2.01 | 0.41 |
| 19:AI:19:VAL:HG21 | 19:AI:44:MET:HE3 | 2.01 | 0.41 |
| 19:AI:41:VAL:HB | 19:AI:42:PRO:HA | 2.02 | 0.41 |
| 20:BI:72:LEU:HA | 20:BI:72:LEU:HD12 | 1.84 | 0.41 |
| 22:2K:19:C:C2' | 22:2K:20:C:H2' | 2.50 | 0.41 |
| 22:3K:8:4SU:S4 | 22:3K:13:G:C8 | 3.14 | 0.41 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 24:1H:91:A:H2' | 24:1H:92:G:C8 | 2.53 | 0.41 |
| 24:1H:773:U:C5' | 27:11:47:GLY:HA3 | 2.51 | 0.41 |
| 24:1H:871:U:H5' | 36:88:69:PHE:CE2 | 2.54 | 0.41 |
| 24:1H:945:A:C4 | 24:1H:2448:A:C2 | 3.08 | 0.41 |
| 24:1H:1002:G:H8 | 24:1H:1002:G:O5' | 2.04 | 0.41 |
| 24:1H:1019:U:O2' | 24:1H:1021:A:C2 | 2.73 | 0.41 |
| 24:1H:1964:G:H4' | 24:1H:1965:C:OP2 | 2.20 | 0.41 |
| 24:1H:2074:U:O4 | 57:1H:3707:HOH:O | 2.21 | 0.41 |
| 30:41:101:ILE:HG22 | 30:41:105:LYS:HE2 | 2.02 | 0.41 |
| 32:61:66:GLU:HA | 32:61:69:LYS:HB3 | 2.02 | 0.41 |
| 33:58:15:LEU:HB2 | 33:58:134:ARG:HB2 | 2.02 | 0.41 |
| 35:78:24:GLY:C | 35:78:26:GLY:H | 2.29 | 0.41 |
| 37:98:42:LYS:HA | 37:98:45:ARG:HD2 | 2.02 | 0.41 |
| 38:A8:31:SER:O | 38:A8:97:ARG:NH2 | 2.43 | 0.41 |
| 51:N8:16:ARG:HG3 | 51:N8:17:ASP:N | 2.34 | 0.41 |
| 53:P8:1:MET:O | 53:P8:2:LYS:C | 2.62 | 0.41 |
| 1:1G:95:G:H2' | 1:1G:96:G:O4' | 2.20 | 0.41 |
| 1:1G:246:A:C4 | 1:1G:279:A:N6 | 2.88 | 0.41 |
| 1:1G:384:G:H2' | 1:1G:385:C:C6 | 2.55 | 0.41 |
| 1:1G:539:A:N6 | 1:1G:540:G:O6 | 2.53 | 0.41 |
| 1:1G:748:C:H4' | 1:1G:749:C:O5' | 2.20 | 0.41 |
| 1:1G:781:A:OP2 | 1:1G:800:G:N1 | 2.40 | 0.41 |
| 1:1G:836:G:C6 | 1:1G:851:G:C6 | 3.08 | 0.41 |
| 1:1G:862:C:H2' | 1:1G:863:U:H6 | 1.85 | 0.41 |
| 1:1G:1055:A:C8 | 1:1G:1206:G:C2 | 3.08 | 0.41 |
| 1:1G:1124:G:O2' | 1:1G:1145:C:N4 | 2.54 | 0.41 |
| 2:12:102:LEU:HD23 | 2:12:182:ILE:HD12 | 2.01 | 0.41 |
| 7:62:16:LEU:HD12 | 9:82:42:ARG:HA | 2.03 | 0.41 |
| 24:14:28:A:C2 | 24:14:513:A:C8 | 3.09 | 0.41 |
| 24:14:82:G:N1 | 24:14:103:A:OP2 | 2.50 | 0.41 |
| 24:14:451:C:P | 29:39:52:LYS:HD2 | 2.60 | 0.41 |
| 24:14:1040:C:H2' | 24:14:1041:C:O4' | 2.21 | 0.41 |
| 24:14:1050:A:O2' | 24:14:2752:C:O2 | 2.37 | 0.41 |
| 24:14:1077:A:O2' | 24:14:1078:U:O4' | 2.30 | 0.41 |
| 24:14:1131:G:C2 | 24:14:1132:A:C4 | 3.08 | 0.41 |
| 24:14:1488:G:H5" | 24:14:1488:G:C8 | 2.55 | 0.41 |
| 24:14:1657:C:H2' | 24:14:1658:C:H6 | 1.85 | 0.41 |
| 24:14:2540:C:O2' | 24:14:2740:A:N3 | 2.50 | 0.41 |
| 24:14:2572:A:N7 | 28:29:144:ARG:HD2 | 2.34 | 0.41 |
| 25:1J:13:A:O2' | 25:1J:15:A:O5' | 2.38 | 0.41 |
| 26:79:52:ARG:HH21 | 26:79:167:LYS:HE2 | 1.84 | 0.41 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 31:59:82:GLY:HA3 | 31:59:135:GLY:O | 2.21 | 0.41 |
| 35:35:61:ARG:HG2 | 35:35:61:ARG:H | 1.61 | 0.41 |
| 36:45:138:ASP:OD1 | 36:45:138:ASP:N | 2.52 | 0.41 |
| 38:65:3:ARG:NE | 38:65:4:LEU:N | 2.68 | 0.41 |
| 38:65:17:ARG:HH11 | 38:65:17:ARG:HG3 | 1.84 | 0.41 |
| 42:A5:14:PRO:HG2 | 42:A5:78:GLU:HB2 | 2.02 | 0.41 |
| 43:B5:69:TYR:HD1 | 43:B5:70:LEU:N | 2.17 | 0.41 |
| 44:C5:48:ALA:HB3 | 44:C5:59:GLY:CA | 2.44 | 0.41 |
| 45:D5:62:PRO:C | 45:D5:64:GLY:H | 2.28 | 0.41 |
| 47:F5:82:LEU:HB2 | 47:F5:83:GLU:H | 1.74 | 0.41 |
| 54:M5:54:GLU:HG3 | 54:M5:57:ARG:HH12 | 1.85 | 0.41 |
| 1:13:222:U:H2' | 1:13:223:U:H6 | 1.84 | 0.41 |
| 1:13:363:A:C5 | 12:3I:31:PRO:HD2 | 2.55 | 0.41 |
| 1:13:451:A:H61 | 1:13:480:U:H2' | 1.85 | 0.41 |
| 1:13:1266:G:N2 | 1:13:1270:C:C2 | 2.89 | 0.41 |
| 1:13:1428:A:H2' | 1:13:1429:C:C6 | 2.55 | 0.41 |
| 2:1E:14:GLY:N | 2:1E:16:HIS:CE1 | 2.86 | 0.41 |
| 2:1E:84:GLU:OE1 | 2:1E:216:SER:HA | 2.21 | 0.41 |
| 2:1E:119:GLU:O | 2:1E:122:PHE:HB3 | 2.20 | 0.41 |
| 5:4E:48:ALA:HB3 | 5:4E:54:ALA:HB2 | 2.03 | 0.41 |
| 20:BI:53:LEU:HB2 | 20:BI:100:ILE:CG2 | 2.50 | 0.41 |
| 22:2K:22:A:C2 | 22:2K:57:C:C5 | 3.08 | 0.41 |
| 23:4K:20:A:H2' | 23:4K:21:A:C8 | 2.55 | 0.41 |
| 24:1H:306:U:H2' | 24:1H:307:G:O4' | 2.20 | 0.41 |
| 24:1H:862:G:H2' | 24:1H:863:A:O4' | 2.20 | 0.41 |
| 24:1H:973:A:O4' | 24:1H:1188:U:C6 | 2.73 | 0.41 |
| 24:1H:1007:C:O2' | 33:58:108:PRO:HA | 2.20 | 0.41 |
| 24:1H:2175:C:H4' | 26:71:218:MET:O | 2.20 | 0.41 |
| 24:1H:2257:U:O2' | 24:1H:2258:C:H5' | 2.20 | 0.41 |
| 24:1H:2260:C:H2' | 24:1H:2261:C:H5' | 2.02 | 0.41 |
| 24:1H:2636:U:H1' | 24:1H:2783:G:N2 | 2.36 | 0.41 |
| 24:1H:2723:C:O3' | 37:98:1:MET:HE1 | 2.20 | 0.41 |
| 24:1H:2841:C:H2' | 24:1H:2842:G:C8 | 2.56 | 0.41 |
| 25:16:48:A:H4' | 38:A8:95:HIS:ND1 | 2.35 | 0.41 |
| 31:51:140:LYS:HE3 | 31:51:140:LYS:HB2 | 1.85 | 0.41 |
| 35:78:46:LYS:HE2 | 35:78:46:LYS:HB3 | 1.87 | 0.41 |
| 40:C8:95:LEU:HA | 40:C8:95:LEU:HD13 | 1.81 | 0.41 |
| 44:G8:96:ILE:HG22 | 44:G8:97:ARG:N | 2.36 | 0.41 |
| 45:H8:48:PHE:CE1 | 45:H8:52:SER:HA | 2.55 | 0.41 |
| 48:K8:61:LEU:HD23 | 48:K8:61:LEU:HA | 1.91 | 0.41 |
| 54:Q8:40:GLU:H | 54:Q8:43:GLN:H | 1.68 | 0.41 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 1:1G:440:A:OP2 | 1:1G:440:A:H8 | 2.04 | 0.41 |
| 1:1G:448:A:O2' | 1:1G:449:C:H5' | 2.20 | 0.41 |
| 1:1G:542:G:N2 | 1:1G:543:C:C2 | 2.89 | 0.41 |
| 1:1G:1015:A:C6 | 1:1G:1016:A:C6 | 3.09 | 0.41 |
| 1:1G:1497:G:C2' | 1:1G:1498:U:H5' | 2.47 | 0.41 |
| 4:32:102:ASP:HB2 | 4:32:118:ARG:HA | 2.02 | 0.41 |
| 5:42:96:PRO:HA | 5:42:117:ASP:OD2 | 2.21 | 0.41 |
| 5:42:123:LEU:HD23 | 5:42:123:LEU:HA | 1.80 | 0.41 |
| 8:72:16:ALA:HB2 | 8:72:24:THR:HG21 | 2.03 | 0.41 |
| 11:2A:112:THR:HA | 11:2A:113:PRO:HD3 | 1.81 | 0.41 |
| 14:5A:26:ARG:NH1 | 14:5A:47:LEU:HD21 | 2.34 | 0.41 |
| 17:8A:81:ARG:CZ | 17:8A:84:LEU:HD21 | 2.51 | 0.41 |
| 22:2L:63:5MU:H72 | 22:2L:64:PSU:HN1 | 1.84 | 0.41 |
| 24:14:761:A:C8 | 57:14:3606:HOH:O | 2.73 | 0.41 |
| 24:14:768:G:C6 | 24:14:769:G:C5 | 3.08 | 0.41 |
| 24:14:1142:U:H5" | 24:14:1142(A):A:H5' | 2.02 | 0.41 |
| 24:14:1438:U:O2' | 24:14:1439:A:H5' | 2.21 | 0.41 |
| 24:14:1570:A:H2' | 24:14:1571:A:C8 | 2.55 | 0.41 |
| 24:14:1636:C:H2' | 24:14:1637:A:C8 | 2.56 | 0.41 |
| 24:14:1803:A:N1 | 24:14:1822:G:O2' | 2.51 | 0.41 |
| 24:14:2287:A:C4 | 24:14:2289:G:C8 | 3.09 | 0.41 |
| 24:14:2722:G:H5' | 37:55:4:LEU:HD12 | 2.02 | 0.41 |
| 24:14:2860:A:N7 | 24:14:2861:G:H1' | 2.36 | 0.41 |
| 24:14:2861:G:C4 | 24:14:2862:G:C8 | 3.09 | 0.41 |
| 25:1J:118:G:C2 | 25:1J:119:A:H1' | 2.56 | 0.41 |
| 27:19:79:VAL:HG21 | 27:19:111:LEU:HD11 | 2.03 | 0.41 |
| 28:29:48:GLN:O | 28:29:79:ARG:O | 2.38 | 0.41 |
| 28:29:70:ALA:N | 28:29:71:GLY:HA3 | 2.36 | 0.41 |
| 32:69:75:LEU:HD13 | 32:69:139:GLN:HG3 | 2.03 | 0.41 |
| 35:35:2:LYS:HG3 | 35:35:5:ASP:CG | 2.46 | 0.41 |
| 39:75:121:ILE:O | 39:75:124:ASP:HB2 | 2.21 | 0.41 |
| 45:D5:44:PHE:CE2 | 45:D5:86:VAL:HG21 | 2.56 | 0.41 |
| 1:13:658:G:C2 | 1:13:659:U:C2 | 3.07 | 0.41 |
| 1:13:698:G:C6 | 1:13:699:C:C4 | 3.09 | 0.41 |
| 1:13:811:C:H4' | 1:13:900:A:N6 | 2.35 | 0.41 |
| 1:13:815:A:N6 | 1:13:1509:C:H1' | 2.35 | 0.41 |
| 1:13:960:U:O2 | 1:13:960:U:H2' | 2.21 | 0.41 |
| 1:13:1196:U:C4 | 23:4K:23:A:H8 | 2.39 | 0.41 |
| 1:13:1272:G:C6 | 1:13:1273:G:C4 | 3.08 | 0.41 |
| 1:13:1321:C:C5 | 1:13:1322:C:C2 | 3.08 | 0.41 |
| 2:1E:21:ARG:CB | 2:1E:39:ILE:HA | 2.42 | 0.41 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 3:2E:15:THR:O | 3:2E:15:THR:HG22 | 2.20 | 0.41 |
| 3:2E:139:GLN:NE2 | 3:2E:143:GLU:OE2 | 2.51 | 0.41 |
| 5:4E:36:ASP:CG | 5:4E:38:GLN:H | 2.26 | 0.41 |
| 5:4E:50:GLU:HB3 | 5:4E:53:LEU:HD13 | 2.03 | 0.41 |
| 8:7E:5:PRO:O | 8:7E:8:ASP:HB3 | 2.21 | 0.41 |
| 8:7E:118:VAL:C | 8:7E:119:LEU:HD23 | 2.46 | 0.41 |
| 10:1I:9:ARG:NH2 | 10:1I:97:GLU:HG3 | 2.36 | 0.41 |
| 11:2I:23:ALA:HA | 11:2I:28:THR:HG23 | 2.02 | 0.41 |
| 12:3I:34:ARG:HD3 | 12:3I:105:TYR:CZ | 2.55 | 0.41 |
| 19:AI:40:ILE:HG22 | 19:AI:69:HIS:O | 2.20 | 0.41 |
| 24:1H:7:G:C2 | 24:1H:8:A:C4 | 3.08 | 0.41 |
| 24:1H:784:A:C8 | 24:1H:792:G:C5 | 3.09 | 0.41 |
| 24:1H:831:G:H8 | 24:1H:831:G:O5' | 2.02 | 0.41 |
| 24:1H:1022:G:N2 | 24:1H:1024:G:C2 | 2.88 | 0.41 |
| 24:1H:1222:C:H2' | 24:1H:1223:C:C6 | 2.54 | 0.41 |
| 24:1H:2239:G:H5' | 27:11:251:GLY:HA3 | 2.03 | 0.41 |
| 24:1H:2583:G:C6 | 24:1H:2584:U:C4 | 3.09 | 0.41 |
| 24:1H:2751:G:H8 | 24:1H:2751:G:OP1 | 2.03 | 0.41 |
| 27:11:28:GLU:O | 27:11:29:PRO:C | 2.60 | 0.41 |
| 27:11:228:PRO:HG3 | 27:11:234:GLY:O | 2.21 | 0.41 |
| 28:21:24:THR:HG21 | 28:21:188:VAL:HG13 | 2.03 | 0.41 |
| 28:21:135:HIS:CE1 | 57:21:401:HOH:O | 2.66 | 0.41 |
| 30:41:77:ILE:O | 30:41:81:LYS:O | 2.38 | 0.41 |
| 31:51:7:LEU:H | 31:51:7:LEU:HG | 1.56 | 0.41 |
| 31:51:130:ARG:NH1 | 31:51:130:ARG:HB3 | 2.35 | 0.41 |
| 31:51:153:LYS:H | 31:51:153:LYS:CD | 2.31 | 0.41 |
| 33:58:55:VAL:HG12 | 33:58:127:ASP:O | 2.21 | 0.41 |
| 40:C8:91:ASP:O | 40:C8:95:LEU:HB2 | 2.20 | 0.41 |
| 42:E8:84:ARG:HB2 | 42:E8:96:ILE:HD13 | 2.03 | 0.41 |
| 1:1G:938:A:N6 | 1:1G:939:G:C6 | 2.88 | 0.41 |
| 1:1G:1162:C:N3 | 1:1G:1175:G:C2 | 2.88 | 0.41 |
| 1:1G:1193:G:C2' | 1:1G:1194:U:H5' | 2.50 | 0.41 |
| 1:1G:1323:G:N2 | 1:1G:1361:G:O2' | 2.49 | 0.41 |
| 1:1G:1466:C:H2' | 1:1G:1467:G:O4' | 2.21 | 0.41 |
| 1:1G:1521:G:H2' | 1:1G:1522:U:O4' | 2.21 | 0.41 |
| 2:12:219:VAL:O | 2:12:222:ILE:HB | 2.20 | 0.41 |
| 3:22:58:GLU:O | 3:22:59:ARG:HD2 | 2.19 | 0.41 |
| 4:32:178:VAL:C | 4:32:180:GLY:N | 2.78 | 0.41 |
| 6:52:95:GLU:HA | 6:52:96:PRO:HD3 | 1.81 | 0.41 |
| 14:5A:53:LEU:HD23 | 14:5A:53:LEU:HA | 1.86 | 0.41 |
| 15:6A:10:LYS:HA | 15:6A:10:LYS:HD2 | 1.70 | 0.41 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 22:3L:59:A:H2' | 22:3L:60:A:O4' | 2.21 | 0.41 |
| 24:14:273(C):C:H5' | 24:14:273(D):C:OP2 | 2.21 | 0.41 |
| 24:14:321:G:C4 | 24:14:341:G:H4' | 2.56 | 0.41 |
| 24:14:389:G:H8 | 24:14:389:G:O5' | 2.03 | 0.41 |
| 24:14:491:G:H2' | 24:14:492:A:H8 | 1.84 | 0.41 |
| 24:14:573:G:H1 | 24:14:2031:A:P | 2.44 | 0.41 |
| 24:14:635:C:H2' | 24:14:636:G:O4' | 2.20 | 0.41 |
| 24:14:686:G:H1 | 53:L5:16:HIS:CD2 | 2.39 | 0.41 |
| 24:14:996:A:H4' | 40:85:92:ARG:HE | 1.85 | 0.41 |
| 24:14:1027:A:C6 | 24:14:1126:A:C4 | 3.09 | 0.41 |
| 24:14:1055:G:H2' | 24:14:1056:G:O4' | 2.20 | 0.41 |
| 24:14:1123:C:H2' | 24:14:1124:C:C6 | 2.56 | 0.41 |
| 24:14:1319:G:C6 | 24:14:1320:C:N4 | 2.89 | 0.41 |
| 24:14:1858:G:H1' | 24:14:1884:A:H61 | 1.85 | 0.41 |
| 24:14:2065:C:H1' | 24:14:2449:U:H3 | 1.84 | 0.41 |
| 24:14:2786:U:H4' | 28:29:63:LEU:O | 2.20 | 0.41 |
| 25:1J:30:C:C5 | 25:1J:31:C:C2 | 3.09 | 0.41 |
| 27:19:62:TYR:CE2 | 27:19:64:ILE:HA | 2.56 | 0.41 |
| 28:29:96:PHE:O | 28:29:175:VAL:HG11 | 2.21 | 0.41 |
| 33:15:10:GLU:HG3 | 33:15:11:PRO:HD2 | 2.01 | 0.41 |
| 33:15:61:ARG:HE | 33:15:61:ARG:HA | 1.85 | 0.41 |
| 39:75:10:VAL:O | 39:75:11:GLU:HB2 | 2.21 | 0.41 |
| 40:85:65:ILE:HG12 | 40:85:96:ALA:CB | 2.51 | 0.41 |
| 43:B5:12:VAL:HG12 | 43:B5:29:TRP:N | 2.36 | 0.41 |
| 47:F5:3:LYS:O | 47:F5:12:PRO:HD3 | 2.21 | 0.41 |
| 51:J5:19:ARG:O | 51:J5:19:ARG:HG2 | 2.21 | 0.41 |
| 1:13:171:A:C2 | 1:13:172:A:C5 | 3.08 | 0.41 |
| 1:13:543:C:O2' | 1:13:544:G:H5' | 2.20 | 0.41 |
| 1:13:1053:G:O6 | 1:13:1199:U:H2' | 2.20 | 0.41 |
| 1:13:1239:A:O2' | 7:6E:114:ARG:O | 2.34 | 0.41 |
| 1:13:1260:C:H4' | 1:13:1284:C:H5' | 2.03 | 0.41 |
| 1:13:1308:U:H5" | 13:4I:98:VAL:HG22 | 2.03 | 0.41 |
| 3:2E:154:SER:HB3 | 3:2E:165:THR:HB | 2.03 | 0.41 |
| 5:4E:41:VAL:HG22 | 5:4E:113:ALA:HB2 | 2.02 | 0.41 |
| 11:2I:20:TYR:O | 11:2I:30:VAL:HG23 | 2.20 | 0.41 |
| 15:6I:62:GLN:O | 15:6I:66:LEU:HD13 | 2.21 | 0.41 |
| 20:BI:53:LEU:HD12 | 20:BI:100:ILE:HG22 | 2.03 | 0.41 |
| 22:2K:54:C:H2' | 22:2K:55:U:C6 | 2.55 | 0.41 |
| 24:1H:41:C:H2' | 24:1H:43:G:O4' | 2.21 | 0.41 |
| 24:1H:241:A:H4' | 24:1H:242:G:OP1 | 2.20 | 0.41 |
| 24:1H:299:A:H5' | 24:1H:300:A:OP2 | 2.21 | 0.41 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 24:1H:773:U:H5' | 27:11:47:GLY:HA3 | 2.03 | 0.41 |
| 24:1H:819:A:OP2 | 24:1H:1187:G:N2 | 2.49 | 0.41 |
| 24:1H:1103:A:H3' | 24:1H:1104:C:C5 | 2.56 | 0.41 |
| 24:1H:1312:U:C2 | 24:1H:1603:A:C2 | 3.09 | 0.41 |
| 24:1H:1324:G:C2 | 24:1H:1331:A:C2 | 3.08 | 0.41 |
| 24:1H:1530:G:H1 | 24:1H:1541:U:H3 | 1.68 | 0.41 |
| 24:1H:1844:C:O3' | 27:11:258:LYS:NZ | 2.44 | 0.41 |
| 24:1H:2172:U:H5' | 24:1H:2173:A:OP2 | 2.21 | 0.41 |
| 24:1H:2333:A:O4' | 24:1H:2335:A:C5 | 2.73 | 0.41 |
| 24:1H:2739:U:O2' | 24:1H:2740:A:H5' | 2.21 | 0.41 |
| 28:21:45:THR:O | 28:21:46:ALA:HB2 | 2.21 | 0.41 |
| 29:31:32:LEU:CD2 | 29:31:105:VAL:HG13 | 2.51 | 0.41 |
| 29:31:129:PHE:HA | 29:31:142:TRP:NE1 | 2.36 | 0.41 |
| 30:41:125:PHE:CD1 | 30:41:131:TYR:HB2 | 2.55 | 0.41 |
| 33:58:68:GLU:H | 33:58:68:GLU:HG3 | 1.71 | 0.41 |
| 36:88:5:ARG:H | 36:88:5:ARG:HG3 | 1.40 | 0.41 |
| 37:98:75:LEU:O | 37:98:79:LEU:HB2 | 2.21 | 0.41 |
| 37:98:117:VAL:HG22 | 37:98:118:GLU:N | 2.35 | 0.41 |
| 38:A8:21:THR:O | 38:A8:21:THR:OG1 | 2.37 | 0.41 |
| 39:B8:90:GLN:HG3 | 39:B8:91:ARG:N | 2.35 | 0.41 |
| 40:C8:8:VAL:HG23 | 40:C8:11:ARG:NH2 | 2.35 | 0.41 |
| 41:D8:47:VAL:HG22 | 41:D8:48:GLY:N | 2.36 | 0.41 |
| 42:E8:11:ARG:NH1 | 42:E8:11:ARG:HB3 | 2.36 | 0.41 |
| 48:K8:14:ARG:NH1 | 48:K8:66:GLU:OE2 | 2.54 | 0.41 |
| 1:1G:145:G:C2 | 1:1G:178:C:N3 | 2.88 | 0.41 |
| 1:1G:186(D):C:H2' | 1:1G:186(E):C:H6 | 1.85 | 0.41 |
| 1:1G:252:U:H2' | 1:1G:275:G:N2 | 2.36 | 0.41 |
| 1:1G:428:G:O4' | 1:1G:430:A:C8 | 2.74 | 0.41 |
| 1:1G:474:G:H5" | 16:7A:81:ARG:CZ | 2.51 | 0.41 |
| 1:1G:510:A:H5" | 1:1G:511:C:P | 2.60 | 0.41 |
| 1:1G:604:G:H2' | 1:1G:605:U:O4' | 2.20 | 0.41 |
| 1:1G:927:G:OP2 | 1:1G:927:G:H4' | 2.20 | 0.41 |
| 1:1G:1123:A:H1' | 10:1A:39:PRO:HD3 | 2.01 | 0.41 |
| 1:1G:1446:A:H3' | 1:1G:1446:A:N3 | 2.36 | 0.41 |
| 2:12:56:ARG:HA | 2:12:56:ARG:HH11 | 1.85 | 0.41 |
| 2:12:80:ILE:HD11 | 2:12:208:ILE:HG23 | 2.02 | 0.41 |
| 3:22:50:ALA:HB2 | 3:22:75:VAL:CB | 2.45 | 0.41 |
| 3:22:74:GLY:HA2 | 3:22:77:ILE:HB | 2.03 | 0.41 |
| 4:32:3:ARG:HG3 | 4:32:5:ILE:HD11 | 2.03 | 0.41 |
| 5:42:12:LEU:HD22 | 5:42:13:ILE:N | 2.36 | 0.41 |
| 8:72:33:GLU:O | 8:72:36:LEU:HB2 | 2.21 | 0.41 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 16:7A:1:MET:HE1 | 16:7A:3:LYS:HE2 | 2.02 | 0.41 |
| 16:7A:17:TYR:HE2 | 16:7A:41:PRO:HG3 | 1.85 | 0.41 |
| 19:AA:23:ASN:HA | 19:AA:27:GLU:OE2 | 2.21 | 0.41 |
| 20:BA:66:ALA:HB1 | 20:BA:71:THR:CG2 | 2.50 | 0.41 |
| 22:2L:20:C:C6 | 22:2L:22:A:C8 | 3.07 | 0.41 |
| 24:14:270(M):U:O2 | 24:14:270(M):U:H2' | 2.20 | 0.41 |
| 24:14:480:A:H3' | 24:14:481:G:H5" | 2.03 | 0.41 |
| 24:14:522:G:H2' | 24:14:523:C:H6 | 1.86 | 0.41 |
| 24:14:994:C:O2' | 24:14:996:A:OP1 | 2.31 | 0.41 |
| 24:14:1138:G:N2 | 33:15:106:MET:HE2 | 2.35 | 0.41 |
| 24:14:1141:U:H4' | 24:14:1142(A):A:O4' | 2.20 | 0.41 |
| 24:14:1568:G:H5" | 27:19:61:LEU:HD22 | 2.03 | 0.41 |
| 24:14:1576:U:H2' | 24:14:1577:C:H6 | 1.85 | 0.41 |
| 24:14:1710:C:H2' | 24:14:1711:C:C6 | 2.55 | 0.41 |
| 24:14:2002:G:C5 | 57:14:3587:HOH:O | 2.73 | 0.41 |
| 24:14:2086:U:H2' | 24:14:2087:G:C8 | 2.56 | 0.41 |
| 24:14:2133:G:H2' | 24:14:2157:G:O6 | 2.21 | 0.41 |
| 24:14:2172:U:O2' | 24:14:2174:C:OP2 | 2.30 | 0.41 |
| 24:14:2579:C:H2' | 24:14:2580:U:O4' | 2.21 | 0.41 |
| 24:14:2584:U:C6 | 24:14:2585:U:C5 | 3.09 | 0.41 |
| 24:14:2749:A:H1' | 31:59:63:SER:HB3 | 2.02 | 0.41 |
| 24:14:2863:C:O2' | 24:14:2864:G:H5' | 2.21 | 0.41 |
| 25:1J:56:G:H4' | 25:1J:57:A:C8 | 2.56 | 0.41 |
| 28:29:11:MET:HG3 | 28:29:23:VAL:O | 2.21 | 0.41 |
| 28:29:135:HIS:CD2 | 28:29:135:HIS:H | 2.38 | 0.41 |
| 28:29:147:PRO:HB2 | 28:29:149:ARG:HG2 | 2.02 | 0.41 |
| 30:49:16:ARG:N | 30:49:17:PRO:HD2 | 2.35 | 0.41 |
| 31:59:26:VAL:CG1 | 31:59:33:LEU:H | 2.33 | 0.41 |
| 32:69:140:LEU:HD12 | 32:69:141:LYS:N | 2.36 | 0.41 |
| 37:55:13:HIS:NE2 | 37:55:15:SER:OG | 2.53 | 0.41 |
| 39:75:5:ALA:N | 39:75:7:ILE:O | 2.49 | 0.41 |
| 39:75:10:VAL:HG12 | 39:75:11:GLU:H | 1.85 | 0.41 |
| 39:75:86:ILE:O | 39:75:86:ILE:HG12 | 2.19 | 0.41 |
| 43:B5:28:PHE:O | 43:B5:30:VAL:HG13 | 2.21 | 0.41 |
| 1:13:22:G:C5 | 1:13:23:C:C4 | 3.09 | 0.41 |
| 1:13:166:G:H2' | 1:13:167:G:C8 | 2.55 | 0.41 |
| 1:13:191:G:C6 | 1:13:192:U:C4 | 3.09 | 0.41 |
| 1:13:407:G:N2 | 1:13:436:C:C2 | 2.89 | 0.41 |
| 1:13:665:A:N3 | 1:13:732:C:H2' | 2.36 | 0.41 |
| 1:13:716:A:C6 | 1:13:717:C:N3 | 2.88 | 0.41 |
| 1:13:780:A:C2 | 1:13:803:G:N1 | 2.89 | 0.41 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 1:13:818:G:O2' | 1:13:819:A:H5' | 2.21 | 0.41 |
| 1:13:827:U:C5 | 1:13:870:U:C5 | 3.08 | 0.41 |
| 1:13:922:G:C6 | 1:13:923:A:C6 | 3.09 | 0.41 |
| 1:13:958:A:C6 | 1:13:959:A:C6 | 3.09 | 0.41 |
| 1:13:1213:A:C8 | 1:13:1215:G:C6 | 3.09 | 0.41 |
| 1:13:1226:C:H4' | 1:13:1227:A:OP1 | 2.21 | 0.41 |
| 1:13:1504:G:H3' | 57:13:1821:HOH:O | 2.20 | 0.41 |
| 2:1E:150:SER:OG | 2:1E:151:GLY:N | 2.52 | 0.41 |
| 2:1E:211:ILE:HG22 | 2:1E:215:LEU:HD23 | 2.03 | 0.41 |
| 2:1E:237:ALA:C | 2:1E:239:VAL:H | 2.29 | 0.41 |
| 3:2E:50:ALA:HB1 | 3:2E:70:VAL:HG11 | 2.03 | 0.41 |
| 5:4E:139:LEU:HA | 5:4E:142:LEU:CD1 | 2.51 | 0.41 |
| 6:5E:14:LEU:HD13 | 6:5E:19:LEU:HA | 2.03 | 0.41 |
| 6:5E:43:LEU:HD12 | 6:5E:43:LEU:N | 2.36 | 0.41 |
| 8:7E:56:LYS:HA | 8:7E:57:PRO:HD2 | 1.81 | 0.41 |
| 10:1I:3:LYS:HD2 | 10:1I:3:LYS:N | 2.35 | 0.41 |
| 10:1I:6:ILE:HD11 | 10:1I:72:VAL:HG12 | 2.02 | 0.41 |
| 15:6I:39:LEU:HD13 | 15:6I:56:LEU:HB2 | 2.02 | 0.41 |
| 17:8I:32:TYR:O | 17:8I:34:LYS:N | 2.54 | 0.41 |
| 24:1H:173:G:H2' | 24:1H:174:C:C6 | 2.56 | 0.41 |
| 24:1H:562:U:C4 | 24:1H:2036:C:O4' | 2.73 | 0.41 |
| 24:1H:601:C:OP1 | 29:31:108:LYS:HE3 | 2.21 | 0.41 |
| 24:1H:806:C:P | 35:78:41:ARG:HH21 | 2.44 | 0.41 |
| 24:1H:817:C:O2' | 24:1H:839:U:OP1 | 2.32 | 0.41 |
| 24:1H:884:C:H2' | 24:1H:885:C:O4' | 2.20 | 0.41 |
| 24:1H:954:G:N3 | 24:1H:2274:A:H2 | 2.19 | 0.41 |
| 24:1H:1152:C:H5' | 40:C8:77:SER:O | 2.20 | 0.41 |
| 24:1H:1813:G:H1' | 27:11:50:THR:OG1 | 2.21 | 0.41 |
| 24:1H:2016:U:H1' | 51:N8:6:VAL:HG13 | 2.03 | 0.41 |
| 24:1H:2132:U:H3 | 26:71:5:LYS:HB3 | 1.86 | 0.41 |
| 24:1H:2237:G:H8 | 24:1H:2237:G:O5' | 2.04 | 0.41 |
| 24:1H:2791:C:OP2 | 24:1H:2893:G:N2 | 2.54 | 0.41 |
| 24:1H:2889:C:H2' | 24:1H:2891:G:O4' | 2.21 | 0.41 |
| 25:16:20:C:H2' | 25:16:21:G:O4' | 2.21 | 0.41 |
| 25:16:72:G:N2 | 25:16:103:U:C5 | 2.89 | 0.41 |
| 25:16:111:U:H2' | 25:16:112:G:C8 | 2.49 | 0.41 |
| 27:11:79:VAL:HG21 | 27:11:111:LEU:HD21 | 2.02 | 0.41 |
| 27:11:108:PRO:HB3 | 27:11:143:HIS:HE1 | 1.86 | 0.41 |
| 28:21:48:GLN:NE2 | 28:21:77:ILE:HD12 | 2.34 | 0.41 |
| 28:21:96:PHE:O | 28:21:175:VAL:HG11 | 2.19 | 0.41 |
| 29:31:29:ASN:H | 29:31:112:MET:HE1 | 1.85 | 0.41 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 29:31:99:TYR:HE1 | 29:31:101:LEU:HD13 | 1.86 | 0.41 |
| 35:78:49:ARG:HB2 | 54:Q8:60:LEU:HD11 | 2.03 | 0.41 |
| 36:88:87:LYS:HB3 | 36:88:88:GLY:H | 1.73 | 0.41 |
| 37:98:65:LEU:HD12 | 37:98:65:LEU:HA | 1.81 | 0.41 |
| 37:98:98:LEU:O | 37:98:113:LEU:N | 2.53 | 0.41 |
| 38:A8:11:LYS:HD2 | 38:A8:15:ARG:NH2 | 2.36 | 0.41 |
| 39:B8:48:ILE:O | 39:B8:63:VAL:HA | 2.21 | 0.41 |
| 39:B8:70:VAL:HG12 | 39:B8:71:GLY:O | 2.21 | 0.41 |
| 39:B8:77:PRO:O | 39:B8:80:SER:HB2 | 2.20 | 0.41 |
| 40:C8:76:TYR:CD1 | 40:C8:76:TYR:C | 2.99 | 0.41 |
| 46:I8:41:ARG:NE | 46:I8:41:ARG:HA | 2.35 | 0.41 |
| 1:1G:45:U:H2' | 1:1G:46:G:H8 | 1.83 | 0.41 |
| 1:1G:102:G:O2' | 1:1G:151:A:N3 | 2.50 | 0.41 |
| 1:1G:154:C:N4 | 1:1G:168:G:O6 | 2.53 | 0.41 |
| 1:1G:191(E):G:H2' | 1:1G:191(F):U:H6 | 1.86 | 0.41 |
| 1:1G:340:U:H2' | 1:1G:341:C:C6 | 2.56 | 0.41 |
| 1:1G:646:U:H2' | 1:1G:647:C:C6 | 2.56 | 0.41 |
| 1:1G:760:G:H2' | 1:1G:761:G:H5' | 2.01 | 0.41 |
| 1:1G:947:G:OP1 | 13:4A:108:ARG:HG2 | 2.20 | 0.41 |
| 1:1G:963:G:N2 | 10:1A:55:LYS:HE2 | 2.23 | 0.41 |
| 1:1G:971:G:C4 | 1:1G:1365:G:H4' | 2.56 | 0.41 |
| 1:1G:1105:A:C2 | 1:1G:1106:G:N7 | 2.89 | 0.41 |
| 1:1G:1131:G:H2' | 1:1G:1132:C:C6 | 2.54 | 0.41 |
| 1:1G:1153:C:P | 10:1A:13:HIS:HE2 | 2.42 | 0.41 |
| 1:1G:1259:C:C4 | 1:1G:1260:C:H1' | 2.56 | 0.41 |
| 1:1G:1324:A:H2' | 1:1G:1325:C:C6 | 2.56 | 0.41 |
| 1:1G:1346:A:H1' | 1:1G:1347:G:OP2 | 2.21 | 0.41 |
| 1:1G:1512:U:H2' | 1:1G:1513:A:C8 | 2.56 | 0.41 |
| 2:12:204:ASN:N | 2:12:204:ASN:OD1 | 2.54 | 0.41 |
| 3:22:14:ILE:C | 3:22:16:ARG:H | 2.29 | 0.41 |
| 3:22:36:ASP:OD2 | 3:22:57:ILE:HG21 | 2.21 | 0.41 |
| 5:42:12:LEU:O | 5:42:30:ALA:HA | 2.21 | 0.41 |
| 5:42:78:HIS:CE1 | 5:42:142:LEU:HD23 | 2.54 | 0.41 |
| 5:42:122:GLU:O | 5:42:123:LEU:HD23 | 2.20 | 0.41 |
| 5:42:129:ILE:O | 5:42:132:ALA:HB3 | 2.20 | 0.41 |
| 6:52:35:ALA:HA | 6:52:67:MET:HB3 | 2.03 | 0.41 |
| 6:52:61:LEU:HA | 6:52:61:LEU:HD12 | 1.84 | 0.41 |
| 6:52:62:TRP:CE2 | 18:9A:35:ARG:NH2 | 2.88 | 0.41 |
| 7:62:20:ASP:HB3 | 7:62:23:VAL:CG2 | 2.51 | 0.41 |
| 12:3A:85:ILE:HD13 | 12:3A:85:ILE:HA | 1.82 | 0.41 |
| 13:4A:118:ALA:HB2 | 22:2L:29:C:O2' | 2.20 | 0.41 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 17:8A:15:MET:HB2 | 17:8A:15:MET:HE3 | 1.59 | 0.41 |
| 17:8A:16:GLN:O | 17:8A:17:LYS:HB2 | 2.21 | 0.41 |
| 19:AA:18:LYS:O | 19:AA:22:LEU:HD13 | 2.20 | 0.41 |
| 22:2L:69:U:H3' | 22:2L:70:C:H5' | 2.03 | 0.41 |
| 24:14:8:A:H2 | 24:14:2895:U:H3 | 1.68 | 0.41 |
| 24:14:84:A:N1 | 24:14:98:G:O2' | 2.47 | 0.41 |
| 24:14:250:G:P | 35:35:60:MET:HE1 | 2.60 | 0.41 |
| 24:14:289:A:N3 | 24:14:289:A:H2' | 2.36 | 0.41 |
| 24:14:309:G:O3' | 44:C5:18:GLY:HA2 | 2.20 | 0.41 |
| 24:14:468:G:H2' | 24:14:469:G:O4' | 2.20 | 0.41 |
| 24:14:535:C:O2' | 24:14:536:A:H5' | 2.20 | 0.41 |
| 24:14:654(F):C:O2 | 24:14:654(P):G:N2 | 2.53 | 0.41 |
| 24:14:775:G:C4 | 24:14:794:G:C8 | 3.09 | 0.41 |
| 24:14:956:G:OP1 | 36:45:88:GLY:N | 2.54 | 0.41 |
| 24:14:960:A:H4' | 24:14:961:C:OP1 | 2.20 | 0.41 |
| 24:14:1164:G:H1 | 24:14:1185:C:H42 | 1.68 | 0.41 |
| 24:14:1375:C:H2' | 24:14:1376:C:H6 | 1.85 | 0.41 |
| 24:14:1416:G:H21 | 24:14:1586:A:N6 | 2.19 | 0.41 |
| 24:14:1448:G:O2' | 24:14:1528:A:N6 | 2.54 | 0.41 |
| 24:14:1773:A:C5 | 24:14:1829:A:H1' | 2.56 | 0.41 |
| 24:14:1953:A:N1 | 24:14:2549:G:O2' | 2.49 | 0.41 |
| 24:14:2112:G:H2' | 24:14:2113:U:C5 | 2.55 | 0.41 |
| 24:14:2655:G:H1' | 24:14:2656:U:H5 | 1.86 | 0.41 |
| 24:14:2733:A:N1 | 28:29:203:LYS:HA | 2.36 | 0.41 |
| 24:14:2749:A:N1 | 24:14:2750:A:N6 | 2.69 | 0.41 |
| 25:1J:50:G:H2' | 25:1J:51:G:O4' | 2.20 | 0.41 |
| 25:1J:52:A:N6 | 38:65:33:LYS:HG2 | 2.36 | 0.41 |
| 26:79:186:ALA:O | 26:79:190:ARG:NH1 | 2.54 | 0.41 |
| 26:79:192:PHE:O | 26:79:196:LEU:HD22 | 2.21 | 0.41 |
| 27:19:40:THR:C | 27:19:41:GLY:O | 2.60 | 0.41 |
| 29:39:7:TYR:CE2 | 29:39:10:PRO:HG3 | 2.55 | 0.41 |
| 29:39:84:VAL:O | 29:39:85:GLY:C | 2.62 | 0.41 |
| 29:39:132:VAL:C | 29:39:134:GLY:N | 2.78 | 0.41 |
| 30:49:129:GLY:HA2 | 30:49:166:ASP:HA | 2.03 | 0.41 |
| 31:59:86:GLU:HA | 31:59:132:ARG:HB2 | 2.03 | 0.41 |
| 32:69:84:GLY:O | 32:69:85:GLU:HB3 | 2.19 | 0.41 |
| 35:35:36:LYS:HB3 | 35:35:40:SER:OG | 2.20 | 0.41 |
| 36:45:65:PHE:O | 36:45:104:PHE:HA | 2.20 | 0.41 |
| 37:55:12:ARG:HG2 | 37:55:16:HIS:CG | 2.56 | 0.41 |
| 37:55:13:HIS:CD2 | 37:55:16:HIS:H | 2.39 | 0.41 |
| 39:75:6:LEU:HD12 | 39:75:6:LEU:O | 2.21 | 0.41 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 39:75:16:ARG:NH1 | 39:75:80:SER:O | 2.53 | 0.41 |
| 39:75:47:GLY:O | 39:75:63:VAL:HG13 | 2.21 | 0.41 |
| 39:75:106:SER:HA | 39:75:110:ILE:HD11 | 2.03 | 0.41 |
| 39:75:124:ASP:O | 39:75:128:GLU:HB2 | 2.20 | 0.41 |
| 42:A5:14:PRO:O | 42:A5:18:ARG:HB2 | 2.20 | 0.41 |
| 43:B5:47:PHE:CD2 | 43:B5:89:ILE:HD13 | 2.55 | 0.41 |
| 44:C5:5:MET:HE1 | 44:C5:69:ALA:HB1 | 2.03 | 0.41 |
| 48:G5:17:SER:HB2 | 48:G5:18:PRO:C | 2.46 | 0.41 |
| 51:J5:16:ARG:HH11 | 51:J5:16:ARG:HB3 | 1.86 | 0.41 |
| 1:13:193:C:H2' | 1:13:194:C:C6 | 2.56 | 0.41 |
| 1:13:344:A:H2' | 1:13:346:G:N7 | 2.36 | 0.41 |
| 1:13:393:A:OP2 | 16:7I:12:LYS:NZ | 2.45 | 0.41 |
| 1:13:519:C:H2' | 1:13:520:A:C8 | 2.56 | 0.41 |
| 1:13:715:A:O2' | 1:13:716:A:H5' | 2.20 | 0.41 |
| 1:13:803:G:C6 | 1:13:804:U:N3 | 2.89 | 0.41 |
| 1:13:827:U:C5 | 1:13:872:A:N1 | 2.88 | 0.41 |
| 1:13:1149:C:O2' | 1:13:1280:A:N1 | 2.50 | 0.41 |
| 5:4E:80:ILE:HD12 | 8:7E:104:ARG:NH2 | 2.35 | 0.41 |
| 7:6E:120:ILE:HG22 | 7:6E:124:LEU:HD12 | 2.03 | 0.41 |
| 9:8E:48:GLU:N | 9:8E:49:PRO:HD2 | 2.36 | 0.41 |
| 10:1I:78:ASN:O | 10:1I:81:THR:OG1 | 2.34 | 0.41 |
| 11:2I:31:THR:OG1 | 11:2I:42:TRP:HB3 | 2.21 | 0.41 |
| 16:7I:26:ARG:HH11 | 16:7I:26:ARG:CG | 2.26 | 0.41 |
| 22:3K:11:C:H2' | 22:3K:12:C:O4' | 2.20 | 0.41 |
| 24:1H:136:G:H2' | 24:1H:137:C:H6 | 1.85 | 0.41 |
| 24:1H:323:G:C8 | 29:31:171:PRO:HG3 | 2.56 | 0.41 |
| 24:1H:440:G:H2' | 24:1H:441:U:C6 | 2.55 | 0.41 |
| 24:1H:573:G:O2' | 24:1H:574:C:H3' | 2.20 | 0.41 |
| 24:1H:654(N):G:H2' | 24:1H:654(O):G:C8 | 2.56 | 0.41 |
| 24:1H:1173:G:C2 | 24:1H:1175:U:C4 | 3.08 | 0.41 |
| 24:1H:1392:A:C6 | 24:1H:1393:A:C6 | 3.08 | 0.41 |
| 24:1H:1636:C:H2' | 24:1H:1637:A:C8 | 2.56 | 0.41 |
| 24:1H:2590:A:H2' | 24:1H:2591:C:C6 | 2.56 | 0.41 |
| 24:1H:2799:A:H2' | 24:1H:2801:A:C8 | 2.56 | 0.41 |
| 25:16:19:G:N2 | 25:16:65:C:N3 | 2.69 | 0.41 |
| 28:21:13:ARG:HA | 28:21:21:VAL:O | 2.21 | 0.41 |
| 29:31:64:ILE:HD13 | 29:31:64:ILE:HA | 1.72 | 0.41 |
| 29:31:110:LEU:HA | 29:31:110:LEU:HD12 | 1.54 | 0.41 |
| 30:41:20:ILE:HG13 | 30:41:20:ILE:H | 1.72 | 0.41 |
| 38:A8:62:LYS:HA | 38:A8:65:VAL:HB | 2.02 | 0.41 |
| 40:C8:9:VAL:H | 40:C8:9:VAL:HG23 | 1.56 | 0.41 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 45:H8:49:ARG:HD3 | 45:H8:49:ARG:HA | 1.78 | 0.41 |
| 51:N8:40:LYS:HG2 | 51:N8:46:CYS:HA | 2.03 | 0.41 |
| 1:1G:448:A:N7 | 1:1G:486:U:O4 | 2.54 | 0.41 |
| 1:1G:605:U:H2' | 1:1G:606:G:O4' | 2.21 | 0.41 |
| 1:1G:833:U:H2' | 1:1G:834:C:C6 | 2.56 | 0.41 |
| 1:1G:1127:G:H21 | 1:1G:1147:C:H5 | 1.67 | 0.41 |
| 1:1G:1379:G:OP1 | 7:62:6:ARG:NH1 | 2.54 | 0.41 |
| 1:1G:1446:A:N7 | 39:75:118:ARG:NH1 | 2.69 | 0.41 |
| 1:1G:1530:G:H8 | 1:1G:1530:G:H5" | 1.86 | 0.41 |
| 2:12:119:GLU:CD | 2:12:153:ARG:HH12 | 2.28 | 0.41 |
| 3:22:113:ALA:HB1 | 3:22:185:GLY:H | 1.86 | 0.41 |
| 4:32:26:CYS:HA | 4:32:31:CYS:SG | 2.60 | 0.41 |
| 4:32:204:ILE:HD13 | 5:42:97:GLY:O | 2.21 | 0.41 |
| 5:42:88:LYS:HG2 | 5:42:123:LEU:HB2 | 2.02 | 0.41 |
| 10:1A:25:GLU:O | 10:1A:29:ARG:HB3 | 2.21 | 0.41 |
| 11:2A:50:TYR:HD2 | 11:2A:60:ALA:HB2 | 1.86 | 0.41 |
| 15:6A:84:LYS:HE2 | 15:6A:84:LYS:HB2 | 1.84 | 0.41 |
| 16:7A:75:ARG:HG3 | 16:7A:80:PHE:CD2 | 2.56 | 0.41 |
| 24:14:65:C:H2' | 24:14:66:C:C6 | 2.56 | 0.41 |
| 24:14:411:G:OP2 | 24:14:2406:U:O2' | 2.35 | 0.41 |
| 24:14:611:C:H2' | 24:14:612:G:O4' | 2.21 | 0.41 |
| 24:14:879:G:C2 | 24:14:880:G:H1' | 2.56 | 0.41 |
| 24:14:1084:A:N3 | 24:14:1106:G:H1' | 2.36 | 0.41 |
| 24:14:1133:U:O2 | 24:14:1137:G:H5" | 2.21 | 0.41 |
| 24:14:2116:G:H3' | 24:14:2117:A:H5" | 2.02 | 0.41 |
| 24:14:2206:C:H2' | 24:14:2207:C:C6 | 2.56 | 0.41 |
| 24:14:2228:G:C5 | 24:14:2229:C:C4 | 3.09 | 0.41 |
| 24:14:2291:U:O2' | 24:14:2374:C:O2 | 2.37 | 0.41 |
| 24:14:2517:C:O2' | 24:14:2542:A:H2 | 2.04 | 0.41 |
| 24:14:2526:G:C6 | 24:14:2527:C:C4 | 3.09 | 0.41 |
| 24:14:2538:C:H2' | 24:14:2539:C:H6 | 1.86 | 0.41 |
| 26:79:175:VAL:O | 26:79:188:ASN:ND2 | 2.31 | 0.41 |
| 30:49:29:TRP:HE3 | 30:49:33:ARG:NH1 | 2.19 | 0.41 |
| 33:15:109:LYS:HD3 | 33:15:109:LYS:HA | 1.92 | 0.41 |
| 34:25:7:TYR:CZ | 34:25:44:LYS:HG3 | 2.56 | 0.41 |
| 34:25:87:ILE:HD12 | 34:25:93:PRO:HA | 2.02 | 0.41 |
| 36:45:66:ILE:HG22 | 36:45:67:ARG:N | 2.36 | 0.41 |
| 39:75:88:ILE:HD11 | 39:75:91:ARG:NH2 | 2.36 | 0.41 |
| 45:D5:98:MET:O | 45:D5:125:LEU:HA | 2.21 | 0.41 |
| 48:G5:38:GLN:HG2 | 48:G5:44:LEU:HD23 | 2.03 | 0.41 |
| 50:I5:58:ARG:HH22 | 50:I5:62:ARG:HD2 | 1.85 | 0.41 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 1:13:17:U:O2' | 1:13:1079:G:H1' | 2.21 | 0.40 |
| 1:13:27:G:C6 | 1:13:28:G:C5 | 3.09 | 0.40 |
| 1:13:369:C:O2' | 1:13:370:C:H5' | 2.21 | 0.40 |
| 1:13:649:G:C4 | 1:13:650:G:C8 | 3.09 | 0.40 |
| 1:13:820:U:H4' | 1:13:821:G:OP2 | 2.21 | 0.40 |
| 1:13:983:A:N1 | 1:13:1222:G:N2 | 2.68 | 0.40 |
| 1:13:985:C:N3 | 1:13:1221:G:C2 | 2.89 | 0.40 |
| 1:13:1171:G:H2' | 1:13:1172:C:C6 | 2.56 | 0.40 |
| 1:13:1399:C:C2 | 1:13:1502:A:N6 | 2.89 | 0.40 |
| 1:13:1412:C:H2' | 1:13:1413:A:H8 | 1.85 | 0.40 |
| 3:2E:29:TYR:OH | 14:5I:54:PRO:HD2 | 2.21 | 0.40 |
| 7:6E:73:MET:HA | 7:6E:90:GLU:HA | 2.02 | 0.40 |
| 13:4I:66:LEU:O | 13:4I:69:GLU:HB3 | 2.21 | 0.40 |
| 14:5I:12:ARG:C | 14:5I:14:PRO:HD3 | 2.46 | 0.40 |
| 24:1H:23:G:OP1 | 24:1H:504:U:N3 | 2.54 | 0.40 |
| 24:1H:51:G:N3 | 24:1H:119:A:C2 | 2.89 | 0.40 |
| 24:1H:141(A):C:H2' | 24:1H:142:G:O4' | 2.22 | 0.40 |
| 24:1H:153:C:H2' | 24:1H:154:G:O4' | 2.21 | 0.40 |
| 24:1H:182:A:H2' | 24:1H:183:C:O4' | 2.21 | 0.40 |
| 24:1H:647:G:H8 | 24:1H:647:G:O5' | 2.04 | 0.40 |
| 24:1H:1154:G:H8 | 24:1H:1154:G:O5' | 2.03 | 0.40 |
| 24:1H:1443:G:C2 | 24:1H:1549:C:C2 | 3.09 | 0.40 |
| 24:1H:1479:G:O2' | 24:1H:1558:A:H5' | 2.21 | 0.40 |
| 24:1H:1859:A:N6 | 24:1H:1883:G:O2' | 2.54 | 0.40 |
| 24:1H:2138:C:H2' | 24:1H:2139:C:C6 | 2.56 | 0.40 |
| 24:1H:2408:U:O2' | 24:1H:2409:G:H5' | 2.21 | 0.40 |
| 24:1H:2663:G:C6 | 24:1H:2664:G:C4 | 3.09 | 0.40 |
| 28:21:116:VAL:HG11 | 28:21:138:PRO:HB3 | 2.02 | 0.40 |
| 30:41:121:ASN:O | 30:41:131:TYR:OH | 2.26 | 0.40 |
| 31:51:103:LEU:HD22 | 31:51:131:VAL:HG21 | 2.02 | 0.40 |
| 36:88:20:ALA:O | 45:H8:79:ARG:NH2 | 2.54 | 0.40 |
| 40:C8:88:ILE:HG22 | 40:C8:90:VAL:HG12 | 2.03 | 0.40 |
| 44:G8:28:LYS:HE3 | 44:G8:28:LYS:HB2 | 1.79 | 0.40 |
| 46:I8:36:ILE:HD13 | 46:I8:58:THR:CG2 | 2.51 | 0.40 |
| 1:1G:300:A:H1' | 1:1G:565:U:O2 | 2.21 | 0.40 |
| 1:1G:518:C:C5 | 1:1G:530:G:H5' | 2.56 | 0.40 |
| 1:1G:544:G:OP1 | 4:32:62:GLN:NE2 | 2.29 | 0.40 |
| 3:22:34:LEU:HD12 | 3:22:34:LEU:O | 2.20 | 0.40 |
| 4:32:138:TYR:CD1 | 4:32:138:TYR:C | 2.99 | 0.40 |
| 7:62:51:GLN:HA | 7:62:54:THR:O | 2.21 | 0.40 |
| 10:1A:10:GLY:H | 10:1A:16:LEU:HD11 | 1.86 | 0.40 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 12:3A:59:ARG:HA | 12:3A:65:GLU:HA | 2.03 | 0.40 |
| 16:7A:58:TYR:O | 16:7A:61:SER:HB3 | 2.21 | 0.40 |
| 22:2L:18:G:O4' | 22:2L:66:G:N2 | 2.54 | 0.40 |
| 24:14:236:C:H2' | 24:14:237:C:H6 | 1.86 | 0.40 |
| 24:14:244:A:O3' | 35:35:74:GLU:HB3 | 2.20 | 0.40 |
| 24:14:478:A:H62 | 24:14:502:A:N6 | 2.19 | 0.40 |
| 24:14:729:G:OP2 | 27:19:13:ARG:NH1 | 2.45 | 0.40 |
| 24:14:814:C:H42 | 24:14:1193:G:H1 | 1.69 | 0.40 |
| 24:14:1200:C:P | 57:14:3551:HOH:O | 2.76 | 0.40 |
| 24:14:1366:A:H2' | 24:14:1367:A:O4' | 2.21 | 0.40 |
| 24:14:1581:G:H5" | 24:14:1581:G:C8 | 2.55 | 0.40 |
| 24:14:2012:G:OP1 | 42:A5:11:ARG:NH2 | 2.54 | 0.40 |
| 24:14:2055:C:OP1 | 24:14:2056:G:H4' | 2.21 | 0.40 |
| 24:14:2141:G:C6 | 24:14:2151:G:C6 | 3.09 | 0.40 |
| 24:14:2584:U:H6 | 24:14:2585:U:H5 | 1.68 | 0.40 |
| 24:14:2757:A:N1 | 31:59:67:LEU:HD21 | 2.36 | 0.40 |
| 26:79:26:ALA:O | 26:79:29:VAL:HG12 | 2.21 | 0.40 |
| 26:79:212:VAL:HG21 | 26:79:226:PRO:HD3 | 2.02 | 0.40 |
| 28:29:54:GLN:O | 28:29:55:ASN:ND2 | 2.54 | 0.40 |
| 28:29:105:THR:OG1 | 28:29:199:ARG:NH2 | 2.34 | 0.40 |
| 30:49:81:LYS:HG3 | 30:49:86:MET:HE1 | 2.03 | 0.40 |
| 31:59:9:ILE:HG23 | 31:59:51:ARG:HB3 | 2.03 | 0.40 |
| 31:59:103:LEU:HG | 31:59:115:VAL:HB | 2.03 | 0.40 |
| 32:69:44:LEU:HD23 | 32:69:44:LEU:HA | 1.55 | 0.40 |
| 32:69:68:LEU:HA | 32:69:71:ILE:HG22 | 2.01 | 0.40 |
| 33:15:90:MET:HE2 | 33:15:90:MET:HA | 2.03 | 0.40 |
| 34:25:22:ILE:HA | 34:25:22:ILE:HD13 | 1.43 | 0.40 |
| 36:45:7:MET:HB3 | 36:45:7:MET:HE3 | 1.40 | 0.40 |
| 37:55:24:GLN:HB3 | 37:55:44:LEU:HD11 | 2.03 | 0.40 |
| 40:85:58:ARG:HA | 40:85:61:TRP:CE3 | 2.57 | 0.40 |
| 45:D5:28:MET:HB3 | 45:D5:28:MET:HE2 | 1.82 | 0.40 |
| 45:D5:54:HIS:HB3 | 45:D5:101:PRO:HD3 | 2.02 | 0.40 |
| 45:D5:100:VAL:HG12 | 45:D5:101:PRO:HD2 | 2.03 | 0.40 |
| 48:G5:4:SER:HB3 | 48:G5:5:GLU:OE2 | 2.21 | 0.40 |
| 1:13:235:C:H2' | 1:13:236:G:C8 | 2.57 | 0.40 |
| 1:13:662:G:H2' | 1:13:663:A:C8 | 2.56 | 0.40 |
| 1:13:922:G:C2 | 1:13:923:A:C4 | 3.10 | 0.40 |
| 1:13:1072:G:H2' | 1:13:1073:U:C6 | 2.56 | 0.40 |
| 1:13:1121:U:C4 | 1:13:1122:U:C4 | 3.09 | 0.40 |
| 1:13:1304:G:OP1 | 21:1F:2:GLY:N | 2.54 | 0.40 |
| 6:5E:97:PHE:O | 18:9I:31:LEU:N | 2.35 | 0.40 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 8:7E:82:HIS:CD2 | 8:7E:82:HIS:C | 2.98 | 0.40 |
| 9:8E:4:TYR:CZ | 9:8E:88:TYR:HB2 | 2.56 | 0.40 |
| 22:2K:19:C:H3' | 22:2K:20:C:H3' | 2.03 | 0.40 |
| 24:1H:107:C:O2' | 24:1H:108:U:H5' | 2.22 | 0.40 |
| 24:1H:705:A:O3' | 27:11:7:LYS:HD2 | 2.21 | 0.40 |
| 24:1H:1048:A:C6 | 24:1H:1049:C:C4 | 3.09 | 0.40 |
| 24:1H:1688:U:O2 | 24:1H:1700:A:H8 | 2.05 | 0.40 |
| 24:1H:1728:G:N2 | 24:1H:1730:U:OP2 | 2.54 | 0.40 |
| 24:1H:2077:A:H2' | 24:1H:2078:C:C6 | 2.53 | 0.40 |
| 24:1H:2115:G:H8 | 24:1H:2115:G:O5' | 2.04 | 0.40 |
| 24:1H:2303:G:C6 | 24:1H:2314:C:N4 | 2.90 | 0.40 |
| 24:1H:2751:G:N2 | 31:51:3:ARG:HG2 | 2.35 | 0.40 |
| 26:71:6:ARG:HG2 | 26:71:34:THR:HB | 2.02 | 0.40 |
| 28:21:100:GLU:O | 28:21:172:VAL:HG23 | 2.20 | 0.40 |
| 29:31:112:MET:HB3 | 29:31:112:MET:HE3 | 1.85 | 0.40 |
| 36:88:12:GLN:HE21 | 36:88:72:LYS:HG3 | 1.87 | 0.40 |
| 36:88:54:MET:O | 36:88:57:HIS:N | 2.51 | 0.40 |
| 37:98:60:LEU:O | 37:98:64:ARG:HG3 | 2.21 | 0.40 |
| 45:H8:76:LEU:HD23 | 45:H8:76:LEU:N | 2.36 | 0.40 |
| 1:1G:38:G:H22 | 1:1G:397:A:H5" | 1.85 | 0.40 |
| 1:1G:255:G:OP1 | 17:8A:69:LYS:NZ | 2.51 | 0.40 |
| 1:1G:390:C:H2' | 1:1G:391:G:C8 | 2.56 | 0.40 |
| 1:1G:474:G:H2' | 1:1G:475:G:H8 | 1.86 | 0.40 |
| 1:1G:711:G:P | 6:52:54:LYS:HZ1 | 2.35 | 0.40 |
| 1:1G:1355:G:H2' | 1:1G:1356:G:O4' | 2.21 | 0.40 |
| 1:1G:1394:A:C5 | 1:1G:1501:C:H4' | 2.56 | 0.40 |
| 1:1G:1481:U:H2' | 1:1G:1482:G:C8 | 2.56 | 0.40 |
| 2:12:128:GLU:HG3 | 2:12:129:GLU:CD | 2.47 | 0.40 |
| 4:32:12:CYS:HA | 4:32:19:LEU:HD12 | 2.04 | 0.40 |
| 4:32:38:TYR:CD2 | 4:32:45:GLN:HB3 | 2.57 | 0.40 |
| 4:32:108:LEU:HD12 | 4:32:108:LEU:HA | 1.74 | 0.40 |
| 5:42:137:GLU:O | 5:42:141:GLN:HB2 | 2.21 | 0.40 |
| 6:52:45:LEU:HD13 | 6:52:57:GLN:OE1 | 2.21 | 0.40 |
| 7:62:69:VAL:HG13 | 7:62:134:ALA:O | 2.21 | 0.40 |
| 10:1A:63:PHE:CD1 | 14:5A:58:LYS:HA | 2.57 | 0.40 |
| 15:6A:88:ARG:HB3 | 15:6A:89:GLY:H | 1.74 | 0.40 |
| 20:BA:54:LYS:HB2 | 20:BA:54:LYS:HE3 | 1.82 | 0.40 |
| 22:3L:35:QUO:H101 | 22:3L:35:QUO:H162 | 1.82 | 0.40 |
| 24:14:839:U:H1' | 24:14:1191:G:H1' | 2.03 | 0.40 |
| 24:14:1274:A:N1 | 24:14:1644:C:O2' | 2.49 | 0.40 |
| 24:14:1528:A:C2 | 24:14:1543:A:C2 | 3.09 | 0.40 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 24:14:1808:U:H2' | 24:14:1809:A:O4' | 2.21 | 0.40 |
| 24:14:2191:G:C5 | 24:14:2192:G:C8 | 3.09 | 0.40 |
| 24:14:2212:A:H1' | 24:14:2215:G:C5 | 2.56 | 0.40 |
| 24:14:2303:G:O2' | 30:49:132:ASN:HB2 | 2.21 | 0.40 |
| 24:14:2485:G:H5" | 36:45:46:GLN:HE21 | 1.86 | 0.40 |
| 24:14:2584:U:H6 | 24:14:2585:U:C5 | 2.39 | 0.40 |
| 24:14:2652:C:C2 | 24:14:2669:G:C2 | 3.09 | 0.40 |
| 24:14:2778:A:H4' | 24:14:2779:U:OP2 | 2.20 | 0.40 |
| 24:14:2861:G:H2' | 24:14:2862:G:C8 | 2.54 | 0.40 |
| 28:29:111:ARG:HA | 37:55:2:ARG:HH12 | 1.86 | 0.40 |
| 31:59:3:ARG:CG | 31:59:4:ILE:HG13 | 2.51 | 0.40 |
| 31:59:7:LEU:HD12 | 31:59:8:PRO:HD3 | 2.03 | 0.40 |
| 35:35:52:GLU:OE2 | 35:35:53:GLY:N | 2.54 | 0.40 |
| 35:35:96:THR:HG23 | 35:35:99:LEU:HB2 | 2.03 | 0.40 |
| 37:55:84:ALA:HB3 | 37:55:85:PRO:HD3 | 2.04 | 0.40 |
| 38:65:50:SER:O | 38:65:76:LYS:NZ | 2.52 | 0.40 |
| 43:B5:49:VAL:HB | 43:B5:83:VAL:CG2 | 2.49 | 0.40 |
| 50:I5:37:SER:HG | 50:I5:38:LYS:H | 1.58 | 0.40 |
| 1:13:62:U:O2' | 1:13:379:C:O2 | 2.34 | 0.40 |
| 1:13:198:G:C6 | 1:13:220:G:C2 | 3.09 | 0.40 |
| 1:13:894:G:H2' | 1:13:895:G:O4' | 2.21 | 0.40 |
| 1:13:1000:A:H2' | 1:13:1001:G:O4' | 2.21 | 0.40 |
| 1:13:1288:A:H8 | 1:13:1288:A:O5' | 2.05 | 0.40 |
| 1:13:1348:U:N3 | 1:13:1374:A:H2 | 1.97 | 0.40 |
| 1:13:1399:C:H4' | 1:13:1400:C:O5' | 2.20 | 0.40 |
| 4:3E:64:LEU:O | 4:3E:67:ILE:HB | 2.21 | 0.40 |
| 5:4E:137:GLU:HG2 | 5:4E:140:ARG:HH21 | 1.85 | 0.40 |
| 7:6E:65:ALA:HB1 | 7:6E:127:ALA:HB3 | 2.03 | 0.40 |
| 8:7E:82:HIS:NE2 | 8:7E:136:GLU:OE2 | 2.54 | 0.40 |
| 10:1I:55:LYS:HB3 | 10:1I:56:HIS:CD2 | 2.56 | 0.40 |
| 11:2I:15:ALA:HA | 11:2I:76:GLY:O | 2.20 | 0.40 |
| 14:5I:44:LEU:O | 14:5I:44:LEU:HD12 | 2.22 | 0.40 |
| 20:BI:71:THR:HB | 20:BI:72:LEU:H | 1.57 | 0.40 |
| 22:2K:38:MIA:H112 | 22:2K:39:A:H1' | 2.04 | 0.40 |
| 24:1H:164:U:H6 | 24:1H:165:U:C6 | 2.40 | 0.40 |
| 24:1H:248:G:H5' | 24:1H:250:G:N7 | 2.37 | 0.40 |
| 24:1H:638:G:H2' | 24:1H:639:U:C6 | 2.56 | 0.40 |
| 24:1H:640:C:H42 | 24:1H:648:G:H1 | 1.69 | 0.40 |
| 24:1H:1231:G:H2' | 24:1H:1232:G:H8 | 1.85 | 0.40 |
| 24:1H:1528:A:C2 | 24:1H:1542:G:C2 | 3.09 | 0.40 |
| 24:1H:1729:A:H2' | 24:1H:1731:G:N7 | 2.36 | 0.40 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 24:1H:2095:C:C4 | 24:1H:2096:U:C5 | 3.09 | 0.40 |
| 24:1H:2129:C:H2' | 24:1H:2130:U:O4' | 2.22 | 0.40 |
| 24:1H:2370:G:H2' | 24:1H:2371:G:O4' | 2.21 | 0.40 |
| 24:1H:2756:U:H4' | 24:1H:2757:A:OP1 | 2.20 | 0.40 |
| 24:1H:2771:C:H4' | 28:21:202:LYS:HG2 | 2.03 | 0.40 |
| 26:71:202:GLU:C | 26:71:204:ALA:H | 2.29 | 0.40 |
| 29:31:33:LEU:HD12 | 29:31:33:LEU:HA | 1.96 | 0.40 |
| 30:41:6:ALA:HB3 | 50:M8:23:GLU:HG3 | 2.03 | 0.40 |
| 30:41:105:LYS:O | 30:41:109:VAL:HB | 2.21 | 0.40 |
| 31:51:40:GLU:OE1 | 31:51:61:HIS:NE2 | 2.37 | 0.40 |
| 31:51:154:PRO:HD3 | 31:51:162:ILE:O | 2.22 | 0.40 |
| 35:78:59:LEU:HD21 | 54:Q8:10:ALA:HA | 2.03 | 0.40 |
| 36:88:29:PHE:HB3 | 36:88:65:PHE:CE1 | 2.56 | 0.40 |
| 39:B8:86:ILE:HD13 | 39:B8:86:ILE:HG21 | 1.73 | 0.40 |
| 51:N8:49:CYS:HB3 | 51:N8:56:LYS:HD2 | 2.03 | 0.40 |
| 1:1G:409:G:C6 | 1:1G:410:G:C4 | 3.10 | 0.40 |
| 1:1G:518:C:C4 | 1:1G:530:G:C5 | 3.10 | 0.40 |
| 1:1G:624:C:O3' | 16:7A:10:GLY:HA2 | 2.21 | 0.40 |
| 1:1G:922:G:H4' | 5:42:20:GLN:HA | 2.03 | 0.40 |
| 1:1G:953:G:C6 | 1:1G:954:G:C4 | 3.10 | 0.40 |
| 1:1G:979:C:C5 | 1:1G:980:C:C6 | 3.10 | 0.40 |
| 1:1G:1199:U:H5' | 10:1A:54:PHE:CE2 | 2.56 | 0.40 |
| 9:82:104:ARG:HD2 | 9:82:104:ARG:C | 2.47 | 0.40 |
| 19:AA:81:ARG:HE | 19:AA:81:ARG:HB2 | 1.25 | 0.40 |
| 24:14:106:C:HO2' | 24:14:294:A:HO2' | 1.65 | 0.40 |
| 24:14:370:G:OP2 | 24:14:370:G:H8 | 2.04 | 0.40 |
| 24:14:489:G:C6 | 24:14:491:G:C5 | 3.09 | 0.40 |
| 24:14:699:A:H4' | 24:14:1634:A:N7 | 2.36 | 0.40 |
| 24:14:839:U:H2' | 24:14:840:C:C6 | 2.57 | 0.40 |
| 24:14:1060:U:H1' | 24:14:1062:G:H5' | 2.02 | 0.40 |
| 24:14:1072:C:H42 | 24:14:1092:C:H41 | 1.70 | 0.40 |
| 24:14:1301:A:H2 | 24:14:1626:G:H21 | 1.69 | 0.40 |
| 24:14:1329:U:H5" | 24:14:1330:C:C5 | 2.49 | 0.40 |
| 24:14:1385:G:C4 | 24:14:1386:C:C5 | 3.09 | 0.40 |
| 24:14:1444(A):A:H5" | 24:14:1445:C:H5 | 1.86 | 0.40 |
| 24:14:2118:U:H5" | 24:14:2119:A:OP1 | 2.21 | 0.40 |
| 24:14:2494:G:O2' | 36:45:80:GLU:HA | 2.22 | 0.40 |
| 24:14:2876:G:O5' | 39:75:2:ASN:HA | 2.21 | 0.40 |
| 25:1J:25:A:H2' | 25:1J:26:A:O4' | 2.21 | 0.40 |
| 26:79:185:LEU:HD23 | 26:79:185:LEU:HA | 1.94 | 0.40 |
| 27:19:68:LYS:HB3 | 27:19:70:TRP:CZ3 | 2.56 | 0.40 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 28:29:5:LEU:HD23 | 28:29:5:LEU:N | 2.36 | 0.40 |
| 28:29:63:LEU:O | 28:29:66:HIS:ND1 | 2.54 | 0.40 |
| 29:39:125:LEU:HD21 | 29:39:199:TRP:CD1 | 2.56 | 0.40 |
| 31:59:4:ILE:HD12 | 31:59:5:GLY:H | 1.85 | 0.40 |
| 31:59:74:ASN:OD1 | 31:59:74:ASN:N | 2.55 | 0.40 |
| 32:69:91:SER:HB3 | 32:69:121:LYS:CD | 2.51 | 0.40 |
| 34:25:20:MET:HE3 | 34:25:20:MET:HB2 | 1.75 | 0.40 |
| 46:E5:24:LYS:HA | 46:E5:24:LYS:HD3 | 1.84 | 0.40 |
| 1:13:55:A:H2 | 32:69:82:ARG:HG3 | 1.86 | 0.40 |
| 1:13:60:A:N1 | 1:13:107:G:O2' | 2.44 | 0.40 |
| 1:13:140:A:C5 | 1:13:141:A:N7 | 2.90 | 0.40 |
| 1:13:654:G:H8 | 1:13:654:G:O5' | 2.03 | 0.40 |
| 1:13:659:U:C2 | 1:13:660:G:C8 | 3.09 | 0.40 |
| 1:13:688:G:H2' | 1:13:689:C:C6 | 2.54 | 0.40 |
| 1:13:791:G:O2' | 1:13:792:A:H5' | 2.21 | 0.40 |
| 1:13:877:C:H5" | 8:7E:88:LYS:CD | 2.51 | 0.40 |
| 1:13:878:G:H1' | 8:7E:3:THR:HG21 | 2.02 | 0.40 |
| 2:1E:39:ILE:HG22 | 2:1E:40:HIS:O | 2.21 | 0.40 |
| 4:3E:25:ARG:NH1 | 4:3E:30:LYS:HZ2 | 2.14 | 0.40 |
| 5:4E:36:ASP:CG | 5:4E:38:GLN:HB2 | 2.46 | 0.40 |
| 6:5E:2:ARG:O | 6:5E:66:GLU:HA | 2.21 | 0.40 |
| 8:7E:87:SER:CB | 8:7E:93:VAL:H | 2.35 | 0.40 |
| 9:8E:18:PHE:HB2 | 9:8E:62:TYR:O | 2.21 | 0.40 |
| 9:8E:95:LYS:HB2 | 9:8E:95:LYS:HE3 | 1.82 | 0.40 |
| 9:8E:117:HIS:HB2 | 9:8E:121:ARG:O | 2.22 | 0.40 |
| 10:1I:13:HIS:CE1 | 10:1I:14:LYS:HG2 | 2.57 | 0.40 |
| 12:3I:110:VAL:HG23 | 12:3I:120:TYR:HB3 | 2.01 | 0.40 |
| 15:6I:13:GLN:H | 15:6I:13:GLN:HG3 | 1.73 | 0.40 |
| 19:AI:6:LYS:HB3 | 19:AI:7:LYS:H | 1.77 | 0.40 |
| 24:1H:36:G:C5 | 24:1H:37:C:C5 | 3.10 | 0.40 |
| 24:1H:57:C:H2' | 24:1H:58:G:O4' | 2.20 | 0.40 |
| 24:1H:619:G:H5" | 24:1H:620:G:OP2 | 2.22 | 0.40 |
| 24:1H:649:G:H2' | 24:1H:650:C:C6 | 2.57 | 0.40 |
| 24:1H:782:A:H5' | 24:1H:783:A:C2 | 2.57 | 0.40 |
| 24:1H:930:U:O2 | 24:1H:930:U:O4' | 2.39 | 0.40 |
| 24:1H:1049:C:C2' | 24:1H:1050:A:H5' | 2.52 | 0.40 |
| 24:1H:1142(A):A:C4 | 24:1H:1144:G:C8 | 3.09 | 0.40 |
| 24:1H:1488:G:C5 | 24:1H:1489:U:C5 | 3.10 | 0.40 |
| 24:1H:1658:C:H2' | 24:1H:1659:U:C6 | 2.55 | 0.40 |
| 24:1H:1668:A:H4' | 24:1H:1669:A:O5' | 2.22 | 0.40 |
| 24:1H:1826:G:H2' | 24:1H:1827:C:H6 | 1.87 | 0.40 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 24:1H:2029:G:H2' | 24:1H:2031:A:OP1 | 2.21 | 0.40 |
| 24:1H:2314:C:C2 | 24:1H:2315:G:C8 | 3.09 | 0.40 |
| 24:1H:2492:U:H2' | 24:1H:2493:U:C6 | 2.56 | 0.40 |
| 24:1H:2773:C:H5" | 28:21:164:ARG:HG2 | 2.02 | 0.40 |
| 24:1H:2815:C:H2' | 24:1H:2816:C:C6 | 2.56 | 0.40 |
| 24:1H:2881:C:H2' | 24:1H:2882:A:C8 | 2.56 | 0.40 |
| 25:16:81:G:C6 | 25:16:82:G:C5 | 3.09 | 0.40 |
| 27:11:122:ASP:O | 27:11:123:ALA:HB3 | 2.21 | 0.40 |
| 28:21:46:ALA:HB2 | 28:21:82:ARG:HA | 2.03 | 0.40 |
| 28:21:101:ARG:HD2 | 28:21:101:ARG:HA | 1.84 | 0.40 |
| 29:31:33:LEU:HD13 | 29:31:112:MET:HE2 | 2.03 | 0.40 |
| 29:31:68:LYS:HE3 | 29:31:68:LYS:HB3 | 1.69 | 0.40 |
| 31:51:54:ARG:HA | 31:51:55:PRO:HD3 | 1.73 | 0.40 |
| 32:61:118:LYS:HG3 | 32:61:119:PRO:HD2 | 2.03 | 0.40 |
| 40:C8:92:ARG:HA | 40:C8:95:LEU:HB2 | 2.04 | 0.40 |
| 41:D8:93:GLU:O | 41:D8:94:LEU:HD23 | 2.21 | 0.40 |
| 45:H8:52:SER:O | 45:H8:54:HIS:N | 2.54 | 0.40 |
| 45:H8:52:SER:C | 45:H8:54:HIS:N | 2.79 | 0.40 |
| 45:H8:102:LEU:HG | 45:H8:123:ASP:HA | 2.02 | 0.40 |
| 46:I8:45:PHE:CE2 | 46:I8:69:PHE:HE2 | 2.40 | 0.40 |
| 1:1G:8:A:C5 | 4:32:209:ARG:HA | 2.57 | 0.40 |
| 1:1G:309:G:O2' | 1:1G:607:A:N1 | 2.53 | 0.40 |
| 1:1G:623:C:C4 | 1:1G:624:C:C5 | 3.10 | 0.40 |
| 1:1G:1106:G:H4' | 3:22:171:GLY:O | 2.21 | 0.40 |
| 3:22:164:ARG:HG2 | 3:22:165:THR:H | 1.86 | 0.40 |
| 5:42:19:MET:HE2 | 5:42:19:MET:HB2 | 1.92 | 0.40 |
| 6:52:87:ARG:HG3 | 6:52:87:ARG:NH1 | 2.05 | 0.40 |
| 7:62:73:MET:HG3 | 7:62:89:MET:O | 2.22 | 0.40 |
| 9:82:42:ARG:O | 9:82:43:ALA:C | 2.64 | 0.40 |
| 12:3A:62:SER:HB2 | 12:3A:64:TYR:HB2 | 2.03 | 0.40 |
| 16:7A:58:TYR:O | 16:7A:62:VAL:HG22 | 2.22 | 0.40 |
| 22:2L:35:QUO:C6 | 22:2L:36:U:C4 | 3.04 | 0.40 |
| 22:3L:16:C:N4 | 22:3L:68:A:C4 | 2.90 | 0.40 |
| 24:14:105:C:H2' | 24:14:106:C:C6 | 2.56 | 0.40 |
| 24:14:224:G:N7 | 24:14:420:C:H4' | 2.37 | 0.40 |
| 24:14:638:G:C5 | 24:14:651:G:C2 | 3.09 | 0.40 |
| 24:14:649:G:H2' | 24:14:650:C:O4' | 2.22 | 0.40 |
| 24:14:1111:A:H4' | 31:59:3:ARG:H | 1.86 | 0.40 |
| 24:14:1416:G:HO2' | 24:14:1417:C:H6 | 1.68 | 0.40 |
| 24:14:2365:G:H2' | 24:14:2366:A:C8 | 2.57 | 0.40 |
| 24:14:2839:G:C5' | 37:55:46:GLY:HA2 | 2.52 | 0.40 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 24:14:2859:G:C8 | 24:14:2859:G:C3' | 3.04 | 0.40 |
| 28:29:111:ARG:HB2 | 28:29:160:TYR:O | 2.22 | 0.40 |
| 32:69:120:ILE:HD12 | 32:69:126:TYR:CD2 | 2.57 | 0.40 |
| 33:15:112:LEU:HA | 33:15:112:LEU:HD12 | 1.76 | 0.40 |
| 34:25:68:GLU:H | 34:25:68:GLU:CD | 2.29 | 0.40 |
| 36:45:70:PRO:HA | 36:45:94:VAL:O | 2.22 | 0.40 |
| 37:55:57:ARG:HH11 | 37:55:57:ARG:CG | 2.26 | 0.40 |
| 37:55:70:LEU:HA | 37:55:70:LEU:HD23 | 1.79 | 0.40 |
| 44:C5:31:LEU:HD12 | 44:C5:36:ALA:HB3 | 2.04 | 0.40 |
| 48:G5:28:LYS:HD3 | 48:G5:28:LYS:HA | 1.91 | 0.40 |
| 53:L5:30:VAL:H | 53:L5:30:VAL:HG23 | 1.67 | 0.40 |
| 1:13:109:A:H2' | 1:13:326:G:N2 | 2.37 | 0.40 |
| 1:13:123:C:OP1 | 1:13:312:C:H5' | 2.21 | 0.40 |
| 1:13:391:G:C6 | 1:13:392:G:C5 | 3.09 | 0.40 |
| 1:13:452:A:H62 | 1:13:480:U:H3 | 1.68 | 0.40 |
| 1:13:836:G:OP1 | 18:9I:61:LYS:NZ | 2.54 | 0.40 |
| 1:13:1057:G:H2' | 1:13:1058:G:O4' | 2.21 | 0.40 |
| 1:13:1335:C:H5" | 1:13:1336:C:OP1 | 2.21 | 0.40 |
| 1:13:1369:C:H2' | 1:13:1370:G:C8 | 2.56 | 0.40 |
| 2:1E:219:VAL:HA | 2:1E:222:ILE:CD1 | 2.51 | 0.40 |
| 6:5E:67:MET:HB2 | 6:5E:68:PRO:HD2 | 2.04 | 0.40 |
| 6:5E:96:PRO:HB3 | 18:9I:30:ASP:CG | 2.47 | 0.40 |
| 9:8E:28:VAL:HA | 9:8E:63:ILE:O | 2.22 | 0.40 |
| 10:1I:48:THR:CG2 | 10:1I:62:HIS:HB3 | 2.38 | 0.40 |
| 15:6I:4:THR:OG1 | 15:6I:6:GLU:HG2 | 2.21 | 0.40 |
| 22:2K:17:OMG:H5" | 22:2K:69:U:O2 | 2.21 | 0.40 |
| 22:2K:17:OMG:C5 | 22:2K:66:G:C6 | 3.10 | 0.40 |
| 24:1H:66:C:H2' | 24:1H:67:U:C6 | 2.57 | 0.40 |
| 24:1H:307:G:H22 | 24:1H:310:A:P | 2.45 | 0.40 |
| 24:1H:630:G:N2 | 24:1H:632:A:H3' | 2.36 | 0.40 |
| 24:1H:868:U:H2' | 24:1H:869:G:O4' | 2.21 | 0.40 |
| 24:1H:1575:C:H2' | 24:1H:1576:U:O4' | 2.21 | 0.40 |
| 24:1H:2179:C:H2' | 24:1H:2180:U:C6 | 2.56 | 0.40 |
| 24:1H:2210:G:H5" | 24:1H:2211:G:C5 | 2.55 | 0.40 |
| 24:1H:2433:A:H5" | 24:1H:2434:A:OP1 | 2.22 | 0.40 |
| 24:1H:2556:C:H2' | 24:1H:2557:G:O4' | 2.21 | 0.40 |
| 24:1H:2676:C:N4 | 57:1H:3852:HOH:O | 2.53 | 0.40 |
| 24:1H:2861:G:H2' | 24:1H:2862:G:C8 | 2.57 | 0.40 |
| 25:16:63:G:H2' | 25:16:64:C:H6 | 1.83 | 0.40 |
| 27:11:182:LEU:HA | 27:11:182:LEU:HD23 | 1.83 | 0.40 |
| 28:21:26:ILE:HD13 | 28:21:26:ILE:C | 2.47 | 0.40 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 31:51:10:PRO:HD3 | 31:51:69:ARG:CD | 2.51 | 0.40 |
| 31:51:90:LYS:O | 31:51:94:TYR:HD2 | 2.05 | 0.40 |
| 31:51:150:ALA:O | 31:51:153:LYS:HG3 | 2.21 | 0.40 |
| 33:58:40:PRO:HB3 | 40:C8:68:ALA:HB2 | 2.04 | 0.40 |
| 36:88:66:ILE:HG22 | 36:88:67:ARG:N | 2.37 | 0.40 |
| 37:98:44:LEU:HA | 37:98:44:LEU:HD23 | 1.88 | 0.40 |
| 38:A8:10:ARG:HG3 | 38:A8:13:ARG:NH1 | 2.36 | 0.40 |
| 42:E8:72:LYS:HB3 | 42:E8:106:ILE:HD11 | 2.01 | 0.40 |
| 51:N8:56:LYS:C | 51:N8:58:LEU:H | 2.30 | 0.40 |
| 1:1G:486:U:O2 | 1:1G:486:U:H2' | 2.22 | 0.40 |
| 1:1G:865:A:H5' | 1:1G:1078:U:C5 | 2.56 | 0.40 |
| 1:1G:1409:C:C2' | 1:1G:1410:G:H5' | 2.52 | 0.40 |
| 2:12:10:LEU:HD12 | 2:12:10:LEU:HA | 1.87 | 0.40 |
| 2:12:16:HIS:HD2 | 2:12:209:ARG:CZ | 2.35 | 0.40 |
| 5:42:107:ARG:O | 5:42:108:ALA:C | 2.64 | 0.40 |
| 10:1A:80:LYS:HA | 10:1A:80:LYS:HD2 | 1.90 | 0.40 |
| 18:9A:36:ASN:OD1 | 18:9A:36:ASN:N | 2.53 | 0.40 |
| 22:3L:25:G:H2' | 22:3L:26:G:C8 | 2.46 | 0.40 |
| 24:14:63:U:H6 | 24:14:63:U:H2' | 1.72 | 0.40 |
| 24:14:150:C:H2' | 24:14:151:C:H6 | 1.85 | 0.40 |
| 24:14:459:U:H4' | 53:L5:40:TRP:CZ3 | 2.56 | 0.40 |
| 24:14:511:U:H3' | 24:14:512:G:H5" | 2.03 | 0.40 |
| 24:14:837:C:H6 | 24:14:837:C:O5' | 2.05 | 0.40 |
| 24:14:951:C:O2' | 24:14:952:G:H5' | 2.21 | 0.40 |
| 24:14:1000:A:C6 | 24:14:1001:A:C6 | 3.09 | 0.40 |
| 24:14:1050:A:C6 | 24:14:2751:G:N7 | 2.89 | 0.40 |
| 24:14:1385:G:O2' | 24:14:1396:U:C6 | 2.73 | 0.40 |
| 24:14:1461:G:H2' | 24:14:1462:C:C6 | 2.56 | 0.40 |
| 24:14:1805:U:O2 | 27:19:50:THR:HB | 2.21 | 0.40 |
| 24:14:2286:A:C8 | 24:14:2287:A:C6 | 3.09 | 0.40 |
| 24:14:2469:A:H3' | 24:14:2470:G:H8 | 1.86 | 0.40 |
| 24:14:2479:G:H2' | 24:14:2480:C:O4' | 2.21 | 0.40 |
| 24:14:2694:G:H2' | 24:14:2695:C:H6 | 1.86 | 0.40 |
| 24:14:2850:A:H3' | 24:14:2851:A:H8 | 1.87 | 0.40 |
| 25:1J:13:A:O2' | 25:1J:14:U:H3' | 2.22 | 0.40 |
| 27:19:112:GLN:HB2 | 27:19:115:GLN:HE21 | 1.86 | 0.40 |
| 27:19:244:ARG:HB2 | 27:19:245:PRO:HD2 | 2.04 | 0.40 |
| 32:69:56:LYS:O | 32:69:56:LYS:HG2 | 2.21 | 0.40 |
| 36:45:51:ARG:O | 36:45:54:MET:N | 2.50 | 0.40 |
| 36:45:74:TYR:O | 36:45:90:VAL:HA | 2.21 | 0.40 |
| 38:65:3:ARG:HE | 38:65:4:LEU:N | 2.18 | 0.40 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 38:65:40:ILE:HG23 | 38:65:47:THR:HA | 2.03 | 0.40 |
| 40:85:92:ARG:HD2 | 41:95:11:GLN:CD | 2.46 | 0.40 |
| 40:85:92:ARG:CG | 40:85:94:ASN:HB3 | 2.51 | 0.40 |
| 40:85:98:LEU:O | 40:85:99:ALA:CB | 2.69 | 0.40 |
| 44:C5:6:HIS:CE1 | 44:C5:7:VAL:HG13 | 2.56 | 0.40 |
| 44:C5:50:ARG:HE | 44:C5:50:ARG:HB2 | 1.75 | 0.40 |
| 44:C5:75:ILE:HD12 | 44:C5:75:ILE:HA | 1.87 | 0.40 |

