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

Mar 6, 2026 – 10:23 PM UTC

| | | |
|---|---|---|
| PDB ID | : | 7AZS / pdb_00007azs |
| Title | : | 70S thermus thermophilus ribosome with bound antibiotic lead SEQ-569 |
| Authors | : | Jenner, L.B.; Yusupov, M.; Yusupova, G.; Rak, A. |
| Deposited on | : | 2020-11-17 |
| 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:

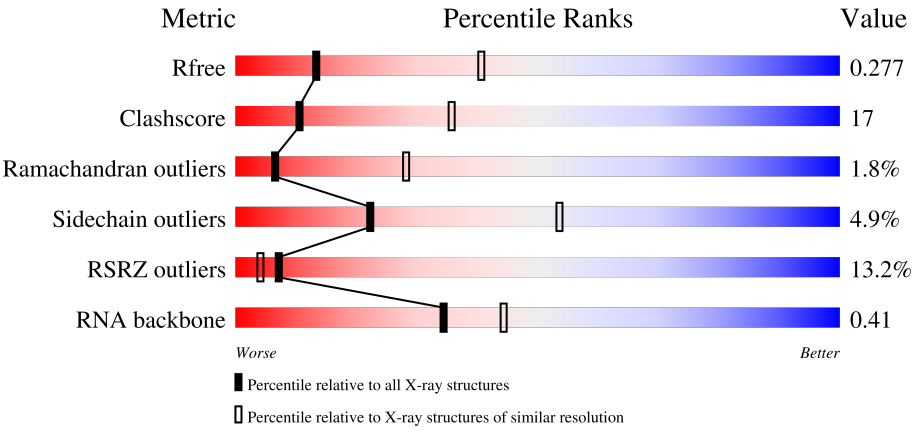
| | | |
|---|---|---|
| MolProbity | : | 4-5-2 with Phenix2.0 |
| Mogul | : | 2022.3.0, CSD as543be (2022) |
| Xtriage (Phenix) | : | 2.0 |
| EDS | : | 3.0 |
| Buster-report | : | wwPDB partial adaption of 1.1.7 (2018) |
| Percentile statistics | : | 20250101.v01 (using entries in the PDB archive January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

# 1 Overall quality at a glance (i)

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

The reported resolution of this entry is 3.10 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 | 16SA | 1512 | 4% 76% 23% |
| 1 | 16SB | 1512 | 2% 76% 23% |
| 2 | S2A | 256 | 34% 53% 35% 5% 7% |
| 2 | S2B | 256 | 36% 46% 43% 7% |

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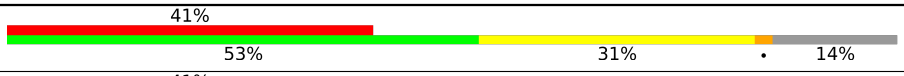
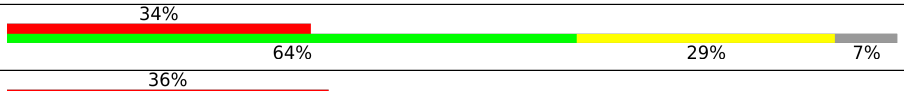
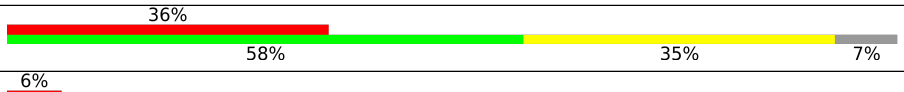
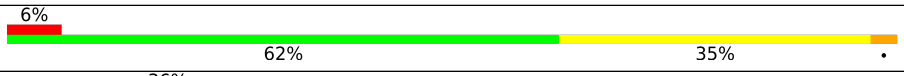
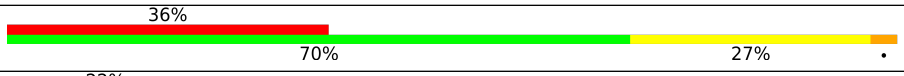
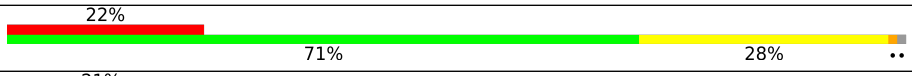
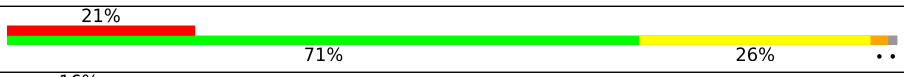
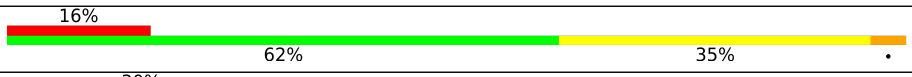
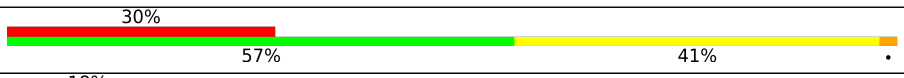
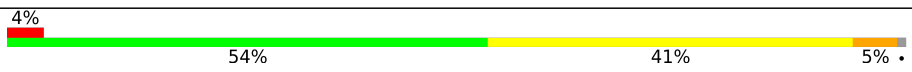
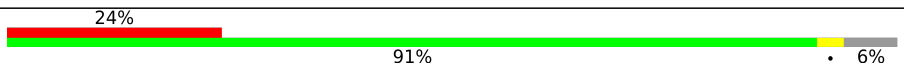
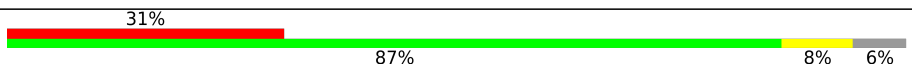
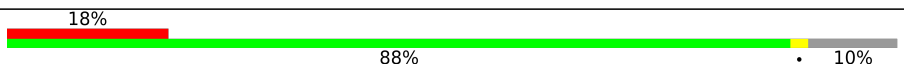
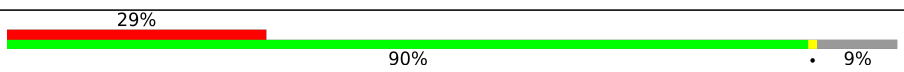
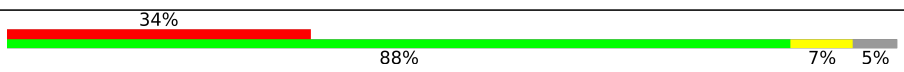
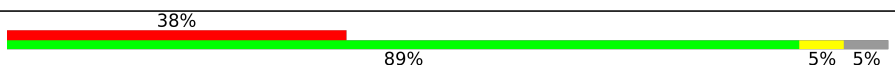
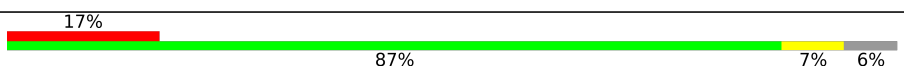
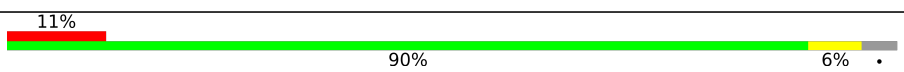
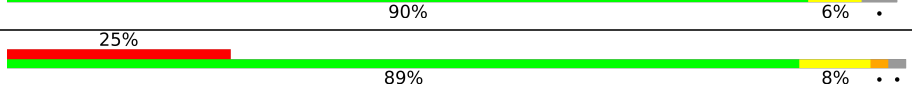
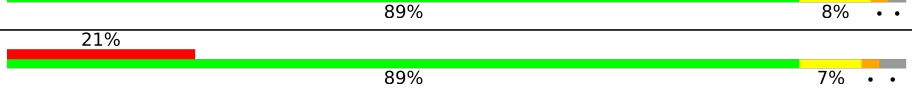
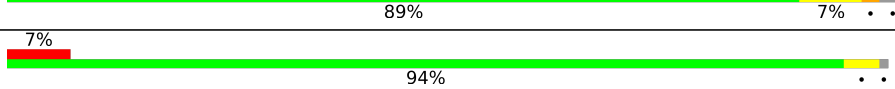
| Mol | Chain | Length | Quality of chain |
|---|---|---|---|
| 3 | S3A | 239 |   |
| 3 | S3B | 239 | |
| 4 | S4A | 209 | |
| 4 | S4B | 209 | |
| 5 | S5A | 162 |   |
| 5 | S5B | 162 |   |
| 6 | S6A | 101 |   |
| 6 | S6B | 101 |   |
| 7 | S7A | 156 |   |
| 7 | S7B | 156 |   |
| 8 | S8A | 138 |   |
| 8 | S8B | 138 |   |
| 9 | S9A | 128 | |
| 9 | S9B | 128 |   |
| 10 | S10A | 105 |   |
| 10 | S10B | 105 |   |
| 11 | S11A | 129 |   |
| 11 | S11B | 129 |   |
| 12 | S12A | 132 |   |
| 12 | S12B | 132 |   |
| 13 | S13A | 126 |   |
| 13 | S13B | 126 |   |
| 14 | S14A | 61 |   |
| 14 | S14B | 61 |   |
| 15 | S15A | 89 |   |

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| Mol | Chain | Length | Quality of chain |
|---|---|---|---|
| 15 | S15B | 89 | 9% 96% |
| 16 | S16A | 88 | 25% 90% 5% 6% |
| 16 | S16B | 88 | 43% 93% 5% |
| 17 | S17A | 105 | 4% 91% 5% |
| 17 | S17B | 105 | 12% 91% 5% |
| 18 | S18A | 88 | 8% 77% 19% |
| 18 | S18B | 88 | 30% 76% 20% |
| 19 | S19A | 93 | 37% 82% 8% 10% |
| 19 | S19B | 93 | 11% 86% 6% 8% |
| 20 | S20A | 106 | 22% 88% 6% 7% |
| 20 | S20B | 106 | 9% 89% 7% |
| 21 | THXA | 27 | 11% 89% 11% |
| 21 | THXB | 27 | 85% 7% 7% |
| 22 | ASIA | 76 | 62% 38% 57% 5% |
| 23 | PSIA | 76 | 18% 64% 28% 8% |
| 23 | PSIB | 76 | 7% 53% 42% 5% |
| 24 | ESIA | 76 | 33% 55% 45% |
| 24 | ESIB | 76 | 16% 67% 32% |
| 25 | MRNA | 30 | 33% 73% 27% |
| 25 | MRNB | 30 | 17% 60% 40% |
| 26 | TRNA | 76 | 7% 45% 45% 7% |
| 27 | 23SA | 2911 | 2% 76% 23% |
| 27 | 23SB | 2911 | 2% 75% 24% |
| 28 | 5SA | 124 | % 60% 25% 13% |
| 28 | 5SB | 124 | 3% 46% 37% 15% |

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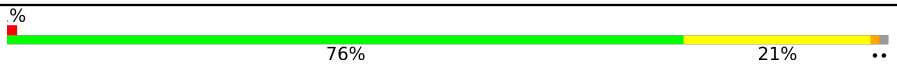
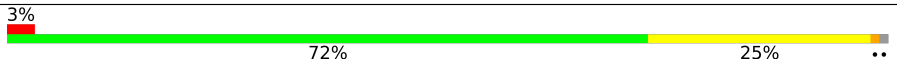
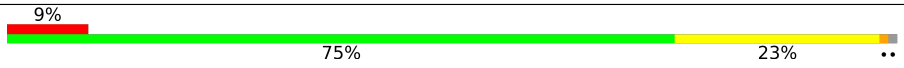
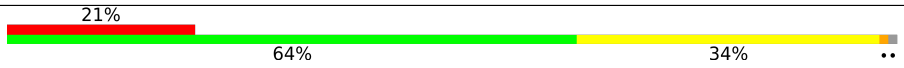
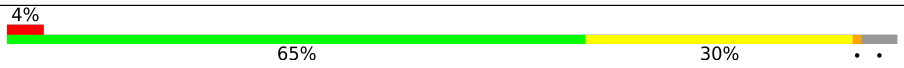
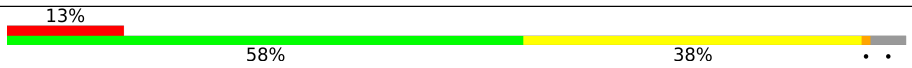
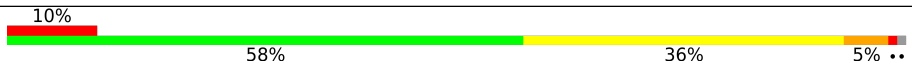
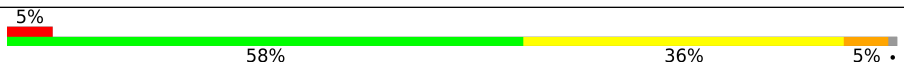
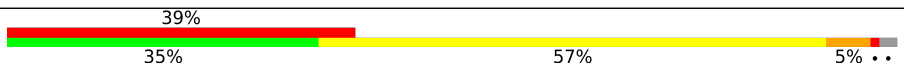
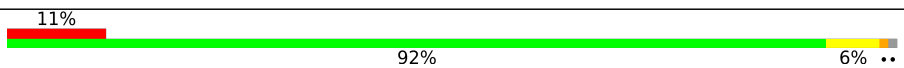
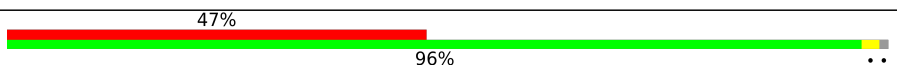
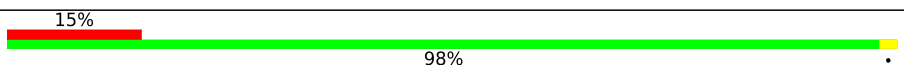
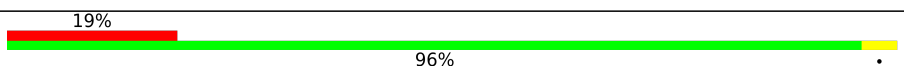
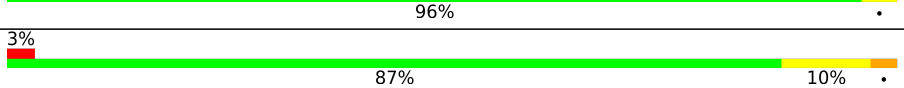
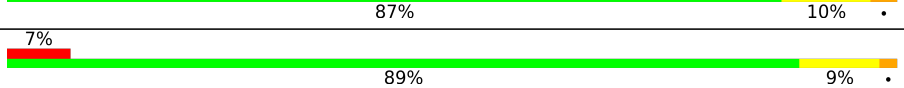
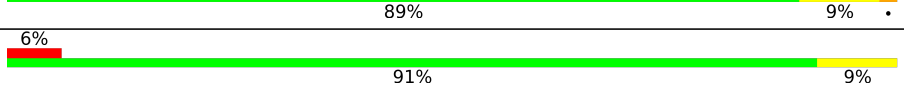
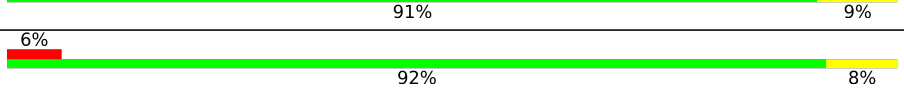
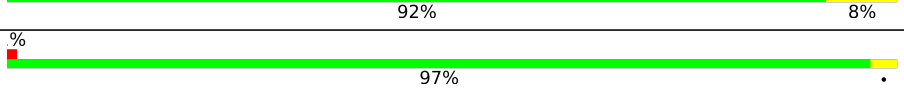
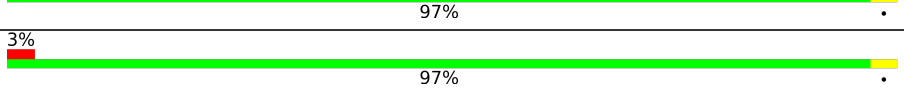
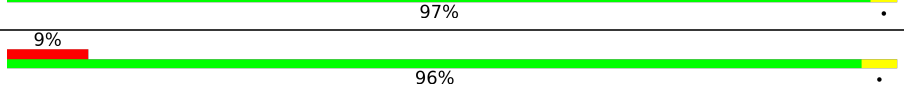
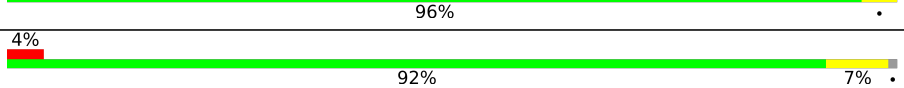
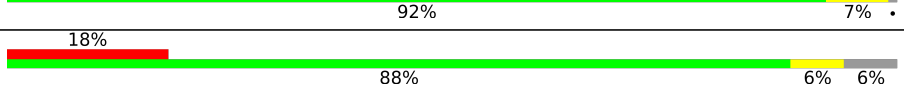
| Mol | Chain | Length | Quality of chain |
|---|---|---|---|
| 29 | L2A | 276 |   |
| 29 | L2B | 276 |   |
| 30 | L3A | 206 |   |
| 30 | L3B | 206 |   |
| 31 | L4A | 210 |   |
| 31 | L4B | 210 |   |
| 32 | L5A | 182 |   |
| 32 | L5B | 182 |   |
| 33 | L6A | 180 | |
| 33 | L6B | 180 | |
| 34 | L9A | 148 |   |
| 34 | L9B | 148 | |
| 35 | L13A | 140 |   |
| 35 | L13B | 140 |   |
| 36 | L14A | 122 |   |
| 36 | L14B | 122 |   |
| 37 | L15A | 150 |   |
| 37 | L15B | 150 |   |
| 38 | L16A | 141 |   |
| 38 | L16B | 141 |   |
| 39 | L17A | 118 |   |
| 39 | L17B | 118 |   |
| 40 | L18A | 112 |   |
| 40 | L18B | 112 |   |
| 41 | L19A | 146 |   |

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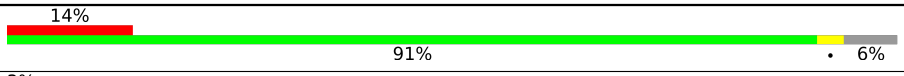
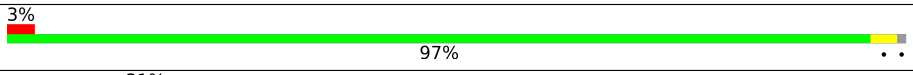
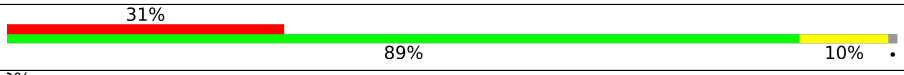
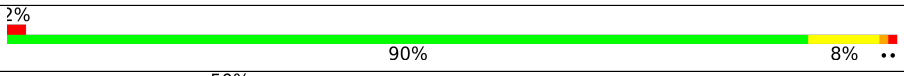
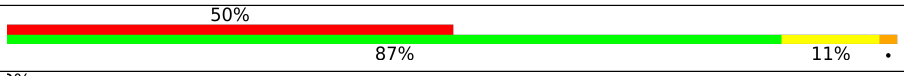
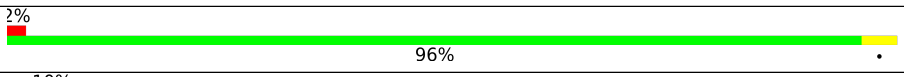
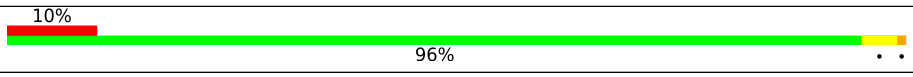
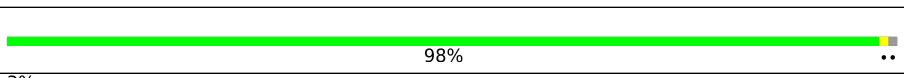
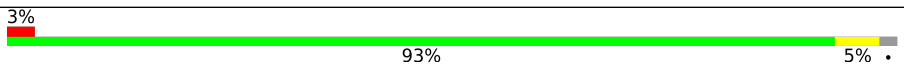
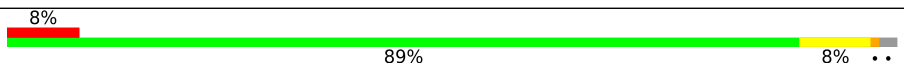
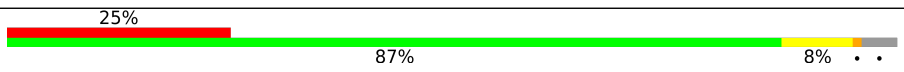
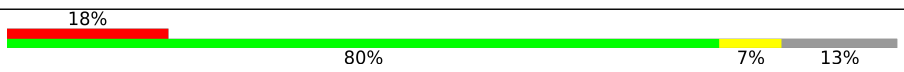
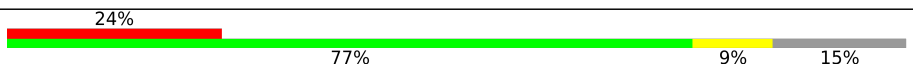
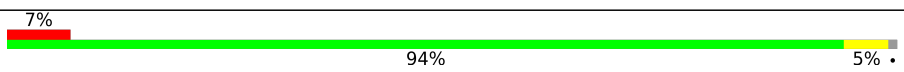
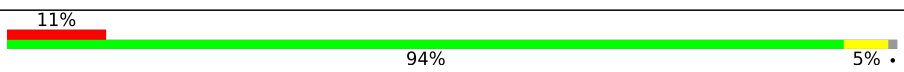
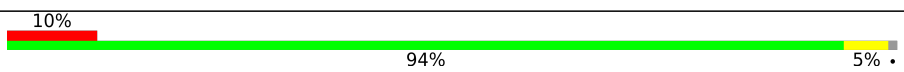
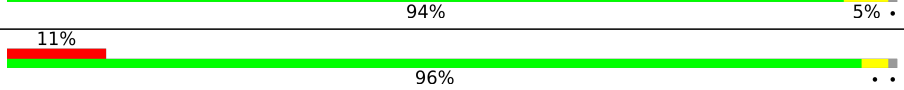
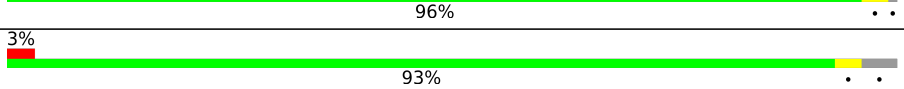
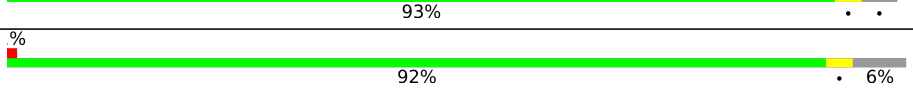
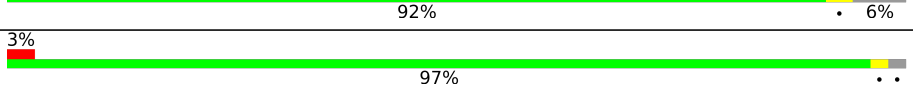
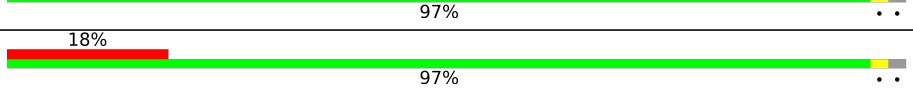
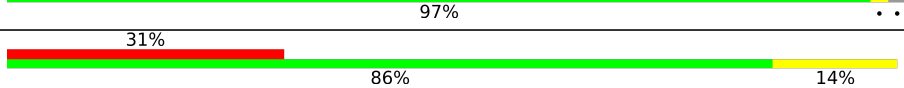
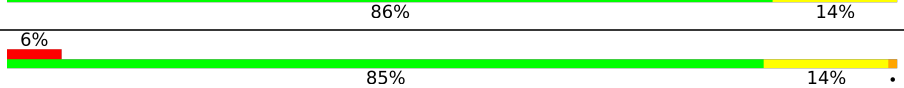
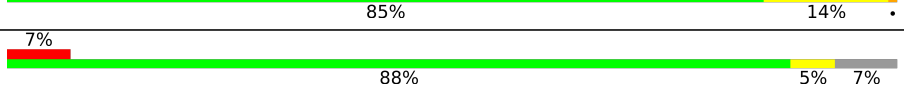
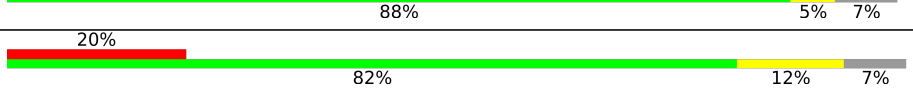
| Mol | Chain | Length | Quality of chain |
|---|---|---|---|
| 41 | L19B | 146 |   |
| 42 | L20A | 118 |   |
| 42 | L20B | 118 |   |
| 43 | L21A | 101 |   |
| 43 | L21B | 101 |   |
| 44 | L22A | 113 |   |
| 44 | L22B | 113 |   |
| 45 | L23A | 96 |   |
| 45 | L23B | 96 |   |
| 46 | L24A | 110 |   |
| 46 | L24B | 110 |   |
| 47 | L25A | 206 |   |
| 47 | L25B | 206 |   |
| 48 | L27A | 85 |   |
| 48 | L27B | 85 |   |
| 49 | L28A | 98 |   |
| 49 | L28B | 98 |   |
| 50 | L29A | 72 |   |
| 50 | L29B | 72 |   |
| 51 | L30A | 60 |   |
| 51 | L30B | 60 |   |
| 52 | L31A | 71 |   |
| 52 | L31B | 71 |   |
| 53 | L32A | 60 |   |
| 53 | L32B | 60 |   |

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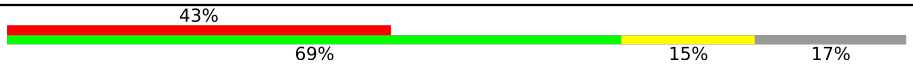
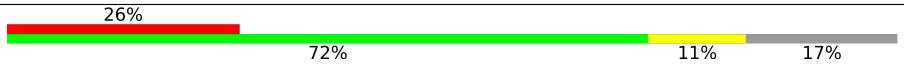
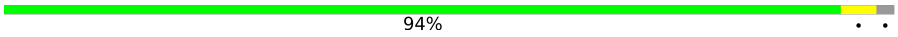
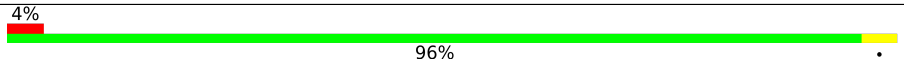
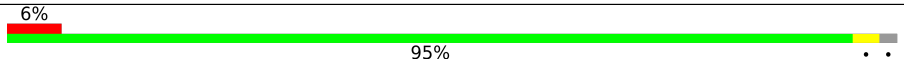
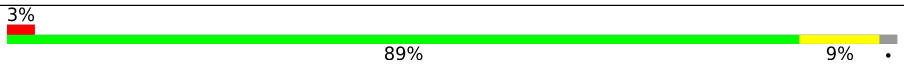
| Mol | Chain | Length | Quality of chain |
|---|---|---|---|
| 54 | L33A | 54 |   |
| 54 | L33B | 54 |   |
| 55 | L34A | 49 |   |
| 55 | L34B | 49 |   |
| 56 | L35A | 65 |   |
| 56 | L35B | 65 |   |
| 57 | ASIB | 76 | |

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 |
|---|---|---|---|---|---|---|---|
| 58 | MG | 16SA | 2217 | - | - | - | X |
| 58 | MG | 16SB | 2248 | - | - | - | X |
| 58 | MG | 23SA | 3015 | - | - | - | X |
| 58 | MG | 23SB | 3087 | - | - | - | X |
| 59 | K | 23SA | 3390 | - | - | - | X |

# 2 Entry composition (i)

There are 62 unique types of molecules in this entry. The entry contains 306277 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 rRNA.

| Mol | Chain | Residues | Atoms | | | | | ZeroOcc | AltConf | Trace |
|---|---|---|---|---|---|---|---|---|---|---|
| 1 | 16SA | 1511 | Total | C | N | O | P | 0 | 0 | 0 |
| | | | 32489 | 14469 | 6014 | 10495 | 1511 | | | |
| 1 | 16SB | 1507 | Total | C | N | O | P | 0 | 0 | 0 |
| | | | 32409 | 14433 | 6005 | 10464 | 1507 | | | |