All (1) symmetry-related close contacts are listed below. The label for Atom-2 includes the symmetry operator and encoded unit-cell translations to be applied.

| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 6:5E:15:ASP:OD1 | 4:32:27:TYR:OH[4_555] | 2.04 | 0.16 |

## 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 |
|---|---|---|---|---|---|---|
| 2 | 12 | 235/256 (92%) | 196 (83%) | 35 (15%) | 4 (2%) | 7 30 |
| 2 | 1E | 235/256 (92%) | 199 (85%) | 32 (14%) | 4 (2%) | 7 30 |
| 3 | 22 | 204/239 (85%) | 175 (86%) | 29 (14%) | 0 | 100 100 |
| 3 | 2E | 203/239 (85%) | 185 (91%) | 18 (9%) | 0 | 100 100 |
| 4 | 32 | 206/209 (99%) | 176 (85%) | 26 (13%) | 4 (2%) | 6 27 |
| 4 | 3E | 206/209 (99%) | 191 (93%) | 15 (7%) | 0 | 100 100 |
| 5 | 42 | 149/162 (92%) | 142 (95%) | 7 (5%) | 0 | 100 100 |
| 5 | 4E | 149/162 (92%) | 141 (95%) | 7 (5%) | 1 (1%) | 18 49 |
| 6 | 52 | 99/101 (98%) | 95 (96%) | 4 (4%) | 0 | 100 100 |
| 6 | 5E | 99/101 (98%) | 93 (94%) | 6 (6%) | 0 | 100 100 |

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| Mol | Chain | Analysed | Favoured | Allowed | Outliers | Percentiles | |
|---|---|---|---|---|---|---|---|
| 7 | 62 | 153/156 (98%) | 145 (95%) | 8 (5%) | 0 | 100 | 100 |
| 7 | 6E | 153/156 (98%) | 142 (93%) | 11 (7%) | 0 | 100 | 100 |
| 8 | 72 | 136/138 (99%) | 127 (93%) | 7 (5%) | 2 (2%) | 8 | 32 |
| 8 | 7E | 136/138 (99%) | 125 (92%) | 11 (8%) | 0 | 100 | 100 |
| 9 | 82 | 125/128 (98%) | 112 (90%) | 12 (10%) | 1 (1%) | 16 | 47 |
| 9 | 8E | 125/128 (98%) | 114 (91%) | 11 (9%) | 0 | 100 | 100 |
| 10 | 1A | 97/105 (92%) | 85 (88%) | 12 (12%) | 0 | 100 | 100 |
| 10 | 1I | 97/105 (92%) | 84 (87%) | 13 (13%) | 0 | 100 | 100 |
| 11 | 2A | 114/129 (88%) | 102 (90%) | 12 (10%) | 0 | 100 | 100 |
| 11 | 2I | 114/129 (88%) | 102 (90%) | 11 (10%) | 1 (1%) | 14 | 44 |
| 12 | 3A | 123/132 (93%) | 111 (90%) | 12 (10%) | 0 | 100 | 100 |
| 12 | 3I | 123/132 (93%) | 112 (91%) | 11 (9%) | 0 | 100 | 100 |
| 13 | 4A | 115/126 (91%) | 98 (85%) | 12 (10%) | 5 (4%) | 2 | 12 |
| 13 | 4I | 114/126 (90%) | 98 (86%) | 16 (14%) | 0 | 100 | 100 |
| 14 | 5A | 58/61 (95%) | 48 (83%) | 10 (17%) | 0 | 100 | 100 |
| 14 | 5I | 58/61 (95%) | 52 (90%) | 5 (9%) | 1 (2%) | 7 | 30 |
| 15 | 6A | 86/89 (97%) | 80 (93%) | 6 (7%) | 0 | 100 | 100 |
| 15 | 6I | 86/89 (97%) | 77 (90%) | 9 (10%) | 0 | 100 | 100 |
| 16 | 7A | 82/88 (93%) | 76 (93%) | 5 (6%) | 1 (1%) | 10 | 37 |
| 16 | 7I | 82/88 (93%) | 79 (96%) | 3 (4%) | 0 | 100 | 100 |
| 17 | 8A | 98/105 (93%) | 92 (94%) | 6 (6%) | 0 | 100 | 100 |
| 17 | 8I | 98/105 (93%) | 90 (92%) | 7 (7%) | 1 (1%) | 12 | 41 |
| 18 | 9A | 70/88 (80%) | 65 (93%) | 5 (7%) | 0 | 100 | 100 |
| 18 | 9I | 70/88 (80%) | 63 (90%) | 6 (9%) | 1 (1%) | 9 | 34 |
| 19 | AA | 77/93 (83%) | 57 (74%) | 17 (22%) | 3 (4%) | 2 | 14 |
| 19 | AI | 81/93 (87%) | 66 (82%) | 13 (16%) | 2 (2%) | 4 | 21 |
| 20 | BA | 97/106 (92%) | 83 (86%) | 14 (14%) | 0 | 100 | 100 |
| 20 | BI | 97/106 (92%) | 84 (87%) | 13 (13%) | 0 | 100 | 100 |
| 21 | 1B | 23/27 (85%) | 22 (96%) | 1 (4%) | 0 | 100 | 100 |
| 21 | 1F | 23/27 (85%) | 21 (91%) | 2 (9%) | 0 | 100 | 100 |
| 26 | 71 | 131/229 (57%) | 130 (99%) | 1 (1%) | 0 | 100 | 100 |

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| Mol | Chain | Analysed | Favoured | Allowed | Outliers | Percentiles |
|---|---|---|---|---|---|---|
| 26 | 79 | 131/229 (57%) | 129 (98%) | 2 (2%) | 0 | 100 100 |
| 27 | 11 | 270/276 (98%) | 254 (94%) | 12 (4%) | 4 (2%) | 8 32 |
| 27 | 19 | 271/276 (98%) | 253 (93%) | 15 (6%) | 3 (1%) | 11 39 |
| 28 | 21 | 203/206 (98%) | 174 (86%) | 28 (14%) | 1 (0%) | 24 57 |
| 28 | 29 | 203/206 (98%) | 160 (79%) | 34 (17%) | 9 (4%) | 2 12 |
| 29 | 31 | 200/210 (95%) | 189 (94%) | 10 (5%) | 1 (0%) | 24 57 |
| 29 | 39 | 206/210 (98%) | 176 (85%) | 21 (10%) | 9 (4%) | 2 12 |
| 30 | 41 | 179/182 (98%) | 154 (86%) | 24 (13%) | 1 (1%) | 21 52 |
| 30 | 49 | 179/182 (98%) | 151 (84%) | 25 (14%) | 3 (2%) | 7 30 |
| 31 | 51 | 172/180 (96%) | 146 (85%) | 20 (12%) | 6 (4%) | 3 16 |
| 31 | 59 | 169/180 (94%) | 133 (79%) | 35 (21%) | 1 (1%) | 21 52 |
| 32 | 61 | 144/148 (97%) | 120 (83%) | 21 (15%) | 3 (2%) | 5 25 |
| 32 | 69 | 144/148 (97%) | 122 (85%) | 19 (13%) | 3 (2%) | 5 25 |
| 33 | 15 | 136/140 (97%) | 128 (94%) | 7 (5%) | 1 (1%) | 18 49 |
| 33 | 58 | 136/140 (97%) | 116 (85%) | 13 (10%) | 7 (5%) | 1 10 |
| 34 | 25 | 120/122 (98%) | 111 (92%) | 9 (8%) | 0 | 100 100 |
| 34 | 68 | 120/122 (98%) | 115 (96%) | 4 (3%) | 1 (1%) | 16 47 |
| 35 | 35 | 148/150 (99%) | 118 (80%) | 24 (16%) | 6 (4%) | 2 13 |
| 35 | 78 | 148/150 (99%) | 117 (79%) | 28 (19%) | 3 (2%) | 6 25 |
| 36 | 45 | 139/141 (99%) | 114 (82%) | 20 (14%) | 5 (4%) | 2 16 |
| 36 | 88 | 139/141 (99%) | 111 (80%) | 23 (16%) | 5 (4%) | 2 16 |
| 37 | 55 | 115/118 (98%) | 103 (90%) | 11 (10%) | 1 (1%) | 14 44 |
| 37 | 98 | 116/118 (98%) | 104 (90%) | 10 (9%) | 2 (2%) | 7 30 |
| 38 | 65 | 109/112 (97%) | 93 (85%) | 14 (13%) | 2 (2%) | 6 28 |
| 38 | A8 | 109/112 (97%) | 94 (86%) | 13 (12%) | 2 (2%) | 6 28 |
| 39 | 75 | 135/146 (92%) | 113 (84%) | 19 (14%) | 3 (2%) | 5 24 |
| 39 | B8 | 135/146 (92%) | 117 (87%) | 18 (13%) | 0 | 100 100 |
| 40 | 85 | 115/118 (98%) | 106 (92%) | 9 (8%) | 0 | 100 100 |
| 40 | C8 | 115/118 (98%) | 109 (95%) | 6 (5%) | 0 | 100 100 |
| 41 | 95 | 99/101 (98%) | 82 (83%) | 12 (12%) | 5 (5%) | 1 10 |
| 41 | D8 | 99/101 (98%) | 89 (90%) | 9 (9%) | 1 (1%) | 12 41 |

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| Mol | Chain | Analysed | Favoured | Allowed | Outliers | Percentiles |
|---|---|---|---|---|---|---|
| 42 | A5 | 111/113 (98%) | 104 (94%) | 7 (6%) | 0 | 100 100 |
| 42 | E8 | 111/113 (98%) | 103 (93%) | 8 (7%) | 0 | 100 100 |
| 43 | B5 | 91/96 (95%) | 86 (94%) | 4 (4%) | 1 (1%) | 11 39 |
| 43 | F8 | 90/96 (94%) | 84 (93%) | 4 (4%) | 2 (2%) | 5 24 |
| 44 | C5 | 102/110 (93%) | 72 (71%) | 27 (26%) | 3 (3%) | 3 19 |
| 44 | G8 | 102/110 (93%) | 84 (82%) | 12 (12%) | 6 (6%) | 1 8 |
| 45 | D5 | 177/206 (86%) | 145 (82%) | 25 (14%) | 7 (4%) | 2 13 |
| 45 | H8 | 173/206 (84%) | 134 (78%) | 32 (18%) | 7 (4%) | 2 13 |
| 46 | E5 | 75/85 (88%) | 73 (97%) | 2 (3%) | 0 | 100 100 |
| 46 | I8 | 81/85 (95%) | 70 (86%) | 11 (14%) | 0 | 100 100 |
| 47 | F5 | 95/98 (97%) | 87 (92%) | 7 (7%) | 1 (1%) | 11 39 |
| 47 | J8 | 95/98 (97%) | 83 (87%) | 10 (10%) | 2 (2%) | 5 25 |
| 48 | G5 | 67/72 (93%) | 56 (84%) | 11 (16%) | 0 | 100 100 |
| 48 | K8 | 64/72 (89%) | 61 (95%) | 0 | 3 (5%) | 2 11 |
| 49 | H5 | 57/60 (95%) | 55 (96%) | 2 (4%) | 0 | 100 100 |
| 49 | L8 | 57/60 (95%) | 54 (95%) | 3 (5%) | 0 | 100 100 |
| 50 | I5 | 61/71 (86%) | 33 (54%) | 24 (39%) | 4 (7%) | 1 6 |
| 50 | M8 | 64/71 (90%) | 45 (70%) | 17 (27%) | 2 (3%) | 3 18 |
| 51 | J5 | 57/60 (95%) | 48 (84%) | 8 (14%) | 1 (2%) | 6 28 |
| 51 | N8 | 57/60 (95%) | 49 (86%) | 6 (10%) | 2 (4%) | 3 16 |
| 52 | K5 | 43/54 (80%) | 28 (65%) | 15 (35%) | 0 | 100 100 |
| 52 | O8 | 43/54 (80%) | 32 (74%) | 11 (26%) | 0 | 100 100 |
| 53 | L5 | 47/49 (96%) | 47 (100%) | 0 | 0 | 100 100 |
| 53 | P8 | 45/49 (92%) | 39 (87%) | 4 (9%) | 2 (4%) | 2 12 |
| 54 | M5 | 60/65 (92%) | 51 (85%) | 6 (10%) | 3 (5%) | 1 11 |
| 54 | Q8 | 60/65 (92%) | 51 (85%) | 7 (12%) | 2 (3%) | 3 17 |
| All | All | 11616/12512 (93%) | 10210 (88%) | 1239 (11%) | 167 (1%) | 9 34 |

All (167) Ramachandran outliers are listed below:

| Mol | Chain | Res | Type |
|---|---|---|---|
| 18 | 9I | 22 | VAL |
| 27 | 11 | 240 | ALA |

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| Mol | Chain | Res | Type |
|---|---|---|---|
| 36 | 88 | 87 | LYS |
| 43 | F8 | 68 | ARG |
| 44 | G8 | 53 | PRO |
| 44 | G8 | 81 | LYS |
| 48 | K8 | 43 | GLN |
| 48 | K8 | 48 | HIS |
| 53 | P8 | 45 | ALA |
| 53 | P8 | 46 | VAL |
| 9 | 82 | 41 | VAL |
| 28 | 29 | 51 | PHE |
| 28 | 29 | 72 | VAL |
| 30 | 49 | 36 | LYS |
| 35 | 35 | 48 | PRO |
| 35 | 35 | 49 | ARG |
| 38 | 65 | 110 | LEU |
| 39 | 75 | 106 | SER |
| 44 | C5 | 40 | GLU |
| 45 | D5 | 53 | ILE |
| 50 | I5 | 5 | ILE |
| 33 | 58 | 97 | ARG |
| 36 | 88 | 66 | ILE |
| 38 | A8 | 82 | ILE |
| 45 | H8 | 53 | ILE |
| 47 | J8 | 90 | ILE |
| 51 | N8 | 57 | VAL |
| 2 | 12 | 22 | LYS |
| 4 | 32 | 32 | ALA |
| 28 | 29 | 81 | ILE |
| 28 | 29 | 82 | ARG |
| 29 | 39 | 22 | ALA |
| 29 | 39 | 25 | PRO |
| 29 | 39 | 84 | VAL |
| 32 | 69 | 144 | VAL |
| 35 | 35 | 55 | ARG |
| 35 | 35 | 56 | SER |
| 36 | 45 | 21 | THR |
| 41 | 95 | 79 | VAL |
| 41 | 95 | 84 | LYS |
| 44 | C5 | 29 | GLU |
| 45 | D5 | 60 | GLU |
| 2 | 1E | 237 | ALA |
| 31 | 51 | 8 | PRO |

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| Mol | Chain | Res | Type |
|---|---|---|---|
| 31 | 51 | 9 | ILE |
| 31 | 51 | 83 | TYR |
| 33 | 58 | 9 | VAL |
| 33 | 58 | 128 | HIS |
| 36 | 88 | 6 | ARG |
| 36 | 88 | 79 | LEU |
| 44 | G8 | 94 | LYS |
| 45 | H8 | 6 | LYS |
| 45 | H8 | 151 | HIS |
| 45 | H8 | 165 | VAL |
| 2 | 12 | 234 | PRO |
| 13 | 4A | 99 | ARG |
| 27 | 19 | 33 | LEU |
| 28 | 29 | 9 | VAL |
| 29 | 39 | 23 | ASP |
| 29 | 39 | 133 | ASN |
| 35 | 35 | 46 | LYS |
| 36 | 45 | 7 | MET |
| 45 | D5 | 135 | GLU |
| 45 | D5 | 161 | VAL |
| 54 | M5 | 32 | LEU |
| 2 | 1E | 194 | PRO |
| 14 | 5I | 16 | PHE |
| 27 | 11 | 26 | LYS |
| 31 | 51 | 167 | GLU |
| 33 | 58 | 22 | THR |
| 36 | 88 | 90 | VAL |
| 38 | A8 | 4 | LEU |
| 41 | D8 | 45 | THR |
| 43 | F8 | 67 | GLY |
| 44 | G8 | 54 | LYS |
| 44 | G8 | 84 | ARG |
| 45 | H8 | 60 | GLU |
| 45 | H8 | 141 | VAL |
| 45 | H8 | 171 | ILE |
| 48 | K8 | 47 | ASN |
| 50 | M8 | 34 | GLU |
| 19 | AA | 9 | VAL |
| 32 | 69 | 83 | ALA |
| 37 | 55 | 3 | HIS |
| 38 | 65 | 111 | GLU |
| 39 | 75 | 5 | ALA |

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| Mol | Chain | Res | Type |
|---|---|---|---|
| 41 | 95 | 45 | THR |
| 2 | 1E | 95 | GLN |
| 2 | 1E | 238 | LEU |
| 17 | 8I | 82 | MET |
| 37 | 98 | 71 | GLN |
| 51 | N8 | 6 | VAL |
| 54 | Q8 | 33 | ASN |
| 54 | Q8 | 34 | TRP |
| 4 | 32 | 189 | PRO |
| 13 | 4A | 5 | ALA |
| 19 | AA | 29 | ARG |
| 27 | 19 | 240 | ALA |
| 28 | 29 | 187 | ALA |
| 29 | 39 | 85 | GLY |
| 29 | 39 | 123 | LEU |
| 30 | 49 | 139 | LEU |
| 32 | 69 | 117 | GLU |
| 35 | 35 | 7 | ARG |
| 39 | 75 | 7 | ILE |
| 41 | 95 | 85 | LYS |
| 43 | B5 | 51 | VAL |
| 45 | D5 | 8 | TYR |
| 11 | 2I | 82 | VAL |
| 32 | 61 | 133 | HIS |
| 33 | 58 | 95 | PRO |
| 34 | 68 | 97 | ARG |
| 35 | 78 | 95 | VAL |
| 37 | 98 | 45 | ARG |
| 44 | G8 | 76 | CYS |
| 47 | J8 | 86 | SER |
| 27 | 19 | 3 | VAL |
| 28 | 29 | 49 | LEU |
| 29 | 39 | 28 | ILE |
| 36 | 45 | 78 | PRO |
| 36 | 45 | 127 | ILE |
| 50 | I5 | 31 | ILE |
| 54 | M5 | 31 | HIS |
| 54 | M5 | 62 | LEU |
| 19 | AI | 9 | VAL |
| 27 | 11 | 3 | VAL |
| 30 | 41 | 5 | VAL |
| 8 | 72 | 100 | ILE |

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| Mol | Chain | Res | Type |
|---|---|---|---|
| 13 | 4A | 117 | VAL |
| 36 | 45 | 90 | VAL |
| 45 | D5 | 141 | VAL |
| 47 | F5 | 30 | VAL |
| 50 | I5 | 22 | ILE |
| 27 | 11 | 123 | ALA |
| 2 | 12 | 39 | ILE |
| 16 | 7A | 53 | VAL |
| 19 | AA | 67 | VAL |
| 30 | 49 | 5 | VAL |
| 50 | I5 | 33 | VAL |
| 51 | J5 | 57 | VAL |
| 5 | 4E | 115 | VAL |
| 28 | 21 | 72 | VAL |
| 29 | 31 | 132 | VAL |
| 32 | 61 | 118 | LYS |
| 35 | 78 | 47 | ASP |
| 2 | 12 | 232 | PRO |
| 8 | 72 | 103 | VAL |
| 13 | 4A | 4 | ILE |
| 13 | 4A | 84 | ILE |
| 28 | 29 | 25 | VAL |
| 28 | 29 | 52 | LEU |
| 19 | AI | 41 | VAL |
| 31 | 51 | 92 | ILE |
| 32 | 61 | 145 | VAL |
| 33 | 58 | 135 | PRO |
| 35 | 78 | 7 | ARG |
| 50 | M8 | 5 | ILE |
| 29 | 39 | 66 | PRO |
| 31 | 59 | 151 | ILE |
| 41 | 95 | 99 | ILE |
| 44 | C5 | 76 | CYS |
| 33 | 58 | 11 | PRO |
| 4 | 32 | 5 | ILE |
| 4 | 32 | 105 | VAL |
| 33 | 15 | 128 | HIS |
| 45 | D5 | 61 | LEU |
| 31 | 51 | 173 | PRO |

### 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 |
|---|---|---|---|---|---|
| 2 | 12 | 205/220 (93%) | 162 (79%) | 43 (21%) | 1 5 |
| 2 | 1E | 205/220 (93%) | 148 (72%) | 57 (28%) | 0 1 |
| 3 | 22 | 160/188 (85%) | 121 (76%) | 39 (24%) | 1 3 |
| 3 | 2E | 159/188 (85%) | 128 (80%) | 31 (20%) | 1 6 |
| 4 | 32 | 180/181 (99%) | 141 (78%) | 39 (22%) | 1 5 |
| 4 | 3E | 180/181 (99%) | 143 (79%) | 37 (21%) | 1 5 |
| 5 | 42 | 116/123 (94%) | 86 (74%) | 30 (26%) | 0 2 |
| 5 | 4E | 116/123 (94%) | 85 (73%) | 31 (27%) | 0 2 |
| 6 | 52 | 90/90 (100%) | 74 (82%) | 16 (18%) | 2 9 |
| 6 | 5E | 90/90 (100%) | 71 (79%) | 19 (21%) | 1 5 |
| 7 | 62 | 126/127 (99%) | 97 (77%) | 29 (23%) | 1 4 |
| 7 | 6E | 126/127 (99%) | 96 (76%) | 30 (24%) | 1 3 |
| 8 | 72 | 119/119 (100%) | 97 (82%) | 22 (18%) | 1 8 |
| 8 | 7E | 119/119 (100%) | 98 (82%) | 21 (18%) | 2 9 |
| 9 | 82 | 98/99 (99%) | 77 (79%) | 21 (21%) | 1 5 |
| 9 | 8E | 98/99 (99%) | 80 (82%) | 18 (18%) | 1 8 |
| 10 | 1A | 89/92 (97%) | 64 (72%) | 25 (28%) | 0 1 |
| 10 | 1I | 89/92 (97%) | 73 (82%) | 16 (18%) | 2 8 |
| 11 | 2A | 88/99 (89%) | 70 (80%) | 18 (20%) | 1 5 |
| 11 | 2I | 88/99 (89%) | 73 (83%) | 15 (17%) | 2 10 |
| 12 | 3A | 104/109 (95%) | 89 (86%) | 15 (14%) | 3 14 |
| 12 | 3I | 104/109 (95%) | 87 (84%) | 17 (16%) | 2 11 |
| 13 | 4A | 94/101 (93%) | 73 (78%) | 21 (22%) | 1 4 |
| 13 | 4I | 94/101 (93%) | 74 (79%) | 20 (21%) | 1 5 |
| 14 | 5A | 49/50 (98%) | 44 (90%) | 5 (10%) | 7 28 |
| 14 | 5I | 49/50 (98%) | 37 (76%) | 12 (24%) | 1 3 |

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| Mol | Chain | Analysed | Rotameric | Outliers | Percentiles |
|---|---|---|---|---|---|
| 15 | 6A | 79/80 (99%) | 66 (84%) | 13 (16%) | 2 11 |
| 15 | 6I | 79/80 (99%) | 64 (81%) | 15 (19%) | 1 7 |
| 16 | 7A | 72/74 (97%) | 56 (78%) | 16 (22%) | 1 4 |
| 16 | 7I | 72/74 (97%) | 55 (76%) | 17 (24%) | 1 3 |
| 17 | 8A | 95/97 (98%) | 75 (79%) | 20 (21%) | 1 5 |
| 17 | 8I | 95/97 (98%) | 77 (81%) | 18 (19%) | 1 7 |
| 18 | 9A | 63/77 (82%) | 53 (84%) | 10 (16%) | 2 12 |
| 18 | 9I | 63/77 (82%) | 54 (86%) | 9 (14%) | 3 14 |
| 19 | AA | 68/80 (85%) | 50 (74%) | 18 (26%) | 0 2 |
| 19 | AI | 72/80 (90%) | 54 (75%) | 18 (25%) | 0 2 |
| 20 | BA | 76/82 (93%) | 62 (82%) | 14 (18%) | 1 8 |
| 20 | BI | 76/82 (93%) | 60 (79%) | 16 (21%) | 1 5 |
| 21 | 1B | 20/22 (91%) | 18 (90%) | 2 (10%) | 7 29 |
| 21 | 1F | 20/22 (91%) | 19 (95%) | 1 (5%) | 22 53 |
| 26 | 71 | 111/181 (61%) | 104 (94%) | 7 (6%) | 16 45 |
| 26 | 79 | 111/181 (61%) | 97 (87%) | 14 (13%) | 4 19 |
| 27 | 11 | 214/218 (98%) | 170 (79%) | 44 (21%) | 1 5 |
| 27 | 19 | 214/218 (98%) | 172 (80%) | 42 (20%) | 1 6 |
| 28 | 21 | 165/166 (99%) | 127 (77%) | 38 (23%) | 1 4 |
| 28 | 29 | 165/166 (99%) | 122 (74%) | 43 (26%) | 0 2 |
| 29 | 31 | 161/166 (97%) | 117 (73%) | 44 (27%) | 0 1 |
| 29 | 39 | 165/166 (99%) | 121 (73%) | 44 (27%) | 0 2 |
| 30 | 41 | 155/156 (99%) | 125 (81%) | 30 (19%) | 1 7 |
| 30 | 49 | 155/156 (99%) | 115 (74%) | 40 (26%) | 0 2 |
| 31 | 51 | 145/148 (98%) | 105 (72%) | 40 (28%) | 0 1 |
| 31 | 59 | 142/148 (96%) | 106 (75%) | 36 (25%) | 0 2 |
| 32 | 61 | 122/124 (98%) | 92 (75%) | 30 (25%) | 1 3 |
| 32 | 69 | 122/124 (98%) | 86 (70%) | 36 (30%) | 0 1 |
| 33 | 15 | 117/119 (98%) | 88 (75%) | 29 (25%) | 1 2 |
| 33 | 58 | 117/119 (98%) | 81 (69%) | 36 (31%) | 0 0 |
| 34 | 25 | 100/100 (100%) | 75 (75%) | 25 (25%) | 0 2 |

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| Mol | Chain | Analysed | Rotameric | Outliers | Percentiles |
|---|---|---|---|---|---|
| 34 | 68 | 100/100 (100%) | 78 (78%) | 22 (22%) | 1 4 |
| 35 | 35 | 116/116 (100%) | 78 (67%) | 38 (33%) | 0 0 |
| 35 | 78 | 116/116 (100%) | 70 (60%) | 46 (40%) | 0 0 |
| 36 | 45 | 111/111 (100%) | 86 (78%) | 25 (22%) | 1 4 |
| 36 | 88 | 111/111 (100%) | 86 (78%) | 25 (22%) | 1 4 |
| 37 | 55 | 100/101 (99%) | 77 (77%) | 23 (23%) | 1 4 |
| 37 | 98 | 101/101 (100%) | 79 (78%) | 22 (22%) | 1 5 |
| 38 | 65 | 87/88 (99%) | 55 (63%) | 32 (37%) | 0 0 |
| 38 | A8 | 87/88 (99%) | 67 (77%) | 20 (23%) | 1 4 |
| 39 | 75 | 117/127 (92%) | 91 (78%) | 26 (22%) | 1 4 |
| 39 | B8 | 120/127 (94%) | 83 (69%) | 37 (31%) | 0 0 |
| 40 | 85 | 93/94 (99%) | 76 (82%) | 17 (18%) | 2 8 |
| 40 | C8 | 93/94 (99%) | 74 (80%) | 19 (20%) | 1 5 |
| 41 | 95 | 82/82 (100%) | 62 (76%) | 20 (24%) | 1 3 |
| 41 | D8 | 82/82 (100%) | 53 (65%) | 29 (35%) | 0 0 |
| 42 | A5 | 92/92 (100%) | 70 (76%) | 22 (24%) | 1 3 |
| 42 | E8 | 92/92 (100%) | 64 (70%) | 28 (30%) | 0 0 |
| 43 | B5 | 74/78 (95%) | 57 (77%) | 17 (23%) | 1 4 |
| 43 | F8 | 74/78 (95%) | 53 (72%) | 21 (28%) | 0 1 |
| 44 | C5 | 85/91 (93%) | 62 (73%) | 23 (27%) | 0 2 |
| 44 | G8 | 85/91 (93%) | 58 (68%) | 27 (32%) | 0 0 |
| 45 | D5 | 158/179 (88%) | 120 (76%) | 38 (24%) | 1 3 |
| 45 | H8 | 154/179 (86%) | 116 (75%) | 38 (25%) | 1 2 |
| 46 | E5 | 62/67 (92%) | 49 (79%) | 13 (21%) | 1 5 |
| 46 | I8 | 66/67 (98%) | 48 (73%) | 18 (27%) | 0 1 |
| 47 | F5 | 82/83 (99%) | 56 (68%) | 26 (32%) | 0 0 |
| 47 | J8 | 82/83 (99%) | 54 (66%) | 28 (34%) | 0 0 |
| 48 | G5 | 64/67 (96%) | 47 (73%) | 17 (27%) | 0 2 |
| 48 | K8 | 62/67 (92%) | 45 (73%) | 17 (27%) | 0 1 |
| 49 | H5 | 51/52 (98%) | 43 (84%) | 8 (16%) | 2 12 |
| 49 | L8 | 51/52 (98%) | 37 (72%) | 14 (28%) | 0 1 |

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| Mol | Chain | Analysed | Rotameric | Outliers | Percentiles |
|---|---|---|---|---|---|
| 50 | I5 | 57/63 (90%) | 43 (75%) | 14 (25%) | 1 3 |
| 50 | M8 | 59/63 (94%) | 50 (85%) | 9 (15%) | 3 12 |
| 51 | J5 | 51/52 (98%) | 36 (71%) | 15 (29%) | 0 1 |
| 51 | N8 | 51/52 (98%) | 37 (72%) | 14 (28%) | 0 1 |
| 52 | K5 | 44/52 (85%) | 27 (61%) | 17 (39%) | 0 0 |
| 52 | O8 | 44/52 (85%) | 33 (75%) | 11 (25%) | 0 2 |
| 53 | L5 | 42/42 (100%) | 32 (76%) | 10 (24%) | 1 3 |
| 53 | P8 | 40/42 (95%) | 32 (80%) | 8 (20%) | 1 6 |
| 54 | M5 | 52/55 (94%) | 36 (69%) | 16 (31%) | 0 0 |
| 54 | Q8 | 50/55 (91%) | 30 (60%) | 20 (40%) | 0 0 |
| All | All | 9806/10360 (95%) | 7504 (76%) | 2302 (24%) | 1 3 |

All (2302) residues with a non-rotameric sidechain are listed below:

| Mol | Chain | Res | Type |
|---|---|---|---|
| 2 | 1E | 4 | GLU |
| 2 | 1E | 5 | ILE |
| 2 | 1E | 6 | THR |
| 2 | 1E | 8 | LYS |
| 2 | 1E | 9 | GLU |
| 2 | 1E | 12 | GLU |
| 2 | 1E | 16 | HIS |
| 2 | 1E | 17 | PHE |
| 2 | 1E | 21 | ARG |
| 2 | 1E | 32 | ILE |
| 2 | 1E | 41 | ILE |
| 2 | 1E | 42 | ILE |
| 2 | 1E | 49 | GLU |
| 2 | 1E | 53 | ARG |
| 2 | 1E | 68 | ILE |
| 2 | 1E | 71 | VAL |
| 2 | 1E | 79 | ASP |
| 2 | 1E | 81 | VAL |
| 2 | 1E | 83 | MET |
| 2 | 1E | 87 | ARG |
| 2 | 1E | 90 | MET |
| 2 | 1E | 103 | THR |
| 2 | 1E | 106 | LYS |

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| Mol | Chain | Res | Type |
|---|---|---|---|
| 2 | 1E | 108 | ILE |
| 2 | 1E | 111 | ARG |
| 2 | 1E | 112 | VAL |
| 2 | 1E | 118 | LEU |
| 2 | 1E | 127 | ILE |
| 2 | 1E | 136 | VAL |
| 2 | 1E | 139 | LYS |
| 2 | 1E | 140 | HIS |
| 2 | 1E | 145 | LEU |
| 2 | 1E | 150 | SER |
| 2 | 1E | 157 | ARG |
| 2 | 1E | 165 | VAL |
| 2 | 1E | 168 | THR |
| 2 | 1E | 169 | LYS |
| 2 | 1E | 170 | GLU |
| 2 | 1E | 172 | ILE |
| 2 | 1E | 178 | ARG |
| 2 | 1E | 185 | ILE |
| 2 | 1E | 187 | LEU |
| 2 | 1E | 192 | SER |
| 2 | 1E | 196 | LEU |
| 2 | 1E | 197 | VAL |
| 2 | 1E | 200 | ILE |
| 2 | 1E | 208 | ILE |
| 2 | 1E | 210 | SER |
| 2 | 1E | 211 | ILE |
| 2 | 1E | 213 | LEU |
| 2 | 1E | 214 | ILE |
| 2 | 1E | 215 | LEU |
| 2 | 1E | 217 | ARG |
| 2 | 1E | 221 | LEU |
| 2 | 1E | 222 | ILE |
| 2 | 1E | 223 | ILE |
| 2 | 1E | 230 | VAL |
| 3 | 2E | 3 | ASN |
| 3 | 2E | 8 | ILE |
| 3 | 2E | 12 | LEU |
| 3 | 2E | 17 | ASP |
| 3 | 2E | 27 | LYS |
| 3 | 2E | 30 | ARG |
| 3 | 2E | 38 | ARG |
| 3 | 2E | 45 | LYS |

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| Mol | Chain | Res | Type |
|---|---|---|---|
| 3 | 2E | 46 | GLU |
| 3 | 2E | 49 | SER |
| 3 | 2E | 58 | GLU |
| 3 | 2E | 64 | VAL |
| 3 | 2E | 67 | THR |
| 3 | 2E | 95 | THR |
| 3 | 2E | 102 | ASN |
| 3 | 2E | 104 | GLN |
| 3 | 2E | 107 | GLN |
| 3 | 2E | 115 | LEU |
| 3 | 2E | 116 | VAL |
| 3 | 2E | 143 | GLU |
| 3 | 2E | 154 | SER |
| 3 | 2E | 165 | THR |
| 3 | 2E | 178 | LEU |
| 3 | 2E | 179 | ARG |
| 3 | 2E | 184 | TYR |
| 3 | 2E | 188 | LEU |
| 3 | 2E | 191 | THR |
| 3 | 2E | 195 | VAL |
| 3 | 2E | 196 | LEU |
| 3 | 2E | 202 | ILE |
| 3 | 2E | 206 | GLU |
| 4 | 3E | 3 | ARG |
| 4 | 3E | 8 | VAL |
| 4 | 3E | 13 | ARG |
| 4 | 3E | 15 | GLU |
| 4 | 3E | 30 | LYS |
| 4 | 3E | 33 | MET |
| 4 | 3E | 35 | ARG |
| 4 | 3E | 45 | GLN |
| 4 | 3E | 47 | ARG |
| 4 | 3E | 58 | LEU |
| 4 | 3E | 59 | ARG |
| 4 | 3E | 61 | LYS |
| 4 | 3E | 84 | LYS |
| 4 | 3E | 86 | LYS |
| 4 | 3E | 89 | THR |
| 4 | 3E | 92 | VAL |
| 4 | 3E | 96 | LEU |
| 4 | 3E | 104 | VAL |
| 4 | 3E | 106 | TYR |

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| Mol | Chain | Res | Type |
|---|---|---|---|
| 4 | 3E | 108 | LEU |
| 4 | 3E | 114 | ARG |
| 4 | 3E | 122 | ARG |
| 4 | 3E | 127 | THR |
| 4 | 3E | 135 | LEU |
| 4 | 3E | 141 | ARG |
| 4 | 3E | 146 | ILE |
| 4 | 3E | 150 | GLU |
| 4 | 3E | 154 | ASN |
| 4 | 3E | 165 | MET |
| 4 | 3E | 166 | LYS |
| 4 | 3E | 178 | VAL |
| 4 | 3E | 179 | GLU |
| 4 | 3E | 184 | LYS |
| 4 | 3E | 188 | LEU |
| 4 | 3E | 192 | GLU |
| 4 | 3E | 200 | GLU |
| 4 | 3E | 204 | ILE |
| 5 | 4E | 8 | GLU |
| 5 | 4E | 11 | ILE |
| 5 | 4E | 12 | LEU |
| 5 | 4E | 13 | ILE |
| 5 | 4E | 14 | ARG |
| 5 | 4E | 18 | ARG |
| 5 | 4E | 19 | MET |
| 5 | 4E | 25 | ARG |
| 5 | 4E | 27 | ARG |
| 5 | 4E | 31 | LEU |
| 5 | 4E | 41 | VAL |
| 5 | 4E | 45 | PHE |
| 5 | 4E | 50 | GLU |
| 5 | 4E | 51 | VAL |
| 5 | 4E | 53 | LEU |
| 5 | 4E | 55 | VAL |
| 5 | 4E | 64 | ARG |
| 5 | 4E | 68 | GLU |
| 5 | 4E | 71 | LEU |
| 5 | 4E | 72 | GLN |
| 5 | 4E | 78 | HIS |
| 5 | 4E | 79 | GLU |
| 5 | 4E | 81 | GLU |
| 5 | 4E | 87 | SER |

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| Mol | Chain | Res | Type |
|---|---|---|---|
| 5 | 4E | 91 | LEU |
| 5 | 4E | 101 | ILE |
| 5 | 4E | 121 | LYS |
| 5 | 4E | 122 | GLU |
| 5 | 4E | 126 | ARG |
| 5 | 4E | 131 | ILE |
| 5 | 4E | 153 | LYS |
| 6 | 5E | 7 | ASN |
| 6 | 5E | 10 | LEU |
| 6 | 5E | 13 | ASN |
| 6 | 5E | 16 | GLN |
| 6 | 5E | 21 | LEU |
| 6 | 5E | 23 | LYS |
| 6 | 5E | 24 | GLU |
| 6 | 5E | 55 | ASP |
| 6 | 5E | 62 | TRP |
| 6 | 5E | 63 | TYR |
| 6 | 5E | 64 | GLN |
| 6 | 5E | 65 | VAL |
| 6 | 5E | 72 | VAL |
| 6 | 5E | 74 | ASP |
| 6 | 5E | 75 | LEU |
| 6 | 5E | 81 | ILE |
| 6 | 5E | 87 | ARG |
| 6 | 5E | 92 | LYS |
| 6 | 5E | 98 | LEU |
| 7 | 6E | 5 | ARG |
| 7 | 6E | 6 | ARG |
| 7 | 6E | 8 | GLU |
| 7 | 6E | 12 | LEU |
| 7 | 6E | 16 | LEU |
| 7 | 6E | 23 | VAL |
| 7 | 6E | 24 | THR |
| 7 | 6E | 27 | ILE |
| 7 | 6E | 38 | LEU |
| 7 | 6E | 41 | ARG |
| 7 | 6E | 47 | CYS |
| 7 | 6E | 52 | GLU |
| 7 | 6E | 63 | LYS |
| 7 | 6E | 66 | VAL |
| 7 | 6E | 73 | MET |
| 7 | 6E | 75 | VAL |

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| Mol | Chain | Res | Type |
|---|---|---|---|
| 7 | 6E | 78 | ARG |
| 7 | 6E | 90 | GLU |
| 7 | 6E | 91 | VAL |
| 7 | 6E | 95 | ARG |
| 7 | 6E | 98 | SER |
| 7 | 6E | 104 | LEU |
| 7 | 6E | 109 | ASN |
| 7 | 6E | 111 | ARG |
| 7 | 6E | 113 | GLU |
| 7 | 6E | 120 | ILE |
| 7 | 6E | 122 | HIS |
| 7 | 6E | 139 | GLU |
| 7 | 6E | 143 | ARG |
| 7 | 6E | 155 | ARG |
| 8 | 7E | 1 | MET |
| 8 | 7E | 3 | THR |
| 8 | 7E | 6 | ILE |
| 8 | 7E | 21 | LYS |
| 8 | 7E | 24 | THR |
| 8 | 7E | 26 | VAL |
| 8 | 7E | 29 | SER |
| 8 | 7E | 45 | ILE |
| 8 | 7E | 68 | ARG |
| 8 | 7E | 69 | ARG |
| 8 | 7E | 82 | HIS |
| 8 | 7E | 84 | ARG |
| 8 | 7E | 85 | ARG |
| 8 | 7E | 95 | VAL |
| 8 | 7E | 97 | VAL |
| 8 | 7E | 102 | ARG |
| 8 | 7E | 112 | LEU |
| 8 | 7E | 115 | SER |
| 8 | 7E | 118 | VAL |
| 8 | 7E | 121 | ASP |
| 8 | 7E | 129 | VAL |
| 9 | 8E | 2 | GLU |
| 9 | 8E | 9 | ARG |
| 9 | 8E | 14 | VAL |
| 9 | 8E | 17 | VAL |
| 9 | 8E | 38 | GLN |
| 9 | 8E | 42 | ARG |
| 9 | 8E | 44 | VAL |

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| Mol | Chain | Res | Type |
|---|---|---|---|
| 9 | 8E | 47 | LEU |
| 9 | 8E | 53 | VAL |
| 9 | 8E | 70 | LYS |
| 9 | 8E | 75 | ASP |
| 9 | 8E | 85 | LEU |
| 9 | 8E | 86 | VAL |
| 9 | 8E | 92 | TYR |
| 9 | 8E | 108 | VAL |
| 9 | 8E | 111 | ARG |
| 9 | 8E | 114 | TYR |
| 9 | 8E | 117 | HIS |
| 10 | 1I | 6 | ILE |
| 10 | 1I | 23 | ILE |
| 10 | 1I | 24 | VAL |
| 10 | 1I | 29 | ARG |
| 10 | 1I | 34 | VAL |
| 10 | 1I | 38 | ILE |
| 10 | 1I | 48 | THR |
| 10 | 1I | 56 | HIS |
| 10 | 1I | 62 | HIS |
| 10 | 1I | 66 | ARG |
| 10 | 1I | 70 | ARG |
| 10 | 1I | 75 | ILE |
| 10 | 1I | 78 | ASN |
| 10 | 1I | 84 | GLN |
| 10 | 1I | 96 | ILE |
| 10 | 1I | 98 | ILE |
| 11 | 2I | 13 | GLN |
| 11 | 2I | 14 | VAL |
| 11 | 2I | 25 | TYR |
| 11 | 2I | 29 | ILE |
| 11 | 2I | 32 | ILE |
| 11 | 2I | 40 | ILE |
| 11 | 2I | 91 | ARG |
| 11 | 2I | 93 | GLN |
| 11 | 2I | 98 | LEU |
| 11 | 2I | 99 | GLN |
| 11 | 2I | 103 | LEU |
| 11 | 2I | 108 | ILE |
| 11 | 2I | 109 | VAL |
| 11 | 2I | 123 | LYS |
| 11 | 2I | 124 | LYS |

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| Mol | Chain | Res | Type |
|---|---|---|---|
| 12 | 3I | 11 | VAL |
| 12 | 3I | 21 | LYS |
| 12 | 3I | 23 | LYS |
| 12 | 3I | 33 | ARG |
| 12 | 3I | 39 | VAL |
| 12 | 3I | 47 | LYS |
| 12 | 3I | 55 | VAL |
| 12 | 3I | 62 | SER |
| 12 | 3I | 66 | VAL |
| 12 | 3I | 70 | ILE |
| 12 | 3I | 93 | LEU |
| 12 | 3I | 97 | ARG |
| 12 | 3I | 110 | VAL |
| 12 | 3I | 114 | LYS |
| 12 | 3I | 116 | SER |
| 12 | 3I | 118 | SER |
| 12 | 3I | 127 | GLU |
| 13 | 4I | 19 | LEU |
| 13 | 4I | 21 | TYR |
| 13 | 4I | 34 | LEU |
| 13 | 4I | 45 | VAL |
| 13 | 4I | 47 | ASP |
| 13 | 4I | 56 | LEU |
| 13 | 4I | 63 | THR |
| 13 | 4I | 64 | TRP |
| 13 | 4I | 66 | LEU |
| 13 | 4I | 70 | LEU |
| 13 | 4I | 74 | VAL |
| 13 | 4I | 84 | ILE |
| 13 | 4I | 88 | ARG |
| 13 | 4I | 93 | ARG |
| 13 | 4I | 102 | ARG |
| 13 | 4I | 103 | THR |
| 13 | 4I | 105 | THR |
| 13 | 4I | 108 | ARG |
| 13 | 4I | 114 | ARG |
| 13 | 4I | 115 | LYS |
| 14 | 5I | 3 | ARG |
| 14 | 5I | 9 | LYS |
| 14 | 5I | 17 | LYS |
| 14 | 5I | 18 | VAL |
| 14 | 5I | 22 | THR |

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| Mol | Chain | Res | Type |
|---|---|---|---|
| 14 | 5I | 23 | ARG |
| 14 | 5I | 32 | SER |
| 14 | 5I | 33 | VAL |
| 14 | 5I | 44 | LEU |
| 14 | 5I | 56 | VAL |
| 14 | 5I | 58 | LYS |
| 14 | 5I | 60 | SER |
| 15 | 6I | 6 | GLU |
| 15 | 6I | 10 | LYS |
| 15 | 6I | 22 | THR |
| 15 | 6I | 26 | GLU |
| 15 | 6I | 31 | LEU |
| 15 | 6I | 34 | LEU |
| 15 | 6I | 38 | ARG |
| 15 | 6I | 39 | LEU |
| 15 | 6I | 47 | LYS |
| 15 | 6I | 48 | LYS |
| 15 | 6I | 58 | MET |
| 15 | 6I | 65 | ARG |
| 15 | 6I | 67 | LEU |
| 15 | 6I | 82 | ILE |
| 15 | 6I | 87 | ILE |
| 16 | 7I | 1 | MET |
| 16 | 7I | 2 | VAL |
| 16 | 7I | 4 | ILE |
| 16 | 7I | 6 | LEU |
| 16 | 7I | 8 | ARG |
| 16 | 7I | 11 | SER |
| 16 | 7I | 20 | VAL |
| 16 | 7I | 25 | ARG |
| 16 | 7I | 26 | ARG |
| 16 | 7I | 28 | ARG |
| 16 | 7I | 36 | ILE |
| 16 | 7I | 49 | LEU |
| 16 | 7I | 55 | ARG |
| 16 | 7I | 69 | THR |
| 16 | 7I | 71 | ARG |
| 16 | 7I | 75 | ARG |
| 16 | 7I | 82 | GLN |
| 17 | 8I | 9 | VAL |
| 17 | 8I | 14 | LYS |
| 17 | 8I | 15 | MET |

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| Mol | Chain | Res | Type |
|---|---|---|---|
| 17 | 8I | 27 | PHE |
| 17 | 8I | 38 | ARG |
| 17 | 8I | 39 | SER |
| 17 | 8I | 48 | GLU |
| 17 | 8I | 53 | LEU |
| 17 | 8I | 57 | VAL |
| 17 | 8I | 60 | ILE |
| 17 | 8I | 63 | ARG |
| 17 | 8I | 74 | LEU |
| 17 | 8I | 77 | VAL |
| 17 | 8I | 89 | LEU |
| 17 | 8I | 90 | ILE |
| 17 | 8I | 91 | ARG |
| 17 | 8I | 97 | SER |
| 17 | 8I | 99 | SER |
| 18 | 9I | 26 | LEU |
| 18 | 9I | 39 | VAL |
| 18 | 9I | 42 | ARG |
| 18 | 9I | 47 | THR |
| 18 | 9I | 54 | ARG |
| 18 | 9I | 55 | ARG |
| 18 | 9I | 56 | THR |
| 18 | 9I | 76 | LEU |
| 18 | 9I | 85 | LEU |
| 19 | AI | 7 | LYS |
| 19 | AI | 12 | ASP |
| 19 | AI | 15 | LEU |
| 19 | AI | 29 | ARG |
| 19 | AI | 31 | ILE |
| 19 | AI | 36 | ARG |
| 19 | AI | 37 | ARG |
| 19 | AI | 41 | VAL |
| 19 | AI | 51 | VAL |
| 19 | AI | 58 | VAL |
| 19 | AI | 60 | VAL |
| 19 | AI | 61 | TYR |
| 19 | AI | 62 | ILE |
| 19 | AI | 64 | GLU |
| 19 | AI | 65 | ASN |
| 19 | AI | 67 | VAL |
| 19 | AI | 71 | LEU |
| 19 | AI | 78 | ARG |

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| Mol | Chain | Res | Type |
|---|---|---|---|
| 20 | BI | 9 | ASN |
| 20 | BI | 10 | LEU |
| 20 | BI | 17 | ARG |
| 20 | BI | 23 | ARG |
| 20 | BI | 24 | LEU |
| 20 | BI | 26 | ASN |
| 20 | BI | 30 | LYS |
| 20 | BI | 53 | LEU |
| 20 | BI | 54 | LYS |
| 20 | BI | 62 | LEU |
| 20 | BI | 63 | ILE |
| 20 | BI | 73 | HIS |
| 20 | BI | 75 | ASN |
| 20 | BI | 83 | ARG |
| 20 | BI | 87 | LYS |
| 20 | BI | 105 | SER |
| 21 | 1F | 15 | ARG |
| 26 | 71 | 28 | LEU |
| 26 | 71 | 34 | THR |
| 26 | 71 | 168 | THR |
| 26 | 71 | 172 | HIS |
| 26 | 71 | 183 | GLU |
| 26 | 71 | 207 | THR |
| 26 | 71 | 216 | THR |
| 27 | 11 | 4 | LYS |
| 27 | 11 | 14 | ARG |
| 27 | 11 | 17 | THR |
| 27 | 11 | 23 | GLU |
| 27 | 11 | 25 | THR |
| 27 | 11 | 27 | THR |
| 27 | 11 | 28 | GLU |
| 27 | 11 | 31 | LYS |
| 27 | 11 | 38 | LYS |
| 27 | 11 | 39 | LYS |
| 27 | 11 | 59 | LYS |
| 27 | 11 | 61 | LEU |
| 27 | 11 | 64 | ILE |
| 27 | 11 | 65 | ILE |
| 27 | 11 | 68 | LYS |
| 27 | 11 | 73 | VAL |
| 27 | 11 | 83 | GLU |
| 27 | 11 | 94 | LEU |

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| Mol | Chain | Res | Type |
|---|---|---|---|
| 27 | 11 | 103 | ARG |
| 27 | 11 | 105 | ILE |
| 27 | 11 | 106 | ILE |
| 27 | 11 | 111 | LEU |
| 27 | 11 | 112 | GLN |
| 27 | 11 | 136 | ILE |
| 27 | 11 | 141 | VAL |
| 27 | 11 | 155 | LEU |
| 27 | 11 | 165 | ILE |
| 27 | 11 | 171 | ASP |
| 27 | 11 | 173 | VAL |
| 27 | 11 | 176 | ARG |
| 27 | 11 | 192 | THR |
| 27 | 11 | 193 | VAL |
| 27 | 11 | 205 | VAL |
| 27 | 11 | 212 | SER |
| 27 | 11 | 213 | ARG |
| 27 | 11 | 217 | ARG |
| 27 | 11 | 218 | ARG |
| 27 | 11 | 221 | VAL |
| 27 | 11 | 228 | PRO |
| 27 | 11 | 229 | VAL |
| 27 | 11 | 242 | ARG |
| 27 | 11 | 253 | GLN |
| 27 | 11 | 259 | THR |
| 27 | 11 | 271 | ILE |
| 28 | 21 | 2 | LYS |
| 28 | 21 | 4 | ILE |
| 28 | 21 | 5 | LEU |
| 28 | 21 | 7 | VAL |
| 28 | 21 | 13 | ARG |
| 28 | 21 | 14 | ILE |
| 28 | 21 | 26 | ILE |
| 28 | 21 | 33 | VAL |
| 28 | 21 | 34 | VAL |
| 28 | 21 | 36 | ARG |
| 28 | 21 | 37 | ARG |
| 28 | 21 | 47 | VAL |
| 28 | 21 | 59 | VAL |
| 28 | 21 | 61 | ARG |
| 28 | 21 | 64 | LYS |
| 28 | 21 | 66 | HIS |

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| Mol | Chain | Res | Type |
|---|---|---|---|
| 28 | 21 | 78 | LEU |
| 28 | 21 | 80 | GLU |
| 28 | 21 | 87 | GLU |
| 28 | 21 | 116 | VAL |
| 28 | 21 | 117 | MET |
| 28 | 21 | 119 | ARG |
| 28 | 21 | 144 | ARG |
| 28 | 21 | 146 | THR |
| 28 | 21 | 149 | ARG |
| 28 | 21 | 152 | LYS |
| 28 | 21 | 154 | LYS |
| 28 | 21 | 167 | VAL |
| 28 | 21 | 175 | VAL |
| 28 | 21 | 178 | GLU |
| 28 | 21 | 179 | GLU |
| 28 | 21 | 180 | ASN |
| 28 | 21 | 181 | LEU |
| 28 | 21 | 184 | VAL |
| 28 | 21 | 188 | VAL |
| 28 | 21 | 196 | VAL |
| 28 | 21 | 197 | ILE |
| 28 | 21 | 202 | LYS |
| 29 | 31 | 7 | TYR |
| 29 | 31 | 8 | GLN |
| 29 | 31 | 9 | ILE |
| 29 | 31 | 13 | SER |
| 29 | 31 | 23 | ASP |
| 29 | 31 | 24 | LEU |
| 29 | 31 | 28 | ILE |
| 29 | 31 | 32 | LEU |
| 29 | 31 | 33 | LEU |
| 29 | 31 | 37 | VAL |
| 29 | 31 | 38 | ARG |
| 29 | 31 | 45 | ARG |
| 29 | 31 | 50 | SER |
| 29 | 31 | 56 | GLU |
| 29 | 31 | 57 | VAL |
| 29 | 31 | 60 | SER |
| 29 | 31 | 64 | ILE |
| 29 | 31 | 68 | LYS |
| 29 | 31 | 78 | ILE |
| 29 | 31 | 82 | ILE |

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| Mol | Chain | Res | Type |
|---|---|---|---|
| 29 | 31 | 88 | VAL |
| 29 | 31 | 106 | ARG |
| 29 | 31 | 107 | LYS |
| 29 | 31 | 108 | LYS |
| 29 | 31 | 117 | ARG |
| 29 | 31 | 127 | GLU |
| 29 | 31 | 135 | LYS |
| 29 | 31 | 136 | THR |
| 29 | 31 | 140 | LEU |
| 29 | 31 | 145 | GLU |
| 29 | 31 | 153 | SER |
| 29 | 31 | 158 | THR |
| 29 | 31 | 170 | LEU |
| 29 | 31 | 174 | VAL |
| 29 | 31 | 175 | THR |
| 29 | 31 | 176 | LEU |
| 29 | 31 | 181 | LEU |
| 29 | 31 | 183 | VAL |
| 29 | 31 | 188 | ARG |
| 29 | 31 | 191 | ARG |
| 29 | 31 | 192 | LEU |
| 29 | 31 | 194 | MET |
| 29 | 31 | 200 | GLU |
| 29 | 31 | 201 | VAL |
| 30 | 41 | 20 | ILE |
| 30 | 41 | 28 | VAL |
| 30 | 41 | 31 | VAL |
| 30 | 41 | 49 | ASP |
| 30 | 41 | 52 | ILE |
| 30 | 41 | 53 | LEU |
| 30 | 41 | 60 | LEU |
| 30 | 41 | 67 | LYS |
| 30 | 41 | 70 | VAL |
| 30 | 41 | 71 | THR |
| 30 | 41 | 81 | LYS |
| 30 | 41 | 82 | LEU |
| 30 | 41 | 83 | ARG |
| 30 | 41 | 86 | MET |
| 30 | 41 | 88 | ILE |
| 30 | 41 | 90 | LEU |
| 30 | 41 | 91 | ARG |
| 30 | 41 | 104 | GLU |

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| Mol | Chain | Res | Type |
|---|---|---|---|
| 30 | 41 | 116 | ASP |
| 30 | 41 | 120 | LEU |
| 30 | 41 | 121 | ASN |
| 30 | 41 | 128 | ARG |
| 30 | 41 | 130 | ASN |
| 30 | 41 | 133 | LEU |
| 30 | 41 | 140 | ILE |
| 30 | 41 | 153 | ARG |
| 30 | 41 | 161 | THR |
| 30 | 41 | 162 | THR |
| 30 | 41 | 167 | GLU |
| 30 | 41 | 172 | LEU |
| 31 | 51 | 4 | ILE |
| 31 | 51 | 7 | LEU |
| 31 | 51 | 9 | ILE |
| 31 | 51 | 13 | LYS |
| 31 | 51 | 17 | VAL |
| 31 | 51 | 24 | VAL |
| 31 | 51 | 32 | GLU |
| 31 | 51 | 34 | GLU |
| 31 | 51 | 43 | VAL |
| 31 | 51 | 45 | VAL |
| 31 | 51 | 47 | GLU |
| 31 | 51 | 49 | VAL |
| 31 | 51 | 50 | VAL |
| 31 | 51 | 53 | GLU |
| 31 | 51 | 71 | LEU |
| 31 | 51 | 72 | ILE |
| 31 | 51 | 77 | LYS |
| 31 | 51 | 84 | SER |
| 31 | 51 | 87 | LEU |
| 31 | 51 | 95 | ARG |
| 31 | 51 | 98 | LEU |
| 31 | 51 | 104 | GLU |
| 31 | 51 | 105 | LEU |
| 31 | 51 | 115 | VAL |
| 31 | 51 | 121 | ILE |
| 31 | 51 | 122 | THR |
| 31 | 51 | 125 | VAL |
| 31 | 51 | 129 | THR |
| 31 | 51 | 130 | ARG |
| 31 | 51 | 131 | VAL |

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| Mol | Chain | Res | Type |
|---|---|---|---|
| 31 | 51 | 133 | VAL |
| 31 | 51 | 134 | SER |
| 31 | 51 | 136 | ILE |
| 31 | 51 | 139 | GLN |
| 31 | 51 | 141 | VAL |
| 31 | 51 | 151 | ILE |
| 31 | 51 | 153 | LYS |
| 31 | 51 | 169 | VAL |
| 31 | 51 | 170 | ARG |
| 31 | 51 | 172 | LYS |
| 32 | 61 | 1 | MET |
| 32 | 61 | 3 | VAL |
| 32 | 61 | 7 | GLU |
| 32 | 61 | 9 | LEU |
| 32 | 61 | 15 | VAL |
| 32 | 61 | 35 | LEU |
| 32 | 61 | 37 | VAL |
| 32 | 61 | 40 | THR |
| 32 | 61 | 41 | GLU |
| 32 | 61 | 44 | LEU |
| 32 | 61 | 50 | ARG |
| 32 | 61 | 51 | ILE |
| 32 | 61 | 60 | GLU |
| 32 | 61 | 62 | LYS |
| 32 | 61 | 64 | GLU |
| 32 | 61 | 68 | LEU |
| 32 | 61 | 70 | GLU |
| 32 | 61 | 71 | ILE |
| 32 | 61 | 79 | ILE |
| 32 | 61 | 85 | GLU |
| 32 | 61 | 92 | VAL |
| 32 | 61 | 95 | LYS |
| 32 | 61 | 114 | LEU |
| 32 | 61 | 116 | LEU |
| 32 | 61 | 121 | LYS |
| 32 | 61 | 128 | LEU |
| 32 | 61 | 135 | GLU |
| 32 | 61 | 136 | VAL |
| 32 | 61 | 142 | VAL |
| 32 | 61 | 144 | VAL |
| 33 | 58 | 1 | MET |
| 33 | 58 | 3 | THR |

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| Mol | Chain | Res | Type |
|---|---|---|---|
| 33 | 58 | 5 | VAL |
| 33 | 58 | 8 | GLN |
| 33 | 58 | 10 | GLU |
| 33 | 58 | 15 | LEU |
| 33 | 58 | 16 | ILE |
| 33 | 58 | 28 | THR |
| 33 | 58 | 30 | ILE |
| 33 | 58 | 32 | THR |
| 33 | 58 | 34 | LEU |
| 33 | 58 | 35 | ARG |
| 33 | 58 | 39 | ARG |
| 33 | 58 | 42 | TRP |
| 33 | 58 | 43 | THR |
| 33 | 58 | 45 | ASN |
| 33 | 58 | 48 | MET |
| 33 | 58 | 58 | ASP |
| 33 | 58 | 60 | ILE |
| 33 | 58 | 63 | THR |
| 33 | 58 | 65 | LYS |
| 33 | 58 | 67 | LEU |
| 33 | 58 | 68 | GLU |
| 33 | 58 | 70 | LYS |
| 33 | 58 | 85 | ILE |
| 33 | 58 | 87 | LEU |
| 33 | 58 | 90 | MET |
| 33 | 58 | 96 | GLU |
| 33 | 58 | 99 | LEU |
| 33 | 58 | 106 | MET |
| 33 | 58 | 122 | VAL |
| 33 | 58 | 127 | ASP |
| 33 | 58 | 128 | HIS |
| 33 | 58 | 130 | HIS |
| 33 | 58 | 131 | GLN |
| 33 | 58 | 134 | ARG |
| 34 | 68 | 1 | MET |
| 34 | 68 | 5 | GLN |
| 34 | 68 | 8 | LEU |
| 34 | 68 | 9 | GLU |
| 34 | 68 | 20 | MET |
| 34 | 68 | 22 | ILE |
| 34 | 68 | 24 | VAL |
| 34 | 68 | 25 | LEU |

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| Mol | Chain | Res | Type |
|---|---|---|---|
| 34 | 68 | 26 | LYS |
| 34 | 68 | 28 | SER |
| 34 | 68 | 53 | LYS |
| 34 | 68 | 58 | VAL |
| 34 | 68 | 66 | LYS |
| 34 | 68 | 77 | ILE |
| 34 | 68 | 78 | ARG |
| 34 | 68 | 94 | ARG |
| 34 | 68 | 97 | ARG |
| 34 | 68 | 108 | GLU |
| 34 | 68 | 114 | ILE |
| 34 | 68 | 115 | VAL |
| 34 | 68 | 116 | SER |
| 34 | 68 | 117 | LEU |
| 35 | 78 | 1 | MET |
| 35 | 78 | 4 | SER |
| 35 | 78 | 6 | LEU |
| 35 | 78 | 7 | ARG |
| 35 | 78 | 10 | PRO |
| 35 | 78 | 16 | ARG |
| 35 | 78 | 19 | VAL |
| 35 | 78 | 21 | ARG |
| 35 | 78 | 27 | HIS |
| 35 | 78 | 36 | LYS |
| 35 | 78 | 38 | GLN |
| 35 | 78 | 39 | LYS |
| 35 | 78 | 41 | ARG |
| 35 | 78 | 42 | SER |
| 35 | 78 | 45 | LEU |
| 35 | 78 | 46 | LYS |
| 35 | 78 | 49 | ARG |
| 35 | 78 | 50 | ARG |
| 35 | 78 | 52 | GLU |
| 35 | 78 | 56 | SER |
| 35 | 78 | 59 | LEU |
| 35 | 78 | 62 | LEU |
| 35 | 78 | 64 | LYS |
| 35 | 78 | 70 | GLN |
| 35 | 78 | 71 | VAL |
| 35 | 78 | 75 | ILE |
| 35 | 78 | 85 | LEU |
| 35 | 78 | 88 | LEU |

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| Mol | Chain | Res | Type |
|---|---|---|---|
| 35 | 78 | 96 | THR |
| 35 | 78 | 99 | LEU |
| 35 | 78 | 100 | LEU |
| 35 | 78 | 101 | VAL |
| 35 | 78 | 105 | LEU |
| 35 | 78 | 106 | LEU |
| 35 | 78 | 112 | LEU |
| 35 | 78 | 114 | ILE |
| 35 | 78 | 115 | LEU |
| 35 | 78 | 117 | GLU |
| 35 | 78 | 126 | VAL |
| 35 | 78 | 132 | LYS |
| 35 | 78 | 133 | SER |
| 35 | 78 | 138 | LEU |
| 35 | 78 | 144 | GLU |
| 35 | 78 | 146 | VAL |
| 35 | 78 | 147 | LEU |
| 35 | 78 | 148 | LEU |
| 36 | 88 | 3 | MET |
| 36 | 88 | 5 | ARG |
| 36 | 88 | 7 | MET |
| 36 | 88 | 18 | LYS |
| 36 | 88 | 25 | ASP |
| 36 | 88 | 26 | TYR |
| 36 | 88 | 43 | THR |
| 36 | 88 | 45 | GLN |
| 36 | 88 | 51 | ARG |
| 36 | 88 | 52 | VAL |
| 36 | 88 | 55 | VAL |
| 36 | 88 | 59 | ARG |
| 36 | 88 | 60 | ARG |
| 36 | 88 | 79 | LEU |
| 36 | 88 | 82 | ARG |
| 36 | 88 | 85 | LYS |
| 36 | 88 | 89 | ASN |
| 36 | 88 | 91 | GLU |
| 36 | 88 | 97 | VAL |
| 36 | 88 | 99 | PRO |
| 36 | 88 | 103 | MET |
| 36 | 88 | 110 | THR |
| 36 | 88 | 112 | GLU |
| 36 | 88 | 131 | ILE |

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| Mol | Chain | Res | Type |
|---|---|---|---|
| 36 | 88 | 139 | GLU |
| 37 | 98 | 6 | SER |
| 37 | 98 | 10 | LEU |
| 37 | 98 | 17 | ARG |
| 37 | 98 | 18 | LEU |
| 37 | 98 | 28 | LEU |
| 37 | 98 | 29 | LEU |
| 37 | 98 | 36 | THR |
| 37 | 98 | 40 | LYS |
| 37 | 98 | 44 | LEU |
| 37 | 98 | 65 | LEU |
| 37 | 98 | 67 | LEU |
| 37 | 98 | 74 | LYS |
| 37 | 98 | 75 | LEU |
| 37 | 98 | 76 | VAL |
| 37 | 98 | 79 | LEU |
| 37 | 98 | 91 | GLN |
| 37 | 98 | 96 | ARG |
| 37 | 98 | 100 | LEU |
| 37 | 98 | 105 | ARG |
| 37 | 98 | 107 | ASP |
| 37 | 98 | 113 | LEU |
| 37 | 98 | 114 | VAL |
| 38 | A8 | 4 | LEU |
| 38 | A8 | 14 | VAL |
| 38 | A8 | 15 | ARG |
| 38 | A8 | 17 | ARG |
| 38 | A8 | 19 | LYS |
| 38 | A8 | 21 | THR |
| 38 | A8 | 26 | LEU |
| 38 | A8 | 35 | ILE |
| 38 | A8 | 39 | ILE |
| 38 | A8 | 43 | GLU |
| 38 | A8 | 46 | VAL |
| 38 | A8 | 47 | THR |
| 38 | A8 | 49 | VAL |
| 38 | A8 | 52 | SER |
| 38 | A8 | 53 | SER |
| 38 | A8 | 69 | VAL |
| 38 | A8 | 82 | ILE |
| 38 | A8 | 98 | VAL |
| 38 | A8 | 101 | LEU |

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| Mol | Chain | Res | Type |
|---|---|---|---|
| 38 | A8 | 107 | GLU |
| 39 | B8 | 6 | LEU |
| 39 | B8 | 9 | LEU |
| 39 | B8 | 10 | VAL |
| 39 | B8 | 12 | SER |
| 39 | B8 | 15 | VAL |
| 39 | B8 | 16 | ARG |
| 39 | B8 | 17 | THR |
| 39 | B8 | 18 | ASP |
| 39 | B8 | 19 | LEU |
| 39 | B8 | 21 | GLU |
| 39 | B8 | 27 | THR |
| 39 | B8 | 30 | VAL |
| 39 | B8 | 38 | ASN |
| 39 | B8 | 39 | ARG |
| 39 | B8 | 40 | THR |
| 39 | B8 | 44 | ASP |
| 39 | B8 | 49 | VAL |
| 39 | B8 | 50 | ILE |
| 39 | B8 | 62 | THR |
| 39 | B8 | 73 | GLU |
| 39 | B8 | 74 | ARG |
| 39 | B8 | 80 | SER |
| 39 | B8 | 86 | ILE |
| 39 | B8 | 87 | ASP |
| 39 | B8 | 88 | ILE |
| 39 | B8 | 89 | VAL |
| 39 | B8 | 96 | ARG |
| 39 | B8 | 98 | LYS |
| 39 | B8 | 105 | LEU |
| 39 | B8 | 106 | SER |
| 39 | B8 | 109 | GLU |
| 39 | B8 | 110 | ILE |
| 39 | B8 | 118 | ARG |
| 39 | B8 | 121 | ILE |
| 39 | B8 | 125 | ARG |
| 39 | B8 | 132 | LYS |
| 39 | B8 | 136 | GLN |
| 40 | C8 | 5 | LYS |
| 40 | C8 | 9 | VAL |
| 40 | C8 | 27 | LEU |
| 40 | C8 | 34 | LYS |

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| Mol | Chain | Res | Type |
|---|---|---|---|
| 40 | C8 | 52 | ARG |
| 40 | C8 | 60 | LEU |
| 40 | C8 | 70 | ARG |
| 40 | C8 | 74 | LEU |
| 40 | C8 | 75 | ASN |
| 40 | C8 | 81 | HIS |
| 40 | C8 | 84 | LYS |
| 40 | C8 | 89 | GLU |
| 40 | C8 | 90 | VAL |
| 40 | C8 | 92 | ARG |
| 40 | C8 | 95 | LEU |
| 40 | C8 | 98 | LEU |
| 40 | C8 | 108 | GLU |
| 40 | C8 | 109 | LEU |
| 40 | C8 | 111 | GLU |
| 41 | D8 | 5 | VAL |
| 41 | D8 | 6 | LYS |
| 41 | D8 | 7 | THR |
| 41 | D8 | 12 | TYR |
| 41 | D8 | 13 | ARG |
| 41 | D8 | 18 | LEU |
| 41 | D8 | 20 | LEU |
| 41 | D8 | 22 | VAL |
| 41 | D8 | 23 | GLU |
| 41 | D8 | 24 | LYS |
| 41 | D8 | 25 | LEU |
| 41 | D8 | 28 | GLU |
| 41 | D8 | 35 | LEU |
| 41 | D8 | 37 | VAL |
| 41 | D8 | 39 | LEU |
| 41 | D8 | 40 | LEU |
| 41 | D8 | 45 | THR |
| 41 | D8 | 47 | VAL |
| 41 | D8 | 49 | THR |
| 41 | D8 | 52 | VAL |
| 41 | D8 | 57 | VAL |
| 41 | D8 | 58 | VAL |
| 41 | D8 | 62 | LEU |
| 41 | D8 | 70 | ILE |
| 41 | D8 | 72 | VAL |
| 41 | D8 | 78 | LYS |
| 41 | D8 | 88 | ARG |

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| Mol | Chain | Res | Type |
|---|---|---|---|
| 41 | D8 | 95 | LEU |
| 41 | D8 | 98 | GLU |
| 42 | E8 | 1 | MET |
| 42 | E8 | 2 | GLU |
| 42 | E8 | 6 | ILE |
| 42 | E8 | 11 | ARG |
| 42 | E8 | 19 | LEU |
| 42 | E8 | 20 | VAL |
| 42 | E8 | 21 | VAL |
| 42 | E8 | 27 | LYS |
| 42 | E8 | 37 | ARG |
| 42 | E8 | 39 | THR |
| 42 | E8 | 51 | LEU |
| 42 | E8 | 52 | GLU |
| 42 | E8 | 64 | MET |
| 42 | E8 | 69 | LEU |
| 42 | E8 | 76 | VAL |
| 42 | E8 | 77 | ASP |
| 42 | E8 | 78 | GLU |
| 42 | E8 | 83 | LYS |
| 42 | E8 | 88 | ARG |
| 42 | E8 | 94 | ASP |
| 42 | E8 | 95 | ILE |
| 42 | E8 | 96 | ILE |
| 42 | E8 | 97 | LYS |
| 42 | E8 | 98 | LYS |
| 42 | E8 | 100 | THR |
| 42 | E8 | 106 | ILE |
| 42 | E8 | 107 | LEU |
| 42 | E8 | 111 | HIS |
| 43 | F8 | 3 | THR |
| 43 | F8 | 8 | ILE |
| 43 | F8 | 12 | VAL |
| 43 | F8 | 15 | GLU |
| 43 | F8 | 23 | GLU |
| 43 | F8 | 27 | THR |
| 43 | F8 | 33 | LYS |
| 43 | F8 | 35 | THR |
| 43 | F8 | 37 | THR |
| 43 | F8 | 40 | LYS |
| 43 | F8 | 53 | LYS |
| 43 | F8 | 57 | LEU |

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| Mol | Chain | Res | Type |
|---|---|---|---|
| 43 | F8 | 65 | ARG |
| 43 | F8 | 68 | ARG |
| 43 | F8 | 76 | ARG |
| 43 | F8 | 78 | LYS |
| 43 | F8 | 80 | ILE |
| 43 | F8 | 81 | VAL |
| 43 | F8 | 89 | ILE |
| 43 | F8 | 90 | GLU |
| 43 | F8 | 92 | LEU |
| 44 | G8 | 4 | LYS |
| 44 | G8 | 7 | VAL |
| 44 | G8 | 14 | LEU |
| 44 | G8 | 21 | LYS |
| 44 | G8 | 24 | VAL |
| 44 | G8 | 27 | VAL |
| 44 | G8 | 29 | GLU |
| 44 | G8 | 31 | LEU |
| 44 | G8 | 33 | LYS |
| 44 | G8 | 38 | ILE |
| 44 | G8 | 39 | VAL |
| 44 | G8 | 40 | GLU |
| 44 | G8 | 42 | VAL |
| 44 | G8 | 47 | LYS |
| 44 | G8 | 49 | VAL |
| 44 | G8 | 52 | SER |
| 44 | G8 | 54 | LYS |
| 44 | G8 | 57 | GLN |
| 44 | G8 | 64 | GLU |
| 44 | G8 | 67 | LEU |
| 44 | G8 | 75 | ILE |
| 44 | G8 | 84 | ARG |
| 44 | G8 | 85 | VAL |
| 44 | G8 | 86 | ARG |
| 44 | G8 | 90 | LEU |
| 44 | G8 | 94 | LYS |
| 44 | G8 | 99 | CYS |
| 45 | H8 | 2 | GLU |
| 45 | H8 | 9 | TYR |
| 45 | H8 | 16 | SER |
| 45 | H8 | 18 | LEU |
| 45 | H8 | 19 | ARG |
| 45 | H8 | 20 | ARG |

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| Mol | Chain | Res | Type |
|---|---|---|---|
| 45 | H8 | 24 | LEU |
| 45 | H8 | 33 | LEU |
| 45 | H8 | 34 | ASN |
| 45 | H8 | 35 | ARG |
| 45 | H8 | 37 | VAL |
| 45 | H8 | 47 | VAL |
| 45 | H8 | 52 | SER |
| 45 | H8 | 53 | ILE |
| 45 | H8 | 59 | LEU |
| 45 | H8 | 61 | LEU |
| 45 | H8 | 71 | VAL |
| 45 | H8 | 72 | ARG |
| 45 | H8 | 74 | VAL |
| 45 | H8 | 76 | LEU |
| 45 | H8 | 77 | ASP |
| 45 | H8 | 81 | ARG |
| 45 | H8 | 82 | ARG |
| 45 | H8 | 91 | LEU |
| 45 | H8 | 94 | GLU |
| 45 | H8 | 97 | GLU |
| 45 | H8 | 105 | VAL |
| 45 | H8 | 107 | THR |
| 45 | H8 | 111 | VAL |
| 45 | H8 | 120 | ILE |
| 45 | H8 | 121 | HIS |
| 45 | H8 | 132 | ASN |
| 45 | H8 | 140 | ASP |
| 45 | H8 | 155 | LEU |
| 45 | H8 | 163 | LEU |
| 45 | H8 | 165 | VAL |
| 45 | H8 | 168 | GLU |
| 45 | H8 | 169 | GLU |
| 46 | I8 | 3 | HIS |
| 46 | I8 | 4 | LYS |
| 46 | I8 | 5 | LYS |
| 46 | I8 | 10 | THR |
| 46 | I8 | 20 | ARG |
| 46 | I8 | 36 | ILE |
| 46 | I8 | 40 | GLN |
| 46 | I8 | 41 | ARG |
| 46 | I8 | 43 | THR |
| 46 | I8 | 53 | MET |

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| Mol | Chain | Res | Type |
|---|---|---|---|
| 46 | I8 | 64 | ASP |
| 46 | I8 | 66 | VAL |
| 46 | I8 | 67 | VAL |
| 46 | I8 | 68 | GLU |
| 46 | I8 | 72 | ARG |
| 46 | I8 | 79 | VAL |
| 46 | I8 | 80 | HIS |
| 46 | I8 | 81 | VAL |
| 47 | J8 | 4 | VAL |
| 47 | J8 | 6 | GLU |
| 47 | J8 | 13 | ILE |
| 47 | J8 | 14 | VAL |
| 47 | J8 | 19 | GLN |
| 47 | J8 | 26 | ARG |
| 47 | J8 | 40 | ARG |
| 47 | J8 | 41 | ARG |
| 47 | J8 | 46 | LEU |
| 47 | J8 | 51 | VAL |
| 47 | J8 | 53 | VAL |
| 47 | J8 | 62 | VAL |
| 47 | J8 | 65 | SER |
| 47 | J8 | 69 | LYS |
| 47 | J8 | 73 | LEU |
| 47 | J8 | 74 | VAL |
| 47 | J8 | 78 | LYS |
| 47 | J8 | 80 | LEU |
| 47 | J8 | 81 | LYS |
| 47 | J8 | 82 | LEU |
| 47 | J8 | 83 | GLU |
| 47 | J8 | 85 | LEU |
| 47 | J8 | 86 | SER |
| 47 | J8 | 89 | GLU |
| 47 | J8 | 91 | LYS |
| 47 | J8 | 93 | GLU |
| 47 | J8 | 94 | LEU |
| 47 | J8 | 96 | LYS |
| 48 | K8 | 4 | SER |
| 48 | K8 | 5 | GLU |
| 48 | K8 | 6 | VAL |
| 48 | K8 | 10 | LEU |
| 48 | K8 | 11 | GLU |
| 48 | K8 | 16 | LEU |

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| Mol | Chain | Res | Type |
|---|---|---|---|
| 48 | K8 | 24 | LEU |
| 48 | K8 | 28 | LYS |
| 48 | K8 | 32 | LEU |
| 48 | K8 | 35 | LEU |
| 48 | K8 | 44 | LEU |
| 48 | K8 | 47 | ASN |
| 48 | K8 | 53 | LEU |
| 48 | K8 | 54 | LYS |
| 48 | K8 | 64 | LEU |
| 48 | K8 | 65 | ASN |
| 48 | K8 | 66 | GLU |
| 49 | L8 | 6 | VAL |
| 49 | L8 | 8 | LEU |
| 49 | L8 | 11 | SER |
| 49 | L8 | 18 | ASP |
| 49 | L8 | 23 | LEU |
| 49 | L8 | 31 | LEU |
| 49 | L8 | 34 | GLU |
| 49 | L8 | 35 | ARG |
| 49 | L8 | 37 | LEU |
| 49 | L8 | 38 | GLU |
| 49 | L8 | 40 | THR |
| 49 | L8 | 43 | ILE |
| 49 | L8 | 53 | LEU |
| 49 | L8 | 58 | VAL |
| 50 | M8 | 6 | HIS |
| 50 | M8 | 10 | VAL |
| 50 | M8 | 35 | VAL |
| 50 | M8 | 48 | ARG |
| 50 | M8 | 50 | VAL |
| 50 | M8 | 57 | GLU |
| 50 | M8 | 60 | GLN |
| 50 | M8 | 61 | ARG |
| 50 | M8 | 63 | TYR |
| 51 | N8 | 5 | PRO |
| 51 | N8 | 6 | VAL |
| 51 | N8 | 9 | LYS |
| 51 | N8 | 10 | LYS |
| 51 | N8 | 11 | THR |
| 51 | N8 | 16 | ARG |
| 51 | N8 | 26 | THR |
| 51 | N8 | 29 | THR |

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| Mol | Chain | Res | Type |
|---|---|---|---|
| 51 | N8 | 33 | CYS |
| 51 | N8 | 36 | CYS |
| 51 | N8 | 40 | LYS |
| 51 | N8 | 44 | THR |
| 51 | N8 | 51 | TYR |
| 51 | N8 | 52 | TYR |
| 52 | O8 | 9 | LEU |
| 52 | O8 | 10 | LEU |
| 52 | O8 | 23 | THR |
| 52 | O8 | 28 | ARG |
| 52 | O8 | 30 | THR |
| 52 | O8 | 32 | ASN |
| 52 | O8 | 34 | LEU |
| 52 | O8 | 36 | LEU |
| 52 | O8 | 43 | CYS |
| 52 | O8 | 44 | ARG |
| 52 | O8 | 51 | GLU |
| 53 | P8 | 4 | THR |
| 53 | P8 | 8 | ASN |
| 53 | P8 | 11 | LYS |
| 53 | P8 | 14 | LYS |
| 53 | P8 | 23 | ARG |
| 53 | P8 | 24 | THR |
| 53 | P8 | 43 | THR |
| 53 | P8 | 46 | VAL |
| 54 | Q8 | 4 | MET |
| 54 | Q8 | 8 | LYS |
| 54 | Q8 | 11 | LYS |
| 54 | Q8 | 13 | ARG |
| 54 | Q8 | 14 | VAL |
| 54 | Q8 | 19 | SER |
| 54 | Q8 | 22 | VAL |
| 54 | Q8 | 23 | VAL |
| 54 | Q8 | 25 | MET |
| 54 | Q8 | 26 | LYS |
| 54 | Q8 | 29 | LYS |
| 54 | Q8 | 40 | GLU |
| 54 | Q8 | 49 | VAL |
| 54 | Q8 | 54 | GLU |
| 54 | Q8 | 56 | GLU |
| 54 | Q8 | 57 | ARG |
| 54 | Q8 | 58 | ILE |

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| Mol | Chain | Res | Type |
|---|---|---|---|
| 54 | Q8 | 59 | LYS |
| 54 | Q8 | 60 | LEU |
| 54 | Q8 | 62 | LEU |
| 2 | 12 | 6 | THR |
| 2 | 12 | 7 | VAL |
| 2 | 12 | 8 | LYS |
| 2 | 12 | 19 | HIS |
| 2 | 12 | 20 | GLU |
| 2 | 12 | 23 | ARG |
| 2 | 12 | 32 | ILE |
| 2 | 12 | 36 | ARG |
| 2 | 12 | 41 | ILE |
| 2 | 12 | 44 | LEU |
| 2 | 12 | 47 | THR |
| 2 | 12 | 48 | MET |
| 2 | 12 | 56 | ARG |
| 2 | 12 | 58 | ILE |
| 2 | 12 | 67 | THR |
| 2 | 12 | 69 | LEU |
| 2 | 12 | 71 | VAL |
| 2 | 12 | 76 | GLN |
| 2 | 12 | 86 | GLU |
| 2 | 12 | 87 | ARG |
| 2 | 12 | 90 | MET |
| 2 | 12 | 98 | LEU |
| 2 | 12 | 107 | THR |
| 2 | 12 | 108 | ILE |
| 2 | 12 | 111 | ARG |
| 2 | 12 | 112 | VAL |
| 2 | 12 | 118 | LEU |
| 2 | 12 | 132 | LYS |
| 2 | 12 | 164 | VAL |
| 2 | 12 | 168 | THR |
| 2 | 12 | 172 | ILE |
| 2 | 12 | 176 | GLU |
| 2 | 12 | 185 | ILE |
| 2 | 12 | 196 | LEU |
| 2 | 12 | 200 | ILE |
| 2 | 12 | 205 | ASP |
| 2 | 12 | 212 | GLN |
| 2 | 12 | 215 | LEU |
| 2 | 12 | 223 | ILE |

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| Mol | Chain | Res | Type |
|---|---|---|---|
| 2 | 12 | 230 | VAL |
| 2 | 12 | 233 | SER |
| 2 | 12 | 238 | LEU |
| 2 | 12 | 239 | VAL |
| 3 | 22 | 3 | ASN |
| 3 | 22 | 4 | LYS |
| 3 | 22 | 12 | LEU |
| 3 | 22 | 14 | ILE |
| 3 | 22 | 15 | THR |
| 3 | 22 | 21 | ARG |
| 3 | 22 | 27 | LYS |
| 3 | 22 | 28 | GLN |
| 3 | 22 | 34 | LEU |
| 3 | 22 | 39 | ILE |
| 3 | 22 | 40 | ARG |
| 3 | 22 | 42 | LEU |
| 3 | 22 | 46 | GLU |
| 3 | 22 | 47 | LEU |
| 3 | 22 | 59 | ARG |
| 3 | 22 | 64 | VAL |
| 3 | 22 | 72 | LYS |
| 3 | 22 | 79 | ARG |
| 3 | 22 | 84 | ILE |
| 3 | 22 | 88 | ARG |
| 3 | 22 | 89 | GLU |
| 3 | 22 | 94 | LEU |
| 3 | 22 | 104 | GLN |
| 3 | 22 | 115 | LEU |
| 3 | 22 | 118 | GLN |
| 3 | 22 | 119 | ARG |
| 3 | 22 | 122 | GLU |
| 3 | 22 | 142 | MET |
| 3 | 22 | 151 | VAL |
| 3 | 22 | 153 | VAL |
| 3 | 22 | 167 | TRP |
| 3 | 22 | 173 | VAL |
| 3 | 22 | 175 | LEU |
| 3 | 22 | 178 | LEU |
| 3 | 22 | 184 | TYR |
| 3 | 22 | 188 | LEU |
| 3 | 22 | 202 | ILE |
| 3 | 22 | 204 | LEU |

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| Mol | Chain | Res | Type |
|---|---|---|---|
| 3 | 22 | 207 | VAL |
| 4 | 32 | 12 | CYS |
| 4 | 32 | 15 | GLU |
| 4 | 32 | 18 | LYS |
| 4 | 32 | 24 | GLU |
| 4 | 32 | 25 | ARG |
| 4 | 32 | 30 | LYS |
| 4 | 32 | 35 | ARG |
| 4 | 32 | 36 | ARG |
| 4 | 32 | 38 | TYR |
| 4 | 32 | 42 | GLN |
| 4 | 32 | 49 | ARG |
| 4 | 32 | 50 | ARG |
| 4 | 32 | 53 | ASP |
| 4 | 32 | 58 | LEU |
| 4 | 32 | 59 | ARG |
| 4 | 32 | 64 | LEU |
| 4 | 32 | 66 | ARG |
| 4 | 32 | 76 | ARG |
| 4 | 32 | 85 | LYS |
| 4 | 32 | 108 | LEU |
| 4 | 32 | 119 | GLN |
| 4 | 32 | 122 | ARG |
| 4 | 32 | 132 | ARG |
| 4 | 32 | 134 | ASP |
| 4 | 32 | 135 | LEU |
| 4 | 32 | 139 | ARG |
| 4 | 32 | 141 | ARG |
| 4 | 32 | 154 | ASN |
| 4 | 32 | 156 | GLU |
| 4 | 32 | 158 | ILE |
| 4 | 32 | 170 | VAL |
| 4 | 32 | 175 | SER |
| 4 | 32 | 178 | VAL |
| 4 | 32 | 184 | LYS |
| 4 | 32 | 187 | ARG |
| 4 | 32 | 191 | ARG |
| 4 | 32 | 192 | GLU |
| 4 | 32 | 194 | LEU |
| 4 | 32 | 200 | GLU |
| 5 | 42 | 9 | LYS |
| 5 | 42 | 12 | LEU |

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| Mol | Chain | Res | Type |
|---|---|---|---|
| 5 | 42 | 16 | THR |
| 5 | 42 | 33 | VAL |
| 5 | 42 | 47 | LYS |
| 5 | 42 | 50 | GLU |
| 5 | 42 | 51 | VAL |
| 5 | 42 | 60 | TYR |
| 5 | 42 | 63 | ARG |
| 5 | 42 | 66 | MET |
| 5 | 42 | 73 | ASN |
| 5 | 42 | 75 | THR |
| 5 | 42 | 78 | HIS |
| 5 | 42 | 79 | GLU |
| 5 | 42 | 80 | ILE |
| 5 | 42 | 81 | GLU |
| 5 | 42 | 82 | VAL |
| 5 | 42 | 90 | VAL |
| 5 | 42 | 91 | LEU |
| 5 | 42 | 92 | LYS |
| 5 | 42 | 101 | ILE |
| 5 | 42 | 107 | ARG |
| 5 | 42 | 112 | LEU |
| 5 | 42 | 115 | VAL |
| 5 | 42 | 120 | THR |
| 5 | 42 | 121 | LYS |
| 5 | 42 | 131 | ILE |
| 5 | 42 | 135 | THR |
| 5 | 42 | 144 | THR |
| 5 | 42 | 147 | ASP |
| 6 | 52 | 3 | ARG |
| 6 | 52 | 16 | GLN |
| 6 | 52 | 21 | LEU |
| 6 | 52 | 23 | LYS |
| 6 | 52 | 24 | GLU |
| 6 | 52 | 27 | GLN |
| 6 | 52 | 40 | VAL |
| 6 | 52 | 46 | ARG |
| 6 | 52 | 61 | LEU |
| 6 | 52 | 69 | GLU |
| 6 | 52 | 71 | ARG |
| 6 | 52 | 83 | ASP |
| 6 | 52 | 87 | ARG |
| 6 | 52 | 92 | LYS |

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| Mol | Chain | Res | Type |
|---|---|---|---|
| 6 | 52 | 95 | GLU |
| 6 | 52 | 98 | LEU |
| 7 | 62 | 6 | ARG |
| 7 | 62 | 8 | GLU |
| 7 | 62 | 9 | VAL |
| 7 | 62 | 12 | LEU |
| 7 | 62 | 21 | VAL |
| 7 | 62 | 24 | THR |
| 7 | 62 | 42 | ILE |
| 7 | 62 | 49 | ILE |
| 7 | 62 | 54 | THR |
| 7 | 62 | 57 | GLU |
| 7 | 62 | 58 | PRO |
| 7 | 62 | 60 | LYS |
| 7 | 62 | 63 | LYS |
| 7 | 62 | 73 | MET |
| 7 | 62 | 80 | VAL |
| 7 | 62 | 85 | TYR |
| 7 | 62 | 89 | MET |
| 7 | 62 | 90 | GLU |
| 7 | 62 | 91 | VAL |
| 7 | 62 | 94 | ARG |
| 7 | 62 | 98 | SER |
| 7 | 62 | 114 | ARG |
| 7 | 62 | 115 | ARG |
| 7 | 62 | 124 | LEU |
| 7 | 62 | 129 | GLU |
| 7 | 62 | 131 | LYS |
| 7 | 62 | 138 | LYS |
| 7 | 62 | 144 | MET |
| 7 | 62 | 149 | ARG |
| 8 | 72 | 1 | MET |
| 8 | 72 | 3 | THR |
| 8 | 72 | 21 | LYS |
| 8 | 72 | 23 | SER |
| 8 | 72 | 33 | GLU |
| 8 | 72 | 39 | LEU |
| 8 | 72 | 41 | ARG |
| 8 | 72 | 49 | GLU |
| 8 | 72 | 82 | HIS |
| 8 | 72 | 91 | ARG |
| 8 | 72 | 92 | ARG |

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| Mol | Chain | Res | Type |
|---|---|---|---|
| 8 | 72 | 97 | VAL |
| 8 | 72 | 100 | ILE |
| 8 | 72 | 103 | VAL |
| 8 | 72 | 109 | ILE |
| 8 | 72 | 111 | ILE |
| 8 | 72 | 112 | LEU |
| 8 | 72 | 115 | SER |
| 8 | 72 | 119 | LEU |
| 8 | 72 | 129 | VAL |
| 8 | 72 | 134 | ILE |
| 8 | 72 | 137 | VAL |
| 9 | 82 | 2 | GLU |
| 9 | 82 | 7 | THR |
| 9 | 82 | 10 | ARG |
| 9 | 82 | 20 | ARG |
| 9 | 82 | 27 | THR |
| 9 | 82 | 37 | PHE |
| 9 | 82 | 38 | GLN |
| 9 | 82 | 40 | LEU |
| 9 | 82 | 44 | VAL |
| 9 | 82 | 64 | THR |
| 9 | 82 | 65 | VAL |
| 9 | 82 | 75 | ASP |
| 9 | 82 | 77 | ILE |
| 9 | 82 | 79 | LEU |
| 9 | 82 | 88 | TYR |
| 9 | 82 | 89 | ASN |
| 9 | 82 | 95 | LYS |
| 9 | 82 | 97 | LYS |
| 9 | 82 | 104 | ARG |
| 9 | 82 | 108 | VAL |
| 9 | 82 | 118 | LYS |
| 10 | 1A | 4 | ILE |
| 10 | 1A | 6 | ILE |
| 10 | 1A | 19 | SER |
| 10 | 1A | 22 | LYS |
| 10 | 1A | 29 | ARG |
| 10 | 1A | 38 | ILE |
| 10 | 1A | 40 | LEU |
| 10 | 1A | 48 | THR |
| 10 | 1A | 50 | ILE |
| 10 | 1A | 55 | LYS |

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| Mol | Chain | Res | Type |
|---|---|---|---|
| 10 | 1A | 57 | LYS |
| 10 | 1A | 58 | ASP |
| 10 | 1A | 59 | SER |
| 10 | 1A | 61 | GLU |
| 10 | 1A | 62 | HIS |
| 10 | 1A | 66 | ARG |
| 10 | 1A | 68 | HIS |
| 10 | 1A | 75 | ILE |
| 10 | 1A | 78 | ASN |
| 10 | 1A | 79 | ARG |
| 10 | 1A | 83 | GLU |
| 10 | 1A | 90 | LEU |
| 10 | 1A | 92 | THR |
| 10 | 1A | 95 | GLU |
| 10 | 1A | 99 | LYS |
| 11 | 2A | 12 | ARG |
| 11 | 2A | 13 | GLN |
| 11 | 2A | 14 | VAL |
| 11 | 2A | 21 | ILE |
| 11 | 2A | 24 | SER |
| 11 | 2A | 28 | THR |
| 11 | 2A | 29 | ILE |
| 11 | 2A | 30 | VAL |
| 11 | 2A | 48 | ILE |
| 11 | 2A | 63 | LEU |
| 11 | 2A | 70 | LYS |
| 11 | 2A | 77 | MET |
| 11 | 2A | 78 | GLN |
| 11 | 2A | 83 | ILE |
| 11 | 2A | 93 | GLN |
| 11 | 2A | 103 | LEU |
| 11 | 2A | 112 | THR |
| 11 | 2A | 114 | VAL |
| 12 | 3A | 24 | VAL |
| 12 | 3A | 28 | LYS |
| 12 | 3A | 38 | THR |
| 12 | 3A | 41 | ARG |
| 12 | 3A | 43 | VAL |
| 12 | 3A | 44 | THR |
| 12 | 3A | 53 | ARG |
| 12 | 3A | 54 | LYS |
| 12 | 3A | 57 | LYS |

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| Mol | Chain | Res | Type |
|---|---|---|---|
| 12 | 3A | 60 | LEU |
| 12 | 3A | 64 | TYR |
| 12 | 3A | 83 | VAL |
| 12 | 3A | 84 | LEU |
| 12 | 3A | 97 | ARG |
| 12 | 3A | 111 | LYS |
| 13 | 4A | 3 | ARG |
| 13 | 4A | 4 | ILE |
| 13 | 4A | 7 | VAL |
| 13 | 4A | 12 | ASN |
| 13 | 4A | 19 | LEU |
| 13 | 4A | 43 | THR |
| 13 | 4A | 44 | ARG |
| 13 | 4A | 60 | VAL |
| 13 | 4A | 63 | THR |
| 13 | 4A | 64 | TRP |
| 13 | 4A | 66 | LEU |
| 13 | 4A | 70 | LEU |
| 13 | 4A | 71 | ARG |
| 13 | 4A | 73 | GLU |
| 13 | 4A | 74 | VAL |
| 13 | 4A | 82 | MET |
| 13 | 4A | 101 | GLN |
| 13 | 4A | 103 | THR |
| 13 | 4A | 106 | ASN |
| 13 | 4A | 108 | ARG |
| 13 | 4A | 109 | THR |
| 14 | 5A | 6 | LEU |
| 14 | 5A | 8 | GLU |
| 14 | 5A | 33 | VAL |
| 14 | 5A | 44 | LEU |
| 14 | 5A | 58 | LYS |
| 15 | 6A | 3 | ILE |
| 15 | 6A | 10 | LYS |
| 15 | 6A | 27 | VAL |
| 15 | 6A | 34 | LEU |
| 15 | 6A | 39 | LEU |
| 15 | 6A | 40 | SER |
| 15 | 6A | 42 | HIS |
| 15 | 6A | 65 | ARG |
| 15 | 6A | 66 | LEU |
| 15 | 6A | 82 | ILE |

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| Mol | Chain | Res | Type |
|---|---|---|---|
| 15 | 6A | 83 | GLU |
| 15 | 6A | 84 | LYS |
| 15 | 6A | 88 | ARG |
| 16 | 7A | 1 | MET |
| 16 | 7A | 2 | VAL |
| 16 | 7A | 5 | ARG |
| 16 | 7A | 11 | SER |
| 16 | 7A | 19 | ILE |
| 16 | 7A | 20 | VAL |
| 16 | 7A | 21 | VAL |
| 16 | 7A | 25 | ARG |
| 16 | 7A | 27 | LYS |
| 16 | 7A | 35 | LYS |
| 16 | 7A | 45 | THR |
| 16 | 7A | 47 | ASP |
| 16 | 7A | 53 | VAL |
| 16 | 7A | 67 | THR |
| 16 | 7A | 73 | LEU |
| 16 | 7A | 74 | LEU |
| 17 | 8A | 6 | LEU |
| 17 | 8A | 12 | SER |
| 17 | 8A | 13 | ASP |
| 17 | 8A | 26 | GLN |
| 17 | 8A | 34 | LYS |
| 17 | 8A | 36 | ILE |
| 17 | 8A | 48 | GLU |
| 17 | 8A | 49 | GLU |
| 17 | 8A | 50 | LYS |
| 17 | 8A | 52 | LYS |
| 17 | 8A | 53 | LEU |
| 17 | 8A | 57 | VAL |
| 17 | 8A | 63 | ARG |
| 17 | 8A | 68 | ARG |
| 17 | 8A | 69 | LYS |
| 17 | 8A | 73 | VAL |
| 17 | 8A | 74 | LEU |
| 17 | 8A | 84 | LEU |
| 17 | 8A | 96 | GLU |
| 17 | 8A | 100 | LYS |
| 18 | 9A | 26 | LEU |
| 18 | 9A | 31 | LEU |
| 18 | 9A | 32 | ARG |

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| Mol | Chain | Res | Type |
|---|---|---|---|
| 18 | 9A | 36 | ASN |
| 18 | 9A | 39 | VAL |
| 18 | 9A | 42 | ARG |
| 18 | 9A | 44 | LEU |
| 18 | 9A | 82 | THR |
| 18 | 9A | 84 | LYS |
| 18 | 9A | 86 | VAL |
| 19 | AA | 7 | LYS |
| 19 | AA | 10 | PHE |
| 19 | AA | 14 | HIS |
| 19 | AA | 23 | ASN |
| 19 | AA | 28 | LYS |
| 19 | AA | 37 | ARG |
| 19 | AA | 40 | ILE |
| 19 | AA | 43 | GLU |
| 19 | AA | 51 | VAL |
| 19 | AA | 55 | LYS |
| 19 | AA | 58 | VAL |
| 19 | AA | 60 | VAL |
| 19 | AA | 63 | THR |
| 19 | AA | 64 | GLU |
| 19 | AA | 70 | LYS |
| 19 | AA | 78 | ARG |
| 19 | AA | 81 | ARG |
| 19 | AA | 83 | HIS |
| 20 | BA | 10 | LEU |
| 20 | BA | 36 | LEU |
| 20 | BA | 37 | SER |
| 20 | BA | 39 | LYS |
| 20 | BA | 41 | ILE |
| 20 | BA | 43 | LEU |
| 20 | BA | 56 | MET |
| 20 | BA | 71 | THR |
| 20 | BA | 72 | LEU |
| 20 | BA | 75 | ASN |
| 20 | BA | 80 | ARG |
| 20 | BA | 84 | LEU |
| 20 | BA | 86 | ARG |
| 20 | BA | 87 | LYS |
| 21 | 1B | 24 | ARG |
| 21 | 1B | 25 | LYS |
| 26 | 79 | 10 | LEU |

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| Mol | Chain | Res | Type |
|---|---|---|---|
| 26 | 79 | 14 | VAL |
| 26 | 79 | 21 | THR |
| 26 | 79 | 31 | GLU |
| 26 | 79 | 44 | HIS |
| 26 | 79 | 55 | ASP |
| 26 | 79 | 167 | LYS |
| 26 | 79 | 168 | THR |
| 26 | 79 | 172 | HIS |
| 26 | 79 | 183 | GLU |
| 26 | 79 | 196 | LEU |
| 26 | 79 | 205 | LYS |
| 26 | 79 | 212 | VAL |
| 26 | 79 | 224 | ILE |
| 27 | 19 | 7 | LYS |
| 27 | 19 | 23 | GLU |
| 27 | 19 | 28 | GLU |
| 27 | 19 | 30 | GLU |
| 27 | 19 | 32 | SER |
| 27 | 19 | 33 | LEU |
| 27 | 19 | 34 | VAL |
| 27 | 19 | 37 | LEU |
| 27 | 19 | 43 | ARG |
| 27 | 19 | 49 | ILE |
| 27 | 19 | 61 | LEU |
| 27 | 19 | 64 | ILE |
| 27 | 19 | 65 | ILE |
| 27 | 19 | 89 | SER |
| 27 | 19 | 94 | LEU |
| 27 | 19 | 101 | GLU |
| 27 | 19 | 103 | ARG |
| 27 | 19 | 105 | ILE |
| 27 | 19 | 112 | GLN |
| 27 | 19 | 127 | VAL |
| 27 | 19 | 136 | ILE |
| 27 | 19 | 138 | VAL |
| 27 | 19 | 141 | VAL |
| 27 | 19 | 147 | LEU |
| 27 | 19 | 157 | ARG |
| 27 | 19 | 165 | ILE |
| 27 | 19 | 166 | GLN |
| 27 | 19 | 173 | VAL |
| 27 | 19 | 192 | THR |

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| Mol | Chain | Res | Type |
|---|---|---|---|
| 27 | 19 | 193 | VAL |
| 27 | 19 | 200 | ASP |
| 27 | 19 | 204 | ILE |
| 27 | 19 | 211 | ARG |
| 27 | 19 | 217 | ARG |
| 27 | 19 | 218 | ARG |
| 27 | 19 | 242 | ARG |
| 27 | 19 | 244 | ARG |
| 27 | 19 | 255 | LYS |
| 27 | 19 | 257 | LEU |
| 27 | 19 | 262 | ARG |
| 27 | 19 | 263 | ARG |
| 27 | 19 | 271 | ILE |
| 28 | 29 | 4 | ILE |
| 28 | 29 | 5 | LEU |
| 28 | 29 | 11 | MET |
| 28 | 29 | 25 | VAL |
| 28 | 29 | 26 | ILE |
| 28 | 29 | 27 | LEU |
| 28 | 29 | 33 | VAL |
| 28 | 29 | 38 | THR |
| 28 | 29 | 41 | LYS |
| 28 | 29 | 45 | THR |
| 28 | 29 | 48 | GLN |
| 28 | 29 | 51 | PHE |
| 28 | 29 | 59 | VAL |
| 28 | 29 | 60 | ASN |
| 28 | 29 | 63 | LEU |
| 28 | 29 | 69 | LYS |
| 28 | 29 | 76 | ARG |
| 28 | 29 | 77 | ILE |
| 28 | 29 | 78 | LEU |
| 28 | 29 | 82 | ARG |
| 28 | 29 | 87 | GLU |
| 28 | 29 | 101 | ARG |
| 28 | 29 | 107 | THR |
| 28 | 29 | 116 | VAL |
| 28 | 29 | 119 | ARG |
| 28 | 29 | 140 | SER |
| 28 | 29 | 144 | ARG |
| 28 | 29 | 146 | THR |
| 28 | 29 | 152 | LYS |

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| Mol | Chain | Res | Type |
|---|---|---|---|
| 28 | 29 | 154 | LYS |
| 28 | 29 | 165 | VAL |
| 28 | 29 | 166 | THR |
| 28 | 29 | 171 | GLU |
| 28 | 29 | 175 | VAL |
| 28 | 29 | 181 | LEU |
| 28 | 29 | 182 | LEU |
| 28 | 29 | 184 | VAL |
| 28 | 29 | 188 | VAL |
| 28 | 29 | 197 | ILE |
| 28 | 29 | 199 | ARG |
| 28 | 29 | 200 | GLU |
| 28 | 29 | 201 | THR |
| 28 | 29 | 203 | LYS |
| 29 | 39 | 1 | MET |
| 29 | 39 | 2 | LYS |
| 29 | 39 | 3 | GLU |
| 29 | 39 | 6 | VAL |
| 29 | 39 | 7 | TYR |
| 29 | 39 | 8 | GLN |
| 29 | 39 | 11 | VAL |
| 29 | 39 | 13 | SER |
| 29 | 39 | 19 | GLU |
| 29 | 39 | 20 | LEU |
| 29 | 39 | 23 | ASP |
| 29 | 39 | 33 | LEU |
| 29 | 39 | 38 | ARG |
| 29 | 39 | 40 | GLN |
| 29 | 39 | 41 | LEU |
| 29 | 39 | 53 | THR |
| 29 | 39 | 57 | VAL |
| 29 | 39 | 63 | LYS |
| 29 | 39 | 64 | ILE |
| 29 | 39 | 68 | LYS |
| 29 | 39 | 70 | THR |
| 29 | 39 | 74 | ARG |
| 29 | 39 | 82 | ILE |
| 29 | 39 | 88 | VAL |
| 29 | 39 | 98 | SER |
| 29 | 39 | 104 | LYS |
| 29 | 39 | 108 | LYS |
| 29 | 39 | 110 | LEU |

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| Mol | Chain | Res | Type |
|---|---|---|---|
| 29 | 39 | 114 | VAL |
| 29 | 39 | 123 | LEU |
| 29 | 39 | 124 | LEU |
| 29 | 39 | 127 | GLU |
| 29 | 39 | 151 | SER |
| 29 | 39 | 154 | VAL |
| 29 | 39 | 158 | THR |
| 29 | 39 | 171 | PRO |
| 29 | 39 | 175 | THR |
| 29 | 39 | 181 | LEU |
| 29 | 39 | 183 | VAL |
| 29 | 39 | 191 | ARG |
| 29 | 39 | 192 | LEU |
| 29 | 39 | 196 | LEU |
| 29 | 39 | 200 | GLU |
| 29 | 39 | 201 | VAL |
| 30 | 49 | 3 | LEU |
| 30 | 49 | 5 | VAL |
| 30 | 49 | 7 | LEU |
| 30 | 49 | 14 | GLU |
| 30 | 49 | 16 | ARG |
| 30 | 49 | 25 | TYR |
| 30 | 49 | 26 | GLN |
| 30 | 49 | 31 | VAL |
| 30 | 49 | 37 | VAL |
| 30 | 49 | 39 | ILE |
| 30 | 49 | 40 | ASN |
| 30 | 49 | 41 | GLN |
| 30 | 49 | 43 | LEU |
| 30 | 49 | 45 | GLU |
| 30 | 49 | 48 | GLU |
| 30 | 49 | 59 | GLU |
| 30 | 49 | 60 | LEU |
| 30 | 49 | 63 | ILE |
| 30 | 49 | 64 | THR |
| 30 | 49 | 71 | THR |
| 30 | 49 | 79 | ASN |
| 30 | 49 | 80 | PHE |
| 30 | 49 | 86 | MET |
| 30 | 49 | 88 | ILE |
| 30 | 49 | 91 | ARG |
| 30 | 49 | 94 | LEU |

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| Mol | Chain | Res | Type |
|---|---|---|---|
| 30 | 49 | 95 | ARG |
| 30 | 49 | 116 | ASP |
| 30 | 49 | 128 | ARG |
| 30 | 49 | 130 | ASN |
| 30 | 49 | 133 | LEU |
| 30 | 49 | 138 | GLN |
| 30 | 49 | 140 | ILE |
| 30 | 49 | 148 | MET |
| 30 | 49 | 149 | VAL |
| 30 | 49 | 150 | ASP |
| 30 | 49 | 160 | VAL |
| 30 | 49 | 164 | GLU |
| 30 | 49 | 172 | LEU |
| 30 | 49 | 173 | LEU |
| 31 | 59 | 4 | ILE |
| 31 | 59 | 9 | ILE |
| 31 | 59 | 19 | VAL |
| 31 | 59 | 26 | VAL |
| 31 | 59 | 30 | LYS |
| 31 | 59 | 32 | GLU |
| 31 | 59 | 35 | VAL |
| 31 | 59 | 41 | MET |
| 31 | 59 | 44 | VAL |
| 31 | 59 | 45 | VAL |
| 31 | 59 | 47 | GLU |
| 31 | 59 | 49 | VAL |
| 31 | 59 | 51 | ARG |
| 31 | 59 | 52 | VAL |
| 31 | 59 | 56 | SER |
| 31 | 59 | 57 | ASP |
| 31 | 59 | 83 | TYR |
| 31 | 59 | 88 | LEU |
| 31 | 59 | 95 | ARG |
| 31 | 59 | 101 | ARG |
| 31 | 59 | 103 | LEU |
| 31 | 59 | 104 | GLU |
| 31 | 59 | 105 | LEU |
| 31 | 59 | 107 | VAL |
| 31 | 59 | 122 | THR |
| 31 | 59 | 123 | PHE |
| 31 | 59 | 127 | GLU |
| 31 | 59 | 129 | THR |

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| Mol | Chain | Res | Type |
|---|---|---|---|
| 31 | 59 | 136 | ILE |
| 31 | 59 | 143 | GLN |
| 31 | 59 | 144 | VAL |
| 31 | 59 | 157 | TYR |
| 31 | 59 | 159 | GLU |
| 31 | 59 | 160 | LYS |
| 31 | 59 | 164 | TYR |
| 31 | 59 | 171 | LEU |
| 32 | 69 | 4 | ILE |
| 32 | 69 | 7 | GLU |
| 32 | 69 | 9 | LEU |
| 32 | 69 | 10 | GLU |
| 32 | 69 | 14 | ASP |
| 32 | 69 | 18 | VAL |
| 32 | 69 | 19 | VAL |
| 32 | 69 | 38 | LEU |
| 32 | 69 | 40 | THR |
| 32 | 69 | 47 | LEU |
| 32 | 69 | 50 | ARG |
| 32 | 69 | 58 | LEU |
| 32 | 69 | 62 | LYS |
| 32 | 69 | 67 | ARG |
| 32 | 69 | 76 | THR |
| 32 | 69 | 77 | LEU |
| 32 | 69 | 82 | ARG |
| 32 | 69 | 85 | GLU |
| 32 | 69 | 86 | THR |
| 32 | 69 | 87 | LYS |
| 32 | 69 | 101 | LEU |
| 32 | 69 | 102 | SER |
| 32 | 69 | 103 | ARG |
| 32 | 69 | 109 | ILE |
| 32 | 69 | 114 | LEU |
| 32 | 69 | 116 | LEU |
| 32 | 69 | 120 | ILE |
| 32 | 69 | 122 | GLU |
| 32 | 69 | 125 | GLU |
| 32 | 69 | 128 | LEU |
| 32 | 69 | 133 | HIS |
| 32 | 69 | 136 | VAL |
| 32 | 69 | 139 | GLN |
| 32 | 69 | 140 | LEU |

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| Mol | Chain | Res | Type |
|---|---|---|---|
| 32 | 69 | 142 | VAL |
| 32 | 69 | 145 | VAL |
| 33 | 15 | 7 | LYS |
| 33 | 15 | 9 | VAL |
| 33 | 15 | 15 | LEU |
| 33 | 15 | 30 | ILE |
| 33 | 15 | 32 | THR |
| 33 | 15 | 33 | LEU |
| 33 | 15 | 34 | LEU |
| 33 | 15 | 38 | HIS |
| 33 | 15 | 42 | TRP |
| 33 | 15 | 50 | ASP |
| 33 | 15 | 60 | ILE |
| 33 | 15 | 62 | VAL |
| 33 | 15 | 63 | THR |
| 33 | 15 | 67 | LEU |
| 33 | 15 | 68 | GLU |
| 33 | 15 | 74 | ARG |
| 33 | 15 | 87 | LEU |
| 33 | 15 | 93 | THR |
| 33 | 15 | 94 | HIS |
| 33 | 15 | 98 | VAL |
| 33 | 15 | 99 | LEU |
| 33 | 15 | 104 | LYS |
| 33 | 15 | 106 | MET |
| 33 | 15 | 116 | LEU |
| 33 | 15 | 120 | LEU |
| 33 | 15 | 127 | ASP |
| 33 | 15 | 131 | GLN |
| 33 | 15 | 134 | ARG |
| 33 | 15 | 137 | LYS |
| 34 | 25 | 1 | MET |
| 34 | 25 | 5 | GLN |
| 34 | 25 | 8 | LEU |
| 34 | 25 | 10 | VAL |
| 34 | 25 | 22 | ILE |
| 34 | 25 | 23 | ARG |
| 34 | 25 | 24 | VAL |
| 34 | 25 | 26 | LYS |
| 34 | 25 | 29 | ASN |
| 34 | 25 | 31 | LYS |
| 34 | 25 | 47 | ILE |

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| Mol | Chain | Res | Type |
|---|---|---|---|
| 34 | 25 | 52 | VAL |
| 34 | 25 | 66 | LYS |
| 34 | 25 | 70 | LYS |
| 34 | 25 | 71 | ARG |
| 34 | 25 | 78 | ARG |
| 34 | 25 | 82 | ASN |
| 34 | 25 | 86 | ILE |
| 34 | 25 | 87 | ILE |
| 34 | 25 | 89 | ASN |
| 34 | 25 | 91 | LEU |
| 34 | 25 | 96 | THR |
| 34 | 25 | 98 | VAL |
| 34 | 25 | 108 | GLU |
| 34 | 25 | 117 | LEU |
| 35 | 35 | 2 | LYS |
| 35 | 35 | 3 | LEU |
| 35 | 35 | 5 | ASP |
| 35 | 35 | 6 | LEU |
| 35 | 35 | 15 | ARG |
| 35 | 35 | 21 | ARG |
| 35 | 35 | 30 | THR |
| 35 | 35 | 36 | LYS |
| 35 | 35 | 41 | ARG |
| 35 | 35 | 45 | LEU |
| 35 | 35 | 46 | LYS |
| 35 | 35 | 49 | ARG |
| 35 | 35 | 50 | ARG |
| 35 | 35 | 52 | GLU |
| 35 | 35 | 59 | LEU |
| 35 | 35 | 65 | ARG |
| 35 | 35 | 70 | GLN |
| 35 | 35 | 71 | VAL |
| 35 | 35 | 75 | ILE |
| 35 | 35 | 83 | VAL |
| 35 | 35 | 85 | LEU |
| 35 | 35 | 90 | ARG |
| 35 | 35 | 91 | PHE |
| 35 | 35 | 95 | VAL |
| 35 | 35 | 96 | THR |
| 35 | 35 | 98 | GLU |
| 35 | 35 | 105 | LEU |
| 35 | 35 | 111 | ARG |

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| Mol | Chain | Res | Type |
|---|---|---|---|
| 35 | 35 | 112 | LEU |
| 35 | 35 | 114 | ILE |
| 35 | 35 | 125 | VAL |
| 35 | 35 | 126 | VAL |
| 35 | 35 | 133 | SER |
| 35 | 35 | 138 | LEU |
| 35 | 35 | 139 | LYS |
| 35 | 35 | 144 | GLU |
| 35 | 35 | 146 | VAL |
| 35 | 35 | 147 | LEU |
| 36 | 45 | 3 | MET |
| 36 | 45 | 5 | ARG |
| 36 | 45 | 7 | MET |
| 36 | 45 | 10 | ARG |
| 36 | 45 | 22 | LYS |
| 36 | 45 | 35 | VAL |
| 36 | 45 | 42 | ILE |
| 36 | 45 | 45 | GLN |
| 36 | 45 | 47 | ILE |
| 36 | 45 | 52 | VAL |
| 36 | 45 | 56 | ARG |
| 36 | 45 | 60 | ARG |
| 36 | 45 | 64 | ILE |
| 36 | 45 | 81 | VAL |
| 36 | 45 | 83 | MET |
| 36 | 45 | 90 | VAL |
| 36 | 45 | 103 | MET |
| 36 | 45 | 109 | VAL |
| 36 | 45 | 110 | THR |
| 36 | 45 | 118 | LEU |
| 36 | 45 | 127 | ILE |
| 36 | 45 | 129 | THR |
| 36 | 45 | 131 | ILE |
| 36 | 45 | 132 | VAL |
| 36 | 45 | 137 | TYR |
| 37 | 55 | 18 | LEU |
| 37 | 55 | 28 | LEU |
| 37 | 55 | 29 | LEU |
| 37 | 55 | 33 | ARG |
| 37 | 55 | 34 | ILE |
| 37 | 55 | 36 | THR |
| 37 | 55 | 37 | THR |

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| Mol | Chain | Res | Type |
|---|---|---|---|
| 37 | 55 | 44 | LEU |
| 37 | 55 | 48 | VAL |
| 37 | 55 | 54 | LEU |
| 37 | 55 | 57 | ARG |
| 37 | 55 | 65 | LEU |
| 37 | 55 | 66 | VAL |
| 37 | 55 | 67 | LEU |
| 37 | 55 | 73 | VAL |
| 37 | 55 | 75 | LEU |
| 37 | 55 | 79 | LEU |
| 37 | 55 | 88 | ARG |
| 37 | 55 | 95 | THR |
| 37 | 55 | 102 | GLU |
| 37 | 55 | 105 | ARG |
| 37 | 55 | 107 | ASP |
| 37 | 55 | 117 | VAL |
| 38 | 65 | 3 | ARG |
| 38 | 65 | 14 | VAL |
| 38 | 65 | 15 | ARG |
| 38 | 65 | 18 | ILE |
| 38 | 65 | 25 | ARG |
| 38 | 65 | 26 | LEU |
| 38 | 65 | 28 | VAL |
| 38 | 65 | 30 | ARG |
| 38 | 65 | 36 | TYR |
| 38 | 65 | 40 | ILE |
| 38 | 65 | 41 | ASP |
| 38 | 65 | 42 | ASP |
| 38 | 65 | 44 | LYS |
| 38 | 65 | 50 | SER |
| 38 | 65 | 56 | LEU |
| 38 | 65 | 57 | LYS |
| 38 | 65 | 58 | LEU |
| 38 | 65 | 59 | LYS |
| 38 | 65 | 61 | ASN |
| 38 | 65 | 64 | GLU |
| 38 | 65 | 65 | VAL |
| 38 | 65 | 69 | VAL |
| 38 | 65 | 71 | ARG |
| 38 | 65 | 73 | LEU |
| 38 | 65 | 78 | LEU |
| 38 | 65 | 83 | LYS |

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| Mol | Chain | Res | Type |
|---|---|---|---|
| 38 | 65 | 97 | ARG |
| 38 | 65 | 98 | VAL |
| 38 | 65 | 101 | LEU |
| 38 | 65 | 106 | ARG |
| 38 | 65 | 107 | GLU |
| 38 | 65 | 110 | LEU |
| 39 | 75 | 3 | ARG |
| 39 | 75 | 12 | SER |
| 39 | 75 | 13 | ARG |
| 39 | 75 | 15 | VAL |
| 39 | 75 | 17 | THR |
| 39 | 75 | 27 | THR |
| 39 | 75 | 30 | VAL |
| 39 | 75 | 40 | THR |
| 39 | 75 | 49 | VAL |
| 39 | 75 | 50 | ILE |
| 39 | 75 | 51 | ARG |
| 39 | 75 | 54 | ARG |
| 39 | 75 | 55 | ASN |
| 39 | 75 | 57 | PHE |
| 39 | 75 | 59 | THR |
| 39 | 75 | 62 | THR |
| 39 | 75 | 74 | ARG |
| 39 | 75 | 85 | LYS |
| 39 | 75 | 86 | ILE |
| 39 | 75 | 89 | VAL |
| 39 | 75 | 93 | ARG |
| 39 | 75 | 105 | LEU |
| 39 | 75 | 107 | ASP |
| 39 | 75 | 112 | ARG |
| 39 | 75 | 118 | ARG |
| 39 | 75 | 121 | ILE |
| 40 | 85 | 5 | LYS |
| 40 | 85 | 15 | LYS |
| 40 | 85 | 17 | ILE |
| 40 | 85 | 20 | LEU |
| 40 | 85 | 27 | LEU |
| 40 | 85 | 31 | SER |
| 40 | 85 | 33 | ARG |
| 40 | 85 | 55 | ARG |
| 40 | 85 | 64 | ARG |
| 40 | 85 | 74 | LEU |

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| Mol | Chain | Res | Type |
|---|---|---|---|
| 40 | 85 | 83 | LEU |
| 40 | 85 | 88 | ILE |
| 40 | 85 | 92 | ARG |
| 40 | 85 | 97 | ASP |
| 40 | 85 | 98 | LEU |
| 40 | 85 | 100 | VAL |
| 40 | 85 | 101 | ARG |
| 41 | 95 | 7 | THR |
| 41 | 95 | 19 | LYS |
| 41 | 95 | 21 | ARG |
| 41 | 95 | 26 | ASP |
| 41 | 95 | 32 | THR |
| 41 | 95 | 47 | VAL |
| 41 | 95 | 53 | GLU |
| 41 | 95 | 57 | VAL |
| 41 | 95 | 61 | VAL |
| 41 | 95 | 62 | LEU |
| 41 | 95 | 68 | LYS |
| 41 | 95 | 70 | ILE |
| 41 | 95 | 80 | GLN |
| 41 | 95 | 81 | TYR |
| 41 | 95 | 82 | ARG |
| 41 | 95 | 83 | ARG |
| 41 | 95 | 84 | LYS |
| 41 | 95 | 88 | ARG |
| 41 | 95 | 95 | LEU |
| 41 | 95 | 100 | ARG |
| 42 | A5 | 11 | ARG |
| 42 | A5 | 15 | ARG |
| 42 | A5 | 19 | LEU |
| 42 | A5 | 20 | VAL |
| 42 | A5 | 23 | LEU |
| 42 | A5 | 27 | LYS |
| 42 | A5 | 41 | LYS |
| 42 | A5 | 50 | VAL |
| 42 | A5 | 51 | LEU |
| 42 | A5 | 52 | GLU |
| 42 | A5 | 59 | VAL |
| 42 | A5 | 60 | ASN |
| 42 | A5 | 65 | LEU |
| 42 | A5 | 70 | TYR |
| 42 | A5 | 71 | VAL |

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| Mol | Chain | Res | Type |
|---|---|---|---|
| 42 | A5 | 76 | VAL |
| 42 | A5 | 90 | ARG |
| 42 | A5 | 94 | ASP |
| 42 | A5 | 106 | ILE |
| 42 | A5 | 107 | LEU |
| 42 | A5 | 110 | LYS |
| 42 | A5 | 111 | HIS |
| 43 | B5 | 8 | ILE |
| 43 | B5 | 12 | VAL |
| 43 | B5 | 35 | THR |
| 43 | B5 | 40 | LYS |
| 43 | B5 | 43 | VAL |
| 43 | B5 | 48 | LYS |
| 43 | B5 | 51 | VAL |
| 43 | B5 | 52 | VAL |
| 43 | B5 | 53 | LYS |
| 43 | B5 | 54 | VAL |
| 43 | B5 | 57 | LEU |
| 43 | B5 | 60 | ARG |
| 43 | B5 | 63 | LYS |
| 43 | B5 | 66 | LEU |
| 43 | B5 | 76 | ARG |
| 43 | B5 | 80 | ILE |
| 43 | B5 | 92 | LEU |
| 44 | C5 | 2 | ARG |
| 44 | C5 | 5 | MET |
| 44 | C5 | 6 | HIS |
| 44 | C5 | 14 | LEU |
| 44 | C5 | 23 | ARG |
| 44 | C5 | 31 | LEU |
| 44 | C5 | 35 | TYR |
| 44 | C5 | 38 | ILE |
| 44 | C5 | 44 | ILE |
| 44 | C5 | 45 | VAL |
| 44 | C5 | 47 | LYS |
| 44 | C5 | 51 | VAL |
| 44 | C5 | 60 | PHE |
| 44 | C5 | 62 | GLU |
| 44 | C5 | 70 | SER |
| 44 | C5 | 75 | ILE |
| 44 | C5 | 86 | ARG |
| 44 | C5 | 87 | LYS |

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| Mol | Chain | Res | Type |
|---|---|---|---|
| 44 | C5 | 88 | LYS |
| 44 | C5 | 89 | PHE |
| 44 | C5 | 97 | ARG |
| 44 | C5 | 98 | VAL |
| 44 | C5 | 99 | CYS |
| 45 | D5 | 2 | GLU |
| 45 | D5 | 14 | LYS |
| 45 | D5 | 16 | SER |
| 45 | D5 | 18 | LEU |
| 45 | D5 | 19 | ARG |
| 45 | D5 | 24 | LEU |
| 45 | D5 | 32 | HIS |
| 45 | D5 | 41 | LEU |
| 45 | D5 | 42 | VAL |
| 45 | D5 | 53 | ILE |
| 45 | D5 | 58 | VAL |
| 45 | D5 | 59 | LEU |
| 45 | D5 | 71 | VAL |
| 45 | D5 | 72 | ARG |
| 45 | D5 | 74 | VAL |
| 45 | D5 | 77 | ASP |
| 45 | D5 | 90 | VAL |
| 45 | D5 | 93 | ASP |
| 45 | D5 | 98 | MET |
| 45 | D5 | 100 | VAL |
| 45 | D5 | 105 | VAL |
| 45 | D5 | 107 | THR |
| 45 | D5 | 117 | LEU |
| 45 | D5 | 118 | GLN |
| 45 | D5 | 120 | ILE |
| 45 | D5 | 123 | ASP |
| 45 | D5 | 132 | ASN |
| 45 | D5 | 133 | ILE |
| 45 | D5 | 138 | GLU |
| 45 | D5 | 140 | ASP |
| 45 | D5 | 144 | LEU |
| 45 | D5 | 161 | VAL |
| 45 | D5 | 163 | LEU |
| 45 | D5 | 165 | VAL |
| 45 | D5 | 171 | ILE |
| 45 | D5 | 174 | VAL |
| 45 | D5 | 175 | VAL |

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| Mol | Chain | Res | Type |
|---|---|---|---|
| 45 | D5 | 179 | ASP |
| 46 | E5 | 9 | SER |
| 46 | E5 | 11 | ARG |
| 46 | E5 | 12 | ASN |
| 46 | E5 | 25 | ARG |
| 46 | E5 | 36 | ILE |
| 46 | E5 | 41 | ARG |
| 46 | E5 | 44 | ARG |
| 46 | E5 | 49 | LYS |
| 46 | E5 | 50 | ASN |
| 46 | E5 | 51 | VAL |
| 46 | E5 | 63 | VAL |
| 46 | E5 | 74 | ARG |
| 46 | E5 | 80 | HIS |
| 47 | F5 | 3 | LYS |
| 47 | F5 | 4 | VAL |
| 47 | F5 | 6 | GLU |
| 47 | F5 | 8 | SER |
| 47 | F5 | 25 | LYS |
| 47 | F5 | 37 | ILE |
| 47 | F5 | 38 | SER |
| 47 | F5 | 39 | LYS |
| 47 | F5 | 41 | ARG |
| 47 | F5 | 42 | GLN |
| 47 | F5 | 59 | THR |
| 47 | F5 | 62 | VAL |
| 47 | F5 | 67 | ILE |
| 47 | F5 | 70 | VAL |
| 47 | F5 | 72 | GLU |
| 47 | F5 | 76 | ARG |
| 47 | F5 | 80 | LEU |
| 47 | F5 | 81 | LYS |
| 47 | F5 | 82 | LEU |
| 47 | F5 | 83 | GLU |
| 47 | F5 | 85 | LEU |
| 47 | F5 | 89 | GLU |
| 47 | F5 | 91 | LYS |
| 47 | F5 | 93 | GLU |
| 47 | F5 | 97 | LEU |
| 47 | F5 | 98 | LEU |
| 48 | G5 | 5 | GLU |
| 48 | G5 | 7 | ARG |

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| Mol | Chain | Res | Type |
|---|---|---|---|
| 48 | G5 | 16 | LEU |
| 48 | G5 | 19 | VAL |
| 48 | G5 | 20 | GLU |
| 48 | G5 | 21 | LEU |
| 48 | G5 | 24 | LEU |
| 48 | G5 | 32 | LEU |
| 48 | G5 | 40 | SER |
| 48 | G5 | 44 | LEU |
| 48 | G5 | 46 | GLN |
| 48 | G5 | 47 | ASN |
| 48 | G5 | 53 | LEU |
| 48 | G5 | 59 | ARG |
| 48 | G5 | 60 | LEU |
| 48 | G5 | 64 | LEU |
| 48 | G5 | 65 | ASN |
| 49 | H5 | 8 | LEU |
| 49 | H5 | 17 | LYS |
| 49 | H5 | 18 | ASP |
| 49 | H5 | 30 | ARG |
| 49 | H5 | 33 | GLN |
| 49 | H5 | 40 | THR |
| 49 | H5 | 50 | VAL |
| 49 | H5 | 55 | ARG |
| 50 | I5 | 5 | ILE |
| 50 | I5 | 9 | LEU |
| 50 | I5 | 14 | ILE |
| 50 | I5 | 15 | ILE |
| 50 | I5 | 18 | CYS |
| 50 | I5 | 22 | ILE |
| 50 | I5 | 31 | ILE |
| 50 | I5 | 32 | TYR |
| 50 | I5 | 42 | PHE |
| 50 | I5 | 44 | THR |
| 50 | I5 | 50 | VAL |
| 50 | I5 | 53 | GLU |
| 50 | I5 | 55 | ARG |
| 50 | I5 | 62 | ARG |
| 51 | J5 | 6 | VAL |
| 51 | J5 | 9 | LYS |
| 51 | J5 | 12 | SER |
| 51 | J5 | 16 | ARG |
| 51 | J5 | 26 | THR |

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| Mol | Chain | Res | Type |
|---|---|---|---|
| 51 | J5 | 29 | THR |
| 51 | J5 | 33 | CYS |
| 51 | J5 | 35 | GLU |
| 51 | J5 | 37 | LYS |
| 51 | J5 | 48 | GLU |
| 51 | J5 | 49 | CYS |
| 51 | J5 | 51 | TYR |
| 51 | J5 | 55 | ARG |
| 51 | J5 | 56 | LYS |
| 51 | J5 | 57 | VAL |
| 52 | K5 | 11 | LEU |
| 52 | K5 | 12 | GLU |
| 52 | K5 | 13 | CYS |
| 52 | K5 | 18 | ARG |
| 52 | K5 | 23 | THR |
| 52 | K5 | 24 | GLU |
| 52 | K5 | 27 | LYS |
| 52 | K5 | 30 | THR |
| 52 | K5 | 32 | ASN |
| 52 | K5 | 37 | ARG |
| 52 | K5 | 38 | LYS |
| 52 | K5 | 42 | TRP |
| 52 | K5 | 43 | CYS |
| 52 | K5 | 45 | LYS |
| 52 | K5 | 48 | VAL |
| 52 | K5 | 50 | ARG |
| 52 | K5 | 52 | VAL |
| 53 | L5 | 1 | MET |
| 53 | L5 | 4 | THR |
| 53 | L5 | 8 | ASN |
| 53 | L5 | 11 | LYS |
| 53 | L5 | 14 | LYS |
| 53 | L5 | 24 | THR |
| 53 | L5 | 43 | THR |
| 53 | L5 | 46 | VAL |
| 53 | L5 | 47 | ARG |
| 53 | L5 | 48 | LYS |
| 54 | M5 | 4 | MET |
| 54 | M5 | 11 | LYS |
| 54 | M5 | 14 | VAL |
| 54 | M5 | 22 | VAL |
| 54 | M5 | 30 | ARG |

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| Mol | Chain | Res | Type |
|---|---|---|---|
| 54 | M5 | 32 | LEU |
| 54 | M5 | 36 | LYS |
| 54 | M5 | 40 | GLU |
| 54 | M5 | 41 | ILE |
| 54 | M5 | 46 | ARG |
| 54 | M5 | 49 | VAL |
| 54 | M5 | 50 | LEU |
| 54 | M5 | 52 | LYS |
| 54 | M5 | 57 | ARG |
| 54 | M5 | 59 | LYS |
| 54 | M5 | 62 | LEU |

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (58) such sidechains are listed below:

| Mol | Chain | Res | Type |
|---|---|---|---|
| 2 | 1E | 212 | GLN |
| 3 | 2E | 6 | HIS |
| 3 | 2E | 69 | HIS |
| 4 | 3E | 43 | HIS |
| 5 | 4E | 78 | HIS |
| 6 | 5E | 7 | ASN |
| 6 | 5E | 18 | GLN |
| 9 | 8E | 124 | GLN |
| 11 | 2I | 38 | ASN |
| 11 | 2I | 93 | GLN |
| 17 | 8I | 16 | GLN |
| 20 | BI | 9 | ASN |
| 27 | 11 | 143 | HIS |
| 27 | 11 | 253 | GLN |
| 30 | 41 | 108 | ASN |
| 31 | 51 | 147 | ASN |
| 32 | 61 | 17 | GLN |
| 32 | 61 | 28 | ASN |
| 32 | 61 | 43 | ASN |
| 34 | 68 | 29 | ASN |
| 35 | 78 | 38 | GLN |
| 37 | 98 | 13 | HIS |
| 37 | 98 | 61 | HIS |
| 37 | 98 | 91 | GLN |
| 39 | B8 | 79 | HIS |
| 40 | C8 | 75 | ASN |
| 40 | C8 | 81 | HIS |

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| Mol | Chain | Res | Type |
|---|---|---|---|
| 41 | D8 | 87 | HIS |
| 43 | F8 | 55 | ASN |
| 49 | L8 | 32 | GLN |
| 50 | M8 | 60 | GLN |
| 2 | 12 | 16 | HIS |
| 2 | 12 | 37 | ASN |
| 3 | 22 | 6 | HIS |
| 3 | 22 | 110 | ASN |
| 4 | 32 | 42 | GLN |
| 4 | 32 | 119 | GLN |
| 5 | 42 | 78 | HIS |
| 6 | 52 | 7 | ASN |
| 7 | 62 | 96 | GLN |
| 8 | 72 | 81 | HIS |
| 9 | 82 | 3 | GLN |
| 9 | 82 | 34 | ASN |
| 19 | AA | 57 | HIS |
| 26 | 79 | 227 | HIS |
| 27 | 19 | 58 | HIS |
| 27 | 19 | 116 | GLN |
| 30 | 49 | 26 | GLN |
| 30 | 49 | 41 | GLN |
| 30 | 49 | 58 | GLN |
| 32 | 69 | 105 | HIS |
| 37 | 55 | 31 | HIS |
| 39 | 75 | 136 | GLN |
| 41 | 95 | 11 | GLN |
| 45 | D5 | 32 | HIS |
| 45 | D5 | 118 | GLN |
| 50 | I5 | 47 | GLN |
| 51 | J5 | 23 | HIS |

### 5.3.3 RNA

| Mol | Chain | Analysed | Backbone Outliers | Pucker Outliers |
|---|---|---|---|---|
| 1 | 13 | 1492/1522 (98%) | 354 (23%) | 26 (1%) |
| 1 | 1G | 1502/1522 (98%) | 372 (24%) | 39 (2%) |
| 22 | 2K | 79/85 (92%) | 34 (43%) | 5 (6%) |
| 22 | 2L | 76/85 (89%) | 26 (34%) | 8 (10%) |
| 22 | 3K | 83/85 (97%) | 25 (30%) | 3 (3%) |
| 22 | 3L | 84/85 (98%) | 24 (28%) | 3 (3%) |

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| Mol | Chain | Analysed | Backbone Outliers | Pucker Outliers |
|---|---|---|---|---|
| 23 | 4K | 16/30 (53%) | 7 (43%) | 3 (18%) |
| 23 | 4L | 7/30 (23%) | 4 (57%) | 1 (14%) |
| 24 | 14 | 2908/2917 (99%) | 688 (23%) | 48 (1%) |
| 24 | 1H | 2911/2917 (99%) | 704 (24%) | 56 (1%) |
| 25 | 16 | 121/122 (99%) | 38 (31%) | 0 |
| 25 | 1J | 121/122 (99%) | 34 (28%) | 0 |
| All | All | 9400/9522 (98%) | 2310 (24%) | 192 (2%) |

All (2310) RNA backbone outliers are listed below:

| Mol | Chain | Res | Type |
|---|---|---|---|
| 1 | 13 | 5 | U |
| 1 | 13 | 6 | G |
| 1 | 13 | 7 | G |
| 1 | 13 | 9 | G |
| 1 | 13 | 32 | A |
| 1 | 13 | 39 | G |
| 1 | 13 | 44 | G |
| 1 | 13 | 48 | C |
| 1 | 13 | 50 | A |
| 1 | 13 | 51 | A |
| 1 | 13 | 59 | A |
| 1 | 13 | 60 | A |
| 1 | 13 | 61 | G |
| 1 | 13 | 65 | U |
| 1 | 13 | 66 | G |
| 1 | 13 | 76 | G |
| 1 | 13 | 78 | G |
| 1 | 13 | 89 | U |
| 1 | 13 | 91 | C |
| 1 | 13 | 95 | G |
| 1 | 13 | 96 | G |
| 1 | 13 | 101 | A |
| 1 | 13 | 108 | G |
| 1 | 13 | 113 | G |
| 1 | 13 | 115 | G |
| 1 | 13 | 121 | C |
| 1 | 13 | 131 | C |
| 1 | 13 | 143 | A |
| 1 | 13 | 144 | G |
| 1 | 13 | 156 | G |
| 1 | 13 | 158 | G |