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

| Mol | Chain | Residues | Atoms | | | | | ZeroOcc | AltConf | Trace |
|---|---|---|---|---|---|---|---|---|---|---|
| 2 | S2A | 237 | Total | C | N | O | S | 0 | 0 | 0 |
| | | | 1924 | 1228 | 344 | 347 | 5 | | | |
| 2 | S2B | 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 | S3A | 205 | Total | C | N | O | S | 0 | 0 | 0 |
| | | | 1605 | 1011 | 313 | 280 | 1 | | | |
| 3 | S3B | 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 | S4A | 208 | Total | C | N | O | S | 0 | 0 | 0 |
| | | | 1702 | 1066 | 339 | 290 | 7 | | | |
| 4 | S4B | 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 | S5A | 151 | Total | C | N | O | S | 0 | 0 | 0 |
| | | | 1155 | 729 | 218 | 204 | 4 | | | |
| 5 | S5B | 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 | S6A | 101 | Total | C | N | O | S | 0 | 0 | 0 |
| | | | 842 | 531 | 155 | 153 | 3 | | | |
| 6 | S6B | 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 | S7A | 155 | Total | C | N | O | S | 0 | 0 | 0 |
| | | | 1256 | 781 | 252 | 217 | 6 | | | |
| 7 | S7B | 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 | S8A | 138 | Total | C | N | O | S | 0 | 0 | 0 |
| | | | 1115 | 705 | 215 | 192 | 3 | | | |
| 8 | S8B | 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 | S9A | 127 | Total | C | N | O | 0 | 0 | 0 |
| | | | 1009 | 639 | 197 | 173 | | | |
| 9 | S9B | 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 | S10A | 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 | S10B | 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 | S11A | 116 | Total | C | N | O | S | 0 | 0 | 0 |
| | | | 864 | 537 | 164 | 160 | 3 | | | |
| 11 | S11B | 117 | Total | C | N | O | S | 0 | 0 | 0 |
| | | | 873 | 543 | 166 | 161 | 3 | | | |

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

| Mol | Chain | Residues | Atoms | | | | | ZeroOcc | AltConf | Trace |
|---|---|---|---|---|---|---|---|---|---|---|
| 12 | S12A | 125 | Total | C | N | O | S | 0 | 0 | 0 |
| | | | 977 | 615 | 196 | 164 | 2 | | | |
| 12 | S12B | 125 | Total | C | N | O | S | 0 | 0 | 0 |
| | | | 977 | 615 | 196 | 164 | 2 | | | |

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

| Mol | Chain | Residues | Atoms | | | | | ZeroOcc | AltConf | Trace |
|---|---|---|---|---|---|---|---|---|---|---|
| 13 | S13A | 119 | Total | C | N | O | S | 0 | 0 | 0 |
| | | | 946 | 585 | 195 | 164 | 2 | | | |
| 13 | S13B | 121 | Total | C | N | O | S | 0 | 0 | 0 |
| | | | 964 | 597 | 199 | 166 | 2 | | | |

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

| Mol | Chain | Residues | Atoms | | | | | ZeroOcc | AltConf | Trace |
|---|---|---|---|---|---|---|---|---|---|---|
| 14 | S14A | 60 | Total | C | N | O | S | 0 | 0 | 0 |
| | | | 491 | 312 | 104 | 71 | 4 | | | |
| 14 | S14B | 59 | Total | C | N | O | S | 0 | 0 | 0 |
| | | | 486 | 309 | 103 | 70 | 4 | | | |

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

| Mol | Chain | Residues | Atoms | | | | | ZeroOcc | AltConf | Trace |
|---|---|---|---|---|---|---|---|---|---|---|
| 15 | S15A | 88 | Total | C | N | O | S | 0 | 0 | 0 |
| | | | 733 | 459 | 147 | 125 | 2 | | | |
| 15 | S15B | 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 | S16A | 83 | Total | C | N | O | S | 0 | 0 | 0 |
| | | | 700 | 443 | 139 | 117 | 1 | | | |
| 16 | S16B | 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 | S17A | 100 | Total | C | N | O | S | 0 | 0 | 0 |
| | | | 834 | 534 | 155 | 143 | 2 | | | |
| 17 | S17B | 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 | S18A | 71 | Total | C | N | O | 0 | 0 | 0 |
| | | | 584 | 373 | 116 | 95 | | | |
| 18 | S18B | 70 | Total | C | N | O | 0 | 0 | 0 |
| | | | 573 | 367 | 112 | 94 | | | |

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

| Mol | Chain | Residues | Atoms | | | | | ZeroOcc | AltConf | Trace |
|---|---|---|---|---|---|---|---|---|---|---|
| 19 | S19A | 84 | Total | C | N | O | S | 0 | 0 | 0 |
| | | | 674 | 430 | 126 | 116 | 2 | | | |
| 19 | S19B | 86 | Total | C | N | O | S | 0 | 0 | 0 |
| | | | 684 | 436 | 126 | 120 | 2 | | | |

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

| Mol | Chain | Residues | Atoms | | | | | ZeroOcc | AltConf | Trace |
|---|---|---|---|---|---|---|---|---|---|---|
| 20 | S20A | 99 | Total | C | N | O | S | 0 | 0 | 0 |
| | | | 762 | 470 | 162 | 128 | 2 | | | |
| 20 | S20B | 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 | THXA | 24 | Total<br>208 | C<br>128 | N<br>50 | O<br>30 | 0 | 0 | 0 |
| 21 | THXB | 25 | Total<br>217 | C<br>134 | N<br>52 | O<br>31 | 0 | 0 | 0 |

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

| Mol | Chain | Residues | Atoms | | | | | | ZeroOcc | AltConf | Trace |
|---|---|---|---|---|---|---|---|---|---|---|---|
| 22 | ASIA | 76 | Total<br>1628 | C<br>731 | N<br>290 | O<br>530 | P<br>75 | S<br>2 | 0 | 0 | 0 |

- Molecule 23 is a RNA chain called Phe-tRNA.

| Mol | Chain | Residues | Atoms | | | | | | ZeroOcc | AltConf | Trace |
|---|---|---|---|---|---|---|---|---|---|---|---|
| 23 | PSIA | 76 | Total<br>1635 | C<br>735 | N<br>291 | O<br>532 | P<br>75 | S<br>2 | 0 | 0 | 0 |
| 23 | PSIB | 76 | Total<br>1635 | C<br>735 | N<br>291 | O<br>532 | P<br>75 | S<br>2 | 0 | 0 | 0 |

- Molecule 24 is a RNA chain called Phe-tRNA.

| Mol | Chain | Residues | Atoms | | | | | | ZeroOcc | AltConf | Trace |
|---|---|---|---|---|---|---|---|---|---|---|---|
| 24 | ESIA | 76 | Total<br>1626 | C<br>729 | N<br>290 | O<br>531 | P<br>75 | S<br>1 | 0 | 0 | 0 |
| 24 | ESIB | 76 | Total<br>1626 | C<br>729 | N<br>290 | O<br>531 | P<br>75 | S<br>1 | 0 | 0 | 0 |

- Molecule 25 is a RNA chain called mRNA.

| Mol | Chain | Residues | Atoms | | | | | ZeroOcc | AltConf | Trace |
|---|---|---|---|---|---|---|---|---|---|---|
| 25 | MRNA | 30 | Total<br>621 | C<br>279 | N<br>88 | O<br>225 | P<br>29 | 0 | 0 | 0 |
| 25 | MRNB | 30 | Total<br>621 | C<br>279 | N<br>88 | O<br>225 | P<br>29 | 0 | 0 | 0 |

- Molecule 26 is a RNA chain called Phe-tRNA.

| Mol | Chain | Residues | Atoms | | | | | | ZeroOcc | AltConf | Trace |
|---|---|---|---|---|---|---|---|---|---|---|---|
| 26 | TRNA | 73 | Total<br>1565 | C<br>702 | N<br>279 | O<br>510 | P<br>72 | S<br>2 | 0 | 0 | 0 |

- Molecule 27 is a RNA chain called 23S rRNA.

| Mol | Chain | Residues | Atoms | | | | | ZeroOcc | AltConf | Trace |
|---|---|---|---|---|---|---|---|---|---|---|
| 27 | 23SA | 2889 | Total<br>62225 | C<br>27699 | N<br>11629 | O<br>20008 | P<br>2889 | 0 | 0 | 0 |
| 27 | 23SB | 2875 | Total<br>61926 | C<br>27566 | N<br>11578 | O<br>19907 | P<br>2875 | 0 | 0 | 0 |

- Molecule 28 is a RNA chain called 5S rRNA.

| Mol | Chain | Residues | Atoms | | | | | ZeroOcc | AltConf | Trace |
|---|---|---|---|---|---|---|---|---|---|---|
| 28 | 5SA | 122 | Total<br>2617 | C<br>1166 | N<br>486 | O<br>844 | P<br>121 | 0 | 0 | 0 |
| 28 | 5SB | 121 | Total<br>2598 | C<br>1156 | N<br>481 | O<br>840 | P<br>121 | 0 | 0 | 0 |

- Molecule 29 is a protein called 50S ribosomal protein L2.

| Mol | Chain | Residues | Atoms | | | | | ZeroOcc | AltConf | Trace |
|---|---|---|---|---|---|---|---|---|---|---|
| 29 | L2A | 272 | Total<br>2115 | C<br>1335 | N<br>420 | O<br>357 | S<br>3 | 0 | 0 | 0 |
| 29 | L2B | 272 | Total<br>2115 | C<br>1335 | N<br>420 | O<br>357 | S<br>3 | 0 | 0 | 0 |

- Molecule 30 is a protein called 50S ribosomal protein L3.

| Mol | Chain | Residues | Atoms | | | | | ZeroOcc | AltConf | Trace |
|---|---|---|---|---|---|---|---|---|---|---|
| 30 | L3A | 204 | Total<br>1563 | C<br>988 | N<br>299 | O<br>270 | S<br>6 | 0 | 0 | 0 |
| 30 | L3B | 204 | Total<br>1563 | C<br>988 | N<br>299 | O<br>270 | S<br>6 | 0 | 0 | 0 |

- Molecule 31 is a protein called 50S ribosomal protein L4.

| Mol | Chain | Residues | Atoms | | | | | ZeroOcc | AltConf | Trace |
|---|---|---|---|---|---|---|---|---|---|---|
| 31 | L4A | 202 | Total<br>1585 | C<br>1011 | N<br>297 | O<br>275 | S<br>2 | 0 | 0 | 0 |
| 31 | L4B | 202 | Total<br>1585 | C<br>1011 | N<br>297 | O<br>275 | S<br>2 | 0 | 0 | 0 |

- Molecule 32 is a protein called 50S ribosomal protein L5.

| Mol | Chain | Residues | Atoms | | | | | ZeroOcc | AltConf | Trace |
|---|---|---|---|---|---|---|---|---|---|---|
| 32 | L5A | 181 | Total<br>1473 | C<br>942 | N<br>268 | O<br>259 | S<br>4 | 0 | 0 | 0 |

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| Mol | Chain | Residues | Atoms | | | | | ZeroOcc | AltConf | Trace |
|---|---|---|---|---|---|---|---|---|---|---|
| 32 | L5B | 181 | Total | C | N | O | S | 0 | 0 | 0 |
| | | | 1473 | 942 | 268 | 259 | 4 | | | |

- Molecule 33 is a protein called 50S ribosomal protein L6.

| Mol | Chain | Residues | Atoms | | | | | ZeroOcc | AltConf | Trace |
|---|---|---|---|---|---|---|---|---|---|---|
| 33 | L6A | 174 | Total | C | N | O | S | 0 | 0 | 0 |
| | | | 1336 | 848 | 251 | 236 | 1 | | | |
| 33 | L6B | 173 | Total | C | N | O | S | 0 | 0 | 0 |
| | | | 1327 | 842 | 249 | 235 | 1 | | | |

- Molecule 34 is a protein called 50S ribosomal protein L9.

| Mol | Chain | Residues | Atoms | | | | | ZeroOcc | AltConf | Trace |
|---|---|---|---|---|---|---|---|---|---|---|
| 34 | L9A | 145 | Total | C | N | O | S | 0 | 0 | 0 |
| | | | 1131 | 723 | 200 | 207 | 1 | | | |
| 34 | L9B | 146 | Total | C | N | O | S | 0 | 0 | 0 |
| | | | 1136 | 726 | 201 | 208 | 1 | | | |

- Molecule 35 is a protein called 50S ribosomal protein L13.

| Mol | Chain | Residues | Atoms | | | | | ZeroOcc | AltConf | Trace |
|---|---|---|---|---|---|---|---|---|---|---|
| 35 | L13A | 138 | Total | C | N | O | S | 0 | 0 | 0 |
| | | | 1104 | 712 | 206 | 182 | 4 | | | |
| 35 | L13B | 138 | Total | C | N | O | S | 0 | 0 | 0 |
| | | | 1104 | 712 | 206 | 182 | 4 | | | |

- Molecule 36 is a protein called 50S ribosomal protein L14.

| Mol | Chain | Residues | Atoms | | | | | ZeroOcc | AltConf | Trace |
|---|---|---|---|---|---|---|---|---|---|---|
| 36 | L14A | 122 | Total | C | N | O | S | 0 | 0 | 0 |
| | | | 932 | 588 | 171 | 169 | 4 | | | |
| 36 | L14B | 122 | Total | C | N | O | S | 0 | 0 | 0 |
| | | | 932 | 588 | 171 | 169 | 4 | | | |

- Molecule 37 is a protein called 50S ribosomal protein L15.

| Mol | Chain | Residues | Atoms | | | | | ZeroOcc | AltConf | Trace |
|---|---|---|---|---|---|---|---|---|---|---|
| 37 | L15A | 150 | Total | C | N | O | S | 0 | 0 | 0 |
| | | | 1144 | 712 | 232 | 197 | 3 | | | |
| 37 | L15B | 150 | Total | C | N | O | S | 0 | 0 | 0 |
| | | | 1144 | 712 | 232 | 197 | 3 | | | |

- Molecule 38 is a protein called 50S ribosomal protein L16.

| Mol | Chain | Residues | Atoms | | | | | ZeroOcc | AltConf | Trace |
|---|---|---|---|---|---|---|---|---|---|---|
| 38 | L16A | 141 | Total | C | N | O | S | 0 | 0 | 0 |
| | | | 1121 | 715 | 212 | 187 | 7 | | | |
| 38 | L16B | 141 | Total | C | N | O | S | 0 | 0 | 0 |
| | | | 1121 | 715 | 212 | 187 | 7 | | | |

- Molecule 39 is a protein called 50S ribosomal protein L17.

| Mol | Chain | Residues | Atoms | | | | | ZeroOcc | AltConf | Trace |
|---|---|---|---|---|---|---|---|---|---|---|
| 39 | L17A | 118 | Total | C | N | O | S | 0 | 0 | 0 |
| | | | 967 | 604 | 203 | 159 | 1 | | | |
| 39 | L17B | 118 | Total | C | N | O | S | 0 | 0 | 0 |
| | | | 967 | 604 | 203 | 159 | 1 | | | |

- Molecule 40 is a protein called 50S ribosomal protein L18.

| Mol | Chain | Residues | Atoms | | | | | ZeroOcc | AltConf | Trace |
|---|---|---|---|---|---|---|---|---|---|---|
| 40 | L18A | 112 | Total | C | N | O | S | 0 | 0 | 0 |
| | | | 889 | 561 | 177 | 150 | 1 | | | |
| 40 | L18B | 111 | Total | C | N | O | | 0 | 0 | 0 |
| | | | 881 | 556 | 176 | 149 | | | | |

- Molecule 41 is a protein called 50S ribosomal protein L19.

| Mol | Chain | Residues | Atoms | | | | | ZeroOcc | AltConf | Trace |
|---|---|---|---|---|---|---|---|---|---|---|
| 41 | L19A | 137 | Total | C | N | O | S | 0 | 0 | 0 |
| | | | 1141 | 710 | 234 | 196 | 1 | | | |
| 41 | L19B | 137 | Total | C | N | O | S | 0 | 0 | 0 |
| | | | 1141 | 710 | 234 | 196 | 1 | | | |

- Molecule 42 is a protein called 50S ribosomal protein L20.

| Mol | Chain | Residues | Atoms | | | | | ZeroOcc | AltConf | Trace |
|---|---|---|---|---|---|---|---|---|---|---|
| 42 | L20A | 117 | Total | C | N | O | S | 0 | 0 | 0 |
| | | | 963 | 610 | 202 | 150 | 1 | | | |
| 42 | L20B | 117 | Total | C | N | O | S | 0 | 0 | 0 |
| | | | 963 | 610 | 202 | 150 | 1 | | | |

- Molecule 43 is a protein called 50S ribosomal protein L21.

| Mol | Chain | Residues | Atoms | | | | | ZeroOcc | AltConf | Trace |
|---|---|---|---|---|---|---|---|---|---|---|
| 43 | L21A | 101 | Total | C | N | O | S | 0 | 0 | 0 |
| | | | 778 | 501 | 142 | 134 | 1 | | | |
| 43 | L21B | 101 | Total | C | N | O | S | 0 | 0 | 0 |
| | | | 778 | 501 | 142 | 134 | 1 | | | |

- Molecule 44 is a protein called 50S ribosomal protein L22.

| Mol | Chain | Residues | Atoms | | | | | ZeroOcc | AltConf | Trace |
|---|---|---|---|---|---|---|---|---|---|---|
| 44 | L22A | 113 | Total | C | N | O | S | 0 | 0 | 0 |
| | | | 899 | 566 | 177 | 154 | 2 | | | |
| 44 | L22B | 113 | Total | C | N | O | S | 0 | 0 | 0 |
| | | | 899 | 566 | 177 | 154 | 2 | | | |

- Molecule 45 is a protein called 50S ribosomal protein L23.

| Mol | Chain | Residues | Atoms | | | | | ZeroOcc | AltConf | Trace |
|---|---|---|---|---|---|---|---|---|---|---|
| 45 | L23A | 95 | Total | C | N | O | S | 0 | 0 | 0 |
| | | | 747 | 485 | 135 | 126 | 1 | | | |
| 45 | L23B | 94 | Total | C | N | O | S | 0 | 0 | 0 |
| | | | 742 | 482 | 134 | 125 | 1 | | | |

- Molecule 46 is a protein called 50S ribosomal protein L24.

| Mol | Chain | Residues | Atoms | | | | | ZeroOcc | AltConf | Trace |
|---|---|---|---|---|---|---|---|---|---|---|
| 46 | L24A | 108 | Total | C | N | O | S | 0 | 0 | 0 |
| | | | 824 | 528 | 153 | 138 | 5 | | | |
| 46 | L24B | 106 | Total | C | N | O | S | 0 | 0 | 0 |
| | | | 775 | 494 | 147 | 129 | 5 | | | |

- Molecule 47 is a protein called 50S ribosomal protein L25.

| Mol | Chain | Residues | Atoms | | | | | ZeroOcc | AltConf | Trace |
|---|---|---|---|---|---|---|---|---|---|---|
| 47 | L25A | 179 | Total | C | N | O | S | 0 | 0 | 0 |
| | | | 1428 | 911 | 255 | 259 | 3 | | | |
| 47 | L25B | 176 | Total | C | N | O | S | 0 | 0 | 0 |
| | | | 1404 | 897 | 252 | 252 | 3 | | | |

- Molecule 48 is a protein called 50S ribosomal protein L27.

| Mol | Chain | Residues | Atoms | | | | | ZeroOcc | AltConf | Trace |
|---|---|---|---|---|---|---|---|---|---|---|
| 48 | L27A | 84 | Total | C | N | O | S | 0 | 0 | 0 |
| | | | 661 | 410 | 140 | 110 | 1 | | | |

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| Mol | Chain | Residues | Atoms | | | | | ZeroOcc | AltConf | Trace |
|---|---|---|---|---|---|---|---|---|---|---|
| 48 | L27B | 84 | Total<br>661 | C<br>410 | N<br>140 | O<br>110 | S<br>1 | 0 | 0 | 0 |

- Molecule 49 is a protein called 50S ribosomal protein L28.

| Mol | Chain | Residues | Atoms | | | | | ZeroOcc | AltConf | Trace |
|---|---|---|---|---|---|---|---|---|---|---|
| 49 | L28A | 97 | Total<br>762 | C<br>481 | N<br>150 | O<br>130 | S<br>1 | 0 | 0 | 0 |
| 49 | L28B | 97 | Total<br>762 | C<br>481 | N<br>150 | O<br>130 | S<br>1 | 0 | 0 | 0 |

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

| Mol | Chain | Residues | Atoms | | | | | ZeroOcc | AltConf | Trace |
|---|---|---|---|---|---|---|---|---|---|---|
| 50 | L29A | 69 | Total<br>583 | C<br>363 | N<br>117 | O<br>101 | S<br>2 | 0 | 0 | 0 |
| 50 | L29B | 68 | Total<br>575 | C<br>358 | N<br>116 | O<br>100 | S<br>1 | 0 | 0 | 0 |

- Molecule 51 is a protein called 50S ribosomal protein L30.

| Mol | Chain | Residues | Atoms | | | | ZeroOcc | AltConf | Trace |
|---|---|---|---|---|---|---|---|---|---|
| 51 | L30A | 59 | Total<br>468 | C<br>298 | N<br>90 | O<br>80 | 0 | 0 | 0 |
| 51 | L30B | 59 | Total<br>468 | C<br>298 | N<br>90 | O<br>80 | 0 | 0 | 0 |

- Molecule 52 is a protein called 50S ribosomal protein L31.

| Mol | Chain | Residues | Atoms | | | | | ZeroOcc | AltConf | Trace |
|---|---|---|---|---|---|---|---|---|---|---|
| 52 | L31A | 71 | Total<br>580 | C<br>364 | N<br>108 | O<br>103 | S<br>5 | 0 | 0 | 0 |
| 52 | L31B | 71 | Total<br>580 | C<br>364 | N<br>108 | O<br>103 | S<br>5 | 0 | 0 | 0 |

- Molecule 53 is a protein called 50S ribosomal protein L32.

| Mol | Chain | Residues | Atoms | | | | | ZeroOcc | AltConf | Trace |
|---|---|---|---|---|---|---|---|---|---|---|
| 53 | L32A | 56 | Total<br>434 | C<br>272 | N<br>87 | O<br>70 | S<br>5 | 0 | 0 | 0 |
| 53 | L32B | 56 | Total<br>434 | C<br>272 | N<br>87 | O<br>70 | S<br>5 | 0 | 0 | 0 |

- Molecule 54 is a protein called 50S ribosomal protein L33.

| Mol | Chain | Residues | Atoms | | | | | ZeroOcc | AltConf | Trace |
|---|---|---|---|---|---|---|---|---|---|---|
| 54 | L33A | 45 | Total | C | N | O | S | 0 | 0 | 0 |
| | | | 389 | 241 | 79 | 65 | 4 | | | |
| 54 | L33B | 45 | Total | C | N | O | S | 0 | 0 | 0 |
| | | | 389 | 241 | 79 | 65 | 4 | | | |

- Molecule 55 is a protein called 50S ribosomal protein L34.

| Mol | Chain | Residues | Atoms | | | | | ZeroOcc | AltConf | Trace |
|---|---|---|---|---|---|---|---|---|---|---|
| 55 | L34A | 48 | Total | C | N | O | S | 0 | 0 | 0 |
| | | | 418 | 257 | 104 | 55 | 2 | | | |
| 55 | L34B | 49 | Total | C | N | O | S | 0 | 0 | 0 |
| | | | 429 | 263 | 108 | 56 | 2 | | | |

- Molecule 56 is a protein called 50S ribosomal protein L35.

| Mol | Chain | Residues | Atoms | | | | | ZeroOcc | AltConf | Trace |
|---|---|---|---|---|---|---|---|---|---|---|
| 56 | L35A | 64 | Total | C | N | O | S | 0 | 0 | 0 |
| | | | 516 | 331 | 102 | 81 | 2 | | | |
| 56 | L35B | 64 | Total | C | N | O | S | 0 | 0 | 0 |
| | | | 516 | 331 | 102 | 81 | 2 | | | |

- Molecule 57 is a RNA chain called Phe-tRNA.

| Mol | Chain | Residues | Atoms | | | | | | ZeroOcc | AltConf | Trace |
|---|---|---|---|---|---|---|---|---|---|---|---|
| 57 | ASIB | 76 | Total | C | N | O | P | S | 0 | 0 | 0 |
| | | | 1627 | 730 | 290 | 531 | 75 | 1 | | | |

- Molecule 58 is MAGNESIUM ION (CCD ID: MG) (formula: Mg).

| Mol | Chain | Residues | Atoms | | ZeroOcc | AltConf |
|---|---|---|---|---|---|---|
| 58 | 16SA | 90 | Total | Mg | 0 | 0 |
| | | | 90 | 90 | | |
| 58 | S4A | 1 | Total | Mg | 0 | 0 |
| | | | 1 | 1 | | |
| 58 | PSIA | 2 | Total | Mg | 0 | 0 |
| | | | 2 | 2 | | |
| 58 | MRNA | 1 | Total | Mg | 0 | 0 |
| | | | 1 | 1 | | |
| 58 | 23SA | 334 | Total | Mg | 0 | 0 |
| | | | 334 | 334 | | |

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| Mol | Chain | Residues | Atoms | ZeroOcc | AltConf |
|---|---|---|---|---|---|
| 58 | 5SA | 6 | Total Mg<br>6 6 | 0 | 0 |
| 58 | L3A | 2 | Total Mg<br>2 2 | 0 | 0 |
| 58 | L4A | 2 | Total Mg<br>2 2 | 0 | 0 |
| 58 | L5A | 1 | Total Mg<br>1 1 | 0 | 0 |
| 58 | L15A | 2 | Total Mg<br>2 2 | 0 | 0 |
| 58 | L17A | 1 | Total Mg<br>1 1 | 0 | 0 |
| 58 | L23A | 1 | Total Mg<br>1 1 | 0 | 0 |
| 58 | L27A | 2 | Total Mg<br>2 2 | 0 | 0 |
| 58 | L30A | 1 | Total Mg<br>1 1 | 0 | 0 |
| 58 | L32A | 1 | Total Mg<br>1 1 | 0 | 0 |
| 58 | L33A | 1 | Total Mg<br>1 1 | 0 | 0 |
| 58 | L34A | 1 | Total Mg<br>1 1 | 0 | 0 |
| 58 | L35A | 1 | Total Mg<br>1 1 | 0 | 0 |
| 58 | 16SB | 85 | Total Mg<br>86 86 | 0 | 1 |
| 58 | S5B | 2 | Total Mg<br>2 2 | 0 | 0 |
| 58 | PSIB | 3 | Total Mg<br>3 3 | 0 | 0 |
| 58 | 23SB | 239 | Total Mg<br>240 240 | 0 | 1 |
| 58 | 5SB | 4 | Total Mg<br>4 4 | 0 | 0 |
| 58 | L2B | 1 | Total Mg<br>1 1 | 0 | 0 |
| 58 | L3B | 2 | Total Mg<br>2 2 | 0 | 0 |
| 58 | L5B | 1 | Total Mg<br>1 1 | 0 | 0 |

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| Mol | Chain | Residues | Atoms | ZeroOcc | AltConf |
|---|---|---|---|---|---|
| 58 | L27B | 1 | Total Mg<br>1 1 | 0 | 0 |
| 58 | L35B | 2 | Total Mg<br>2 2 | 0 | 0 |

- Molecule 59 is POTASSIUM ION (CCD ID: K) (formula: K).

| Mol | Chain | Residues | Atoms | ZeroOcc | AltConf |
|---|---|---|---|---|---|
| 59 | 16SA | 46 | Total K<br>46 46 | 0 | 0 |
| 59 | S6A | 1 | Total K<br>1 1 | 0 | 0 |
| 59 | S13A | 1 | Total K<br>1 1 | 0 | 0 |
| 59 | S20A | 1 | Total K<br>1 1 | 0 | 0 |
| 59 | PSIA | 2 | Total K<br>2 2 | 0 | 0 |
| 59 | 23SA | 101 | Total K<br>101 101 | 0 | 0 |
| 59 | 5SA | 2 | Total K<br>2 2 | 0 | 0 |
| 59 | L2A | 1 | Total K<br>1 1 | 0 | 0 |
| 59 | L3A | 1 | Total K<br>1 1 | 0 | 0 |
| 59 | L4A | 1 | Total K<br>1 1 | 0 | 0 |
| 59 | L5A | 1 | Total K<br>1 1 | 0 | 0 |
| 59 | L16A | 1 | Total K<br>1 1 | 0 | 0 |
| 59 | 16SB | 36 | Total K<br>36 36 | 0 | 0 |
| 59 | S4B | 1 | Total K<br>1 1 | 0 | 0 |
| 59 | S6B | 1 | Total K<br>1 1 | 0 | 0 |
| 59 | S13B | 1 | Total K<br>1 1 | 0 | 0 |
| 59 | S20B | 1 | Total K<br>1 1 | 0 | 0 |