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| Mol | Chain | Res | Type |
|---|---|---|---|
| 1 | 13 | 160 | A |
| 1 | 13 | 163 | C |
| 1 | 13 | 169 | C |
| 1 | 13 | 173 | U |
| 1 | 13 | 174 | C |
| 1 | 13 | 182 | U |
| 1 | 13 | 189 | U |
| 1 | 13 | 190 | G |
| 1 | 13 | 191(A) | G |
| 1 | 13 | 192 | U |
| 1 | 13 | 195 | A |
| 1 | 13 | 197 | A |
| 1 | 13 | 199 | G |
| 1 | 13 | 201 | C |
| 1 | 13 | 208 | U |
| 1 | 13 | 209 | U |
| 1 | 13 | 210 | U |
| 1 | 13 | 216 | G |
| 1 | 13 | 226 | G |
| 1 | 13 | 244 | U |
| 1 | 13 | 245 | C |
| 1 | 13 | 247 | G |
| 1 | 13 | 251 | G |
| 1 | 13 | 257 | G |
| 1 | 13 | 262 | A |
| 1 | 13 | 266 | G |
| 1 | 13 | 267 | C |
| 1 | 13 | 281 | G |
| 1 | 13 | 289 | G |
| 1 | 13 | 313 | A |
| 1 | 13 | 321 | A |
| 1 | 13 | 328 | C |
| 1 | 13 | 329 | A |
| 1 | 13 | 332 | G |
| 1 | 13 | 344 | A |
| 1 | 13 | 345 | C |
| 1 | 13 | 346 | G |
| 1 | 13 | 347 | G |
| 1 | 13 | 351 | G |
| 1 | 13 | 352 | C |
| 1 | 13 | 353 | A |
| 1 | 13 | 354 | G |

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| Mol | Chain | Res | Type |
|---|---|---|---|
| 1 | 13 | 355 | C |
| 1 | 13 | 362 | G |
| 1 | 13 | 367 | U |
| 1 | 13 | 372 | C |
| 1 | 13 | 373 | A |
| 1 | 13 | 382 | A |
| 1 | 13 | 383 | A |
| 1 | 13 | 384 | G |
| 1 | 13 | 388 | G |
| 1 | 13 | 390 | C |
| 1 | 13 | 397 | A |
| 1 | 13 | 398 | C |
| 1 | 13 | 406 | G |
| 1 | 13 | 411 | A |
| 1 | 13 | 412 | A |
| 1 | 13 | 413 | G |
| 1 | 13 | 419 | C |
| 1 | 13 | 422 | C |
| 1 | 13 | 424 | G |
| 1 | 13 | 429 | U |
| 1 | 13 | 430 | A |
| 1 | 13 | 439 | A |
| 1 | 13 | 442 | C |
| 1 | 13 | 454 | C |
| 1 | 13 | 455 | C |
| 1 | 13 | 466 | C |
| 1 | 13 | 467 | G |
| 1 | 13 | 477 | G |
| 1 | 13 | 482 | A |
| 1 | 13 | 484 | G |
| 1 | 13 | 485 | G |
| 1 | 13 | 487 | A |
| 1 | 13 | 496 | A |
| 1 | 13 | 497 | U |
| 1 | 13 | 498 | A |
| 1 | 13 | 505 | G |
| 1 | 13 | 508 | C |
| 1 | 13 | 509 | A |
| 1 | 13 | 510 | A |
| 1 | 13 | 511 | C |
| 1 | 13 | 513 | C |
| 1 | 13 | 518 | C |

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| Mol | Chain | Res | Type |
|---|---|---|---|
| 1 | 13 | 522 | C |
| 1 | 13 | 527 | G |
| 1 | 13 | 531 | U |
| 1 | 13 | 533 | A |
| 1 | 13 | 536 | C |
| 1 | 13 | 545 | C |
| 1 | 13 | 547 | A |
| 1 | 13 | 559 | A |
| 1 | 13 | 561 | U |
| 1 | 13 | 569 | C |
| 1 | 13 | 572 | A |
| 1 | 13 | 573 | A |
| 1 | 13 | 576 | G |
| 1 | 13 | 577 | G |
| 1 | 13 | 580 | U |
| 1 | 13 | 587 | G |
| 1 | 13 | 596 | C |
| 1 | 13 | 602 | A |
| 1 | 13 | 607 | A |
| 1 | 13 | 610 | G |
| 1 | 13 | 620 | C |
| 1 | 13 | 630 | G |
| 1 | 13 | 631 | G |
| 1 | 13 | 632 | A |
| 1 | 13 | 633 | G |
| 1 | 13 | 642 | A |
| 1 | 13 | 651 | C |
| 1 | 13 | 653 | A |
| 1 | 13 | 659 | U |
| 1 | 13 | 665 | A |
| 1 | 13 | 679 | C |
| 1 | 13 | 686 | U |
| 1 | 13 | 687 | A |
| 1 | 13 | 702 | A |
| 1 | 13 | 703 | G |
| 1 | 13 | 704 | A |
| 1 | 13 | 711 | G |
| 1 | 13 | 723 | U |
| 1 | 13 | 724 | G |
| 1 | 13 | 731 | G |
| 1 | 13 | 748 | C |
| 1 | 13 | 749 | C |

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| Mol | Chain | Res | Type |
|---|---|---|---|
| 1 | 13 | 753 | A |
| 1 | 13 | 755 | G |
| 1 | 13 | 763 | G |
| 1 | 13 | 777 | A |
| 1 | 13 | 785 | G |
| 1 | 13 | 788 | U |
| 1 | 13 | 792 | A |
| 1 | 13 | 793 | U |
| 1 | 13 | 794 | A |
| 1 | 13 | 796 | C |
| 1 | 13 | 798 | G |
| 1 | 13 | 805 | C |
| 1 | 13 | 812 | C |
| 1 | 13 | 813 | U |
| 1 | 13 | 815 | A |
| 1 | 13 | 817 | C |
| 1 | 13 | 818 | G |
| 1 | 13 | 828 | A |
| 1 | 13 | 836 | G |
| 1 | 13 | 841 | U |
| 1 | 13 | 842 | C |
| 1 | 13 | 843 | U |
| 1 | 13 | 848 | C |
| 1 | 13 | 870 | U |
| 1 | 13 | 874 | G |
| 1 | 13 | 885 | G |
| 1 | 13 | 902 | G |
| 1 | 13 | 914 | A |
| 1 | 13 | 916 | G |
| 1 | 13 | 926 | G |
| 1 | 13 | 927 | G |
| 1 | 13 | 929 | G |
| 1 | 13 | 934 | C |
| 1 | 13 | 935 | A |
| 1 | 13 | 936 | C |
| 1 | 13 | 941 | G |
| 1 | 13 | 942 | G |
| 1 | 13 | 948 | C |
| 1 | 13 | 960 | U |
| 1 | 13 | 966 | G |
| 1 | 13 | 968 | A |
| 1 | 13 | 969 | A |

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| Mol | Chain | Res | Type |
|---|---|---|---|
| 1 | 13 | 974 | A |
| 1 | 13 | 975 | A |
| 1 | 13 | 976 | G |
| 1 | 13 | 977 | A |
| 1 | 13 | 978 | A |
| 1 | 13 | 982 | U |
| 1 | 13 | 983 | A |
| 1 | 13 | 991 | U |
| 1 | 13 | 993 | G |
| 1 | 13 | 1001 | G |
| 1 | 13 | 1002 | G |
| 1 | 13 | 1004 | A |
| 1 | 13 | 1006 | C |
| 1 | 13 | 1009 | G |
| 1 | 13 | 1011 | G |
| 1 | 13 | 1012 | U |
| 1 | 13 | 1017 | G |
| 1 | 13 | 1020 | U |
| 1 | 13 | 1021 | G |
| 1 | 13 | 1024 | G |
| 1 | 13 | 1025 | U |
| 1 | 13 | 1026 | G |
| 1 | 13 | 1027 | C |
| 1 | 13 | 1028 | C |
| 1 | 13 | 1029 | G |
| 1 | 13 | 1030 | C |
| 1 | 13 | 1032(A) | G |
| 1 | 13 | 1036 | G |
| 1 | 13 | 1044 | A |
| 1 | 13 | 1046 | A |
| 1 | 13 | 1052 | U |
| 1 | 13 | 1054 | C |
| 1 | 13 | 1065 | U |
| 1 | 13 | 1066 | C |
| 1 | 13 | 1081 | G |
| 1 | 13 | 1088 | G |
| 1 | 13 | 1094 | G |
| 1 | 13 | 1095 | U |
| 1 | 13 | 1099 | G |
| 1 | 13 | 1101 | A |
| 1 | 13 | 1108 | G |
| 1 | 13 | 1124 | G |

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| Mol | Chain | Res | Type |
|---|---|---|---|
| 1 | 13 | 1125 | U |
| 1 | 13 | 1126 | U |
| 1 | 13 | 1127 | G |
| 1 | 13 | 1129 | C |
| 1 | 13 | 1130 | A |
| 1 | 13 | 1131 | G |
| 1 | 13 | 1132 | C |
| 1 | 13 | 1136 | U |
| 1 | 13 | 1137 | C |
| 1 | 13 | 1138 | G |
| 1 | 13 | 1139 | G |
| 1 | 13 | 1146 | A |
| 1 | 13 | 1151 | A |
| 1 | 13 | 1152 | A |
| 1 | 13 | 1157 | A |
| 1 | 13 | 1158 | C |
| 1 | 13 | 1159 | U |
| 1 | 13 | 1160 | G |
| 1 | 13 | 1177 | G |
| 1 | 13 | 1181 | G |
| 1 | 13 | 1182 | G |
| 1 | 13 | 1183 | A |
| 1 | 13 | 1184 | G |
| 1 | 13 | 1188 | A |
| 1 | 13 | 1189 | C |
| 1 | 13 | 1191 | A |
| 1 | 13 | 1193 | G |
| 1 | 13 | 1195 | C |
| 1 | 13 | 1196 | U |
| 1 | 13 | 1197 | G |
| 1 | 13 | 1211 | U |
| 1 | 13 | 1213 | A |
| 1 | 13 | 1218 | C |
| 1 | 13 | 1225 | A |
| 1 | 13 | 1227 | A |
| 1 | 13 | 1233 | G |
| 1 | 13 | 1238 | A |
| 1 | 13 | 1240 | U |
| 1 | 13 | 1252 | A |
| 1 | 13 | 1253 | G |
| 1 | 13 | 1256 | A |
| 1 | 13 | 1257 | U |

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| Mol | Chain | Res | Type |
|---|---|---|---|
| 1 | 13 | 1258 | G |
| 1 | 13 | 1260 | C |
| 1 | 13 | 1270 | C |
| 1 | 13 | 1272 | G |
| 1 | 13 | 1273 | G |
| 1 | 13 | 1278 | U |
| 1 | 13 | 1279 | A |
| 1 | 13 | 1280 | A |
| 1 | 13 | 1281 | U |
| 1 | 13 | 1282 | C |
| 1 | 13 | 1286 | A |
| 1 | 13 | 1287 | A |
| 1 | 13 | 1290 | G |
| 1 | 13 | 1291 | G |
| 1 | 13 | 1299 | A |
| 1 | 13 | 1300 | G |
| 1 | 13 | 1302 | U |
| 1 | 13 | 1303 | C |
| 1 | 13 | 1305 | G |
| 1 | 13 | 1310 | G |
| 1 | 13 | 1312 | G |
| 1 | 13 | 1317 | C |
| 1 | 13 | 1319 | A |
| 1 | 13 | 1320 | C |
| 1 | 13 | 1322 | C |
| 1 | 13 | 1323 | G |
| 1 | 13 | 1331 | G |
| 1 | 13 | 1335 | C |
| 1 | 13 | 1336 | C |
| 1 | 13 | 1337 | G |
| 1 | 13 | 1338 | G |
| 1 | 13 | 1339 | A |
| 1 | 13 | 1346 | A |
| 1 | 13 | 1347 | G |
| 1 | 13 | 1350 | A |
| 1 | 13 | 1353 | G |
| 1 | 13 | 1356 | G |
| 1 | 13 | 1358 | U |
| 1 | 13 | 1359 | C |
| 1 | 13 | 1361 | G |
| 1 | 13 | 1362(A) | C |
| 1 | 13 | 1364 | U |

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| Mol | Chain | Res | Type |
|---|---|---|---|
| 1 | 13 | 1370 | G |
| 1 | 13 | 1379 | G |
| 1 | 13 | 1381 | U |
| 1 | 13 | 1398 | A |
| 1 | 13 | 1401 | G |
| 1 | 13 | 1416 | G |
| 1 | 13 | 1419 | G |
| 1 | 13 | 1422 | G |
| 1 | 13 | 1435 | G |
| 1 | 13 | 1442 | G |
| 1 | 13 | 1443 | G |
| 1 | 13 | 1446 | A |
| 1 | 13 | 1451 | A |
| 1 | 13 | 1452 | C |
| 1 | 13 | 1453 | G |
| 1 | 13 | 1454 | G |
| 1 | 13 | 1459 | C |
| 1 | 13 | 1469 | G |
| 1 | 13 | 1487 | G |
| 1 | 13 | 1497 | G |
| 1 | 13 | 1498 | U |
| 1 | 13 | 1499 | A |
| 1 | 13 | 1503 | A |
| 1 | 13 | 1504 | G |
| 1 | 13 | 1506 | U |
| 1 | 13 | 1517 | G |
| 1 | 13 | 1529 | G |
| 1 | 13 | 1530 | G |
| 1 | 13 | 1531 | A |
| 22 | 2K | 2 | G |
| 22 | 2K | 6 | G |
| 22 | 2K | 7 | G |
| 22 | 2K | 8 | 4SU |
| 22 | 2K | 9 | U |
| 22 | 2K | 10 | C |
| 22 | 2K | 14 | A |
| 22 | 2K | 15 | G |
| 22 | 2K | 19 | C |
| 22 | 2K | 20 | C |
| 22 | 2K | 21 | A |
| 22 | 2K | 24 | G |
| 22 | 2K | 25 | G |

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| Mol | Chain | Res | Type |
|---|---|---|---|
| 22 | 2K | 34 | U |
| 22 | 2K | 35 | QUO |
| 22 | 2K | 40 | PSU |
| 22 | 2K | 45 | C |
| 22 | 2K | 47 | U |
| 22 | 2K | 49 | A |
| 22 | 2K | 54 | C |
| 22 | 2K | 55 | U |
| 22 | 2K | 60 | A |
| 22 | 2K | 61 | G |
| 22 | 2K | 62 | G |
| 22 | 2K | 63 | 5MU |
| 22 | 2K | 64 | PSU |
| 22 | 2K | 65 | C |
| 22 | 2K | 69 | U |
| 22 | 2K | 71 | C |
| 22 | 2K | 72 | U |
| 22 | 2K | 73 | U |
| 22 | 2K | 74 | C |
| 22 | 2K | 82 | A |
| 22 | 2K | 85 | A |
| 22 | 3K | 6 | G |
| 22 | 3K | 7 | G |
| 22 | 3K | 8 | 4SU |
| 22 | 3K | 9 | U |
| 22 | 3K | 14 | A |
| 22 | 3K | 15 | G |
| 22 | 3K | 18 | G |
| 22 | 3K | 19 | C |
| 22 | 3K | 20 | C |
| 22 | 3K | 21 | A |
| 22 | 3K | 22 | A |
| 22 | 3K | 25 | G |
| 22 | 3K | 31 | G |
| 22 | 3K | 34 | U |
| 22 | 3K | 35 | QUO |
| 22 | 3K | 38 | MIA |
| 22 | 3K | 41 | C |
| 22 | 3K | 46 | G |
| 22 | 3K | 48 | C |
| 22 | 3K | 52 | G |
| 22 | 3K | 56 | U |

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| Mol | Chain | Res | Type |
|---|---|---|---|
| 22 | 3K | 68 | A |
| 22 | 3K | 69 | U |
| 22 | 3K | 79 | A |
| 22 | 3K | 85 | A |
| 23 | 4K | 10 | G |
| 23 | 4K | 11 | U |
| 23 | 4K | 12 | A |
| 23 | 4K | 13 | A |
| 23 | 4K | 14 | A |
| 23 | 4K | 19 | A |
| 23 | 4K | 23 | A |
| 24 | 1H | 2 | G |
| 24 | 1H | 4 | C |
| 24 | 1H | 5 | A |
| 24 | 1H | 9 | U |
| 24 | 1H | 23 | G |
| 24 | 1H | 34 | C |
| 24 | 1H | 35 | G |
| 24 | 1H | 46 | C |
| 24 | 1H | 51 | G |
| 24 | 1H | 55 | G |
| 24 | 1H | 59 | U |
| 24 | 1H | 63 | U |
| 24 | 1H | 70 | G |
| 24 | 1H | 71 | A |
| 24 | 1H | 74 | A |
| 24 | 1H | 75 | G |
| 24 | 1H | 83 | G |
| 24 | 1H | 85 | G |
| 24 | 1H | 92 | G |
| 24 | 1H | 93 | C |
| 24 | 1H | 95 | G |
| 24 | 1H | 102 | G |
| 24 | 1H | 118 | A |
| 24 | 1H | 119 | A |
| 24 | 1H | 120 | U |
| 24 | 1H | 123 | G |
| 24 | 1H | 125 | G |
| 24 | 1H | 126 | A |
| 24 | 1H | 129 | C |
| 24 | 1H | 131 | G |
| 24 | 1H | 138 | G |

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| Mol | Chain | Res | Type |
|---|---|---|---|
| 24 | 1H | 155 | C |
| 24 | 1H | 163 | U |
| 24 | 1H | 164 | U |
| 24 | 1H | 165 | U |
| 24 | 1H | 180 | G |
| 24 | 1H | 181 | A |
| 24 | 1H | 196 | A |
| 24 | 1H | 197 | A |
| 24 | 1H | 199 | A |
| 24 | 1H | 200 | U |
| 24 | 1H | 214 | G |
| 24 | 1H | 215 | G |
| 24 | 1H | 216 | A |
| 24 | 1H | 221 | A |
| 24 | 1H | 222 | A |
| 24 | 1H | 223 | A |
| 24 | 1H | 224 | G |
| 24 | 1H | 228 | A |
| 24 | 1H | 229 | A |
| 24 | 1H | 230 | U |
| 24 | 1H | 233 | A |
| 24 | 1H | 245 | G |
| 24 | 1H | 248 | G |
| 24 | 1H | 250 | G |
| 24 | 1H | 252 | G |
| 24 | 1H | 266 | G |
| 24 | 1H | 269 | U |
| 24 | 1H | 270(K) | C |
| 24 | 1H | 270(M) | U |
| 24 | 1H | 270(N) | G |
| 24 | 1H | 271(C) | U |
| 24 | 1H | 271 | G |
| 24 | 1H | 273(D) | C |
| 24 | 1H | 274 | G |
| 24 | 1H | 275 | G |
| 24 | 1H | 277 | C |
| 24 | 1H | 278 | A |
| 24 | 1H | 299 | A |
| 24 | 1H | 310 | A |
| 24 | 1H | 311 | A |
| 24 | 1H | 316 | C |
| 24 | 1H | 323 | G |

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| Mol | Chain | Res | Type |
|---|---|---|---|
| 24 | 1H | 324 | A |
| 24 | 1H | 329 | G |
| 24 | 1H | 330 | A |
| 24 | 1H | 334 | C |
| 24 | 1H | 340 | A |
| 24 | 1H | 345 | A |
| 24 | 1H | 352 | G |
| 24 | 1H | 353 | G |
| 24 | 1H | 360 | G |
| 24 | 1H | 363(D) | G |
| 24 | 1H | 372 | G |
| 24 | 1H | 386 | G |
| 24 | 1H | 389 | G |
| 24 | 1H | 396 | G |
| 24 | 1H | 405 | U |
| 24 | 1H | 407 | G |
| 24 | 1H | 411 | G |
| 24 | 1H | 412 | A |
| 24 | 1H | 428 | A |
| 24 | 1H | 443 | A |
| 24 | 1H | 444 | C |
| 24 | 1H | 448 | U |
| 24 | 1H | 449 | A |
| 24 | 1H | 451 | C |
| 24 | 1H | 452 | G |
| 24 | 1H | 454 | A |
| 24 | 1H | 455 | C |
| 24 | 1H | 457 | A |
| 24 | 1H | 463 | G |
| 24 | 1H | 481 | G |
| 24 | 1H | 482 | A |
| 24 | 1H | 501 | A |
| 24 | 1H | 505 | A |
| 24 | 1H | 508 | G |
| 24 | 1H | 509 | C |
| 24 | 1H | 528 | A |
| 24 | 1H | 529 | A |
| 24 | 1H | 530 | G |
| 24 | 1H | 531 | C |
| 24 | 1H | 532 | A |
| 24 | 1H | 533 | G |
| 24 | 1H | 537 | C |

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| Mol | Chain | Res | Type |
|---|---|---|---|
| 24 | 1H | 546 | C |
| 24 | 1H | 547 | A |
| 24 | 1H | 556 | G |
| 24 | 1H | 563 | G |
| 24 | 1H | 564 | C |
| 24 | 1H | 567 | A |
| 24 | 1H | 573 | G |
| 24 | 1H | 574 | C |
| 24 | 1H | 575 | A |
| 24 | 1H | 577 | G |
| 24 | 1H | 586 | A |
| 24 | 1H | 592 | G |
| 24 | 1H | 593 | G |
| 24 | 1H | 595 | C |
| 24 | 1H | 603 | A |
| 24 | 1H | 607 | U |
| 24 | 1H | 614 | U |
| 24 | 1H | 615 | G |
| 24 | 1H | 617 | G |
| 24 | 1H | 618 | G |
| 24 | 1H | 621 | A |
| 24 | 1H | 622 | G |
| 24 | 1H | 626 | U |
| 24 | 1H | 627 | A |
| 24 | 1H | 634 | C |
| 24 | 1H | 637 | A |
| 24 | 1H | 643 | A |
| 24 | 1H | 644 | A |
| 24 | 1H | 645 | C |
| 24 | 1H | 646 | A |
| 24 | 1H | 654(A) | A |
| 24 | 1H | 654(B) | C |
| 24 | 1H | 654(G) | C |
| 24 | 1H | 654(H) | G |
| 24 | 1H | 654(I) | C |
| 24 | 1H | 654(L) | G |
| 24 | 1H | 654(N) | G |
| 24 | 1H | 654(T) | A |
| 24 | 1H | 654(V) | A |
| 24 | 1H | 666 | G |
| 24 | 1H | 667 | U |
| 24 | 1H | 668 | G |

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| Mol | Chain | Res | Type |
|---|---|---|---|
| 24 | 1H | 685 | A |
| 24 | 1H | 686 | G |
| 24 | 1H | 717 | G |
| 24 | 1H | 730 | C |
| 24 | 1H | 731 | C |
| 24 | 1H | 738 | G |
| 24 | 1H | 740 | U |
| 24 | 1H | 746 | A |
| 24 | 1H | 747 | U |
| 24 | 1H | 752 | A |
| 24 | 1H | 753 | C |
| 24 | 1H | 764 | A |
| 24 | 1H | 765 | G |
| 24 | 1H | 776 | G |
| 24 | 1H | 782 | A |
| 24 | 1H | 784 | A |
| 24 | 1H | 785 | G |
| 24 | 1H | 790 | C |
| 24 | 1H | 792 | G |
| 24 | 1H | 805 | G |
| 24 | 1H | 812 | C |
| 24 | 1H | 819 | A |
| 24 | 1H | 827 | U |
| 24 | 1H | 828 | U |
| 24 | 1H | 836 | G |
| 24 | 1H | 845 | G |
| 24 | 1H | 847 | U |
| 24 | 1H | 859 | G |
| 24 | 1H | 860 | U |
| 24 | 1H | 861 | A |
| 24 | 1H | 866 | A |
| 24 | 1H | 870 | A |
| 24 | 1H | 880 | G |
| 24 | 1H | 881 | G |
| 24 | 1H | 882 | G |
| 24 | 1H | 883 | G |
| 24 | 1H | 885 | C |
| 24 | 1H | 886 | C |
| 24 | 1H | 887 | A |
| 24 | 1H | 888 | C |
| 24 | 1H | 890 | A |
| 24 | 1H | 893 | C |

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| Mol | Chain | Res | Type |
|---|---|---|---|
| 24 | 1H | 894 | C |
| 24 | 1H | 895 | U |
| 24 | 1H | 897 | C |
| 24 | 1H | 898 | C |
| 24 | 1H | 901 | A |
| 24 | 1H | 904 | C |
| 24 | 1H | 910 | A |
| 24 | 1H | 917 | A |
| 24 | 1H | 925 | C |
| 24 | 1H | 926 | A |
| 24 | 1H | 932 | G |
| 24 | 1H | 938 | G |
| 24 | 1H | 941 | A |
| 24 | 1H | 946 | G |
| 24 | 1H | 953 | A |
| 24 | 1H | 957 | A |
| 24 | 1H | 959 | A |
| 24 | 1H | 961 | C |
| 24 | 1H | 968 | G |
| 24 | 1H | 974 | G |
| 24 | 1H | 974(A) | C |
| 24 | 1H | 975 | G |
| 24 | 1H | 982 | C |
| 24 | 1H | 983 | A |
| 24 | 1H | 986 | C |
| 24 | 1H | 990 | A |
| 24 | 1H | 991 | C |
| 24 | 1H | 996 | A |
| 24 | 1H | 998 | C |
| 24 | 1H | 1002 | G |
| 24 | 1H | 1003 | G |
| 24 | 1H | 1005 | C |
| 24 | 1H | 1008 | C |
| 24 | 1H | 1010 | A |
| 24 | 1H | 1011 | G |
| 24 | 1H | 1012 | U |
| 24 | 1H | 1013 | C |
| 24 | 1H | 1019 | U |
| 24 | 1H | 1020 | A |
| 24 | 1H | 1022 | G |
| 24 | 1H | 1023 | U |
| 24 | 1H | 1025 | G |

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| Mol | Chain | Res | Type |
|---|---|---|---|
| 24 | 1H | 1026 | U |
| 24 | 1H | 1027 | A |
| 24 | 1H | 1033 | U |
| 24 | 1H | 1037 | G |
| 24 | 1H | 1043 | C |
| 24 | 1H | 1045 | A |
| 24 | 1H | 1046 | A |
| 24 | 1H | 1047 | G |
| 24 | 1H | 1053 | C |
| 24 | 1H | 1055 | G |
| 24 | 1H | 1056 | G |
| 24 | 1H | 1057 | A |
| 24 | 1H | 1058 | U |
| 24 | 1H | 1061 | U |
| 24 | 1H | 1062 | G |
| 24 | 1H | 1066 | U |
| 24 | 1H | 1067 | A |
| 24 | 1H | 1068 | G |
| 24 | 1H | 1070 | A |
| 24 | 1H | 1071 | G |
| 24 | 1H | 1073 | A |
| 24 | 1H | 1074 | G |
| 24 | 1H | 1076 | C |
| 24 | 1H | 1077 | A |
| 24 | 1H | 1078 | U |
| 24 | 1H | 1080 | A |
| 24 | 1H | 1083 | U |
| 24 | 1H | 1087 | G |
| 24 | 1H | 1088 | A |
| 24 | 1H | 1090 | U |
| 24 | 1H | 1092 | C |
| 24 | 1H | 1095 | A |
| 24 | 1H | 1097 | U |
| 24 | 1H | 1104 | C |
| 24 | 1H | 1105 | U |
| 24 | 1H | 1110 | G |
| 24 | 1H | 1112 | G |
| 24 | 1H | 1121 | C |
| 24 | 1H | 1126 | A |
| 24 | 1H | 1129 | A |
| 24 | 1H | 1130 | U |
| 24 | 1H | 1135 | C |

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| Mol | Chain | Res | Type |
|---|---|---|---|
| 24 | 1H | 1136 | G |
| 24 | 1H | 1139 | G |
| 24 | 1H | 1142 | U |
| 24 | 1H | 1142(A) | A |
| 24 | 1H | 1148 | A |
| 24 | 1H | 1149 | G |
| 24 | 1H | 1151 | G |
| 24 | 1H | 1155 | A |
| 24 | 1H | 1156 | A |
| 24 | 1H | 1170 | G |
| 24 | 1H | 1173 | G |
| 24 | 1H | 1176 | G |
| 24 | 1H | 1177 | A |
| 24 | 1H | 1178 | C |
| 24 | 1H | 1179 | C |
| 24 | 1H | 1180 | C |
| 24 | 1H | 1187 | G |
| 24 | 1H | 1188 | U |
| 24 | 1H | 1200 | C |
| 24 | 1H | 1205 | U |
| 24 | 1H | 1210 | A |
| 24 | 1H | 1218 | C |
| 24 | 1H | 1220 | A |
| 24 | 1H | 1221 | C |
| 24 | 1H | 1225 | C |
| 24 | 1H | 1244 | G |
| 24 | 1H | 1250 | G |
| 24 | 1H | 1253 | A |
| 24 | 1H | 1256 | G |
| 24 | 1H | 1265 | A |
| 24 | 1H | 1267 | U |
| 24 | 1H | 1271 | G |
| 24 | 1H | 1272 | A |
| 24 | 1H | 1273 | U |
| 24 | 1H | 1282 | U |
| 24 | 1H | 1286 | A |
| 24 | 1H | 1287 | A |
| 24 | 1H | 1288 | U |
| 24 | 1H | 1293 | C |
| 24 | 1H | 1300 | U |
| 24 | 1H | 1301 | A |
| 24 | 1H | 1312 | U |

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| Mol | Chain | Res | Type |
|---|---|---|---|
| 24 | 1H | 1313 | U |
| 24 | 1H | 1314 | C |
| 24 | 1H | 1319 | G |
| 24 | 1H | 1329 | U |
| 24 | 1H | 1332 | G |
| 24 | 1H | 1338 | G |
| 24 | 1H | 1344 | G |
| 24 | 1H | 1345 | C |
| 24 | 1H | 1348 | G |
| 24 | 1H | 1349 | A |
| 24 | 1H | 1359 | A |
| 24 | 1H | 1360 | A |
| 24 | 1H | 1365 | A |
| 24 | 1H | 1379 | A |
| 24 | 1H | 1380 | G |
| 24 | 1H | 1385 | G |
| 24 | 1H | 1388 | G |
| 24 | 1H | 1395 | A |
| 24 | 1H | 1411 | C |
| 24 | 1H | 1416 | G |
| 24 | 1H | 1417 | C |
| 24 | 1H | 1420 | U |
| 24 | 1H | 1421 | G |
| 24 | 1H | 1427 | A |
| 24 | 1H | 1428 | C |
| 24 | 1H | 1430 | C |
| 24 | 1H | 1437 | C |
| 24 | 1H | 1444(A) | A |
| 24 | 1H | 1449 | A |
| 24 | 1H | 1453 | A |
| 24 | 1H | 1455 | G |
| 24 | 1H | 1459 | G |
| 24 | 1H | 1460 | A |
| 24 | 1H | 1461 | G |
| 24 | 1H | 1467 | C |
| 24 | 1H | 1471 | A |
| 24 | 1H | 1483 | G |
| 24 | 1H | 1493 | C |
| 24 | 1H | 1494 | A |
| 24 | 1H | 1495 | A |
| 24 | 1H | 1497 | U |
| 24 | 1H | 1500 | G |

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| Mol | Chain | Res | Type |
|---|---|---|---|
| 24 | 1H | 1507 | A |
| 24 | 1H | 1509 | C |
| 24 | 1H | 1510 | A |
| 24 | 1H | 1511 | A |
| 24 | 1H | 1520 | U |
| 24 | 1H | 1522 | G |
| 24 | 1H | 1523 | U |
| 24 | 1H | 1526 | G |
| 24 | 1H | 1533 | C |
| 24 | 1H | 1534 | G |
| 24 | 1H | 1535 | U |
| 24 | 1H | 1536 | A |
| 24 | 1H | 1537 | C |
| 24 | 1H | 1540 | G |
| 24 | 1H | 1543 | A |
| 24 | 1H | 1544 | C |
| 24 | 1H | 1545 | A |
| 24 | 1H | 1548 | C |
| 24 | 1H | 1554 | A |
| 24 | 1H | 1558 | A |
| 24 | 1H | 1559 | G |
| 24 | 1H | 1566 | A |
| 24 | 1H | 1569 | A |
| 24 | 1H | 1578 | U |
| 24 | 1H | 1580 | A |
| 24 | 1H | 1581 | G |
| 24 | 1H | 1585 | C |
| 24 | 1H | 1586 | A |
| 24 | 1H | 1608 | A |
| 24 | 1H | 1609 | A |
| 24 | 1H | 1610 | A |
| 24 | 1H | 1616 | A |
| 24 | 1H | 1617 | C |
| 24 | 1H | 1618 | A |
| 24 | 1H | 1639 | U |
| 24 | 1H | 1647 | G |
| 24 | 1H | 1648 | C |
| 24 | 1H | 1651 | G |
| 24 | 1H | 1653 | G |
| 24 | 1H | 1654 | A |
| 24 | 1H | 1655 | A |
| 24 | 1H | 1674 | G |

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| Mol | Chain | Res | Type |
|---|---|---|---|
| 24 | 1H | 1678 | G |
| 24 | 1H | 1728 | G |
| 24 | 1H | 1729 | A |
| 24 | 1H | 1730 | U |
| 24 | 1H | 1731 | G |
| 24 | 1H | 1733 | G |
| 24 | 1H | 1742 | C |
| 24 | 1H | 1743 | G |
| 24 | 1H | 1750 | G |
| 24 | 1H | 1756 | G |
| 24 | 1H | 1762 | A |
| 24 | 1H | 1763 | G |
| 24 | 1H | 1764 | G |
| 24 | 1H | 1773 | A |
| 24 | 1H | 1782 | C |
| 24 | 1H | 1791 | A |
| 24 | 1H | 1798 | U |
| 24 | 1H | 1799 | G |
| 24 | 1H | 1800 | C |
| 24 | 1H | 1801 | G |
| 24 | 1H | 1816 | G |
| 24 | 1H | 1827 | C |
| 24 | 1H | 1829 | A |
| 24 | 1H | 1839 | G |
| 24 | 1H | 1847 | A |
| 24 | 1H | 1848 | A |
| 24 | 1H | 1856 | G |
| 24 | 1H | 1858 | G |
| 24 | 1H | 1870 | C |
| 24 | 1H | 1871 | A |
| 24 | 1H | 1878 | G |
| 24 | 1H | 1882 | C |
| 24 | 1H | 1886 | C |
| 24 | 1H | 1900 | A |
| 24 | 1H | 1906 | G |
| 24 | 1H | 1912 | A |
| 24 | 1H | 1913 | A |
| 24 | 1H | 1914 | C |
| 24 | 1H | 1919 | A |
| 24 | 1H | 1920 | C |
| 24 | 1H | 1929 | G |
| 24 | 1H | 1930 | G |

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| Mol | Chain | Res | Type |
|---|---|---|---|
| 24 | 1H | 1931 | U |
| 24 | 1H | 1936 | A |
| 24 | 1H | 1938 | A |
| 24 | 1H | 1941 | C |
| 24 | 1H | 1955 | U |
| 24 | 1H | 1960 | A |
| 24 | 1H | 1963 | U |
| 24 | 1H | 1967 | C |
| 24 | 1H | 1968 | G |
| 24 | 1H | 1969 | A |
| 24 | 1H | 1970 | A |
| 24 | 1H | 1971 | A |
| 24 | 1H | 1972 | A |
| 24 | 1H | 1976 | U |
| 24 | 1H | 1982 | C |
| 24 | 1H | 1985 | G |
| 24 | 1H | 1993 | U |
| 24 | 1H | 2020 | A |
| 24 | 1H | 2023 | G |
| 24 | 1H | 2030 | A |
| 24 | 1H | 2031 | A |
| 24 | 1H | 2032 | G |
| 24 | 1H | 2033 | A |
| 24 | 1H | 2035 | G |
| 24 | 1H | 2043 | C |
| 24 | 1H | 2051 | A |
| 24 | 1H | 2052 | G |
| 24 | 1H | 2054 | A |
| 24 | 1H | 2055 | C |
| 24 | 1H | 2056 | G |
| 24 | 1H | 2057 | A |
| 24 | 1H | 2061 | G |
| 24 | 1H | 2062 | A |
| 24 | 1H | 2063 | C |
| 24 | 1H | 2068 | U |
| 24 | 1H | 2069 | G |
| 24 | 1H | 2071 | A |
| 24 | 1H | 2099 | U |
| 24 | 1H | 2110 | G |
| 24 | 1H | 2111 | C |
| 24 | 1H | 2112 | G |
| 24 | 1H | 2113 | U |

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| Mol | Chain | Res | Type |
|---|---|---|---|
| 24 | 1H | 2114 | A |
| 24 | 1H | 2115 | G |
| 24 | 1H | 2117 | A |
| 24 | 1H | 2119 | A |
| 24 | 1H | 2126 | A |
| 24 | 1H | 2128 | C |
| 24 | 1H | 2129 | C |
| 24 | 1H | 2131 | G |
| 24 | 1H | 2132 | U |
| 24 | 1H | 2133 | G |
| 24 | 1H | 2134 | A |
| 24 | 1H | 2135 | A |
| 24 | 1H | 2137 | C |
| 24 | 1H | 2139 | C |
| 24 | 1H | 2141 | G |
| 24 | 1H | 2145 | C |
| 24 | 1H | 2146 | C |
| 24 | 1H | 2147 | G |
| 24 | 1H | 2148 | G |
| 24 | 1H | 2151 | G |
| 24 | 1H | 2158 | A |
| 24 | 1H | 2165 | G |
| 24 | 1H | 2167 | U |
| 24 | 1H | 2168 | G |
| 24 | 1H | 2170 | A |
| 24 | 1H | 2171 | A |
| 24 | 1H | 2173 | A |
| 24 | 1H | 2189 | U |
| 24 | 1H | 2190 | G |
| 24 | 1H | 2191 | G |
| 24 | 1H | 2198 | A |
| 24 | 1H | 2199 | A |
| 24 | 1H | 2210 | G |
| 24 | 1H | 2211 | G |
| 24 | 1H | 2212 | A |
| 24 | 1H | 2213 | U |
| 24 | 1H | 2215 | G |
| 24 | 1H | 2219 | G |
| 24 | 1H | 2225 | A |
| 24 | 1H | 2226 | C |
| 24 | 1H | 2238 | G |
| 24 | 1H | 2239 | G |

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| Mol | Chain | Res | Type |
|---|---|---|---|
| 24 | 1H | 2240 | C |
| 24 | 1H | 2252 | G |
| 24 | 1H | 2261 | C |
| 24 | 1H | 2264 | C |
| 24 | 1H | 2267 | A |
| 24 | 1H | 2268 | A |
| 24 | 1H | 2269 | A |
| 24 | 1H | 2275 | C |
| 24 | 1H | 2280 | G |
| 24 | 1H | 2283 | C |
| 24 | 1H | 2284 | C |
| 24 | 1H | 2287 | A |
| 24 | 1H | 2288 | A |
| 24 | 1H | 2298 | A |
| 24 | 1H | 2305 | A |
| 24 | 1H | 2307 | G |
| 24 | 1H | 2308 | G |
| 24 | 1H | 2310 | A |
| 24 | 1H | 2311 | A |
| 24 | 1H | 2314 | C |
| 24 | 1H | 2315 | G |
| 24 | 1H | 2320 | A |
| 24 | 1H | 2321 | G |
| 24 | 1H | 2324 | C |
| 24 | 1H | 2325 | G |
| 24 | 1H | 2326 | C |
| 24 | 1H | 2327 | A |
| 24 | 1H | 2334 | G |
| 24 | 1H | 2336 | A |
| 24 | 1H | 2343 | C |
| 24 | 1H | 2346 | A |
| 24 | 1H | 2347 | C |
| 24 | 1H | 2350 | C |
| 24 | 1H | 2352 | A |
| 24 | 1H | 2355 | C |
| 24 | 1H | 2360 | A |
| 24 | 1H | 2361 | A |
| 24 | 1H | 2372 | G |
| 24 | 1H | 2376 | A |
| 24 | 1H | 2383 | G |
| 24 | 1H | 2385 | C |
| 24 | 1H | 2389 | G |

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| Mol | Chain | Res | Type |
|---|---|---|---|
| 24 | 1H | 2402 | C |
| 24 | 1H | 2403 | C |
| 24 | 1H | 2405 | G |
| 24 | 1H | 2406 | U |
| 24 | 1H | 2407 | G |
| 24 | 1H | 2415 | G |
| 24 | 1H | 2418 | A |
| 24 | 1H | 2422 | A |
| 24 | 1H | 2424 | C |
| 24 | 1H | 2425 | A |
| 24 | 1H | 2426 | A |
| 24 | 1H | 2428 | G |
| 24 | 1H | 2429 | G |
| 24 | 1H | 2430 | A |
| 24 | 1H | 2431 | U |
| 24 | 1H | 2434 | A |
| 24 | 1H | 2435 | A |
| 24 | 1H | 2439 | A |
| 24 | 1H | 2440 | C |
| 24 | 1H | 2441 | C |
| 24 | 1H | 2442 | C |
| 24 | 1H | 2445 | G |
| 24 | 1H | 2447 | G |
| 24 | 1H | 2448 | A |
| 24 | 1H | 2468 | G |
| 24 | 1H | 2474 | C |
| 24 | 1H | 2477 | C |
| 24 | 1H | 2478 | A |
| 24 | 1H | 2484 | G |
| 24 | 1H | 2497 | A |
| 24 | 1H | 2502 | G |
| 24 | 1H | 2505 | G |
| 24 | 1H | 2506 | U |
| 24 | 1H | 2507 | C |
| 24 | 1H | 2518 | A |
| 24 | 1H | 2525 | G |
| 24 | 1H | 2529 | G |
| 24 | 1H | 2531 | A |
| 24 | 1H | 2549 | G |
| 24 | 1H | 2554 | U |
| 24 | 1H | 2564 | A |
| 24 | 1H | 2567 | G |

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| Mol | Chain | Res | Type |
|---|---|---|---|
| 24 | 1H | 2569 | G |
| 24 | 1H | 2573 | C |
| 24 | 1H | 2582 | G |
| 24 | 1H | 2599 | G |
| 24 | 1H | 2601 | C |
| 24 | 1H | 2602 | A |
| 24 | 1H | 2603 | G |
| 24 | 1H | 2608 | G |
| 24 | 1H | 2609 | U |
| 24 | 1H | 2611 | U |
| 24 | 1H | 2612 | C |
| 24 | 1H | 2614 | A |
| 24 | 1H | 2615 | U |
| 24 | 1H | 2621 | A |
| 24 | 1H | 2629 | A |
| 24 | 1H | 2636 | U |
| 24 | 1H | 2641 | G |
| 24 | 1H | 2663 | G |
| 24 | 1H | 2665 | A |
| 24 | 1H | 2672 | G |
| 24 | 1H | 2673 | G |
| 24 | 1H | 2678 | C |
| 24 | 1H | 2682 | U |
| 24 | 1H | 2689 | U |
| 24 | 1H | 2690 | C |
| 24 | 1H | 2691 | C |
| 24 | 1H | 2702 | U |
| 24 | 1H | 2703 | C |
| 24 | 1H | 2705 | A |
| 24 | 1H | 2706 | G |
| 24 | 1H | 2707 | G |
| 24 | 1H | 2710 | C |
| 24 | 1H | 2712(A) | A |
| 24 | 1H | 2713 | A |
| 24 | 1H | 2714 | G |
| 24 | 1H | 2726 | U |
| 24 | 1H | 2733 | A |
| 24 | 1H | 2738 | A |
| 24 | 1H | 2739 | U |
| 24 | 1H | 2744 | G |
| 24 | 1H | 2747 | G |
| 24 | 1H | 2748 | A |

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| Mol | Chain | Res | Type |
|---|---|---|---|
| 24 | 1H | 2751 | G |
| 24 | 1H | 2757 | A |
| 24 | 1H | 2758 | A |
| 24 | 1H | 2764 | A |
| 24 | 1H | 2765 | A |
| 24 | 1H | 2766 | G |
| 24 | 1H | 2770 | G |
| 24 | 1H | 2777 | G |
| 24 | 1H | 2778 | A |
| 24 | 1H | 2779 | U |
| 24 | 1H | 2780 | G |
| 24 | 1H | 2781 | A |
| 24 | 1H | 2783 | G |
| 24 | 1H | 2789 | C |
| 24 | 1H | 2790 | A |
| 24 | 1H | 2791 | C |
| 24 | 1H | 2792 | G |
| 24 | 1H | 2793 | G |
| 24 | 1H | 2794 | C |
| 24 | 1H | 2795 | G |
| 24 | 1H | 2797 | U |
| 24 | 1H | 2801 | A |
| 24 | 1H | 2802 | G |
| 24 | 1H | 2803 | C |
| 24 | 1H | 2805 | G |
| 24 | 1H | 2808 | U |
| 24 | 1H | 2818 | G |
| 24 | 1H | 2820 | A |
| 24 | 1H | 2821 | A |
| 24 | 1H | 2830 | G |
| 24 | 1H | 2833 | G |
| 24 | 1H | 2834 | G |
| 24 | 1H | 2835 | A |
| 24 | 1H | 2850 | A |
| 24 | 1H | 2851 | A |
| 24 | 1H | 2860 | A |
| 24 | 1H | 2871 | C |
| 24 | 1H | 2872 | G |
| 24 | 1H | 2883 | A |
| 24 | 1H | 2885 | C |
| 24 | 1H | 2891 | G |
| 24 | 1H | 2892 | A |

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| Mol | Chain | Res | Type |
|---|---|---|---|
| 24 | 1H | 2893 | G |
| 25 | 16 | 3 | C |
| 25 | 16 | 7 | G |
| 25 | 16 | 9 | G |
| 25 | 16 | 12 | C |
| 25 | 16 | 13 | A |
| 25 | 16 | 15 | A |
| 25 | 16 | 16 | G |
| 25 | 16 | 18 | G |
| 25 | 16 | 19 | G |
| 25 | 16 | 21 | G |
| 25 | 16 | 23 | G |
| 25 | 16 | 24 | G |
| 25 | 16 | 25 | A |
| 25 | 16 | 32 | C |
| 25 | 16 | 38 | C |
| 25 | 16 | 39 | A |
| 25 | 16 | 40 | U |
| 25 | 16 | 41 | U |
| 25 | 16 | 42 | C |
| 25 | 16 | 44 | G |
| 25 | 16 | 45 | A |
| 25 | 16 | 46 | A |
| 25 | 16 | 52 | A |
| 25 | 16 | 53 | A |
| 25 | 16 | 56 | G |
| 25 | 16 | 73 | A |
| 25 | 16 | 74 | U |
| 25 | 16 | 76 | G |
| 25 | 16 | 77 | U |
| 25 | 16 | 81 | G |
| 25 | 16 | 84 | C |
| 25 | 16 | 89 | G |
| 25 | 16 | 95 | U |
| 25 | 16 | 105 | G |
| 25 | 16 | 109 | G |
| 25 | 16 | 115 | G |
| 25 | 16 | 116 | G |
| 25 | 16 | 117 | G |
| 1 | 1G | 5 | U |
| 1 | 1G | 6 | G |
| 1 | 1G | 7 | G |

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| Mol | Chain | Res | Type |
|---|---|---|---|
| 1 | 1G | 9 | G |
| 1 | 1G | 10 | A |
| 1 | 1G | 15 | G |
| 1 | 1G | 22 | G |
| 1 | 1G | 26 | A |
| 1 | 1G | 31 | G |
| 1 | 1G | 32 | A |
| 1 | 1G | 33 | A |
| 1 | 1G | 39 | G |
| 1 | 1G | 41 | G |
| 1 | 1G | 42 | G |
| 1 | 1G | 44 | G |
| 1 | 1G | 47 | C |
| 1 | 1G | 48 | C |
| 1 | 1G | 50 | A |
| 1 | 1G | 51 | A |
| 1 | 1G | 54 | C |
| 1 | 1G | 66 | G |
| 1 | 1G | 76 | G |
| 1 | 1G | 77 | C |
| 1 | 1G | 79 | G |
| 1 | 1G | 81 | G |
| 1 | 1G | 90 | C |
| 1 | 1G | 91 | C |
| 1 | 1G | 92 | G |
| 1 | 1G | 95 | G |
| 1 | 1G | 101 | A |
| 1 | 1G | 105 | G |
| 1 | 1G | 115 | G |
| 1 | 1G | 116 | A |
| 1 | 1G | 120 | A |
| 1 | 1G | 121 | C |
| 1 | 1G | 131 | C |
| 1 | 1G | 144 | G |
| 1 | 1G | 145 | G |
| 1 | 1G | 163 | C |
| 1 | 1G | 169 | C |
| 1 | 1G | 173 | U |
| 1 | 1G | 174 | C |
| 1 | 1G | 182 | U |
| 1 | 1G | 186 | C |
| 1 | 1G | 186(A) | C |

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| Mol | Chain | Res | Type |
|---|---|---|---|
| 1 | 1G | 186(F) | C |
| 1 | 1G | 188 | U |
| 1 | 1G | 189 | U |
| 1 | 1G | 190 | G |
| 1 | 1G | 191(D) | U |
| 1 | 1G | 195 | A |
| 1 | 1G | 196 | A |
| 1 | 1G | 197 | A |
| 1 | 1G | 198 | G |
| 1 | 1G | 208 | U |
| 1 | 1G | 209 | U |
| 1 | 1G | 210 | U |
| 1 | 1G | 216 | G |
| 1 | 1G | 220 | G |
| 1 | 1G | 243 | A |
| 1 | 1G | 245 | C |
| 1 | 1G | 247 | G |
| 1 | 1G | 250 | A |
| 1 | 1G | 251 | G |
| 1 | 1G | 262 | A |
| 1 | 1G | 266 | G |
| 1 | 1G | 267 | C |
| 1 | 1G | 274 | A |
| 1 | 1G | 281 | G |
| 1 | 1G | 288 | A |
| 1 | 1G | 289 | G |
| 1 | 1G | 318 | G |
| 1 | 1G | 321 | A |
| 1 | 1G | 328 | C |
| 1 | 1G | 329 | A |
| 1 | 1G | 332 | G |
| 1 | 1G | 340 | U |
| 1 | 1G | 342 | C |
| 1 | 1G | 345 | C |
| 1 | 1G | 346 | G |
| 1 | 1G | 347 | G |
| 1 | 1G | 350 | G |
| 1 | 1G | 351 | G |
| 1 | 1G | 352 | C |
| 1 | 1G | 353 | A |
| 1 | 1G | 354 | G |
| 1 | 1G | 363 | A |

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| Mol | Chain | Res | Type |
|---|---|---|---|
| 1 | 1G | 367 | U |
| 1 | 1G | 369 | C |
| 1 | 1G | 372 | C |
| 1 | 1G | 378 | G |
| 1 | 1G | 384 | G |
| 1 | 1G | 388 | G |
| 1 | 1G | 397 | A |
| 1 | 1G | 398 | C |
| 1 | 1G | 406 | G |
| 1 | 1G | 411 | A |
| 1 | 1G | 412 | A |
| 1 | 1G | 413 | G |
| 1 | 1G | 414 | A |
| 1 | 1G | 419 | C |
| 1 | 1G | 421 | U |
| 1 | 1G | 422 | C |
| 1 | 1G | 423 | G |
| 1 | 1G | 429 | U |
| 1 | 1G | 431 | A |
| 1 | 1G | 435 | C |
| 1 | 1G | 439 | A |
| 1 | 1G | 452 | A |
| 1 | 1G | 466 | C |
| 1 | 1G | 467 | G |
| 1 | 1G | 484 | G |
| 1 | 1G | 485 | G |
| 1 | 1G | 486 | U |
| 1 | 1G | 494 | U |
| 1 | 1G | 495 | A |
| 1 | 1G | 496 | A |
| 1 | 1G | 497 | U |
| 1 | 1G | 500 | G |
| 1 | 1G | 505 | G |
| 1 | 1G | 509 | A |
| 1 | 1G | 510 | A |
| 1 | 1G | 511 | C |
| 1 | 1G | 518 | C |
| 1 | 1G | 519 | C |
| 1 | 1G | 520 | A |
| 1 | 1G | 521 | G |
| 1 | 1G | 527 | G |
| 1 | 1G | 530 | G |

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| Mol | Chain | Res | Type |
|---|---|---|---|
| 1 | 1G | 531 | U |
| 1 | 1G | 532 | A |
| 1 | 1G | 533 | A |
| 1 | 1G | 536 | C |
| 1 | 1G | 547 | A |
| 1 | 1G | 549 | C |
| 1 | 1G | 552 | U |
| 1 | 1G | 559 | A |
| 1 | 1G | 561 | U |
| 1 | 1G | 562 | C |
| 1 | 1G | 563 | A |
| 1 | 1G | 564 | C |
| 1 | 1G | 572 | A |
| 1 | 1G | 573 | A |
| 1 | 1G | 576 | G |
| 1 | 1G | 577 | G |
| 1 | 1G | 591 | U |
| 1 | 1G | 596 | C |
| 1 | 1G | 607 | A |
| 1 | 1G | 615 | C |
| 1 | 1G | 617 | G |
| 1 | 1G | 630 | G |
| 1 | 1G | 632 | A |
| 1 | 1G | 633 | G |
| 1 | 1G | 640 | A |
| 1 | 1G | 653 | A |
| 1 | 1G | 661 | G |
| 1 | 1G | 665 | A |
| 1 | 1G | 670 | G |
| 1 | 1G | 687 | A |
| 1 | 1G | 688 | G |
| 1 | 1G | 702 | A |
| 1 | 1G | 715 | A |
| 1 | 1G | 722 | A |
| 1 | 1G | 723 | U |
| 1 | 1G | 724 | G |
| 1 | 1G | 731 | G |
| 1 | 1G | 734 | G |
| 1 | 1G | 735 | C |
| 1 | 1G | 749 | C |
| 1 | 1G | 754 | C |
| 1 | 1G | 755 | G |

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| Mol | Chain | Res | Type |
|---|---|---|---|
| 1 | 1G | 760 | G |
| 1 | 1G | 773 | G |
| 1 | 1G | 777 | A |
| 1 | 1G | 787 | A |
| 1 | 1G | 792 | A |
| 1 | 1G | 793 | U |
| 1 | 1G | 794 | A |
| 1 | 1G | 801 | U |
| 1 | 1G | 802 | A |
| 1 | 1G | 813 | U |
| 1 | 1G | 816 | A |
| 1 | 1G | 817 | C |
| 1 | 1G | 819 | A |
| 1 | 1G | 825 | G |
| 1 | 1G | 826 | C |
| 1 | 1G | 827 | U |
| 1 | 1G | 828 | A |
| 1 | 1G | 834 | C |
| 1 | 1G | 842 | C |
| 1 | 1G | 843 | U |
| 1 | 1G | 848 | C |
| 1 | 1G | 859 | A |
| 1 | 1G | 860 | A |
| 1 | 1G | 885 | G |
| 1 | 1G | 889 | A |
| 1 | 1G | 912 | C |
| 1 | 1G | 913 | A |
| 1 | 1G | 914 | A |
| 1 | 1G | 916 | G |
| 1 | 1G | 921 | U |
| 1 | 1G | 922 | G |
| 1 | 1G | 926 | G |
| 1 | 1G | 927 | G |
| 1 | 1G | 934 | C |
| 1 | 1G | 935 | A |
| 1 | 1G | 944 | G |
| 1 | 1G | 954 | G |
| 1 | 1G | 957 | U |
| 1 | 1G | 958 | A |
| 1 | 1G | 960 | U |
| 1 | 1G | 961 | U |
| 1 | 1G | 967 | C |

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| Mol | Chain | Res | Type |
|---|---|---|---|
| 1 | 1G | 968 | A |
| 1 | 1G | 969 | A |
| 1 | 1G | 971 | G |
| 1 | 1G | 972 | C |
| 1 | 1G | 974 | A |
| 1 | 1G | 975 | A |
| 1 | 1G | 976 | G |
| 1 | 1G | 977 | A |
| 1 | 1G | 980 | C |
| 1 | 1G | 983 | A |
| 1 | 1G | 988 | G |
| 1 | 1G | 989 | C |
| 1 | 1G | 991 | U |
| 1 | 1G | 992 | U |
| 1 | 1G | 993 | G |
| 1 | 1G | 994 | A |
| 1 | 1G | 1002 | G |
| 1 | 1G | 1004 | A |
| 1 | 1G | 1006 | C |
| 1 | 1G | 1009 | G |
| 1 | 1G | 1016 | A |
| 1 | 1G | 1023 | G |
| 1 | 1G | 1024 | G |
| 1 | 1G | 1028 | C |
| 1 | 1G | 1029 | G |
| 1 | 1G | 1030 | C |
| 1 | 1G | 1031 | G |
| 1 | 1G | 1032(A) | G |
| 1 | 1G | 1032(B) | G |
| 1 | 1G | 1033 | G |
| 1 | 1G | 1036 | G |
| 1 | 1G | 1040 | U |
| 1 | 1G | 1046 | A |
| 1 | 1G | 1052 | U |
| 1 | 1G | 1054 | C |
| 1 | 1G | 1055 | A |
| 1 | 1G | 1066 | C |
| 1 | 1G | 1067 | A |
| 1 | 1G | 1081 | G |
| 1 | 1G | 1082 | G |
| 1 | 1G | 1094 | G |
| 1 | 1G | 1095 | U |

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| Mol | Chain | Res | Type |
|---|---|---|---|
| 1 | 1G | 1101 | A |
| 1 | 1G | 1109 | C |
| 1 | 1G | 1110 | A |
| 1 | 1G | 1113 | C |
| 1 | 1G | 1117 | G |
| 1 | 1G | 1124 | G |
| 1 | 1G | 1126 | U |
| 1 | 1G | 1127 | G |
| 1 | 1G | 1129 | C |
| 1 | 1G | 1137 | C |
| 1 | 1G | 1138 | G |
| 1 | 1G | 1139 | G |
| 1 | 1G | 1140 | C |
| 1 | 1G | 1146 | A |
| 1 | 1G | 1147 | C |
| 1 | 1G | 1148 | U |
| 1 | 1G | 1154 | G |
| 1 | 1G | 1157 | A |
| 1 | 1G | 1159 | U |
| 1 | 1G | 1160 | G |
| 1 | 1G | 1163 | C |
| 1 | 1G | 1171 | G |
| 1 | 1G | 1178 | G |
| 1 | 1G | 1179 | A |
| 1 | 1G | 1181 | G |
| 1 | 1G | 1182 | G |
| 1 | 1G | 1184 | G |
| 1 | 1G | 1188 | A |
| 1 | 1G | 1190 | G |
| 1 | 1G | 1193 | G |
| 1 | 1G | 1194 | U |
| 1 | 1G | 1196 | U |
| 1 | 1G | 1197 | G |
| 1 | 1G | 1200 | C |
| 1 | 1G | 1201 | A |
| 1 | 1G | 1202 | G |
| 1 | 1G | 1212 | U |
| 1 | 1G | 1215 | G |
| 1 | 1G | 1225 | A |
| 1 | 1G | 1233 | G |
| 1 | 1G | 1238 | A |
| 1 | 1G | 1257 | U |

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| Mol | Chain | Res | Type |
|---|---|---|---|
| 1 | 1G | 1263 | C |
| 1 | 1G | 1267 | C |
| 1 | 1G | 1269 | A |
| 1 | 1G | 1270 | C |
| 1 | 1G | 1273 | G |
| 1 | 1G | 1278 | U |
| 1 | 1G | 1279 | A |
| 1 | 1G | 1280 | A |
| 1 | 1G | 1281 | U |
| 1 | 1G | 1285 | A |
| 1 | 1G | 1287 | A |
| 1 | 1G | 1288 | A |
| 1 | 1G | 1291 | G |
| 1 | 1G | 1293 | G |
| 1 | 1G | 1297 | C |
| 1 | 1G | 1298 | C |
| 1 | 1G | 1299 | A |
| 1 | 1G | 1300 | G |
| 1 | 1G | 1301 | U |
| 1 | 1G | 1303 | C |
| 1 | 1G | 1305 | G |
| 1 | 1G | 1312 | G |
| 1 | 1G | 1316 | G |
| 1 | 1G | 1317 | C |
| 1 | 1G | 1318 | A |
| 1 | 1G | 1319 | A |
| 1 | 1G | 1320 | C |
| 1 | 1G | 1322 | C |
| 1 | 1G | 1323 | G |
| 1 | 1G | 1325 | C |
| 1 | 1G | 1326 | C |
| 1 | 1G | 1331 | G |
| 1 | 1G | 1335 | C |
| 1 | 1G | 1336 | C |
| 1 | 1G | 1338 | G |
| 1 | 1G | 1346 | A |
| 1 | 1G | 1347 | G |
| 1 | 1G | 1353 | G |
| 1 | 1G | 1358 | U |
| 1 | 1G | 1363 | A |
| 1 | 1G | 1364 | U |
| 1 | 1G | 1368 | G |

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| Mol | Chain | Res | Type |
|---|---|---|---|
| 1 | 1G | 1370 | G |
| 1 | 1G | 1379 | G |
| 1 | 1G | 1402 | C |
| 1 | 1G | 1410 | G |
| 1 | 1G | 1419 | G |
| 1 | 1G | 1442 | G |
| 1 | 1G | 1443 | G |
| 1 | 1G | 1446 | A |
| 1 | 1G | 1449 | C |
| 1 | 1G | 1450 | U |
| 1 | 1G | 1452 | C |
| 1 | 1G | 1453 | G |
| 1 | 1G | 1454 | G |
| 1 | 1G | 1465 | C |
| 1 | 1G | 1468 | A |
| 1 | 1G | 1469 | G |
| 1 | 1G | 1477 | C |
| 1 | 1G | 1487 | G |
| 1 | 1G | 1492 | A |
| 1 | 1G | 1493 | A |
| 1 | 1G | 1494 | G |
| 1 | 1G | 1497 | G |
| 1 | 1G | 1498 | U |
| 1 | 1G | 1499 | A |
| 1 | 1G | 1502 | A |
| 1 | 1G | 1503 | A |
| 1 | 1G | 1504 | G |
| 1 | 1G | 1506 | U |
| 1 | 1G | 1517 | G |
| 1 | 1G | 1520 | G |
| 1 | 1G | 1529 | G |
| 1 | 1G | 1530 | G |
| 1 | 1G | 1532 | U |
| 22 | 2L | 6 | G |
| 22 | 2L | 8 | 4SU |
| 22 | 2L | 9 | U |
| 22 | 2L | 15 | G |
| 22 | 2L | 18 | G |
| 22 | 2L | 19 | C |
| 22 | 2L | 20 | C |
| 22 | 2L | 21 | A |
| 22 | 2L | 22 | A |

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| Mol | Chain | Res | Type |
|---|---|---|---|
| 22 | 2L | 23 | A |
| 22 | 2L | 43 | G |
| 22 | 2L | 48 | C |
| 22 | 2L | 56 | U |
| 22 | 2L | 57 | C |
| 22 | 2L | 58 | G |
| 22 | 2L | 61 | G |
| 22 | 2L | 62 | G |
| 22 | 2L | 63 | 5MU |
| 22 | 2L | 64 | PSU |
| 22 | 2L | 67 | A |
| 22 | 2L | 69 | U |
| 22 | 2L | 70 | C |
| 22 | 2L | 71 | C |
| 22 | 2L | 72 | U |
| 22 | 2L | 73 | U |
| 22 | 2L | 85 | A |
| 22 | 3L | 6 | G |
| 22 | 3L | 8 | 4SU |
| 22 | 3L | 14 | A |
| 22 | 3L | 15 | G |
| 22 | 3L | 17 | OMG |
| 22 | 3L | 18 | G |
| 22 | 3L | 19 | C |
| 22 | 3L | 20 | C |
| 22 | 3L | 21 | A |
| 22 | 3L | 25 | G |
| 22 | 3L | 35 | QUO |
| 22 | 3L | 36 | U |
| 22 | 3L | 38 | MIA |
| 22 | 3L | 46 | G |
| 22 | 3L | 49 | A |
| 22 | 3L | 51 | C |
| 22 | 3L | 52 | G |
| 22 | 3L | 53 | A |
| 22 | 3L | 56 | U |
| 22 | 3L | 57 | C |
| 22 | 3L | 58 | G |
| 22 | 3L | 67 | A |
| 22 | 3L | 77 | C |
| 22 | 3L | 85 | A |
| 23 | 4L | 12 | A |

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| Mol | Chain | Res | Type |
|---|---|---|---|
| 23 | 4L | 13 | A |
| 23 | 4L | 14 | A |
| 23 | 4L | 18 | C |
| 24 | 14 | 2 | G |
| 24 | 14 | 3 | U |
| 24 | 14 | 4 | C |
| 24 | 14 | 5 | A |
| 24 | 14 | 6 | A |
| 24 | 14 | 9 | U |
| 24 | 14 | 10 | G |
| 24 | 14 | 11 | G |
| 24 | 14 | 15 | G |
| 24 | 14 | 30 | G |
| 24 | 14 | 33 | U |
| 24 | 14 | 34 | C |
| 24 | 14 | 35 | G |
| 24 | 14 | 36 | G |
| 24 | 14 | 46 | C |
| 24 | 14 | 51 | G |
| 24 | 14 | 58 | G |
| 24 | 14 | 71 | A |
| 24 | 14 | 72 | U |
| 24 | 14 | 74 | A |
| 24 | 14 | 75 | G |
| 24 | 14 | 89 | G |
| 24 | 14 | 90 | U |
| 24 | 14 | 91 | A |
| 24 | 14 | 92 | G |
| 24 | 14 | 95 | G |
| 24 | 14 | 101 | G |
| 24 | 14 | 102 | G |
| 24 | 14 | 108 | U |
| 24 | 14 | 118 | A |
| 24 | 14 | 119 | A |
| 24 | 14 | 120 | U |
| 24 | 14 | 129 | C |
| 24 | 14 | 131 | G |
| 24 | 14 | 153 | C |
| 24 | 14 | 154 | G |
| 24 | 14 | 155 | C |
| 24 | 14 | 161 | U |
| 24 | 14 | 174 | C |

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| Mol | Chain | Res | Type |
|---|---|---|---|
| 24 | 14 | 175 | G |
| 24 | 14 | 181 | A |
| 24 | 14 | 188 | G |
| 24 | 14 | 196 | A |
| 24 | 14 | 197 | A |
| 24 | 14 | 199 | A |
| 24 | 14 | 200 | U |
| 24 | 14 | 214 | G |
| 24 | 14 | 215 | G |
| 24 | 14 | 216 | A |
| 24 | 14 | 222 | A |
| 24 | 14 | 229 | A |
| 24 | 14 | 233 | A |
| 24 | 14 | 248 | G |
| 24 | 14 | 250 | G |
| 24 | 14 | 252 | G |
| 24 | 14 | 265 | A |
| 24 | 14 | 270(K) | C |
| 24 | 14 | 270(L) | U |
| 24 | 14 | 270(M) | U |
| 24 | 14 | 270(O) | U |
| 24 | 14 | 271(B) | G |
| 24 | 14 | 271(C) | U |
| 24 | 14 | 271 | G |
| 24 | 14 | 273(C) | C |
| 24 | 14 | 273(D) | C |
| 24 | 14 | 274 | G |
| 24 | 14 | 277 | C |
| 24 | 14 | 278 | A |
| 24 | 14 | 279 | C |
| 24 | 14 | 283 | A |
| 24 | 14 | 288 | C |
| 24 | 14 | 289 | A |
| 24 | 14 | 290 | G |
| 24 | 14 | 292 | C |
| 24 | 14 | 299 | A |
| 24 | 14 | 307 | G |
| 24 | 14 | 311 | A |
| 24 | 14 | 315 | G |
| 24 | 14 | 323 | G |
| 24 | 14 | 324 | A |
| 24 | 14 | 329 | G |

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| Mol | Chain | Res | Type |
|---|---|---|---|
| 24 | 14 | 330 | A |
| 24 | 14 | 333 | G |
| 24 | 14 | 342 | G |
| 24 | 14 | 352 | G |
| 24 | 14 | 355 | G |
| 24 | 14 | 363(E) | U |
| 24 | 14 | 370 | G |
| 24 | 14 | 372 | G |
| 24 | 14 | 386 | G |
| 24 | 14 | 395 | U |
| 24 | 14 | 396 | G |
| 24 | 14 | 405 | U |
| 24 | 14 | 406 | G |
| 24 | 14 | 407 | G |
| 24 | 14 | 411 | G |
| 24 | 14 | 412 | A |
| 24 | 14 | 428 | A |
| 24 | 14 | 443 | A |
| 24 | 14 | 444 | C |
| 24 | 14 | 447 | A |
| 24 | 14 | 448 | U |
| 24 | 14 | 451 | C |
| 24 | 14 | 454 | A |
| 24 | 14 | 455 | C |
| 24 | 14 | 457 | A |
| 24 | 14 | 470 | A |
| 24 | 14 | 480 | A |
| 24 | 14 | 481 | G |
| 24 | 14 | 505 | A |
| 24 | 14 | 508 | G |
| 24 | 14 | 509 | C |
| 24 | 14 | 512 | G |
| 24 | 14 | 513 | A |
| 24 | 14 | 528 | A |
| 24 | 14 | 530 | G |
| 24 | 14 | 531 | C |
| 24 | 14 | 532 | A |
| 24 | 14 | 533 | G |
| 24 | 14 | 546 | C |
| 24 | 14 | 547 | A |
| 24 | 14 | 549 | G |
| 24 | 14 | 556 | G |

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| Mol | Chain | Res | Type |
|---|---|---|---|
| 24 | 14 | 563 | G |
| 24 | 14 | 573 | G |
| 24 | 14 | 575 | A |
| 24 | 14 | 579 | G |
| 24 | 14 | 580 | C |
| 24 | 14 | 586 | A |
| 24 | 14 | 599 | G |
| 24 | 14 | 603 | A |
| 24 | 14 | 607 | U |
| 24 | 14 | 614 | U |
| 24 | 14 | 617 | G |
| 24 | 14 | 618 | G |
| 24 | 14 | 618(A) | C |
| 24 | 14 | 620 | G |
| 24 | 14 | 621 | A |
| 24 | 14 | 622 | G |
| 24 | 14 | 627 | A |
| 24 | 14 | 634 | C |
| 24 | 14 | 637 | A |
| 24 | 14 | 645 | C |
| 24 | 14 | 646 | A |
| 24 | 14 | 654 | A |
| 24 | 14 | 654(G) | C |
| 24 | 14 | 654(I) | C |
| 24 | 14 | 654(J) | A |
| 24 | 14 | 654(K) | C |
| 24 | 14 | 654(L) | G |
| 24 | 14 | 654(N) | G |
| 24 | 14 | 654(O) | G |
| 24 | 14 | 654(Q) | C |
| 24 | 14 | 654(T) | A |
| 24 | 14 | 656 | G |
| 24 | 14 | 665 | C |
| 24 | 14 | 666 | G |
| 24 | 14 | 669 | G |
| 24 | 14 | 685 | A |
| 24 | 14 | 686 | G |
| 24 | 14 | 699 | A |
| 24 | 14 | 717 | G |
| 24 | 14 | 730 | C |
| 24 | 14 | 738 | G |
| 24 | 14 | 741 | G |

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| Mol | Chain | Res | Type |
|---|---|---|---|
| 24 | 14 | 745 | G |
| 24 | 14 | 748 | G |
| 24 | 14 | 758 | C |
| 24 | 14 | 762 | U |
| 24 | 14 | 764 | A |
| 24 | 14 | 765 | G |
| 24 | 14 | 775 | G |
| 24 | 14 | 776 | G |
| 24 | 14 | 779 | U |
| 24 | 14 | 782 | A |
| 24 | 14 | 784 | A |
| 24 | 14 | 785 | G |
| 24 | 14 | 790 | C |
| 24 | 14 | 792 | G |
| 24 | 14 | 797 | C |
| 24 | 14 | 805 | G |
| 24 | 14 | 812 | C |
| 24 | 14 | 819 | A |
| 24 | 14 | 827 | U |
| 24 | 14 | 828 | U |
| 24 | 14 | 832 | G |
| 24 | 14 | 843 | G |
| 24 | 14 | 857 | C |
| 24 | 14 | 859 | G |
| 24 | 14 | 860 | U |
| 24 | 14 | 861 | A |
| 24 | 14 | 865 | C |
| 24 | 14 | 866 | A |
| 24 | 14 | 869 | G |
| 24 | 14 | 878 | A |
| 24 | 14 | 880 | G |
| 24 | 14 | 882 | G |
| 24 | 14 | 883 | G |
| 24 | 14 | 885 | C |
| 24 | 14 | 887 | A |
| 24 | 14 | 888 | C |
| 24 | 14 | 889 | C |
| 24 | 14 | 890 | A |
| 24 | 14 | 892 | G |
| 24 | 14 | 894 | C |
| 24 | 14 | 895 | U |
| 24 | 14 | 896 | A |

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| Mol | Chain | Res | Type |
|---|---|---|---|
| 24 | 14 | 897 | C |
| 24 | 14 | 898 | C |
| 24 | 14 | 899 | A |
| 24 | 14 | 901 | A |
| 24 | 14 | 902 | C |
| 24 | 14 | 904 | C |
| 24 | 14 | 907 | U |
| 24 | 14 | 909 | A |
| 24 | 14 | 910 | A |
| 24 | 14 | 914 | C |
| 24 | 14 | 917 | A |
| 24 | 14 | 918 | A |
| 24 | 14 | 925 | C |
| 24 | 14 | 926 | A |
| 24 | 14 | 928 | G |
| 24 | 14 | 932 | G |
| 24 | 14 | 938 | G |
| 24 | 14 | 941 | A |
| 24 | 14 | 945 | A |
| 24 | 14 | 946 | G |
| 24 | 14 | 961 | C |
| 24 | 14 | 972 | G |
| 24 | 14 | 974 | G |
| 24 | 14 | 980 | A |
| 24 | 14 | 983 | A |
| 24 | 14 | 996 | A |
| 24 | 14 | 1005 | C |
| 24 | 14 | 1009 | A |
| 24 | 14 | 1010 | A |
| 24 | 14 | 1011 | G |
| 24 | 14 | 1012 | U |
| 24 | 14 | 1013 | C |
| 24 | 14 | 1020 | A |
| 24 | 14 | 1022 | G |
| 24 | 14 | 1023 | U |
| 24 | 14 | 1025 | G |
| 24 | 14 | 1026 | U |
| 24 | 14 | 1033 | U |
| 24 | 14 | 1037 | G |
| 24 | 14 | 1040 | C |
| 24 | 14 | 1043 | C |
| 24 | 14 | 1045 | A |

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| Mol | Chain | Res | Type |
|---|---|---|---|
| 24 | 14 | 1047 | G |
| 24 | 14 | 1048 | A |
| 24 | 14 | 1049 | C |
| 24 | 14 | 1054 | A |
| 24 | 14 | 1060 | U |
| 24 | 14 | 1061 | U |
| 24 | 14 | 1062 | G |
| 24 | 14 | 1063 | G |
| 24 | 14 | 1064 | C |
| 24 | 14 | 1065 | U |
| 24 | 14 | 1067 | A |
| 24 | 14 | 1068 | G |
| 24 | 14 | 1070 | A |
| 24 | 14 | 1071 | G |
| 24 | 14 | 1075 | C |
| 24 | 14 | 1076 | C |
| 24 | 14 | 1079 | C |
| 24 | 14 | 1082 | U |
| 24 | 14 | 1083 | U |
| 24 | 14 | 1085 | A |
| 24 | 14 | 1086 | A |
| 24 | 14 | 1087 | G |
| 24 | 14 | 1088 | A |
| 24 | 14 | 1089 | G |
| 24 | 14 | 1094 | U |
| 24 | 14 | 1096 | A |
| 24 | 14 | 1097 | U |
| 24 | 14 | 1099 | G |
| 24 | 14 | 1104 | C |
| 24 | 14 | 1105 | U |
| 24 | 14 | 1112 | G |
| 24 | 14 | 1128 | A |
| 24 | 14 | 1129 | A |
| 24 | 14 | 1130 | U |
| 24 | 14 | 1135 | C |
| 24 | 14 | 1136 | G |
| 24 | 14 | 1139 | G |
| 24 | 14 | 1143 | A |
| 24 | 14 | 1147 | C |
| 24 | 14 | 1148 | A |
| 24 | 14 | 1151 | G |
| 24 | 14 | 1155 | A |

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| Mol | Chain | Res | Type |
|---|---|---|---|
| 24 | 14 | 1170 | G |
| 24 | 14 | 1173 | G |
| 24 | 14 | 1175 | U |
| 24 | 14 | 1177 | A |
| 24 | 14 | 1178 | C |
| 24 | 14 | 1180 | C |
| 24 | 14 | 1204 | A |
| 24 | 14 | 1205 | U |
| 24 | 14 | 1212 | G |
| 24 | 14 | 1220 | A |
| 24 | 14 | 1237 | A |
| 24 | 14 | 1244 | G |
| 24 | 14 | 1253 | A |
| 24 | 14 | 1256 | G |
| 24 | 14 | 1271 | G |
| 24 | 14 | 1272 | A |
| 24 | 14 | 1273 | U |
| 24 | 14 | 1284 | A |
| 24 | 14 | 1287 | A |
| 24 | 14 | 1289 | C |
| 24 | 14 | 1298 | C |
| 24 | 14 | 1300 | U |
| 24 | 14 | 1301 | A |
| 24 | 14 | 1303 | G |
| 24 | 14 | 1314 | C |
| 24 | 14 | 1319 | G |
| 24 | 14 | 1325 | G |
| 24 | 14 | 1328 | G |
| 24 | 14 | 1329 | U |
| 24 | 14 | 1332 | G |
| 24 | 14 | 1338 | G |
| 24 | 14 | 1345 | C |
| 24 | 14 | 1349 | A |
| 24 | 14 | 1359 | A |
| 24 | 14 | 1360 | A |
| 24 | 14 | 1365 | A |
| 24 | 14 | 1378 | A |
| 24 | 14 | 1380 | G |
| 24 | 14 | 1384 | A |
| 24 | 14 | 1385 | G |
| 24 | 14 | 1386 | C |
| 24 | 14 | 1403 | C |

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| Mol | Chain | Res | Type |
|---|---|---|---|
| 24 | 14 | 1404 | C |
| 24 | 14 | 1416 | G |
| 24 | 14 | 1417 | C |
| 24 | 14 | 1420 | U |
| 24 | 14 | 1421 | G |
| 24 | 14 | 1427 | A |
| 24 | 14 | 1428 | C |
| 24 | 14 | 1437 | C |
| 24 | 14 | 1444(A) | A |
| 24 | 14 | 1445 | C |
| 24 | 14 | 1449 | A |
| 24 | 14 | 1449(A) | G |
| 24 | 14 | 1458 | C |
| 24 | 14 | 1459 | G |
| 24 | 14 | 1460 | A |
| 24 | 14 | 1467 | C |
| 24 | 14 | 1471 | A |
| 24 | 14 | 1474 | C |
| 24 | 14 | 1475 | G |
| 24 | 14 | 1476 | C |
| 24 | 14 | 1480 | G |
| 24 | 14 | 1482 | U |
| 24 | 14 | 1483 | G |
| 24 | 14 | 1487 | G |
| 24 | 14 | 1488 | G |
| 24 | 14 | 1490 | A |
| 24 | 14 | 1493 | C |
| 24 | 14 | 1494 | A |
| 24 | 14 | 1497 | U |
| 24 | 14 | 1500 | G |
| 24 | 14 | 1509 | C |
| 24 | 14 | 1510 | A |
| 24 | 14 | 1526 | G |
| 24 | 14 | 1534 | G |
| 24 | 14 | 1535 | U |
| 24 | 14 | 1536 | A |
| 24 | 14 | 1537 | C |
| 24 | 14 | 1540 | G |
| 24 | 14 | 1543 | A |
| 24 | 14 | 1547 | C |
| 24 | 14 | 1554 | A |
| 24 | 14 | 1558 | A |

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| Mol | Chain | Res | Type |
|---|---|---|---|
| 24 | 14 | 1559 | G |
| 24 | 14 | 1560 | G |
| 24 | 14 | 1566 | A |
| 24 | 14 | 1569 | A |
| 24 | 14 | 1578 | U |
| 24 | 14 | 1580 | A |
| 24 | 14 | 1581 | G |
| 24 | 14 | 1586 | A |
| 24 | 14 | 1587 | A |
| 24 | 14 | 1588 | C |
| 24 | 14 | 1598 | C |
| 24 | 14 | 1608 | A |
| 24 | 14 | 1609 | A |
| 24 | 14 | 1610 | A |
| 24 | 14 | 1612 | C |
| 24 | 14 | 1616 | A |
| 24 | 14 | 1618 | A |
| 24 | 14 | 1641 | A |
| 24 | 14 | 1647 | G |
| 24 | 14 | 1648 | C |
| 24 | 14 | 1649 | G |
| 24 | 14 | 1672 | C |
| 24 | 14 | 1673 | U |
| 24 | 14 | 1674 | G |
| 24 | 14 | 1676 | A |
| 24 | 14 | 1678 | G |
| 24 | 14 | 1695 | G |
| 24 | 14 | 1697 | G |
| 24 | 14 | 1698 | A |
| 24 | 14 | 1700 | A |
| 24 | 14 | 1701 | A |
| 24 | 14 | 1725 | G |
| 24 | 14 | 1729 | A |
| 24 | 14 | 1730 | U |
| 24 | 14 | 1731 | G |
| 24 | 14 | 1732 | A |
| 24 | 14 | 1743 | G |
| 24 | 14 | 1756 | G |
| 24 | 14 | 1762 | A |
| 24 | 14 | 1763 | G |
| 24 | 14 | 1764 | G |
| 24 | 14 | 1773 | A |

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| Mol | Chain | Res | Type |
|---|---|---|---|
| 24 | 14 | 1782 | C |
| 24 | 14 | 1791 | A |
| 24 | 14 | 1800 | C |
| 24 | 14 | 1801 | G |
| 24 | 14 | 1802 | A |
| 24 | 14 | 1806 | C |
| 24 | 14 | 1811 | G |
| 24 | 14 | 1816 | G |
| 24 | 14 | 1829 | A |
| 24 | 14 | 1834 | U |
| 24 | 14 | 1835 | G |
| 24 | 14 | 1839 | G |
| 24 | 14 | 1847 | A |
| 24 | 14 | 1848 | A |
| 24 | 14 | 1850 | G |
| 24 | 14 | 1858 | G |
| 24 | 14 | 1859 | A |
| 24 | 14 | 1861 | G |
| 24 | 14 | 1869 | G |
| 24 | 14 | 1871 | A |
| 24 | 14 | 1878 | G |
| 24 | 14 | 1887 | C |
| 24 | 14 | 1889 | A |
| 24 | 14 | 1900 | A |
| 24 | 14 | 1906 | G |
| 24 | 14 | 1911 | U |
| 24 | 14 | 1912 | A |
| 24 | 14 | 1913 | A |
| 24 | 14 | 1914 | C |
| 24 | 14 | 1917 | U |
| 24 | 14 | 1929 | G |
| 24 | 14 | 1930 | G |
| 24 | 14 | 1931 | U |
| 24 | 14 | 1934 | C |
| 24 | 14 | 1936 | A |
| 24 | 14 | 1938 | A |
| 24 | 14 | 1952 | A |
| 24 | 14 | 1955 | U |
| 24 | 14 | 1963 | U |
| 24 | 14 | 1967 | C |
| 24 | 14 | 1970 | A |
| 24 | 14 | 1971 | A |

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| Mol | Chain | Res | Type |
|---|---|---|---|
| 24 | 14 | 1972 | A |
| 24 | 14 | 1984 | G |
| 24 | 14 | 1993 | U |
| 24 | 14 | 2000 | G |
| 24 | 14 | 2023 | G |
| 24 | 14 | 2024 | G |
| 24 | 14 | 2025 | C |
| 24 | 14 | 2027 | G |
| 24 | 14 | 2030 | A |
| 24 | 14 | 2031 | A |
| 24 | 14 | 2032 | G |
| 24 | 14 | 2033 | A |
| 24 | 14 | 2036 | C |
| 24 | 14 | 2043 | C |
| 24 | 14 | 2049 | G |
| 24 | 14 | 2055 | C |
| 24 | 14 | 2056 | G |
| 24 | 14 | 2059 | A |
| 24 | 14 | 2060 | A |
| 24 | 14 | 2061 | G |
| 24 | 14 | 2062 | A |
| 24 | 14 | 2063 | C |
| 24 | 14 | 2069 | G |
| 24 | 14 | 2071 | A |
| 24 | 14 | 2074 | U |
| 24 | 14 | 2093 | G |
| 24 | 14 | 2099 | U |
| 24 | 14 | 2100 | G |
| 24 | 14 | 2103 | C |
| 24 | 14 | 2111 | C |
| 24 | 14 | 2112 | G |
| 24 | 14 | 2114 | A |
| 24 | 14 | 2115 | G |
| 24 | 14 | 2117 | A |
| 24 | 14 | 2120 | G |
| 24 | 14 | 2123 | G |
| 24 | 14 | 2125 | G |
| 24 | 14 | 2126 | A |
| 24 | 14 | 2127 | G |
| 24 | 14 | 2128 | C |
| 24 | 14 | 2131 | G |
| 24 | 14 | 2132 | U |

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| Mol | Chain | Res | Type |
|---|---|---|---|
| 24 | 14 | 2133 | G |
| 24 | 14 | 2136 | C |
| 24 | 14 | 2145 | C |
| 24 | 14 | 2146 | C |
| 24 | 14 | 2147 | G |
| 24 | 14 | 2159 | G |
| 24 | 14 | 2162 | G |
| 24 | 14 | 2165 | G |
| 24 | 14 | 2166 | G |
| 24 | 14 | 2167 | U |
| 24 | 14 | 2169 | A |
| 24 | 14 | 2170 | A |
| 24 | 14 | 2171 | A |
| 24 | 14 | 2173 | A |
| 24 | 14 | 2174 | C |
| 24 | 14 | 2175 | C |
| 24 | 14 | 2181 | G |
| 24 | 14 | 2189 | U |
| 24 | 14 | 2192 | G |
| 24 | 14 | 2198 | A |
| 24 | 14 | 2210 | G |
| 24 | 14 | 2211 | G |
| 24 | 14 | 2212 | A |
| 24 | 14 | 2213 | U |
| 24 | 14 | 2215 | G |
| 24 | 14 | 2225 | A |
| 24 | 14 | 2238 | G |
| 24 | 14 | 2268 | A |
| 24 | 14 | 2273 | A |
| 24 | 14 | 2275 | C |
| 24 | 14 | 2283 | C |
| 24 | 14 | 2286 | A |
| 24 | 14 | 2287 | A |
| 24 | 14 | 2288 | A |
| 24 | 14 | 2298 | A |
| 24 | 14 | 2305 | A |
| 24 | 14 | 2307 | G |
| 24 | 14 | 2308 | G |
| 24 | 14 | 2309 | A |
| 24 | 14 | 2310 | A |
| 24 | 14 | 2312 | U |
| 24 | 14 | 2316 | C |

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| Mol | Chain | Res | Type |
|---|---|---|---|
| 24 | 14 | 2320 | A |
| 24 | 14 | 2321 | G |
| 24 | 14 | 2322 | A |
| 24 | 14 | 2325 | G |
| 24 | 14 | 2327 | A |
| 24 | 14 | 2334 | G |
| 24 | 14 | 2336 | A |
| 24 | 14 | 2337 | G |
| 24 | 14 | 2342 | C |
| 24 | 14 | 2346 | A |
| 24 | 14 | 2347 | C |
| 24 | 14 | 2350 | C |
| 24 | 14 | 2354 | G |
| 24 | 14 | 2355 | C |
| 24 | 14 | 2361 | A |
| 24 | 14 | 2379 | G |
| 24 | 14 | 2383 | G |
| 24 | 14 | 2385 | C |
| 24 | 14 | 2388 | A |
| 24 | 14 | 2389 | G |
| 24 | 14 | 2392 | A |
| 24 | 14 | 2402 | C |
| 24 | 14 | 2403 | C |
| 24 | 14 | 2406 | U |
| 24 | 14 | 2407 | G |
| 24 | 14 | 2410 | G |
| 24 | 14 | 2414 | G |
| 24 | 14 | 2422 | A |
| 24 | 14 | 2423 | U |
| 24 | 14 | 2424 | C |
| 24 | 14 | 2425 | A |
| 24 | 14 | 2428 | G |
| 24 | 14 | 2429 | G |
| 24 | 14 | 2430 | A |
| 24 | 14 | 2431 | U |
| 24 | 14 | 2434 | A |
| 24 | 14 | 2435 | A |
| 24 | 14 | 2439 | A |
| 24 | 14 | 2440 | C |
| 24 | 14 | 2441 | C |
| 24 | 14 | 2448 | A |
| 24 | 14 | 2449 | U |

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| Mol | Chain | Res | Type |
|---|---|---|---|
| 24 | 14 | 2468 | G |
| 24 | 14 | 2474 | C |
| 24 | 14 | 2476 | A |
| 24 | 14 | 2477 | C |
| 24 | 14 | 2487 | G |
| 24 | 14 | 2491 | U |
| 24 | 14 | 2492 | U |
| 24 | 14 | 2502 | G |
| 24 | 14 | 2504 | U |
| 24 | 14 | 2505 | G |
| 24 | 14 | 2506 | U |
| 24 | 14 | 2518 | A |
| 24 | 14 | 2529 | G |
| 24 | 14 | 2535 | G |
| 24 | 14 | 2542 | A |
| 24 | 14 | 2554 | U |
| 24 | 14 | 2555 | U |
| 24 | 14 | 2566 | A |
| 24 | 14 | 2567 | G |
| 24 | 14 | 2569 | G |
| 24 | 14 | 2572 | A |
| 24 | 14 | 2573 | C |
| 24 | 14 | 2574 | G |
| 24 | 14 | 2578 | G |
| 24 | 14 | 2579 | C |
| 24 | 14 | 2584 | U |
| 24 | 14 | 2585 | U |
| 24 | 14 | 2602 | A |
| 24 | 14 | 2603 | G |
| 24 | 14 | 2604 | U |
| 24 | 14 | 2608 | G |
| 24 | 14 | 2609 | U |
| 24 | 14 | 2611 | U |
| 24 | 14 | 2612 | C |
| 24 | 14 | 2615 | U |
| 24 | 14 | 2629 | A |
| 24 | 14 | 2630 | G |
| 24 | 14 | 2635 | C |
| 24 | 14 | 2636 | U |
| 24 | 14 | 2644 | G |
| 24 | 14 | 2654 | A |
| 24 | 14 | 2660 | A |

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| Mol | Chain | Res | Type |
|---|---|---|---|
| 24 | 14 | 2661 | G |
| 24 | 14 | 2663 | G |
| 24 | 14 | 2665 | A |
| 24 | 14 | 2673 | G |
| 24 | 14 | 2679 | A |
| 24 | 14 | 2689 | U |
| 24 | 14 | 2690 | C |
| 24 | 14 | 2700 | C |
| 24 | 14 | 2702 | U |
| 24 | 14 | 2707 | G |
| 24 | 14 | 2708 | G |
| 24 | 14 | 2709 | G |
| 24 | 14 | 2712(A) | A |
| 24 | 14 | 2713 | A |
| 24 | 14 | 2714 | G |
| 24 | 14 | 2725 | A |
| 24 | 14 | 2726 | U |
| 24 | 14 | 2733 | A |
| 24 | 14 | 2743 | C |
| 24 | 14 | 2744 | G |
| 24 | 14 | 2748 | A |
| 24 | 14 | 2750 | A |
| 24 | 14 | 2751 | G |
| 24 | 14 | 2752 | C |
| 24 | 14 | 2761 | G |
| 24 | 14 | 2762 | G |
| 24 | 14 | 2764 | A |
| 24 | 14 | 2765 | A |
| 24 | 14 | 2766 | G |
| 24 | 14 | 2769 | C |
| 24 | 14 | 2777 | G |
| 24 | 14 | 2778 | A |
| 24 | 14 | 2789 | C |
| 24 | 14 | 2791 | C |
| 24 | 14 | 2793 | G |
| 24 | 14 | 2795 | G |
| 24 | 14 | 2797 | U |
| 24 | 14 | 2798 | C |
| 24 | 14 | 2799 | A |
| 24 | 14 | 2801 | A |
| 24 | 14 | 2802 | G |
| 24 | 14 | 2808 | U |

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| Mol | Chain | Res | Type |
|---|---|---|---|
| 24 | 14 | 2810 | A |
| 24 | 14 | 2812 | G |
| 24 | 14 | 2818 | G |
| 24 | 14 | 2820 | A |
| 24 | 14 | 2821 | A |
| 24 | 14 | 2833 | G |
| 24 | 14 | 2834 | G |
| 24 | 14 | 2835 | A |
| 24 | 14 | 2846 | G |
| 24 | 14 | 2847 | U |
| 24 | 14 | 2849 | U |
| 24 | 14 | 2859 | G |
| 24 | 14 | 2860 | A |
| 24 | 14 | 2872 | G |
| 24 | 14 | 2876 | G |
| 24 | 14 | 2879 | C |
| 24 | 14 | 2892 | A |
| 24 | 14 | 2894 | G |
| 24 | 14 | 2896 | C |
| 25 | 1J | 0 | A |
| 25 | 1J | 3 | C |
| 25 | 1J | 7 | G |
| 25 | 1J | 12 | C |
| 25 | 1J | 13 | A |
| 25 | 1J | 15 | A |
| 25 | 1J | 16 | G |
| 25 | 1J | 17 | C |
| 25 | 1J | 25 | A |
| 25 | 1J | 26 | A |
| 25 | 1J | 27 | C |
| 25 | 1J | 28 | C |
| 25 | 1J | 29 | A |
| 25 | 1J | 30 | C |
| 25 | 1J | 40 | U |
| 25 | 1J | 41 | U |
| 25 | 1J | 42 | C |
| 25 | 1J | 44 | G |
| 25 | 1J | 45 | A |
| 25 | 1J | 47 | C |
| 25 | 1J | 58 | A |
| 25 | 1J | 59 | A |
| 25 | 1J | 60 | C |

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| Mol | Chain | Res | Type |
|---|---|---|---|
| 25 | 1J | 64 | C |
| 25 | 1J | 67 | G |
| 25 | 1J | 73 | A |
| 25 | 1J | 74 | U |
| 25 | 1J | 75 | G |
| 25 | 1J | 88 | C |
| 25 | 1J | 89(A) | A |
| 25 | 1J | 90 | C |
| 25 | 1J | 100 | G |
| 25 | 1J | 109 | G |
| 25 | 1J | 116 | G |

All (192) RNA pucker outliers are listed below:

| Mol | Chain | Res | Type |
|---|---|---|---|
| 1 | 13 | 5 | U |
| 1 | 13 | 181 | G |
| 1 | 13 | 210 | U |
| 1 | 13 | 243 | A |
| 1 | 13 | 244 | U |
| 1 | 13 | 266 | G |
| 1 | 13 | 412 | A |
| 1 | 13 | 429 | U |
| 1 | 13 | 484 | G |
| 1 | 13 | 509 | A |
| 1 | 13 | 560 | U |
| 1 | 13 | 686 | U |
| 1 | 13 | 703 | G |
| 1 | 13 | 748 | C |
| 1 | 13 | 793 | U |
| 1 | 13 | 811 | C |
| 1 | 13 | 812 | C |
| 1 | 13 | 913 | A |
| 1 | 13 | 1027 | C |
| 1 | 13 | 1054 | C |
| 1 | 13 | 1065 | U |
| 1 | 13 | 1126 | U |
| 1 | 13 | 1285 | A |
| 1 | 13 | 1302 | U |
| 1 | 13 | 1336 | C |
| 1 | 13 | 1498 | U |
| 22 | 2K | 9 | U |

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| Mol | Chain | Res | Type |
|---|---|---|---|
| 22 | 2K | 20 | C |
| 22 | 2K | 44 | C |
| 22 | 2K | 54 | C |
| 22 | 2K | 61 | G |
| 22 | 3K | 17 | OMG |
| 22 | 3K | 18 | G |
| 22 | 3K | 21 | A |
| 23 | 4K | 9 | G |
| 23 | 4K | 11 | U |
| 23 | 4K | 13 | A |
| 24 | 1H | 125 | G |
| 24 | 1H | 196 | A |
| 24 | 1H | 199 | A |
| 24 | 1H | 222 | A |
| 24 | 1H | 229 | A |
| 24 | 1H | 249 | C |
| 24 | 1H | 270(M) | U |
| 24 | 1H | 310 | A |
| 24 | 1H | 404 | C |
| 24 | 1H | 621 | A |
| 24 | 1H | 654(S) | G |
| 24 | 1H | 685 | A |
| 24 | 1H | 746 | A |
| 24 | 1H | 752 | A |
| 24 | 1H | 764 | A |
| 24 | 1H | 776 | G |
| 24 | 1H | 858 | U |
| 24 | 1H | 859 | G |
| 24 | 1H | 897 | C |
| 24 | 1H | 961 | C |
| 24 | 1H | 974 | G |
| 24 | 1H | 974(A) | C |
| 24 | 1H | 990 | A |
| 24 | 1H | 1022 | G |
| 24 | 1H | 1026 | U |
| 24 | 1H | 1060 | U |
| 24 | 1H | 1178 | C |
| 24 | 1H | 1286 | A |
| 24 | 1H | 1312 | U |
| 24 | 1H | 1378 | A |
| 24 | 1H | 1379 | A |
| 24 | 1H | 1396 | U |

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| Mol | Chain | Res | Type |
|---|---|---|---|
| 24 | 1H | 1427 | A |
| 24 | 1H | 1508 | A |
| 24 | 1H | 1536 | A |
| 24 | 1H | 1558 | A |
| 24 | 1H | 1608 | A |
| 24 | 1H | 1609 | A |
| 24 | 1H | 1617 | C |
| 24 | 1H | 1647 | G |
| 24 | 1H | 1653 | G |
| 24 | 1H | 1799 | G |
| 24 | 1H | 1899 | G |
| 24 | 1H | 1912 | A |
| 24 | 1H | 2210 | G |
| 24 | 1H | 2212 | A |
| 24 | 1H | 2225 | A |
| 24 | 1H | 2351 | G |
| 24 | 1H | 2402 | C |
| 24 | 1H | 2422 | A |
| 24 | 1H | 2439 | A |
| 24 | 1H | 2477 | C |
| 24 | 1H | 2566 | A |
| 24 | 1H | 2611 | U |
| 24 | 1H | 2689 | U |
| 24 | 1H | 2756 | U |
| 1 | 1G | 4 | U |
| 1 | 1G | 7 | G |
| 1 | 1G | 80 | G |
| 1 | 1G | 89 | U |
| 1 | 1G | 115 | G |
| 1 | 1G | 197 | A |
| 1 | 1G | 201 | C |
| 1 | 1G | 250 | A |
| 1 | 1G | 327 | A |
| 1 | 1G | 345 | C |
| 1 | 1G | 412 | A |
| 1 | 1G | 485 | G |
| 1 | 1G | 509 | A |
| 1 | 1G | 560 | U |
| 1 | 1G | 632 | A |
| 1 | 1G | 652 | U |
| 1 | 1G | 687 | A |
| 1 | 1G | 748 | C |

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| Mol | Chain | Res | Type |
|---|---|---|---|
| 1 | 1G | 793 | U |
| 1 | 1G | 812 | C |
| 1 | 1G | 884 | U |
| 1 | 1G | 913 | A |
| 1 | 1G | 974 | A |
| 1 | 1G | 991 | U |
| 1 | 1G | 992 | U |
| 1 | 1G | 1054 | C |
| 1 | 1G | 1094 | G |
| 1 | 1G | 1126 | U |
| 1 | 1G | 1137 | C |
| 1 | 1G | 1145 | C |
| 1 | 1G | 1181 | G |
| 1 | 1G | 1183 | A |
| 1 | 1G | 1211 | U |
| 1 | 1G | 1300 | G |
| 1 | 1G | 1330 | U |
| 1 | 1G | 1346 | A |
| 1 | 1G | 1442 | G |
| 1 | 1G | 1453 | G |
| 1 | 1G | 1498 | U |
| 22 | 2L | 9 | U |
| 22 | 2L | 17 | OMG |
| 22 | 2L | 18 | G |
| 22 | 2L | 22 | A |
| 22 | 2L | 57 | C |
| 22 | 2L | 60 | A |
| 22 | 2L | 70 | C |
| 22 | 2L | 71 | C |
| 22 | 3L | 17 | OMG |
| 22 | 3L | 18 | G |
| 22 | 3L | 57 | C |
| 23 | 4L | 12 | A |
| 24 | 14 | 128 | C |
| 24 | 14 | 196 | A |
| 24 | 14 | 197 | A |
| 24 | 14 | 199 | A |
| 24 | 14 | 249 | C |
| 24 | 14 | 278 | A |
| 24 | 14 | 310 | A |
| 24 | 14 | 385 | C |
| 24 | 14 | 503 | A |

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| Mol | Chain | Res | Type |
|---|---|---|---|
| 24 | 14 | 654(S) | G |
| 24 | 14 | 685 | A |
| 24 | 14 | 764 | A |
| 24 | 14 | 774 | A |
| 24 | 14 | 856 | C |
| 24 | 14 | 886 | C |
| 24 | 14 | 888 | C |
| 24 | 14 | 945 | A |
| 24 | 14 | 960 | A |
| 24 | 14 | 971 | C |
| 24 | 14 | 1022 | G |
| 24 | 14 | 1085 | A |
| 24 | 14 | 1088 | A |
| 24 | 14 | 1378 | A |
| 24 | 14 | 1379 | A |
| 24 | 14 | 1396 | U |
| 24 | 14 | 1420 | U |
| 24 | 14 | 1427 | A |
| 24 | 14 | 1497 | U |
| 24 | 14 | 1558 | A |
| 24 | 14 | 1608 | A |
| 24 | 14 | 1609 | A |
| 24 | 14 | 1672 | C |
| 24 | 14 | 1912 | A |
| 24 | 14 | 2166 | G |
| 24 | 14 | 2212 | A |
| 24 | 14 | 2335 | A |
| 24 | 14 | 2402 | C |
| 24 | 14 | 2406 | U |
| 24 | 14 | 2430 | A |
| 24 | 14 | 2439 | A |
| 24 | 14 | 2448 | A |
| 24 | 14 | 2602 | A |
| 24 | 14 | 2689 | U |
| 24 | 14 | 2726 | U |
| 24 | 14 | 2776 | A |
| 24 | 14 | 2801 | A |
| 24 | 14 | 2859 | G |
| 24 | 14 | 2893 | G |

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

28 non-standard protein/DNA/RNA residues are modelled in this entry.

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

| Mol | Type | Chain | Res | Link | Bond lengths | | | Bond angles | | |
|---|---|---|---|---|---|---|---|---|---|---|
| | | | | | Counts | RMSZ | $\#\|Z\| > 2$ | Counts | RMSZ | $\#\|Z\| > 2$ |
| 22 | PSU | 3K | 40 | 22 | 18,21,22 | 1.16 | 1 (5%) | 21,30,33 | 1.66 | 2 (9%) |
| 22 | PSU | 2K | 40 | 22 | 18,21,22 | 1.05 | 1 (5%) | 21,30,33 | 1.92 | 4 (19%) |
| 22 | MIA | 3K | 38 | 22 | 28,31,32 | 2.32 | 3 (10%) | 38,44,47 | 2.94 | 14 (36%) |
| 22 | MIA | 2K | 38 | 22 | 28,31,32 | 2.29 | 3 (10%) | 38,44,47 | 3.55 | 11 (28%) |
| 22 | 4SU | 3L | 8 | 22,55 | 18,21,22 | 2.07 | 5 (27%) | 25,30,33 | 2.04 | 4 (16%) |
| 22 | QUO | 3K | 35 | 22 | 32,35,36 | 4.91 | 13 (40%) | 36,52,55 | 5.06 | 11 (30%) |
| 22 | MIA | 2L | 38 | 22 | 28,31,32 | 2.19 | 3 (10%) | 38,44,47 | 2.74 | 12 (31%) |
| 22 | MIA | 3L | 38 | 22 | 28,31,32 | 2.36 | 4 (14%) | 38,44,47 | 3.11 | 17 (44%) |
| 22 | 4SU | 2L | 8 | 22 | 18,21,22 | 1.79 | 4 (22%) | 25,30,33 | 2.16 | 7 (28%) |
| 22 | 4SU | 2K | 8 | 22 | 18,21,22 | 2.13 | 3 (16%) | 25,30,33 | 2.96 | 7 (28%) |
| 22 | PSU | 2L | 64 | 22 | 18,21,22 | 1.33 | 2 (11%) | 21,30,33 | 1.68 | 4 (19%) |
| 22 | PSU | 2L | 40 | 22 | 18,21,22 | 1.37 | 1 (5%) | 21,30,33 | 1.69 | 4 (19%) |
| 22 | QUO | 3L | 35 | 22 | 32,35,36 | 4.82 | 13 (40%) | 36,52,55 | 4.75 | 13 (36%) |
| 22 | 4SU | 3K | 8 | 22 | 18,21,22 | 1.85 | 3 (16%) | 25,30,33 | 2.69 | 4 (16%) |
| 22 | PSU | 3K | 64 | 22 | 18,21,22 | 1.26 | 2 (11%) | 21,30,33 | 1.90 | 3 (14%) |
| 22 | 5MU | 3L | 63 | 22 | 19,22,23 | 3.95 | 5 (26%) | 27,32,35 | 3.32 | 9 (33%) |
| 22 | PSU | 2K | 64 | 22,55 | 18,21,22 | 1.35 | 2 (11%) | 21,30,33 | 2.16 | 6 (28%) |
| 22 | QUO | 2L | 35 | 22,23 | 32,35,36 | 4.80 | 12 (37%) | 36,52,55 | 4.83 | 13 (36%) |
| 22 | QUO | 2K | 35 | 22,23 | 32,35,36 | 4.80 | 13 (40%) | 36,52,55 | 4.61 | 11 (30%) |
| 22 | PSU | 3L | 64 | 22 | 18,21,22 | 1.35 | 1 (5%) | 21,30,33 | 1.66 | 2 (9%) |
| 22 | PSU | 3L | 40 | 22 | 18,21,22 | 1.27 | 1 (5%) | 21,30,33 | 1.79 | 3 (14%) |
| 22 | OMG | 2L | 17 | 22 | 23,26,27 | 4.92 | 10 (43%) | 32,38,41 | 4.55 | 18 (56%) |
| 22 | OMG | 2K | 17 | 22 | 23,26,27 | 5.05 | 11 (47%) | 32,38,41 | 4.59 | 18 (56%) |
| 22 | 5MU | 2L | 63 | 22 | 19,22,23 | 3.90 | 5 (26%) | 27,32,35 | 3.54 | 10 (37%) |
| 22 | OMG | 3K | 17 | 22 | 23,26,27 | 5.23 | 11 (47%) | 32,38,41 | 4.83 | 16 (50%) |
| 22 | OMG | 3L | 17 | 22 | 23,26,27 | 5.20 | 11 (47%) | 32,38,41 | 4.74 | 17 (53%) |

| Mol | Type | Chain | Res | Link | Bond lengths | | | Bond angles | | |
|---|---|---|---|---|---|---|---|---|---|---|
| | | | | | Counts | RMSZ | $\#\|Z\|>2$ | Counts | RMSZ | $\#\|Z\|>2$ |
| 22 | 5MU | 3K | 63 | 22 | 19,22,23 | 3.89 | 5 (26%) | 27,32,35 | 3.09 | 10 (37%) |
| 22 | 5MU | 2K | 63 | 22 | 19,22,23 | 4.14 | 5 (26%) | 27,32,35 | 3.60 | 10 (37%) |

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 |
|---|---|---|---|---|---|---|---|
| 22 | PSU | 3K | 40 | 22 | - | 0/7/25/26 | 0/2/2/2 |
| 22 | PSU | 2K | 40 | 22 | - | 0/7/25/26 | 0/2/2/2 |
| 22 | MIA | 3K | 38 | 22 | - | 8/15/33/34 | 0/3/3/3 |
| 22 | MIA | 2K | 38 | 22 | - | 5/15/33/34 | 0/3/3/3 |
| 22 | 4SU | 3L | 8 | 22,55 | - | 0/7/25/26 | 0/2/2/2 |
| 22 | QUO | 3K | 35 | 22 | - | 3/12/43/44 | 0/4/4/4 |
| 22 | MIA | 2L | 38 | 22 | - | 3/15/33/34 | 0/3/3/3 |
| 22 | MIA | 3L | 38 | 22 | - | 8/15/33/34 | 0/3/3/3 |
| 22 | 4SU | 2L | 8 | 22 | - | 0/7/25/26 | 0/2/2/2 |
| 22 | 4SU | 2K | 8 | 22 | - | 0/7/25/26 | 0/2/2/2 |
| 22 | PSU | 2L | 64 | 22 | - | 0/7/25/26 | 0/2/2/2 |
| 22 | PSU | 2L | 40 | 22 | - | 0/7/25/26 | 0/2/2/2 |
| 22 | QUO | 3L | 35 | 22 | - | 4/12/43/44 | 0/4/4/4 |
| 22 | 4SU | 3K | 8 | 22 | - | 0/7/25/26 | 0/2/2/2 |
| 22 | PSU | 3K | 64 | 22 | - | 0/7/25/26 | 0/2/2/2 |
| 22 | 5MU | 3L | 63 | 22 | - | 0/7/25/26 | 0/2/2/2 |
| 22 | PSU | 2K | 64 | 22,55 | - | 2/7/25/26 | 0/2/2/2 |
| 22 | QUO | 2L | 35 | 22,23 | - | 1/12/43/44 | 0/4/4/4 |
| 22 | QUO | 2K | 35 | 22,23 | - | 2/12/43/44 | 0/4/4/4 |
| 22 | PSU | 3L | 64 | 22 | - | 4/7/25/26 | 0/2/2/2 |
| 22 | PSU | 3L | 40 | 22 | - | 0/7/25/26 | 0/2/2/2 |
| 22 | OMG | 2L | 17 | 22 | - | 1/9/27/28 | 0/3/3/3 |
| 22 | OMG | 2K | 17 | 22 | - | 3/9/27/28 | 0/3/3/3 |
| 22 | 5MU | 2L | 63 | 22 | - | 3/7/25/26 | 0/2/2/2 |
| 22 | OMG | 3K | 17 | 22 | - | 2/9/27/28 | 0/3/3/3 |
| 22 | OMG | 3L | 17 | 22 | - | 3/9/27/28 | 0/3/3/3 |
| 22 | 5MU | 3K | 63 | 22 | - | 0/7/25/26 | 0/2/2/2 |
| 22 | 5MU | 2K | 63 | 22 | - | 5/7/25/26 | 0/2/2/2 |

All (153) bond length outliers are listed below:

| Mol | Chain | Res | Type | Atoms | Z | Observed(Å) | Ideal(Å) |
|---|---|---|---|---|---|---|---|
| 22 | 2L | 35 | QUO | C4-N3 | 16.38 | 1.71 | 1.34 |
| 22 | 3L | 35 | QUO | C4-N3 | 16.33 | 1.71 | 1.34 |
| 22 | 3K | 35 | QUO | C4-N3 | 16.30 | 1.71 | 1.34 |
| 22 | 2K | 35 | QUO | C4-N3 | 15.16 | 1.68 | 1.34 |
| 22 | 2K | 63 | 5MU | C2-N1 | 14.02 | 1.60 | 1.38 |
| 22 | 3L | 63 | 5MU | C2-N1 | 12.89 | 1.58 | 1.38 |
| 22 | 2K | 35 | QUO | C6-N1 | -12.88 | 1.14 | 1.38 |
| 22 | 2L | 63 | 5MU | C2-N1 | 12.81 | 1.58 | 1.38 |
| 22 | 3K | 35 | QUO | C6-N1 | -12.57 | 1.15 | 1.38 |
| 22 | 3L | 35 | QUO | C6-N1 | -12.51 | 1.15 | 1.38 |
| 22 | 3K | 63 | 5MU | C2-N1 | 12.42 | 1.57 | 1.38 |
| 22 | 2L | 35 | QUO | C6-N1 | -12.05 | 1.16 | 1.38 |
| 22 | 3K | 17 | OMG | C5-N7 | -11.95 | 1.15 | 1.39 |
| 22 | 3K | 17 | OMG | C4-N3 | 11.92 | 1.61 | 1.34 |
| 22 | 2L | 17 | OMG | C5-N7 | -11.86 | 1.15 | 1.39 |
| 22 | 3L | 17 | OMG | C4-N3 | 11.75 | 1.61 | 1.34 |
| 22 | 2K | 17 | OMG | C4-N3 | 11.75 | 1.61 | 1.34 |
| 22 | 3L | 17 | OMG | C5-N7 | -11.69 | 1.15 | 1.39 |
| 22 | 2K | 17 | OMG | C5-N7 | -11.36 | 1.16 | 1.39 |
| 22 | 2L | 17 | OMG | C4-N3 | 10.94 | 1.59 | 1.34 |
| 22 | 3L | 17 | OMG | C4-N9 | 9.04 | 1.61 | 1.38 |
| 22 | 3K | 17 | OMG | C4-N9 | 8.94 | 1.60 | 1.38 |
| 22 | 3K | 35 | QUO | C8-N9 | -8.83 | 1.22 | 1.38 |
| 22 | 3K | 17 | OMG | C8-N7 | -8.80 | 1.07 | 1.32 |
| 22 | 2K | 17 | OMG | C4-N9 | 8.75 | 1.60 | 1.38 |
| 22 | 2L | 17 | OMG | C8-N7 | -8.74 | 1.08 | 1.32 |
| 22 | 3L | 17 | OMG | C8-N7 | -8.55 | 1.08 | 1.32 |
| 22 | 2K | 17 | OMG | C8-N7 | -8.47 | 1.08 | 1.32 |
| 22 | 2L | 35 | QUO | C8-N9 | -8.43 | 1.23 | 1.38 |
| 22 | 2K | 35 | QUO | C8-N9 | -8.31 | 1.23 | 1.38 |
| 22 | 3K | 17 | OMG | C5-C4 | 8.31 | 1.61 | 1.38 |
| 22 | 3L | 17 | OMG | C5-C4 | 8.29 | 1.61 | 1.38 |
| 22 | 2K | 38 | MIA | C13-C14 | 8.26 | 1.57 | 1.32 |
| 22 | 2K | 17 | OMG | C5-C4 | 8.26 | 1.61 | 1.38 |
| 22 | 2L | 38 | MIA | C13-C14 | 8.22 | 1.57 | 1.32 |
| 22 | 3K | 38 | MIA | C13-C14 | 8.20 | 1.57 | 1.32 |
| 22 | 3L | 38 | MIA | C13-C14 | 8.19 | 1.56 | 1.32 |
| 22 | 3L | 17 | OMG | C6-N1 | -8.14 | 1.23 | 1.38 |
| 22 | 2L | 17 | OMG | C5-C4 | 7.86 | 1.60 | 1.38 |
| 22 | 3L | 35 | QUO | C8-N9 | -7.83 | 1.24 | 1.38 |
| 22 | 3K | 35 | QUO | C2-N3 | 7.81 | 1.52 | 1.33 |
| 22 | 3K | 17 | OMG | C6-N1 | -7.59 | 1.24 | 1.38 |
| 22 | 2L | 35 | QUO | C2-N3 | 7.58 | 1.51 | 1.33 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(Å) | Ideal(Å) |
|---|---|---|---|---|---|---|---|
| 22 | 3L | 35 | QUO | C2-N3 | 7.44 | 1.51 | 1.33 |
| 22 | 2K | 35 | QUO | C4-N9 | -7.21 | 1.19 | 1.38 |
| 22 | 2L | 17 | OMG | C6-N1 | -7.20 | 1.25 | 1.38 |
| 22 | 3L | 38 | MIA | C6-N6 | 7.20 | 1.45 | 1.34 |
| 22 | 2L | 17 | OMG | C4-N9 | 7.20 | 1.56 | 1.38 |
| 22 | 2K | 17 | OMG | C6-N1 | -7.18 | 1.25 | 1.38 |
| 22 | 2K | 8 | 4SU | C5-C4 | 7.12 | 1.51 | 1.42 |
| 22 | 2K | 35 | QUO | C2-N3 | 7.11 | 1.50 | 1.33 |
| 22 | 3K | 38 | MIA | C6-N6 | 6.83 | 1.45 | 1.34 |
| 22 | 2K | 38 | MIA | C6-N6 | 6.73 | 1.44 | 1.34 |
| 22 | 3L | 35 | QUO | C8-C7 | 6.73 | 1.50 | 1.37 |
| 22 | 3K | 35 | QUO | C4-N9 | -6.64 | 1.21 | 1.38 |
| 22 | 2K | 35 | QUO | C5-C6 | -6.62 | 1.29 | 1.44 |
| 22 | 2L | 35 | QUO | C4-N9 | -6.56 | 1.21 | 1.38 |
| 22 | 3L | 8 | 4SU | C5-C4 | 6.51 | 1.50 | 1.42 |
| 22 | 3K | 35 | QUO | C5-C6 | -6.39 | 1.30 | 1.44 |
| 22 | 2K | 35 | QUO | C8-C7 | 6.36 | 1.49 | 1.37 |
| 22 | 3L | 35 | QUO | C4-N9 | -6.28 | 1.22 | 1.38 |
| 22 | 2L | 38 | MIA | C6-N6 | 6.26 | 1.44 | 1.34 |
| 22 | 3L | 35 | QUO | C5-C6 | -6.23 | 1.30 | 1.44 |
| 22 | 3K | 35 | QUO | C8-C7 | 6.21 | 1.49 | 1.37 |
| 22 | 2L | 63 | 5MU | C4-N3 | -6.21 | 1.27 | 1.38 |
| 22 | 2L | 35 | QUO | C8-C7 | 6.12 | 1.49 | 1.37 |
| 22 | 3K | 63 | 5MU | C4-N3 | -6.08 | 1.27 | 1.38 |
| 22 | 2L | 35 | QUO | C5-C6 | -6.06 | 1.31 | 1.44 |
| 22 | 3L | 63 | 5MU | C4-N3 | -6.05 | 1.27 | 1.38 |
| 22 | 3L | 63 | 5MU | C2-N3 | 6.01 | 1.48 | 1.38 |
| 22 | 3K | 63 | 5MU | C2-N3 | 5.97 | 1.48 | 1.38 |
| 22 | 2K | 63 | 5MU | C2-N3 | 5.87 | 1.48 | 1.38 |
| 22 | 2K | 63 | 5MU | C4-N3 | -5.84 | 1.27 | 1.38 |
| 22 | 2L | 63 | 5MU | C2-N3 | 5.78 | 1.48 | 1.38 |
| 22 | 2L | 35 | QUO | C13-C12 | -5.58 | 1.47 | 1.53 |
| 22 | 3K | 63 | 5MU | C6-N1 | 5.56 | 1.47 | 1.38 |
| 22 | 2K | 35 | QUO | C13-C12 | -5.55 | 1.47 | 1.53 |
| 22 | 3K | 35 | QUO | C13-C12 | -5.53 | 1.47 | 1.53 |
| 22 | 3L | 63 | 5MU | C6-N1 | 5.49 | 1.47 | 1.38 |
| 22 | 3L | 35 | QUO | C13-C12 | -5.49 | 1.47 | 1.53 |
| 22 | 3K | 8 | 4SU | C5-C4 | 5.46 | 1.49 | 1.42 |
| 22 | 2L | 63 | 5MU | C6-N1 | 5.43 | 1.47 | 1.38 |
| 22 | 2K | 63 | 5MU | C6-N1 | 5.39 | 1.47 | 1.38 |
| 22 | 2K | 63 | 5MU | C4-C5 | 5.16 | 1.53 | 1.44 |
| 22 | 3K | 63 | 5MU | C4-C5 | 5.06 | 1.53 | 1.44 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(Å) | Ideal(Å) |
|---|---|---|---|---|---|---|---|
| 22 | 3L | 63 | 5MU | C4-C5 | 4.99 | 1.52 | 1.44 |
| 22 | 2L | 8 | 4SU | C5-C4 | 4.98 | 1.48 | 1.42 |
| 22 | 2L | 40 | PSU | C6-C5 | 4.79 | 1.40 | 1.35 |
| 22 | 3K | 17 | OMG | C8-N9 | -4.74 | 1.26 | 1.37 |
| 22 | 2L | 17 | OMG | C8-N9 | -4.72 | 1.26 | 1.37 |
| 22 | 3L | 64 | PSU | C6-C5 | 4.70 | 1.40 | 1.35 |
| 22 | 3L | 17 | OMG | C8-N9 | -4.61 | 1.27 | 1.37 |
| 22 | 2K | 64 | PSU | C6-C5 | 4.61 | 1.40 | 1.35 |
| 22 | 3K | 38 | MIA | C2-S10 | 4.54 | 1.79 | 1.75 |
| 22 | 2K | 17 | OMG | C8-N9 | -4.52 | 1.27 | 1.37 |
| 22 | 2L | 63 | 5MU | C4-C5 | 4.40 | 1.52 | 1.44 |
| 22 | 3L | 40 | PSU | C6-C5 | 4.28 | 1.40 | 1.35 |
| 22 | 3K | 64 | PSU | C6-C5 | 4.28 | 1.40 | 1.35 |
| 22 | 2L | 64 | PSU | C6-C5 | 4.22 | 1.40 | 1.35 |
| 22 | 3L | 38 | MIA | C2-S10 | 4.12 | 1.79 | 1.75 |
| 22 | 3K | 35 | QUO | C2-N2 | 4.12 | 1.43 | 1.34 |
| 22 | 3L | 8 | 4SU | C2-N1 | 3.96 | 1.44 | 1.38 |
| 22 | 3K | 40 | PSU | C6-C5 | 3.93 | 1.39 | 1.35 |
| 22 | 2L | 8 | 4SU | C2-N1 | 3.90 | 1.44 | 1.38 |
| 22 | 2K | 35 | QUO | C2-N2 | 3.82 | 1.43 | 1.34 |
| 22 | 3K | 8 | 4SU | C2-N1 | 3.78 | 1.44 | 1.38 |
| 22 | 2L | 35 | QUO | C2-N2 | 3.71 | 1.42 | 1.34 |
| 22 | 2K | 8 | 4SU | C2-N1 | 3.66 | 1.44 | 1.38 |
| 22 | 3L | 35 | QUO | C2-N2 | 3.60 | 1.42 | 1.34 |
| 22 | 2K | 38 | MIA | C5-N7 | -3.44 | 1.32 | 1.39 |
| 22 | 2K | 40 | PSU | C6-C5 | 3.44 | 1.39 | 1.35 |
| 22 | 2L | 38 | MIA | C5-N7 | -3.13 | 1.33 | 1.39 |
| 22 | 2K | 17 | OMG | C2-N2 | 3.13 | 1.41 | 1.34 |
| 22 | 3K | 17 | OMG | C2-N3 | 3.13 | 1.40 | 1.33 |
| 22 | 3L | 17 | OMG | C2-N3 | 3.12 | 1.40 | 1.33 |
| 22 | 3K | 17 | OMG | C2-N2 | 3.12 | 1.41 | 1.34 |
| 22 | 2L | 17 | OMG | O6-C6 | -3.06 | 1.17 | 1.23 |
| 22 | 2K | 17 | OMG | C2-N3 | 3.03 | 1.40 | 1.33 |
| 22 | 2K | 35 | QUO | C14-C13 | -2.99 | 1.48 | 1.53 |
| 22 | 3L | 17 | OMG | O6-C6 | -2.93 | 1.18 | 1.23 |
| 22 | 3L | 8 | 4SU | C6-N1 | 2.90 | 1.45 | 1.38 |
| 22 | 2K | 8 | 4SU | C6-N1 | 2.84 | 1.44 | 1.38 |
| 22 | 3K | 8 | 4SU | C6-N1 | 2.82 | 1.44 | 1.38 |
| 22 | 3K | 17 | OMG | O6-C6 | -2.82 | 1.18 | 1.23 |
| 22 | 3L | 17 | OMG | C2-N2 | 2.79 | 1.40 | 1.34 |
| 22 | 3L | 35 | QUO | C14-C13 | -2.76 | 1.49 | 1.53 |
| 22 | 3K | 35 | QUO | C16-C15 | 2.70 | 1.61 | 1.54 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(Å) | Ideal(Å) |
|---|---|---|---|---|---|---|---|
| 22 | 2L | 35 | QUO | C16-C15 | 2.64 | 1.61 | 1.54 |
| 22 | 2L | 17 | OMG | C2-N2 | 2.63 | 1.40 | 1.34 |
| 22 | 2K | 35 | QUO | C2-N1 | -2.57 | 1.31 | 1.37 |
| 22 | 2L | 8 | 4SU | C6-N1 | 2.57 | 1.44 | 1.38 |
| 22 | 3L | 35 | QUO | C16-C15 | 2.53 | 1.60 | 1.54 |
| 22 | 2K | 35 | QUO | C5-C7 | 2.53 | 1.55 | 1.43 |
| 22 | 2L | 35 | QUO | C5-C7 | 2.52 | 1.55 | 1.43 |
| 22 | 3K | 35 | QUO | C5-C7 | 2.52 | 1.55 | 1.43 |
| 22 | 3L | 17 | OMG | C2-N1 | -2.46 | 1.31 | 1.37 |
| 22 | 2K | 64 | PSU | C4-C5 | -2.43 | 1.37 | 1.44 |
| 22 | 3L | 35 | QUO | C2-N1 | -2.40 | 1.31 | 1.37 |
| 22 | 3L | 38 | MIA | C5-N7 | -2.38 | 1.34 | 1.39 |
| 22 | 2K | 17 | OMG | O6-C6 | -2.37 | 1.19 | 1.23 |
| 22 | 2L | 8 | 4SU | C4-N3 | 2.35 | 1.40 | 1.37 |
| 22 | 2L | 17 | OMG | C2-N3 | 2.34 | 1.38 | 1.33 |
| 22 | 3K | 35 | QUO | C2-N1 | -2.33 | 1.32 | 1.37 |
| 22 | 3L | 35 | QUO | C5-C7 | 2.31 | 1.54 | 1.43 |
| 22 | 2K | 35 | QUO | C16-C15 | 2.25 | 1.60 | 1.54 |
| 22 | 2L | 35 | QUO | C2-N1 | -2.21 | 1.32 | 1.37 |
| 22 | 3L | 8 | 4SU | C2-N3 | 2.14 | 1.41 | 1.38 |
| 22 | 2L | 64 | PSU | C2-N1 | 2.14 | 1.39 | 1.36 |
| 22 | 3K | 35 | QUO | C14-C13 | -2.13 | 1.50 | 1.53 |
| 22 | 3L | 8 | 4SU | C4-N3 | 2.10 | 1.39 | 1.37 |
| 22 | 3K | 17 | OMG | C2-N1 | -2.09 | 1.32 | 1.37 |
| 22 | 2K | 17 | OMG | C2-N1 | -2.05 | 1.32 | 1.37 |
| 22 | 3K | 64 | PSU | C2-N1 | 2.01 | 1.39 | 1.36 |

All (260) bond angle outliers are listed below:

| Mol | Chain | Res | Type | Atoms | Z | Observed($^o$) | Ideal($^o$) |
|---|---|---|---|---|---|---|---|
| 22 | 3L | 35 | QUO | C5-C4-N3 | -19.71 | 104.90 | 127.53 |
| 22 | 3K | 35 | QUO | C5-C4-N3 | -19.34 | 105.33 | 127.53 |
| 22 | 2K | 35 | QUO | C5-C4-N3 | -18.53 | 106.26 | 127.53 |
| 22 | 2L | 35 | QUO | C5-C4-N3 | -18.15 | 106.69 | 127.53 |
| 22 | 2K | 38 | MIA | C11-S10-C2 | 15.14 | 113.61 | 102.25 |
| 22 | 3K | 35 | QUO | C1'-N9-C8 | -12.68 | 111.35 | 125.72 |
| 22 | 3K | 35 | QUO | N9-C4-N3 | 12.23 | 150.41 | 125.95 |
| 22 | 2K | 63 | 5MU | C5-C4-N3 | 11.96 | 125.72 | 115.32 |
| 22 | 2L | 63 | 5MU | C5-C4-N3 | 11.80 | 125.58 | 115.32 |
| 22 | 2L | 17 | OMG | C6-C5-N7 | 11.66 | 151.51 | 130.29 |
| 22 | 2L | 35 | QUO | N9-C4-N3 | 11.54 | 149.03 | 125.95 |
| 22 | 3L | 35 | QUO | N9-C4-N3 | 11.33 | 148.60 | 125.95 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed($^o$) | Ideal($^o$) |
|---|---|---|---|---|---|---|---|
| 22 | 2K | 17 | OMG | C6-C5-N7 | 11.27 | 150.81 | 130.29 |
| 22 | 2K | 35 | QUO | N9-C4-N3 | 11.05 | 148.04 | 125.95 |
| 22 | 2L | 35 | QUO | C7-C8-N9 | -11.00 | 100.81 | 111.08 |
| 22 | 2L | 35 | QUO | C1'-N9-C8 | -10.80 | 113.48 | 125.72 |
| 22 | 3L | 17 | OMG | C6-C5-N7 | 10.73 | 149.82 | 130.29 |
| 22 | 3L | 63 | 5MU | C5-C4-N3 | 10.57 | 124.51 | 115.32 |
| 22 | 3K | 17 | OMG | N9-C4-N3 | 10.50 | 146.94 | 125.95 |
| 22 | 3K | 17 | OMG | C6-C5-N7 | 10.35 | 149.13 | 130.29 |
| 22 | 3L | 17 | OMG | N9-C4-N3 | 10.25 | 146.46 | 125.95 |
| 22 | 2K | 8 | 4SU | C4-N3-C2 | -10.20 | 117.54 | 127.31 |
| 22 | 3K | 35 | QUO | C7-C8-N9 | -10.20 | 101.56 | 111.08 |
| 22 | 3L | 17 | OMG | C8-N7-C5 | 10.15 | 122.33 | 104.26 |
| 22 | 3L | 35 | QUO | C7-C8-N9 | -10.02 | 101.73 | 111.08 |
| 22 | 2K | 17 | OMG | C8-N7-C5 | 9.96 | 122.00 | 104.26 |
| 22 | 3K | 63 | 5MU | C5-C4-N3 | 9.86 | 123.89 | 115.32 |
| 22 | 2K | 35 | QUO | C7-C8-N9 | -9.74 | 101.99 | 111.08 |
| 22 | 3K | 17 | OMG | C8-N7-C5 | 9.73 | 121.60 | 104.26 |
| 22 | 3K | 38 | MIA | C11-S10-C2 | 9.52 | 109.39 | 102.25 |
| 22 | 3K | 17 | OMG | C1'-N9-C4 | 9.46 | 154.44 | 126.49 |
| 22 | 2L | 17 | OMG | C8-N7-C5 | 9.45 | 121.10 | 104.26 |
| 22 | 2K | 17 | OMG | N9-C4-N3 | 9.33 | 144.61 | 125.95 |
| 22 | 2K | 35 | QUO | C1'-N9-C8 | -8.96 | 115.57 | 125.72 |
| 22 | 2L | 38 | MIA | C12-C13-C14 | -8.94 | 110.96 | 127.01 |
| 22 | 2K | 38 | MIA | C12-C13-C14 | -8.89 | 111.05 | 127.01 |
| 22 | 3L | 38 | MIA | C11-S10-C2 | 8.86 | 108.89 | 102.25 |
| 22 | 2L | 17 | OMG | C6-C5-C4 | -8.84 | 105.53 | 118.83 |
| 22 | 3L | 38 | MIA | C12-C13-C14 | -8.43 | 111.88 | 127.01 |
| 22 | 2L | 17 | OMG | N9-C4-N3 | 8.38 | 142.70 | 125.95 |
| 22 | 3K | 8 | 4SU | C4-N3-C2 | -8.35 | 119.31 | 127.31 |
| 22 | 3L | 17 | OMG | C1'-N9-C4 | 8.23 | 150.81 | 126.49 |
| 22 | 2K | 17 | OMG | C6-C5-C4 | -8.07 | 106.69 | 118.83 |
| 22 | 2K | 8 | 4SU | C5-C4-N3 | 7.67 | 121.88 | 114.75 |
| 22 | 2L | 38 | MIA | C5-C4-N3 | -7.57 | 119.21 | 127.18 |
| 22 | 3L | 35 | QUO | C7-C5-C4 | -7.49 | 104.09 | 112.68 |
| 22 | 3K | 38 | MIA | C12-C13-C14 | -7.46 | 113.63 | 127.01 |
| 22 | 3K | 8 | 4SU | C5-C4-N3 | 7.43 | 121.67 | 114.75 |
| 22 | 2K | 38 | MIA | C5-C4-N3 | -7.40 | 119.38 | 127.18 |
| 22 | 3K | 17 | OMG | C6-C5-C4 | -7.39 | 107.72 | 118.83 |
| 22 | 3L | 38 | MIA | C5-C4-N3 | -7.24 | 119.56 | 127.18 |
| 22 | 3L | 17 | OMG | C6-C5-C4 | -7.17 | 108.04 | 118.83 |
| 22 | 2L | 35 | QUO | C7-C5-C4 | -7.08 | 104.57 | 112.68 |
| 22 | 3L | 8 | 4SU | C4-N3-C2 | -6.95 | 120.65 | 127.31 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed($^o$) | Ideal($^o$) |
|---|---|---|---|---|---|---|---|
| 22 | 2K | 17 | OMG | C1'-N9-C4 | 6.91 | 146.90 | 126.49 |
| 22 | 2K | 35 | QUO | C7-C5-C4 | -6.88 | 104.79 | 112.68 |
| 22 | 3K | 35 | QUO | C7-C5-C4 | -6.86 | 104.81 | 112.68 |
| 22 | 2L | 17 | OMG | C1'-N9-C4 | 6.82 | 146.64 | 126.49 |
| 22 | 3K | 17 | OMG | C1'-N9-C8 | -6.82 | 107.36 | 126.73 |
| 22 | 2L | 63 | 5MU | O4-C4-C5 | -6.56 | 117.41 | 124.92 |
| 22 | 2K | 63 | 5MU | C4-N3-C2 | -6.54 | 118.76 | 127.34 |
| 22 | 3K | 17 | OMG | C5-C6-N1 | 6.49 | 129.77 | 113.25 |
| 22 | 2L | 63 | 5MU | C4-N3-C2 | -6.48 | 118.84 | 127.34 |
| 22 | 2L | 17 | OMG | C5-C6-N1 | 6.47 | 129.72 | 113.25 |
| 22 | 3L | 17 | OMG | C5-C6-N1 | 6.46 | 129.69 | 113.25 |
| 22 | 3L | 17 | OMG | C5-C4-N3 | -6.42 | 118.18 | 128.39 |
| 22 | 3K | 38 | MIA | C5-C4-N3 | -6.34 | 120.50 | 127.18 |
| 22 | 3K | 17 | OMG | C5-C4-N9 | -6.31 | 94.35 | 105.66 |
| 22 | 2K | 17 | OMG | C5-C6-N1 | 6.27 | 129.20 | 113.25 |
| 22 | 3L | 63 | 5MU | C4-N3-C2 | -6.26 | 119.13 | 127.34 |
| 22 | 2K | 63 | 5MU | O4-C4-C5 | -6.12 | 117.92 | 124.92 |
| 22 | 3K | 17 | OMG | C5-C4-N3 | -6.09 | 118.69 | 128.39 |
| 22 | 2L | 8 | 4SU | C4-N3-C2 | -5.95 | 121.61 | 127.31 |
| 22 | 2L | 17 | OMG | C5-C4-N9 | -5.89 | 95.10 | 105.66 |
| 22 | 2K | 63 | 5MU | C5-C6-N1 | -5.88 | 116.92 | 123.31 |
| 22 | 2K | 17 | OMG | C5-C4-N9 | -5.88 | 95.13 | 105.66 |
| 22 | 3K | 63 | 5MU | C4-N3-C2 | -5.85 | 119.67 | 127.34 |
| 22 | 2L | 38 | MIA | N3-C4-N9 | 5.83 | 134.39 | 126.99 |
| 22 | 3L | 63 | 5MU | C5-C6-N1 | -5.83 | 116.98 | 123.31 |
| 22 | 3L | 63 | 5MU | C6-C5-C4 | 5.77 | 122.78 | 118.02 |
| 22 | 3L | 17 | OMG | C5-C4-N9 | -5.75 | 95.36 | 105.66 |
| 22 | 3K | 8 | 4SU | C5-C4-S4 | -5.68 | 117.82 | 124.31 |
| 22 | 3L | 35 | QUO | C1'-N9-C8 | -5.60 | 119.37 | 125.72 |
| 22 | 3L | 38 | MIA | N3-C4-N9 | 5.58 | 134.07 | 126.99 |
| 22 | 2L | 63 | 5MU | C5-C6-N1 | -5.53 | 117.31 | 123.31 |
| 22 | 3K | 63 | 5MU | C6-C5-C4 | 5.46 | 122.52 | 118.02 |
| 22 | 3K | 63 | 5MU | C5-C6-N1 | -5.41 | 117.43 | 123.31 |
| 22 | 3L | 17 | OMG | C4-C5-N7 | -5.38 | 102.14 | 110.67 |
| 22 | 3L | 17 | OMG | C1'-N9-C8 | -5.33 | 111.58 | 126.73 |
| 22 | 3L | 63 | 5MU | O4-C4-C5 | -5.31 | 118.84 | 124.92 |
| 22 | 2K | 64 | PSU | N1-C2-N3 | 5.19 | 120.64 | 115.17 |
| 22 | 2K | 17 | OMG | C4-C5-N7 | -5.16 | 102.49 | 110.67 |
| 22 | 2K | 17 | OMG | C5-C4-N3 | -5.12 | 120.24 | 128.39 |
| 22 | 3K | 38 | MIA | C15-C14-C13 | -5.09 | 107.38 | 122.66 |
| 22 | 3K | 64 | PSU | C4-N3-C2 | -5.08 | 119.37 | 126.37 |
| 22 | 3K | 17 | OMG | N9-C8-N7 | 5.04 | 122.75 | 113.40 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed($^o$) | Ideal($^o$) |
|---|---|---|---|---|---|---|---|
| 22 | 2K | 63 | 5MU | C6-C5-C4 | 5.02 | 122.16 | 118.02 |
| 22 | 3L | 17 | OMG | N9-C8-N7 | 4.95 | 122.58 | 113.40 |
| 22 | 2L | 17 | OMG | C4-C5-N7 | -4.87 | 102.96 | 110.67 |
| 22 | 3K | 17 | OMG | O6-C6-C5 | -4.84 | 113.74 | 126.53 |
| 22 | 2L | 63 | 5MU | C6-C5-C4 | 4.84 | 122.01 | 118.02 |
| 22 | 2L | 63 | 5MU | C5M-C5-C6 | -4.84 | 116.30 | 122.85 |
| 22 | 2K | 64 | PSU | C4-N3-C2 | -4.79 | 119.78 | 126.37 |
| 22 | 3L | 8 | 4SU | C5-C4-N3 | 4.78 | 119.20 | 114.75 |
| 22 | 2K | 63 | 5MU | C5M-C5-C6 | -4.78 | 116.38 | 122.85 |
| 22 | 3L | 63 | 5MU | C5M-C5-C6 | -4.76 | 116.40 | 122.85 |
| 22 | 2L | 17 | OMG | O6-C6-C5 | -4.76 | 113.98 | 126.53 |
| 22 | 2K | 40 | PSU | N1-C2-N3 | 4.75 | 120.18 | 115.17 |
| 22 | 3K | 17 | OMG | C4-C5-N7 | -4.74 | 103.15 | 110.67 |
| 22 | 2L | 64 | PSU | C4-N3-C2 | -4.73 | 119.85 | 126.37 |
| 22 | 3L | 35 | QUO | C5-C6-N1 | 4.68 | 127.99 | 115.10 |
| 22 | 3L | 40 | PSU | C4-N3-C2 | -4.65 | 119.97 | 126.37 |
| 22 | 3L | 38 | MIA | C16-C14-C13 | -4.61 | 108.81 | 122.66 |
| 22 | 2K | 17 | OMG | N9-C8-N7 | 4.61 | 121.95 | 113.40 |
| 22 | 2K | 8 | 4SU | N3-C2-N1 | 4.57 | 120.84 | 114.89 |
| 22 | 2K | 38 | MIA | N3-C4-N9 | 4.53 | 132.75 | 126.99 |
| 22 | 3L | 17 | OMG | C8-N9-C4 | -4.51 | 97.57 | 106.03 |
| 22 | 2K | 35 | QUO | C5-C6-N1 | 4.49 | 127.46 | 115.10 |
| 22 | 2L | 17 | OMG | C1'-N9-C8 | -4.46 | 114.07 | 126.73 |
| 22 | 3K | 64 | PSU | N1-C2-N3 | 4.44 | 119.85 | 115.17 |
| 22 | 3K | 63 | 5MU | O4-C4-C5 | -4.43 | 119.85 | 124.92 |
| 22 | 3K | 35 | QUO | C5-C6-N1 | 4.42 | 127.29 | 115.10 |
| 22 | 2L | 38 | MIA | C16-C14-C13 | -4.41 | 109.42 | 122.66 |
| 22 | 2L | 17 | OMG | N9-C8-N7 | 4.40 | 121.57 | 113.40 |
| 22 | 3K | 40 | PSU | C4-N3-C2 | -4.39 | 120.32 | 126.37 |
| 22 | 2L | 8 | 4SU | C5-C4-N3 | 4.35 | 118.80 | 114.75 |
| 22 | 3L | 38 | MIA | C5-N7-C8 | 4.34 | 110.27 | 103.45 |
| 22 | 2K | 38 | MIA | C15-C14-C13 | -4.33 | 109.65 | 122.66 |
| 22 | 2K | 40 | PSU | C4-N3-C2 | -4.27 | 120.48 | 126.37 |
| 22 | 3L | 64 | PSU | C4-N3-C2 | -4.25 | 120.52 | 126.37 |
| 22 | 2K | 17 | OMG | C1'-N9-C8 | -4.25 | 114.66 | 126.73 |
| 22 | 3K | 63 | 5MU | C5M-C5-C6 | -4.25 | 117.10 | 122.85 |
| 22 | 3K | 17 | OMG | C8-N9-C4 | -4.21 | 98.13 | 106.03 |
| 22 | 3K | 38 | MIA | N3-C4-N9 | 4.13 | 132.23 | 126.99 |
| 22 | 2L | 8 | 4SU | C5-C4-S4 | -4.13 | 119.59 | 124.31 |
| 22 | 3L | 17 | OMG | O6-C6-C5 | -4.12 | 115.66 | 126.53 |
| 22 | 2L | 35 | QUO | C5-C6-N1 | 4.12 | 126.44 | 115.10 |
| 22 | 3L | 40 | PSU | N1-C2-N3 | 4.11 | 119.51 | 115.17 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed($^o$) | Ideal($^o$) |
|---|---|---|---|---|---|---|---|
| 22 | 2K | 17 | OMG | C8-N9-C4 | -4.06 | 98.42 | 106.03 |
| 22 | 2K | 17 | OMG | O6-C6-C5 | -4.06 | 115.82 | 126.53 |
| 22 | 2L | 17 | OMG | N2-C2-N1 | 4.05 | 125.32 | 116.76 |
| 22 | 3L | 35 | QUO | C1'-N9-C4 | -4.02 | 114.62 | 126.49 |
| 22 | 2L | 40 | PSU | N1-C2-N3 | 3.95 | 119.33 | 115.17 |
| 22 | 2L | 17 | OMG | C5-C4-N3 | -3.89 | 122.19 | 128.39 |
| 22 | 3K | 40 | PSU | N1-C2-N3 | 3.87 | 119.25 | 115.17 |
| 22 | 2L | 8 | 4SU | N3-C2-N1 | 3.82 | 119.86 | 114.89 |
| 22 | 2L | 38 | MIA | C15-C14-C13 | -3.81 | 111.23 | 122.66 |
| 22 | 2L | 38 | MIA | C5-N7-C8 | 3.80 | 109.42 | 103.45 |
| 22 | 3L | 38 | MIA | C15-C14-C13 | -3.79 | 111.28 | 122.66 |
| 22 | 3L | 8 | 4SU | N3-C2-N1 | 3.77 | 119.80 | 114.89 |
| 22 | 3L | 38 | MIA | C4-C5-N7 | -3.75 | 106.29 | 110.58 |
| 22 | 3L | 64 | PSU | N1-C2-N3 | 3.69 | 119.06 | 115.17 |
| 22 | 2K | 63 | 5MU | C1'-N1-C2 | 3.68 | 124.20 | 117.59 |
| 22 | 2L | 40 | PSU | C4-N3-C2 | -3.68 | 121.31 | 126.37 |
| 22 | 3K | 38 | MIA | C5-N7-C8 | 3.66 | 109.21 | 103.45 |
| 22 | 3K | 38 | MIA | C6-C5-N7 | 3.65 | 136.41 | 132.43 |
| 22 | 3K | 35 | QUO | N1-C2-N3 | -3.65 | 116.65 | 123.32 |
| 22 | 2L | 17 | OMG | C8-N9-C4 | -3.61 | 99.25 | 106.03 |
| 22 | 3L | 35 | QUO | N1-C2-N3 | -3.59 | 116.76 | 123.32 |
| 22 | 2K | 40 | PSU | C6-N1-C2 | -3.55 | 119.40 | 122.69 |
| 22 | 2K | 64 | PSU | C6-N1-C2 | -3.55 | 119.40 | 122.69 |
| 22 | 2K | 40 | PSU | O2-C2-N1 | -3.55 | 119.13 | 122.79 |
| 22 | 3L | 35 | QUO | O6-C6-N1 | -3.53 | 113.47 | 120.11 |
| 22 | 3K | 38 | MIA | C16-C14-C13 | -3.52 | 112.08 | 122.66 |
| 22 | 3L | 38 | MIA | N9-C8-N7 | -3.45 | 109.03 | 113.94 |
| 22 | 3K | 38 | MIA | C4-C5-N7 | -3.45 | 106.64 | 110.58 |
| 22 | 3K | 8 | 4SU | N3-C2-N1 | 3.43 | 119.36 | 114.89 |
| 22 | 2K | 38 | MIA | C16-C14-C13 | -3.42 | 112.40 | 122.66 |
| 22 | 2K | 8 | 4SU | C5-C4-S4 | -3.40 | 120.42 | 124.31 |
| 22 | 2L | 35 | QUO | N1-C2-N3 | -3.35 | 117.19 | 123.32 |
| 22 | 2K | 17 | OMG | C2-N1-C6 | 3.24 | 130.99 | 125.11 |
| 22 | 2K | 35 | QUO | C1'-N9-C4 | -3.19 | 117.06 | 126.49 |
| 22 | 2L | 63 | 5MU | C1'-N1-C2 | 3.19 | 123.32 | 117.59 |
| 22 | 3K | 38 | MIA | C2-N3-C4 | 3.15 | 120.55 | 112.29 |
| 22 | 2K | 38 | MIA | C2-N3-C4 | 3.14 | 120.50 | 112.29 |
| 22 | 2L | 38 | MIA | C4-C5-N7 | -3.13 | 107.00 | 110.58 |
| 22 | 2K | 35 | QUO | N1-C2-N3 | -3.12 | 117.62 | 123.32 |
| 22 | 2K | 63 | 5MU | C1'-N1-C6 | -3.11 | 116.04 | 121.15 |
| 22 | 2L | 40 | PSU | C6-N1-C2 | -3.10 | 119.81 | 122.69 |
| 22 | 2L | 35 | QUO | C1'-N9-C4 | -3.01 | 117.59 | 126.49 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed($^o$) | Ideal($^o$) |
|---|---|---|---|---|---|---|---|
| 22 | 3K | 35 | QUO | C10-N11-C12 | -2.99 | 108.73 | 114.83 |
| 22 | 2L | 38 | MIA | N9-C8-N7 | -2.98 | 109.71 | 113.94 |
| 22 | 2K | 38 | MIA | C5-N7-C8 | 2.96 | 108.10 | 103.45 |
| 22 | 2L | 8 | 4SU | C6-N1-C2 | -2.95 | 117.40 | 121.00 |
| 22 | 2K | 35 | QUO | O6-C6-N1 | -2.94 | 114.58 | 120.11 |
| 22 | 3K | 17 | OMG | C2-N1-C6 | 2.93 | 130.44 | 125.11 |
| 22 | 3K | 63 | 5MU | C6-N1-C2 | -2.91 | 118.41 | 121.30 |
| 22 | 3L | 17 | OMG | O6-C6-N1 | -2.90 | 114.65 | 120.11 |
| 22 | 2K | 38 | MIA | C4-C5-N7 | -2.90 | 107.26 | 110.58 |
| 22 | 2L | 38 | MIA | C4-C5-C6 | 2.88 | 119.17 | 116.78 |
| 22 | 2K | 64 | PSU | C6-C5-C4 | 2.87 | 120.11 | 118.17 |
| 22 | 2L | 17 | OMG | C2-N1-C6 | 2.83 | 130.25 | 125.11 |
| 22 | 3K | 38 | MIA | N9-C8-N7 | -2.81 | 109.95 | 113.94 |
| 22 | 3K | 38 | MIA | N3-C2-N1 | -2.80 | 121.89 | 127.00 |
| 22 | 3L | 8 | 4SU | C5-C4-S4 | -2.79 | 121.12 | 124.31 |
| 22 | 3L | 38 | MIA | C2-N3-C4 | 2.76 | 119.52 | 112.29 |
| 22 | 2K | 17 | OMG | O6-C6-N1 | -2.74 | 114.97 | 120.11 |
| 22 | 2K | 8 | 4SU | C5-C6-N1 | -2.73 | 117.41 | 121.84 |
| 22 | 2L | 35 | QUO | O6-C6-N1 | -2.73 | 114.99 | 120.11 |
| 22 | 2L | 63 | 5MU | C5M-C5-C4 | 2.72 | 121.69 | 118.78 |
| 22 | 2L | 38 | MIA | C2-N3-C4 | 2.70 | 119.37 | 112.29 |
| 22 | 2L | 8 | 4SU | C1'-N1-C2 | 2.70 | 122.44 | 117.59 |
| 22 | 3L | 17 | OMG | C2-N1-C6 | 2.70 | 130.01 | 125.11 |
| 22 | 3K | 35 | QUO | O6-C6-N1 | -2.69 | 115.06 | 120.11 |
| 22 | 3K | 35 | QUO | O6-C6-C5 | -2.68 | 117.66 | 125.69 |
| 22 | 3K | 17 | OMG | N1-C2-N3 | -2.66 | 118.45 | 123.32 |
| 22 | 2L | 64 | PSU | N1-C2-N3 | 2.66 | 117.97 | 115.17 |
| 22 | 2L | 35 | QUO | O14-C14-C15 | -2.65 | 105.21 | 111.43 |
| 22 | 2K | 17 | OMG | N1-C2-N3 | -2.64 | 118.49 | 123.32 |
| 22 | 2L | 35 | QUO | C10-N11-C12 | -2.60 | 109.53 | 114.83 |
| 22 | 2K | 35 | QUO | N2-C2-N1 | 2.59 | 122.22 | 116.76 |
| 22 | 2K | 35 | QUO | O6-C6-C5 | -2.58 | 117.95 | 125.69 |
| 22 | 3L | 38 | MIA | C4-C5-C6 | 2.58 | 118.92 | 116.78 |
| 22 | 2L | 38 | MIA | N6-C6-N1 | 2.56 | 121.77 | 118.33 |
| 22 | 2L | 64 | PSU | C5-C4-N3 | 2.52 | 122.10 | 116.55 |
| 22 | 2K | 64 | PSU | O2-C2-N1 | -2.52 | 120.19 | 122.79 |
| 22 | 2K | 63 | 5MU | C5M-C5-C4 | 2.51 | 121.46 | 118.78 |
| 22 | 2K | 64 | PSU | O4-C4-C5 | -2.50 | 117.78 | 124.01 |
| 22 | 2L | 38 | MIA | C16-C14-C15 | -2.50 | 108.83 | 114.59 |
| 22 | 3L | 35 | QUO | O3'-C3'-C2' | 2.46 | 119.69 | 111.82 |
| 22 | 3K | 63 | 5MU | N3-C2-N1 | 2.44 | 118.07 | 114.89 |
| 22 | 3L | 35 | QUO | N2-C2-N1 | 2.44 | 121.91 | 116.76 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed($^o$) | Ideal($^o$) |
|---|---|---|---|---|---|---|---|
| 22 | 2K | 38 | MIA | N6-C6-N1 | 2.40 | 121.55 | 118.33 |
| 22 | 2K | 8 | 4SU | S4-C4-N3 | -2.40 | 117.70 | 120.20 |
| 22 | 2L | 64 | PSU | O4-C4-C5 | -2.39 | 118.07 | 124.01 |
| 22 | 3L | 35 | QUO | O6-C6-C5 | -2.38 | 118.54 | 125.69 |
| 22 | 2L | 35 | QUO | O13-C13-C12 | -2.38 | 106.56 | 112.92 |
| 22 | 2L | 35 | QUO | O6-C6-C5 | -2.37 | 118.56 | 125.69 |
| 22 | 3L | 63 | 5MU | C6-N1-C2 | -2.35 | 118.97 | 121.30 |
| 22 | 2K | 17 | OMG | N2-C2-N1 | 2.35 | 121.71 | 116.76 |
| 22 | 3L | 38 | MIA | C2-N1-C6 | 2.32 | 121.94 | 117.54 |
| 22 | 2K | 17 | OMG | C3'-C2'-C1' | -2.31 | 98.38 | 102.81 |
| 22 | 3K | 17 | OMG | N2-C2-N1 | 2.30 | 121.62 | 116.76 |
| 22 | 2L | 17 | OMG | N1-C2-N3 | -2.26 | 119.18 | 123.32 |
| 22 | 3L | 40 | PSU | O2-C2-N1 | -2.25 | 120.46 | 122.79 |
| 22 | 3L | 38 | MIA | N3-C2-N1 | -2.25 | 122.89 | 127.00 |
| 22 | 3L | 63 | 5MU | C1'-N1-C2 | 2.24 | 121.61 | 117.59 |
| 22 | 2L | 63 | 5MU | C1'-N1-C6 | -2.22 | 117.50 | 121.15 |
| 22 | 3L | 17 | OMG | N1-C2-N3 | -2.20 | 119.30 | 123.32 |
| 22 | 3K | 35 | QUO | C1'-N9-C4 | -2.19 | 120.01 | 126.49 |
| 22 | 2L | 40 | PSU | C6-C5-C4 | -2.19 | 116.70 | 118.17 |
| 22 | 3L | 17 | OMG | C3'-C2'-C1' | -2.18 | 98.63 | 102.81 |
| 22 | 3L | 38 | MIA | C4-N9-C8 | 2.18 | 108.03 | 105.74 |
| 22 | 3K | 38 | MIA | C16-C14-C15 | -2.17 | 109.58 | 114.59 |
| 22 | 2L | 8 | 4SU | O2-C2-N3 | -2.17 | 117.49 | 121.49 |
| 22 | 3L | 38 | MIA | C6-C5-N7 | 2.16 | 134.79 | 132.43 |
| 22 | 2K | 8 | 4SU | O2-C2-N1 | -2.16 | 119.99 | 122.80 |
| 22 | 2L | 17 | OMG | N2-C2-N3 | -2.14 | 115.50 | 119.67 |
| 22 | 2L | 63 | 5MU | C6-N1-C2 | -2.14 | 119.18 | 121.30 |
| 22 | 3L | 35 | QUO | C2-N3-C4 | 2.13 | 115.96 | 112.30 |
| 22 | 3L | 63 | 5MU | N3-C2-N1 | 2.11 | 117.64 | 114.89 |
| 22 | 3K | 63 | 5MU | O2-C2-N1 | -2.06 | 120.12 | 122.80 |
| 22 | 3K | 63 | 5MU | O4-C4-N3 | -2.06 | 116.25 | 120.11 |
| 22 | 3K | 64 | PSU | O4-C4-C5 | -2.05 | 118.91 | 124.01 |
| 22 | 2K | 38 | MIA | N3-C2-N1 | -2.05 | 123.26 | 127.00 |
| 22 | 2L | 17 | OMG | O6-C6-N1 | -2.03 | 116.30 | 120.11 |
| 22 | 3L | 38 | MIA | N6-C6-N1 | 2.02 | 121.04 | 118.33 |
| 22 | 3L | 38 | MIA | C16-C14-C15 | -2.02 | 109.94 | 114.59 |
| 22 | 3K | 38 | MIA | C2-N1-C6 | 2.01 | 121.35 | 117.54 |
| 22 | 2K | 63 | 5MU | O4-C4-N3 | -2.00 | 116.35 | 120.11 |

There are no chirality outliers.