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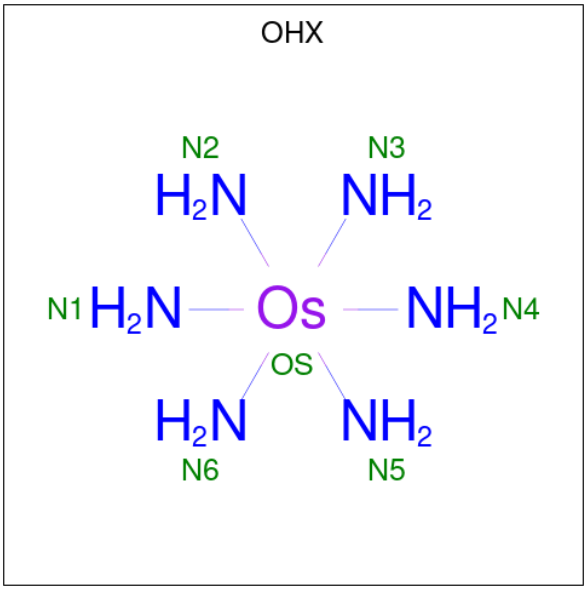
| Mol | Chain | Residues | Atoms | ZeroOcc | AltConf |
|---|---|---|---|---|---|
| 59 | 23SB | 83 | Total K<br>83 83 | 0 | 0 |
| 59 | 5SB | 1 | Total K<br>1 1 | 0 | 0 |
| 59 | L2B | 1 | Total K<br>1 1 | 0 | 0 |
| 59 | L3B | 1 | Total K<br>1 1 | 0 | 0 |
| 59 | L4B | 1 | Total K<br>1 1 | 0 | 0 |
| 59 | L5B | 1 | Total K<br>1 1 | 0 | 0 |
| 59 | L16B | 1 | Total K<br>1 1 | 0 | 0 |

- Molecule 60 is osmium (III) hexammine (CCD ID: OHX) (formula: $H_{12}N_6Os$).




| Mol | Chain | Residues | Atoms | ZeroOcc | AltConf |
|---|---|---|---|---|---|
| 60 | 16SA | 1 | Total N Os<br>7 6 1 | 0 | 0 |
| 60 | 16SA | 1 | Total N Os<br>7 6 1 | 0 | 0 |
| 60 | 16SA | 1 | Total N Os<br>7 6 1 | 0 | 0 |
| 60 | 16SA | 1 | Total N Os<br>7 6 1 | 0 | 0 |

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| Mol | Chain | Residues | Atoms | ZeroOcc | AltConf |
|---|---|---|---|---|---|
| 60 | 16SA | 1 | Total N Os<br>7 6 1 | 0 | 0 |
| 60 | 16SA | 1 | Total N Os<br>7 6 1 | 0 | 0 |
| 60 | 16SA | 1 | Total N Os<br>7 6 1 | 0 | 0 |
| 60 | 16SA | 1 | Total N Os<br>7 6 1 | 0 | 0 |
| 60 | 16SA | 1 | Total N Os<br>7 6 1 | 0 | 0 |
| 60 | 16SA | 1 | Total N Os<br>7 6 1 | 0 | 0 |
| 60 | 16SA | 1 | Total N Os<br>7 6 1 | 0 | 0 |
| 60 | 16SA | 1 | Total N Os<br>7 6 1 | 0 | 0 |
| 60 | 16SA | 1 | Total N Os<br>7 6 1 | 0 | 0 |
| 60 | 16SA | 1 | Total N Os<br>7 6 1 | 0 | 0 |
| 60 | 16SA | 1 | Total N Os<br>7 6 1 | 0 | 0 |
| 60 | 16SA | 1 | Total N Os<br>7 6 1 | 0 | 0 |
| 60 | 16SA | 1 | Total N Os<br>7 6 1 | 0 | 0 |
| 60 | 16SA | 1 | Total N Os<br>7 6 1 | 0 | 0 |
| 60 | 16SA | 1 | Total N Os<br>7 6 1 | 0 | 0 |
| 60 | 16SA | 1 | Total N Os<br>7 6 1 | 0 | 0 |
| 60 | 16SA | 1 | Total N Os<br>7 6 1 | 0 | 0 |
| 60 | 16SA | 1 | Total N Os<br>7 6 1 | 0 | 0 |
| 60 | 16SA | 1 | Total N Os<br>7 6 1 | 0 | 0 |
| 60 | 16SA | 1 | Total N Os<br>7 6 1 | 0 | 0 |
| 60 | 16SA | 1 | Total N Os<br>7 6 1 | 0 | 0 |

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| Mol | Chain | Residues | Atoms | ZeroOcc | AltConf |
|---|---|---|---|---|---|
| 60 | 16SA | 1 | Total N Os<br>7 6 1 | 0 | 0 |
| 60 | 16SA | 1 | Total N Os<br>7 6 1 | 0 | 0 |
| 60 | 16SA | 1 | Total N Os<br>7 6 1 | 0 | 0 |
| 60 | 16SA | 1 | Total N Os<br>7 6 1 | 0 | 0 |
| 60 | 16SA | 1 | Total N Os<br>7 6 1 | 0 | 0 |
| 60 | 16SA | 1 | Total N Os<br>7 6 1 | 0 | 0 |
| 60 | 16SA | 1 | Total N Os<br>7 6 1 | 0 | 0 |
| 60 | 16SA | 1 | Total N Os<br>7 6 1 | 0 | 0 |
| 60 | 16SA | 1 | Total N Os<br>7 6 1 | 0 | 0 |
| 60 | 16SA | 1 | Total N Os<br>7 6 1 | 0 | 0 |
| 60 | 16SA | 1 | Total N Os<br>7 6 1 | 0 | 0 |
| 60 | 16SA | 1 | Total N Os<br>7 6 1 | 0 | 0 |
| 60 | 16SA | 1 | Total N Os<br>7 6 1 | 0 | 0 |
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| 60 | 16SA | 1 | Total N Os<br>7 6 1 | 0 | 0 |
| 60 | 16SA | 1 | Total N Os<br>7 6 1 | 0 | 0 |
| 60 | 16SA | 1 | Total N Os<br>7 6 1 | 0 | 0 |
| 60 | 16SA | 1 | Total N Os<br>7 6 1 | 0 | 0 |
| 60 | 16SA | 1 | Total N Os<br>7 6 1 | 0 | 0 |
| 60 | 16SA | 1 | Total N Os<br>7 6 1 | 0 | 0 |
| 60 | 16SA | 1 | Total N Os<br>7 6 1 | 0 | 0 |

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| Mol | Chain | Residues | Atoms | | | ZeroOcc | AltConf |
|---|---|---|---|---|---|---|---|
| 60 | 16SA | 1 | Total | N | Os | 0 | 0 |
| | | | 7 | 6 | 1 | | |
| 60 | 16SA | 1 | Total | N | Os | 0 | 0 |
| | | | 7 | 6 | 1 | | |
| 60 | 16SA | 1 | Total | N | Os | 0 | 0 |
| | | | 7 | 6 | 1 | | |
| 60 | 16SA | 1 | Total | N | Os | 0 | 0 |
| | | | 7 | 6 | 1 | | |
| 60 | 16SA | 1 | Total | N | Os | 0 | 0 |
| | | | 7 | 6 | 1 | | |
| 60 | 16SA | 1 | Total | N | Os | 0 | 0 |
| | | | 7 | 6 | 1 | | |
| 60 | 16SA | 1 | Total | N | Os | 0 | 0 |
| | | | 7 | 6 | 1 | | |
| 60 | 16SA | 1 | Total | N | Os | 0 | 0 |
| | | | 7 | 6 | 1 | | |
| 60 | 16SA | 1 | Total | N | Os | 0 | 0 |
| | | | 7 | 6 | 1 | | |
| 60 | 16SA | 1 | Total | N | Os | 0 | 0 |
| | | | 7 | 6 | 1 | | |
| 60 | 16SA | 1 | Total | N | Os | 0 | 0 |
| | | | 7 | 6 | 1 | | |
| 60 | 16SA | 1 | Total | N | Os | 0 | 0 |
| | | | 7 | 6 | 1 | | |
| 60 | 16SA | 1 | Total | N | Os | 0 | 0 |
| | | | 7 | 6 | 1 | | |
| 60 | 16SA | 1 | Total | N | Os | 0 | 0 |
| | | | 7 | 6 | 1 | | |
| 60 | 16SA | 1 | Total | N | Os | 0 | 0 |
| | | | 7 | 6 | 1 | | |
| 60 | 16SA | 1 | Total | N | Os | 0 | 0 |
| | | | 7 | 6 | 1 | | |
| 60 | 16SA | 1 | Total | N | Os | 0 | 0 |
| | | | 7 | 6 | 1 | | |
| 60 | 16SA | 1 | Total | N | Os | 0 | 0 |
| | | | 7 | 6 | 1 | | |
| 60 | 16SA | 1 | Total | N | Os | 0 | 0 |
| | | | 7 | 6 | 1 | | |
| 60 | 16SA | 1 | Total | N | Os | 0 | 0 |
| | | | 7 | 6 | 1 | | |

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| Mol | Chain | Residues | Atoms | ZeroOcc | AltConf |
|---|---|---|---|---|---|
| 60 | 16SA | 1 | Total N Os<br>7 6 1 | 0 | 0 |
| 60 | 16SA | 1 | Total N Os<br>7 6 1 | 0 | 0 |
| 60 | 16SA | 1 | Total N Os<br>7 6 1 | 0 | 0 |
| 60 | 16SA | 1 | Total N Os<br>7 6 1 | 0 | 0 |
| 60 | 16SA | 1 | Total N Os<br>7 6 1 | 0 | 0 |
| 60 | 16SA | 1 | Total N Os<br>7 6 1 | 0 | 0 |
| 60 | 16SA | 1 | Total N Os<br>7 6 1 | 0 | 0 |
| 60 | 16SA | 1 | Total N Os<br>7 6 1 | 0 | 0 |
| 60 | 16SA | 1 | Total N Os<br>7 6 1 | 0 | 0 |
| 60 | 16SA | 1 | Total N Os<br>7 6 1 | 0 | 0 |
| 60 | 16SA | 1 | Total N Os<br>7 6 1 | 0 | 0 |
| 60 | 16SA | 1 | Total N Os<br>7 6 1 | 0 | 0 |
| 60 | 16SA | 1 | Total N Os<br>7 6 1 | 0 | 0 |
| 60 | S19A | 1 | Total N Os<br>7 6 1 | 0 | 0 |
| 60 | ASIA | 1 | Total N Os<br>7 6 1 | 0 | 0 |
| 60 | ASIA | 1 | Total N Os<br>7 6 1 | 0 | 0 |
| 60 | ASIA | 1 | Total N Os<br>7 6 1 | 0 | 0 |
| 60 | PSIA | 1 | Total N Os<br>7 6 1 | 0 | 0 |
| 60 | ESIA | 1 | Total N Os<br>7 6 1 | 0 | 0 |
| 60 | MRNA | 1 | Total N Os<br>7 6 1 | 0 | 0 |
| 60 | TRNA | 1 | Total N Os<br>7 6 1 | 0 | 0 |

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| Mol | Chain | Residues | Atoms | ZeroOcc | AltConf |
|---|---|---|---|---|---|
| 60 | TRNA | 1 | Total N Os<br>7 6 1 | 0 | 0 |
| 60 | 23SA | 1 | Total N Os<br>7 6 1 | 0 | 0 |
| 60 | 23SA | 1 | Total N Os<br>7 6 1 | 0 | 0 |
| 60 | 23SA | 1 | Total N Os<br>7 6 1 | 0 | 0 |
| 60 | 23SA | 1 | Total N Os<br>7 6 1 | 0 | 0 |
| 60 | 23SA | 1 | Total N Os<br>7 6 1 | 0 | 0 |
| 60 | 23SA | 1 | Total N Os<br>7 6 1 | 0 | 0 |
| 60 | 23SA | 1 | Total N Os<br>7 6 1 | 0 | 0 |
| 60 | 23SA | 1 | Total N Os<br>7 6 1 | 0 | 0 |
| 60 | 23SA | 1 | Total N Os<br>7 6 1 | 0 | 0 |
| 60 | 23SA | 1 | Total N Os<br>7 6 1 | 0 | 0 |
| 60 | 23SA | 1 | Total N Os<br>7 6 1 | 0 | 0 |
| 60 | 23SA | 1 | Total N Os<br>7 6 1 | 0 | 0 |
| 60 | 23SA | 1 | Total N Os<br>7 6 1 | 0 | 0 |
| 60 | 23SA | 1 | Total N Os<br>7 6 1 | 0 | 0 |
| 60 | 23SA | 1 | Total N Os<br>7 6 1 | 0 | 0 |
| 60 | 23SA | 1 | Total N Os<br>7 6 1 | 0 | 0 |
| 60 | 23SA | 1 | Total N Os<br>7 6 1 | 0 | 0 |
| 60 | 23SA | 1 | Total N Os<br>7 6 1 | 0 | 0 |
| 60 | 23SA | 1 | Total N Os<br>7 6 1 | 0 | 0 |
| 60 | 23SA | 1 | Total N Os<br>7 6 1 | 0 | 0 |

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| Mol | Chain | Residues | Atoms | ZeroOcc | AltConf |
|---|---|---|---|---|---|
| 60 | 23SA | 1 | Total N Os<br>7 6 1 | 0 | 0 |
| 60 | 23SA | 1 | Total N Os<br>7 6 1 | 0 | 0 |
| 60 | 23SA | 1 | Total N Os<br>7 6 1 | 0 | 0 |
| 60 | 23SA | 1 | Total N Os<br>7 6 1 | 0 | 0 |
| 60 | 23SA | 1 | Total N Os<br>7 6 1 | 0 | 0 |
| 60 | 23SA | 1 | Total N Os<br>7 6 1 | 0 | 0 |
| 60 | 23SA | 1 | Total N Os<br>7 6 1 | 0 | 0 |
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| 60 | 23SA | 1 | Total N Os<br>7 6 1 | 0 | 0 |
| 60 | 23SA | 1 | Total N Os<br>7 6 1 | 0 | 0 |
| 60 | 23SA | 1 | Total N Os<br>7 6 1 | 0 | 0 |
| 60 | 23SA | 1 | Total N Os<br>7 6 1 | 0 | 0 |
| 60 | 23SA | 1 | Total N Os<br>7 6 1 | 0 | 0 |
| 60 | 23SA | 1 | Total N Os<br>7 6 1 | 0 | 0 |
| 60 | 23SA | 1 | Total N Os<br>7 6 1 | 0 | 0 |
| 60 | 23SA | 1 | Total N Os<br>7 6 1 | 0 | 0 |
| 60 | 23SA | 1 | Total N Os<br>7 6 1 | 0 | 0 |
| 60 | 23SA | 1 | Total N Os<br>7 6 1 | 0 | 0 |
| 60 | 23SA | 1 | Total N Os<br>7 6 1 | 0 | 0 |
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| Mol | Chain | Residues | Atoms | ZeroOcc | AltConf |
|---|---|---|---|---|---|
| 60 | 23SA | 1 | Total N Os<br>7 6 1 | 0 | 0 |
| 60 | 23SA | 1 | Total N Os<br>7 6 1 | 0 | 0 |
| 60 | 23SA | 1 | Total N Os<br>7 6 1 | 0 | 0 |
| 60 | 23SA | 1 | Total N Os<br>7 6 1 | 0 | 0 |
| 60 | 23SA | 1 | Total N Os<br>7 6 1 | 0 | 0 |
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| 60 | 23SA | 1 | Total N Os<br>7 6 1 | 0 | 0 |
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| 60 | 23SA | 1 | Total N Os<br>7 6 1 | 0 | 0 |
| 60 | 23SA | 1 | Total N Os<br>7 6 1 | 0 | 0 |
| 60 | 23SA | 1 | Total N Os<br>7 6 1 | 0 | 0 |
| 60 | 23SA | 1 | Total N Os<br>7 6 1 | 0 | 0 |
| 60 | 23SA | 1 | Total N Os<br>7 6 1 | 0 | 0 |
| 60 | 23SA | 1 | Total N Os<br>7 6 1 | 0 | 0 |
| 60 | 23SA | 1 | Total N Os<br>7 6 1 | 0 | 0 |
| 60 | 23SA | 1 | Total N Os<br>7 6 1 | 0 | 0 |
| 60 | 23SA | 1 | Total N Os<br>7 6 1 | 0 | 0 |
| 60 | 23SA | 1 | Total N Os<br>7 6 1 | 0 | 0 |
| 60 | 23SA | 1 | Total N Os<br>7 6 1 | 0 | 0 |
| 60 | 23SA | 1 | Total N Os<br>7 6 1 | 0 | 0 |

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| Mol | Chain | Residues | Atoms | ZeroOcc | AltConf |
|---|---|---|---|---|---|
| 60 | 23SA | 1 | Total N Os<br>7 6 1 | 0 | 0 |
| 60 | 23SA | 1 | Total N Os<br>7 6 1 | 0 | 0 |
| 60 | 23SA | 1 | Total N Os<br>7 6 1 | 0 | 0 |
| 60 | 23SA | 1 | Total N Os<br>7 6 1 | 0 | 0 |
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| 60 | 23SA | 1 | Total N Os<br>7 6 1 | 0 | 0 |
| 60 | 23SA | 1 | Total N Os<br>7 6 1 | 0 | 0 |
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| 60 | 23SA | 1 | Total N Os<br>7 6 1 | 0 | 0 |
| 60 | 23SA | 1 | Total N Os<br>7 6 1 | 0 | 0 |
| 60 | 23SA | 1 | Total N Os<br>7 6 1 | 0 | 0 |
| 60 | 23SA | 1 | Total N Os<br>7 6 1 | 0 | 0 |

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| Mol | Chain | Residues | Atoms | ZeroOcc | AltConf |
|---|---|---|---|---|---|
| 60 | 23SA | 1 | Total N Os<br>7 6 1 | 0 | 0 |
| 60 | 23SA | 1 | Total N Os<br>7 6 1 | 0 | 0 |
| 60 | 23SA | 1 | Total N Os<br>7 6 1 | 0 | 0 |
| 60 | 23SA | 1 | Total N Os<br>7 6 1 | 0 | 0 |
| 60 | 23SA | 1 | Total N Os<br>7 6 1 | 0 | 0 |
| 60 | 23SA | 1 | Total N Os<br>7 6 1 | 0 | 0 |
| 60 | 23SA | 1 | Total N Os<br>7 6 1 | 0 | 0 |
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| 60 | 23SA | 1 | Total N Os<br>7 6 1 | 0 | 0 |
| 60 | 23SA | 1 | Total N Os<br>7 6 1 | 0 | 0 |
| 60 | 23SA | 1 | Total N Os<br>7 6 1 | 0 | 0 |
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| 60 | 23SA | 1 | Total N Os<br>7 6 1 | 0 | 0 |
| 60 | 23SA | 1 | Total N Os<br>7 6 1 | 0 | 0 |
| 60 | 23SA | 1 | Total N Os<br>7 6 1 | 0 | 0 |
| 60 | 23SA | 1 | Total N Os<br>7 6 1 | 0 | 0 |
| 60 | 23SA | 1 | Total N Os<br>7 6 1 | 0 | 0 |
| 60 | 23SA | 1 | Total N Os<br>7 6 1 | 0 | 0 |
| 60 | 23SA | 1 | Total N Os<br>7 6 1 | 0 | 0 |
| 60 | 23SA | 1 | Total N Os<br>7 6 1 | 0 | 0 |

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| Mol | Chain | Residues | Atoms | ZeroOcc | AltConf |
|---|---|---|---|---|---|
| 60 | 23SA | 1 | Total N Os<br>7 6 1 | 0 | 0 |
| 60 | 23SA | 1 | Total N Os<br>7 6 1 | 0 | 0 |
| 60 | 23SA | 1 | Total N Os<br>7 6 1 | 0 | 0 |
| 60 | 23SA | 1 | Total N Os<br>7 6 1 | 0 | 0 |
| 60 | 23SA | 1 | Total N Os<br>7 6 1 | 0 | 0 |
| 60 | 23SA | 1 | Total N Os<br>7 6 1 | 0 | 0 |
| 60 | 23SA | 1 | Total N Os<br>7 6 1 | 0 | 0 |
| 60 | 23SA | 1 | Total N Os<br>7 6 1 | 0 | 0 |
| 60 | 23SA | 1 | Total N Os<br>7 6 1 | 0 | 0 |
| 60 | 23SA | 1 | Total N Os<br>7 6 1 | 0 | 0 |
| 60 | 23SA | 1 | Total N Os<br>7 6 1 | 0 | 0 |
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| 60 | 23SA | 1 | Total N Os<br>7 6 1 | 0 | 0 |
| 60 | 23SA | 1 | Total N Os<br>7 6 1 | 0 | 0 |
| 60 | 23SA | 1 | Total N Os<br>7 6 1 | 0 | 0 |
| 60 | 23SA | 1 | Total N Os<br>7 6 1 | 0 | 0 |
| 60 | 23SA | 1 | Total N Os<br>7 6 1 | 0 | 0 |
| 60 | 23SA | 1 | Total N Os<br>7 6 1 | 0 | 0 |
| 60 | 23SA | 1 | Total N Os<br>7 6 1 | 0 | 0 |
| 60 | 23SA | 1 | Total N Os<br>7 6 1 | 0 | 0 |

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| Mol | Chain | Residues | Atoms | ZeroOcc | AltConf |
|---|---|---|---|---|---|
| 60 | 23SA | 1 | Total N Os<br>7 6 1 | 0 | 0 |
| 60 | 23SA | 1 | Total N Os<br>7 6 1 | 0 | 0 |
| 60 | 23SA | 1 | Total N Os<br>7 6 1 | 0 | 0 |
| 60 | 23SA | 1 | Total N Os<br>7 6 1 | 0 | 0 |
| 60 | 23SA | 1 | Total N Os<br>7 6 1 | 0 | 0 |
| 60 | 23SA | 1 | Total N Os<br>7 6 1 | 0 | 0 |
| 60 | 23SA | 1 | Total N Os<br>7 6 1 | 0 | 0 |
| 60 | 23SA | 1 | Total N Os<br>7 6 1 | 0 | 0 |
| 60 | 23SA | 1 | Total N Os<br>7 6 1 | 0 | 0 |
| 60 | 23SA | 1 | Total N Os<br>7 6 1 | 0 | 0 |
| 60 | 23SA | 1 | Total N Os<br>7 6 1 | 0 | 0 |
| 60 | 23SA | 1 | Total N Os<br>7 6 1 | 0 | 0 |
| 60 | 23SA | 1 | Total N Os<br>7 6 1 | 0 | 0 |
| 60 | 23SA | 1 | Total N Os<br>7 6 1 | 0 | 0 |
| 60 | 23SA | 1 | Total N Os<br>7 6 1 | 0 | 0 |
| 60 | 23SA | 1 | Total N Os<br>7 6 1 | 0 | 0 |
| 60 | 23SA | 1 | Total N Os<br>7 6 1 | 0 | 0 |
| 60 | 23SA | 1 | Total N Os<br>7 6 1 | 0 | 0 |
| 60 | 23SA | 1 | Total N Os<br>7 6 1 | 0 | 0 |
| 60 | 23SA | 1 | Total N Os<br>7 6 1 | 0 | 0 |
| 60 | 23SA | 1 | Total N Os<br>7 6 1 | 0 | 0 |

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| Mol | Chain | Residues | Atoms | ZeroOcc | AltConf |
|---|---|---|---|---|---|
| 60 | 23SA | 1 | Total N Os<br>7 6 1 | 0 | 0 |
| 60 | 23SA | 1 | Total N Os<br>7 6 1 | 0 | 0 |
| 60 | 23SA | 1 | Total N Os<br>7 6 1 | 0 | 0 |
| 60 | 23SA | 1 | Total N Os<br>7 6 1 | 0 | 0 |
| 60 | 23SA | 1 | Total N Os<br>7 6 1 | 0 | 0 |
| 60 | 23SA | 1 | Total N Os<br>7 6 1 | 0 | 0 |
| 60 | 23SA | 1 | Total N Os<br>7 6 1 | 0 | 0 |
| 60 | 23SA | 1 | Total N Os<br>7 6 1 | 0 | 0 |
| 60 | 23SA | 1 | Total N Os<br>7 6 1 | 0 | 0 |
| 60 | 23SA | 1 | Total N Os<br>7 6 1 | 0 | 0 |
| 60 | 23SA | 1 | Total N Os<br>7 6 1 | 0 | 0 |
| 60 | 23SA | 1 | Total N Os<br>7 6 1 | 0 | 0 |
| 60 | 23SA | 1 | Total N Os<br>7 6 1 | 0 | 0 |
| 60 | 23SA | 1 | Total N Os<br>7 6 1 | 0 | 0 |
| 60 | 23SA | 1 | Total N Os<br>7 6 1 | 0 | 0 |
| 60 | 23SA | 1 | Total N Os<br>7 6 1 | 0 | 0 |
| 60 | 23SA | 1 | Total N Os<br>7 6 1 | 0 | 0 |
| 60 | 23SA | 1 | Total N Os<br>7 6 1 | 0 | 0 |
| 60 | 23SA | 1 | Total N Os<br>7 6 1 | 0 | 0 |
| 60 | 23SA | 1 | Total N Os<br>7 6 1 | 0 | 0 |

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| Mol | Chain | Residues | Atoms | ZeroOcc | AltConf |
|---|---|---|---|---|---|
| 60 | 23SA | 1 | Total N Os<br>7 6 1 | 0 | 0 |
| 60 | 23SA | 1 | Total N Os<br>7 6 1 | 0 | 0 |
| 60 | 23SA | 1 | Total N Os<br>7 6 1 | 0 | 0 |
| 60 | 23SA | 1 | Total N Os<br>7 6 1 | 0 | 0 |
| 60 | 23SA | 1 | Total N Os<br>7 6 1 | 0 | 0 |
| 60 | 23SA | 1 | Total N Os<br>7 6 1 | 0 | 0 |
| 60 | 23SA | 1 | Total N Os<br>7 6 1 | 0 | 0 |
| 60 | 23SA | 1 | Total N Os<br>7 6 1 | 0 | 0 |
| 60 | 23SA | 1 | Total N Os<br>7 6 1 | 0 | 0 |
| 60 | 23SA | 1 | Total N Os<br>7 6 1 | 0 | 0 |
| 60 | 23SA | 1 | Total N Os<br>7 6 1 | 0 | 0 |
| 60 | 23SA | 1 | Total N Os<br>7 6 1 | 0 | 0 |
| 60 | 23SA | 1 | Total N Os<br>7 6 1 | 0 | 0 |
| 60 | 23SA | 1 | Total N Os<br>7 6 1 | 0 | 0 |
| 60 | 23SA | 1 | Total N Os<br>7 6 1 | 0 | 0 |
| 60 | 23SA | 1 | Total N Os<br>7 6 1 | 0 | 0 |
| 60 | 23SA | 1 | Total N Os<br>7 6 1 | 0 | 0 |
| 60 | 23SA | 1 | Total N Os<br>7 6 1 | 0 | 0 |
| 60 | 23SA | 1 | Total N Os<br>7 6 1 | 0 | 0 |
| 60 | 23SA | 1 | Total N Os<br>7 6 1 | 0 | 0 |

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| Mol | Chain | Residues | Atoms | ZeroOcc | AltConf |
|---|---|---|---|---|---|
| 60 | 23SA | 1 | Total N Os<br>7 6 1 | 0 | 0 |
| 60 | 23SA | 1 | Total N Os<br>7 6 1 | 0 | 0 |
| 60 | 23SA | 1 | Total N Os<br>7 6 1 | 0 | 0 |
| 60 | 23SA | 1 | Total N Os<br>7 6 1 | 0 | 0 |
| 60 | 23SA | 1 | Total N Os<br>7 6 1 | 0 | 0 |
| 60 | 23SA | 1 | Total N Os<br>7 6 1 | 0 | 0 |
| 60 | 23SA | 1 | Total N Os<br>7 6 1 | 0 | 0 |
| 60 | 23SA | 1 | Total N Os<br>7 6 1 | 0 | 0 |
| 60 | 23SA | 1 | Total N Os<br>7 6 1 | 0 | 0 |
| 60 | 5SA | 1 | Total N Os<br>7 6 1 | 0 | 0 |
| 60 | 5SA | 1 | Total N Os<br>7 6 1 | 0 | 0 |
| 60 | 5SA | 1 | Total N Os<br>7 6 1 | 0 | 0 |
| 60 | 5SA | 1 | Total N Os<br>7 6 1 | 0 | 0 |
| 60 | 5SA | 1 | Total N Os<br>7 6 1 | 0 | 0 |
| 60 | 5SA | 1 | Total N Os<br>7 6 1 | 0 | 0 |
| 60 | 5SA | 1 | Total N Os<br>7 6 1 | 0 | 0 |
| 60 | 5SA | 1 | Total N Os<br>7 6 1 | 0 | 0 |
| 60 | 5SA | 1 | Total N Os<br>7 6 1 | 0 | 0 |
| 60 | 5SA | 1 | Total N Os<br>7 6 1 | 0 | 0 |
| 60 | L4A | 1 | Total N Os<br>7 6 1 | 0 | 0 |
| 60 | L15A | 1 | Total N Os<br>7 6 1 | 0 | 0 |

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| Mol | Chain | Residues | Atoms | ZeroOcc | AltConf |
|---|---|---|---|---|---|
| 60 | L17A | 1 | Total N Os<br>7 6 1 | 0 | 0 |
| 60 | L19A | 1 | Total N Os<br>7 6 1 | 0 | 0 |
| 60 | L27A | 1 | Total N Os<br>7 6 1 | 0 | 0 |
| 60 | L27A | 1 | Total N Os<br>7 6 1 | 0 | 0 |
| 60 | L28A | 1 | Total N Os<br>7 6 1 | 0 | 0 |
| 60 | L35A | 1 | Total N Os<br>7 6 1 | 0 | 0 |
| 60 | 16SB | 1 | Total N Os<br>7 6 1 | 0 | 0 |
| 60 | 16SB | 1 | Total N Os<br>7 6 1 | 0 | 0 |
| 60 | 16SB | 1 | Total N Os<br>7 6 1 | 0 | 0 |
| 60 | 16SB | 1 | Total N Os<br>7 6 1 | 0 | 0 |
| 60 | 16SB | 1 | Total N Os<br>7 6 1 | 0 | 0 |
| 60 | 16SB | 1 | Total N Os<br>7 6 1 | 0 | 0 |
| 60 | 16SB | 1 | Total N Os<br>7 6 1 | 0 | 0 |
| 60 | 16SB | 1 | Total N Os<br>7 6 1 | 0 | 0 |
| 60 | 16SB | 1 | Total N Os<br>7 6 1 | 0 | 0 |
| 60 | 16SB | 1 | Total N Os<br>7 6 1 | 0 | 0 |
| 60 | 16SB | 1 | Total N Os<br>7 6 1 | 0 | 0 |
| 60 | 16SB | 1 | Total N Os<br>7 6 1 | 0 | 0 |
| 60 | 16SB | 1 | Total N Os<br>7 6 1 | 0 | 0 |
| 60 | 16SB | 1 | Total N Os<br>7 6 1 | 0 | 0 |

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| Mol | Chain | Residues | Atoms | ZeroOcc | AltConf |
|---|---|---|---|---|---|
| 60 | 16SB | 1 | Total N Os<br>7 6 1 | 0 | 0 |
| 60 | 16SB | 1 | Total N Os<br>7 6 1 | 0 | 0 |
| 60 | 16SB | 1 | Total N Os<br>7 6 1 | 0 | 0 |
| 60 | 16SB | 1 | Total N Os<br>7 6 1 | 0 | 0 |
| 60 | 16SB | 1 | Total N Os<br>7 6 1 | 0 | 0 |
| 60 | 16SB | 1 | Total N Os<br>7 6 1 | 0 | 0 |
| 60 | 16SB | 1 | Total N Os<br>7 6 1 | 0 | 0 |
| 60 | 16SB | 1 | Total N Os<br>7 6 1 | 0 | 0 |
| 60 | 16SB | 1 | Total N Os<br>7 6 1 | 0 | 0 |
| 60 | 16SB | 1 | Total N Os<br>7 6 1 | 0 | 0 |
| 60 | 16SB | 1 | Total N Os<br>7 6 1 | 0 | 0 |
| 60 | 16SB | 1 | Total N Os<br>7 6 1 | 0 | 0 |
| 60 | 16SB | 1 | Total N Os<br>7 6 1 | 0 | 0 |
| 60 | 16SB | 1 | Total N Os<br>7 6 1 | 0 | 0 |
| 60 | 16SB | 1 | Total N Os<br>7 6 1 | 0 | 0 |
| 60 | 16SB | 1 | Total N Os<br>7 6 1 | 0 | 0 |
| 60 | 16SB | 1 | Total N Os<br>7 6 1 | 0 | 0 |
| 60 | 16SB | 1 | Total N Os<br>7 6 1 | 0 | 0 |
| 60 | 16SB | 1 | Total N Os<br>7 6 1 | 0 | 0 |
| 60 | 16SB | 1 | Total N Os<br>7 6 1 | 0 | 0 |

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| Mol | Chain | Residues | Atoms | ZeroOcc | AltConf |
|---|---|---|---|---|---|
| 60 | 16SB | 1 | Total N Os<br>7 6 1 | 0 | 0 |
| 60 | 16SB | 1 | Total N Os<br>7 6 1 | 0 | 0 |
| 60 | 16SB | 1 | Total N Os<br>7 6 1 | 0 | 0 |
| 60 | 16SB | 1 | Total N Os<br>7 6 1 | 0 | 0 |
| 60 | 16SB | 1 | Total N Os<br>7 6 1 | 0 | 0 |
| 60 | 16SB | 1 | Total N Os<br>7 6 1 | 0 | 0 |
| 60 | 16SB | 1 | Total N Os<br>7 6 1 | 0 | 0 |
| 60 | 16SB | 1 | Total N Os<br>7 6 1 | 0 | 0 |
| 60 | 16SB | 1 | Total N Os<br>7 6 1 | 0 | 0 |
| 60 | 16SB | 1 | Total N Os<br>7 6 1 | 0 | 0 |
| 60 | 16SB | 1 | Total N Os<br>7 6 1 | 0 | 0 |
| 60 | 16SB | 1 | Total N Os<br>7 6 1 | 0 | 0 |
| 60 | 16SB | 1 | Total N Os<br>7 6 1 | 0 | 0 |
| 60 | 16SB | 1 | Total N Os<br>7 6 1 | 0 | 0 |
| 60 | 16SB | 1 | Total N Os<br>7 6 1 | 0 | 0 |
| 60 | 16SB | 1 | Total N Os<br>7 6 1 | 0 | 0 |
| 60 | 16SB | 1 | Total N Os<br>7 6 1 | 0 | 0 |
| 60 | 16SB | 1 | Total N Os<br>7 6 1 | 0 | 0 |
| 60 | 16SB | 1 | Total N Os<br>7 6 1 | 0 | 0 |
| 60 | 16SB | 1 | Total N Os<br>7 6 1 | 0 | 0 |

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| Mol | Chain | Residues | Atoms | ZeroOcc | AltConf |
|---|---|---|---|---|---|
| 60 | 16SB | 1 | Total N Os<br>7 6 1 | 0 | 0 |
| 60 | 16SB | 1 | Total N Os<br>7 6 1 | 0 | 0 |
| 60 | 16SB | 1 | Total N Os<br>7 6 1 | 0 | 0 |
| 60 | 16SB | 1 | Total N Os<br>7 6 1 | 0 | 0 |
| 60 | 16SB | 1 | Total N Os<br>7 6 1 | 0 | 0 |
| 60 | 16SB | 1 | Total N Os<br>7 6 1 | 0 | 0 |
| 60 | 16SB | 1 | Total N Os<br>7 6 1 | 0 | 0 |
| 60 | 16SB | 1 | Total N Os<br>7 6 1 | 0 | 0 |
| 60 | 16SB | 1 | Total N Os<br>7 6 1 | 0 | 0 |
| 60 | 16SB | 1 | Total N Os<br>7 6 1 | 0 | 0 |
| 60 | 16SB | 1 | Total N Os<br>7 6 1 | 0 | 0 |
| 60 | 16SB | 1 | Total N Os<br>7 6 1 | 0 | 0 |
| 60 | 16SB | 1 | Total N Os<br>7 6 1 | 0 | 0 |
| 60 | 16SB | 1 | Total N Os<br>7 6 1 | 0 | 0 |
| 60 | 16SB | 1 | Total N Os<br>7 6 1 | 0 | 0 |
| 60 | 16SB | 1 | Total N Os<br>7 6 1 | 0 | 0 |
| 60 | 16SB | 1 | Total N Os<br>7 6 1 | 0 | 0 |
| 60 | 16SB | 1 | Total N Os<br>7 6 1 | 0 | 0 |
| 60 | 16SB | 1 | Total N Os<br>7 6 1 | 0 | 0 |
| 60 | 16SB | 1 | Total N Os<br>7 6 1 | 0 | 0 |

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| Mol | Chain | Residues | Atoms | ZeroOcc | AltConf |
|---|---|---|---|---|---|
| 60 | S4B | 1 | Total N Os<br>7 6 1 | 0 | 0 |
| 60 | S8B | 1 | Total N Os<br>7 6 1 | 0 | 0 |
| 60 | S14B | 1 | Total N Os<br>7 6 1 | 0 | 0 |
| 60 | ASIB | 1 | Total N Os<br>7 6 1 | 0 | 0 |
| 60 | ASIB | 1 | Total N Os<br>7 6 1 | 0 | 0 |
| 60 | ASIB | 1 | Total N Os<br>7 6 1 | 0 | 0 |
| 60 | PSIB | 1 | Total N Os<br>7 6 1 | 0 | 0 |
| 60 | PSIB | 1 | Total N Os<br>7 6 1 | 0 | 0 |
| 60 | PSIB | 1 | Total N Os<br>7 6 1 | 0 | 0 |
| 60 | ESIB | 1 | Total N Os<br>7 6 1 | 0 | 0 |
| 60 | MRNB | 1 | Total N Os<br>7 6 1 | 0 | 0 |
| 60 | 23SB | 1 | Total N Os<br>7 6 1 | 0 | 0 |
| 60 | 23SB | 1 | Total N Os<br>7 6 1 | 0 | 0 |
| 60 | 23SB | 1 | Total N Os<br>7 6 1 | 0 | 0 |
| 60 | 23SB | 1 | Total N Os<br>7 6 1 | 0 | 0 |
| 60 | 23SB | 1 | Total N Os<br>7 6 1 | 0 | 0 |
| 60 | 23SB | 1 | Total N Os<br>7 6 1 | 0 | 0 |
| 60 | 23SB | 1 | Total N Os<br>7 6 1 | 0 | 0 |
| 60 | 23SB | 1 | Total N Os<br>7 6 1 | 0 | 0 |
| 60 | 23SB | 1 | Total N Os<br>7 6 1 | 0 | 0 |
| 60 | 23SB | 1 | Total N Os<br>7 6 1 | 0 | 0 |

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| Mol | Chain | Residues | Atoms | ZeroOcc | AltConf |
|---|---|---|---|---|---|
| 60 | 23SB | 1 | Total N Os<br>7 6 1 | 0 | 0 |
| 60 | 23SB | 1 | Total N Os<br>7 6 1 | 0 | 0 |
| 60 | 23SB | 1 | Total N Os<br>7 6 1 | 0 | 0 |
| 60 | 23SB | 1 | Total N Os<br>7 6 1 | 0 | 0 |
| 60 | 23SB | 1 | Total N Os<br>7 6 1 | 0 | 0 |
| 60 | 23SB | 1 | Total N Os<br>7 6 1 | 0 | 0 |
| 60 | 23SB | 1 | Total N Os<br>7 6 1 | 0 | 0 |
| 60 | 23SB | 1 | Total N Os<br>7 6 1 | 0 | 0 |
| 60 | 23SB | 1 | Total N Os<br>7 6 1 | 0 | 0 |
| 60 | 23SB | 1 | Total N Os<br>7 6 1 | 0 | 0 |
| 60 | 23SB | 1 | Total N Os<br>7 6 1 | 0 | 0 |
| 60 | 23SB | 1 | Total N Os<br>7 6 1 | 0 | 0 |
| 60 | 23SB | 1 | Total N Os<br>7 6 1 | 0 | 0 |
| 60 | 23SB | 1 | Total N Os<br>7 6 1 | 0 | 0 |
| 60 | 23SB | 1 | Total N Os<br>7 6 1 | 0 | 0 |
| 60 | 23SB | 1 | Total N Os<br>7 6 1 | 0 | 0 |
| 60 | 23SB | 1 | Total N Os<br>7 6 1 | 0 | 0 |
| 60 | 23SB | 1 | Total N Os<br>7 6 1 | 0 | 0 |
| 60 | 23SB | 1 | Total N Os<br>7 6 1 | 0 | 0 |
| 60 | 23SB | 1 | Total N Os<br>7 6 1 | 0 | 0 |

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| Mol | Chain | Residues | Atoms | ZeroOcc | AltConf |
|---|---|---|---|---|---|
| 60 | 23SB | 1 | Total N Os<br>7 6 1 | 0 | 0 |
| 60 | 23SB | 1 | Total N Os<br>7 6 1 | 0 | 0 |
| 60 | 23SB | 1 | Total N Os<br>7 6 1 | 0 | 0 |
| 60 | 23SB | 1 | Total N Os<br>7 6 1 | 0 | 0 |
| 60 | 23SB | 1 | Total N Os<br>7 6 1 | 0 | 0 |
| 60 | 23SB | 1 | Total N Os<br>7 6 1 | 0 | 0 |
| 60 | 23SB | 1 | Total N Os<br>7 6 1 | 0 | 0 |
| 60 | 23SB | 1 | Total N Os<br>7 6 1 | 0 | 0 |
| 60 | 23SB | 1 | Total N Os<br>7 6 1 | 0 | 0 |
| 60 | 23SB | 1 | Total N Os<br>7 6 1 | 0 | 0 |
| 60 | 23SB | 1 | Total N Os<br>7 6 1 | 0 | 0 |
| 60 | 23SB | 1 | Total N Os<br>7 6 1 | 0 | 0 |
| 60 | 23SB | 1 | Total N Os<br>7 6 1 | 0 | 0 |
| 60 | 23SB | 1 | Total N Os<br>7 6 1 | 0 | 0 |
| 60 | 23SB | 1 | Total N Os<br>7 6 1 | 0 | 0 |
| 60 | 23SB | 1 | Total N Os<br>7 6 1 | 0 | 0 |
| 60 | 23SB | 1 | Total N Os<br>7 6 1 | 0 | 0 |
| 60 | 23SB | 1 | Total N Os<br>7 6 1 | 0 | 0 |
| 60 | 23SB | 1 | Total N Os<br>7 6 1 | 0 | 0 |
| 60 | 23SB | 1 | Total N Os<br>7 6 1 | 0 | 0 |

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| Mol | Chain | Residues | Atoms | ZeroOcc | AltConf |
|---|---|---|---|---|---|
| 60 | 23SB | 1 | Total N Os<br>7 6 1 | 0 | 0 |
| 60 | 23SB | 1 | Total N Os<br>7 6 1 | 0 | 0 |
| 60 | 23SB | 1 | Total N Os<br>7 6 1 | 0 | 0 |
| 60 | 23SB | 1 | Total N Os<br>7 6 1 | 0 | 0 |
| 60 | 23SB | 1 | Total N Os<br>7 6 1 | 0 | 0 |
| 60 | 23SB | 1 | Total N Os<br>7 6 1 | 0 | 0 |
| 60 | 23SB | 1 | Total N Os<br>7 6 1 | 0 | 0 |
| 60 | 23SB | 1 | Total N Os<br>7 6 1 | 0 | 0 |
| 60 | 23SB | 1 | Total N Os<br>7 6 1 | 0 | 0 |
| 60 | 23SB | 1 | Total N Os<br>7 6 1 | 0 | 0 |
| 60 | 23SB | 1 | Total N Os<br>7 6 1 | 0 | 0 |
| 60 | 23SB | 1 | Total N Os<br>7 6 1 | 0 | 0 |
| 60 | 23SB | 1 | Total N Os<br>7 6 1 | 0 | 0 |
| 60 | 23SB | 1 | Total N Os<br>7 6 1 | 0 | 0 |
| 60 | 23SB | 1 | Total N Os<br>7 6 1 | 0 | 0 |
| 60 | 23SB | 1 | Total N Os<br>7 6 1 | 0 | 0 |
| 60 | 23SB | 1 | Total N Os<br>7 6 1 | 0 | 0 |
| 60 | 23SB | 1 | Total N Os<br>7 6 1 | 0 | 0 |
| 60 | 23SB | 1 | Total N Os<br>7 6 1 | 0 | 0 |
| 60 | 23SB | 1 | Total N Os<br>7 6 1 | 0 | 0 |

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| Mol | Chain | Residues | Atoms | ZeroOcc | AltConf |
|---|---|---|---|---|---|
| 60 | 23SB | 1 | Total N Os<br>7 6 1 | 0 | 0 |
| 60 | 23SB | 1 | Total N Os<br>7 6 1 | 0 | 0 |
| 60 | 23SB | 1 | Total N Os<br>7 6 1 | 0 | 0 |
| 60 | 23SB | 1 | Total N Os<br>7 6 1 | 0 | 0 |
| 60 | 23SB | 1 | Total N Os<br>7 6 1 | 0 | 0 |
| 60 | 23SB | 1 | Total N Os<br>7 6 1 | 0 | 0 |
| 60 | 23SB | 1 | Total N Os<br>7 6 1 | 0 | 0 |
| 60 | 23SB | 1 | Total N Os<br>7 6 1 | 0 | 0 |
| 60 | 23SB | 1 | Total N Os<br>7 6 1 | 0 | 0 |
| 60 | 23SB | 1 | Total N Os<br>7 6 1 | 0 | 0 |
| 60 | 23SB | 1 | Total N Os<br>7 6 1 | 0 | 0 |
| 60 | 23SB | 1 | Total N Os<br>7 6 1 | 0 | 0 |
| 60 | 23SB | 1 | Total N Os<br>7 6 1 | 0 | 0 |
| 60 | 23SB | 1 | Total N Os<br>7 6 1 | 0 | 0 |
| 60 | 23SB | 1 | Total N Os<br>7 6 1 | 0 | 0 |
| 60 | 23SB | 1 | Total N Os<br>7 6 1 | 0 | 0 |
| 60 | 23SB | 1 | Total N Os<br>7 6 1 | 0 | 0 |
| 60 | 23SB | 1 | Total N Os<br>7 6 1 | 0 | 0 |
| 60 | 23SB | 1 | Total N Os<br>7 6 1 | 0 | 0 |
| 60 | 23SB | 1 | Total N Os<br>7 6 1 | 0 | 0 |

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| Mol | Chain | Residues | Atoms | ZeroOcc | AltConf |
|---|---|---|---|---|---|
| 60 | 23SB | 1 | Total N Os<br>7 6 1 | 0 | 0 |
| 60 | 23SB | 1 | Total N Os<br>7 6 1 | 0 | 0 |
| 60 | 23SB | 1 | Total N Os<br>7 6 1 | 0 | 0 |
| 60 | 23SB | 1 | Total N Os<br>7 6 1 | 0 | 0 |
| 60 | 23SB | 1 | Total N Os<br>7 6 1 | 0 | 0 |
| 60 | 23SB | 1 | Total N Os<br>7 6 1 | 0 | 0 |
| 60 | 23SB | 1 | Total N Os<br>7 6 1 | 0 | 0 |
| 60 | 23SB | 1 | Total N Os<br>7 6 1 | 0 | 0 |
| 60 | 23SB | 1 | Total N Os<br>7 6 1 | 0 | 0 |
| 60 | 23SB | 1 | Total N Os<br>7 6 1 | 0 | 0 |
| 60 | 23SB | 1 | Total N Os<br>7 6 1 | 0 | 0 |
| 60 | 23SB | 1 | Total N Os<br>7 6 1 | 0 | 0 |
| 60 | 23SB | 1 | Total N Os<br>7 6 1 | 0 | 0 |
| 60 | 23SB | 1 | Total N Os<br>7 6 1 | 0 | 0 |
| 60 | 23SB | 1 | Total N Os<br>7 6 1 | 0 | 0 |
| 60 | 23SB | 1 | Total N Os<br>7 6 1 | 0 | 0 |
| 60 | 23SB | 1 | Total N Os<br>7 6 1 | 0 | 0 |
| 60 | 23SB | 1 | Total N Os<br>7 6 1 | 0 | 0 |
| 60 | 23SB | 1 | Total N Os<br>7 6 1 | 0 | 0 |
| 60 | 23SB | 1 | Total N Os<br>7 6 1 | 0 | 0 |

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| Mol | Chain | Residues | Atoms | | | ZeroOcc | AltConf |
|---|---|---|---|---|---|---|---|
| 60 | 23SB | 1 | Total | N | Os | 0 | 0 |
| | | | 7 | 6 | 1 | | |
| 60 | 23SB | 1 | Total | N | Os | 0 | 0 |
| | | | 7 | 6 | 1 | | |
| 60 | 23SB | 1 | Total | N | Os | 0 | 0 |
| | | | 7 | 6 | 1 | | |
| 60 | 23SB | 1 | Total | N | Os | 0 | 0 |
| | | | 7 | 6 | 1 | | |
| 60 | 23SB | 1 | Total | N | Os | 0 | 0 |
| | | | 7 | 6 | 1 | | |
| 60 | 23SB | 1 | Total | N | Os | 0 | 0 |
| | | | 7 | 6 | 1 | | |
| 60 | 23SB | 1 | Total | N | Os | 0 | 0 |
| | | | 7 | 6 | 1 | | |
| 60 | 23SB | 1 | Total | N | Os | 0 | 0 |
| | | | 7 | 6 | 1 | | |
| 60 | 23SB | 1 | Total | N | Os | 0 | 0 |
| | | | 7 | 6 | 1 | | |
| 60 | 23SB | 1 | Total | N | Os | 0 | 0 |
| | | | 7 | 6 | 1 | | |
| 60 | 23SB | 1 | Total | N | Os | 0 | 0 |
| | | | 7 | 6 | 1 | | |
| 60 | 23SB | 1 | Total | N | Os | 0 | 0 |
| | | | 7 | 6 | 1 | | |
| 60 | 23SB | 1 | Total | N | Os | 0 | 0 |
| | | | 7 | 6 | 1 | | |
| 60 | 23SB | 1 | Total | N | Os | 0 | 0 |
| | | | 7 | 6 | 1 | | |
| 60 | 23SB | 1 | Total | N | Os | 0 | 0 |
| | | | 7 | 6 | 1 | | |
| 60 | 23SB | 1 | Total | N | Os | 0 | 0 |
| | | | 7 | 6 | 1 | | |
| 60 | 23SB | 1 | Total | N | Os | 0 | 0 |
| | | | 7 | 6 | 1 | | |
| 60 | 23SB | 1 | Total | N | Os | 0 | 0 |
| | | | 7 | 6 | 1 | | |
| 60 | 23SB | 1 | Total | N | Os | 0 | 0 |
| | | | 7 | 6 | 1 | | |
| 60 | 23SB | 1 | Total | N | Os | 0 | 0 |
| | | | 7 | 6 | 1 | | |

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| Mol | Chain | Residues | Atoms | ZeroOcc | AltConf |
|---|---|---|---|---|---|
| 60 | 23SB | 1 | Total N Os<br>7 6 1 | 0 | 0 |
| 60 | 23SB | 1 | Total N Os<br>7 6 1 | 0 | 0 |
| 60 | 23SB | 1 | Total N Os<br>7 6 1 | 0 | 0 |
| 60 | 23SB | 1 | Total N Os<br>7 6 1 | 0 | 0 |
| 60 | 23SB | 1 | Total N Os<br>7 6 1 | 0 | 0 |
| 60 | 23SB | 1 | Total N Os<br>7 6 1 | 0 | 0 |
| 60 | 23SB | 1 | Total N Os<br>7 6 1 | 0 | 0 |
| 60 | 23SB | 1 | Total N Os<br>7 6 1 | 0 | 0 |
| 60 | 23SB | 1 | Total N Os<br>7 6 1 | 0 | 0 |
| 60 | 23SB | 1 | Total N Os<br>7 6 1 | 0 | 0 |
| 60 | 23SB | 1 | Total N Os<br>7 6 1 | 0 | 0 |
| 60 | 23SB | 1 | Total N Os<br>7 6 1 | 0 | 0 |
| 60 | 23SB | 1 | Total N Os<br>7 6 1 | 0 | 0 |
| 60 | 23SB | 1 | Total N Os<br>7 6 1 | 0 | 0 |
| 60 | 23SB | 1 | Total N Os<br>7 6 1 | 0 | 0 |
| 60 | 23SB | 1 | Total N Os<br>7 6 1 | 0 | 0 |
| 60 | 23SB | 1 | Total N Os<br>7 6 1 | 0 | 0 |
| 60 | 23SB | 1 | Total N Os<br>7 6 1 | 0 | 0 |
| 60 | 23SB | 1 | Total N Os<br>7 6 1 | 0 | 0 |
| 60 | 23SB | 1 | Total N Os<br>7 6 1 | 0 | 0 |

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| Mol | Chain | Residues | Atoms | ZeroOcc | AltConf |
|---|---|---|---|---|---|
| 60 | 23SB | 1 | Total N Os<br>7 6 1 | 0 | 0 |
| 60 | 23SB | 1 | Total N Os<br>7 6 1 | 0 | 0 |
| 60 | 23SB | 1 | Total N Os<br>7 6 1 | 0 | 0 |
| 60 | 23SB | 1 | Total N Os<br>7 6 1 | 0 | 0 |
| 60 | 23SB | 1 | Total N Os<br>7 6 1 | 0 | 0 |
| 60 | 23SB | 1 | Total N Os<br>7 6 1 | 0 | 0 |
| 60 | 23SB | 1 | Total N Os<br>7 6 1 | 0 | 0 |
| 60 | 23SB | 1 | Total N Os<br>7 6 1 | 0 | 0 |
| 60 | 23SB | 1 | Total N Os<br>7 6 1 | 0 | 0 |
| 60 | 23SB | 1 | Total N Os<br>7 6 1 | 0 | 0 |
| 60 | 23SB | 1 | Total N Os<br>7 6 1 | 0 | 0 |
| 60 | 23SB | 1 | Total N Os<br>7 6 1 | 0 | 0 |
| 60 | 23SB | 1 | Total N Os<br>7 6 1 | 0 | 0 |
| 60 | 23SB | 1 | Total N Os<br>7 6 1 | 0 | 0 |
| 60 | 23SB | 1 | Total N Os<br>7 6 1 | 0 | 0 |
| 60 | 23SB | 1 | Total N Os<br>7 6 1 | 0 | 0 |
| 60 | 23SB | 1 | Total N Os<br>7 6 1 | 0 | 0 |
| 60 | 23SB | 1 | Total N Os<br>7 6 1 | 0 | 0 |
| 60 | 23SB | 1 | Total N Os<br>7 6 1 | 0 | 0 |
| 60 | 23SB | 1 | Total N Os<br>7 6 1 | 0 | 0 |

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| Mol | Chain | Residues | Atoms | ZeroOcc | AltConf |
|---|---|---|---|---|---|
| 60 | 23SB | 1 | Total N Os<br>7 6 1 | 0 | 0 |
| 60 | 23SB | 1 | Total N Os<br>7 6 1 | 0 | 0 |
| 60 | 23SB | 1 | Total N Os<br>7 6 1 | 0 | 0 |
| 60 | 23SB | 1 | Total N Os<br>7 6 1 | 0 | 0 |
| 60 | 23SB | 1 | Total N Os<br>7 6 1 | 0 | 0 |
| 60 | 23SB | 1 | Total N Os<br>7 6 1 | 0 | 0 |
| 60 | 23SB | 1 | Total N Os<br>7 6 1 | 0 | 0 |
| 60 | 23SB | 1 | Total N Os<br>7 6 1 | 0 | 0 |
| 60 | 23SB | 1 | Total N Os<br>7 6 1 | 0 | 0 |
| 60 | 23SB | 1 | Total N Os<br>7 6 1 | 0 | 0 |
| 60 | 23SB | 1 | Total N Os<br>7 6 1 | 0 | 0 |
| 60 | 23SB | 1 | Total N Os<br>7 6 1 | 0 | 0 |
| 60 | 23SB | 1 | Total N Os<br>7 6 1 | 0 | 0 |
| 60 | 23SB | 1 | Total N Os<br>7 6 1 | 0 | 0 |
| 60 | 5SB | 1 | Total N Os<br>7 6 1 | 0 | 0 |
| 60 | 5SB | 1 | Total N Os<br>7 6 1 | 0 | 0 |
| 60 | 5SB | 1 | Total N Os<br>7 6 1 | 0 | 0 |
| 60 | 5SB | 1 | Total N Os<br>7 6 1 | 0 | 0 |
| 60 | 5SB | 1 | Total N Os<br>7 6 1 | 0 | 0 |
| 60 | 5SB | 1 | Total N Os<br>7 6 1 | 0 | 0 |
| 60 | 5SB | 1 | Total N Os<br>7 6 1 | 0 | 0 |