All (57) torsion outliers are listed below:

| Mol | Chain | Res | Type | Atoms |
|---|---|---|---|---|
| 22 | 2K | 35 | QUO | O4'-C4'-C5'-O5' |
| 22 | 2K | 35 | QUO | C3'-C4'-C5'-O5' |
| 22 | 2K | 38 | MIA | N1-C2-S10-C11 |
| 22 | 2K | 38 | MIA | N3-C2-S10-C11 |
| 22 | 2K | 38 | MIA | N6-C12-C13-C14 |
| 22 | 2K | 38 | MIA | C12-C13-C14-C15 |
| 22 | 2K | 38 | MIA | C12-C13-C14-C16 |
| 22 | 3K | 17 | OMG | C1'-C2'-O2'-CM2 |
| 22 | 3K | 35 | QUO | O4'-C4'-C5'-O5' |
| 22 | 3K | 35 | QUO | C16-C12-N11-C10 |
| 22 | 3K | 38 | MIA | O4'-C4'-C5'-O5' |
| 22 | 3K | 38 | MIA | C5-C6-N6-C12 |
| 22 | 3K | 38 | MIA | N1-C6-N6-C12 |
| 22 | 3K | 38 | MIA | N1-C2-S10-C11 |
| 22 | 3K | 38 | MIA | N3-C2-S10-C11 |
| 22 | 3K | 38 | MIA | C12-C13-C14-C15 |
| 22 | 3K | 38 | MIA | C12-C13-C14-C16 |
| 22 | 2L | 17 | OMG | C4'-C5'-O5'-P |
| 22 | 2L | 38 | MIA | N1-C2-S10-C11 |
| 22 | 2L | 38 | MIA | N3-C2-S10-C11 |
| 22 | 2L | 38 | MIA | C12-C13-C14-C15 |
| 22 | 2L | 63 | 5MU | C3'-C4'-C5'-O5' |
| 22 | 2L | 63 | 5MU | O4'-C4'-C5'-O5' |
| 22 | 2L | 63 | 5MU | C4'-C5'-O5'-P |
| 22 | 3L | 35 | QUO | C13-C12-N11-C10 |
| 22 | 3L | 35 | QUO | C16-C12-N11-C10 |
| 22 | 3L | 38 | MIA | O4'-C4'-C5'-O5' |
| 22 | 3L | 38 | MIA | N6-C12-C13-C14 |
| 22 | 3L | 38 | MIA | C12-C13-C14-C15 |
| 22 | 3L | 38 | MIA | C12-C13-C14-C16 |
| 22 | 2K | 63 | 5MU | C3'-C4'-C5'-O5' |
| 22 | 3L | 17 | OMG | O4'-C4'-C5'-O5' |
| 22 | 2K | 17 | OMG | O4'-C4'-C5'-O5' |
| 22 | 3K | 38 | MIA | C3'-C4'-C5'-O5' |
| 22 | 3L | 17 | OMG | C3'-C4'-C5'-O5' |
| 22 | 3K | 35 | QUO | C3'-C4'-C5'-O5' |
| 22 | 3L | 38 | MIA | C3'-C4'-C5'-O5' |
| 22 | 2K | 63 | 5MU | O4'-C4'-C5'-O5' |
| 22 | 2K | 17 | OMG | C3'-C4'-C5'-O5' |
| 22 | 3K | 17 | OMG | C4'-C5'-O5'-P |
| 22 | 3L | 38 | MIA | C5-C6-N6-C12 |
| 22 | 3L | 64 | PSU | C3'-C4'-C5'-O5' |
| 22 | 2L | 35 | QUO | C16-C12-N11-C10 |

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| Mol | Chain | Res | Type | Atoms |
|---|---|---|---|---|
| 22 | 3L | 38 | MIA | N1-C6-N6-C12 |
| 22 | 2K | 63 | 5MU | C4'-C5'-O5'-P |
| 22 | 2K | 64 | PSU | C4'-C5'-O5'-P |
| 22 | 3L | 64 | PSU | O4'-C1'-C5-C4 |
| 22 | 2K | 63 | 5MU | C2'-C1'-N1-C2 |
| 22 | 3L | 38 | MIA | C13-C12-N6-C6 |
| 22 | 3L | 35 | QUO | C4'-C5'-O5'-P |
| 22 | 2K | 63 | 5MU | C2'-C1'-N1-C6 |
| 22 | 3L | 17 | OMG | C4'-C5'-O5'-P |
| 22 | 3L | 35 | QUO | N11-C10-C7-C8 |
| 22 | 3L | 64 | PSU | O4'-C1'-C5-C6 |
| 22 | 2K | 17 | OMG | C3'-C2'-O2'-CM2 |
| 22 | 3L | 64 | PSU | O4'-C4'-C5'-O5' |
| 22 | 2K | 64 | PSU | C2'-C1'-C5-C6 |

There are no ring outliers.

21 monomers are involved in 47 short contacts:

| Mol | Chain | Res | Type | Clashes | Symm-Clashes |
|---|---|---|---|---|---|
| 22 | 3K | 38 | MIA | 5 | 0 |
| 22 | 2K | 38 | MIA | 2 | 0 |
| 22 | 3L | 8 | 4SU | 1 | 0 |
| 22 | 3K | 35 | QUO | 2 | 0 |
| 22 | 2L | 38 | MIA | 2 | 0 |
| 22 | 3L | 38 | MIA | 1 | 0 |
| 22 | 2L | 8 | 4SU | 3 | 0 |
| 22 | 2L | 64 | PSU | 2 | 0 |
| 22 | 3L | 35 | QUO | 3 | 0 |
| 22 | 3K | 8 | 4SU | 2 | 0 |
| 22 | 3K | 64 | PSU | 1 | 0 |
| 22 | 2K | 64 | PSU | 4 | 0 |
| 22 | 2L | 35 | QUO | 5 | 0 |
| 22 | 2K | 35 | QUO | 2 | 0 |
| 22 | 3L | 64 | PSU | 1 | 0 |
| 22 | 2L | 17 | OMG | 2 | 0 |
| 22 | 2K | 17 | OMG | 6 | 0 |
| 22 | 2L | 63 | 5MU | 5 | 0 |
| 22 | 3K | 17 | OMG | 1 | 0 |
| 22 | 3L | 17 | OMG | 2 | 0 |
| 22 | 3K | 63 | 5MU | 1 | 0 |

## 5.5 Carbohydrates (i)

There are no oligosaccharides in this entry.

## 5.6 Ligand geometry (i)

Of 1351 ligands modelled in this entry, 1351 are monoatomic - leaving 0 for Mogul analysis.

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

No monomer is involved in short contacts.

## 5.7 Other polymers (i)

There are no such residues in this entry.

## 5.8 Polymer linkage issues (i)

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 | 13 | 1499/1522 (98%) | -0.16 | 10 (0%) 84 68 | 52, 116, 206, 445 | 5 (0%) |
| 1 | 1G | 1503/1522 (98%) | -0.23 | 13 (0%) 81 63 | 68, 115, 190, 453 | 0 |
| 2 | 12 | 237/256 (92%) | 0.46 | 10 (4%) 40 22 | 127, 170, 220, 245 | 0 |
| 2 | 1E | 237/256 (92%) | 0.40 | 4 (1%) 69 48 | 120, 163, 212, 246 | 0 |
| 3 | 22 | 206/239 (86%) | 0.29 | 5 (2%) 59 38 | 120, 147, 179, 189 | 0 |
| 3 | 2E | 205/239 (85%) | 0.23 | 3 (1%) 72 52 | 111, 138, 196, 212 | 0 |
| 4 | 32 | 208/209 (99%) | 0.48 | 9 (4%) 40 22 | 94, 119, 152, 172 | 0 |
| 4 | 3E | 208/209 (99%) | 0.31 | 6 (2%) 53 32 | 87, 119, 147, 176 | 0 |
| 5 | 42 | 151/162 (93%) | 0.08 | 2 (1%) 75 56 | 94, 113, 140, 210 | 0 |
| 5 | 4E | 151/162 (93%) | 0.18 | 1 (0%) 84 68 | 87, 114, 139, 206 | 0 |
| 6 | 52 | 101/101 (100%) | -0.35 | 0 100 100 | 85, 106, 127, 146 | 0 |
| 6 | 5E | 101/101 (100%) | 0.13 | 1 (0%) 79 61 | 95, 122, 138, 154 | 0 |
| 7 | 62 | 155/156 (99%) | 0.10 | 3 (1%) 66 45 | 111, 129, 145, 152 | 0 |
| 7 | 6E | 155/156 (99%) | 0.29 | 5 (3%) 50 30 | 106, 137, 161, 172 | 0 |
| 8 | 72 | 138/138 (100%) | 0.09 | 3 (2%) 62 41 | 98, 117, 133, 158 | 0 |
| 8 | 7E | 138/138 (100%) | 0.09 | 3 (2%) 62 41 | 101, 121, 136, 150 | 0 |
| 9 | 82 | 127/128 (99%) | 1.00 | 15 (11%) 9 5 | 111, 160, 187, 206 | 0 |
| 9 | 8E | 127/128 (99%) | 0.65 | 9 (7%) 22 12 | 104, 155, 177, 184 | 0 |
| 10 | 1A | 99/105 (94%) | 0.96 | 16 (16%) 4 2 | 121, 161, 193, 210 | 0 |
| 10 | 1I | 99/105 (94%) | 0.65 | 4 (4%) 42 23 | 105, 164, 206, 215 | 0 |
| 11 | 2A | 116/129 (89%) | 0.00 | 3 (2%) 57 36 | 81, 110, 134, 164 | 0 |
| 11 | 2I | 116/129 (89%) | 0.18 | 6 (5%) 33 17 | 79, 114, 153, 224 | 0 |
| 12 | 3A | 125/132 (94%) | 0.27 | 5 (4%) 42 23 | 86, 102, 141, 189 | 0 |
| 12 | 3I | 125/132 (94%) | -0.13 | 0 100 100 | 79, 92, 125, 247 | 0 |

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| Mol | Chain | Analysed | <RSRZ> | #RSRZ>2 | OWAB(Å$^2$) | Q<0.9 |
|---|---|---|---|---|---|---|
| 13 | 4A | 117/126 (92%) | 0.54 | 13 (11%) 10 5 | 122, 164, 193, 228 | 0 |
| 13 | 4I | 116/126 (92%) | 0.71 | 8 (6%) 23 12 | 117, 165, 186, 205 | 0 |
| 14 | 5A | 60/61 (98%) | 1.30 | 11 (18%) 3 1 | 131, 150, 178, 185 | 0 |
| 14 | 5I | 60/61 (98%) | 0.73 | 3 (5%) 34 18 | 112, 128, 148, 170 | 0 |
| 15 | 6A | 88/89 (98%) | -0.05 | 1 (1%) 78 59 | 84, 115, 134, 141 | 0 |
| 15 | 6I | 88/89 (98%) | 0.13 | 1 (1%) 78 59 | 92, 112, 133, 151 | 0 |
| 16 | 7A | 84/88 (95%) | 0.30 | 0 100 100 | 94, 108, 132, 195 | 0 |
| 16 | 7I | 84/88 (95%) | 0.79 | 9 (10%) 11 6 | 107, 127, 154, 194 | 0 |
| 17 | 8A | 100/105 (95%) | 0.03 | 2 (2%) 65 44 | 91, 108, 126, 176 | 0 |
| 17 | 8I | 100/105 (95%) | 0.26 | 2 (2%) 65 44 | 97, 119, 133, 142 | 0 |
| 18 | 9A | 72/88 (81%) | -0.17 | 0 100 100 | 91, 112, 166, 208 | 0 |
| 18 | 9I | 72/88 (81%) | -0.04 | 0 100 100 | 100, 121, 150, 227 | 0 |
| 19 | AA | 79/93 (84%) | 0.66 | 7 (8%) 15 8 | 144, 187, 220, 228 | 0 |
| 19 | AI | 83/93 (89%) | 0.56 | 7 (8%) 17 9 | 142, 168, 204, 221 | 0 |
| 20 | BA | 99/106 (93%) | 0.30 | 7 (7%) 22 12 | 86, 114, 153, 193 | 0 |
| 20 | BI | 99/106 (93%) | 0.63 | 7 (7%) 22 12 | 112, 138, 188, 193 | 0 |
| 21 | 1B | 25/27 (92%) | 1.85 | 11 (44%) 0 0 | 117, 140, 171, 190 | 0 |
| 21 | 1F | 25/27 (92%) | 1.12 | 5 (20%) 3 1 | 125, 139, 170, 187 | 0 |
| 22 | 2K | 75/85 (88%) | -0.14 | 0 100 100 | 74, 113, 195, 247 | 0 |
| 22 | 2L | 71/85 (83%) | -0.16 | 1 (1%) 73 53 | 73, 115, 176, 193 | 0 |
| 22 | 3K | 78/85 (91%) | -0.18 | 2 (2%) 57 36 | 85, 189, 296, 344 | 0 |
| 22 | 3L | 78/85 (91%) | -0.13 | 1 (1%) 75 56 | 79, 195, 286, 321 | 0 |
| 23 | 4K | 16/30 (53%) | 0.55 | 1 (6%) 26 14 | 82, 126, 168, 170 | 0 |
| 23 | 4L | 8/30 (26%) | 0.99 | 2 (25%) 2 1 | 93, 107, 190, 231 | 0 |
| 24 | 14 | 2909/2917 (99%) | -0.60 | 10 (0%) 90 80 | 53, 84, 260, 407 | 0 |
| 24 | 1H | 2912/2917 (99%) | -0.60 | 10 (0%) 90 80 | 48, 80, 247, 440 | 0 |
| 25 | 16 | 122/122 (100%) | -0.19 | 0 100 100 | 85, 118, 144, 247 | 0 |
| 25 | 1J | 122/122 (100%) | -0.17 | 2 (1%) 70 49 | 86, 123, 143, 217 | 0 |
| 26 | 71 | 135/229 (58%) | 0.52 | 7 (5%) 33 17 | 156, 219, 251, 258 | 0 |
| 26 | 79 | 135/229 (58%) | 0.48 | 7 (5%) 33 17 | 152, 228, 253, 265 | 0 |
| 27 | 11 | 272/276 (98%) | -0.33 | 2 (0%) 84 68 | 48, 69, 90, 122 | 0 |

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| Mol | Chain | Analysed | <RSRZ> | #RSRZ>2 | OWAB(Å$^2$) | Q<0.9 |
|---|---|---|---|---|---|---|
| 27 | 19 | 273/276 (98%) | -0.26 | 3 (1%) 78 59 | 50, 73, 91, 122 | 0 |
| 28 | 21 | 205/206 (99%) | 0.37 | 17 (8%) 17 9 | 54, 94, 152, 211 | 0 |
| 28 | 29 | 205/206 (99%) | 0.16 | 8 (3%) 43 24 | 57, 88, 164, 238 | 0 |
| 29 | 31 | 202/210 (96%) | -0.30 | 1 (0%) 87 73 | 47, 81, 123, 148 | 0 |
| 29 | 39 | 208/210 (99%) | 0.09 | 5 (2%) 59 38 | 60, 98, 174, 203 | 0 |
| 30 | 41 | 181/182 (99%) | 0.45 | 6 (3%) 49 29 | 123, 154, 197, 210 | 0 |
| 30 | 49 | 181/182 (99%) | 0.21 | 7 (3%) 43 24 | 120, 146, 190, 208 | 0 |
| 31 | 51 | 174/180 (96%) | 0.17 | 5 (2%) 53 32 | 90, 117, 139, 161 | 0 |
| 31 | 59 | 171/180 (95%) | 0.78 | 19 (11%) 10 5 | 141, 208, 248, 354 | 0 |
| 32 | 61 | 146/148 (98%) | 0.04 | 2 (1%) 73 53 | 84, 128, 153, 169 | 0 |
| 32 | 69 | 146/148 (98%) | 0.40 | 11 (7%) 20 11 | 81, 137, 164, 177 | 0 |
| 33 | 15 | 138/140 (98%) | 0.03 | 3 (2%) 62 41 | 72, 101, 142, 174 | 0 |
| 33 | 58 | 138/140 (98%) | 0.21 | 2 (1%) 73 53 | 73, 98, 154, 181 | 0 |
| 34 | 25 | 122/122 (100%) | -0.27 | 0 100 100 | 64, 82, 100, 110 | 0 |
| 34 | 68 | 122/122 (100%) | -0.37 | 0 100 100 | 58, 85, 103, 114 | 0 |
| 35 | 35 | 150/150 (100%) | 0.14 | 5 (3%) 49 29 | 61, 105, 144, 203 | 0 |
| 35 | 78 | 150/150 (100%) | 0.11 | 2 (1%) 75 56 | 55, 91, 117, 251 | 0 |
| 36 | 45 | 141/141 (100%) | 0.18 | 4 (2%) 55 34 | 67, 104, 131, 154 | 0 |
| 36 | 88 | 141/141 (100%) | 0.23 | 8 (5%) 29 16 | 64, 99, 134, 181 | 0 |
| 37 | 55 | 117/118 (99%) | -0.11 | 3 (2%) 57 36 | 62, 82, 99, 121 | 0 |
| 37 | 98 | 118/118 (100%) | -0.11 | 1 (0%) 82 65 | 68, 88, 107, 125 | 0 |
| 38 | 65 | 111/112 (99%) | 0.31 | 3 (2%) 56 35 | 93, 118, 148, 171 | 0 |
| 38 | A8 | 111/112 (99%) | 0.74 | 6 (5%) 31 17 | 97, 119, 163, 218 | 0 |
| 39 | 75 | 137/146 (93%) | 0.14 | 4 (2%) 53 32 | 75, 91, 161, 227 | 0 |
| 39 | B8 | 137/146 (93%) | 0.09 | 5 (3%) 46 26 | 84, 102, 165, 218 | 0 |
| 40 | 85 | 117/118 (99%) | -0.05 | 0 100 100 | 65, 95, 135, 167 | 0 |
| 40 | C8 | 117/118 (99%) | 0.13 | 3 (2%) 57 36 | 57, 83, 130, 183 | 0 |
| 41 | 95 | 101/101 (100%) | 0.32 | 9 (8%) 15 8 | 67, 124, 148, 194 | 0 |
| 41 | D8 | 101/101 (100%) | 0.22 | 2 (1%) 65 44 | 58, 106, 160, 237 | 0 |
| 42 | A5 | 113/113 (100%) | -0.36 | 0 100 100 | 63, 77, 110, 206 | 0 |
| 42 | E8 | 113/113 (100%) | -0.25 | 0 100 100 | 61, 77, 109, 231 | 0 |

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| Mol | Chain | Analysed | <RSRZ> | #RSRZ>2 | OWAB(Å$^2$) | Q<0.9 |
|---|---|---|---|---|---|---|
| 43 | B5 | 93/96 (96%) | -0.07 | 2 (2%) 62 41 | 73, 86, 119, 127 | 0 |
| 43 | F8 | 92/96 (95%) | -0.40 | 0 100 100 | 64, 74, 98, 112 | 0 |
| 44 | C5 | 104/110 (94%) | 0.72 | 6 (5%) 29 16 | 89, 130, 221, 252 | 0 |
| 44 | G8 | 104/110 (94%) | 0.44 | 15 (14%) 6 3 | 71, 96, 149, 186 | 0 |
| 45 | D5 | 179/206 (86%) | 0.45 | 10 (5%) 30 16 | 111, 160, 262, 335 | 0 |
| 45 | H8 | 175/206 (84%) | 0.39 | 5 (2%) 53 32 | 105, 160, 274, 301 | 0 |
| 46 | E5 | 77/85 (90%) | 0.16 | 3 (3%) 43 24 | 74, 89, 109, 178 | 0 |
| 46 | I8 | 83/85 (97%) | 0.42 | 5 (6%) 27 15 | 70, 90, 112, 158 | 0 |
| 47 | F5 | 97/98 (98%) | 0.27 | 7 (7%) 21 11 | 60, 83, 157, 204 | 0 |
| 47 | J8 | 97/98 (98%) | 0.24 | 8 (8%) 17 10 | 57, 82, 168, 218 | 0 |
| 48 | G5 | 69/72 (95%) | 0.18 | 2 (2%) 53 32 | 84, 109, 145, 187 | 0 |
| 48 | K8 | 66/72 (91%) | -0.13 | 3 (4%) 38 20 | 63, 82, 115, 177 | 0 |
| 49 | H5 | 59/60 (98%) | -0.05 | 0 100 100 | 79, 97, 156, 188 | 0 |
| 49 | L8 | 59/60 (98%) | -0.30 | 0 100 100 | 73, 91, 138, 151 | 0 |
| 50 | I5 | 63/71 (88%) | 0.38 | 2 (3%) 50 30 | 161, 233, 263, 283 | 0 |
| 50 | M8 | 66/71 (92%) | 0.48 | 2 (3%) 52 31 | 152, 233, 267, 285 | 0 |
| 51 | J5 | 59/60 (98%) | -0.07 | 2 (3%) 48 28 | 58, 87, 207, 244 | 0 |
| 51 | N8 | 59/60 (98%) | 0.23 | 1 (1%) 69 48 | 52, 92, 216, 240 | 0 |
| 52 | K5 | 45/54 (83%) | 2.69 | 24 (53%) 0 0 | 161, 210, 253, 272 | 0 |
| 52 | O8 | 45/54 (83%) | 1.06 | 7 (15%) 5 2 | 164, 213, 245, 256 | 0 |
| 53 | L5 | 49/49 (100%) | -0.18 | 1 (2%) 65 44 | 56, 61, 106, 147 | 0 |
| 53 | P8 | 47/49 (95%) | -0.40 | 1 (2%) 63 42 | 48, 54, 72, 121 | 0 |
| 54 | M5 | 62/65 (95%) | 0.32 | 6 (9%) 13 7 | 67, 77, 100, 127 | 0 |
| 54 | Q8 | 62/65 (95%) | 0.52 | 3 (4%) 35 19 | 62, 80, 108, 129 | 0 |
| All | All | 21209/22034 (96%) | -0.07 | 534 (2%) 58 37 | 47, 108, 216, 453 | 5 (0%) |

All (534) RSRZ outliers are listed below:

| Mol | Chain | Res | Type | RSRZ |
|---|---|---|---|---|
| 52 | K5 | 23 | THR | 9.5 |
| 9 | 82 | 115 | GLY | 8.9 |
| 52 | K5 | 13 | CYS | 8.8 |
| 52 | K5 | 22 | ALA | 8.6 |
| 7 | 62 | 81 | GLY | 7.2 |

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| Mol | Chain | Res | Type | RSRZ |
|---|---|---|---|---|
| 7 | 6E | 81 | GLY | 6.7 |
| 1 | 13 | 1492[A] | A | 6.6 |
| 47 | J8 | 98 | LEU | 6.6 |
| 38 | 65 | 20 | ARG | 6.0 |
| 52 | K5 | 42 | TRP | 5.6 |
| 9 | 82 | 128 | ARG | 5.5 |
| 31 | 59 | 131 | VAL | 5.3 |
| 24 | 1H | 2113 | U | 5.2 |
| 19 | AI | 2 | PRO | 5.1 |
| 21 | 1B | 13 | ILE | 5.1 |
| 39 | B8 | 1 | MET | 5.0 |
| 52 | K5 | 20 | ASN | 4.9 |
| 52 | O8 | 22 | ALA | 4.9 |
| 39 | B8 | 106 | SER | 4.9 |
| 14 | 5I | 2 | ALA | 4.9 |
| 19 | AA | 82 | GLY | 4.6 |
| 31 | 51 | 171 | LEU | 4.6 |
| 3 | 2E | 39 | ILE | 4.6 |
| 44 | C5 | 49 | VAL | 4.6 |
| 9 | 82 | 127 | LYS | 4.5 |
| 52 | O8 | 23 | THR | 4.4 |
| 13 | 4I | 102 | ARG | 4.4 |
| 40 | C8 | 118 | GLY | 4.4 |
| 9 | 82 | 116 | LYS | 4.3 |
| 13 | 4I | 97 | PRO | 4.3 |
| 8 | 72 | 1 | MET | 4.3 |
| 52 | K5 | 10 | LEU | 4.3 |
| 13 | 4A | 87 | TYR | 4.2 |
| 52 | K5 | 24 | GLU | 4.1 |
| 20 | BI | 12 | ALA | 4.1 |
| 52 | K5 | 14 | THR | 4.0 |
| 10 | 1A | 64 | GLU | 4.0 |
| 9 | 8E | 126 | SER | 4.0 |
| 9 | 8E | 118 | LYS | 4.0 |
| 21 | 1B | 26 | LYS | 4.0 |
| 7 | 6E | 32 | ARG | 3.9 |
| 53 | P8 | 46 | VAL | 3.8 |
| 52 | K5 | 39 | TYR | 3.8 |
| 26 | 79 | 174 | PRO | 3.8 |
| 28 | 21 | 51 | PHE | 3.8 |
| 47 | F5 | 96 | LYS | 3.8 |
| 36 | 88 | 139 | GLU | 3.8 |

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| Mol | Chain | Res | Type | RSRZ |
|---|---|---|---|---|
| 43 | B5 | 69 | TYR | 3.8 |
| 12 | 3A | 64 | TYR | 3.7 |
| 31 | 59 | 71 | LEU | 3.7 |
| 31 | 59 | 98 | LEU | 3.7 |
| 35 | 35 | 110 | TYR | 3.7 |
| 20 | BA | 83 | ARG | 3.7 |
| 52 | K5 | 53 | LYS | 3.7 |
| 1 | 1G | 1532 | U | 3.7 |
| 9 | 82 | 126 | SER | 3.7 |
| 10 | 1A | 67 | THR | 3.7 |
| 28 | 21 | 72 | VAL | 3.7 |
| 38 | 65 | 2 | ALA | 3.6 |
| 52 | K5 | 12 | GLU | 3.6 |
| 2 | 1E | 222 | ILE | 3.6 |
| 52 | K5 | 11 | LEU | 3.6 |
| 9 | 82 | 106 | ALA | 3.6 |
| 54 | M5 | 40 | GLU | 3.6 |
| 38 | A8 | 110 | LEU | 3.6 |
| 47 | J8 | 96 | LYS | 3.6 |
| 52 | K5 | 34 | LEU | 3.6 |
| 41 | 95 | 83 | ARG | 3.5 |
| 44 | C5 | 105 | ALA | 3.5 |
| 32 | 69 | 1 | MET | 3.5 |
| 15 | 6I | 71 | GLN | 3.5 |
| 31 | 59 | 89 | ILE | 3.5 |
| 9 | 82 | 44 | VAL | 3.5 |
| 13 | 4A | 100 | GLY | 3.5 |
| 28 | 21 | 205 | ALA | 3.5 |
| 27 | 19 | 274 | ARG | 3.5 |
| 28 | 21 | 90 | THR | 3.5 |
| 43 | B5 | 86 | GLY | 3.5 |
| 39 | 75 | 106 | SER | 3.5 |
| 52 | K5 | 38 | LYS | 3.4 |
| 17 | 8I | 26 | GLN | 3.4 |
| 47 | F5 | 98 | LEU | 3.4 |
| 36 | 45 | 140 | ALA | 3.4 |
| 31 | 59 | 172 | LYS | 3.4 |
| 32 | 69 | 20 | ASP | 3.4 |
| 32 | 69 | 38 | LEU | 3.4 |
| 14 | 5I | 25 | VAL | 3.4 |
| 26 | 79 | 173 | ALA | 3.4 |
| 32 | 69 | 16 | GLY | 3.3 |

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| Mol | Chain | Res | Type | RSRZ |
|---|---|---|---|---|
| 20 | BA | 25 | ARG | 3.3 |
| 7 | 62 | 80 | VAL | 3.3 |
| 52 | O8 | 9 | LEU | 3.3 |
| 31 | 59 | 72 | ILE | 3.3 |
| 24 | 1H | 2477 | C | 3.3 |
| 9 | 8E | 127 | LYS | 3.3 |
| 50 | M8 | 32 | TYR | 3.3 |
| 45 | H8 | 166 | SER | 3.3 |
| 14 | 5I | 26 | ARG | 3.3 |
| 1 | 1G | 1028(B) | C | 3.3 |
| 29 | 31 | 131 | GLY | 3.3 |
| 45 | D5 | 179 | ASP | 3.2 |
| 17 | 8I | 35 | VAL | 3.2 |
| 30 | 41 | 26 | GLN | 3.2 |
| 44 | G8 | 98 | VAL | 3.2 |
| 52 | K5 | 52 | VAL | 3.2 |
| 4 | 32 | 26 | CYS | 3.2 |
| 27 | 11 | 27 | THR | 3.2 |
| 52 | K5 | 43 | CYS | 3.2 |
| 28 | 21 | 52 | LEU | 3.2 |
| 4 | 3E | 138 | TYR | 3.2 |
| 28 | 29 | 151 | TYR | 3.2 |
| 52 | K5 | 48 | VAL | 3.2 |
| 8 | 72 | 131 | GLY | 3.2 |
| 50 | I5 | 42 | PHE | 3.2 |
| 28 | 21 | 187 | ALA | 3.2 |
| 33 | 58 | 68 | GLU | 3.1 |
| 39 | B8 | 104 | ASN | 3.1 |
| 21 | 1B | 23 | PRO | 3.1 |
| 53 | L5 | 49 | ARG | 3.1 |
| 47 | F5 | 77 | ALA | 3.1 |
| 13 | 4A | 88 | ARG | 3.1 |
| 8 | 7E | 88 | LYS | 3.1 |
| 19 | AA | 79 | THR | 3.1 |
| 31 | 59 | 171 | LEU | 3.1 |
| 21 | 1B | 14 | TRP | 3.1 |
| 26 | 79 | 68 | LEU | 3.1 |
| 28 | 21 | 63 | LEU | 3.1 |
| 16 | 7I | 41 | PRO | 3.1 |
| 32 | 69 | 36 | ALA | 3.1 |
| 45 | D5 | 173 | ALA | 3.1 |
| 30 | 41 | 3 | LEU | 3.1 |

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| Mol | Chain | Res | Type | RSRZ |
|---|---|---|---|---|
| 9 | 8E | 119 | ALA | 3.0 |
| 24 | 1H | 2167 | U | 3.0 |
| 16 | 7I | 39 | TYR | 3.0 |
| 4 | 3E | 9 | CYS | 3.0 |
| 44 | G8 | 106 | LEU | 3.0 |
| 14 | 5A | 2 | ALA | 3.0 |
| 13 | 4I | 2 | ALA | 3.0 |
| 9 | 82 | 75 | ASP | 3.0 |
| 10 | 1A | 55 | LYS | 3.0 |
| 4 | 3E | 31 | CYS | 3.0 |
| 44 | G8 | 89 | PHE | 3.0 |
| 31 | 59 | 148 | ILE | 3.0 |
| 10 | 1I | 66 | ARG | 3.0 |
| 21 | 1F | 10 | ARG | 3.0 |
| 1 | 13 | 877 | C | 3.0 |
| 23 | 4L | 18 | C | 3.0 |
| 40 | C8 | 117 | GLN | 3.0 |
| 4 | 32 | 9 | CYS | 3.0 |
| 10 | 1A | 47 | PHE | 3.0 |
| 26 | 71 | 174 | PRO | 2.9 |
| 36 | 88 | 10 | ARG | 2.9 |
| 32 | 69 | 34 | GLY | 2.9 |
| 46 | I8 | 3 | HIS | 2.9 |
| 47 | F5 | 84 | GLY | 2.9 |
| 2 | 12 | 115 | LEU | 2.9 |
| 39 | 75 | 104 | ASN | 2.9 |
| 52 | K5 | 21 | TYR | 2.9 |
| 19 | AA | 11 | VAL | 2.9 |
| 31 | 59 | 99 | VAL | 2.9 |
| 41 | D8 | 46 | VAL | 2.9 |
| 48 | K8 | 69 | ARG | 2.9 |
| 14 | 5A | 15 | LYS | 2.9 |
| 44 | G8 | 91 | GLU | 2.9 |
| 31 | 59 | 100 | GLY | 2.9 |
| 46 | I8 | 42 | GLY | 2.9 |
| 47 | J8 | 92 | LYS | 2.9 |
| 11 | 2I | 14 | VAL | 2.9 |
| 20 | BI | 62 | LEU | 2.9 |
| 24 | 1H | 2476 | A | 2.9 |
| 2 | 1E | 196 | LEU | 2.9 |
| 38 | A8 | 39 | ILE | 2.9 |
| 29 | 39 | 23 | ASP | 2.8 |

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| Mol | Chain | Res | Type | RSRZ |
|---|---|---|---|---|
| 29 | 39 | 131 | GLY | 2.8 |
| 28 | 21 | 75 | VAL | 2.8 |
| 28 | 21 | 71 | GLY | 2.8 |
| 21 | 1B | 6 | ARG | 2.8 |
| 10 | 1A | 49 | VAL | 2.8 |
| 15 | 6A | 89 | GLY | 2.8 |
| 24 | 14 | 2145 | C | 2.8 |
| 38 | A8 | 92 | TYR | 2.8 |
| 26 | 71 | 175 | VAL | 2.8 |
| 28 | 21 | 59 | VAL | 2.8 |
| 37 | 55 | 73 | VAL | 2.8 |
| 9 | 82 | 103 | THR | 2.8 |
| 11 | 2I | 42 | TRP | 2.8 |
| 19 | AA | 80 | TYR | 2.8 |
| 28 | 29 | 159 | HIS | 2.8 |
| 31 | 51 | 3 | ARG | 2.8 |
| 13 | 4A | 101 | GLN | 2.8 |
| 52 | O8 | 27 | LYS | 2.8 |
| 54 | M5 | 35 | GLN | 2.8 |
| 32 | 61 | 7 | GLU | 2.8 |
| 35 | 35 | 52 | GLU | 2.8 |
| 21 | 1B | 9 | ARG | 2.7 |
| 28 | 29 | 76 | ARG | 2.7 |
| 44 | G8 | 84 | ARG | 2.7 |
| 11 | 2I | 11 | LYS | 2.7 |
| 9 | 82 | 109 | VAL | 2.7 |
| 24 | 14 | 1026 | U | 2.7 |
| 46 | I8 | 7 | LEU | 2.7 |
| 10 | 1A | 54 | PHE | 2.7 |
| 13 | 4A | 8 | GLU | 2.7 |
| 13 | 4A | 4 | ILE | 2.7 |
| 44 | C5 | 29 | GLU | 2.7 |
| 21 | 1B | 15 | ARG | 2.7 |
| 2 | 12 | 101 | MET | 2.7 |
| 28 | 29 | 204 | ALA | 2.7 |
| 54 | Q8 | 63 | PRO | 2.7 |
| 1 | 1G | 1126 | U | 2.7 |
| 9 | 82 | 114 | TYR | 2.7 |
| 44 | G8 | 3 | VAL | 2.7 |
| 47 | J8 | 85 | LEU | 2.7 |
| 19 | AA | 83 | HIS | 2.7 |
| 8 | 7E | 92 | ARG | 2.6 |

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| Mol | Chain | Res | Type | RSRZ |
|---|---|---|---|---|
| 38 | A8 | 12 | PHE | 2.6 |
| 21 | 1F | 26 | LYS | 2.6 |
| 44 | G8 | 83 | THR | 2.6 |
| 52 | K5 | 9 | LEU | 2.6 |
| 16 | 7I | 68 | ASP | 2.6 |
| 10 | 1A | 46 | ARG | 2.6 |
| 28 | 21 | 79 | ARG | 2.6 |
| 4 | 32 | 2 | GLY | 2.6 |
| 31 | 59 | 105 | LEU | 2.6 |
| 13 | 4I | 9 | ILE | 2.6 |
| 19 | AA | 6 | LYS | 2.6 |
| 21 | 1B | 10 | ARG | 2.6 |
| 16 | 7I | 29 | ASP | 2.6 |
| 28 | 21 | 193 | GLY | 2.6 |
| 24 | 1H | 1026 | U | 2.6 |
| 45 | D5 | 144 | LEU | 2.6 |
| 28 | 29 | 150 | VAL | 2.6 |
| 52 | O8 | 42 | TRP | 2.6 |
| 9 | 82 | 9 | ARG | 2.6 |
| 14 | 5A | 58 | LYS | 2.6 |
| 9 | 8E | 117 | HIS | 2.6 |
| 50 | M8 | 63 | TYR | 2.6 |
| 2 | 12 | 70 | PHE | 2.6 |
| 6 | 5E | 89 | MET | 2.6 |
| 1 | 1G | 1400 | C | 2.6 |
| 10 | 1A | 65 | LEU | 2.6 |
| 52 | K5 | 36 | LEU | 2.6 |
| 4 | 32 | 198 | VAL | 2.6 |
| 11 | 2I | 12 | ARG | 2.6 |
| 4 | 32 | 31 | CYS | 2.6 |
| 1 | 1G | 975 | A | 2.6 |
| 29 | 39 | 133 | ASN | 2.6 |
| 3 | 2E | 91 | LEU | 2.6 |
| 4 | 3E | 32 | ALA | 2.6 |
| 2 | 12 | 68 | ILE | 2.5 |
| 2 | 12 | 127 | ILE | 2.5 |
| 52 | K5 | 40 | CYS | 2.5 |
| 3 | 22 | 170 | GLN | 2.5 |
| 26 | 79 | 11 | LEU | 2.5 |
| 21 | 1F | 3 | LYS | 2.5 |
| 1 | 13 | 1451 | A | 2.5 |
| 39 | 75 | 94 | ALA | 2.5 |

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| Mol | Chain | Res | Type | RSRZ |
|---|---|---|---|---|
| 38 | A8 | 35 | ILE | 2.5 |
| 10 | 1I | 47 | PHE | 2.5 |
| 11 | 2A | 25 | TYR | 2.5 |
| 26 | 71 | 173 | ALA | 2.5 |
| 27 | 11 | 30 | GLU | 2.5 |
| 30 | 49 | 35 | GLU | 2.5 |
| 16 | 7I | 13 | HIS | 2.5 |
| 37 | 98 | 21 | TYR | 2.5 |
| 19 | AI | 6 | LYS | 2.5 |
| 21 | 1F | 9 | ARG | 2.5 |
| 22 | 3L | 16 | C | 2.5 |
| 38 | A8 | 20 | ARG | 2.5 |
| 17 | 8A | 65 | ILE | 2.5 |
| 14 | 5A | 44 | LEU | 2.5 |
| 35 | 35 | 36 | LYS | 2.5 |
| 40 | C8 | 116 | ALA | 2.5 |
| 45 | D5 | 171 | ILE | 2.5 |
| 2 | 12 | 163 | PHE | 2.5 |
| 9 | 82 | 64 | THR | 2.5 |
| 17 | 8A | 7 | THR | 2.5 |
| 54 | M5 | 36 | LYS | 2.5 |
| 4 | 32 | 29 | PRO | 2.5 |
| 33 | 15 | 129 | PRO | 2.5 |
| 4 | 32 | 23 | GLY | 2.5 |
| 16 | 7I | 10 | GLY | 2.5 |
| 29 | 39 | 208 | GLY | 2.5 |
| 44 | G8 | 80 | GLY | 2.5 |
| 41 | 95 | 70 | ILE | 2.4 |
| 3 | 22 | 167 | TRP | 2.4 |
| 19 | AI | 13 | ASP | 2.4 |
| 30 | 49 | 160 | VAL | 2.4 |
| 32 | 69 | 37 | VAL | 2.4 |
| 36 | 45 | 100 | GLY | 2.4 |
| 44 | C5 | 98 | VAL | 2.4 |
| 32 | 69 | 83 | ALA | 2.4 |
| 36 | 88 | 141 | GLN | 2.4 |
| 48 | G5 | 4 | SER | 2.4 |
| 20 | BA | 74 | LYS | 2.4 |
| 26 | 79 | 192 | PHE | 2.4 |
| 20 | BA | 80 | ARG | 2.4 |
| 50 | I5 | 44 | THR | 2.4 |
| 46 | I8 | 73 | GLY | 2.4 |

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| Mol | Chain | Res | Type | RSRZ |
|---|---|---|---|---|
| 13 | 4A | 107 | ALA | 2.4 |
| 24 | 14 | 2146 | C | 2.4 |
| 1 | 13 | 631 | G | 2.4 |
| 19 | AA | 10 | PHE | 2.4 |
| 2 | 12 | 93 | VAL | 2.4 |
| 41 | 95 | 81 | TYR | 2.4 |
| 13 | 4A | 2 | ALA | 2.4 |
| 1 | 1G | 1286 | A | 2.4 |
| 2 | 12 | 146 | GLN | 2.4 |
| 9 | 8E | 40 | LEU | 2.4 |
| 22 | 2L | 48 | C | 2.4 |
| 24 | 1H | 34 | C | 2.4 |
| 32 | 61 | 12 | LEU | 2.4 |
| 35 | 78 | 106 | LEU | 2.4 |
| 2 | 12 | 150 | SER | 2.4 |
| 13 | 4A | 97 | PRO | 2.4 |
| 30 | 41 | 142 | PRO | 2.4 |
| 41 | 95 | 91 | TYR | 2.4 |
| 13 | 4A | 99 | ARG | 2.4 |
| 47 | F5 | 82 | LEU | 2.4 |
| 5 | 4E | 83 | GLU | 2.4 |
| 10 | 1A | 59 | SER | 2.4 |
| 32 | 69 | 21 | VAL | 2.4 |
| 33 | 15 | 46 | VAL | 2.4 |
| 44 | C5 | 77 | PRO | 2.4 |
| 13 | 4A | 103 | THR | 2.3 |
| 35 | 35 | 35 | HIS | 2.3 |
| 45 | H8 | 171 | ILE | 2.3 |
| 52 | O8 | 25 | LYS | 2.3 |
| 33 | 15 | 138 | LEU | 2.3 |
| 39 | 75 | 11 | GLU | 2.3 |
| 7 | 6E | 4 | ARG | 2.3 |
| 20 | BA | 76 | ALA | 2.3 |
| 28 | 21 | 77 | ILE | 2.3 |
| 24 | 1H | 2118 | U | 2.3 |
| 30 | 49 | 34 | LEU | 2.3 |
| 13 | 4I | 98 | VAL | 2.3 |
| 45 | H8 | 86 | VAL | 2.3 |
| 45 | D5 | 141 | VAL | 2.3 |
| 20 | BI | 21 | LYS | 2.3 |
| 14 | 5A | 14 | PRO | 2.3 |
| 31 | 59 | 126 | PRO | 2.3 |

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| Mol | Chain | Res | Type | RSRZ |
|---|---|---|---|---|
| 3 | 22 | 171 | GLY | 2.3 |
| 4 | 3E | 12 | CYS | 2.3 |
| 1 | 1G | 994 | A | 2.3 |
| 23 | 4L | 12 | A | 2.3 |
| 45 | D5 | 104 | PHE | 2.3 |
| 39 | B8 | 11 | GLU | 2.3 |
| 1 | 13 | 1066 | C | 2.3 |
| 30 | 49 | 75 | LYS | 2.3 |
| 32 | 69 | 2 | LYS | 2.3 |
| 11 | 2I | 91 | ARG | 2.3 |
| 16 | 7I | 42 | ARG | 2.3 |
| 14 | 5A | 55 | GLY | 2.3 |
| 10 | 1A | 42 | THR | 2.3 |
| 10 | 1I | 40 | LEU | 2.3 |
| 44 | G8 | 90 | LEU | 2.3 |
| 11 | 2I | 25 | TYR | 2.3 |
| 12 | 3A | 28 | LYS | 2.3 |
| 52 | K5 | 25 | LYS | 2.3 |
| 4 | 32 | 34 | GLU | 2.3 |
| 7 | 6E | 80 | VAL | 2.3 |
| 14 | 5A | 26 | ARG | 2.3 |
| 16 | 7I | 25 | ARG | 2.3 |
| 31 | 59 | 97 | ARG | 2.3 |
| 54 | M5 | 63 | PRO | 2.3 |
| 47 | J8 | 84 | GLY | 2.3 |
| 22 | 3K | 19 | C | 2.3 |
| 51 | J5 | 58 | LEU | 2.3 |
| 2 | 1E | 55 | PHE | 2.3 |
| 36 | 45 | 141 | GLN | 2.3 |
| 41 | 95 | 80 | GLN | 2.3 |
| 44 | G8 | 4 | LYS | 2.3 |
| 20 | BI | 57 | ARG | 2.3 |
| 46 | E5 | 71 | ASP | 2.3 |
| 1 | 13 | 933 | G | 2.2 |
| 24 | 1H | 2112 | G | 2.2 |
| 45 | D5 | 120 | ILE | 2.2 |
| 24 | 14 | 3 | U | 2.2 |
| 24 | 14 | 2799 | A | 2.2 |
| 48 | K8 | 4 | SER | 2.2 |
| 14 | 5A | 3 | ARG | 2.2 |
| 4 | 3E | 26 | CYS | 2.2 |
| 44 | G8 | 102 | CYS | 2.2 |

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| Mol | Chain | Res | Type | RSRZ |
|---|---|---|---|---|
| 9 | 8E | 115 | GLY | 2.2 |
| 10 | 1I | 10 | GLY | 2.2 |
| 10 | 1A | 90 | LEU | 2.2 |
| 13 | 4I | 96 | LEU | 2.2 |
| 26 | 79 | 209 | LEU | 2.2 |
| 28 | 21 | 195 | LEU | 2.2 |
| 47 | J8 | 94 | LEU | 2.2 |
| 9 | 82 | 33 | PHE | 2.2 |
| 10 | 1A | 68 | HIS | 2.2 |
| 35 | 78 | 36 | LYS | 2.2 |
| 51 | N8 | 26 | THR | 2.2 |
| 24 | 1H | 1406 | U | 2.2 |
| 29 | 39 | 72 | ARG | 2.2 |
| 24 | 14 | 4 | C | 2.2 |
| 13 | 4I | 6 | GLY | 2.2 |
| 47 | J8 | 77 | ALA | 2.2 |
| 47 | F5 | 85 | LEU | 2.2 |
| 41 | 95 | 76 | LYS | 2.2 |
| 19 | AI | 3 | ARG | 2.2 |
| 41 | D8 | 45 | THR | 2.2 |
| 14 | 5A | 34 | TYR | 2.2 |
| 46 | E5 | 9 | SER | 2.2 |
| 1 | 1G | 950 | U | 2.2 |
| 45 | D5 | 118 | GLN | 2.2 |
| 3 | 22 | 124 | ILE | 2.2 |
| 1 | 1G | 965 | A | 2.2 |
| 1 | 1G | 1224 | G | 2.2 |
| 23 | 4K | 19 | A | 2.2 |
| 47 | F5 | 80 | LEU | 2.2 |
| 52 | K5 | 51 | GLU | 2.2 |
| 10 | 1A | 41 | PRO | 2.2 |
| 20 | BI | 76 | ALA | 2.2 |
| 7 | 62 | 33 | ASP | 2.2 |
| 21 | 1F | 25 | LYS | 2.2 |
| 30 | 49 | 36 | LYS | 2.2 |
| 5 | 42 | 126 | ARG | 2.2 |
| 13 | 4A | 94 | ARG | 2.2 |
| 45 | H8 | 79 | ARG | 2.2 |
| 10 | 1A | 92 | THR | 2.2 |
| 54 | M5 | 31 | HIS | 2.2 |
| 39 | B8 | 100 | TYR | 2.2 |
| 5 | 42 | 20 | GLN | 2.2 |

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| Mol | Chain | Res | Type | RSRZ |
|---|---|---|---|---|
| 41 | 95 | 73 | SER | 2.2 |
| 30 | 49 | 82 | LEU | 2.2 |
| 52 | O8 | 10 | LEU | 2.2 |
| 4 | 32 | 30 | LYS | 2.2 |
| 26 | 71 | 25 | ALA | 2.2 |
| 8 | 72 | 90 | GLY | 2.2 |
| 27 | 19 | 38 | LYS | 2.2 |
| 30 | 41 | 2 | PRO | 2.2 |
| 31 | 59 | 5 | GLY | 2.2 |
| 41 | 95 | 36 | PRO | 2.2 |
| 48 | G5 | 8 | LYS | 2.2 |
| 36 | 45 | 104 | PHE | 2.2 |
| 13 | 4I | 117 | VAL | 2.1 |
| 31 | 59 | 52 | VAL | 2.1 |
| 51 | J5 | 60 | VAL | 2.1 |
| 2 | 1E | 238 | LEU | 2.1 |
| 47 | J8 | 97 | LEU | 2.1 |
| 31 | 59 | 96 | ALA | 2.1 |
| 21 | 1B | 4 | GLY | 2.1 |
| 31 | 51 | 170 | ARG | 2.1 |
| 24 | 14 | 2897 | U | 2.1 |
| 31 | 59 | 129 | THR | 2.1 |
| 33 | 58 | 93 | THR | 2.1 |
| 36 | 88 | 87 | LYS | 2.1 |
| 1 | 13 | 1386 | G | 2.1 |
| 1 | 1G | 973 | G | 2.1 |
| 9 | 8E | 9 | ARG | 2.1 |
| 28 | 21 | 76 | ARG | 2.1 |
| 44 | G8 | 86 | ARG | 2.1 |
| 45 | H8 | 172 | ALA | 2.1 |
| 28 | 21 | 32 | PRO | 2.1 |
| 31 | 59 | 93 | GLY | 2.1 |
| 45 | D5 | 115 | GLY | 2.1 |
| 46 | E5 | 22 | GLY | 2.1 |
| 25 | 1J | 6 | C | 2.1 |
| 44 | G8 | 92 | ASN | 2.1 |
| 44 | C5 | 92 | ASN | 2.1 |
| 10 | 1A | 50 | ILE | 2.1 |
| 11 | 2A | 123 | LYS | 2.1 |
| 16 | 7I | 17 | TYR | 2.1 |
| 26 | 71 | 28 | LEU | 2.1 |
| 54 | M5 | 57 | ARG | 2.1 |

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| Mol | Chain | Res | Type | RSRZ |
|---|---|---|---|---|
| 3 | 2E | 37 | GLN | 2.1 |
| 19 | AI | 84 | GLY | 2.1 |
| 31 | 51 | 5 | GLY | 2.1 |
| 2 | 12 | 71 | VAL | 2.1 |
| 24 | 14 | 2802 | G | 2.1 |
| 24 | 14 | 2899 | G | 2.1 |
| 25 | 1J | 117 | G | 2.1 |
| 26 | 71 | 43 | VAL | 2.1 |
| 24 | 14 | 2402 | C | 2.1 |
| 28 | 29 | 203 | LYS | 2.1 |
| 44 | G8 | 94 | LYS | 2.1 |
| 30 | 41 | 82 | LEU | 2.1 |
| 37 | 55 | 18 | LEU | 2.1 |
| 7 | 6E | 78 | ARG | 2.1 |
| 26 | 79 | 34 | THR | 2.1 |
| 30 | 41 | 25 | TYR | 2.1 |
| 54 | Q8 | 55 | ALA | 2.1 |
| 19 | AI | 56 | GLN | 2.1 |
| 46 | I8 | 40 | GLN | 2.1 |
| 12 | 3A | 16 | GLU | 2.1 |
| 45 | D5 | 139 | VAL | 2.1 |
| 31 | 51 | 175 | LYS | 2.1 |
| 9 | 82 | 102 | LEU | 2.1 |
| 26 | 71 | 171 | ILE | 2.1 |
| 54 | Q8 | 58 | ILE | 2.1 |
| 30 | 49 | 161 | THR | 2.1 |
| 1 | 13 | 108 | G | 2.1 |
| 1 | 1G | 1029 | G | 2.1 |
| 44 | G8 | 105 | ALA | 2.1 |
| 9 | 8E | 87 | GLN | 2.1 |
| 3 | 22 | 186 | PHE | 2.1 |
| 28 | 21 | 73 | GLU | 2.1 |
| 35 | 35 | 74 | GLU | 2.1 |
| 1 | 1G | 82 | U | 2.0 |
| 14 | 5A | 25 | VAL | 2.0 |
| 20 | BA | 14 | LYS | 2.0 |
| 21 | 1B | 3 | LYS | 2.0 |
| 28 | 29 | 7 | VAL | 2.0 |
| 28 | 29 | 59 | VAL | 2.0 |
| 20 | BI | 11 | SER | 2.0 |
| 12 | 3A | 19 | ARG | 2.0 |
| 20 | BA | 26 | ASN | 2.0 |

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| Mol | Chain | Res | Type | RSRZ |
|---|---|---|---|---|
| 38 | 65 | 17 | ARG | 2.0 |
| 1 | 13 | 1350 | A | 2.0 |
| 11 | 2A | 87 | THR | 2.0 |
| 20 | BI | 59 | ALA | 2.0 |
| 24 | 1H | 1536 | A | 2.0 |
| 36 | 88 | 91 | GLU | 2.0 |
| 48 | K8 | 66 | GLU | 2.0 |
| 36 | 88 | 90 | VAL | 2.0 |
| 36 | 88 | 106 | VAL | 2.0 |
| 19 | AI | 5 | LEU | 2.0 |
| 22 | 3K | 18 | G | 2.0 |
| 36 | 88 | 60 | ARG | 2.0 |
| 27 | 19 | 64 | ILE | 2.0 |
| 31 | 59 | 165 | ALA | 2.0 |
| 37 | 55 | 69 | ASP | 2.0 |
| 8 | 7E | 131 | GLY | 2.0 |
| 13 | 4A | 6 | GLY | 2.0 |
| 41 | 95 | 41 | GLY | 2.0 |
| 12 | 3A | 47 | LYS | 2.0 |
| 52 | K5 | 41 | PRO | 2.0 |
| 21 | 1B | 22 | ARG | 2.0 |
| 32 | 69 | 33 | ARG | 2.0 |
| 14 | 5A | 39 | LEU | 2.0 |
| 10 | 1A | 38 | ILE | 2.0 |
| 1 | 13 | 88 | C | 2.0 |

## 6.2 Non-standard residues in protein, DNA, RNA chains (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 |
|---|---|---|---|---|---|---|---|---|
| 22 | PSU | 2L | 64 | 20/21 | 0.66 | 0.10 | 138,148,163,166 | 0 |
| 22 | PSU | 3K | 64 | 20/21 | 0.68 | 0.12 | 182,190,202,202 | 0 |
| 22 | PSU | 3L | 64 | 20/21 | 0.68 | 0.12 | 180,200,211,213 | 0 |
| 22 | 5MU | 3K | 63 | 21/22 | 0.72 | 0.09 | 176,183,187,190 | 0 |
| 22 | 5MU | 3L | 63 | 21/22 | 0.77 | 0.11 | 174,186,190,192 | 0 |
| 22 | OMG | 2K | 17 | 24/25 | 0.79 | 0.10 | 142,148,151,151 | 0 |
| 22 | OMG | 2L | 17 | 24/25 | 0.81 | 0.10 | 136,152,154,155 | 0 |
| 22 | 4SU | 3L | 8 | 20/21 | 0.82 | 0.11 | 184,194,207,207 | 0 |

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| Mol | Type | Chain | Res | Atoms | RSCC | RSR | B-factors(Å$^2$) | Q<0.9 |
|---|---|---|---|---|---|---|---|---|
| 22 | PSU | 2K | 64 | 20/21 | 0.83 | 0.10 | 133,144,150,155 | 0 |
| 22 | 5MU | 2K | 63 | 21/22 | 0.83 | 0.10 | 135,139,149,156 | 0 |
| 22 | OMG | 3K | 17 | 24/25 | 0.84 | 0.12 | 194,212,234,239 | 0 |
| 22 | 5MU | 2L | 63 | 21/22 | 0.84 | 0.10 | 141,149,156,167 | 0 |
| 22 | 4SU | 3K | 8 | 20/21 | 0.85 | 0.07 | 186,202,212,214 | 0 |
| 22 | 4SU | 2K | 8 | 20/21 | 0.87 | 0.09 | 106,112,119,121 | 0 |
| 22 | OMG | 3L | 17 | 24/25 | 0.87 | 0.14 | 200,216,227,230 | 0 |
| 22 | 4SU | 2L | 8 | 20/21 | 0.88 | 0.10 | 112,122,128,139 | 0 |
| 22 | PSU | 3K | 40 | 20/21 | 0.90 | 0.07 | 118,124,129,130 | 0 |
| 22 | QUO | 3L | 35 | 32/33 | 0.91 | 0.12 | 105,114,128,132 | 0 |
| 22 | PSU | 3L | 40 | 20/21 | 0.91 | 0.10 | 107,122,124,127 | 0 |
| 22 | QUO | 2K | 35 | 32/33 | 0.92 | 0.15 | 84,96,115,117 | 6 |
| 22 | QUO | 3K | 35 | 32/33 | 0.93 | 0.13 | 108,114,124,127 | 0 |
| 22 | MIA | 3K | 38 | 29/30 | 0.94 | 0.10 | 114,122,132,135 | 0 |
| 22 | MIA | 3L | 38 | 29/30 | 0.94 | 0.10 | 118,123,131,133 | 0 |
| 22 | MIA | 2K | 38 | 29/30 | 0.94 | 0.10 | 82,94,106,112 | 0 |
| 22 | QUO | 2L | 35 | 32/33 | 0.94 | 0.16 | 91,112,118,124 | 0 |
| 22 | PSU | 2L | 40 | 20/21 | 0.94 | 0.13 | 89,100,105,105 | 0 |
| 22 | MIA | 2L | 38 | 29/30 | 0.96 | 0.10 | 92,101,113,119 | 0 |
| 22 | PSU | 2K | 40 | 20/21 | 0.97 | 0.07 | 83,91,99,105 | 0 |

## 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 |
|---|---|---|---|---|---|---|---|---|
| 55 | MG | 1H | 3360 | 1/1 | -0.08 | 0.43 | 167,167,167,167 | 0 |
| 55 | MG | 1G | 1691 | 1/1 | -0.03 | 0.40 | 132,132,132,132 | 0 |
| 55 | MG | 13 | 1703 | 1/1 | 0.10 | 0.39 | 147,147,147,147 | 0 |
| 55 | MG | 13 | 1712 | 1/1 | 0.30 | 0.28 | 123,123,123,123 | 0 |
| 55 | MG | 14 | 3356 | 1/1 | 0.31 | 0.20 | 195,195,195,195 | 0 |
| 55 | MG | 14 | 3331 | 1/1 | 0.32 | 0.25 | 138,138,138,138 | 0 |
| 55 | MG | 1G | 1708 | 1/1 | 0.32 | 0.30 | 133,133,133,133 | 0 |
| 55 | MG | 1G | 1704 | 1/1 | 0.35 | 0.29 | 117,117,117,117 | 0 |

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| Mol | Type | Chain | Res | Atoms | RSCC | RSR | B-factors(Å$^2$) | Q<0.9 |
|---|---|---|---|---|---|---|---|---|
| 55 | MG | 14 | 3354 | 1/1 | 0.36 | 0.28 | 134,134,134,134 | 0 |
| 55 | MG | 14 | 3113 | 1/1 | 0.39 | 0.36 | 97,97,97,97 | 0 |
| 55 | MG | 13 | 1656 | 1/1 | 0.39 | 0.34 | 120,120,120,120 | 0 |
| 55 | MG | 1G | 1692 | 1/1 | 0.39 | 0.39 | 120,120,120,120 | 0 |
| 55 | MG | 1G | 1721 | 1/1 | 0.39 | 0.44 | 129,129,129,129 | 0 |
| 55 | MG | 2K | 101 | 1/1 | 0.41 | 0.27 | 118,118,118,118 | 0 |
| 55 | MG | 1G | 1726 | 1/1 | 0.41 | 0.38 | 124,124,124,124 | 0 |
| 55 | MG | 1G | 1719 | 1/1 | 0.41 | 0.33 | 104,104,104,104 | 0 |
| 55 | MG | 3E | 301 | 1/1 | 0.43 | 0.14 | 156,156,156,156 | 0 |
| 55 | MG | 1H | 3385 | 1/1 | 0.45 | 0.30 | 97,97,97,97 | 0 |
| 55 | MG | 13 | 1702 | 1/1 | 0.45 | 0.36 | 147,147,147,147 | 0 |
| 55 | MG | 13 | 1692 | 1/1 | 0.45 | 0.45 | 132,132,132,132 | 0 |
| 55 | MG | 13 | 1689 | 1/1 | 0.46 | 0.49 | 116,116,116,116 | 0 |
| 55 | MG | 14 | 3299 | 1/1 | 0.48 | 0.37 | 100,100,100,100 | 0 |
| 55 | MG | 16 | 208 | 1/1 | 0.48 | 0.25 | 113,113,113,113 | 0 |
| 55 | MG | 13 | 1617 | 1/1 | 0.51 | 0.33 | 122,122,122,122 | 0 |
| 55 | MG | 1H | 3396 | 1/1 | 0.52 | 0.32 | 104,104,104,104 | 0 |
| 55 | MG | 13 | 1624 | 1/1 | 0.53 | 0.41 | 107,107,107,107 | 0 |
| 55 | MG | 1G | 1718 | 1/1 | 0.54 | 0.35 | 118,118,118,118 | 0 |
| 55 | MG | 13 | 1695 | 1/1 | 0.54 | 0.28 | 90,90,90,90 | 0 |
| 55 | MG | 1H | 3346 | 1/1 | 0.54 | 0.30 | 113,113,113,113 | 0 |
| 55 | MG | 1H | 3301 | 1/1 | 0.55 | 0.36 | 79,79,79,79 | 0 |
| 55 | MG | 1H | 3379 | 1/1 | 0.55 | 0.15 | 245,245,245,245 | 0 |
| 55 | MG | 13 | 1714 | 1/1 | 0.55 | 0.59 | 117,117,117,117 | 0 |
| 55 | MG | 1H | 3221 | 1/1 | 0.56 | 0.32 | 108,108,108,108 | 0 |
| 55 | MG | 1G | 1694 | 1/1 | 0.56 | 0.28 | 118,118,118,118 | 0 |
| 55 | MG | 1H | 3384 | 1/1 | 0.56 | 0.35 | 108,108,108,108 | 0 |
| 55 | MG | 13 | 1708 | 1/1 | 0.56 | 0.45 | 127,127,127,127 | 0 |
| 55 | MG | 4A | 201 | 1/1 | 0.56 | 0.46 | 115,115,115,115 | 0 |
| 55 | MG | 1H | 3330 | 1/1 | 0.57 | 0.32 | 90,90,90,90 | 0 |
| 55 | MG | 14 | 3186 | 1/1 | 0.57 | 0.31 | 113,113,113,113 | 0 |
| 55 | MG | 13 | 1611 | 1/1 | 0.57 | 0.24 | 83,83,83,83 | 0 |
| 55 | MG | 13 | 1672 | 1/1 | 0.58 | 0.22 | 119,119,119,119 | 0 |
| 55 | MG | 13 | 1644 | 1/1 | 0.59 | 0.37 | 116,116,116,116 | 0 |
| 55 | MG | 1H | 3343 | 1/1 | 0.59 | 0.19 | 90,90,90,90 | 0 |
| 55 | MG | 1H | 3121 | 1/1 | 0.59 | 0.36 | 98,98,98,98 | 0 |
| 55 | MG | 1G | 1685 | 1/1 | 0.59 | 0.36 | 116,116,116,116 | 0 |
| 55 | MG | 14 | 3329 | 1/1 | 0.60 | 0.24 | 101,101,101,101 | 0 |
| 55 | MG | 16 | 211 | 1/1 | 0.61 | 0.23 | 98,98,98,98 | 0 |
| 55 | MG | 16 | 213 | 1/1 | 0.61 | 0.26 | 113,113,113,113 | 0 |
| 55 | MG | 1H | 3364 | 1/1 | 0.61 | 0.23 | 103,103,103,103 | 0 |
| 55 | MG | 1H | 3361 | 1/1 | 0.61 | 0.20 | 155,155,155,155 | 0 |

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| Mol | Type | Chain | Res | Atoms | RSCC | RSR | B-factors(Å$^2$) | Q<0.9 |
|---|---|---|---|---|---|---|---|---|
| 55 | MG | 1H | 3162 | 1/1 | 0.62 | 0.28 | 94,94,94,94 | 0 |
| 55 | MG | 1G | 1667 | 1/1 | 0.62 | 0.27 | 103,103,103,103 | 0 |
| 55 | MG | 1H | 3283 | 1/1 | 0.63 | 0.32 | 104,104,104,104 | 0 |
| 55 | MG | 13 | 1674 | 1/1 | 0.63 | 0.23 | 106,106,106,106 | 0 |
| 55 | MG | 13 | 1688 | 1/1 | 0.64 | 0.49 | 91,91,91,91 | 0 |
| 55 | MG | 1H | 3226 | 1/1 | 0.64 | 0.20 | 114,114,114,114 | 0 |
| 55 | MG | 14 | 3287 | 1/1 | 0.65 | 0.45 | 98,98,98,98 | 0 |
| 55 | MG | 1G | 1703 | 1/1 | 0.65 | 0.38 | 99,99,99,99 | 0 |
| 55 | MG | 1H | 3186 | 1/1 | 0.65 | 0.23 | 70,70,70,70 | 0 |
| 55 | MG | 2L | 102 | 1/1 | 0.65 | 0.38 | 102,102,102,102 | 0 |
| 55 | MG | 1H | 3240 | 1/1 | 0.65 | 0.28 | 92,92,92,92 | 0 |
| 55 | MG | 1G | 1724 | 1/1 | 0.65 | 0.23 | 99,99,99,99 | 0 |
| 55 | MG | 1H | 3194 | 1/1 | 0.66 | 0.35 | 68,68,68,68 | 0 |
| 55 | MG | 14 | 3324 | 1/1 | 0.66 | 0.45 | 101,101,101,101 | 0 |
| 55 | MG | 1H | 3220 | 1/1 | 0.66 | 0.32 | 92,92,92,92 | 0 |
| 55 | MG | 13 | 1658 | 1/1 | 0.66 | 0.27 | 108,108,108,108 | 0 |
| 55 | MG | 1H | 3307 | 1/1 | 0.66 | 0.19 | 83,83,83,83 | 0 |
| 55 | MG | 13 | 1681 | 1/1 | 0.66 | 0.43 | 104,104,104,104 | 0 |
| 55 | MG | 14 | 3373 | 1/1 | 0.66 | 0.24 | 98,98,98,98 | 0 |
| 55 | MG | 14 | 3328 | 1/1 | 0.67 | 0.31 | 115,115,115,115 | 0 |
| 55 | MG | 13 | 1678 | 1/1 | 0.67 | 0.35 | 104,104,104,104 | 0 |
| 55 | MG | 1H | 3203 | 1/1 | 0.67 | 0.44 | 99,99,99,99 | 0 |
| 55 | MG | 1H | 3205 | 1/1 | 0.68 | 0.36 | 103,103,103,103 | 0 |
| 55 | MG | 14 | 3325 | 1/1 | 0.68 | 0.34 | 78,78,78,78 | 0 |
| 55 | MG | 13 | 1673 | 1/1 | 0.68 | 0.27 | 109,109,109,109 | 0 |
| 55 | MG | 32 | 301 | 1/1 | 0.68 | 0.39 | 113,113,113,113 | 0 |
| 55 | MG | 14 | 3300 | 1/1 | 0.69 | 0.20 | 83,83,83,83 | 0 |
| 55 | MG | 1H | 3076 | 1/1 | 0.69 | 0.28 | 77,77,77,77 | 0 |
| 55 | MG | 1H | 3282 | 1/1 | 0.69 | 0.35 | 90,90,90,90 | 0 |
| 55 | MG | 1H | 3043 | 1/1 | 0.69 | 0.29 | 92,92,92,92 | 0 |
| 55 | MG | 1G | 1664 | 1/1 | 0.69 | 0.33 | 104,104,104,104 | 0 |
| 55 | MG | 14 | 3132 | 1/1 | 0.69 | 0.29 | 120,120,120,120 | 0 |
| 55 | MG | 1H | 3398 | 1/1 | 0.69 | 0.20 | 106,106,106,106 | 0 |
| 55 | MG | 1G | 1674 | 1/1 | 0.69 | 0.41 | 111,111,111,111 | 0 |
| 55 | MG | 1G | 1727 | 1/1 | 0.69 | 0.65 | 104,104,104,104 | 0 |
| 55 | MG | 1J | 205 | 1/1 | 0.69 | 0.29 | 122,122,122,122 | 0 |
| 56 | ZN | G8 | 202 | 1/1 | 0.69 | 0.22 | 203,203,203,203 | 0 |
| 55 | MG | 13 | 1700 | 1/1 | 0.70 | 0.47 | 97,97,97,97 | 0 |
| 55 | MG | 1H | 3325 | 1/1 | 0.70 | 0.41 | 97,97,97,97 | 0 |
| 55 | MG | 14 | 3224 | 1/1 | 0.70 | 0.25 | 112,112,112,112 | 0 |
| 55 | MG | 14 | 3357 | 1/1 | 0.70 | 0.22 | 76,76,76,76 | 0 |
| 55 | MG | 14 | 3261 | 1/1 | 0.70 | 0.40 | 105,105,105,105 | 0 |

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| Mol | Type | Chain | Res | Atoms | RSCC | RSR | B-factors(Å$^2$) | Q<0.9 |
|---|---|---|---|---|---|---|---|---|
| 55 | MG | 1H | 3131 | 1/1 | 0.70 | 0.28 | 75,75,75,75 | 0 |
| 55 | MG | 14 | 3296 | 1/1 | 0.70 | 0.27 | 97,97,97,97 | 0 |
| 55 | MG | 4K | 101 | 1/1 | 0.71 | 0.21 | 111,111,111,111 | 0 |
| 55 | MG | 14 | 3119 | 1/1 | 0.71 | 0.46 | 70,70,70,70 | 0 |
| 55 | MG | 14 | 3302 | 1/1 | 0.71 | 0.23 | 91,91,91,91 | 0 |
| 55 | MG | 14 | 3267 | 1/1 | 0.71 | 0.20 | 90,90,90,90 | 0 |
| 55 | MG | 14 | 3286 | 1/1 | 0.71 | 0.32 | 100,100,100,100 | 0 |
| 55 | MG | 1G | 1649 | 1/1 | 0.71 | 0.37 | 93,93,93,93 | 0 |
| 55 | MG | 13 | 1613 | 1/1 | 0.71 | 0.30 | 99,99,99,99 | 0 |
| 55 | MG | 14 | 3171 | 1/1 | 0.72 | 0.32 | 86,86,86,86 | 0 |
| 55 | MG | 1H | 3363 | 1/1 | 0.72 | 0.26 | 104,104,104,104 | 0 |
| 55 | MG | 16 | 204 | 1/1 | 0.72 | 0.28 | 99,99,99,99 | 0 |
| 55 | MG | 14 | 3025 | 1/1 | 0.72 | 0.34 | 86,86,86,86 | 0 |
| 55 | MG | 14 | 3318 | 1/1 | 0.72 | 0.19 | 80,80,80,80 | 0 |
| 55 | MG | 1G | 1653 | 1/1 | 0.72 | 0.39 | 103,103,103,103 | 0 |
| 55 | MG | 1H | 3209 | 1/1 | 0.72 | 0.42 | 99,99,99,99 | 0 |
| 55 | MG | 1H | 3312 | 1/1 | 0.72 | 0.23 | 81,81,81,81 | 0 |
| 55 | MG | 13 | 1659 | 1/1 | 0.73 | 0.29 | 102,102,102,102 | 0 |
| 55 | MG | 13 | 1616 | 1/1 | 0.73 | 0.24 | 141,141,141,141 | 0 |
| 55 | MG | 13 | 1701 | 1/1 | 0.73 | 0.22 | 100,100,100,100 | 0 |
| 55 | MG | 13 | 1621 | 1/1 | 0.73 | 0.30 | 87,87,87,87 | 0 |
| 55 | MG | 14 | 3353 | 1/1 | 0.73 | 0.21 | 84,84,84,84 | 0 |
| 55 | MG | 1G | 1699 | 1/1 | 0.73 | 0.31 | 101,101,101,101 | 0 |
| 55 | MG | 14 | 3169 | 1/1 | 0.73 | 0.40 | 100,100,100,100 | 0 |
| 55 | MG | 1H | 3164 | 1/1 | 0.73 | 0.36 | 90,90,90,90 | 0 |
| 55 | MG | 1H | 3167 | 1/1 | 0.73 | 0.21 | 66,66,66,66 | 0 |
| 55 | MG | 14 | 3218 | 1/1 | 0.73 | 0.26 | 88,88,88,88 | 0 |
| 55 | MG | 1G | 1678 | 1/1 | 0.73 | 0.36 | 102,102,102,102 | 0 |
| 55 | MG | 1H | 3138 | 1/1 | 0.74 | 0.34 | 87,87,87,87 | 0 |
| 55 | MG | 14 | 3304 | 1/1 | 0.74 | 0.40 | 99,99,99,99 | 0 |
| 55 | MG | 14 | 3314 | 1/1 | 0.74 | 0.40 | 105,105,105,105 | 0 |
| 55 | MG | 1G | 1643 | 1/1 | 0.74 | 0.28 | 106,106,106,106 | 0 |
| 55 | MG | 14 | 3323 | 1/1 | 0.74 | 0.20 | 87,87,87,87 | 0 |
| 55 | MG | 1G | 1693 | 1/1 | 0.74 | 0.30 | 95,95,95,95 | 0 |
| 55 | MG | 2K | 103 | 1/1 | 0.74 | 0.30 | 94,94,94,94 | 0 |
| 55 | MG | 1H | 3252 | 1/1 | 0.74 | 0.25 | 98,98,98,98 | 0 |
| 55 | MG | 1H | 3163 | 1/1 | 0.74 | 0.33 | 82,82,82,82 | 0 |
| 55 | MG | 13 | 1663 | 1/1 | 0.74 | 0.32 | 105,105,105,105 | 0 |
| 55 | MG | 14 | 3273 | 1/1 | 0.74 | 0.35 | 87,87,87,87 | 0 |
| 55 | MG | 13 | 1668 | 1/1 | 0.74 | 0.56 | 102,102,102,102 | 0 |
| 55 | MG | 1H | 3168 | 1/1 | 0.74 | 0.41 | 85,85,85,85 | 0 |
| 55 | MG | 14 | 3292 | 1/1 | 0.74 | 0.33 | 90,90,90,90 | 0 |

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| Mol | Type | Chain | Res | Atoms | RSCC | RSR | B-factors(Å$^2$) | Q<0.9 |
|---|---|---|---|---|---|---|---|---|
| 55 | MG | 1H | 3181 | 1/1 | 0.74 | 0.20 | 62,62,62,62 | 0 |
| 55 | MG | 1G | 1720 | 1/1 | 0.74 | 0.34 | 95,95,95,95 | 0 |
| 55 | MG | 14 | 3161 | 1/1 | 0.74 | 0.32 | 89,89,89,89 | 0 |
| 55 | MG | 1G | 1607 | 1/1 | 0.75 | 0.36 | 95,95,95,95 | 0 |
| 55 | MG | 1G | 1609 | 1/1 | 0.75 | 0.34 | 99,99,99,99 | 0 |
| 55 | MG | 1G | 1621 | 1/1 | 0.75 | 0.24 | 91,91,91,91 | 0 |
| 55 | MG | 14 | 3361 | 1/1 | 0.75 | 0.21 | 90,90,90,90 | 0 |
| 55 | MG | 1G | 1632 | 1/1 | 0.75 | 0.34 | 79,79,79,79 | 0 |
| 55 | MG | 1H | 3268 | 1/1 | 0.75 | 0.28 | 100,100,100,100 | 0 |
| 55 | MG | 1H | 3309 | 1/1 | 0.75 | 0.31 | 85,85,85,85 | 0 |
| 55 | MG | 1G | 1644 | 1/1 | 0.76 | 0.27 | 115,115,115,115 | 0 |
| 55 | MG | 13 | 1618 | 1/1 | 0.76 | 0.38 | 96,96,96,96 | 0 |
| 55 | MG | 1G | 1723 | 1/1 | 0.76 | 0.25 | 98,98,98,98 | 0 |
| 55 | MG | 1G | 1675 | 1/1 | 0.76 | 0.35 | 99,99,99,99 | 0 |
| 55 | MG | 14 | 3174 | 1/1 | 0.76 | 0.32 | 107,107,107,107 | 0 |
| 55 | MG | 14 | 3108 | 1/1 | 0.76 | 0.35 | 85,85,85,85 | 0 |
| 55 | MG | 1H | 3362 | 1/1 | 0.76 | 0.30 | 103,103,103,103 | 0 |
| 55 | MG | 1H | 3073 | 1/1 | 0.76 | 0.21 | 77,77,77,77 | 0 |
| 55 | MG | 14 | 3238 | 1/1 | 0.76 | 0.37 | 81,81,81,81 | 0 |
| 55 | MG | 1G | 1654 | 1/1 | 0.77 | 0.35 | 91,91,91,91 | 0 |
| 55 | MG | 1G | 1656 | 1/1 | 0.77 | 0.45 | 94,94,94,94 | 0 |
| 55 | MG | 1H | 3134 | 1/1 | 0.77 | 0.24 | 65,65,65,65 | 0 |
| 55 | MG | 1G | 1640 | 1/1 | 0.77 | 0.30 | 107,107,107,107 | 0 |
| 55 | MG | 1H | 3405 | 1/1 | 0.77 | 0.21 | 74,74,74,74 | 0 |
| 55 | MG | 1G | 1700 | 1/1 | 0.77 | 0.45 | 94,94,94,94 | 0 |
| 55 | MG | 16 | 203 | 1/1 | 0.77 | 0.17 | 92,92,92,92 | 0 |
| 55 | MG | 14 | 3158 | 1/1 | 0.77 | 0.29 | 97,97,97,97 | 0 |
| 55 | MG | 14 | 3372 | 1/1 | 0.77 | 0.31 | 96,96,96,96 | 0 |
| 55 | MG | 14 | 3159 | 1/1 | 0.77 | 0.40 | 85,85,85,85 | 0 |
| 55 | MG | 1H | 3322 | 1/1 | 0.77 | 0.24 | 92,92,92,92 | 0 |
| 55 | MG | 13 | 1610 | 1/1 | 0.77 | 0.28 | 115,115,115,115 | 0 |
| 55 | MG | 1H | 3293 | 1/1 | 0.78 | 0.23 | 95,95,95,95 | 0 |
| 55 | MG | 1G | 1702 | 1/1 | 0.78 | 0.24 | 95,95,95,95 | 0 |
| 55 | MG | 1H | 3296 | 1/1 | 0.78 | 0.30 | 84,84,84,84 | 0 |
| 55 | MG | 1H | 3059 | 1/1 | 0.78 | 0.29 | 83,83,83,83 | 0 |
| 55 | MG | 14 | 3157 | 1/1 | 0.78 | 0.41 | 80,80,80,80 | 0 |
| 55 | MG | 16 | 210 | 1/1 | 0.78 | 0.22 | 96,96,96,96 | 0 |
| 55 | MG | 1H | 3305 | 1/1 | 0.78 | 0.23 | 104,104,104,104 | 0 |
| 55 | MG | 1H | 3151 | 1/1 | 0.78 | 0.31 | 76,76,76,76 | 0 |
| 55 | MG | 1H | 3232 | 1/1 | 0.78 | 0.26 | 103,103,103,103 | 0 |
| 55 | MG | 13 | 1684 | 1/1 | 0.78 | 0.46 | 94,94,94,94 | 0 |
| 55 | MG | 1G | 1682 | 1/1 | 0.78 | 0.24 | 87,87,87,87 | 0 |

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| Mol | Type | Chain | Res | Atoms | RSCC | RSR | B-factors(Å$^2$) | Q<0.9 |
|---|---|---|---|---|---|---|---|---|
| 55 | MG | 1G | 1684 | 1/1 | 0.78 | 0.35 | 99,99,99,99 | 0 |
| 55 | MG | 14 | 3215 | 1/1 | 0.78 | 0.24 | 76,76,76,76 | 0 |
| 55 | MG | 1H | 3320 | 1/1 | 0.78 | 0.35 | 109,109,109,109 | 0 |
| 55 | MG | 14 | 3337 | 1/1 | 0.78 | 0.19 | 105,105,105,105 | 0 |
| 55 | MG | 13 | 1698 | 1/1 | 0.78 | 0.32 | 78,78,78,78 | 0 |
| 55 | MG | 1H | 3389 | 1/1 | 0.78 | 0.68 | 101,101,101,101 | 0 |
| 55 | MG | 14 | 3255 | 1/1 | 0.78 | 0.29 | 92,92,92,92 | 0 |
| 55 | MG | 13 | 1667 | 1/1 | 0.78 | 0.24 | 94,94,94,94 | 0 |
| 55 | MG | 13 | 1707 | 1/1 | 0.78 | 0.29 | 100,100,100,100 | 0 |
| 55 | MG | 14 | 3269 | 1/1 | 0.78 | 0.31 | 68,68,68,68 | 0 |
| 55 | MG | 1H | 3044 | 1/1 | 0.78 | 0.44 | 98,98,98,98 | 0 |
| 55 | MG | 1J | 201 | 1/1 | 0.78 | 0.25 | 100,100,100,100 | 0 |
| 55 | MG | 14 | 3070 | 1/1 | 0.78 | 0.29 | 66,66,66,66 | 0 |
| 55 | MG | 14 | 3082 | 1/1 | 0.78 | 0.20 | 64,64,64,64 | 0 |
| 55 | MG | 14 | 3301 | 1/1 | 0.79 | 0.34 | 82,82,82,82 | 0 |
| 55 | MG | 1G | 1652 | 1/1 | 0.79 | 0.28 | 82,82,82,82 | 0 |
| 55 | MG | 13 | 1625 | 1/1 | 0.79 | 0.26 | 95,95,95,95 | 0 |
| 55 | MG | 1G | 1725 | 1/1 | 0.79 | 0.22 | 93,93,93,93 | 0 |
| 55 | MG | 1H | 3304 | 1/1 | 0.79 | 0.28 | 82,82,82,82 | 0 |
| 55 | MG | 14 | 3182 | 1/1 | 0.79 | 0.38 | 77,77,77,77 | 0 |
| 55 | MG | 1G | 1610 | 1/1 | 0.79 | 0.43 | 99,99,99,99 | 0 |
| 55 | MG | 1G | 1698 | 1/1 | 0.79 | 0.26 | 96,96,96,96 | 0 |
| 55 | MG | 1G | 1659 | 1/1 | 0.79 | 0.29 | 107,107,107,107 | 0 |
| 55 | MG | 1H | 3280 | 1/1 | 0.79 | 0.34 | 70,70,70,70 | 0 |
| 55 | MG | 1G | 1629 | 1/1 | 0.79 | 0.29 | 86,86,86,86 | 0 |
| 55 | MG | 14 | 3335 | 1/1 | 0.79 | 0.30 | 90,90,90,90 | 0 |
| 55 | MG | 13 | 1694 | 1/1 | 0.79 | 0.20 | 92,92,92,92 | 0 |
| 55 | MG | 1G | 1637 | 1/1 | 0.79 | 0.29 | 71,71,71,71 | 0 |
| 55 | MG | 14 | 3105 | 1/1 | 0.79 | 0.46 | 72,72,72,72 | 0 |
| 55 | MG | 1H | 3047 | 1/1 | 0.79 | 0.36 | 76,76,76,76 | 0 |
| 55 | MG | 1G | 1710 | 1/1 | 0.79 | 0.29 | 101,101,101,101 | 0 |
| 55 | MG | 14 | 3117 | 1/1 | 0.79 | 0.38 | 93,93,93,93 | 0 |
| 55 | MG | 1G | 1713 | 1/1 | 0.79 | 0.21 | 107,107,107,107 | 0 |
| 55 | MG | 1H | 3357 | 1/1 | 0.79 | 0.44 | 92,92,92,92 | 0 |
| 55 | MG | 1H | 3031 | 1/1 | 0.79 | 0.36 | 82,82,82,82 | 0 |
| 55 | MG | 1H | 3253 | 1/1 | 0.79 | 0.29 | 71,71,71,71 | 0 |
| 55 | MG | 1G | 1686 | 1/1 | 0.79 | 0.32 | 95,95,95,95 | 0 |
| 55 | MG | 1H | 3340 | 1/1 | 0.80 | 0.26 | 77,77,77,77 | 0 |
| 55 | MG | 1H | 3342 | 1/1 | 0.80 | 0.29 | 89,89,89,89 | 0 |
| 55 | MG | 14 | 3143 | 1/1 | 0.80 | 0.35 | 87,87,87,87 | 0 |
| 55 | MG | 14 | 3297 | 1/1 | 0.80 | 0.23 | 78,78,78,78 | 0 |
| 55 | MG | 1H | 3294 | 1/1 | 0.80 | 0.39 | 85,85,85,85 | 0 |

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| Mol | Type | Chain | Res | Atoms | RSCC | RSR | B-factors(Å$^2$) | Q<0.9 |
|---|---|---|---|---|---|---|---|---|
| 55 | MG | 1G | 1611 | 1/1 | 0.80 | 0.25 | 132,132,132,132 | 0 |
| 55 | MG | 1H | 3390 | 1/1 | 0.80 | 0.32 | 88,88,88,88 | 0 |
| 55 | MG | 1G | 1722 | 1/1 | 0.80 | 0.14 | 91,91,91,91 | 0 |
| 55 | MG | 1G | 1623 | 1/1 | 0.80 | 0.26 | 87,87,87,87 | 0 |
| 55 | MG | 13 | 1647 | 1/1 | 0.80 | 0.29 | 110,110,110,110 | 0 |
| 55 | MG | 14 | 3317 | 1/1 | 0.80 | 0.36 | 83,83,83,83 | 0 |
| 55 | MG | 14 | 3172 | 1/1 | 0.80 | 0.20 | 85,85,85,85 | 0 |
| 55 | MG | 1H | 3349 | 1/1 | 0.80 | 0.21 | 77,77,77,77 | 0 |
| 55 | MG | 1H | 3400 | 1/1 | 0.80 | 0.28 | 84,84,84,84 | 0 |
| 55 | MG | 1H | 3314 | 1/1 | 0.80 | 0.33 | 97,97,97,97 | 0 |
| 55 | MG | 14 | 3206 | 1/1 | 0.80 | 0.34 | 76,76,76,76 | 0 |
| 55 | MG | 1H | 3207 | 1/1 | 0.80 | 0.22 | 67,67,67,67 | 0 |
| 55 | MG | 1H | 3119 | 1/1 | 0.80 | 0.31 | 77,77,77,77 | 0 |
| 55 | MG | 1H | 3323 | 1/1 | 0.80 | 0.29 | 80,80,80,80 | 0 |
| 55 | MG | 1G | 1650 | 1/1 | 0.80 | 0.26 | 90,90,90,90 | 0 |
| 55 | MG | 14 | 3349 | 1/1 | 0.80 | 0.20 | 100,100,100,100 | 0 |
| 55 | MG | 14 | 3252 | 1/1 | 0.80 | 0.23 | 81,81,81,81 | 0 |
| 55 | MG | 13 | 1653 | 1/1 | 0.80 | 0.33 | 104,104,104,104 | 0 |
| 55 | MG | 14 | 3260 | 1/1 | 0.80 | 0.29 | 99,99,99,99 | 0 |
| 55 | MG | 13 | 1655 | 1/1 | 0.80 | 0.30 | 92,92,92,92 | 0 |
| 55 | MG | 1H | 3332 | 1/1 | 0.80 | 0.44 | 87,87,87,87 | 0 |
| 55 | MG | 14 | 3366 | 1/1 | 0.80 | 0.36 | 99,99,99,99 | 0 |
| 55 | MG | I8 | 101 | 1/1 | 0.80 | 0.45 | 83,83,83,83 | 0 |
| 55 | MG | 14 | 3272 | 1/1 | 0.80 | 0.34 | 94,94,94,94 | 0 |
| 55 | MG | I8 | 103 | 1/1 | 0.80 | 0.19 | 92,92,92,92 | 0 |
| 55 | MG | 1J | 204 | 1/1 | 0.80 | 0.26 | 101,101,101,101 | 0 |
| 55 | MG | 14 | 3282 | 1/1 | 0.80 | 0.43 | 87,87,87,87 | 0 |
| 55 | MG | 1G | 1602 | 1/1 | 0.80 | 0.37 | 75,75,75,75 | 0 |
| 55 | MG | 14 | 3069 | 1/1 | 0.81 | 0.35 | 96,96,96,96 | 0 |
| 55 | MG | 1H | 3341 | 1/1 | 0.81 | 0.29 | 76,76,76,76 | 0 |
| 55 | MG | 1G | 1701 | 1/1 | 0.81 | 0.18 | 93,93,93,93 | 0 |
| 55 | MG | 1H | 3397 | 1/1 | 0.81 | 0.13 | 94,94,94,94 | 0 |
| 55 | MG | 1H | 3012 | 1/1 | 0.81 | 0.29 | 57,57,57,57 | 0 |
| 55 | MG | 1H | 3029 | 1/1 | 0.81 | 0.27 | 71,71,71,71 | 0 |
| 55 | MG | Q8 | 102 | 1/1 | 0.81 | 0.49 | 81,81,81,81 | 0 |
| 55 | MG | 14 | 3276 | 1/1 | 0.81 | 0.22 | 73,73,73,73 | 0 |
| 55 | MG | 14 | 3200 | 1/1 | 0.81 | 0.35 | 100,100,100,100 | 0 |
| 55 | MG | 13 | 1693 | 1/1 | 0.81 | 0.33 | 100,100,100,100 | 0 |
| 55 | MG | 14 | 3211 | 1/1 | 0.81 | 0.30 | 77,77,77,77 | 0 |
| 55 | MG | 14 | 3214 | 1/1 | 0.81 | 0.24 | 66,66,66,66 | 0 |
| 55 | MG | 1H | 3264 | 1/1 | 0.81 | 0.33 | 100,100,100,100 | 0 |
| 55 | MG | 1H | 3159 | 1/1 | 0.81 | 0.27 | 66,66,66,66 | 0 |

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| Mol | Type | Chain | Res | Atoms | RSCC | RSR | B-factors(Å$^2$) | Q<0.9 |
|---|---|---|---|---|---|---|---|---|
| 55 | MG | 14 | 3222 | 1/1 | 0.81 | 0.25 | 79,79,79,79 | 0 |
| 55 | MG | 14 | 3362 | 1/1 | 0.81 | 0.24 | 111,111,111,111 | 0 |
| 55 | MG | 14 | 3364 | 1/1 | 0.81 | 0.14 | 68,68,68,68 | 0 |
| 55 | MG | 1H | 3313 | 1/1 | 0.81 | 0.16 | 91,91,91,91 | 0 |
| 55 | MG | 14 | 3228 | 1/1 | 0.81 | 0.31 | 84,84,84,84 | 0 |
| 55 | MG | 14 | 3020 | 1/1 | 0.81 | 0.26 | 72,72,72,72 | 0 |
| 55 | MG | 14 | 3248 | 1/1 | 0.81 | 0.46 | 78,78,78,78 | 0 |
| 55 | MG | 14 | 3308 | 1/1 | 0.81 | 0.24 | 80,80,80,80 | 0 |
| 55 | MG | 14 | 3249 | 1/1 | 0.81 | 0.20 | 87,87,87,87 | 0 |
| 55 | MG | 29 | 304 | 1/1 | 0.81 | 0.54 | 89,89,89,89 | 0 |
| 55 | MG | 13 | 1648 | 1/1 | 0.81 | 0.28 | 105,105,105,105 | 0 |
| 55 | MG | 1H | 3315 | 1/1 | 0.82 | 0.29 | 88,88,88,88 | 0 |
| 55 | MG | 1G | 1745 | 1/1 | 0.82 | 0.19 | 93,93,93,93 | 0 |
| 55 | MG | 1G | 1748 | 1/1 | 0.82 | 0.26 | 90,90,90,90 | 0 |
| 55 | MG | 1H | 3350 | 1/1 | 0.82 | 0.37 | 89,89,89,89 | 0 |
| 55 | MG | 14 | 3185 | 1/1 | 0.82 | 0.29 | 90,90,90,90 | 0 |
| 55 | MG | 42 | 201 | 1/1 | 0.82 | 0.33 | 101,101,101,101 | 0 |
| 55 | MG | 1G | 1608 | 1/1 | 0.82 | 0.20 | 85,85,85,85 | 0 |
| 55 | MG | 13 | 1645 | 1/1 | 0.82 | 0.33 | 98,98,98,98 | 0 |
| 55 | MG | 14 | 3312 | 1/1 | 0.82 | 0.32 | 81,81,81,81 | 0 |
| 55 | MG | 13 | 1711 | 1/1 | 0.82 | 0.40 | 90,90,90,90 | 0 |
| 55 | MG | 1G | 1658 | 1/1 | 0.82 | 0.13 | 99,99,99,99 | 0 |
| 55 | MG | 14 | 3040 | 1/1 | 0.82 | 0.28 | 69,69,69,69 | 0 |
| 55 | MG | 1H | 3057 | 1/1 | 0.82 | 0.27 | 84,84,84,84 | 0 |
| 55 | MG | 14 | 3220 | 1/1 | 0.82 | 0.25 | 89,89,89,89 | 0 |
| 55 | MG | 1G | 1660 | 1/1 | 0.82 | 0.17 | 87,87,87,87 | 0 |
| 55 | MG | 1H | 3150 | 1/1 | 0.82 | 0.31 | 78,78,78,78 | 0 |
| 55 | MG | 14 | 3093 | 1/1 | 0.82 | 0.27 | 84,84,84,84 | 0 |
| 55 | MG | 1H | 3188 | 1/1 | 0.82 | 0.36 | 81,81,81,81 | 0 |
| 55 | MG | 14 | 3333 | 1/1 | 0.82 | 0.17 | 89,89,89,89 | 0 |
| 55 | MG | 1G | 1669 | 1/1 | 0.82 | 0.33 | 86,86,86,86 | 0 |
| 55 | MG | 14 | 3336 | 1/1 | 0.82 | 0.15 | 73,73,73,73 | 0 |
| 55 | MG | 14 | 3111 | 1/1 | 0.82 | 0.16 | 54,54,54,54 | 0 |
| 55 | MG | 1G | 1670 | 1/1 | 0.82 | 0.36 | 92,92,92,92 | 0 |
| 55 | MG | 14 | 3352 | 1/1 | 0.82 | 0.31 | 93,93,93,93 | 0 |
| 55 | MG | 1G | 1627 | 1/1 | 0.82 | 0.35 | 93,93,93,93 | 0 |
| 55 | MG | 14 | 3258 | 1/1 | 0.82 | 0.29 | 70,70,70,70 | 0 |
| 55 | MG | 13 | 1636 | 1/1 | 0.82 | 0.28 | 88,88,88,88 | 0 |
| 55 | MG | 14 | 3123 | 1/1 | 0.82 | 0.21 | 50,50,50,50 | 0 |
| 55 | MG | 1H | 3376 | 1/1 | 0.82 | 0.30 | 94,94,94,94 | 0 |
| 55 | MG | 13 | 1662 | 1/1 | 0.82 | 0.25 | 86,86,86,86 | 0 |
| 55 | MG | 14 | 3271 | 1/1 | 0.82 | 0.28 | 82,82,82,82 | 0 |

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| Mol | Type | Chain | Res | Atoms | RSCC | RSR | B-factors(Å$^2$) | Q<0.9 |
|---|---|---|---|---|---|---|---|---|
| 55 | MG | 14 | 3365 | 1/1 | 0.82 | 0.21 | 78,78,78,78 | 0 |
| 55 | MG | 14 | 3155 | 1/1 | 0.82 | 0.35 | 77,77,77,77 | 0 |
| 55 | MG | 14 | 3369 | 1/1 | 0.82 | 0.27 | 78,78,78,78 | 0 |
| 55 | MG | 14 | 3156 | 1/1 | 0.82 | 0.19 | 75,75,75,75 | 0 |
| 55 | MG | 1H | 3160 | 1/1 | 0.82 | 0.34 | 68,68,68,68 | 0 |
| 55 | MG | 1G | 1642 | 1/1 | 0.82 | 0.24 | 87,87,87,87 | 0 |
| 55 | MG | 14 | 3283 | 1/1 | 0.82 | 0.26 | 87,87,87,87 | 0 |
| 55 | MG | 13 | 1615 | 1/1 | 0.82 | 0.28 | 98,98,98,98 | 0 |
| 55 | MG | 1H | 3032 | 1/1 | 0.82 | 0.23 | 95,95,95,95 | 0 |
| 55 | MG | 13 | 1664 | 1/1 | 0.82 | 0.47 | 93,93,93,93 | 0 |
| 55 | MG | 1G | 1626 | 1/1 | 0.83 | 0.22 | 107,107,107,107 | 0 |
| 55 | MG | 13 | 1704 | 1/1 | 0.83 | 0.15 | 87,87,87,87 | 0 |
| 55 | MG | 13 | 1671 | 1/1 | 0.83 | 0.14 | 70,70,70,70 | 0 |
| 55 | MG | 1H | 3178 | 1/1 | 0.83 | 0.19 | 77,77,77,77 | 0 |
| 55 | MG | 13 | 1699 | 1/1 | 0.83 | 0.30 | 109,109,109,109 | 0 |
| 55 | MG | 1G | 1683 | 1/1 | 0.83 | 0.46 | 103,103,103,103 | 0 |
| 55 | MG | 14 | 3232 | 1/1 | 0.83 | 0.20 | 98,98,98,98 | 0 |
| 55 | MG | 13 | 1665 | 1/1 | 0.83 | 0.16 | 90,90,90,90 | 0 |
| 55 | MG | 14 | 3239 | 1/1 | 0.83 | 0.46 | 87,87,87,87 | 0 |
| 55 | MG | 14 | 3244 | 1/1 | 0.83 | 0.25 | 86,86,86,86 | 0 |
| 55 | MG | 14 | 3127 | 1/1 | 0.83 | 0.30 | 84,84,84,84 | 0 |
| 55 | MG | 1H | 3027 | 1/1 | 0.83 | 0.26 | 86,86,86,86 | 0 |
| 55 | MG | 1H | 3190 | 1/1 | 0.83 | 0.29 | 101,101,101,101 | 0 |
| 55 | MG | 14 | 3150 | 1/1 | 0.83 | 0.34 | 107,107,107,107 | 0 |
| 55 | MG | 13 | 1682 | 1/1 | 0.83 | 0.41 | 85,85,85,85 | 0 |
| 55 | MG | 1H | 3366 | 1/1 | 0.83 | 0.24 | 84,84,84,84 | 0 |
| 55 | MG | 1H | 3375 | 1/1 | 0.83 | 0.16 | 85,85,85,85 | 0 |
| 55 | MG | 14 | 3342 | 1/1 | 0.83 | 0.48 | 94,94,94,94 | 0 |
| 55 | MG | 14 | 3263 | 1/1 | 0.83 | 0.22 | 72,72,72,72 | 0 |
| 55 | MG | 1H | 3153 | 1/1 | 0.83 | 0.25 | 86,86,86,86 | 0 |
| 55 | MG | 1H | 3329 | 1/1 | 0.83 | 0.22 | 85,85,85,85 | 0 |
| 55 | MG | 52 | 201 | 1/1 | 0.83 | 0.13 | 84,84,84,84 | 0 |
| 55 | MG | 14 | 3165 | 1/1 | 0.83 | 0.20 | 74,74,74,74 | 0 |
| 55 | MG | 1H | 3156 | 1/1 | 0.83 | 0.21 | 72,72,72,72 | 0 |
| 55 | MG | 14 | 3275 | 1/1 | 0.83 | 0.35 | 90,90,90,90 | 0 |
| 55 | MG | 13 | 1638 | 1/1 | 0.83 | 0.20 | 85,85,85,85 | 0 |
| 55 | MG | 14 | 3280 | 1/1 | 0.83 | 0.15 | 75,75,75,75 | 0 |
| 55 | MG | 1H | 3093 | 1/1 | 0.83 | 0.36 | 82,82,82,82 | 0 |
| 55 | MG | 1H | 3211 | 1/1 | 0.83 | 0.26 | 79,79,79,79 | 0 |
| 55 | MG | 14 | 3028 | 1/1 | 0.83 | 0.28 | 77,77,77,77 | 0 |
| 55 | MG | 14 | 3036 | 1/1 | 0.83 | 0.26 | 91,91,91,91 | 0 |
| 55 | MG | 1H | 3104 | 1/1 | 0.83 | 0.20 | 85,85,85,85 | 0 |

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| Mol | Type | Chain | Res | Atoms | RSCC | RSR | B-factors(Å$^2$) | Q<0.9 |
|---|---|---|---|---|---|---|---|---|
| 55 | MG | 14 | 3193 | 1/1 | 0.83 | 0.31 | 56,56,56,56 | 0 |
| 55 | MG | 1H | 3108 | 1/1 | 0.83 | 0.39 | 77,77,77,77 | 0 |
| 55 | MG | 1G | 1665 | 1/1 | 0.83 | 0.20 | 69,69,69,69 | 0 |
| 55 | MG | 13 | 1639 | 1/1 | 0.83 | 0.19 | 66,66,66,66 | 0 |
| 55 | MG | 1G | 1624 | 1/1 | 0.83 | 0.28 | 78,78,78,78 | 0 |
| 55 | MG | 21 | 301 | 1/1 | 0.84 | 0.29 | 58,58,58,58 | 0 |
| 55 | MG | 13 | 1686 | 1/1 | 0.84 | 0.40 | 85,85,85,85 | 0 |
| 55 | MG | 1G | 1679 | 1/1 | 0.84 | 0.32 | 97,97,97,97 | 0 |
| 55 | MG | 1H | 3380 | 1/1 | 0.84 | 0.37 | 88,88,88,88 | 0 |
| 55 | MG | 14 | 3087 | 1/1 | 0.84 | 0.27 | 65,65,65,65 | 0 |
| 55 | MG | 1H | 3127 | 1/1 | 0.84 | 0.25 | 60,60,60,60 | 0 |
| 55 | MG | 14 | 3094 | 1/1 | 0.84 | 0.37 | 81,81,81,81 | 0 |
| 55 | MG | 1H | 3284 | 1/1 | 0.84 | 0.30 | 73,73,73,73 | 0 |
| 55 | MG | 1G | 1603 | 1/1 | 0.84 | 0.31 | 76,76,76,76 | 0 |
| 55 | MG | 1H | 3130 | 1/1 | 0.84 | 0.26 | 69,69,69,69 | 0 |
| 55 | MG | 14 | 3208 | 1/1 | 0.84 | 0.20 | 88,88,88,88 | 0 |
| 55 | MG | 1G | 1689 | 1/1 | 0.84 | 0.25 | 90,90,90,90 | 0 |
| 55 | MG | 1H | 3356 | 1/1 | 0.84 | 0.47 | 91,91,91,91 | 0 |
| 55 | MG | 13 | 1660 | 1/1 | 0.84 | 0.25 | 80,80,80,80 | 0 |
| 55 | MG | 1H | 3094 | 1/1 | 0.84 | 0.23 | 60,60,60,60 | 0 |
| 55 | MG | 14 | 3290 | 1/1 | 0.84 | 0.34 | 77,77,77,77 | 0 |
| 55 | MG | 1G | 1657 | 1/1 | 0.84 | 0.29 | 87,87,87,87 | 0 |
| 55 | MG | 1H | 3297 | 1/1 | 0.84 | 0.38 | 81,81,81,81 | 0 |
| 55 | MG | 2K | 104 | 1/1 | 0.84 | 0.38 | 101,101,101,101 | 0 |
| 55 | MG | 14 | 3144 | 1/1 | 0.84 | 0.41 | 98,98,98,98 | 0 |
| 55 | MG | 14 | 3147 | 1/1 | 0.84 | 0.39 | 83,83,83,83 | 0 |
| 55 | MG | 1H | 3106 | 1/1 | 0.84 | 0.33 | 85,85,85,85 | 0 |
| 55 | MG | 1H | 3260 | 1/1 | 0.84 | 0.14 | 70,70,70,70 | 0 |
| 55 | MG | 13 | 1614 | 1/1 | 0.84 | 0.21 | 95,95,95,95 | 0 |
| 55 | MG | 3L | 101 | 1/1 | 0.84 | 0.14 | 180,180,180,180 | 0 |
| 55 | MG | 14 | 3309 | 1/1 | 0.84 | 0.39 | 84,84,84,84 | 0 |
| 55 | MG | 1H | 3369 | 1/1 | 0.84 | 0.20 | 94,94,94,94 | 0 |
| 55 | MG | 1H | 3372 | 1/1 | 0.84 | 0.28 | 94,94,94,94 | 0 |
| 55 | MG | 1H | 3173 | 1/1 | 0.84 | 0.23 | 90,90,90,90 | 0 |
| 55 | MG | 13 | 1604 | 1/1 | 0.84 | 0.14 | 86,86,86,86 | 0 |
| 56 | ZN | C5 | 202 | 1/1 | 0.84 | 0.14 | 219,219,219,219 | 0 |
| 55 | MG | 1H | 3124 | 1/1 | 0.85 | 0.24 | 59,59,59,59 | 0 |
| 55 | MG | 1H | 3407 | 1/1 | 0.85 | 0.40 | 89,89,89,89 | 0 |
| 55 | MG | 1H | 3180 | 1/1 | 0.85 | 0.21 | 86,86,86,86 | 0 |
| 55 | MG | 1H | 3279 | 1/1 | 0.85 | 0.20 | 96,96,96,96 | 0 |
| 55 | MG | 16 | 206 | 1/1 | 0.85 | 0.10 | 101,101,101,101 | 0 |
| 55 | MG | 14 | 3163 | 1/1 | 0.85 | 0.31 | 80,80,80,80 | 0 |

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| Mol | Type | Chain | Res | Atoms | RSCC | RSR | B-factors(Å$^2$) | Q<0.9 |
|---|---|---|---|---|---|---|---|---|
| 55 | MG | 13 | 1685 | 1/1 | 0.85 | 0.12 | 89,89,89,89 | 0 |
| 55 | MG | 16 | 209 | 1/1 | 0.85 | 0.21 | 80,80,80,80 | 0 |
| 55 | MG | 13 | 1676 | 1/1 | 0.85 | 0.25 | 84,84,84,84 | 0 |
| 55 | MG | 1H | 3006 | 1/1 | 0.85 | 0.29 | 67,67,67,67 | 0 |
| 55 | MG | 13 | 1650 | 1/1 | 0.85 | 0.22 | 88,88,88,88 | 0 |
| 55 | MG | 1H | 3353 | 1/1 | 0.85 | 0.29 | 83,83,83,83 | 0 |
| 55 | MG | 14 | 3303 | 1/1 | 0.85 | 0.35 | 99,99,99,99 | 0 |
| 55 | MG | 1H | 3286 | 1/1 | 0.85 | 0.34 | 82,82,82,82 | 0 |
| 55 | MG | 1H | 3193 | 1/1 | 0.85 | 0.29 | 77,77,77,77 | 0 |
| 55 | MG | 14 | 3187 | 1/1 | 0.85 | 0.27 | 94,94,94,94 | 0 |
| 55 | MG | 1H | 3358 | 1/1 | 0.85 | 0.46 | 98,98,98,98 | 0 |
| 55 | MG | 14 | 3195 | 1/1 | 0.85 | 0.24 | 65,65,65,65 | 0 |
| 55 | MG | 1H | 3074 | 1/1 | 0.85 | 0.25 | 82,82,82,82 | 0 |
| 55 | MG | 1H | 3200 | 1/1 | 0.85 | 0.35 | 99,99,99,99 | 0 |
| 55 | MG | 1G | 1605 | 1/1 | 0.85 | 0.37 | 92,92,92,92 | 0 |
| 55 | MG | 1H | 3143 | 1/1 | 0.85 | 0.30 | 73,73,73,73 | 0 |
| 55 | MG | 13 | 1661 | 1/1 | 0.85 | 0.25 | 95,95,95,95 | 0 |
| 55 | MG | 1H | 3077 | 1/1 | 0.85 | 0.18 | 59,59,59,59 | 0 |
| 55 | MG | 14 | 3054 | 1/1 | 0.85 | 0.40 | 81,81,81,81 | 0 |
| 55 | MG | 14 | 3056 | 1/1 | 0.85 | 0.26 | 75,75,75,75 | 0 |
| 55 | MG | 14 | 3221 | 1/1 | 0.85 | 0.23 | 76,76,76,76 | 0 |
| 55 | MG | 1H | 3088 | 1/1 | 0.85 | 0.12 | 52,52,52,52 | 0 |
| 55 | MG | 1H | 3367 | 1/1 | 0.85 | 0.18 | 67,67,67,67 | 0 |
| 55 | MG | 1G | 1619 | 1/1 | 0.85 | 0.39 | 73,73,73,73 | 0 |
| 55 | MG | 13 | 1691 | 1/1 | 0.85 | 0.41 | 83,83,83,83 | 0 |
| 55 | MG | 14 | 3091 | 1/1 | 0.85 | 0.29 | 81,81,81,81 | 0 |
| 55 | MG | 13 | 1607 | 1/1 | 0.85 | 0.31 | 86,86,86,86 | 0 |
| 55 | MG | 14 | 3241 | 1/1 | 0.85 | 0.29 | 89,89,89,89 | 0 |
| 55 | MG | 5E | 201 | 1/1 | 0.85 | 0.20 | 106,106,106,106 | 0 |
| 55 | MG | 14 | 3096 | 1/1 | 0.85 | 0.24 | 94,94,94,94 | 0 |
| 55 | MG | 14 | 3100 | 1/1 | 0.85 | 0.21 | 79,79,79,79 | 0 |
| 55 | MG | 1H | 3223 | 1/1 | 0.85 | 0.37 | 97,97,97,97 | 0 |
| 55 | MG | 1H | 3035 | 1/1 | 0.85 | 0.22 | 75,75,75,75 | 0 |
| 55 | MG | 1H | 3037 | 1/1 | 0.85 | 0.28 | 60,60,60,60 | 0 |
| 55 | MG | 1G | 1631 | 1/1 | 0.85 | 0.22 | 90,90,90,90 | 0 |
| 55 | MG | 1H | 3234 | 1/1 | 0.85 | 0.31 | 88,88,88,88 | 0 |
| 55 | MG | 1H | 3238 | 1/1 | 0.85 | 0.34 | 82,82,82,82 | 0 |
| 55 | MG | 1H | 3112 | 1/1 | 0.85 | 0.29 | 73,73,73,73 | 0 |
| 55 | MG | 1G | 1705 | 1/1 | 0.85 | 0.30 | 96,96,96,96 | 0 |
| 55 | MG | 13 | 1683 | 1/1 | 0.85 | 0.18 | 122,122,122,122 | 0 |
| 55 | MG | 13 | 1608 | 1/1 | 0.85 | 0.31 | 101,101,101,101 | 0 |
| 55 | MG | 1H | 3123 | 1/1 | 0.85 | 0.23 | 78,78,78,78 | 0 |

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| Mol | Type | Chain | Res | Atoms | RSCC | RSR | B-factors(Å$^2$) | Q<0.9 |
|---|---|---|---|---|---|---|---|---|
| 55 | MG | 1J | 206 | 1/1 | 0.85 | 0.23 | 96,96,96,96 | 0 |
| 55 | MG | 1H | 3263 | 1/1 | 0.85 | 0.40 | 84,84,84,84 | 0 |
| 55 | MG | 1H | 3399 | 1/1 | 0.85 | 0.18 | 77,77,77,77 | 0 |
| 55 | MG | 1H | 3334 | 1/1 | 0.85 | 0.24 | 108,108,108,108 | 0 |
| 55 | MG | 14 | 3038 | 1/1 | 0.86 | 0.23 | 86,86,86,86 | 0 |
| 55 | MG | 14 | 3180 | 1/1 | 0.86 | 0.31 | 82,82,82,82 | 0 |
| 55 | MG | 1H | 3100 | 1/1 | 0.86 | 0.25 | 61,61,61,61 | 0 |
| 55 | MG | 14 | 3291 | 1/1 | 0.86 | 0.33 | 82,82,82,82 | 0 |
| 55 | MG | 1H | 3377 | 1/1 | 0.86 | 0.33 | 81,81,81,81 | 0 |
| 55 | MG | 13 | 1705 | 1/1 | 0.86 | 0.20 | 76,76,76,76 | 0 |
| 55 | MG | 1H | 3140 | 1/1 | 0.86 | 0.17 | 52,52,52,52 | 0 |
| 55 | MG | 1H | 3061 | 1/1 | 0.86 | 0.24 | 71,71,71,71 | 0 |
| 55 | MG | 1H | 3146 | 1/1 | 0.86 | 0.18 | 48,48,48,48 | 0 |
| 55 | MG | 14 | 3197 | 1/1 | 0.86 | 0.49 | 81,81,81,81 | 0 |
| 55 | MG | 1H | 3387 | 1/1 | 0.86 | 0.23 | 75,75,75,75 | 0 |
| 55 | MG | 1G | 1709 | 1/1 | 0.86 | 0.30 | 96,96,96,96 | 0 |
| 55 | MG | 1H | 3107 | 1/1 | 0.86 | 0.35 | 81,81,81,81 | 0 |
| 55 | MG | 14 | 3209 | 1/1 | 0.86 | 0.20 | 88,88,88,88 | 0 |
| 55 | MG | 1H | 3025 | 1/1 | 0.86 | 0.40 | 80,80,80,80 | 0 |
| 55 | MG | 1G | 1717 | 1/1 | 0.86 | 0.20 | 107,107,107,107 | 0 |
| 55 | MG | 1H | 3391 | 1/1 | 0.86 | 0.42 | 92,92,92,92 | 0 |
| 55 | MG | 14 | 3216 | 1/1 | 0.86 | 0.27 | 72,72,72,72 | 0 |
| 55 | MG | 1H | 3040 | 1/1 | 0.86 | 0.40 | 71,71,71,71 | 0 |
| 55 | MG | 14 | 3319 | 1/1 | 0.86 | 0.18 | 89,89,89,89 | 0 |
| 55 | MG | 1G | 1614 | 1/1 | 0.86 | 0.27 | 92,92,92,92 | 0 |
| 55 | MG | 1G | 1618 | 1/1 | 0.86 | 0.28 | 79,79,79,79 | 0 |
| 55 | MG | 14 | 3112 | 1/1 | 0.86 | 0.31 | 68,68,68,68 | 0 |
| 55 | MG | 1H | 3118 | 1/1 | 0.86 | 0.39 | 83,83,83,83 | 0 |
| 55 | MG | 13 | 1687 | 1/1 | 0.86 | 0.27 | 77,77,77,77 | 0 |
| 55 | MG | 1H | 3266 | 1/1 | 0.86 | 0.25 | 101,101,101,101 | 0 |
| 55 | MG | 14 | 3236 | 1/1 | 0.86 | 0.51 | 94,94,94,94 | 0 |
| 55 | MG | 1H | 3120 | 1/1 | 0.86 | 0.22 | 69,69,69,69 | 0 |
| 55 | MG | 14 | 3126 | 1/1 | 0.86 | 0.34 | 83,83,83,83 | 0 |
| 55 | MG | 1H | 3271 | 1/1 | 0.86 | 0.18 | 90,90,90,90 | 0 |
| 55 | MG | 1H | 3276 | 1/1 | 0.86 | 0.25 | 88,88,88,88 | 0 |
| 55 | MG | 14 | 3345 | 1/1 | 0.86 | 0.27 | 78,78,78,78 | 0 |
| 55 | MG | 14 | 3247 | 1/1 | 0.86 | 0.14 | 79,79,79,79 | 0 |
| 55 | MG | 13 | 1734 | 1/1 | 0.86 | 0.07 | 178,178,178,178 | 0 |
| 55 | MG | 1H | 3084 | 1/1 | 0.86 | 0.35 | 62,62,62,62 | 0 |
| 55 | MG | 14 | 3251 | 1/1 | 0.86 | 0.20 | 67,67,67,67 | 0 |
| 55 | MG | 14 | 3145 | 1/1 | 0.86 | 0.23 | 78,78,78,78 | 0 |
| 55 | MG | 1H | 3365 | 1/1 | 0.86 | 0.26 | 86,86,86,86 | 0 |

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| Mol | Type | Chain | Res | Atoms | RSCC | RSR | B-factors(Å$^2$) | Q<0.9 |
|---|---|---|---|---|---|---|---|---|
| 55 | MG | 13 | 1633 | 1/1 | 0.86 | 0.25 | 79,79,79,79 | 0 |
| 55 | MG | 1G | 1688 | 1/1 | 0.86 | 0.30 | 102,102,102,102 | 0 |
| 55 | MG | 1G | 1638 | 1/1 | 0.86 | 0.34 | 88,88,88,88 | 0 |
| 55 | MG | 1H | 3049 | 1/1 | 0.86 | 0.26 | 71,71,71,71 | 0 |
| 55 | MG | 13 | 1623 | 1/1 | 0.86 | 0.14 | 107,107,107,107 | 0 |
| 55 | MG | 14 | 3368 | 1/1 | 0.86 | 0.18 | 76,76,76,76 | 0 |
| 55 | MG | 14 | 3014 | 1/1 | 0.86 | 0.26 | 84,84,84,84 | 0 |
| 55 | MG | 14 | 3018 | 1/1 | 0.86 | 0.09 | 64,64,64,64 | 0 |
| 55 | MG | 1H | 3370 | 1/1 | 0.86 | 0.30 | 73,73,73,73 | 0 |
| 55 | MG | 1H | 3096 | 1/1 | 0.86 | 0.35 | 71,71,71,71 | 0 |
| 55 | MG | 1J | 203 | 1/1 | 0.86 | 0.14 | 92,92,92,92 | 0 |
| 55 | MG | 14 | 3166 | 1/1 | 0.86 | 0.14 | 71,71,71,71 | 0 |
| 55 | MG | 14 | 3167 | 1/1 | 0.86 | 0.33 | 83,83,83,83 | 0 |
| 55 | MG | 14 | 3278 | 1/1 | 0.86 | 0.30 | 84,84,84,84 | 0 |
| 55 | MG | 1J | 210 | 1/1 | 0.86 | 0.09 | 144,144,144,144 | 0 |
| 55 | MG | 1G | 1646 | 1/1 | 0.86 | 0.23 | 93,93,93,93 | 0 |
| 55 | MG | 14 | 3031 | 1/1 | 0.86 | 0.28 | 73,73,73,73 | 0 |
| 55 | MG | 1H | 3290 | 1/1 | 0.86 | 0.31 | 80,80,80,80 | 0 |
| 55 | MG | 1G | 1625 | 1/1 | 0.87 | 0.31 | 85,85,85,85 | 0 |
| 55 | MG | 1G | 1747 | 1/1 | 0.87 | 0.20 | 86,86,86,86 | 0 |
| 55 | MG | 1H | 3081 | 1/1 | 0.87 | 0.32 | 73,73,73,73 | 0 |
| 55 | MG | 14 | 3305 | 1/1 | 0.87 | 0.43 | 89,89,89,89 | 0 |
| 55 | MG | 1H | 3239 | 1/1 | 0.87 | 0.31 | 74,74,74,74 | 0 |
| 55 | MG | 1H | 3197 | 1/1 | 0.87 | 0.37 | 85,85,85,85 | 0 |
| 55 | MG | 1H | 3243 | 1/1 | 0.87 | 0.36 | 52,52,52,52 | 0 |
| 55 | MG | 1H | 3244 | 1/1 | 0.87 | 0.27 | 55,55,55,55 | 0 |
| 55 | MG | 1H | 3303 | 1/1 | 0.87 | 0.26 | 63,63,63,63 | 0 |
| 55 | MG | 1H | 3247 | 1/1 | 0.87 | 0.28 | 51,51,51,51 | 0 |
| 55 | MG | 16 | 207 | 1/1 | 0.87 | 0.28 | 85,85,85,85 | 0 |
| 55 | MG | 1H | 3105 | 1/1 | 0.87 | 0.29 | 90,90,90,90 | 0 |
| 55 | MG | 1H | 3060 | 1/1 | 0.87 | 0.23 | 80,80,80,80 | 0 |
| 55 | MG | 1G | 1696 | 1/1 | 0.87 | 0.39 | 92,92,92,92 | 0 |
| 55 | MG | 14 | 3326 | 1/1 | 0.87 | 0.30 | 90,90,90,90 | 0 |
| 55 | MG | 14 | 3327 | 1/1 | 0.87 | 0.36 | 110,110,110,110 | 0 |
| 55 | MG | 1H | 3256 | 1/1 | 0.87 | 0.24 | 78,78,78,78 | 0 |
| 55 | MG | 1H | 3257 | 1/1 | 0.87 | 0.34 | 83,83,83,83 | 0 |
| 55 | MG | 1G | 1648 | 1/1 | 0.87 | 0.29 | 89,89,89,89 | 0 |
| 55 | MG | 14 | 3254 | 1/1 | 0.87 | 0.39 | 85,85,85,85 | 0 |
| 55 | MG | 1H | 3204 | 1/1 | 0.87 | 0.38 | 83,83,83,83 | 0 |
| 55 | MG | 1H | 3171 | 1/1 | 0.87 | 0.33 | 82,82,82,82 | 0 |
| 55 | MG | 14 | 3051 | 1/1 | 0.87 | 0.30 | 62,62,62,62 | 0 |
| 55 | MG | 14 | 3338 | 1/1 | 0.87 | 0.19 | 78,78,78,78 | 0 |

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| Mol | Type | Chain | Res | Atoms | RSCC | RSR | B-factors(Å$^2$) | Q<0.9 |
|---|---|---|---|---|---|---|---|---|
| 55 | MG | 14 | 3340 | 1/1 | 0.87 | 0.17 | 79,79,79,79 | 0 |
| 55 | MG | 1G | 1651 | 1/1 | 0.87 | 0.56 | 96,96,96,96 | 0 |
| 55 | MG | 14 | 3262 | 1/1 | 0.87 | 0.31 | 86,86,86,86 | 0 |
| 55 | MG | 13 | 1713 | 1/1 | 0.87 | 0.33 | 100,100,100,100 | 0 |
| 55 | MG | 14 | 3351 | 1/1 | 0.87 | 0.30 | 87,87,87,87 | 0 |
| 55 | MG | 14 | 3264 | 1/1 | 0.87 | 0.32 | 84,84,84,84 | 0 |
| 55 | MG | 14 | 3067 | 1/1 | 0.87 | 0.30 | 71,71,71,71 | 0 |
| 55 | MG | 1H | 3125 | 1/1 | 0.87 | 0.29 | 73,73,73,73 | 0 |
| 55 | MG | 1H | 3267 | 1/1 | 0.87 | 0.20 | 57,57,57,57 | 0 |
| 55 | MG | 1H | 3126 | 1/1 | 0.87 | 0.34 | 61,61,61,61 | 0 |
| 55 | MG | 1H | 3269 | 1/1 | 0.87 | 0.31 | 82,82,82,82 | 0 |
| 55 | MG | 1G | 1711 | 1/1 | 0.87 | 0.26 | 73,73,73,73 | 0 |
| 55 | MG | 14 | 3191 | 1/1 | 0.87 | 0.34 | 92,92,92,92 | 0 |
| 55 | MG | 1H | 3215 | 1/1 | 0.87 | 0.32 | 91,91,91,91 | 0 |
| 55 | MG | 1H | 3218 | 1/1 | 0.87 | 0.33 | 82,82,82,82 | 0 |
| 55 | MG | 1H | 3277 | 1/1 | 0.87 | 0.36 | 74,74,74,74 | 0 |
| 55 | MG | 1H | 3219 | 1/1 | 0.87 | 0.39 | 72,72,72,72 | 0 |
| 55 | MG | 14 | 3202 | 1/1 | 0.87 | 0.32 | 74,74,74,74 | 0 |
| 55 | MG | 1H | 3339 | 1/1 | 0.87 | 0.29 | 91,91,91,91 | 0 |
| 55 | MG | 13 | 1677 | 1/1 | 0.87 | 0.12 | 83,83,83,83 | 0 |
| 55 | MG | 1H | 3038 | 1/1 | 0.87 | 0.26 | 59,59,59,59 | 0 |
| 55 | MG | 1H | 3116 | 1/1 | 0.87 | 0.45 | 74,74,74,74 | 0 |
| 55 | MG | 14 | 3293 | 1/1 | 0.87 | 0.16 | 75,75,75,75 | 0 |
| 55 | MG | 1H | 3023 | 1/1 | 0.87 | 0.25 | 55,55,55,55 | 0 |
| 55 | MG | 1H | 3192 | 1/1 | 0.87 | 0.21 | 87,87,87,87 | 0 |
| 55 | MG | 29 | 303 | 1/1 | 0.87 | 0.14 | 74,74,74,74 | 0 |
| 55 | MG | 1H | 3348 | 1/1 | 0.87 | 0.26 | 88,88,88,88 | 0 |
| 55 | MG | E5 | 101 | 1/1 | 0.87 | 0.40 | 88,88,88,88 | 0 |
| 55 | MG | 13 | 1706 | 1/1 | 0.87 | 0.50 | 93,93,93,93 | 0 |
| 55 | MG | 14 | 3219 | 1/1 | 0.87 | 0.19 | 67,67,67,67 | 0 |
| 55 | MG | 1H | 3317 | 1/1 | 0.88 | 0.32 | 63,63,63,63 | 0 |
| 55 | MG | 14 | 3129 | 1/1 | 0.88 | 0.34 | 70,70,70,70 | 0 |
| 55 | MG | 14 | 3130 | 1/1 | 0.88 | 0.12 | 72,72,72,72 | 0 |
| 55 | MG | 14 | 3223 | 1/1 | 0.88 | 0.14 | 64,64,64,64 | 0 |
| 55 | MG | 1H | 3285 | 1/1 | 0.88 | 0.15 | 89,89,89,89 | 0 |
| 55 | MG | 14 | 3225 | 1/1 | 0.88 | 0.27 | 75,75,75,75 | 0 |
| 55 | MG | 14 | 3134 | 1/1 | 0.88 | 0.26 | 80,80,80,80 | 0 |
| 55 | MG | 14 | 3137 | 1/1 | 0.88 | 0.24 | 69,69,69,69 | 0 |
| 55 | MG | 14 | 3234 | 1/1 | 0.88 | 0.17 | 51,51,51,51 | 0 |
| 55 | MG | 1G | 1695 | 1/1 | 0.88 | 0.15 | 86,86,86,86 | 0 |
| 55 | MG | 14 | 3321 | 1/1 | 0.88 | 0.34 | 89,89,89,89 | 0 |
| 55 | MG | 1H | 3258 | 1/1 | 0.88 | 0.34 | 91,91,91,91 | 0 |

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| Mol | Type | Chain | Res | Atoms | RSCC | RSR | B-factors(Å$^2$) | Q<0.9 |
|---|---|---|---|---|---|---|---|---|
| 55 | MG | 1G | 1697 | 1/1 | 0.88 | 0.36 | 85,85,85,85 | 0 |
| 55 | MG | 14 | 3017 | 1/1 | 0.88 | 0.25 | 83,83,83,83 | 0 |
| 55 | MG | 14 | 3242 | 1/1 | 0.88 | 0.45 | 86,86,86,86 | 0 |
| 55 | MG | 13 | 1666 | 1/1 | 0.88 | 0.47 | 104,104,104,104 | 0 |
| 55 | MG | 14 | 3154 | 1/1 | 0.88 | 0.32 | 87,87,87,87 | 0 |
| 55 | MG | 1H | 3102 | 1/1 | 0.88 | 0.17 | 49,49,49,49 | 0 |
| 55 | MG | 13 | 1690 | 1/1 | 0.88 | 0.08 | 118,118,118,118 | 0 |
| 55 | MG | 1H | 3295 | 1/1 | 0.88 | 0.39 | 87,87,87,87 | 0 |
| 55 | MG | 1H | 3403 | 1/1 | 0.88 | 0.15 | 111,111,111,111 | 0 |
| 55 | MG | 1H | 3404 | 1/1 | 0.88 | 0.19 | 80,80,80,80 | 0 |
| 55 | MG | 1H | 3236 | 1/1 | 0.88 | 0.31 | 89,89,89,89 | 0 |
| 55 | MG | 1H | 3333 | 1/1 | 0.88 | 0.25 | 81,81,81,81 | 0 |
| 55 | MG | 14 | 3046 | 1/1 | 0.88 | 0.28 | 75,75,75,75 | 0 |
| 55 | MG | 13 | 1637 | 1/1 | 0.88 | 0.49 | 90,90,90,90 | 0 |
| 55 | MG | 1H | 3299 | 1/1 | 0.88 | 0.18 | 57,57,57,57 | 0 |
| 55 | MG | 14 | 3346 | 1/1 | 0.88 | 0.31 | 84,84,84,84 | 0 |
| 55 | MG | 14 | 3348 | 1/1 | 0.88 | 0.20 | 65,65,65,65 | 0 |
| 55 | MG | 1G | 1668 | 1/1 | 0.88 | 0.22 | 82,82,82,82 | 0 |
| 55 | MG | 14 | 3060 | 1/1 | 0.88 | 0.22 | 64,64,64,64 | 0 |
| 55 | MG | 13 | 1697 | 1/1 | 0.88 | 0.45 | 84,84,84,84 | 0 |
| 55 | MG | 1H | 3184 | 1/1 | 0.88 | 0.33 | 85,85,85,85 | 0 |
| 55 | MG | 1G | 1714 | 1/1 | 0.88 | 0.31 | 98,98,98,98 | 0 |
| 55 | MG | 1G | 1673 | 1/1 | 0.88 | 0.19 | 88,88,88,88 | 0 |
| 55 | MG | 1H | 3374 | 1/1 | 0.88 | 0.16 | 67,67,67,67 | 0 |
| 55 | MG | 14 | 3090 | 1/1 | 0.88 | 0.28 | 70,70,70,70 | 0 |
| 55 | MG | 1H | 3083 | 1/1 | 0.88 | 0.25 | 58,58,58,58 | 0 |
| 55 | MG | 13 | 1733 | 1/1 | 0.88 | 0.07 | 141,141,141,141 | 0 |
| 55 | MG | 13 | 1640 | 1/1 | 0.88 | 0.22 | 89,89,89,89 | 0 |
| 55 | MG | 1G | 1681 | 1/1 | 0.88 | 0.47 | 88,88,88,88 | 0 |
| 55 | MG | 14 | 3367 | 1/1 | 0.88 | 0.13 | 72,72,72,72 | 0 |
| 55 | MG | 1H | 3041 | 1/1 | 0.88 | 0.26 | 63,63,63,63 | 0 |
| 55 | MG | 14 | 3284 | 1/1 | 0.88 | 0.20 | 95,95,95,95 | 0 |
| 55 | MG | 14 | 3101 | 1/1 | 0.88 | 0.24 | 65,65,65,65 | 0 |
| 55 | MG | 1H | 3064 | 1/1 | 0.88 | 0.31 | 70,70,70,70 | 0 |
| 55 | MG | 14 | 3465 | 1/1 | 0.88 | 0.30 | 64,64,64,64 | 0 |
| 55 | MG | 1H | 3381 | 1/1 | 0.88 | 0.37 | 62,62,62,62 | 0 |
| 55 | MG | 1J | 202 | 1/1 | 0.88 | 0.40 | 90,90,90,90 | 0 |
| 55 | MG | 14 | 3207 | 1/1 | 0.88 | 0.24 | 77,77,77,77 | 0 |
| 55 | MG | 1H | 3254 | 1/1 | 0.88 | 0.22 | 69,69,69,69 | 0 |
| 55 | MG | 1H | 3030 | 1/1 | 0.88 | 0.27 | 91,91,91,91 | 0 |
| 55 | MG | 14 | 3295 | 1/1 | 0.88 | 0.28 | 72,72,72,72 | 0 |
| 55 | MG | 1G | 1601 | 1/1 | 0.88 | 0.21 | 76,76,76,76 | 0 |

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| Mol | Type | Chain | Res | Atoms | RSCC | RSR | B-factors(Å$^2$) | Q<0.9 |
|---|---|---|---|---|---|---|---|---|
| 55 | MG | 14 | 3115 | 1/1 | 0.88 | 0.14 | 58,58,58,58 | 0 |
| 55 | MG | 1G | 1647 | 1/1 | 0.88 | 0.23 | 80,80,80,80 | 0 |
| 55 | MG | 55 | 201 | 1/1 | 0.88 | 0.27 | 68,68,68,68 | 0 |
| 55 | MG | 1G | 1690 | 1/1 | 0.88 | 0.27 | 98,98,98,98 | 0 |
| 55 | MG | 1H | 3355 | 1/1 | 0.88 | 0.51 | 107,107,107,107 | 0 |
| 55 | MG | 1H | 3099 | 1/1 | 0.88 | 0.32 | 52,52,52,52 | 0 |
| 55 | MG | 14 | 3160 | 1/1 | 0.89 | 0.18 | 74,74,74,74 | 0 |
| 55 | MG | 1G | 1630 | 1/1 | 0.89 | 0.33 | 81,81,81,81 | 0 |
| 55 | MG | 14 | 3061 | 1/1 | 0.89 | 0.25 | 70,70,70,70 | 0 |
| 55 | MG | 1H | 3292 | 1/1 | 0.89 | 0.41 | 82,82,82,82 | 0 |
| 55 | MG | 1H | 3373 | 1/1 | 0.89 | 0.32 | 79,79,79,79 | 0 |
| 55 | MG | 1G | 1680 | 1/1 | 0.89 | 0.35 | 88,88,88,88 | 0 |
| 55 | MG | 1G | 1633 | 1/1 | 0.89 | 0.36 | 80,80,80,80 | 0 |
| 55 | MG | 1H | 3072 | 1/1 | 0.89 | 0.31 | 75,75,75,75 | 0 |
| 55 | MG | 13 | 1632 | 1/1 | 0.89 | 0.39 | 74,74,74,74 | 0 |
| 55 | MG | 16 | 212 | 1/1 | 0.89 | 0.15 | 85,85,85,85 | 0 |
| 55 | MG | 14 | 3259 | 1/1 | 0.89 | 0.22 | 82,82,82,82 | 0 |
| 55 | MG | 1H | 3147 | 1/1 | 0.89 | 0.36 | 60,60,60,60 | 0 |
| 55 | MG | 1H | 3033 | 1/1 | 0.89 | 0.18 | 83,83,83,83 | 0 |
| 55 | MG | 88 | 201 | 1/1 | 0.89 | 0.18 | 98,98,98,98 | 0 |
| 55 | MG | 14 | 3098 | 1/1 | 0.89 | 0.26 | 46,46,46,46 | 0 |
| 55 | MG | 13 | 1606 | 1/1 | 0.89 | 0.20 | 92,92,92,92 | 0 |
| 55 | MG | 14 | 3265 | 1/1 | 0.89 | 0.31 | 76,76,76,76 | 0 |
| 55 | MG | 14 | 3266 | 1/1 | 0.89 | 0.49 | 88,88,88,88 | 0 |
| 55 | MG | 14 | 3189 | 1/1 | 0.89 | 0.26 | 63,63,63,63 | 0 |
| 55 | MG | 1H | 3298 | 1/1 | 0.89 | 0.43 | 87,87,87,87 | 0 |
| 55 | MG | 1H | 3265 | 1/1 | 0.89 | 0.23 | 83,83,83,83 | 0 |
| 55 | MG | 1H | 3187 | 1/1 | 0.89 | 0.17 | 83,83,83,83 | 0 |
| 55 | MG | 1H | 3056 | 1/1 | 0.89 | 0.37 | 68,68,68,68 | 0 |
| 55 | MG | 1H | 3154 | 1/1 | 0.89 | 0.28 | 79,79,79,79 | 0 |
| 55 | MG | 1H | 3155 | 1/1 | 0.89 | 0.28 | 38,38,38,38 | 0 |
| 55 | MG | 13 | 1635 | 1/1 | 0.89 | 0.23 | 95,95,95,95 | 0 |
| 55 | MG | 1H | 3273 | 1/1 | 0.89 | 0.26 | 103,103,103,103 | 0 |
| 55 | MG | 14 | 3281 | 1/1 | 0.89 | 0.39 | 82,82,82,82 | 0 |
| 55 | MG | 14 | 3358 | 1/1 | 0.89 | 0.12 | 85,85,85,85 | 0 |
| 55 | MG | 14 | 3001 | 1/1 | 0.89 | 0.24 | 70,70,70,70 | 0 |
| 55 | MG | 14 | 3002 | 1/1 | 0.89 | 0.16 | 67,67,67,67 | 0 |
| 55 | MG | 14 | 3007 | 1/1 | 0.89 | 0.24 | 58,58,58,58 | 0 |
| 55 | MG | 14 | 3213 | 1/1 | 0.89 | 0.26 | 68,68,68,68 | 0 |
| 55 | MG | 14 | 3009 | 1/1 | 0.89 | 0.22 | 58,58,58,58 | 0 |
| 55 | MG | 1G | 1655 | 1/1 | 0.89 | 0.45 | 74,74,74,74 | 0 |
| 55 | MG | 1H | 3275 | 1/1 | 0.89 | 0.18 | 69,69,69,69 | 0 |

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| Mol | Type | Chain | Res | Atoms | RSCC | RSR | B-factors(Å$^2$) | Q<0.9 |
|---|---|---|---|---|---|---|---|---|
| 55 | MG | 13 | 1675 | 1/1 | 0.89 | 0.27 | 85,85,85,85 | 0 |
| 55 | MG | 13 | 1710 | 1/1 | 0.89 | 0.20 | 103,103,103,103 | 0 |
| 55 | MG | 1H | 3004 | 1/1 | 0.89 | 0.33 | 49,49,49,49 | 0 |
| 55 | MG | 14 | 3026 | 1/1 | 0.89 | 0.24 | 78,78,78,78 | 0 |
| 55 | MG | 1H | 3109 | 1/1 | 0.89 | 0.23 | 76,76,76,76 | 0 |
| 55 | MG | 1H | 3111 | 1/1 | 0.89 | 0.20 | 71,71,71,71 | 0 |
| 55 | MG | 14 | 3034 | 1/1 | 0.89 | 0.30 | 73,73,73,73 | 0 |
| 55 | MG | 13 | 1629 | 1/1 | 0.89 | 0.25 | 60,60,60,60 | 0 |
| 55 | MG | 14 | 3152 | 1/1 | 0.89 | 0.30 | 72,72,72,72 | 0 |
| 55 | MG | 14 | 3231 | 1/1 | 0.89 | 0.21 | 76,76,76,76 | 0 |
| 55 | MG | 1H | 3065 | 1/1 | 0.89 | 0.24 | 64,64,64,64 | 0 |
| 55 | MG | 1H | 3117 | 1/1 | 0.89 | 0.31 | 75,75,75,75 | 0 |
| 55 | MG | 14 | 3235 | 1/1 | 0.89 | 0.10 | 63,63,63,63 | 0 |
| 55 | MG | 1H | 3326 | 1/1 | 0.89 | 0.10 | 78,78,78,78 | 0 |
| 55 | MG | 1H | 3327 | 1/1 | 0.89 | 0.21 | 63,63,63,63 | 0 |
| 55 | MG | 1H | 3142 | 1/1 | 0.89 | 0.20 | 74,74,74,74 | 0 |
| 55 | MG | 1H | 3213 | 1/1 | 0.89 | 0.47 | 84,84,84,84 | 0 |
| 55 | MG | 1H | 3354 | 1/1 | 0.90 | 0.32 | 88,88,88,88 | 0 |
| 55 | MG | 13 | 1622 | 1/1 | 0.90 | 0.35 | 74,74,74,74 | 0 |
| 55 | MG | 14 | 3212 | 1/1 | 0.90 | 0.21 | 66,66,66,66 | 0 |
| 55 | MG | 1G | 1620 | 1/1 | 0.90 | 0.46 | 96,96,96,96 | 0 |
| 55 | MG | 1H | 3007 | 1/1 | 0.90 | 0.28 | 62,62,62,62 | 0 |
| 55 | MG | 1H | 3189 | 1/1 | 0.90 | 0.09 | 83,83,83,83 | 0 |
| 55 | MG | 13 | 1715 | 1/1 | 0.90 | 0.13 | 70,70,70,70 | 0 |
| 55 | MG | 1H | 3316 | 1/1 | 0.90 | 0.10 | 61,61,61,61 | 0 |
| 55 | MG | 14 | 3118 | 1/1 | 0.90 | 0.16 | 84,84,84,84 | 0 |
| 55 | MG | 1H | 3016 | 1/1 | 0.90 | 0.21 | 56,56,56,56 | 0 |
| 55 | MG | 1H | 3087 | 1/1 | 0.90 | 0.22 | 49,49,49,49 | 0 |
| 55 | MG | 14 | 3124 | 1/1 | 0.90 | 0.16 | 56,56,56,56 | 0 |
| 55 | MG | 14 | 3313 | 1/1 | 0.90 | 0.16 | 86,86,86,86 | 0 |
| 55 | MG | 14 | 3125 | 1/1 | 0.90 | 0.30 | 88,88,88,88 | 0 |
| 55 | MG | 14 | 3316 | 1/1 | 0.90 | 0.22 | 70,70,70,70 | 0 |
| 55 | MG | 1G | 1628 | 1/1 | 0.90 | 0.18 | 90,90,90,90 | 0 |
| 55 | MG | 1H | 3514 | 1/1 | 0.90 | 0.20 | 109,109,109,109 | 0 |
| 55 | MG | 1H | 3522 | 1/1 | 0.90 | 0.13 | 68,68,68,68 | 0 |
| 55 | MG | 14 | 3229 | 1/1 | 0.90 | 0.26 | 64,64,64,64 | 0 |
| 55 | MG | 14 | 3230 | 1/1 | 0.90 | 0.29 | 75,75,75,75 | 0 |
| 55 | MG | 16 | 201 | 1/1 | 0.90 | 0.10 | 110,110,110,110 | 0 |
| 55 | MG | 14 | 3131 | 1/1 | 0.90 | 0.14 | 66,66,66,66 | 0 |
| 55 | MG | 13 | 1669 | 1/1 | 0.90 | 0.28 | 77,77,77,77 | 0 |
| 55 | MG | 1H | 3157 | 1/1 | 0.90 | 0.31 | 79,79,79,79 | 0 |
| 55 | MG | 14 | 3135 | 1/1 | 0.90 | 0.18 | 64,64,64,64 | 0 |

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| Mol | Type | Chain | Res | Atoms | RSCC | RSR | B-factors(Å$^2$) | Q<0.9 |
|---|---|---|---|---|---|---|---|---|
| 55 | MG | 16 | 205 | 1/1 | 0.90 | 0.10 | 109,109,109,109 | 0 |
| 55 | MG | 14 | 3330 | 1/1 | 0.90 | 0.24 | 81,81,81,81 | 0 |
| 55 | MG | 14 | 3140 | 1/1 | 0.90 | 0.41 | 77,77,77,77 | 0 |
| 55 | MG | 14 | 3332 | 1/1 | 0.90 | 0.21 | 83,83,83,83 | 0 |
| 55 | MG | 14 | 3240 | 1/1 | 0.90 | 0.20 | 95,95,95,95 | 0 |
| 55 | MG | 1H | 3052 | 1/1 | 0.90 | 0.20 | 73,73,73,73 | 0 |
| 55 | MG | 13 | 1643 | 1/1 | 0.90 | 0.38 | 86,86,86,86 | 0 |
| 55 | MG | 13 | 1738 | 1/1 | 0.90 | 0.10 | 138,138,138,138 | 0 |
| 55 | MG | 14 | 3246 | 1/1 | 0.90 | 0.30 | 83,83,83,83 | 0 |
| 55 | MG | 14 | 3339 | 1/1 | 0.90 | 0.26 | 74,74,74,74 | 0 |
| 55 | MG | 13 | 1679 | 1/1 | 0.90 | 0.25 | 80,80,80,80 | 0 |
| 55 | MG | 13 | 1680 | 1/1 | 0.90 | 0.27 | 77,77,77,77 | 0 |
| 55 | MG | 3I | 201 | 1/1 | 0.90 | 0.14 | 80,80,80,80 | 0 |
| 55 | MG | 14 | 3153 | 1/1 | 0.90 | 0.50 | 82,82,82,82 | 0 |
| 55 | MG | 1H | 3063 | 1/1 | 0.90 | 0.20 | 63,63,63,63 | 0 |
| 55 | MG | 14 | 3029 | 1/1 | 0.90 | 0.32 | 51,51,51,51 | 0 |
| 55 | MG | 1H | 3212 | 1/1 | 0.90 | 0.26 | 78,78,78,78 | 0 |
| 55 | MG | 11 | 301 | 1/1 | 0.90 | 0.19 | 54,54,54,54 | 0 |
| 55 | MG | 14 | 3035 | 1/1 | 0.90 | 0.25 | 57,57,57,57 | 0 |
| 55 | MG | 1H | 3336 | 1/1 | 0.90 | 0.30 | 83,83,83,83 | 0 |
| 55 | MG | 14 | 3037 | 1/1 | 0.90 | 0.34 | 71,71,71,71 | 0 |
| 55 | MG | 13 | 1709 | 1/1 | 0.90 | 0.27 | 78,78,78,78 | 0 |
| 55 | MG | 13 | 1620 | 1/1 | 0.90 | 0.27 | 66,66,66,66 | 0 |
| 55 | MG | 14 | 3359 | 1/1 | 0.90 | 0.11 | 89,89,89,89 | 0 |
| 55 | MG | 14 | 3360 | 1/1 | 0.90 | 0.21 | 74,74,74,74 | 0 |
| 55 | MG | 1H | 3217 | 1/1 | 0.90 | 0.32 | 92,92,92,92 | 0 |
| 55 | MG | 1H | 3300 | 1/1 | 0.90 | 0.23 | 77,77,77,77 | 0 |
| 55 | MG | 14 | 3052 | 1/1 | 0.90 | 0.38 | 65,65,65,65 | 0 |
| 55 | MG | 1G | 1707 | 1/1 | 0.90 | 0.33 | 90,90,90,90 | 0 |
| 55 | MG | 14 | 3170 | 1/1 | 0.90 | 0.20 | 79,79,79,79 | 0 |
| 55 | MG | 14 | 3055 | 1/1 | 0.90 | 0.25 | 61,61,61,61 | 0 |
| 55 | MG | 1H | 3068 | 1/1 | 0.90 | 0.18 | 61,61,61,61 | 0 |
| 55 | MG | 1H | 3344 | 1/1 | 0.90 | 0.43 | 84,84,84,84 | 0 |
| 55 | MG | 13 | 1651 | 1/1 | 0.90 | 0.28 | 73,73,73,73 | 0 |
| 55 | MG | 1H | 3386 | 1/1 | 0.90 | 0.20 | 66,66,66,66 | 0 |
| 55 | MG | 1G | 1712 | 1/1 | 0.90 | 0.14 | 109,109,109,109 | 0 |
| 55 | MG | 14 | 3279 | 1/1 | 0.90 | 0.41 | 84,84,84,84 | 0 |
| 55 | MG | 13 | 1603 | 1/1 | 0.90 | 0.17 | 96,96,96,96 | 0 |
| 55 | MG | 14 | 3078 | 1/1 | 0.90 | 0.28 | 60,60,60,60 | 0 |
| 55 | MG | 1H | 3388 | 1/1 | 0.90 | 0.21 | 74,74,74,74 | 0 |
| 55 | MG | 1G | 1715 | 1/1 | 0.90 | 0.15 | 106,106,106,106 | 0 |
| 55 | MG | 1G | 1663 | 1/1 | 0.90 | 0.31 | 81,81,81,81 | 0 |

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| Mol | Type | Chain | Res | Atoms | RSCC | RSR | B-factors(Å$^2$) | Q<0.9 |
|---|---|---|---|---|---|---|---|---|
| 55 | MG | 1H | 3002 | 1/1 | 0.90 | 0.20 | 53,53,53,53 | 0 |
| 55 | MG | 1H | 3185 | 1/1 | 0.90 | 0.33 | 91,91,91,91 | 0 |
| 55 | MG | 1G | 1666 | 1/1 | 0.90 | 0.31 | 72,72,72,72 | 0 |
| 55 | MG | 1H | 3352 | 1/1 | 0.90 | 0.40 | 97,97,97,97 | 0 |
| 55 | MG | 13 | 1654 | 1/1 | 0.90 | 0.26 | 72,72,72,72 | 0 |
| 55 | MG | 1G | 1615 | 1/1 | 0.90 | 0.19 | 78,78,78,78 | 0 |
| 55 | MG | 1G | 1617 | 1/1 | 0.90 | 0.38 | 71,71,71,71 | 0 |
| 55 | MG | 14 | 3039 | 1/1 | 0.91 | 0.10 | 67,67,67,67 | 0 |
| 55 | MG | 13 | 1612 | 1/1 | 0.91 | 0.27 | 102,102,102,102 | 0 |
| 55 | MG | 14 | 3041 | 1/1 | 0.91 | 0.29 | 58,58,58,58 | 0 |
| 55 | MG | 14 | 3307 | 1/1 | 0.91 | 0.39 | 89,89,89,89 | 0 |
| 55 | MG | 1H | 3225 | 1/1 | 0.91 | 0.33 | 77,77,77,77 | 0 |
| 55 | MG | 21 | 302 | 1/1 | 0.91 | 0.20 | 68,68,68,68 | 0 |
| 55 | MG | 1H | 3289 | 1/1 | 0.91 | 0.25 | 78,78,78,78 | 0 |
| 55 | MG | 1H | 3128 | 1/1 | 0.91 | 0.32 | 63,63,63,63 | 0 |
| 55 | MG | 1H | 3291 | 1/1 | 0.91 | 0.20 | 68,68,68,68 | 0 |
| 55 | MG | 1H | 3324 | 1/1 | 0.91 | 0.33 | 66,66,66,66 | 0 |
| 55 | MG | 14 | 3148 | 1/1 | 0.91 | 0.47 | 86,86,86,86 | 0 |
| 55 | MG | 14 | 3057 | 1/1 | 0.91 | 0.31 | 54,54,54,54 | 0 |
| 55 | MG | 14 | 3059 | 1/1 | 0.91 | 0.21 | 60,60,60,60 | 0 |
| 55 | MG | 1H | 3259 | 1/1 | 0.91 | 0.25 | 93,93,93,93 | 0 |
| 55 | MG | 1G | 1687 | 1/1 | 0.91 | 0.31 | 79,79,79,79 | 0 |
| 55 | MG | 14 | 3062 | 1/1 | 0.91 | 0.32 | 72,72,72,72 | 0 |
| 55 | MG | 14 | 3065 | 1/1 | 0.91 | 0.32 | 50,50,50,50 | 0 |
| 55 | MG | 14 | 3066 | 1/1 | 0.91 | 0.18 | 63,63,63,63 | 0 |
| 55 | MG | 1H | 3228 | 1/1 | 0.91 | 0.27 | 63,63,63,63 | 0 |
| 55 | MG | 14 | 3243 | 1/1 | 0.91 | 0.18 | 78,78,78,78 | 0 |
| 55 | MG | 14 | 3068 | 1/1 | 0.91 | 0.29 | 66,66,66,66 | 0 |
| 55 | MG | 1G | 1741 | 1/1 | 0.91 | 0.14 | 112,112,112,112 | 0 |
| 55 | MG | 1H | 3229 | 1/1 | 0.91 | 0.13 | 54,54,54,54 | 0 |
| 55 | MG | 14 | 3076 | 1/1 | 0.91 | 0.40 | 47,47,47,47 | 0 |
| 55 | MG | 1G | 1604 | 1/1 | 0.91 | 0.11 | 78,78,78,78 | 0 |
| 55 | MG | 1H | 3208 | 1/1 | 0.91 | 0.41 | 69,69,69,69 | 0 |
| 55 | MG | 1H | 3402 | 1/1 | 0.91 | 0.13 | 77,77,77,77 | 0 |
| 55 | MG | 14 | 3253 | 1/1 | 0.91 | 0.21 | 105,105,105,105 | 0 |
| 55 | MG | 1H | 3233 | 1/1 | 0.91 | 0.24 | 72,72,72,72 | 0 |
| 55 | MG | 1H | 3014 | 1/1 | 0.91 | 0.20 | 51,51,51,51 | 0 |
| 55 | MG | 14 | 3092 | 1/1 | 0.91 | 0.39 | 70,70,70,70 | 0 |
| 55 | MG | 13 | 1619 | 1/1 | 0.91 | 0.24 | 74,74,74,74 | 0 |
| 55 | MG | 14 | 3173 | 1/1 | 0.91 | 0.29 | 70,70,70,70 | 0 |
| 55 | MG | 1H | 3003 | 1/1 | 0.91 | 0.22 | 54,54,54,54 | 0 |
| 55 | MG | 14 | 3175 | 1/1 | 0.91 | 0.34 | 85,85,85,85 | 0 |

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| Mol | Type | Chain | Res | Atoms | RSCC | RSR | B-factors(Å$^2$) | Q<0.9 |
|---|---|---|---|---|---|---|---|---|
| 55 | MG | 14 | 3178 | 1/1 | 0.91 | 0.37 | 81,81,81,81 | 0 |
| 55 | MG | 1G | 1612 | 1/1 | 0.91 | 0.10 | 84,84,84,84 | 0 |
| 55 | MG | 1G | 1613 | 1/1 | 0.91 | 0.06 | 92,92,92,92 | 0 |
| 55 | MG | 1H | 3469 | 1/1 | 0.91 | 0.09 | 115,115,115,115 | 0 |
| 55 | MG | 1H | 3502 | 1/1 | 0.91 | 0.09 | 148,148,148,148 | 0 |
| 55 | MG | 14 | 3104 | 1/1 | 0.91 | 0.29 | 59,59,59,59 | 0 |
| 55 | MG | 14 | 3270 | 1/1 | 0.91 | 0.39 | 76,76,76,76 | 0 |
| 55 | MG | 14 | 3188 | 1/1 | 0.91 | 0.31 | 76,76,76,76 | 0 |
| 55 | MG | 13 | 1646 | 1/1 | 0.91 | 0.38 | 90,90,90,90 | 0 |
| 55 | MG | 14 | 3190 | 1/1 | 0.91 | 0.36 | 95,95,95,95 | 0 |
| 55 | MG | 14 | 3107 | 1/1 | 0.91 | 0.34 | 80,80,80,80 | 0 |
| 55 | MG | 14 | 3192 | 1/1 | 0.91 | 0.14 | 56,56,56,56 | 0 |
| 55 | MG | 14 | 3363 | 1/1 | 0.91 | 0.11 | 61,61,61,61 | 0 |
| 55 | MG | 14 | 3277 | 1/1 | 0.91 | 0.31 | 78,78,78,78 | 0 |
| 55 | MG | 1H | 3177 | 1/1 | 0.91 | 0.15 | 69,69,69,69 | 0 |
| 55 | MG | 14 | 3109 | 1/1 | 0.91 | 0.25 | 85,85,85,85 | 0 |
| 55 | MG | 1H | 3241 | 1/1 | 0.91 | 0.18 | 69,69,69,69 | 0 |
| 55 | MG | 14 | 3198 | 1/1 | 0.91 | 0.28 | 70,70,70,70 | 0 |
| 55 | MG | 14 | 3199 | 1/1 | 0.91 | 0.12 | 60,60,60,60 | 0 |
| 55 | MG | 1H | 3216 | 1/1 | 0.91 | 0.39 | 90,90,90,90 | 0 |
| 55 | MG | 13 | 1696 | 1/1 | 0.91 | 0.16 | 86,86,86,86 | 0 |
| 55 | MG | 14 | 3285 | 1/1 | 0.91 | 0.29 | 93,93,93,93 | 0 |
| 55 | MG | 1H | 3306 | 1/1 | 0.91 | 0.15 | 83,83,83,83 | 0 |
| 55 | MG | 14 | 3116 | 1/1 | 0.91 | 0.23 | 49,49,49,49 | 0 |
| 55 | MG | 1H | 3245 | 1/1 | 0.91 | 0.31 | 86,86,86,86 | 0 |
| 55 | MG | 2K | 105 | 1/1 | 0.91 | 0.18 | 76,76,76,76 | 0 |
| 55 | MG | 1H | 3347 | 1/1 | 0.91 | 0.27 | 72,72,72,72 | 0 |
| 55 | MG | 1H | 3250 | 1/1 | 0.91 | 0.09 | 73,73,73,73 | 0 |
| 55 | MG | 14 | 3032 | 1/1 | 0.91 | 0.29 | 64,64,64,64 | 0 |
| 55 | MG | 14 | 3033 | 1/1 | 0.91 | 0.35 | 71,71,71,71 | 0 |
| 55 | MG | 1G | 1671 | 1/1 | 0.91 | 0.20 | 92,92,92,92 | 0 |
| 55 | MG | 15 | 201 | 1/1 | 0.91 | 0.35 | 99,99,99,99 | 0 |
| 55 | MG | 1H | 3039 | 1/1 | 0.91 | 0.27 | 68,68,68,68 | 0 |
| 55 | MG | 1H | 3145 | 1/1 | 0.91 | 0.20 | 46,46,46,46 | 0 |
| 55 | MG | F5 | 101 | 1/1 | 0.91 | 0.29 | 77,77,77,77 | 0 |
| 55 | MG | 1H | 3351 | 1/1 | 0.91 | 0.15 | 90,90,90,90 | 0 |
| 55 | MG | 1H | 3103 | 1/1 | 0.91 | 0.36 | 71,71,71,71 | 0 |
| 55 | MG | 14 | 3294 | 1/1 | 0.92 | 0.17 | 81,81,81,81 | 0 |
| 55 | MG | 14 | 3201 | 1/1 | 0.92 | 0.27 | 61,61,61,61 | 0 |
| 55 | MG | 1H | 3132 | 1/1 | 0.92 | 0.32 | 76,76,76,76 | 0 |
| 55 | MG | 14 | 3204 | 1/1 | 0.92 | 0.35 | 70,70,70,70 | 0 |
| 55 | MG | 14 | 3010 | 1/1 | 0.92 | 0.19 | 47,47,47,47 | 0 |

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| Mol | Type | Chain | Res | Atoms | RSCC | RSR | B-factors(Å$^2$) | Q<0.9 |
|---|---|---|---|---|---|---|---|---|
| 55 | MG | 1H | 3278 | 1/1 | 0.92 | 0.36 | 76,76,76,76 | 0 |
| 55 | MG | 1H | 3010 | 1/1 | 0.92 | 0.29 | 66,66,66,66 | 0 |
| 55 | MG | 1H | 3136 | 1/1 | 0.92 | 0.35 | 85,85,85,85 | 0 |
| 55 | MG | 14 | 3019 | 1/1 | 0.92 | 0.33 | 68,68,68,68 | 0 |
| 55 | MG | 1H | 3196 | 1/1 | 0.92 | 0.35 | 80,80,80,80 | 0 |
| 55 | MG | 14 | 3022 | 1/1 | 0.92 | 0.24 | 60,60,60,60 | 0 |
| 55 | MG | 14 | 3306 | 1/1 | 0.92 | 0.16 | 74,74,74,74 | 0 |
| 55 | MG | 14 | 3023 | 1/1 | 0.92 | 0.20 | 72,72,72,72 | 0 |
| 55 | MG | 1H | 3137 | 1/1 | 0.92 | 0.20 | 60,60,60,60 | 0 |
| 55 | MG | 1H | 3199 | 1/1 | 0.92 | 0.10 | 72,72,72,72 | 0 |
| 55 | MG | 14 | 3122 | 1/1 | 0.92 | 0.18 | 61,61,61,61 | 0 |
| 55 | MG | 1H | 3328 | 1/1 | 0.92 | 0.33 | 85,85,85,85 | 0 |
| 55 | MG | 1H | 3042 | 1/1 | 0.92 | 0.15 | 95,95,95,95 | 0 |
| 55 | MG | 14 | 3030 | 1/1 | 0.92 | 0.24 | 60,60,60,60 | 0 |
| 55 | MG | 1G | 1645 | 1/1 | 0.92 | 0.15 | 79,79,79,79 | 0 |
| 55 | MG | 1H | 3202 | 1/1 | 0.92 | 0.14 | 94,94,94,94 | 0 |
| 55 | MG | 14 | 3128 | 1/1 | 0.92 | 0.32 | 76,76,76,76 | 0 |
| 55 | MG | 1H | 3331 | 1/1 | 0.92 | 0.15 | 84,84,84,84 | 0 |
| 55 | MG | 1H | 3165 | 1/1 | 0.92 | 0.34 | 74,74,74,74 | 0 |
| 55 | MG | 1H | 3166 | 1/1 | 0.92 | 0.18 | 67,67,67,67 | 0 |
| 55 | MG | 1H | 3139 | 1/1 | 0.92 | 0.47 | 69,69,69,69 | 0 |
| 55 | MG | 98 | 201 | 1/1 | 0.92 | 0.54 | 89,89,89,89 | 0 |
| 55 | MG | 1H | 3248 | 1/1 | 0.92 | 0.16 | 61,61,61,61 | 0 |
| 55 | MG | 1G | 1706 | 1/1 | 0.92 | 0.32 | 86,86,86,86 | 0 |
| 55 | MG | 1H | 3382 | 1/1 | 0.92 | 0.12 | 79,79,79,79 | 0 |
| 55 | MG | 14 | 3141 | 1/1 | 0.92 | 0.41 | 85,85,85,85 | 0 |
| 55 | MG | Q8 | 101 | 1/1 | 0.92 | 0.16 | 99,99,99,99 | 0 |
| 55 | MG | 14 | 3042 | 1/1 | 0.92 | 0.35 | 67,67,67,67 | 0 |
| 55 | MG | 14 | 3043 | 1/1 | 0.92 | 0.28 | 62,62,62,62 | 0 |
| 55 | MG | 1H | 3337 | 1/1 | 0.92 | 0.19 | 94,94,94,94 | 0 |
| 55 | MG | 14 | 3048 | 1/1 | 0.92 | 0.29 | 55,55,55,55 | 0 |
| 55 | MG | 14 | 3149 | 1/1 | 0.92 | 0.09 | 66,66,66,66 | 0 |
| 55 | MG | 1H | 3079 | 1/1 | 0.92 | 0.28 | 66,66,66,66 | 0 |
| 55 | MG | 14 | 3245 | 1/1 | 0.92 | 0.32 | 64,64,64,64 | 0 |
| 55 | MG | 1H | 3169 | 1/1 | 0.92 | 0.35 | 83,83,83,83 | 0 |
| 55 | MG | 14 | 3341 | 1/1 | 0.92 | 0.09 | 95,95,95,95 | 0 |
| 55 | MG | 14 | 3053 | 1/1 | 0.92 | 0.19 | 59,59,59,59 | 0 |
| 55 | MG | 13 | 1652 | 1/1 | 0.92 | 0.17 | 88,88,88,88 | 0 |
| 55 | MG | 1H | 3172 | 1/1 | 0.92 | 0.19 | 69,69,69,69 | 0 |
| 55 | MG | 1H | 3255 | 1/1 | 0.92 | 0.10 | 92,92,92,92 | 0 |
| 55 | MG | 1G | 1662 | 1/1 | 0.92 | 0.33 | 84,84,84,84 | 0 |
| 55 | MG | 1G | 1606 | 1/1 | 0.92 | 0.17 | 80,80,80,80 | 0 |

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| Mol | Type | Chain | Res | Atoms | RSCC | RSR | B-factors(Å$^2$) | Q<0.9 |
|---|---|---|---|---|---|---|---|---|
| 55 | MG | 1H | 3026 | 1/1 | 0.92 | 0.16 | 66,66,66,66 | 0 |
| 55 | MG | 1H | 3174 | 1/1 | 0.92 | 0.23 | 89,89,89,89 | 0 |
| 55 | MG | 14 | 3257 | 1/1 | 0.92 | 0.21 | 75,75,75,75 | 0 |
| 55 | MG | 1H | 3392 | 1/1 | 0.92 | 0.27 | 73,73,73,73 | 0 |
| 55 | MG | 1H | 3395 | 1/1 | 0.92 | 0.43 | 76,76,76,76 | 0 |
| 55 | MG | 1H | 3176 | 1/1 | 0.92 | 0.27 | 73,73,73,73 | 0 |
| 55 | MG | 1H | 3144 | 1/1 | 0.92 | 0.34 | 69,69,69,69 | 0 |
| 55 | MG | 1H | 3122 | 1/1 | 0.92 | 0.19 | 82,82,82,82 | 0 |
| 55 | MG | 1H | 3179 | 1/1 | 0.92 | 0.07 | 60,60,60,60 | 0 |
| 55 | MG | 1H | 3045 | 1/1 | 0.92 | 0.20 | 88,88,88,88 | 0 |
| 55 | MG | 14 | 3075 | 1/1 | 0.92 | 0.21 | 52,52,52,52 | 0 |
| 55 | MG | 1H | 3036 | 1/1 | 0.92 | 0.14 | 70,70,70,70 | 0 |
| 55 | MG | 1G | 1739 | 1/1 | 0.92 | 0.12 | 154,154,154,154 | 0 |
| 55 | MG | 14 | 3079 | 1/1 | 0.92 | 0.26 | 82,82,82,82 | 0 |
| 55 | MG | 14 | 3081 | 1/1 | 0.92 | 0.29 | 70,70,70,70 | 0 |
| 55 | MG | 13 | 1627 | 1/1 | 0.92 | 0.44 | 65,65,65,65 | 0 |
| 55 | MG | 14 | 3179 | 1/1 | 0.92 | 0.60 | 88,88,88,88 | 0 |
| 55 | MG | 14 | 3083 | 1/1 | 0.92 | 0.27 | 68,68,68,68 | 0 |
| 55 | MG | 14 | 3181 | 1/1 | 0.92 | 0.32 | 70,70,70,70 | 0 |
| 55 | MG | 14 | 3380 | 1/1 | 0.92 | 0.11 | 79,79,79,79 | 0 |
| 55 | MG | 14 | 3436 | 1/1 | 0.92 | 0.09 | 107,107,107,107 | 0 |
| 55 | MG | 14 | 3450 | 1/1 | 0.92 | 0.15 | 105,105,105,105 | 0 |
| 55 | MG | 14 | 3085 | 1/1 | 0.92 | 0.33 | 72,72,72,72 | 0 |
| 55 | MG | 14 | 3086 | 1/1 | 0.92 | 0.22 | 51,51,51,51 | 0 |
| 55 | MG | 1G | 1676 | 1/1 | 0.92 | 0.34 | 98,98,98,98 | 0 |
| 55 | MG | 1H | 3090 | 1/1 | 0.92 | 0.16 | 47,47,47,47 | 0 |
| 55 | MG | 1H | 3311 | 1/1 | 0.92 | 0.41 | 83,83,83,83 | 0 |
| 55 | MG | 1H | 3092 | 1/1 | 0.92 | 0.30 | 62,62,62,62 | 0 |
| 55 | MG | 1H | 3465 | 1/1 | 0.92 | 0.15 | 87,87,87,87 | 0 |
| 55 | MG | 1H | 3015 | 1/1 | 0.92 | 0.29 | 46,46,46,46 | 0 |
| 55 | MG | 1H | 3227 | 1/1 | 0.92 | 0.35 | 76,76,76,76 | 0 |
| 55 | MG | 1H | 3129 | 1/1 | 0.92 | 0.20 | 63,63,63,63 | 0 |
| 55 | MG | 14 | 3194 | 1/1 | 0.92 | 0.17 | 46,46,46,46 | 0 |
| 55 | MG | 1H | 3518 | 1/1 | 0.92 | 0.07 | 135,135,135,135 | 0 |
| 55 | MG | 13 | 1642 | 1/1 | 0.92 | 0.41 | 66,66,66,66 | 0 |
| 55 | MG | 14 | 3103 | 1/1 | 0.92 | 0.28 | 58,58,58,58 | 0 |
| 55 | MG | 1H | 3021 | 1/1 | 0.92 | 0.17 | 51,51,51,51 | 0 |
| 55 | MG | 1H | 3318 | 1/1 | 0.92 | 0.22 | 75,75,75,75 | 0 |
| 55 | MG | 1H | 3095 | 1/1 | 0.93 | 0.28 | 46,46,46,46 | 0 |
| 55 | MG | 14 | 3050 | 1/1 | 0.93 | 0.10 | 65,65,65,65 | 0 |
| 55 | MG | 14 | 3274 | 1/1 | 0.93 | 0.14 | 69,69,69,69 | 0 |
| 55 | MG | 14 | 3334 | 1/1 | 0.93 | 0.35 | 84,84,84,84 | 0 |

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| Mol | Type | Chain | Res | Atoms | RSCC | RSR | B-factors(Å$^2$) | Q<0.9 |
|---|---|---|---|---|---|---|---|---|
| 55 | MG | 2L | 101 | 1/1 | 0.93 | 0.12 | 77,77,77,77 | 0 |
| 55 | MG | 1H | 3335 | 1/1 | 0.93 | 0.29 | 70,70,70,70 | 0 |
| 55 | MG | 14 | 3168 | 1/1 | 0.93 | 0.34 | 76,76,76,76 | 0 |
| 55 | MG | 13 | 1605 | 1/1 | 0.93 | 0.12 | 84,84,84,84 | 0 |
| 55 | MG | 1H | 3075 | 1/1 | 0.93 | 0.35 | 87,87,87,87 | 0 |
| 55 | MG | 13 | 1634 | 1/1 | 0.93 | 0.27 | 73,73,73,73 | 0 |
| 55 | MG | 14 | 3004 | 1/1 | 0.93 | 0.25 | 57,57,57,57 | 0 |
| 55 | MG | 14 | 3005 | 1/1 | 0.93 | 0.22 | 52,52,52,52 | 0 |
| 55 | MG | 14 | 3058 | 1/1 | 0.93 | 0.13 | 63,63,63,63 | 0 |
| 55 | MG | 13 | 1736 | 1/1 | 0.93 | 0.06 | 132,132,132,132 | 0 |
| 55 | MG | 13 | 1657 | 1/1 | 0.93 | 0.38 | 74,74,74,74 | 0 |
| 55 | MG | 1H | 3191 | 1/1 | 0.93 | 0.40 | 64,64,64,64 | 0 |
| 55 | MG | 14 | 3350 | 1/1 | 0.93 | 0.23 | 77,77,77,77 | 0 |
| 55 | MG | 14 | 3011 | 1/1 | 0.93 | 0.25 | 47,47,47,47 | 0 |
| 55 | MG | 14 | 3289 | 1/1 | 0.93 | 0.15 | 175,175,175,175 | 0 |
| 55 | MG | 14 | 3064 | 1/1 | 0.93 | 0.23 | 52,52,52,52 | 0 |
| 55 | MG | 14 | 3237 | 1/1 | 0.93 | 0.28 | 74,74,74,74 | 0 |
| 55 | MG | 14 | 3355 | 1/1 | 0.93 | 0.25 | 73,73,73,73 | 0 |
| 55 | MG | 14 | 3012 | 1/1 | 0.93 | 0.26 | 53,53,53,53 | 0 |
| 55 | MG | 1G | 1639 | 1/1 | 0.93 | 0.48 | 97,97,97,97 | 0 |
| 55 | MG | 14 | 3015 | 1/1 | 0.93 | 0.10 | 64,64,64,64 | 0 |
| 55 | MG | 1H | 3467 | 1/1 | 0.93 | 0.13 | 72,72,72,72 | 0 |
| 55 | MG | 1G | 1677 | 1/1 | 0.93 | 0.48 | 89,89,89,89 | 0 |
| 55 | MG | 1H | 3281 | 1/1 | 0.93 | 0.30 | 80,80,80,80 | 0 |
| 55 | MG | 14 | 3298 | 1/1 | 0.93 | 0.27 | 69,69,69,69 | 0 |
| 55 | MG | 1H | 3497 | 1/1 | 0.93 | 0.09 | 105,105,105,105 | 0 |
| 55 | MG | 1H | 3501 | 1/1 | 0.93 | 0.10 | 99,99,99,99 | 0 |
| 55 | MG | 1H | 3080 | 1/1 | 0.93 | 0.18 | 62,62,62,62 | 0 |
| 55 | MG | 13 | 1601 | 1/1 | 0.93 | 0.17 | 103,103,103,103 | 0 |
| 55 | MG | 1H | 3170 | 1/1 | 0.93 | 0.25 | 89,89,89,89 | 0 |
| 55 | MG | 1H | 3082 | 1/1 | 0.93 | 0.36 | 72,72,72,72 | 0 |
| 55 | MG | 1H | 3224 | 1/1 | 0.93 | 0.26 | 83,83,83,83 | 0 |
| 55 | MG | 1H | 3287 | 1/1 | 0.93 | 0.36 | 78,78,78,78 | 0 |
| 55 | MG | 1H | 3034 | 1/1 | 0.93 | 0.11 | 54,54,54,54 | 0 |
| 55 | MG | 1H | 3009 | 1/1 | 0.93 | 0.20 | 44,44,44,44 | 0 |
| 55 | MG | 14 | 3413 | 1/1 | 0.93 | 0.09 | 70,70,70,70 | 0 |
| 55 | MG | 14 | 3088 | 1/1 | 0.93 | 0.29 | 70,70,70,70 | 0 |
| 55 | MG | 14 | 3449 | 1/1 | 0.93 | 0.08 | 108,108,108,108 | 0 |
| 55 | MG | 14 | 3311 | 1/1 | 0.93 | 0.32 | 87,87,87,87 | 0 |
| 55 | MG | 14 | 3455 | 1/1 | 0.93 | 0.10 | 108,108,108,108 | 0 |
| 55 | MG | 14 | 3256 | 1/1 | 0.93 | 0.36 | 67,67,67,67 | 0 |
| 55 | MG | 1H | 3152 | 1/1 | 0.93 | 0.30 | 80,80,80,80 | 0 |

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| Mol | Type | Chain | Res | Atoms | RSCC | RSR | B-factors(Å$^2$) | Q<0.9 |
|---|---|---|---|---|---|---|---|---|
| 55 | MG | 13 | 1626 | 1/1 | 0.93 | 0.32 | 65,65,65,65 | 0 |
| 55 | MG | 14 | 3205 | 1/1 | 0.93 | 0.30 | 70,70,70,70 | 0 |
| 55 | MG | 1H | 3067 | 1/1 | 0.93 | 0.16 | 47,47,47,47 | 0 |
| 55 | MG | 1H | 3231 | 1/1 | 0.93 | 0.52 | 88,88,88,88 | 0 |
| 55 | MG | 1H | 3001 | 1/1 | 0.93 | 0.27 | 50,50,50,50 | 0 |
| 55 | MG | 1J | 209 | 1/1 | 0.93 | 0.07 | 128,128,128,128 | 0 |
| 55 | MG | 1H | 3071 | 1/1 | 0.93 | 0.26 | 51,51,51,51 | 0 |
| 55 | MG | 1G | 1622 | 1/1 | 0.93 | 0.39 | 86,86,86,86 | 0 |
| 55 | MG | 1H | 3206 | 1/1 | 0.93 | 0.35 | 72,72,72,72 | 0 |
| 55 | MG | 1H | 3235 | 1/1 | 0.93 | 0.39 | 88,88,88,88 | 0 |
| 55 | MG | 1H | 3135 | 1/1 | 0.93 | 0.19 | 72,72,72,72 | 0 |
| 55 | MG | C5 | 201 | 1/1 | 0.93 | 0.24 | 86,86,86,86 | 0 |
| 55 | MG | 14 | 3268 | 1/1 | 0.93 | 0.40 | 85,85,85,85 | 0 |
| 55 | MG | 1H | 3028 | 1/1 | 0.93 | 0.20 | 53,53,53,53 | 0 |
| 55 | MG | 1H | 3055 | 1/1 | 0.93 | 0.47 | 77,77,77,77 | 0 |
| 55 | MG | 14 | 3217 | 1/1 | 0.93 | 0.24 | 55,55,55,55 | 0 |
| 55 | MG | 1H | 3022 | 1/1 | 0.94 | 0.09 | 60,60,60,60 | 0 |
| 55 | MG | 13 | 1609 | 1/1 | 0.94 | 0.16 | 83,83,83,83 | 0 |
| 55 | MG | 14 | 3347 | 1/1 | 0.94 | 0.17 | 83,83,83,83 | 0 |
| 55 | MG | 13 | 1641 | 1/1 | 0.94 | 0.20 | 67,67,67,67 | 0 |
| 55 | MG | 1H | 3013 | 1/1 | 0.94 | 0.26 | 47,47,47,47 | 0 |
| 55 | MG | 13 | 1670 | 1/1 | 0.94 | 0.09 | 106,106,106,106 | 0 |
| 55 | MG | 1G | 1738 | 1/1 | 0.94 | 0.12 | 140,140,140,140 | 0 |
| 55 | MG | 1H | 3148 | 1/1 | 0.94 | 0.14 | 86,86,86,86 | 0 |
| 55 | MG | 1H | 3242 | 1/1 | 0.94 | 0.17 | 45,45,45,45 | 0 |
| 55 | MG | 1G | 1743 | 1/1 | 0.94 | 0.16 | 105,105,105,105 | 0 |
| 55 | MG | 14 | 3196 | 1/1 | 0.94 | 0.08 | 60,60,60,60 | 0 |
| 55 | MG | 1H | 3274 | 1/1 | 0.94 | 0.40 | 71,71,71,71 | 0 |
| 55 | MG | 1H | 3393 | 1/1 | 0.94 | 0.10 | 62,62,62,62 | 0 |
| 55 | MG | 14 | 3089 | 1/1 | 0.94 | 0.30 | 71,71,71,71 | 0 |
| 55 | MG | 1H | 3113 | 1/1 | 0.94 | 0.16 | 40,40,40,40 | 0 |
| 55 | MG | 1H | 3115 | 1/1 | 0.94 | 0.17 | 51,51,51,51 | 0 |
| 55 | MG | 13 | 1602 | 1/1 | 0.94 | 0.13 | 78,78,78,78 | 0 |
| 55 | MG | 14 | 3203 | 1/1 | 0.94 | 0.20 | 55,55,55,55 | 0 |
| 55 | MG | 1H | 3195 | 1/1 | 0.94 | 0.14 | 79,79,79,79 | 0 |
| 55 | MG | 11 | 302 | 1/1 | 0.94 | 0.18 | 85,85,85,85 | 0 |
| 55 | MG | 14 | 3095 | 1/1 | 0.94 | 0.15 | 65,65,65,65 | 0 |
| 55 | MG | 1H | 3078 | 1/1 | 0.94 | 0.24 | 71,71,71,71 | 0 |
| 55 | MG | 1H | 3222 | 1/1 | 0.94 | 0.30 | 65,65,65,65 | 0 |
| 55 | MG | 14 | 3047 | 1/1 | 0.94 | 0.23 | 57,57,57,57 | 0 |
| 55 | MG | 14 | 3210 | 1/1 | 0.94 | 0.21 | 68,68,68,68 | 0 |
| 55 | MG | 14 | 3371 | 1/1 | 0.94 | 0.22 | 84,84,84,84 | 0 |

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| Mol | Type | Chain | Res | Atoms | RSCC | RSR | B-factors(Å$^2$) | Q<0.9 |
|---|---|---|---|---|---|---|---|---|
| 55 | MG | 1H | 3368 | 1/1 | 0.94 | 0.27 | 72,72,72,72 | 0 |
| 55 | MG | 14 | 3102 | 1/1 | 0.94 | 0.18 | 61,61,61,61 | 0 |
| 55 | MG | 14 | 3376 | 1/1 | 0.94 | 0.09 | 66,66,66,66 | 0 |
| 55 | MG | 1H | 3048 | 1/1 | 0.94 | 0.18 | 58,58,58,58 | 0 |
| 55 | MG | 14 | 3385 | 1/1 | 0.94 | 0.08 | 73,73,73,73 | 0 |
| 55 | MG | 1H | 3198 | 1/1 | 0.94 | 0.25 | 77,77,77,77 | 0 |
| 55 | MG | 1H | 3008 | 1/1 | 0.94 | 0.19 | 44,44,44,44 | 0 |
| 55 | MG | 14 | 3438 | 1/1 | 0.94 | 0.09 | 83,83,83,83 | 0 |
| 55 | MG | 14 | 3322 | 1/1 | 0.94 | 0.13 | 70,70,70,70 | 0 |
| 55 | MG | 1H | 3066 | 1/1 | 0.94 | 0.30 | 70,70,70,70 | 0 |
| 55 | MG | 14 | 3006 | 1/1 | 0.94 | 0.20 | 56,56,56,56 | 0 |
| 55 | MG | 1G | 1635 | 1/1 | 0.94 | 0.44 | 70,70,70,70 | 0 |
| 55 | MG | 14 | 3110 | 1/1 | 0.94 | 0.37 | 63,63,63,63 | 0 |
| 55 | MG | 1G | 1636 | 1/1 | 0.94 | 0.35 | 80,80,80,80 | 0 |
| 55 | MG | 1H | 3425 | 1/1 | 0.94 | 0.12 | 61,61,61,61 | 0 |
| 55 | MG | 1H | 3017 | 1/1 | 0.94 | 0.24 | 47,47,47,47 | 0 |
| 55 | MG | 1H | 3345 | 1/1 | 0.94 | 0.24 | 67,67,67,67 | 0 |
| 55 | MG | 1H | 3054 | 1/1 | 0.94 | 0.19 | 51,51,51,51 | 0 |
| 55 | MG | 1H | 3070 | 1/1 | 0.94 | 0.15 | 60,60,60,60 | 0 |
| 55 | MG | 1H | 3161 | 1/1 | 0.94 | 0.21 | 69,69,69,69 | 0 |
| 55 | MG | 19 | 301 | 1/1 | 0.94 | 0.28 | 67,67,67,67 | 0 |
| 55 | MG | 1H | 3182 | 1/1 | 0.94 | 0.08 | 70,70,70,70 | 0 |
| 55 | MG | 14 | 3177 | 1/1 | 0.94 | 0.35 | 76,76,76,76 | 0 |
| 55 | MG | 39 | 301 | 1/1 | 0.94 | 0.13 | 83,83,83,83 | 0 |
| 55 | MG | 1H | 3508 | 1/1 | 0.94 | 0.06 | 119,119,119,119 | 0 |
| 55 | MG | 1H | 3262 | 1/1 | 0.94 | 0.10 | 71,71,71,71 | 0 |
| 55 | MG | 14 | 3021 | 1/1 | 0.94 | 0.06 | 63,63,63,63 | 0 |
| 55 | MG | 1H | 3141 | 1/1 | 0.94 | 0.29 | 65,65,65,65 | 0 |
| 55 | MG | 1H | 3520 | 1/1 | 0.94 | 0.10 | 103,103,103,103 | 0 |
| 55 | MG | 13 | 1739 | 1/1 | 0.94 | 0.14 | 90,90,90,90 | 0 |
| 55 | MG | 14 | 3071 | 1/1 | 0.94 | 0.15 | 62,62,62,62 | 0 |
| 55 | MG | 1H | 3158 | 1/1 | 0.95 | 0.25 | 71,71,71,71 | 0 |
| 55 | MG | 1H | 3513 | 1/1 | 0.95 | 0.06 | 116,116,116,116 | 0 |
| 55 | MG | 1H | 3058 | 1/1 | 0.95 | 0.31 | 60,60,60,60 | 0 |
| 55 | MG | 14 | 3045 | 1/1 | 0.95 | 0.12 | 41,41,41,41 | 0 |
| 55 | MG | 14 | 3146 | 1/1 | 0.95 | 0.29 | 64,64,64,64 | 0 |
| 55 | MG | 1G | 1672 | 1/1 | 0.95 | 0.33 | 79,79,79,79 | 0 |
| 55 | MG | 1H | 3011 | 1/1 | 0.95 | 0.34 | 54,54,54,54 | 0 |
| 55 | MG | 1H | 3089 | 1/1 | 0.95 | 0.24 | 38,38,38,38 | 0 |
| 55 | MG | 1H | 3046 | 1/1 | 0.95 | 0.21 | 71,71,71,71 | 0 |
| 55 | MG | 14 | 3097 | 1/1 | 0.95 | 0.25 | 54,54,54,54 | 0 |
| 55 | MG | 1G | 1641 | 1/1 | 0.95 | 0.31 | 83,83,83,83 | 0 |

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| Mol | Type | Chain | Res | Atoms | RSCC | RSR | B-factors(Å$^2$) | Q<0.9 |
|---|---|---|---|---|---|---|---|---|
| 55 | MG | 14 | 3099 | 1/1 | 0.95 | 0.14 | 67,67,67,67 | 0 |
| 55 | MG | 14 | 3008 | 1/1 | 0.95 | 0.19 | 53,53,53,53 | 0 |
| 55 | MG | 1H | 3523 | 1/1 | 0.95 | 0.07 | 78,78,78,78 | 0 |
| 55 | MG | 1H | 3394 | 1/1 | 0.95 | 0.08 | 69,69,69,69 | 0 |
| 55 | MG | 16 | 202 | 1/1 | 0.95 | 0.17 | 84,84,84,84 | 0 |
| 55 | MG | 1H | 3018 | 1/1 | 0.95 | 0.16 | 50,50,50,50 | 0 |
| 55 | MG | 14 | 3315 | 1/1 | 0.95 | 0.34 | 85,85,85,85 | 0 |
| 55 | MG | 1H | 3321 | 1/1 | 0.95 | 0.34 | 79,79,79,79 | 0 |
| 55 | MG | 1H | 3020 | 1/1 | 0.95 | 0.21 | 52,52,52,52 | 0 |
| 55 | MG | 13 | 1630 | 1/1 | 0.95 | 0.13 | 61,61,61,61 | 0 |
| 55 | MG | 1H | 3114 | 1/1 | 0.95 | 0.06 | 56,56,56,56 | 0 |
| 55 | MG | 1G | 1616 | 1/1 | 0.95 | 0.10 | 62,62,62,62 | 0 |
| 55 | MG | 1H | 3051 | 1/1 | 0.95 | 0.17 | 47,47,47,47 | 0 |
| 55 | MG | 1H | 3401 | 1/1 | 0.95 | 0.14 | 67,67,67,67 | 0 |
| 55 | MG | 1H | 3230 | 1/1 | 0.95 | 0.30 | 71,71,71,71 | 0 |
| 55 | MG | 14 | 3432 | 1/1 | 0.95 | 0.14 | 100,100,100,100 | 0 |
| 55 | MG | 1H | 3149 | 1/1 | 0.95 | 0.32 | 82,82,82,82 | 0 |
| 55 | MG | 14 | 3024 | 1/1 | 0.95 | 0.20 | 49,49,49,49 | 0 |
| 55 | MG | 1H | 3302 | 1/1 | 0.95 | 0.09 | 74,74,74,74 | 0 |
| 55 | MG | 13 | 1649 | 1/1 | 0.95 | 0.39 | 84,84,84,84 | 0 |
| 55 | MG | 14 | 3454 | 1/1 | 0.95 | 0.10 | 106,106,106,106 | 0 |
| 55 | MG | 1H | 3133 | 1/1 | 0.95 | 0.11 | 49,49,49,49 | 0 |
| 55 | MG | 14 | 3462 | 1/1 | 0.95 | 0.05 | 130,130,130,130 | 0 |
| 55 | MG | 14 | 3463 | 1/1 | 0.95 | 0.09 | 130,130,130,130 | 0 |
| 55 | MG | 13 | 1720 | 1/1 | 0.95 | 0.09 | 129,129,129,129 | 0 |
| 55 | MG | 14 | 3227 | 1/1 | 0.95 | 0.33 | 80,80,80,80 | 0 |
| 55 | MG | 14 | 3176 | 1/1 | 0.95 | 0.25 | 63,63,63,63 | 0 |
| 55 | MG | 14 | 3073 | 1/1 | 0.95 | 0.15 | 58,58,58,58 | 0 |
| 55 | MG | 14 | 3074 | 1/1 | 0.95 | 0.14 | 47,47,47,47 | 0 |
| 55 | MG | 1G | 1740 | 1/1 | 0.95 | 0.08 | 140,140,140,140 | 0 |
| 55 | MG | 1H | 3449 | 1/1 | 0.95 | 0.19 | 94,94,94,94 | 0 |
| 55 | MG | 14 | 3077 | 1/1 | 0.95 | 0.20 | 61,61,61,61 | 0 |
| 55 | MG | 1H | 3457 | 1/1 | 0.95 | 0.12 | 102,102,102,102 | 0 |
| 55 | MG | 1G | 1661 | 1/1 | 0.95 | 0.37 | 76,76,76,76 | 0 |
| 55 | MG | 1H | 3024 | 1/1 | 0.95 | 0.19 | 61,61,61,61 | 0 |
| 55 | MG | 1H | 3069 | 1/1 | 0.95 | 0.17 | 51,51,51,51 | 0 |
| 55 | MG | 1H | 3237 | 1/1 | 0.95 | 0.23 | 67,67,67,67 | 0 |
| 55 | MG | 14 | 3343 | 1/1 | 0.95 | 0.33 | 86,86,86,86 | 0 |
| 55 | MG | 2K | 102 | 1/1 | 0.95 | 0.24 | 93,93,93,93 | 0 |
| 55 | MG | 1H | 3499 | 1/1 | 0.95 | 0.06 | 111,111,111,111 | 0 |
| 55 | MG | 1H | 3005 | 1/1 | 0.95 | 0.15 | 44,44,44,44 | 0 |
| 55 | MG | 14 | 3138 | 1/1 | 0.95 | 0.15 | 58,58,58,58 | 0 |

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| Mol | Type | Chain | Res | Atoms | RSCC | RSR | B-factors(Å$^2$) | Q<0.9 |
|---|---|---|---|---|---|---|---|---|
| 55 | MG | 14 | 3139 | 1/1 | 0.95 | 0.36 | 69,69,69,69 | 0 |
| 55 | MG | 1H | 3086 | 1/1 | 0.95 | 0.17 | 59,59,59,59 | 0 |
| 55 | MG | 14 | 3310 | 1/1 | 0.96 | 0.36 | 75,75,75,75 | 0 |
| 55 | MG | 14 | 3080 | 1/1 | 0.96 | 0.39 | 81,81,81,81 | 0 |
| 55 | MG | 1H | 3439 | 1/1 | 0.96 | 0.11 | 92,92,92,92 | 0 |
| 55 | MG | 14 | 3003 | 1/1 | 0.96 | 0.13 | 47,47,47,47 | 0 |
| 55 | MG | 1H | 3251 | 1/1 | 0.96 | 0.18 | 56,56,56,56 | 0 |
| 55 | MG | 1H | 3452 | 1/1 | 0.96 | 0.07 | 58,58,58,58 | 0 |
| 55 | MG | 1H | 3310 | 1/1 | 0.96 | 0.23 | 72,72,72,72 | 0 |
| 55 | MG | 1H | 3019 | 1/1 | 0.96 | 0.15 | 61,61,61,61 | 0 |
| 55 | MG | 1H | 3359 | 1/1 | 0.96 | 0.21 | 77,77,77,77 | 0 |
| 55 | MG | 13 | 1731 | 1/1 | 0.96 | 0.12 | 153,153,153,153 | 0 |
| 55 | MG | 14 | 3320 | 1/1 | 0.96 | 0.09 | 88,88,88,88 | 0 |
| 55 | MG | 14 | 3049 | 1/1 | 0.96 | 0.12 | 55,55,55,55 | 0 |
| 55 | MG | 14 | 3370 | 1/1 | 0.96 | 0.24 | 75,75,75,75 | 0 |
| 55 | MG | 1H | 3482 | 1/1 | 0.96 | 0.11 | 70,70,70,70 | 0 |
| 55 | MG | 14 | 3183 | 1/1 | 0.96 | 0.25 | 56,56,56,56 | 0 |
| 55 | MG | 1H | 3488 | 1/1 | 0.96 | 0.11 | 66,66,66,66 | 0 |
| 55 | MG | 1H | 3495 | 1/1 | 0.96 | 0.06 | 79,79,79,79 | 0 |
| 55 | MG | 14 | 3013 | 1/1 | 0.96 | 0.13 | 56,56,56,56 | 0 |
| 55 | MG | 14 | 3233 | 1/1 | 0.96 | 0.37 | 67,67,67,67 | 0 |
| 55 | MG | 14 | 3407 | 1/1 | 0.96 | 0.07 | 83,83,83,83 | 0 |
| 55 | MG | 1H | 3097 | 1/1 | 0.96 | 0.25 | 70,70,70,70 | 0 |
| 55 | MG | 14 | 3424 | 1/1 | 0.96 | 0.09 | 81,81,81,81 | 0 |
| 55 | MG | 14 | 3429 | 1/1 | 0.96 | 0.14 | 77,77,77,77 | 0 |
| 55 | MG | 14 | 3431 | 1/1 | 0.96 | 0.05 | 102,102,102,102 | 0 |
| 55 | MG | 13 | 1631 | 1/1 | 0.96 | 0.07 | 60,60,60,60 | 0 |
| 55 | MG | 1H | 3091 | 1/1 | 0.96 | 0.26 | 59,59,59,59 | 0 |
| 55 | MG | 1H | 3270 | 1/1 | 0.96 | 0.06 | 84,84,84,84 | 0 |
| 55 | MG | 14 | 3443 | 1/1 | 0.96 | 0.07 | 103,103,103,103 | 0 |
| 55 | MG | 14 | 3446 | 1/1 | 0.96 | 0.07 | 87,87,87,87 | 0 |
| 55 | MG | 1H | 3383 | 1/1 | 0.96 | 0.15 | 60,60,60,60 | 0 |
| 55 | MG | 1H | 3510 | 1/1 | 0.96 | 0.07 | 111,111,111,111 | 0 |
| 55 | MG | 1H | 3511 | 1/1 | 0.96 | 0.06 | 119,119,119,119 | 0 |
| 55 | MG | 1H | 3214 | 1/1 | 0.96 | 0.21 | 64,64,64,64 | 0 |
| 55 | MG | 14 | 3458 | 1/1 | 0.96 | 0.06 | 108,108,108,108 | 0 |
| 55 | MG | 1H | 3101 | 1/1 | 0.96 | 0.14 | 50,50,50,50 | 0 |
| 55 | MG | 14 | 3063 | 1/1 | 0.96 | 0.20 | 51,51,51,51 | 0 |
| 55 | MG | 1G | 1634 | 1/1 | 0.96 | 0.43 | 80,80,80,80 | 0 |
| 55 | MG | 14 | 3106 | 1/1 | 0.96 | 0.39 | 75,75,75,75 | 0 |
| 55 | MG | 1H | 3517 | 1/1 | 0.96 | 0.05 | 113,113,113,113 | 0 |
| 55 | MG | 1G | 1744 | 1/1 | 0.96 | 0.09 | 128,128,128,128 | 0 |

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| Mol | Type | Chain | Res | Atoms | RSCC | RSR | B-factors(Å$^2$) | Q<0.9 |
|---|---|---|---|---|---|---|---|---|
| 55 | MG | 1H | 3246 | 1/1 | 0.96 | 0.10 | 48,48,48,48 | 0 |
| 55 | MG | 1G | 1746 | 1/1 | 0.96 | 0.09 | 134,134,134,134 | 0 |
| 55 | MG | 14 | 3344 | 1/1 | 0.96 | 0.08 | 95,95,95,95 | 0 |
| 55 | MG | 1H | 3519 | 1/1 | 0.96 | 0.07 | 103,103,103,103 | 0 |
| 55 | MG | 1H | 3085 | 1/1 | 0.96 | 0.12 | 63,63,63,63 | 0 |
| 55 | MG | 1H | 3261 | 1/1 | 0.96 | 0.26 | 72,72,72,72 | 0 |
| 55 | MG | 29 | 301 | 1/1 | 0.96 | 0.22 | 72,72,72,72 | 0 |
| 55 | MG | 29 | 302 | 1/1 | 0.96 | 0.22 | 51,51,51,51 | 0 |
| 55 | MG | 14 | 3114 | 1/1 | 0.96 | 0.15 | 56,56,56,56 | 0 |
| 55 | MG | 7E | 201 | 1/1 | 0.96 | 0.21 | 83,83,83,83 | 0 |
| 55 | MG | 14 | 3164 | 1/1 | 0.96 | 0.25 | 60,60,60,60 | 0 |
| 55 | MG | 1H | 3408 | 1/1 | 0.96 | 0.09 | 54,54,54,54 | 0 |
| 55 | MG | 45 | 201 | 1/1 | 0.96 | 0.29 | 76,76,76,76 | 0 |
| 55 | MG | 1H | 3410 | 1/1 | 0.96 | 0.12 | 52,52,52,52 | 0 |
| 55 | MG | 1H | 3423 | 1/1 | 0.96 | 0.10 | 61,61,61,61 | 0 |
| 55 | MG | 13 | 1628 | 1/1 | 0.96 | 0.23 | 71,71,71,71 | 0 |
| 55 | MG | 14 | 3121 | 1/1 | 0.96 | 0.11 | 54,54,54,54 | 0 |
| 55 | MG | 1H | 3436 | 1/1 | 0.96 | 0.05 | 94,94,94,94 | 0 |
| 55 | MG | 1H | 3438 | 1/1 | 0.96 | 0.12 | 60,60,60,60 | 0 |
| 55 | MG | 1H | 3494 | 1/1 | 0.97 | 0.06 | 81,81,81,81 | 0 |
| 55 | MG | 14 | 3374 | 1/1 | 0.97 | 0.07 | 52,52,52,52 | 0 |
| 55 | MG | 1H | 3371 | 1/1 | 0.97 | 0.05 | 62,62,62,62 | 0 |
| 55 | MG | 1H | 3272 | 1/1 | 0.97 | 0.19 | 76,76,76,76 | 0 |
| 55 | MG | 14 | 3288 | 1/1 | 0.97 | 0.08 | 171,171,171,171 | 0 |
| 55 | MG | 14 | 3391 | 1/1 | 0.97 | 0.07 | 62,62,62,62 | 0 |
| 55 | MG | 1H | 3110 | 1/1 | 0.97 | 0.27 | 47,47,47,47 | 0 |
| 55 | MG | 1H | 3210 | 1/1 | 0.97 | 0.34 | 79,79,79,79 | 0 |
| 55 | MG | 14 | 3414 | 1/1 | 0.97 | 0.07 | 56,56,56,56 | 0 |
| 55 | MG | 14 | 3420 | 1/1 | 0.97 | 0.06 | 89,89,89,89 | 0 |
| 55 | MG | 1H | 3050 | 1/1 | 0.97 | 0.24 | 47,47,47,47 | 0 |
| 55 | MG | 14 | 3425 | 1/1 | 0.97 | 0.06 | 96,96,96,96 | 0 |
| 55 | MG | 1H | 3504 | 1/1 | 0.97 | 0.08 | 80,80,80,80 | 0 |
| 55 | MG | 1H | 3288 | 1/1 | 0.97 | 0.23 | 72,72,72,72 | 0 |
| 55 | MG | 14 | 3250 | 1/1 | 0.97 | 0.22 | 70,70,70,70 | 0 |
| 55 | MG | 1H | 3509 | 1/1 | 0.97 | 0.09 | 85,85,85,85 | 0 |
| 55 | MG | 14 | 3437 | 1/1 | 0.97 | 0.07 | 85,85,85,85 | 0 |
| 55 | MG | 1G | 1732 | 1/1 | 0.97 | 0.04 | 113,113,113,113 | 0 |
| 55 | MG | 14 | 3439 | 1/1 | 0.97 | 0.05 | 101,101,101,101 | 0 |
| 55 | MG | 14 | 3442 | 1/1 | 0.97 | 0.06 | 107,107,107,107 | 0 |
| 55 | MG | 1G | 1733 | 1/1 | 0.97 | 0.05 | 93,93,93,93 | 0 |
| 55 | MG | 1G | 1735 | 1/1 | 0.97 | 0.06 | 96,96,96,96 | 0 |
| 55 | MG | 1G | 1737 | 1/1 | 0.97 | 0.04 | 114,114,114,114 | 0 |

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| Mol | Type | Chain | Res | Atoms | RSCC | RSR | B-factors(Å$^2$) | Q<0.9 |
|---|---|---|---|---|---|---|---|---|
| 55 | MG | 1H | 3429 | 1/1 | 0.97 | 0.07 | 71,71,71,71 | 0 |
| 55 | MG | 14 | 3452 | 1/1 | 0.97 | 0.12 | 100,100,100,100 | 0 |
| 55 | MG | 14 | 3016 | 1/1 | 0.97 | 0.12 | 63,63,63,63 | 0 |
| 55 | MG | 1H | 3183 | 1/1 | 0.97 | 0.40 | 63,63,63,63 | 0 |
| 55 | MG | 14 | 3457 | 1/1 | 0.97 | 0.04 | 125,125,125,125 | 0 |
| 55 | MG | 1H | 3378 | 1/1 | 0.97 | 0.06 | 91,91,91,91 | 0 |
| 55 | MG | 14 | 3460 | 1/1 | 0.97 | 0.06 | 112,112,112,112 | 0 |
| 55 | MG | 1H | 3175 | 1/1 | 0.97 | 0.40 | 74,74,74,74 | 0 |
| 55 | MG | 14 | 3133 | 1/1 | 0.97 | 0.28 | 71,71,71,71 | 0 |
| 55 | MG | 14 | 3464 | 1/1 | 0.97 | 0.10 | 101,101,101,101 | 0 |
| 55 | MG | 1G | 1742 | 1/1 | 0.97 | 0.06 | 112,112,112,112 | 0 |
| 55 | MG | 1H | 3515 | 1/1 | 0.97 | 0.05 | 106,106,106,106 | 0 |
| 55 | MG | 14 | 3136 | 1/1 | 0.97 | 0.28 | 75,75,75,75 | 0 |
| 55 | MG | I8 | 102 | 1/1 | 0.97 | 0.26 | 65,65,65,65 | 0 |
| 55 | MG | 1H | 3443 | 1/1 | 0.97 | 0.05 | 75,75,75,75 | 0 |
| 55 | MG | 1H | 3062 | 1/1 | 0.97 | 0.12 | 48,48,48,48 | 0 |
| 55 | MG | 13 | 1735 | 1/1 | 0.97 | 0.09 | 106,106,106,106 | 0 |
| 55 | MG | 1J | 208 | 1/1 | 0.97 | 0.06 | 97,97,97,97 | 0 |
| 55 | MG | 13 | 1722 | 1/1 | 0.97 | 0.07 | 101,101,101,101 | 0 |
| 55 | MG | 14 | 3184 | 1/1 | 0.97 | 0.20 | 71,71,71,71 | 0 |
| 55 | MG | 14 | 3142 | 1/1 | 0.97 | 0.27 | 72,72,72,72 | 0 |
| 55 | MG | 14 | 3027 | 1/1 | 0.97 | 0.15 | 71,71,71,71 | 0 |
| 55 | MG | 13 | 1737 | 1/1 | 0.97 | 0.06 | 111,111,111,111 | 0 |
| 55 | MG | 1H | 3308 | 1/1 | 0.97 | 0.07 | 106,106,106,106 | 0 |
| 55 | MG | 1H | 3338 | 1/1 | 0.97 | 0.06 | 78,78,78,78 | 0 |
| 55 | MG | 3A | 201 | 1/1 | 0.97 | 0.14 | 81,81,81,81 | 0 |
| 55 | MG | 1H | 3481 | 1/1 | 0.97 | 0.05 | 64,64,64,64 | 0 |
| 55 | MG | 25 | 201 | 1/1 | 0.97 | 0.05 | 111,111,111,111 | 0 |
| 55 | MG | 13 | 1718 | 1/1 | 0.97 | 0.05 | 85,85,85,85 | 0 |
| 55 | MG | 1H | 3484 | 1/1 | 0.97 | 0.05 | 118,118,118,118 | 0 |
| 55 | MG | 14 | 3151 | 1/1 | 0.97 | 0.39 | 78,78,78,78 | 0 |
| 55 | MG | 14 | 3072 | 1/1 | 0.97 | 0.24 | 54,54,54,54 | 0 |
| 55 | MG | 2L | 103 | 1/1 | 0.97 | 0.05 | 130,130,130,130 | 0 |
| 56 | ZN | 3E | 302 | 1/1 | 0.97 | 0.22 | 102,102,102,102 | 0 |
| 55 | MG | 1H | 3249 | 1/1 | 0.97 | 0.41 | 66,66,66,66 | 0 |
| 56 | ZN | 5A | 101 | 1/1 | 0.97 | 0.06 | 133,133,133,133 | 0 |
| 55 | MG | 1H | 3490 | 1/1 | 0.97 | 0.07 | 89,89,89,89 | 0 |
| 55 | MG | 14 | 3400 | 1/1 | 0.98 | 0.06 | 65,65,65,65 | 0 |
| 55 | MG | 14 | 3401 | 1/1 | 0.98 | 0.08 | 82,82,82,82 | 0 |
| 55 | MG | 14 | 3402 | 1/1 | 0.98 | 0.07 | 82,82,82,82 | 0 |
| 55 | MG | 14 | 3406 | 1/1 | 0.98 | 0.04 | 61,61,61,61 | 0 |
| 55 | MG | 1H | 3500 | 1/1 | 0.98 | 0.11 | 65,65,65,65 | 0 |

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| Mol | Type | Chain | Res | Atoms | RSCC | RSR | B-factors(Å$^2$) | Q<0.9 |
|---|---|---|---|---|---|---|---|---|
| 55 | MG | 14 | 3409 | 1/1 | 0.98 | 0.07 | 64,64,64,64 | 0 |
| 55 | MG | 13 | 1732 | 1/1 | 0.98 | 0.06 | 128,128,128,128 | 0 |
| 55 | MG | 13 | 1717 | 1/1 | 0.98 | 0.06 | 66,66,66,66 | 0 |
| 55 | MG | 14 | 3416 | 1/1 | 0.98 | 0.06 | 52,52,52,52 | 0 |
| 55 | MG | 1H | 3430 | 1/1 | 0.98 | 0.05 | 76,76,76,76 | 0 |
| 55 | MG | 1H | 3506 | 1/1 | 0.98 | 0.05 | 110,110,110,110 | 0 |
| 55 | MG | 1H | 3434 | 1/1 | 0.98 | 0.07 | 60,60,60,60 | 0 |
| 55 | MG | 13 | 1721 | 1/1 | 0.98 | 0.04 | 88,88,88,88 | 0 |
| 55 | MG | 1H | 3437 | 1/1 | 0.98 | 0.04 | 66,66,66,66 | 0 |
| 55 | MG | 13 | 1716 | 1/1 | 0.98 | 0.05 | 74,74,74,74 | 0 |
| 55 | MG | 14 | 3434 | 1/1 | 0.98 | 0.04 | 98,98,98,98 | 0 |
| 55 | MG | 1H | 3512 | 1/1 | 0.98 | 0.04 | 115,115,115,115 | 0 |
| 55 | MG | 1G | 1736 | 1/1 | 0.98 | 0.06 | 94,94,94,94 | 0 |
| 55 | MG | 13 | 1724 | 1/1 | 0.98 | 0.07 | 107,107,107,107 | 0 |
| 55 | MG | 13 | 1726 | 1/1 | 0.98 | 0.04 | 89,89,89,89 | 0 |
| 55 | MG | 14 | 3441 | 1/1 | 0.98 | 0.05 | 86,86,86,86 | 0 |
| 55 | MG | 1H | 3447 | 1/1 | 0.98 | 0.05 | 62,62,62,62 | 0 |
| 55 | MG | 1H | 3516 | 1/1 | 0.98 | 0.06 | 88,88,88,88 | 0 |
| 55 | MG | 14 | 3444 | 1/1 | 0.98 | 0.10 | 90,90,90,90 | 0 |
| 55 | MG | 1H | 3448 | 1/1 | 0.98 | 0.05 | 63,63,63,63 | 0 |
| 55 | MG | 14 | 3447 | 1/1 | 0.98 | 0.05 | 102,102,102,102 | 0 |
| 55 | MG | 1H | 3201 | 1/1 | 0.98 | 0.31 | 66,66,66,66 | 0 |
| 55 | MG | 14 | 3162 | 1/1 | 0.98 | 0.28 | 71,71,71,71 | 0 |
| 55 | MG | 1H | 3319 | 1/1 | 0.98 | 0.06 | 60,60,60,60 | 0 |
| 55 | MG | 13 | 1727 | 1/1 | 0.98 | 0.06 | 108,108,108,108 | 0 |
| 55 | MG | 1H | 3461 | 1/1 | 0.98 | 0.06 | 54,54,54,54 | 0 |
| 55 | MG | 14 | 3456 | 1/1 | 0.98 | 0.06 | 102,102,102,102 | 0 |
| 55 | MG | 14 | 3120 | 1/1 | 0.98 | 0.36 | 54,54,54,54 | 0 |
| 55 | MG | 13 | 1729 | 1/1 | 0.98 | 0.04 | 112,112,112,112 | 0 |
| 55 | MG | 14 | 3459 | 1/1 | 0.98 | 0.03 | 130,130,130,130 | 0 |
| 55 | MG | 1H | 3466 | 1/1 | 0.98 | 0.05 | 59,59,59,59 | 0 |
| 55 | MG | 14 | 3461 | 1/1 | 0.98 | 0.09 | 82,82,82,82 | 0 |
| 55 | MG | 13 | 1730 | 1/1 | 0.98 | 0.05 | 115,115,115,115 | 0 |
| 55 | MG | 13 | 1719 | 1/1 | 0.98 | 0.04 | 94,94,94,94 | 0 |
| 55 | MG | 1H | 3470 | 1/1 | 0.98 | 0.10 | 74,74,74,74 | 0 |
| 55 | MG | 1H | 3476 | 1/1 | 0.98 | 0.05 | 59,59,59,59 | 0 |
| 55 | MG | 1H | 3477 | 1/1 | 0.98 | 0.04 | 74,74,74,74 | 0 |
| 55 | MG | 1H | 3409 | 1/1 | 0.98 | 0.05 | 62,62,62,62 | 0 |
| 55 | MG | 1H | 3053 | 1/1 | 0.98 | 0.09 | 61,61,61,61 | 0 |
| 55 | MG | 1H | 3483 | 1/1 | 0.98 | 0.07 | 84,84,84,84 | 0 |
| 55 | MG | 1H | 3412 | 1/1 | 0.98 | 0.05 | 69,69,69,69 | 0 |
| 55 | MG | 2L | 104 | 1/1 | 0.98 | 0.05 | 93,93,93,93 | 0 |

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| Mol | Type | Chain | Res | Atoms | RSCC | RSR | B-factors(Å$^2$) | Q<0.9 |
|---|---|---|---|---|---|---|---|---|
| 55 | MG | 1H | 3486 | 1/1 | 0.98 | 0.09 | 79,79,79,79 | 0 |
| 55 | MG | 14 | 3226 | 1/1 | 0.98 | 0.08 | 55,55,55,55 | 0 |
| 55 | MG | 14 | 3044 | 1/1 | 0.98 | 0.12 | 43,43,43,43 | 0 |
| 55 | MG | 1H | 3487 | 1/1 | 0.98 | 0.11 | 81,81,81,81 | 0 |
| 55 | MG | 1H | 3414 | 1/1 | 0.98 | 0.05 | 59,59,59,59 | 0 |
| 55 | MG | 16 | 215 | 1/1 | 0.98 | 0.04 | 93,93,93,93 | 0 |
| 55 | MG | 1H | 3416 | 1/1 | 0.98 | 0.07 | 71,71,71,71 | 0 |
| 55 | MG | 1H | 3491 | 1/1 | 0.98 | 0.03 | 52,52,52,52 | 0 |
| 55 | MG | 1H | 3493 | 1/1 | 0.98 | 0.05 | 103,103,103,103 | 0 |
| 55 | MG | 1H | 3418 | 1/1 | 0.98 | 0.10 | 63,63,63,63 | 0 |
| 55 | MG | 14 | 3378 | 1/1 | 0.98 | 0.05 | 78,78,78,78 | 0 |
| 55 | MG | 1H | 3421 | 1/1 | 0.98 | 0.06 | 52,52,52,52 | 0 |
| 55 | MG | 14 | 3381 | 1/1 | 0.98 | 0.06 | 52,52,52,52 | 0 |
| 55 | MG | 14 | 3382 | 1/1 | 0.98 | 0.05 | 55,55,55,55 | 0 |
| 55 | MG | 14 | 3383 | 1/1 | 0.98 | 0.05 | 81,81,81,81 | 0 |
| 55 | MG | 1H | 3098 | 1/1 | 0.98 | 0.15 | 42,42,42,42 | 0 |
| 55 | MG | 1H | 3424 | 1/1 | 0.98 | 0.07 | 58,58,58,58 | 0 |
| 56 | ZN | 5I | 101 | 1/1 | 0.98 | 0.03 | 116,116,116,116 | 0 |
| 55 | MG | 14 | 3394 | 1/1 | 0.98 | 0.07 | 89,89,89,89 | 0 |
| 55 | MG | 14 | 3395 | 1/1 | 0.98 | 0.05 | 65,65,65,65 | 0 |
| 55 | MG | 14 | 3396 | 1/1 | 0.98 | 0.05 | 67,67,67,67 | 0 |
| 55 | MG | 14 | 3411 | 1/1 | 0.99 | 0.03 | 63,63,63,63 | 0 |
| 55 | MG | 1H | 3462 | 1/1 | 0.99 | 0.03 | 49,49,49,49 | 0 |
| 55 | MG | 1H | 3505 | 1/1 | 0.99 | 0.07 | 69,69,69,69 | 0 |
| 55 | MG | 14 | 3415 | 1/1 | 0.99 | 0.07 | 62,62,62,62 | 0 |
| 55 | MG | 1H | 3463 | 1/1 | 0.99 | 0.04 | 52,52,52,52 | 0 |
| 55 | MG | 14 | 3417 | 1/1 | 0.99 | 0.03 | 51,51,51,51 | 0 |
| 55 | MG | 14 | 3419 | 1/1 | 0.99 | 0.03 | 94,94,94,94 | 0 |
| 55 | MG | 1H | 3507 | 1/1 | 0.99 | 0.07 | 62,62,62,62 | 0 |
| 55 | MG | 14 | 3421 | 1/1 | 0.99 | 0.07 | 82,82,82,82 | 0 |
| 55 | MG | 1H | 3433 | 1/1 | 0.99 | 0.05 | 54,54,54,54 | 0 |
| 55 | MG | 1H | 3419 | 1/1 | 0.99 | 0.04 | 48,48,48,48 | 0 |
| 55 | MG | 14 | 3426 | 1/1 | 0.99 | 0.04 | 91,91,91,91 | 0 |
| 55 | MG | 14 | 3427 | 1/1 | 0.99 | 0.05 | 75,75,75,75 | 0 |
| 55 | MG | 14 | 3428 | 1/1 | 0.99 | 0.03 | 69,69,69,69 | 0 |
| 55 | MG | 1H | 3435 | 1/1 | 0.99 | 0.04 | 76,76,76,76 | 0 |
| 55 | MG | 14 | 3430 | 1/1 | 0.99 | 0.04 | 67,67,67,67 | 0 |
| 55 | MG | 1H | 3468 | 1/1 | 0.99 | 0.04 | 59,59,59,59 | 0 |
| 55 | MG | 1G | 1728 | 1/1 | 0.99 | 0.04 | 73,73,73,73 | 0 |
| 55 | MG | 1G | 1729 | 1/1 | 0.99 | 0.06 | 93,93,93,93 | 0 |
| 55 | MG | 1G | 1730 | 1/1 | 0.99 | 0.08 | 82,82,82,82 | 0 |
| 55 | MG | 1G | 1731 | 1/1 | 0.99 | 0.10 | 110,110,110,110 | 0 |

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| Mol | Type | Chain | Res | Atoms | RSCC | RSR | B-factors(Å$^2$) | Q<0.9 |
|---|---|---|---|---|---|---|---|---|
| 55 | MG | 1H | 3420 | 1/1 | 0.99 | 0.03 | 52,52,52,52 | 0 |
| 55 | MG | 1H | 3411 | 1/1 | 0.99 | 0.04 | 67,67,67,67 | 0 |
| 55 | MG | 14 | 3440 | 1/1 | 0.99 | 0.03 | 101,101,101,101 | 0 |
| 55 | MG | 1G | 1734 | 1/1 | 0.99 | 0.03 | 81,81,81,81 | 0 |
| 55 | MG | 1H | 3471 | 1/1 | 0.99 | 0.03 | 71,71,71,71 | 0 |
| 55 | MG | 1H | 3472 | 1/1 | 0.99 | 0.03 | 82,82,82,82 | 0 |
| 55 | MG | 1H | 3473 | 1/1 | 0.99 | 0.06 | 64,64,64,64 | 0 |
| 55 | MG | 1H | 3475 | 1/1 | 0.99 | 0.04 | 70,70,70,70 | 0 |
| 55 | MG | 13 | 1723 | 1/1 | 0.99 | 0.04 | 86,86,86,86 | 0 |
| 55 | MG | 14 | 3448 | 1/1 | 0.99 | 0.06 | 87,87,87,87 | 0 |
| 55 | MG | 1H | 3413 | 1/1 | 0.99 | 0.04 | 44,44,44,44 | 0 |
| 55 | MG | 1H | 3478 | 1/1 | 0.99 | 0.07 | 82,82,82,82 | 0 |
| 55 | MG | 14 | 3451 | 1/1 | 0.99 | 0.05 | 74,74,74,74 | 0 |
| 55 | MG | 1H | 3479 | 1/1 | 0.99 | 0.04 | 58,58,58,58 | 0 |
| 55 | MG | 14 | 3453 | 1/1 | 0.99 | 0.05 | 76,76,76,76 | 0 |
| 55 | MG | 1H | 3441 | 1/1 | 0.99 | 0.13 | 63,63,63,63 | 0 |
| 55 | MG | 1H | 3442 | 1/1 | 0.99 | 0.03 | 43,43,43,43 | 0 |
| 55 | MG | 13 | 1725 | 1/1 | 0.99 | 0.03 | 99,99,99,99 | 0 |
| 55 | MG | 1H | 3444 | 1/1 | 0.99 | 0.03 | 59,59,59,59 | 0 |
| 55 | MG | 1H | 3485 | 1/1 | 0.99 | 0.05 | 75,75,75,75 | 0 |
| 55 | MG | 14 | 3084 | 1/1 | 0.99 | 0.12 | 73,73,73,73 | 0 |
| 55 | MG | 1H | 3446 | 1/1 | 0.99 | 0.05 | 52,52,52,52 | 0 |
| 55 | MG | 1H | 3427 | 1/1 | 0.99 | 0.03 | 107,107,107,107 | 0 |
| 55 | MG | 14 | 3375 | 1/1 | 0.99 | 0.04 | 51,51,51,51 | 0 |
| 55 | MG | 1H | 3428 | 1/1 | 0.99 | 0.03 | 74,74,74,74 | 0 |
| 55 | MG | 14 | 3377 | 1/1 | 0.99 | 0.04 | 57,57,57,57 | 0 |
| 55 | MG | 13 | 1728 | 1/1 | 0.99 | 0.04 | 76,76,76,76 | 0 |
| 55 | MG | 14 | 3379 | 1/1 | 0.99 | 0.05 | 53,53,53,53 | 0 |
| 55 | MG | 1H | 3450 | 1/1 | 0.99 | 0.10 | 53,53,53,53 | 0 |
| 55 | MG | 1H | 3492 | 1/1 | 0.99 | 0.02 | 83,83,83,83 | 0 |
| 55 | MG | 1H | 3406 | 1/1 | 0.99 | 0.53 | 91,91,91,91 | 0 |
| 55 | MG | 1H | 3453 | 1/1 | 0.99 | 0.03 | 42,42,42,42 | 0 |
| 55 | MG | 14 | 3384 | 1/1 | 0.99 | 0.05 | 54,54,54,54 | 0 |
| 55 | MG | 1J | 207 | 1/1 | 0.99 | 0.03 | 88,88,88,88 | 0 |
| 55 | MG | 1H | 3454 | 1/1 | 0.99 | 0.04 | 49,49,49,49 | 0 |
| 55 | MG | 14 | 3388 | 1/1 | 0.99 | 0.04 | 61,61,61,61 | 0 |
| 55 | MG | 14 | 3390 | 1/1 | 0.99 | 0.03 | 52,52,52,52 | 0 |
| 55 | MG | 16 | 214 | 1/1 | 0.99 | 0.05 | 86,86,86,86 | 0 |
| 55 | MG | 14 | 3392 | 1/1 | 0.99 | 0.04 | 54,54,54,54 | 0 |
| 55 | MG | 14 | 3393 | 1/1 | 0.99 | 0.03 | 53,53,53,53 | 0 |
| 55 | MG | 1H | 3496 | 1/1 | 0.99 | 0.03 | 78,78,78,78 | 0 |
| 55 | MG | 1H | 3456 | 1/1 | 0.99 | 0.02 | 51,51,51,51 | 0 |

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| Mol | Type | Chain | Res | Atoms | RSCC | RSR | B-factors(Å$^2$) | Q<0.9 |
|---|---|---|---|---|---|---|---|---|
| 55 | MG | 1H | 3498 | 1/1 | 0.99 | 0.05 | 77,77,77,77 | 0 |
| 55 | MG | 14 | 3397 | 1/1 | 0.99 | 0.05 | 70,70,70,70 | 0 |
| 55 | MG | 14 | 3398 | 1/1 | 0.99 | 0.06 | 83,83,83,83 | 0 |
| 55 | MG | 14 | 3399 | 1/1 | 0.99 | 0.04 | 82,82,82,82 | 0 |
| 55 | MG | 1H | 3431 | 1/1 | 0.99 | 0.05 | 70,70,70,70 | 0 |
| 55 | MG | 1H | 3459 | 1/1 | 0.99 | 0.06 | 75,75,75,75 | 0 |
| 55 | MG | 1G | 1716 | 1/1 | 0.99 | 0.04 | 110,110,110,110 | 0 |
| 55 | MG | 14 | 3404 | 1/1 | 0.99 | 0.10 | 79,79,79,79 | 0 |
| 55 | MG | 14 | 3405 | 1/1 | 0.99 | 0.05 | 64,64,64,64 | 0 |
| 55 | MG | 1H | 3460 | 1/1 | 0.99 | 0.04 | 87,87,87,87 | 0 |
| 55 | MG | 1H | 3432 | 1/1 | 0.99 | 0.05 | 68,68,68,68 | 0 |
| 56 | ZN | 32 | 302 | 1/1 | 0.99 | 0.19 | 111,111,111,111 | 0 |
| 55 | MG | G8 | 201 | 1/1 | 0.99 | 0.05 | 77,77,77,77 | 0 |
| 55 | MG | 14 | 3410 | 1/1 | 0.99 | 0.05 | 58,58,58,58 | 0 |
| 55 | MG | 1H | 3464 | 1/1 | 1.00 | 0.01 | 52,52,52,52 | 0 |
| 55 | MG | 1H | 3455 | 1/1 | 1.00 | 0.02 | 47,47,47,47 | 0 |
| 55 | MG | 1H | 3489 | 1/1 | 1.00 | 0.02 | 67,67,67,67 | 0 |
| 55 | MG | 14 | 3418 | 1/1 | 1.00 | 0.04 | 72,72,72,72 | 0 |
| 55 | MG | 14 | 3445 | 1/1 | 1.00 | 0.02 | 58,58,58,58 | 0 |
| 55 | MG | 1H | 3503 | 1/1 | 1.00 | 0.02 | 57,57,57,57 | 0 |
| 55 | MG | 1H | 3422 | 1/1 | 1.00 | 0.03 | 56,56,56,56 | 0 |
| 55 | MG | 1H | 3426 | 1/1 | 1.00 | 0.02 | 67,67,67,67 | 0 |
| 55 | MG | 14 | 3422 | 1/1 | 1.00 | 0.06 | 53,53,53,53 | 0 |
| 55 | MG | 14 | 3423 | 1/1 | 1.00 | 0.02 | 84,84,84,84 | 0 |
| 55 | MG | 1H | 3458 | 1/1 | 1.00 | 0.04 | 70,70,70,70 | 0 |
| 55 | MG | 1H | 3521 | 1/1 | 1.00 | 0.04 | 47,47,47,47 | 0 |
| 55 | MG | 1H | 3480 | 1/1 | 1.00 | 0.03 | 47,47,47,47 | 0 |
| 55 | MG | 14 | 3403 | 1/1 | 1.00 | 0.02 | 69,69,69,69 | 0 |
| 55 | MG | 1H | 3415 | 1/1 | 1.00 | 0.01 | 50,50,50,50 | 0 |
| 55 | MG | 14 | 3386 | 1/1 | 1.00 | 0.02 | 56,56,56,56 | 0 |
| 55 | MG | 14 | 3387 | 1/1 | 1.00 | 0.02 | 58,58,58,58 | 0 |
| 55 | MG | 1H | 3451 | 1/1 | 1.00 | 0.01 | 54,54,54,54 | 0 |
| 55 | MG | 14 | 3408 | 1/1 | 1.00 | 0.04 | 56,56,56,56 | 0 |
| 55 | MG | 14 | 3433 | 1/1 | 1.00 | 0.03 | 87,87,87,87 | 0 |
| 55 | MG | 14 | 3389 | 1/1 | 1.00 | 0.03 | 53,53,53,53 | 0 |
| 55 | MG | 14 | 3435 | 1/1 | 1.00 | 0.02 | 95,95,95,95 | 0 |
| 55 | MG | 1H | 3445 | 1/1 | 1.00 | 0.03 | 59,59,59,59 | 0 |
| 55 | MG | 1H | 3440 | 1/1 | 1.00 | 0.03 | 91,91,91,91 | 0 |
| 55 | MG | 14 | 3412 | 1/1 | 1.00 | 0.03 | 49,49,49,49 | 0 |
| 55 | MG | 1H | 3417 | 1/1 | 1.00 | 0.03 | 40,40,40,40 | 0 |
| 55 | MG | 1H | 3474 | 1/1 | 1.00 | 0.02 | 79,79,79,79 | 0 |

## 6.5 Other polymers (i)

There are no such residues in this entry.