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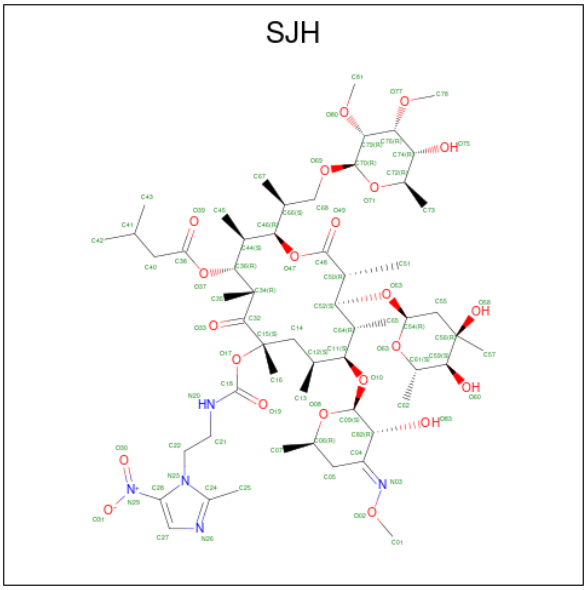
| Mol | Chain | Residues | Atoms | ZeroOcc | AltConf |
|---|---|---|---|---|---|
| 60 | 5SB | 1 | Total N Os<br>7 6 1 | 0 | 0 |
| 60 | 5SB | 1 | Total N Os<br>7 6 1 | 0 | 0 |
| 60 | 5SB | 1 | Total N Os<br>7 6 1 | 0 | 0 |
| 60 | L17B | 1 | Total N Os<br>7 6 1 | 0 | 0 |
| 60 | L20B | 1 | Total N Os<br>7 6 1 | 0 | 0 |
| 60 | L35B | 1 | Total N Os<br>7 6 1 | 0 | 0 |

- Molecule 61 is (2R,3S,4R,5R,7S,9S,10S,11R,12S,13R)-12-(((2R,4R,5S,6S)-4,5-dihydroxy-4,6-dimethyltetrahydro-2H-pyran-2-yl)oxy)-2-((S)-1-(((2R,3R,4R,5R,6R)-5-hydroxy-3,4-dimethoxy-6-methyltetrahydro-2H-pyran-2-yl)oxy)propan-2-yl)-10-(((2S,3R,6R,E)-3-hydroxy-4-(methoxyimino)-6-methyltetrahydro-2H-pyran-2-yl)oxy)-3,5,7,9,11,13-hexamethyl-7-(((2-(2-methyl-5-nitro-1H-imidazol-1-yl)ethyl)carbamoyl)oxy)-6,14-dioxooxacyclotetradecan-4-yl 3-methylbutanoate (CCD ID: SJH) (formula: $C_{56}H_{93}N_5O_{22}$).




| Mol | Chain | Residues | Atoms | ZeroOcc | AltConf |
|---|---|---|---|---|---|
| 61 | 23SA | 1 | Total C N O<br>83 56 5 22 | 0 | 0 |
| 61 | 23SB | 1 | Total C N O<br>83 56 5 22 | 0 | 0 |

- Molecule 62 is water.

| Mol | Chain | Residues | Atoms | ZeroOcc | AltConf |
|---|---|---|---|---|---|
| 62 | 16SA | 173 | Total O<br>173 173 | 0 | 0 |
| 62 | S4A | 2 | Total O<br>2 2 | 0 | 0 |
| 62 | S5A | 1 | Total O<br>1 1 | 0 | 0 |
| 62 | S13A | 1 | Total O<br>1 1 | 0 | 0 |
| 62 | S14A | 1 | Total O<br>1 1 | 0 | 0 |
| 62 | S16A | 1 | Total O<br>1 1 | 0 | 0 |
| 62 | S17A | 1 | Total O<br>1 1 | 0 | 0 |
| 62 | THXA | 3 | Total O<br>3 3 | 0 | 0 |
| 62 | PSIA | 6 | Total O<br>6 6 | 0 | 0 |
| 62 | ESIA | 1 | Total O<br>1 1 | 0 | 0 |
| 62 | 23SA | 801 | Total O<br>801 801 | 0 | 0 |
| 62 | 5SA | 14 | Total O<br>14 14 | 0 | 0 |
| 62 | L2A | 9 | Total O<br>9 9 | 0 | 0 |
| 62 | L3A | 7 | Total O<br>7 7 | 0 | 0 |
| 62 | L4A | 6 | Total O<br>6 6 | 0 | 0 |
| 62 | L15A | 10 | Total O<br>10 10 | 0 | 0 |
| 62 | L16A | 1 | Total O<br>1 1 | 0 | 0 |
| 62 | L17A | 2 | Total O<br>2 2 | 0 | 0 |
| 62 | L18A | 2 | Total O<br>2 2 | 0 | 0 |
| 62 | L19A | 1 | Total O<br>1 1 | 0 | 0 |
| 62 | L23A | 1 | Total O<br>1 1 | 0 | 0 |
| 62 | L27A | 3 | Total O<br>3 3 | 0 | 0 |

*Continued on next page...*

*Continued from previous page...*

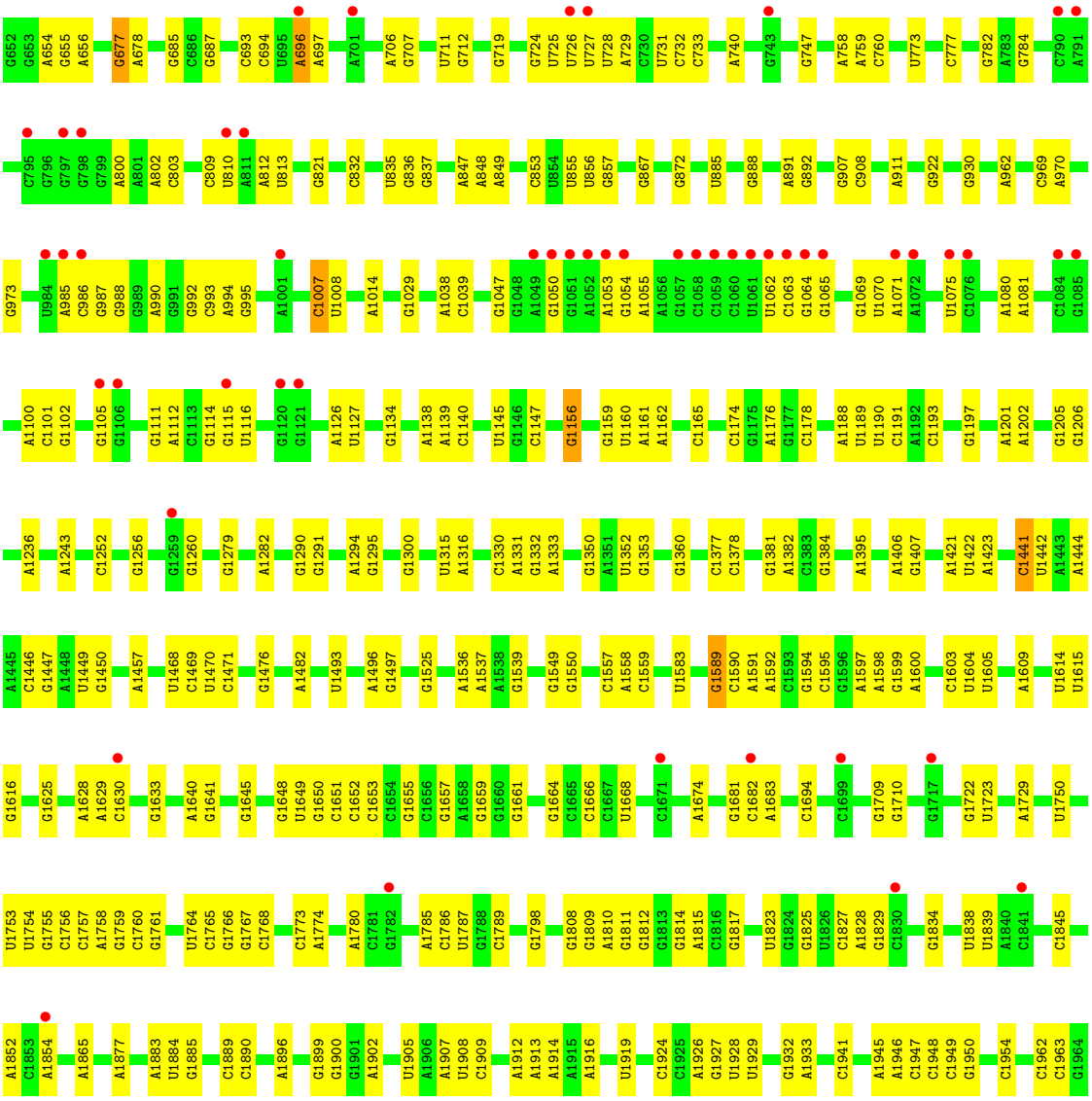
| Mol | Chain | Residues | Atoms | ZeroOcc | AltConf |
|---|---|---|---|---|---|
| 62 | L30A | 1 | Total O<br>1 1 | 0 | 0 |
| 62 | L34A | 1 | Total O<br>1 1 | 0 | 0 |
| 62 | L35A | 1 | Total O<br>1 1 | 0 | 0 |
| 62 | 16SB | 158 | Total O<br>158 158 | 0 | 0 |
| 62 | S4B | 1 | Total O<br>1 1 | 0 | 0 |
| 62 | S5B | 1 | Total O<br>1 1 | 0 | 0 |
| 62 | S9B | 1 | Total O<br>1 1 | 0 | 0 |
| 62 | S12B | 2 | Total O<br>2 2 | 0 | 0 |
| 62 | S14B | 2 | Total O<br>2 2 | 0 | 0 |
| 62 | 23SB | 518 | Total O<br>518 518 | 0 | 0 |
| 62 | 5SB | 5 | Total O<br>5 5 | 0 | 0 |
| 62 | L2B | 13 | Total O<br>13 13 | 0 | 0 |
| 62 | L3B | 6 | Total O<br>6 6 | 0 | 0 |
| 62 | L4B | 1 | Total O<br>1 1 | 0 | 0 |
| 62 | L15B | 7 | Total O<br>7 7 | 0 | 0 |
| 62 | L27B | 2 | Total O<br>2 2 | 0 | 0 |
| 62 | L28B | 1 | Total O<br>1 1 | 0 | 0 |
| 62 | L30B | 2 | Total O<br>2 2 | 0 | 0 |
| 62 | L35B | 6 | Total O<br>6 6 | 0 | 0 |

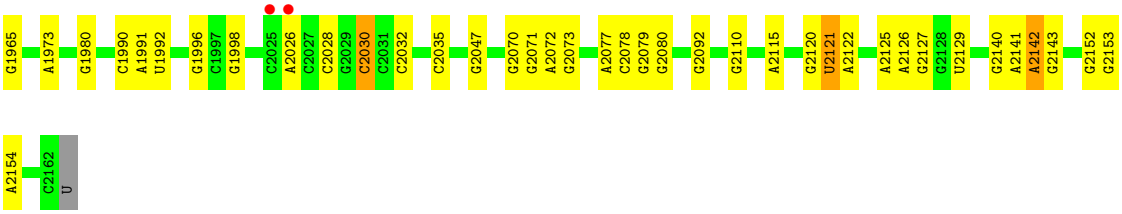
# 3 Residue-property plots (i)

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 rRNA

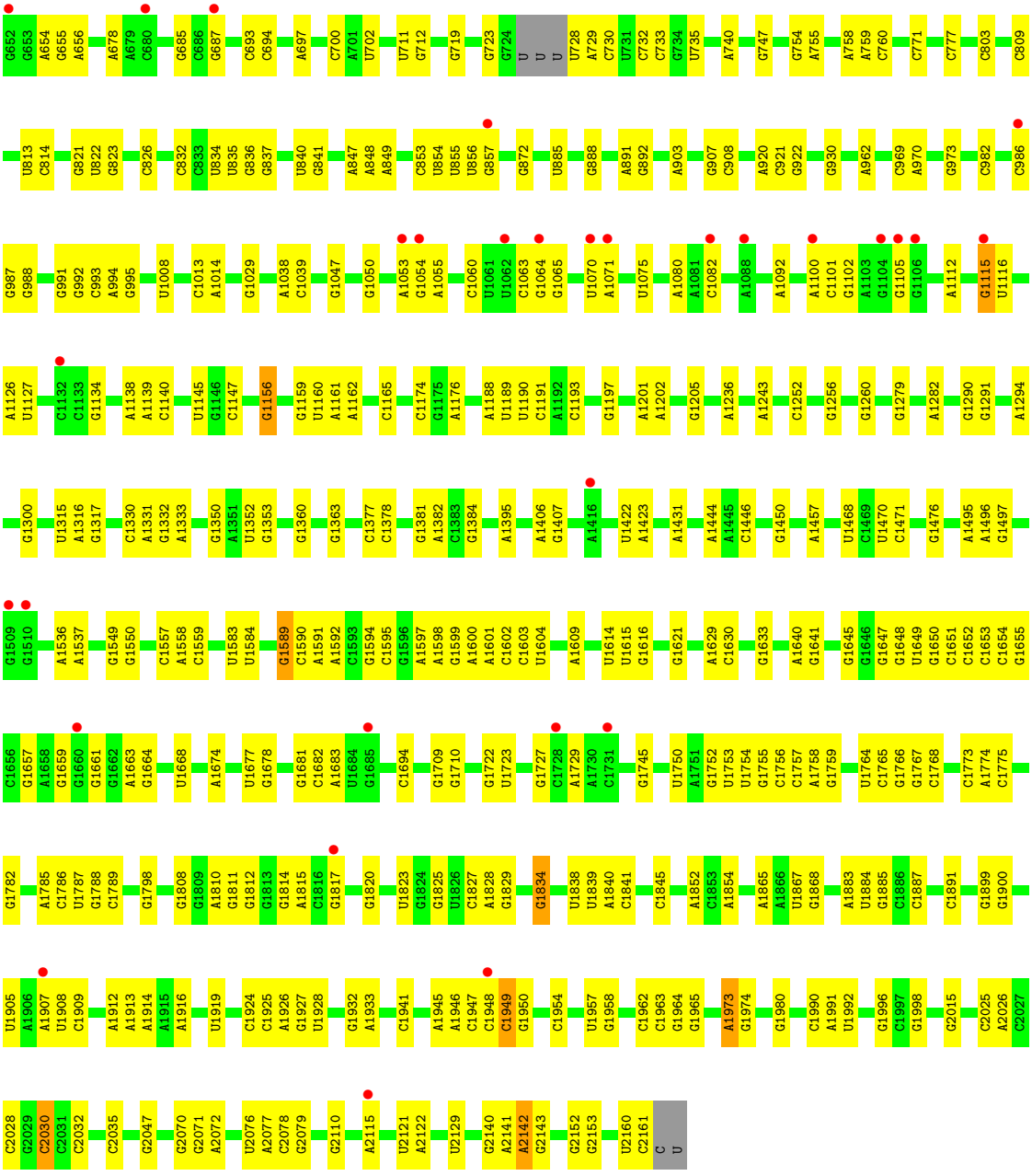
Chain 16SA:





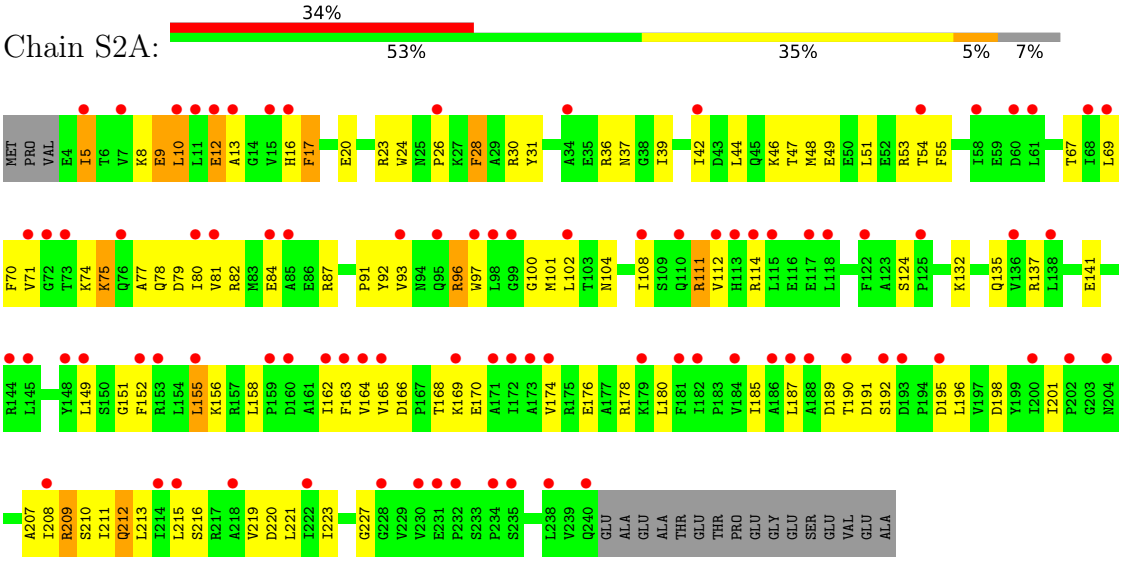
• Molecule 1: 16S rRNA

Chain 16SB:



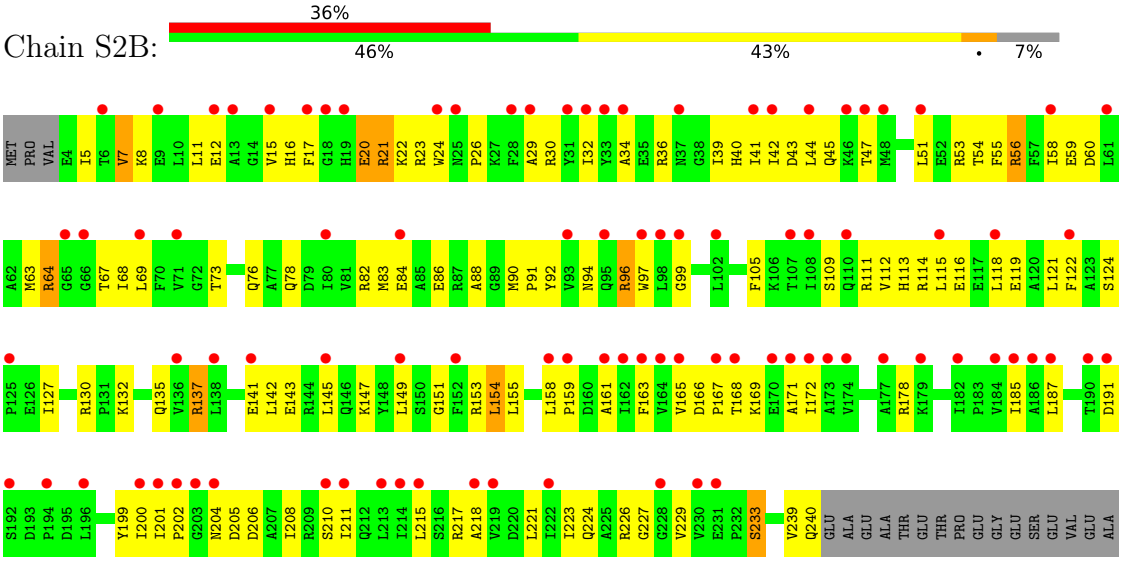
• Molecule 2: 30S ribosomal protein S2

Chain S2A:



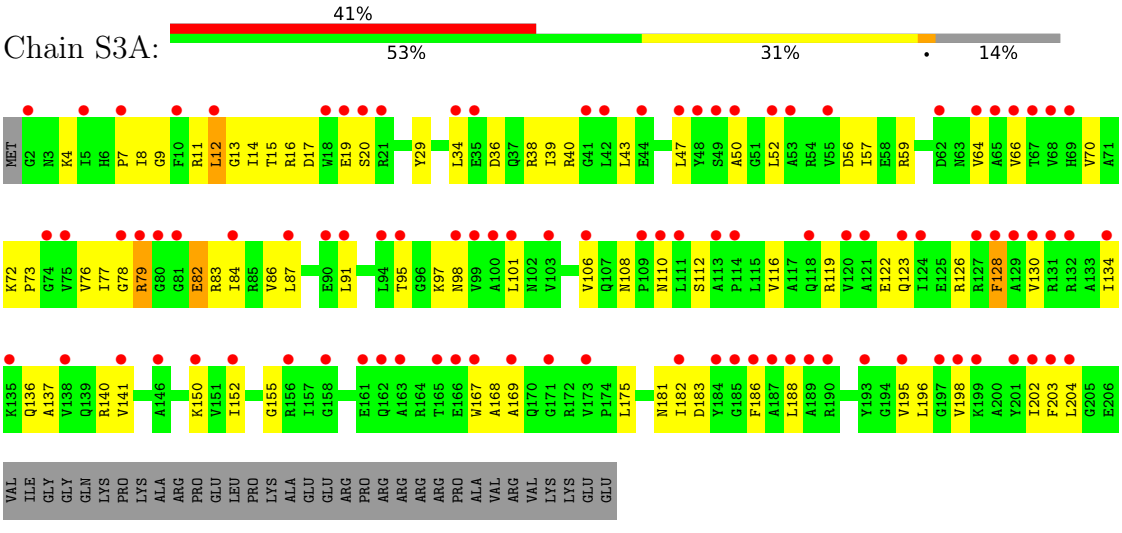

• Molecule 2: 30S ribosomal protein S2

Chain S2B:



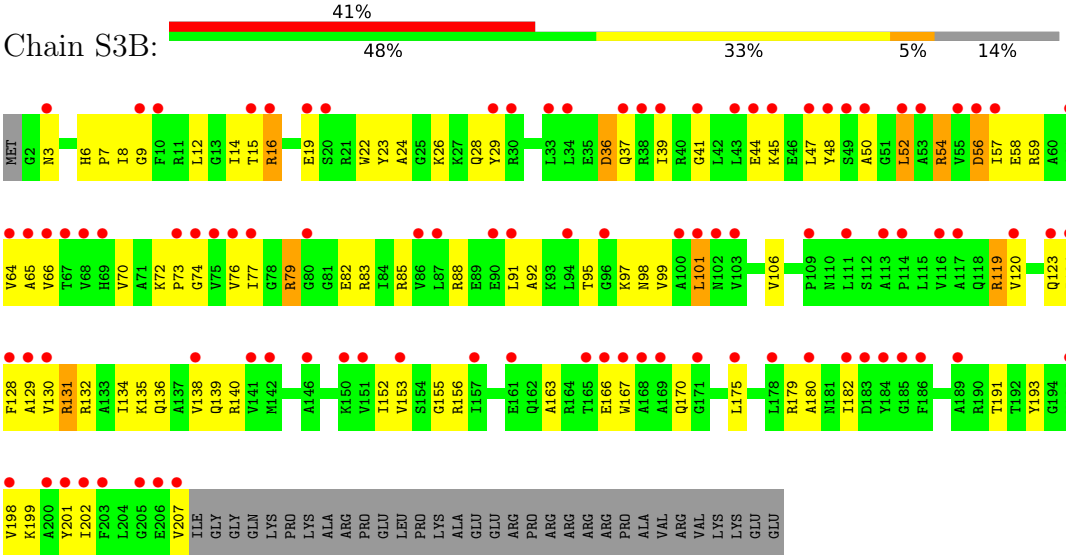

• Molecule 3: 30S ribosomal protein S3

Chain S3A:



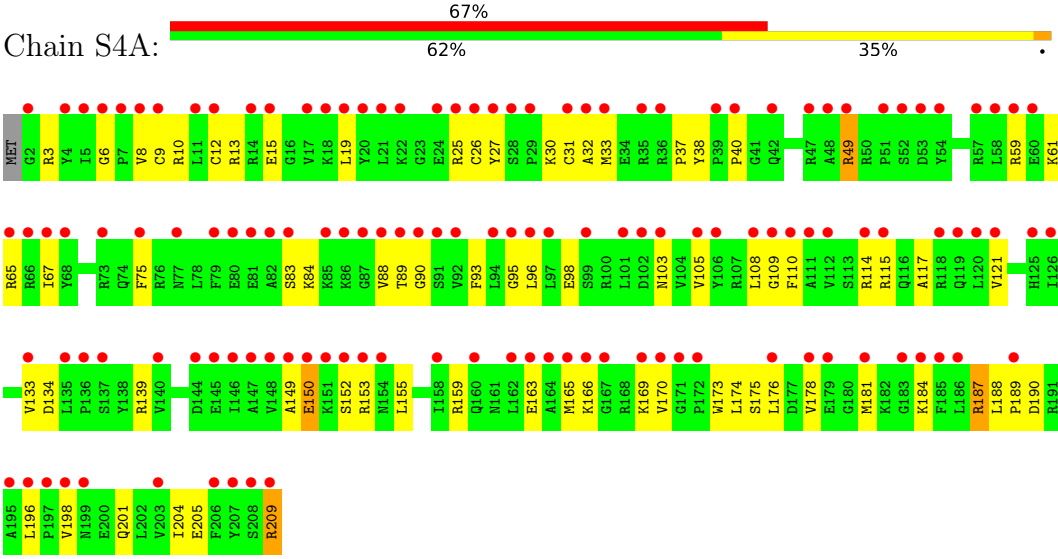
• Molecule 3: 30S ribosomal protein S3

Chain S3B:



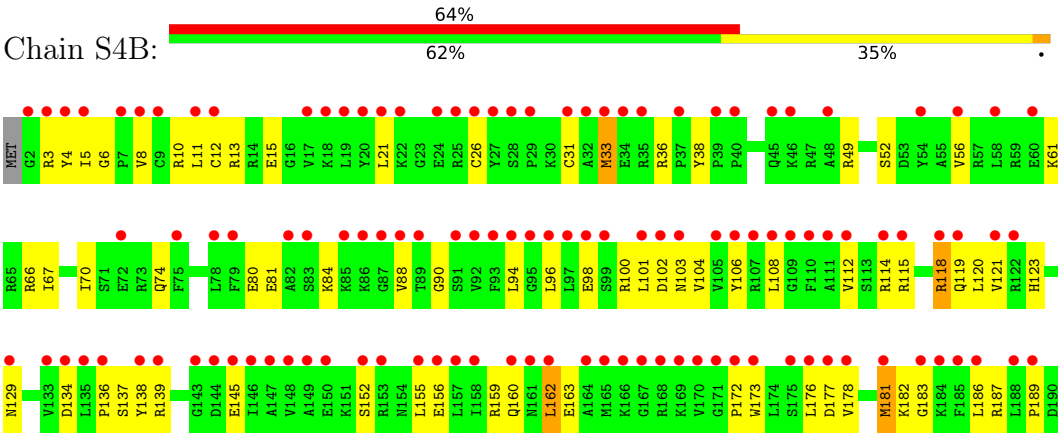

• Molecule 4: 30S ribosomal protein S4

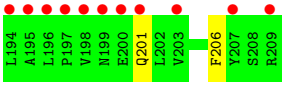
Chain S4A:




• Molecule 4: 30S ribosomal protein S4

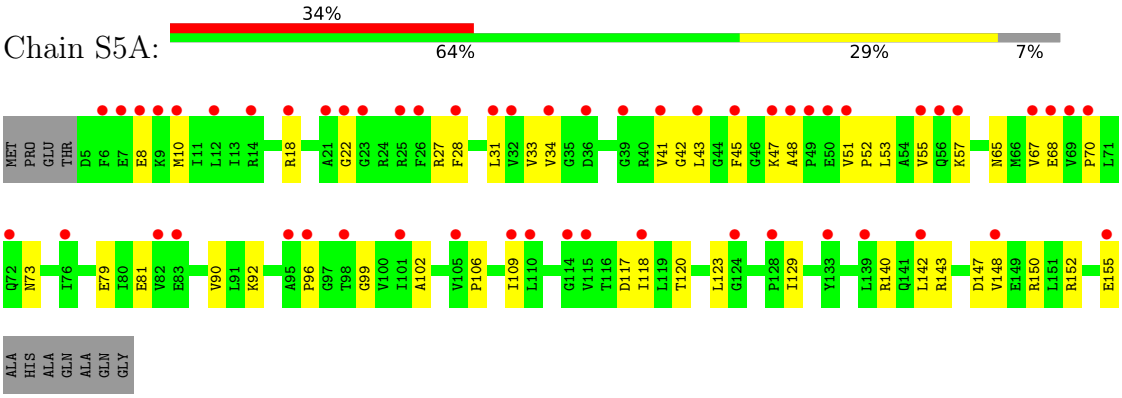
Chain S4B:





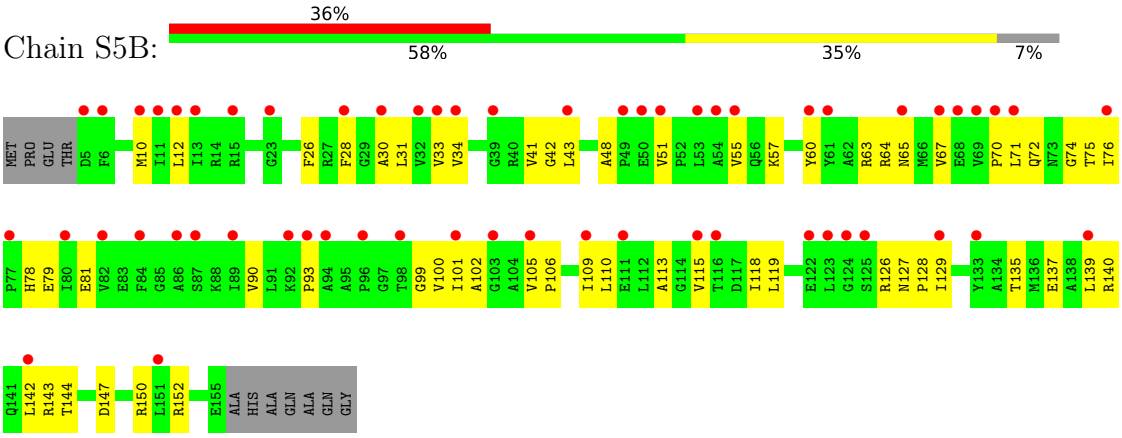

• Molecule 5: 30S ribosomal protein S5

Chain S5A:



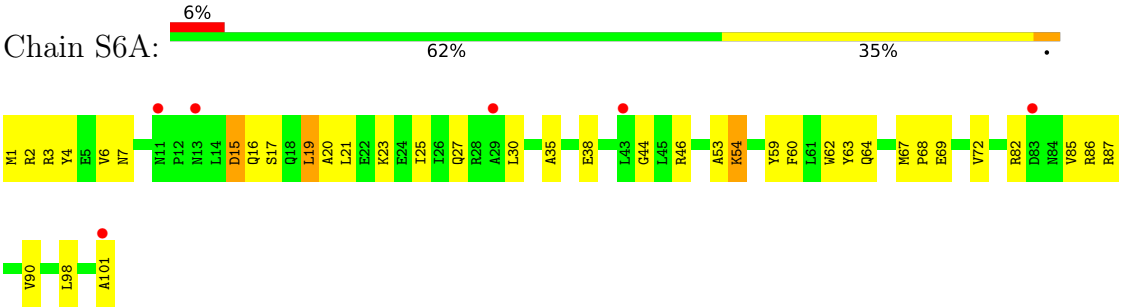

• Molecule 5: 30S ribosomal protein S5

Chain S5B:



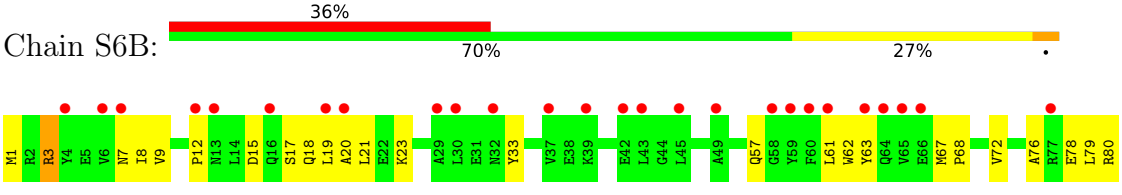

• Molecule 6: 30S ribosomal protein S6

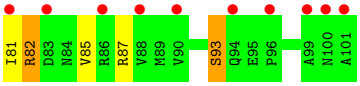
Chain S6A:




• Molecule 6: 30S ribosomal protein S6

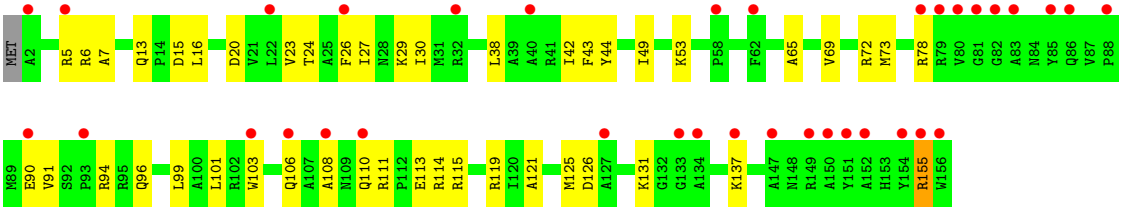
Chain S6B:





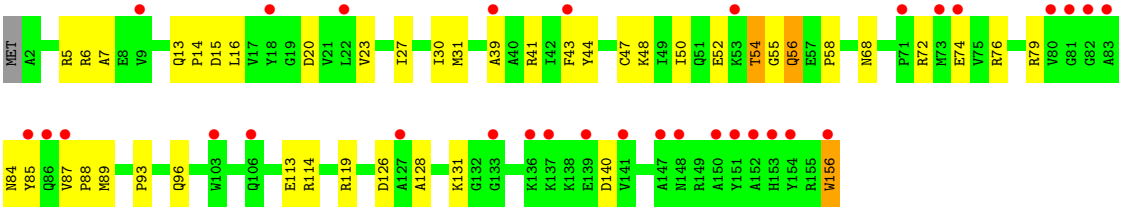

• Molecule 7: 30S ribosomal protein S7

Chain S7A:



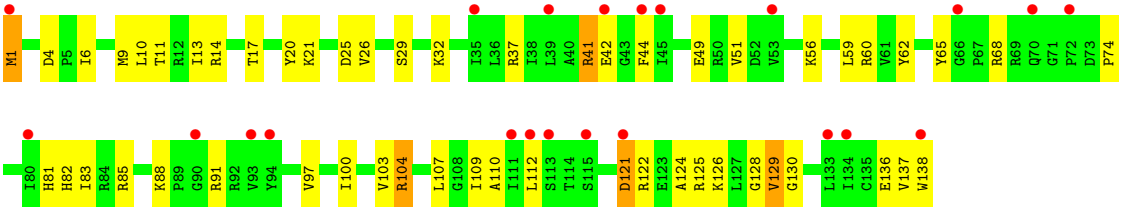

• Molecule 7: 30S ribosomal protein S7

Chain S7B:



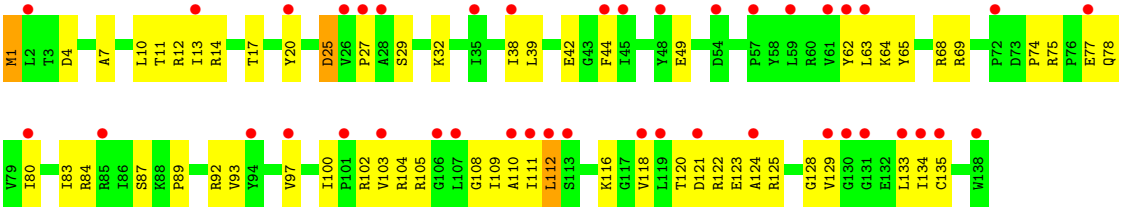

• Molecule 8: 30S ribosomal protein S8

Chain S8A:



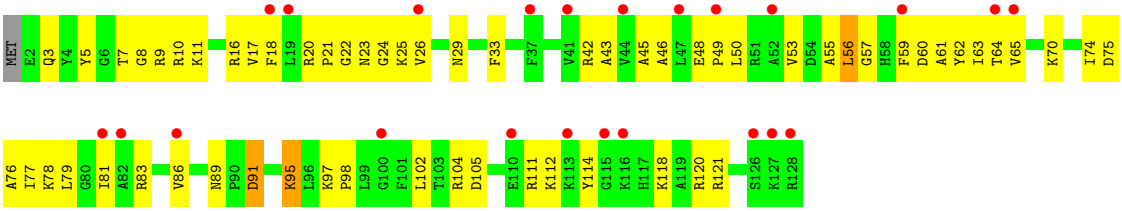

• Molecule 8: 30S ribosomal protein S8

Chain S8B:



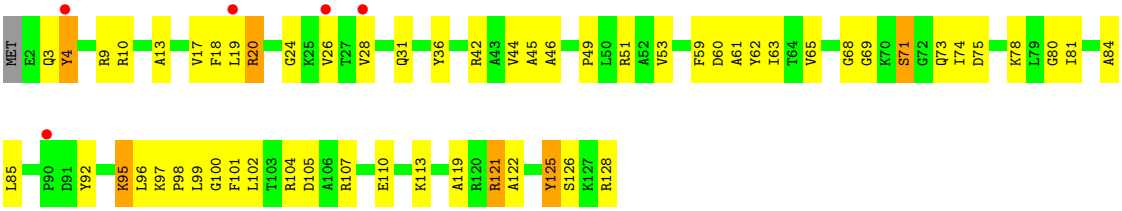

• Molecule 9: 30S ribosomal protein S9

Chain S9A:



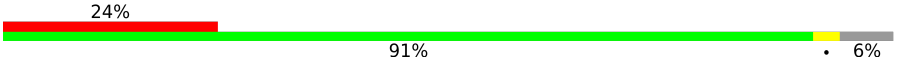

• Molecule 9: 30S ribosomal protein S9

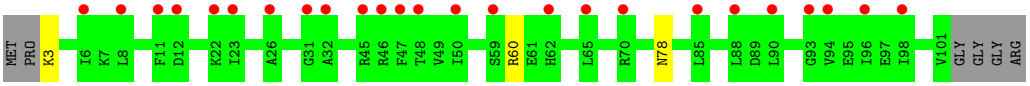
Chain S9B:




• Molecule 10: 30S ribosomal protein S10

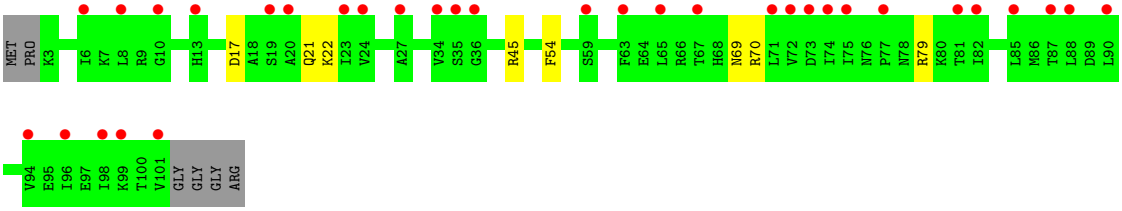
Chain S10A:



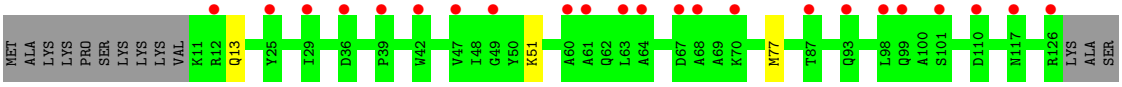

• Molecule 10: 30S ribosomal protein S10

Chain S10B:



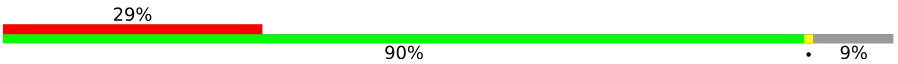

• Molecule 11: 30S ribosomal protein S11

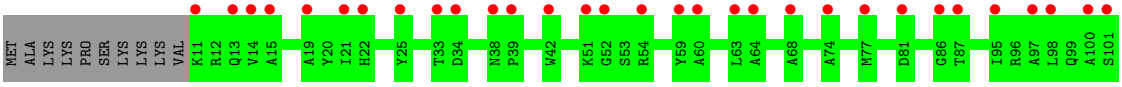
Chain S11A:

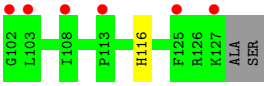



• Molecule 11: 30S ribosomal protein S11

Chain S11B:

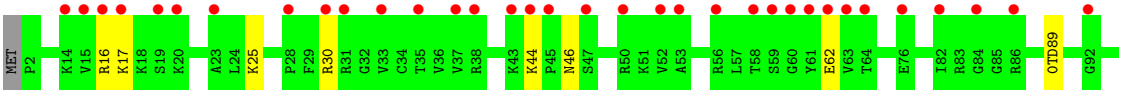


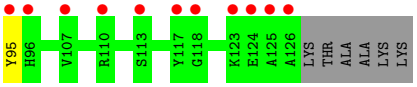






• Molecule 12: 30S ribosomal protein S12

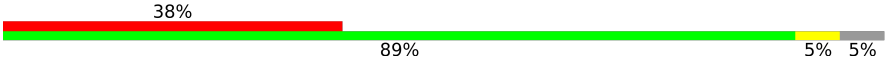
Chain S12A:

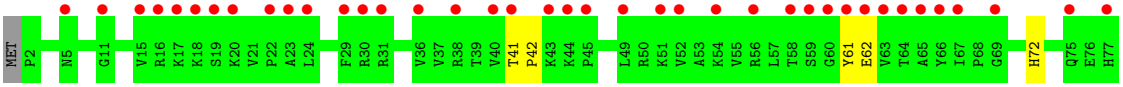


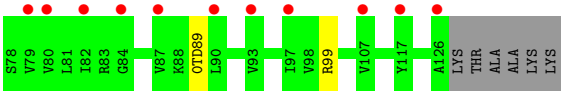




• Molecule 12: 30S ribosomal protein S12

Chain S12B:

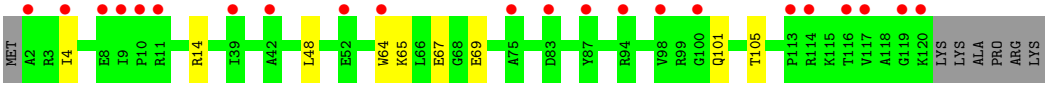


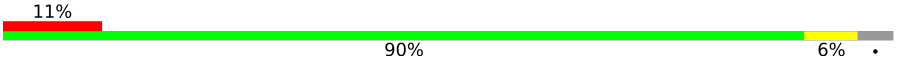

• Molecule 13: 30S ribosomal protein S13

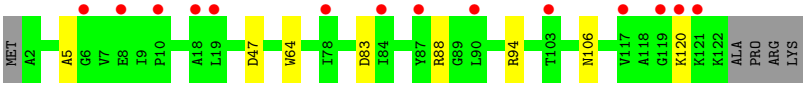
Chain S13A:




• Molecule 13: 30S ribosomal protein S13

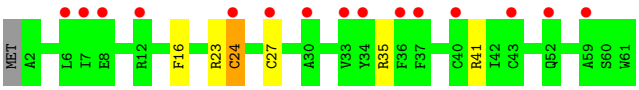
Chain S13B:



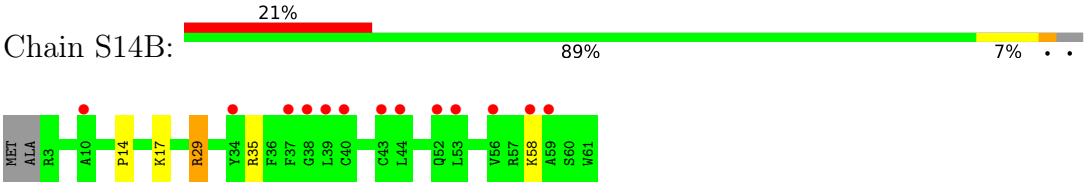

• Molecule 14: 30S ribosomal protein S14 type Z

Chain S14A:



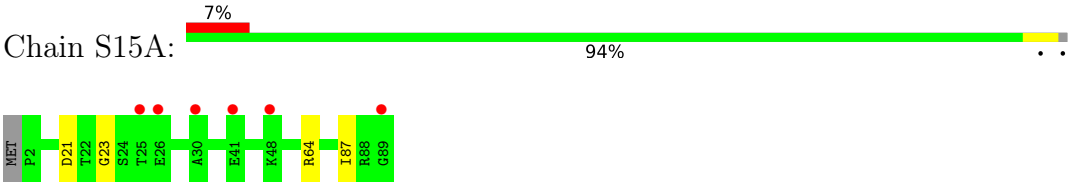

• Molecule 14: 30S ribosomal protein S14 type Z

Chain S14B:



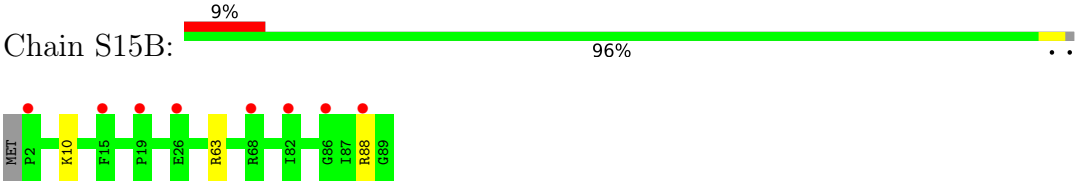

• Molecule 15: 30S ribosomal protein S15

Chain S15A:



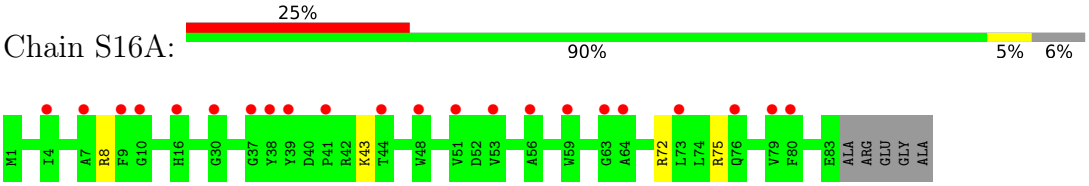

• Molecule 15: 30S ribosomal protein S15

Chain S15B:



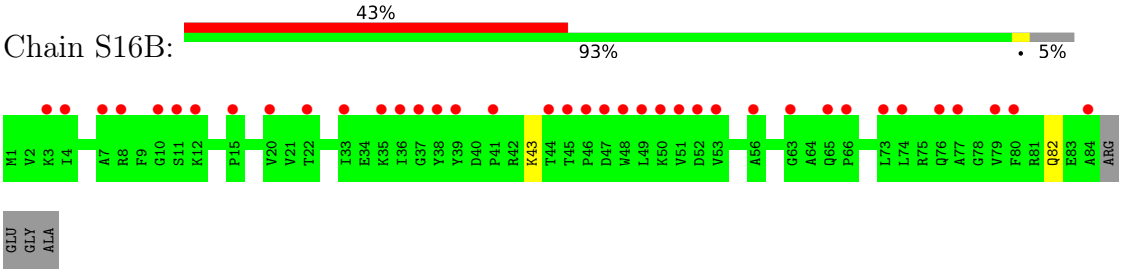

• Molecule 16: 30S ribosomal protein S16

Chain S16A:



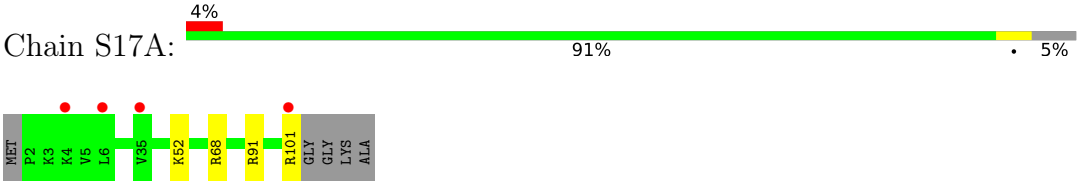

• Molecule 16: 30S ribosomal protein S16

Chain S16B:



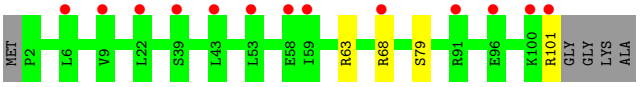

• Molecule 17: 30S ribosomal protein S17

Chain S17A:



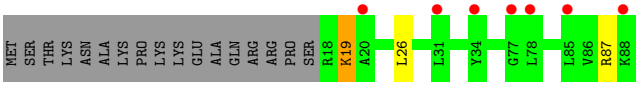

• Molecule 17: 30S ribosomal protein S17

Chain S17B:



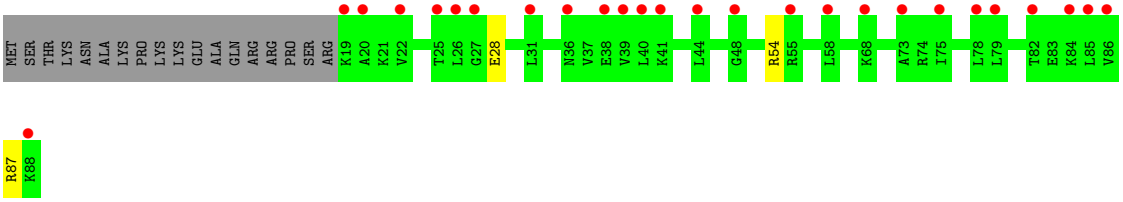

• Molecule 18: 30S ribosomal protein S18

Chain S18A:



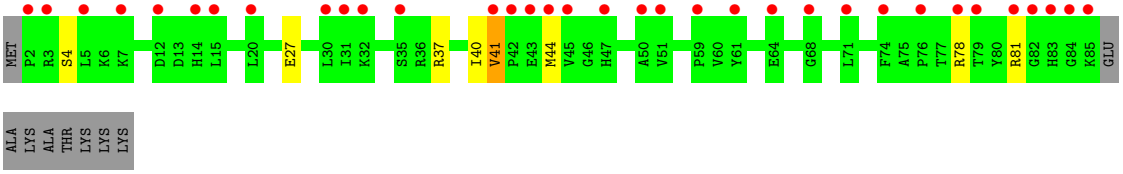

• Molecule 18: 30S ribosomal protein S18

Chain S18B:




• Molecule 19: 30S ribosomal protein S19

Chain S19A:

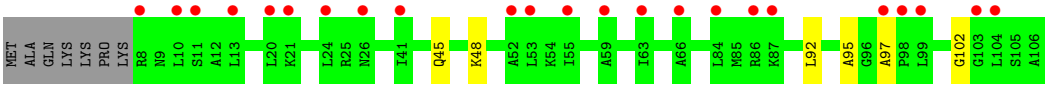



• Molecule 19: 30S ribosomal protein S19

Chain S19B:

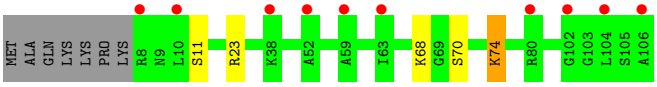
• Molecule 20: 30S ribosomal protein S20

Chain S20A:



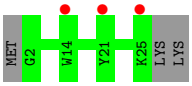

• Molecule 20: 30S ribosomal protein S20

Chain S20B:




• Molecule 21: 30S ribosomal protein Thx

Chain THXA:

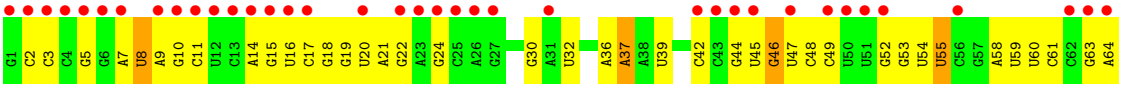


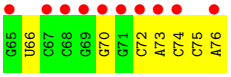

• Molecule 21: 30S ribosomal protein Thx

Chain THXB:

• Molecule 22: Phe-tRNA

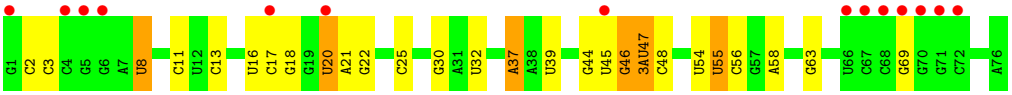
Chain ASIA:



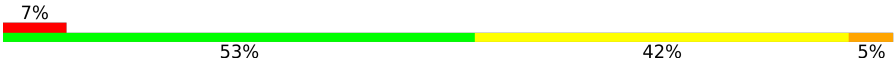

• Molecule 23: Phe-tRNA

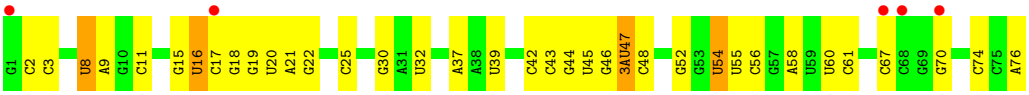
Chain PSIA:




• Molecule 23: Phe-tRNA

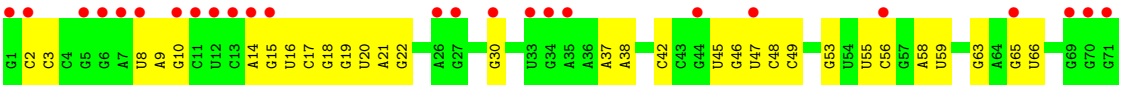
Chain PSIB:



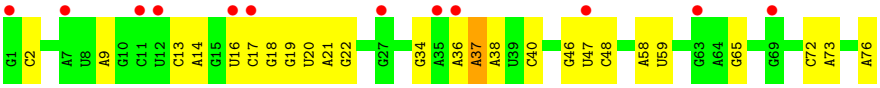

• Molecule 24: Phe-tRNA

Chain ESIA:



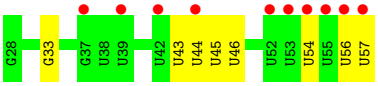
• Molecule 24: Phe-tRNA

Chain ESIB:



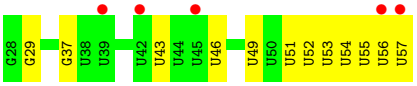

• Molecule 25: mRNA

Chain MRNA:



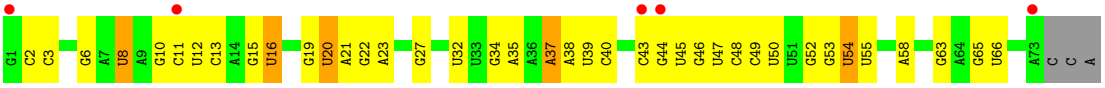

• Molecule 25: mRNA

Chain MRNB:



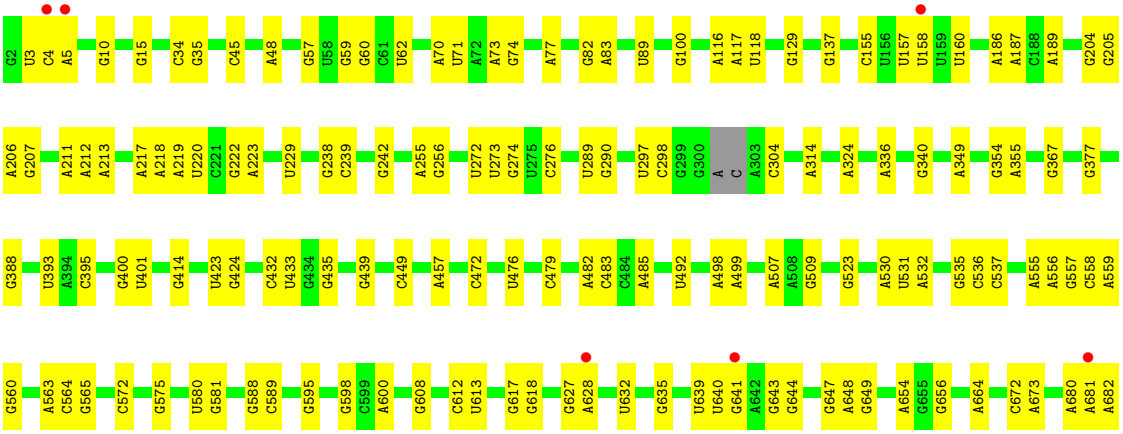

• Molecule 26: Phe-tRNA

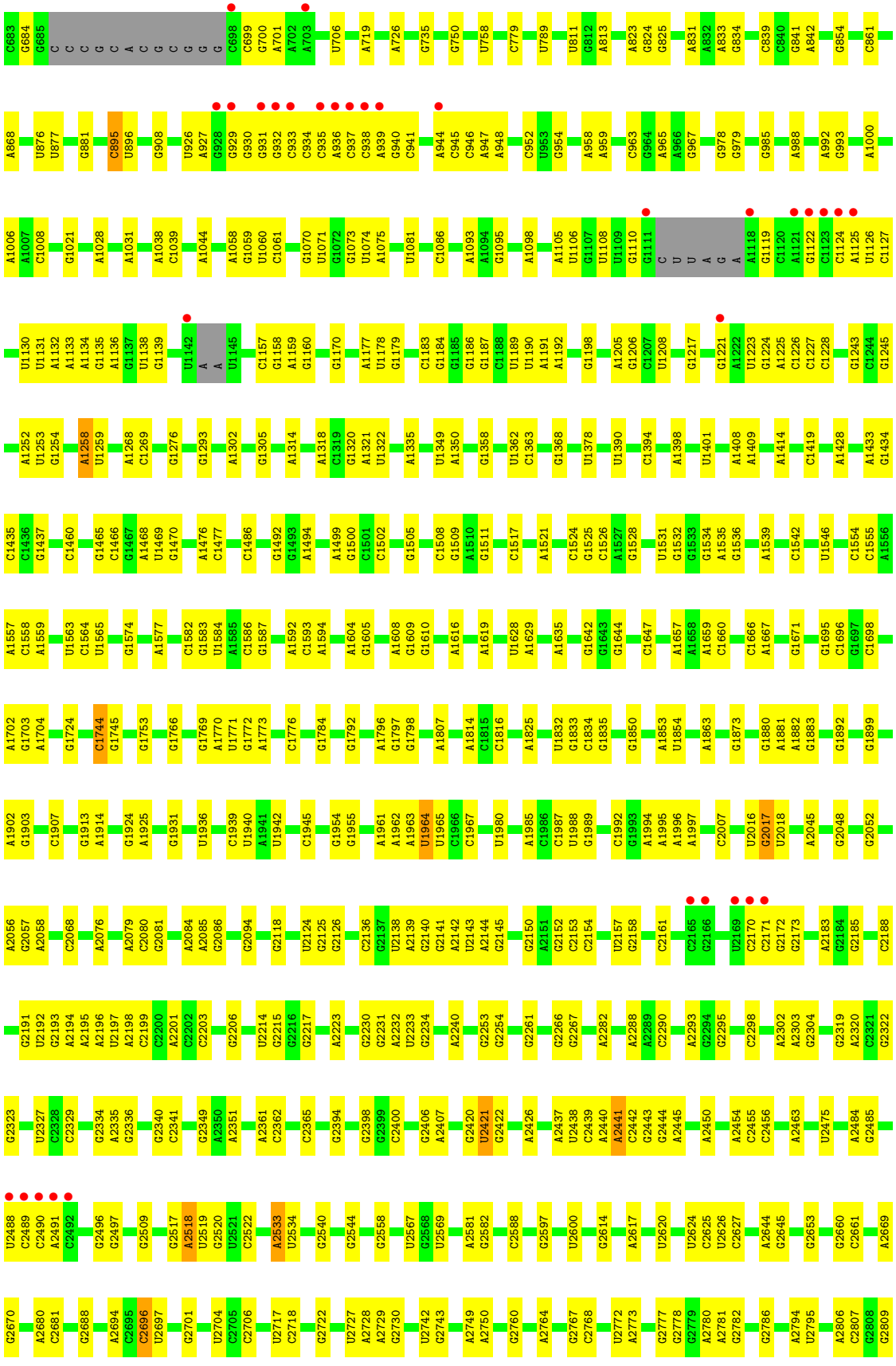
Chain TRNA:




• Molecule 27: 23S rRNA

Chain 23SA:




C683 G684 G685 C C C C G C A C G C G G G C698 C699 G700 A701 A702 A703 U706 A719 A726 G735 G750 U758 C779 U789 U811 G812 A813 A823 G824 G825 A831 A832 A833 G834 C839 C840 G841 A842 G854 C861
A868 U876 U877 G881 C895 U896 G908 U926 A927 G928 G929 G930 G931 G932 C933 C934 C935 A936 C937 C938 A939 G940 C941 A944 C945 C946 A947 A948 C952 U953 G954 A958 A959 C963 G964 A965 A966 G967 G978 G979 G985 A988 A992 G993 A1000
A1006 A1007 C1008 G1021 A1028 A1031 A1038 C1039 A1044 A1058 G1059 U1060 C1061 G1070 U1071 G1072 G1073 U1074 A1075 U1081 C1086 A1093 A1094 G1095 A1098 A1105 U1106 G1107 U1108 U1109 G1110 G1111 C U U A G A A1118 G1119 C1120 A1121 G1122 C1123 C1124 A1125 U1126 C1127
U1130 U1131 A1132 A1133 A1134 G1135 A1136 C1137 U1138 G1139 U1142 A A A U1145 C1157 G1158 A1159 C1160 G1170 A1177 U1178 G1179 C1183 G1184 G1185 G1186 G1187 C1188 U1189 U1190 A1191 A1192 G1198 A1205 G1206 C1207 U1208 G1217 G1221 A1222 U1223 G1224 A1225 C1226 C1227 C1228 G1243 C1244 G1245
A1252 U1253 G1254 A1258 U1259 A1268 C1269 G1276 G1293 A1302 G1305 A1314 A1318 C1319 G1320 A1321 U1322 A1335 U1349 A1350 G1358 U1362 C1363 G1368 U1378 U1390 C1394 A1398 U1401 A1408 A1409 A1414 C1419 A1428 A1433 G1434
C1435 C1436 G1437 C1460 G1465 C1466 C1467 A1468 U1469 G1470 A1476 C1477 C1486 G1492 G1493 A1494 A1499 G1500 C1501 C1502 G1505 C1508 G1509 A1510 G1511 C1517 A1521 C1524 G1525 C1526 A1527 G1528 U1531 G1532 G1533 G1534 A1535 G1536 A1539 C1542 U1546 C1554 C1555 A1556
A1557 C1558 A1559 U1563 C1564 U1565 G1574 A1577 C1582 G1583 U1584 A1585 C1586 G1587 A1592 C1593 A1594 A1604 G1605 A1608 G1609 G1610 A1616 A1619 U1628 A1629 A1635 G1642 G1643 G1644 C1647 A1657 A1658 A1659 C1660 C1666 A1667 G1671 G1695 C1696 G1697 C1698
A1702 G1703 A1704 G1724 C1744 G1745 G1753 G1766 G1769 A1770 U1771 G1772 A1773 C1776 G1784 G1792 A1796 G1797 G1798 A1807 A1814 C1815 C1816 A1825 U1832 G1833 C1834 G1835 G1850 A1853 U1854 A1863 G1873 G1880 A1881 A1882 G1883 G1892 G1899
A1902 G1903 C1907 G1913 A1914 G1924 A1925 G1931 U1936 C1939 U1940 A1941 U1942 C1945 G1954 G1955 A1961 A1962 A1963 U1964 U1965 C1966 C1967 U1980 A1985 C1986 C1987 U1988 G1989 C1992 G1993 A1994 A1995 A1996 A1997 C2007 U2016 G2017 U2018 A2045 G2048 G2052
A2056 G2057 A2058 C2068 A2076 A2079 C2080 G2081 A2084 A2085 G2086 G2094 G2118 U2124 G2125 G2126 C2136 G2137 U2138 A2139 G2140 G2141 A2142 U2143 A2144 G2145 G2150 A2151 G2152 C2153 C2154 U2157 G2158 C2161 C2165 G2166 U2169 C2170 C2171 G2172 G2173 A2183 G2184 C2185 C2188
G2191 U2192 G2193 A2194 A2195 A2196 U2197 A2198 C2199 C2200 A2201 C2202 C2203 G2206 U2214 G2215 G2216 G2217 A2223 G2230 G2231 A2232 U2233 G2234 A2240 G2253 G2254 G2261 G2266 G2267 A2282 A2288 A2289 C2290 A2293 G2294 G2295 C2298 A2302 A2303 G2304 G2319 A2320 C2321 G2322
G2323 U2327 C2328 C2329 G2334 A2335 G2336 G2340 C2341 G2349 A2350 A2351 A2361 C2362 C2365 G2394 G2398 G2399 C2400 G2406 A2407 G2420 U2421 G2422 A2426 A2437 U2438 C2439 A2440 A2441 C2442 G2443 G2444 A2445 A2450 A2454 C2455 C2456 A2463 U2475 A2484 G2485
U2488 C2489 C2490 A2491 C2492 G2496 G2497 G2509 G2517 A2518 U2519 G2520 U2521 C2522 A2533 U2534 G2540 G2544 G2558 U2567 G2568 U2569 A2581 G2582 C2588 G2597 U2600 G2614 A2617 U2620 U2624 C2625 U2626 C2627 A2644 G2645 G2653 G2660 C2661 A2669
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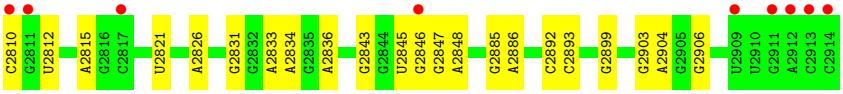
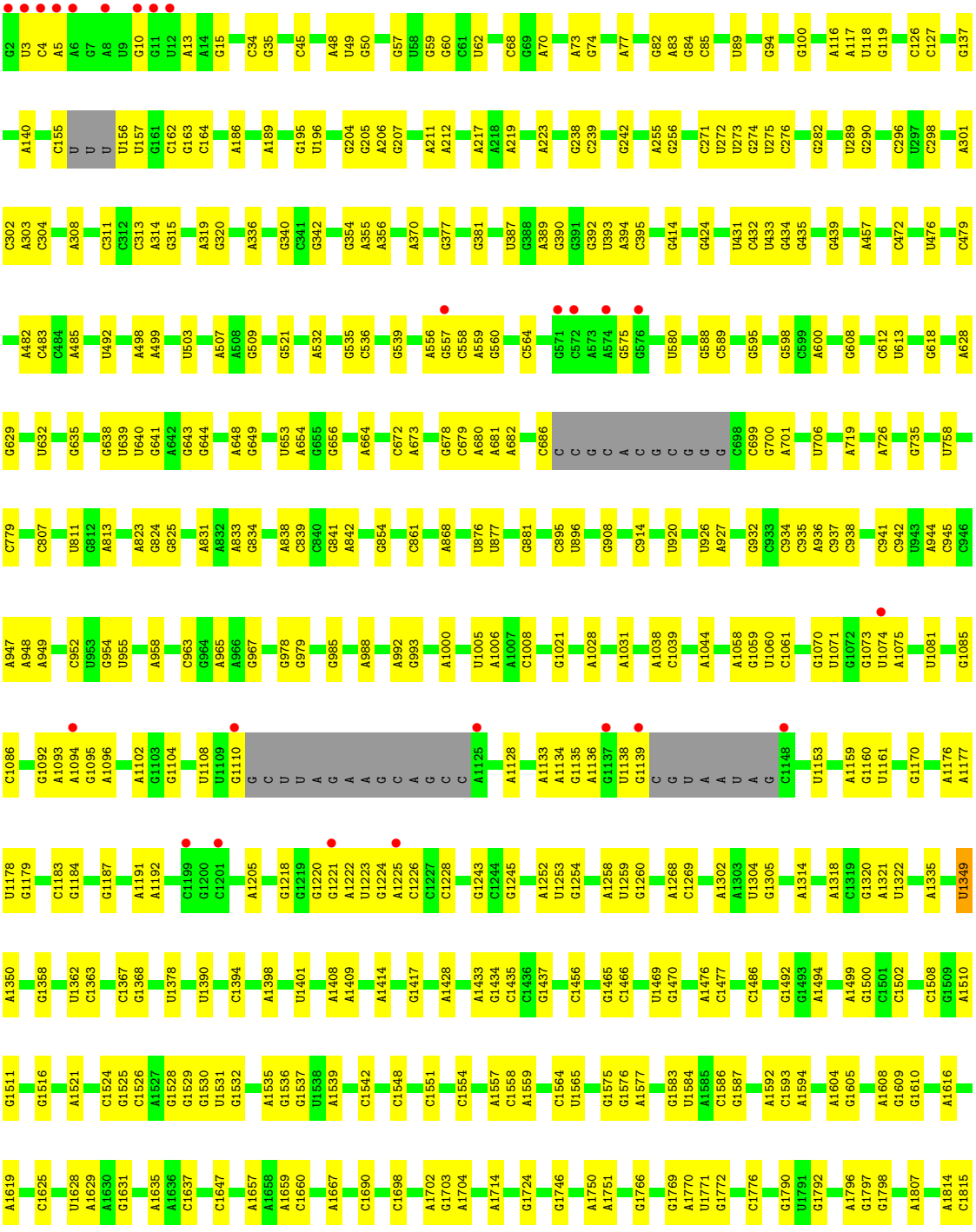
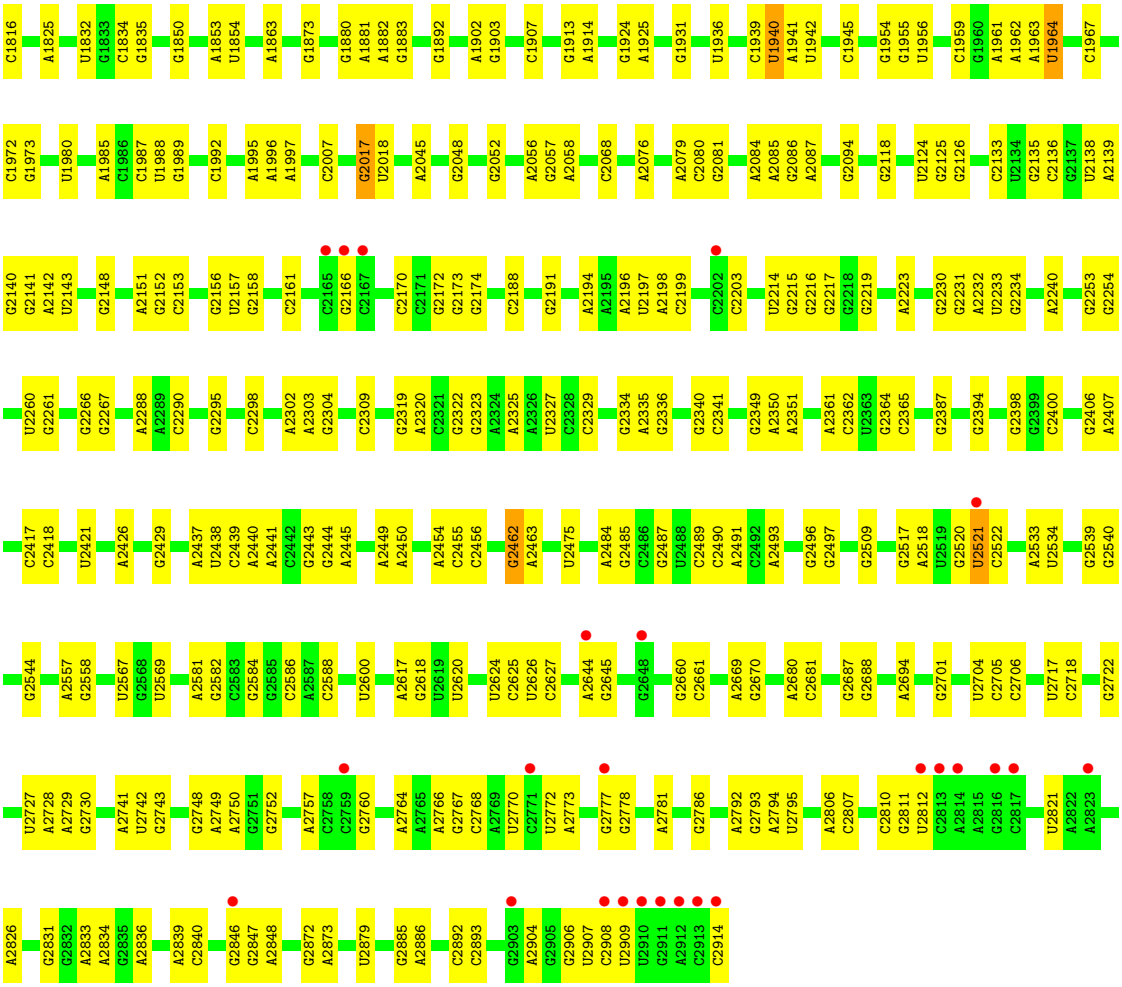



• Molecule 27: 23S rRNA

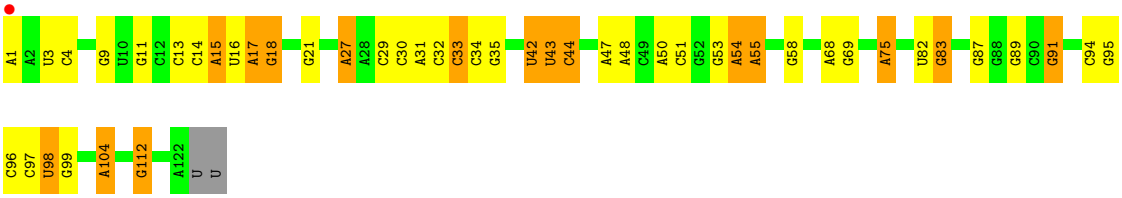
Chain 23SB:





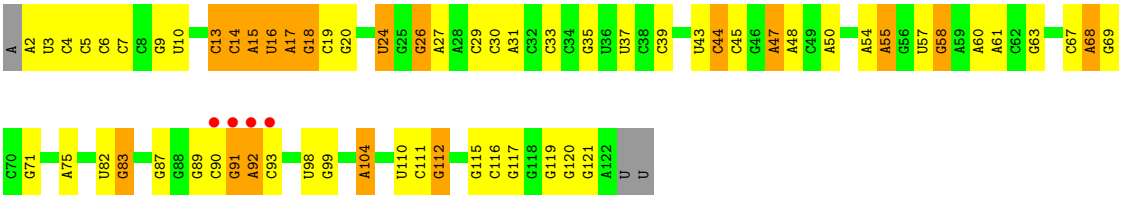
• Molecule 28: 5S rRNA

Chain 5SA:



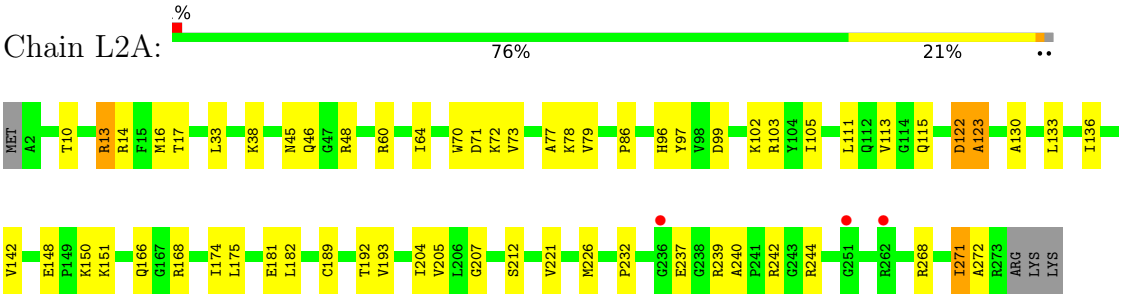
• Molecule 28: 5S rRNA

Chain 5SB:



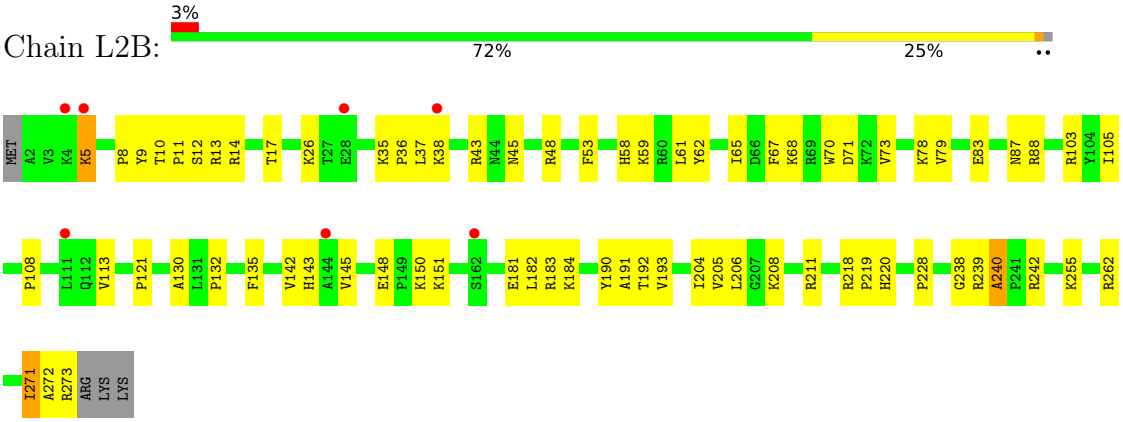
• Molecule 29: 50S ribosomal protein L2

Chain L2A:



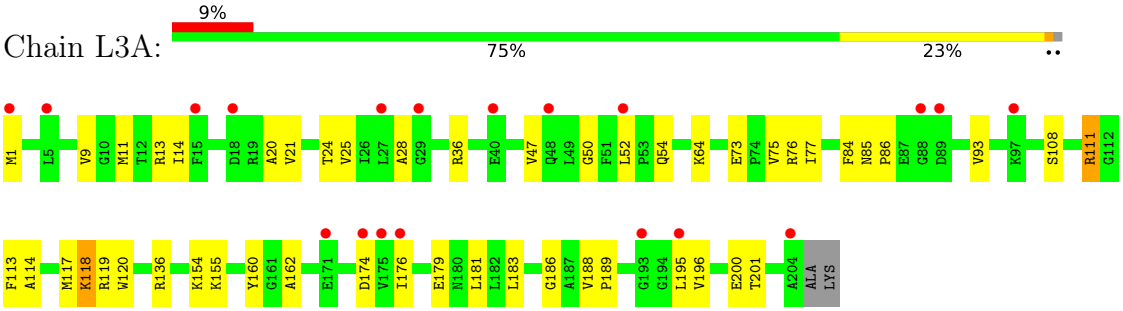

• Molecule 29: 50S ribosomal protein L2

Chain L2B:



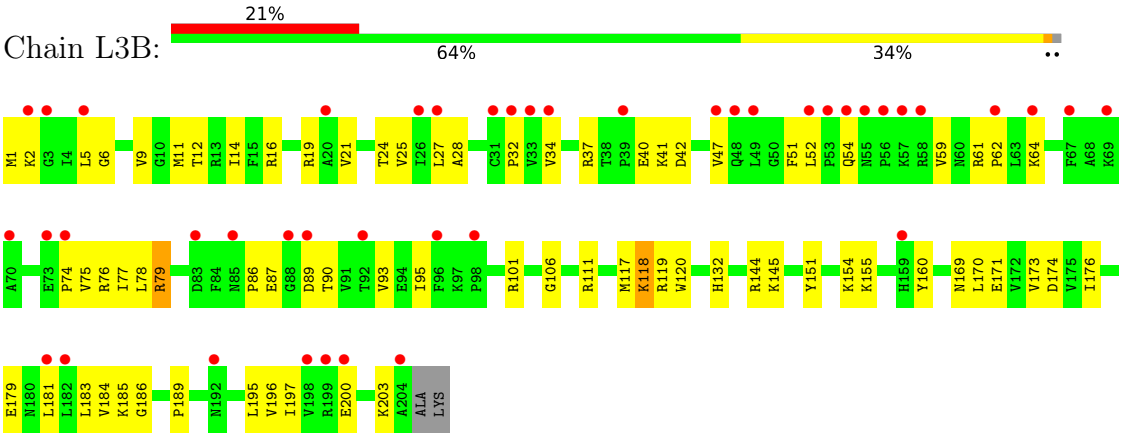

• Molecule 30: 50S ribosomal protein L3

Chain L3A:



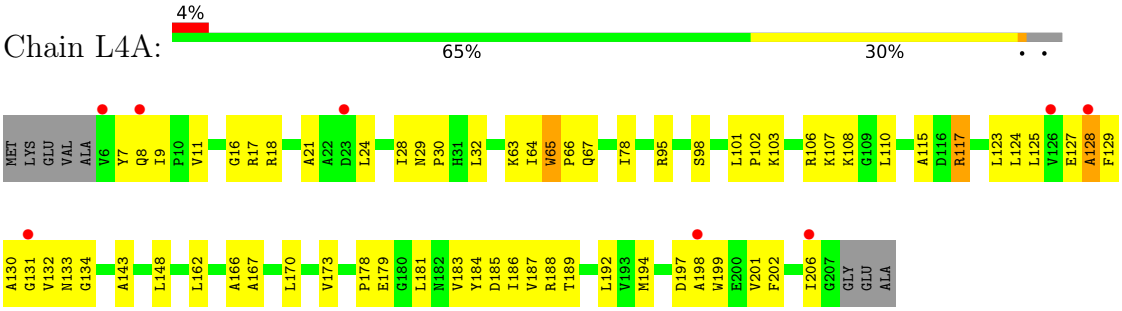

• Molecule 30: 50S ribosomal protein L3

Chain L3B:



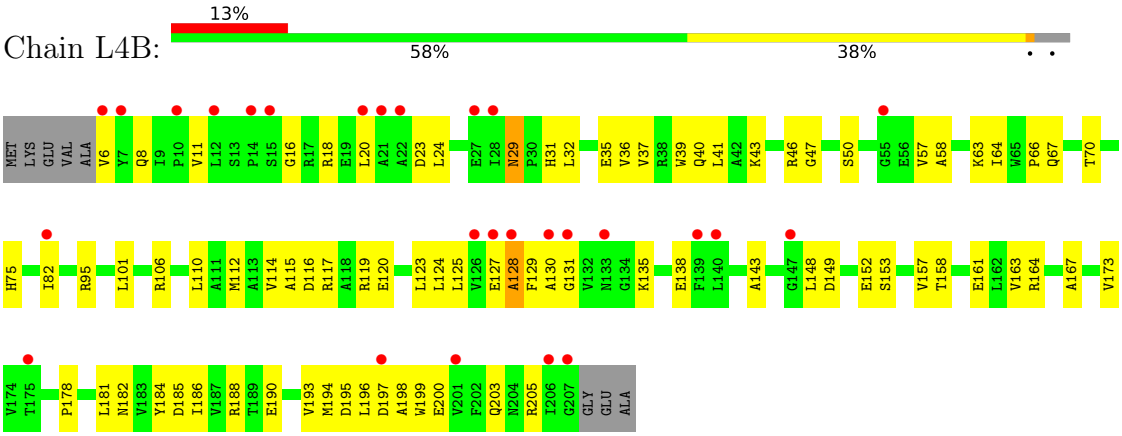

• Molecule 31: 50S ribosomal protein L4

Chain L4A:



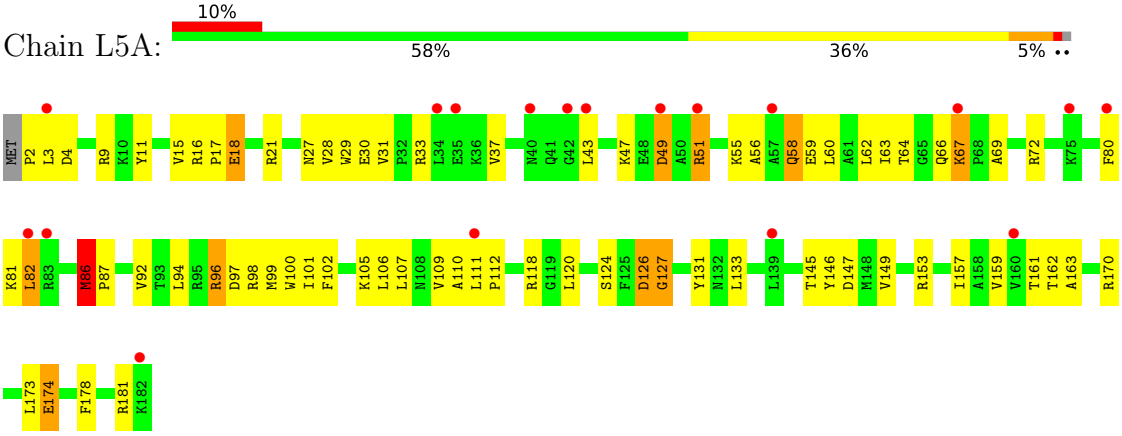

• Molecule 31: 50S ribosomal protein L4

Chain L4B:



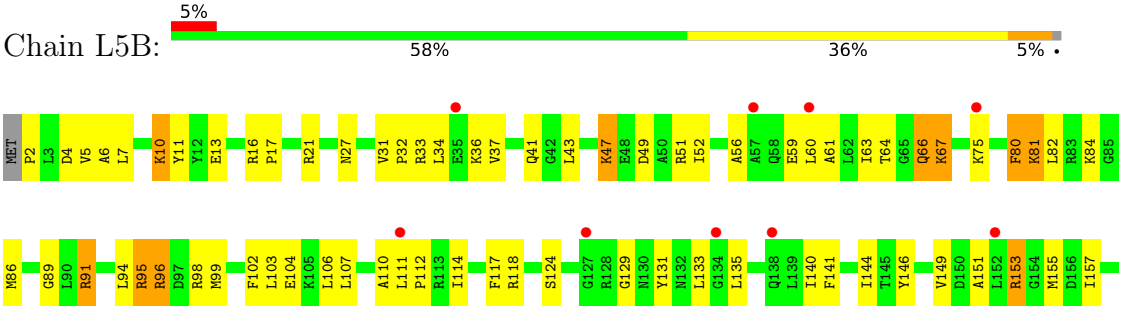

• Molecule 32: 50S ribosomal protein L5

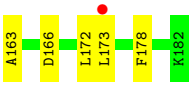
Chain L5A:




• Molecule 32: 50S ribosomal protein L5

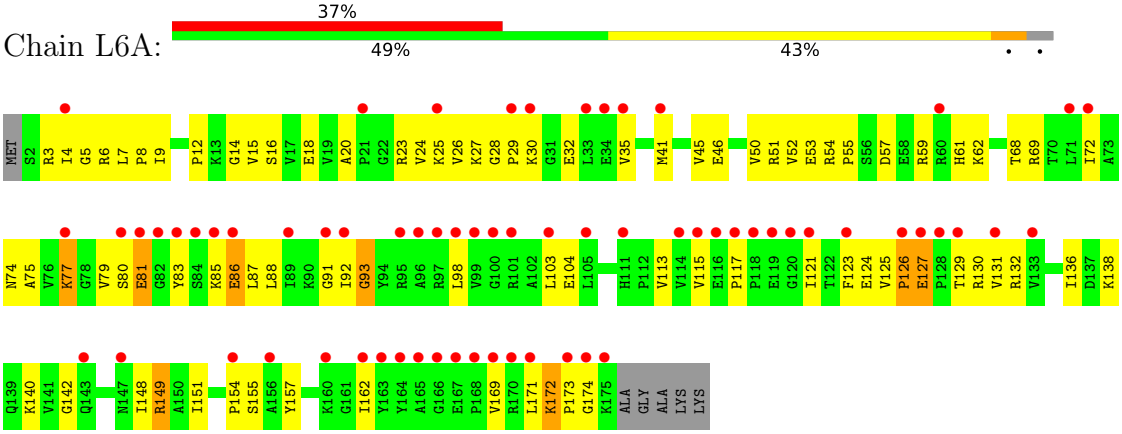
Chain L5B:





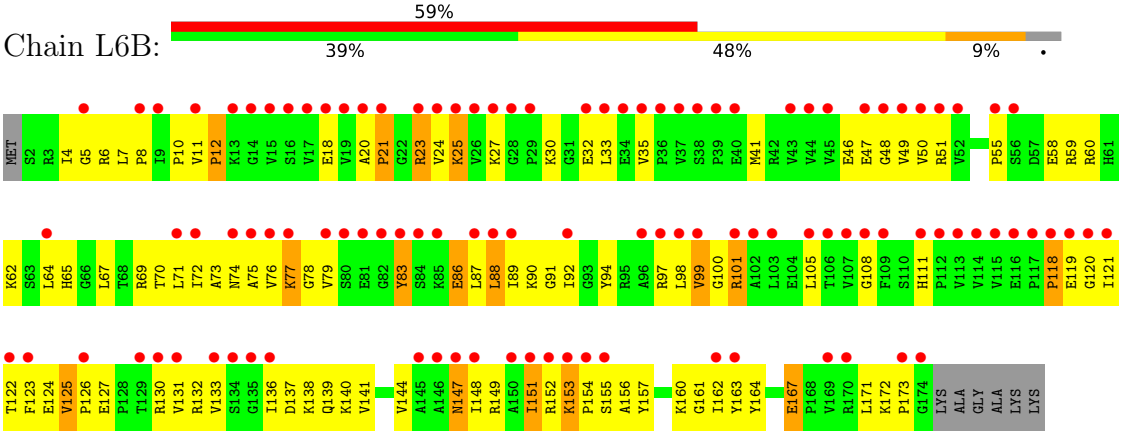

• Molecule 33: 50S ribosomal protein L6

Chain L6A:



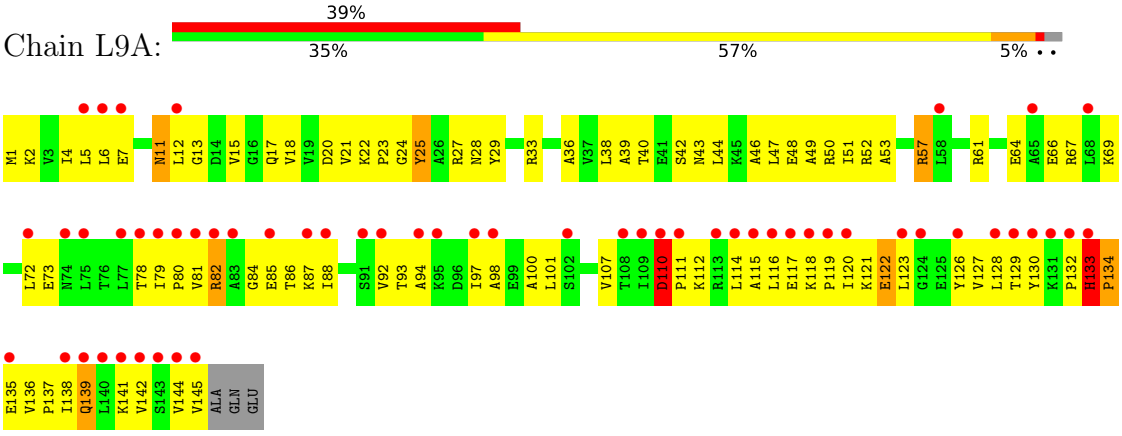

• Molecule 33: 50S ribosomal protein L6

Chain L6B:



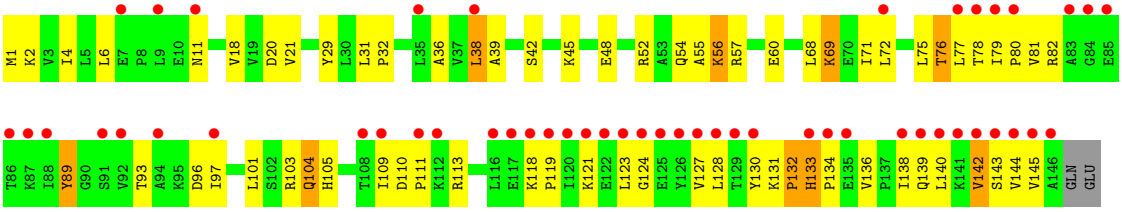

• Molecule 34: 50S ribosomal protein L9

Chain L9A:

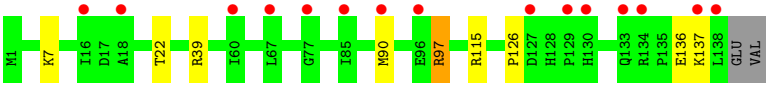



• Molecule 34: 50S ribosomal protein L9

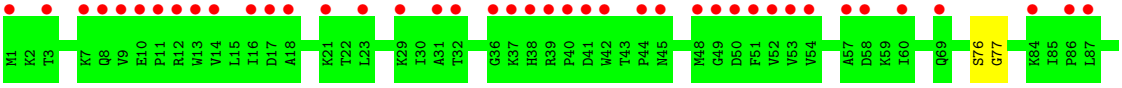
Chain L9B:



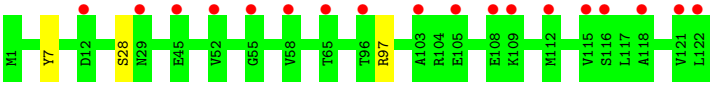

• Molecule 35: 50S ribosomal protein L13



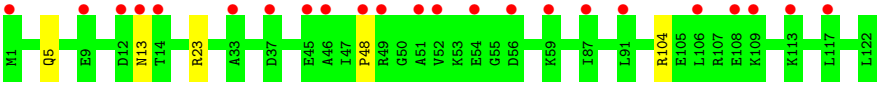

• Molecule 35: 50S ribosomal protein L13



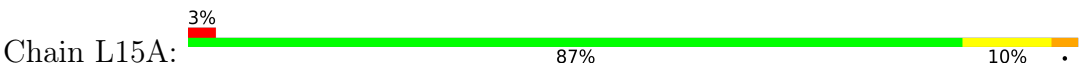

• Molecule 36: 50S ribosomal protein L14

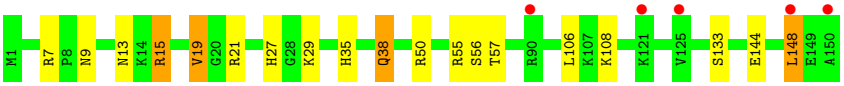



• Molecule 36: 50S ribosomal protein L14



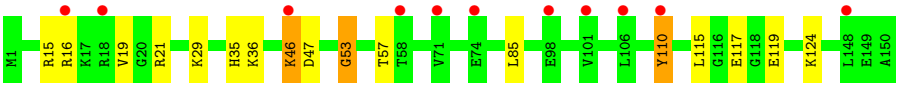

• Molecule 37: 50S ribosomal protein L15



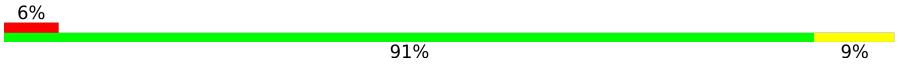

• Molecule 37: 50S ribosomal protein L15

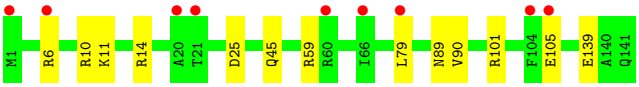
Chain L15B:




• Molecule 38: 50S ribosomal protein L16

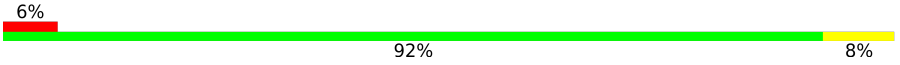
Chain L16A:

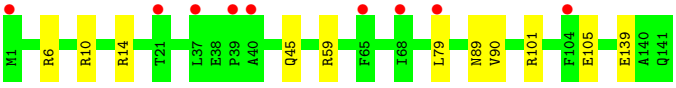



• Molecule 38: 50S ribosomal protein L16

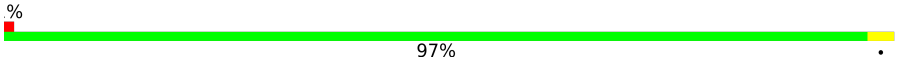
Chain L16B:

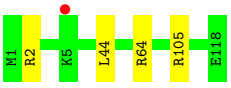



• Molecule 39: 50S ribosomal protein L17

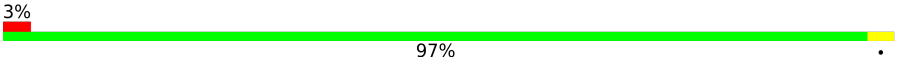
Chain L17A:

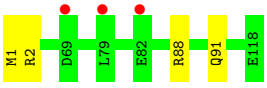



• Molecule 39: 50S ribosomal protein L17

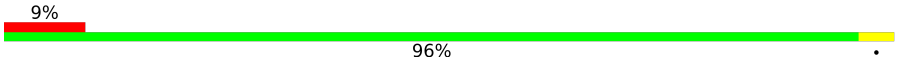
Chain L17B:

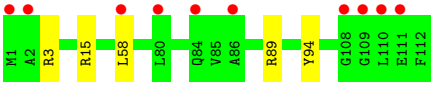



• Molecule 40: 50S ribosomal protein L18

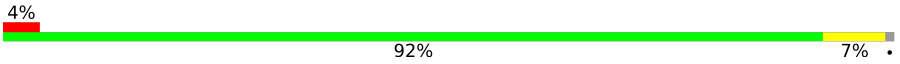
Chain L18A:

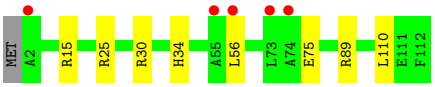



• Molecule 40: 50S ribosomal protein L18

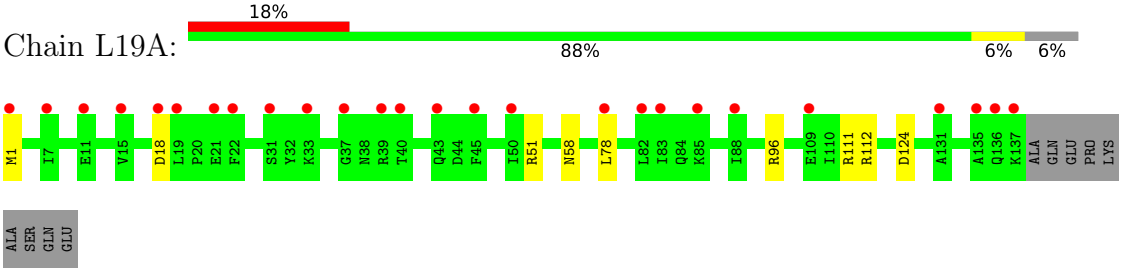
Chain L18B:



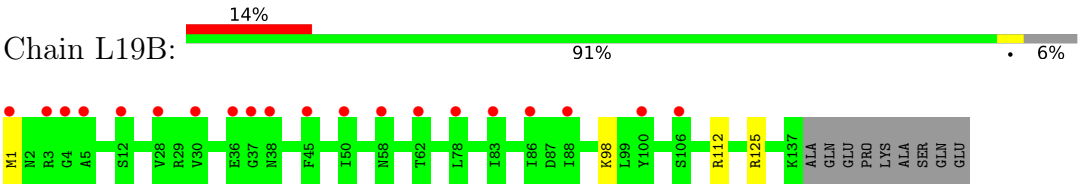
• Molecule 41: 50S ribosomal protein L19

Chain L19A:



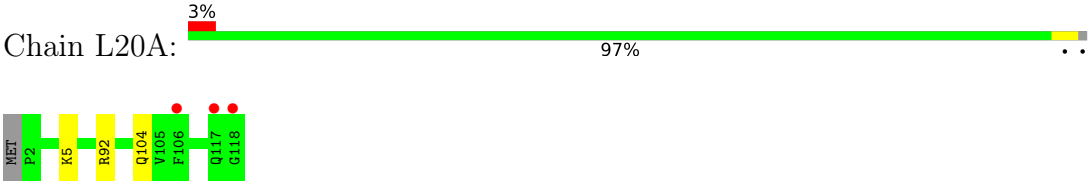

• Molecule 41: 50S ribosomal protein L19

Chain L19B:



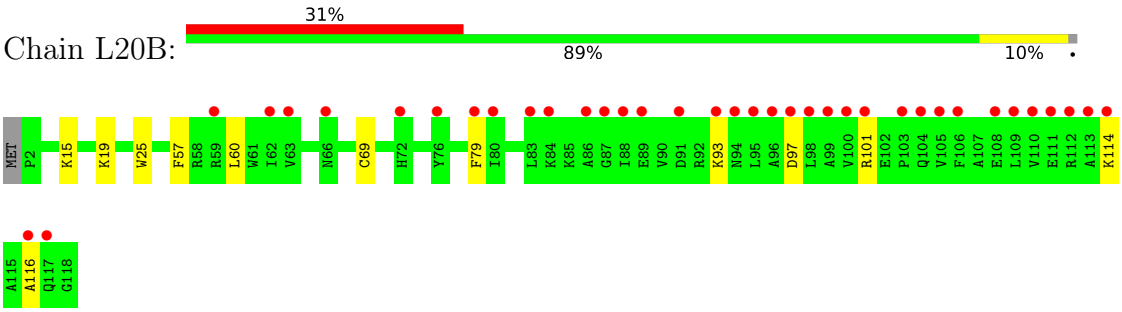

• Molecule 42: 50S ribosomal protein L20

Chain L20A:



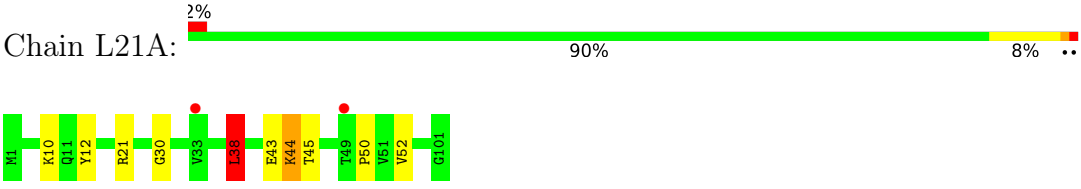

• Molecule 42: 50S ribosomal protein L20

Chain L20B:



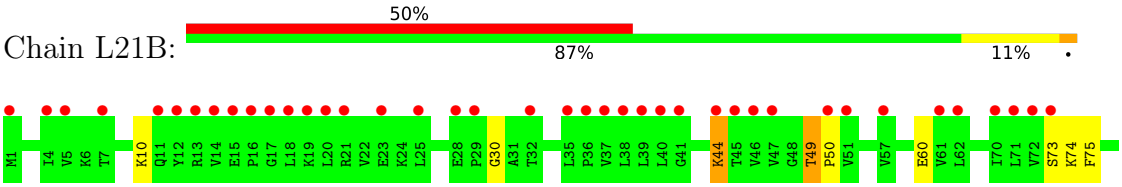

• Molecule 43: 50S ribosomal protein L21

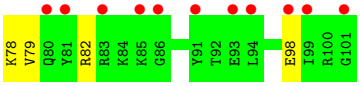
Chain L21A:



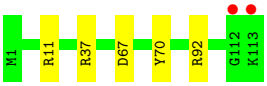

• Molecule 43: 50S ribosomal protein L21

Chain L21B:

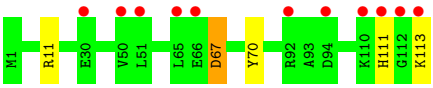




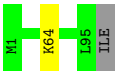

• Molecule 44: 50S ribosomal protein L22



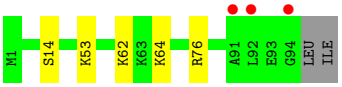

• Molecule 44: 50S ribosomal protein L22



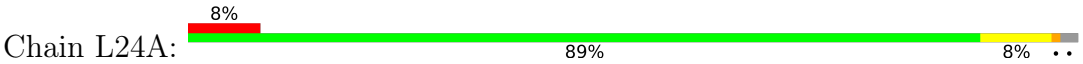

• Molecule 45: 50S ribosomal protein L23

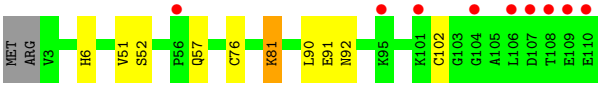



• Molecule 45: 50S ribosomal protein L23

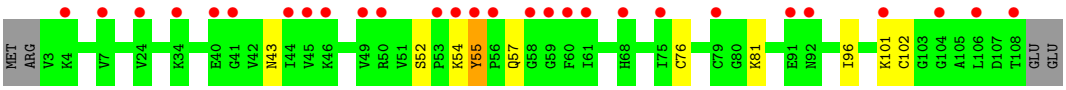



• Molecule 46: 50S ribosomal protein L24



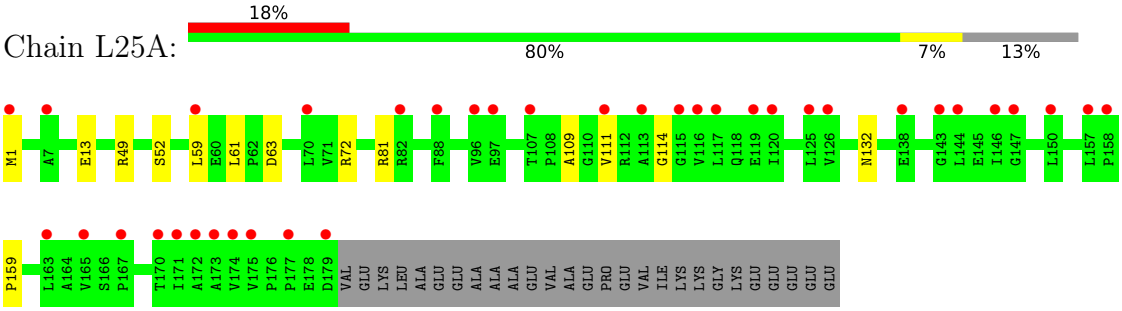




• Molecule 46: 50S ribosomal protein L24



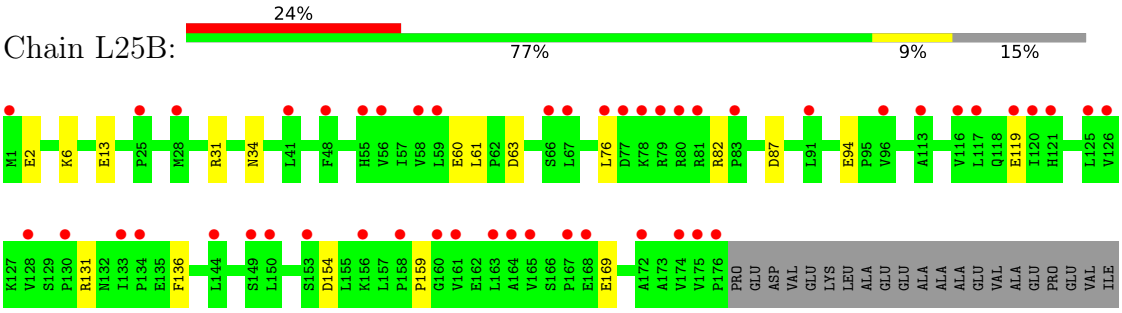

• Molecule 47: 50S ribosomal protein L25

Chain L25A:



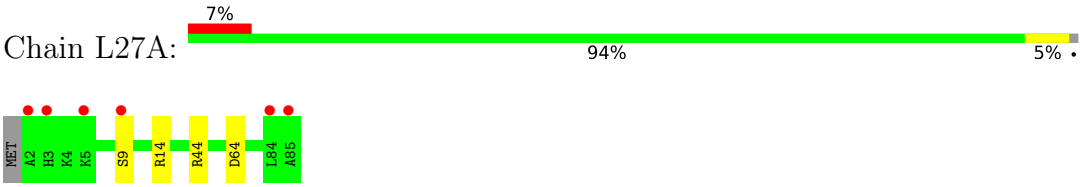

• Molecule 47: 50S ribosomal protein L25

Chain L25B:



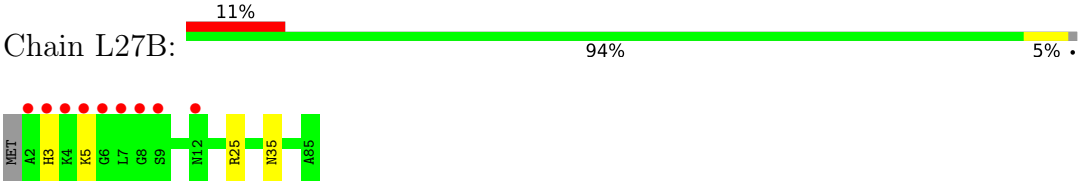

• Molecule 48: 50S ribosomal protein L27

Chain L27A:



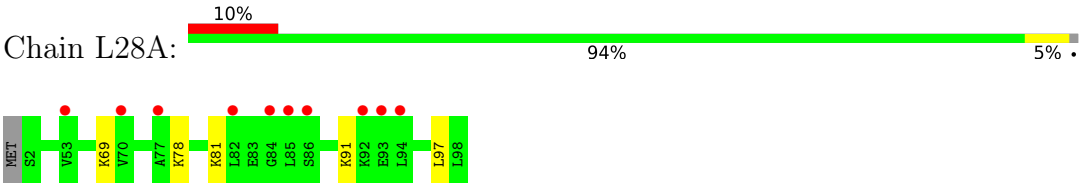

• Molecule 48: 50S ribosomal protein L27

Chain L27B:



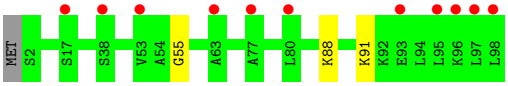

• Molecule 49: 50S ribosomal protein L28

Chain L28A:



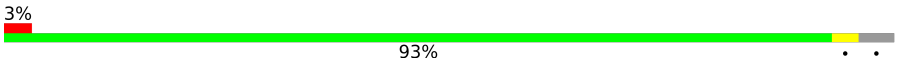

• Molecule 49: 50S ribosomal protein L28

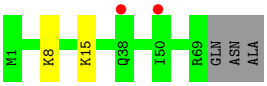
Chain L28B:




• Molecule 50: 50S ribosomal protein L29

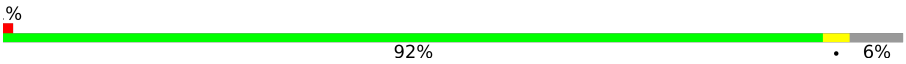
Chain L29A:

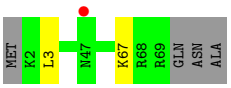



• Molecule 50: 50S ribosomal protein L29

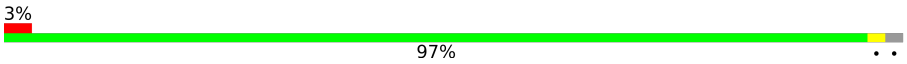
Chain L29B:

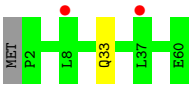



• Molecule 51: 50S ribosomal protein L30

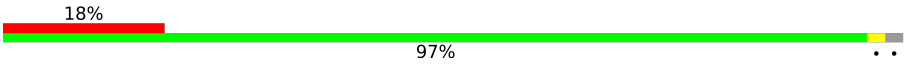
Chain L30A:

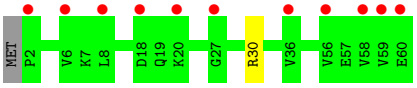



• Molecule 51: 50S ribosomal protein L30

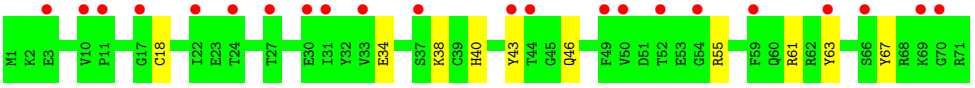
Chain L30B:



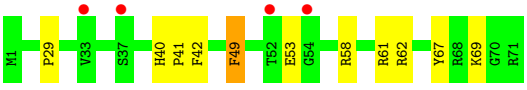

• Molecule 52: 50S ribosomal protein L31

Chain L31A:



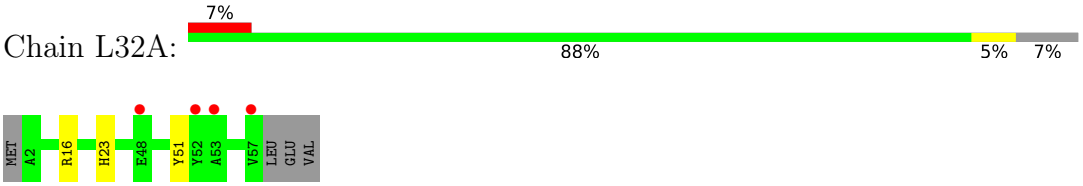

• Molecule 52: 50S ribosomal protein L31

Chain L31B:



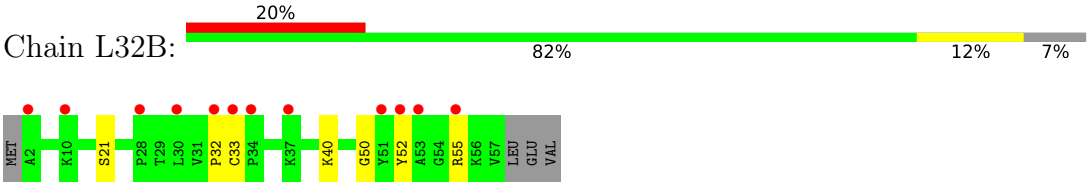

• Molecule 53: 50S ribosomal protein L32

Chain L32A:



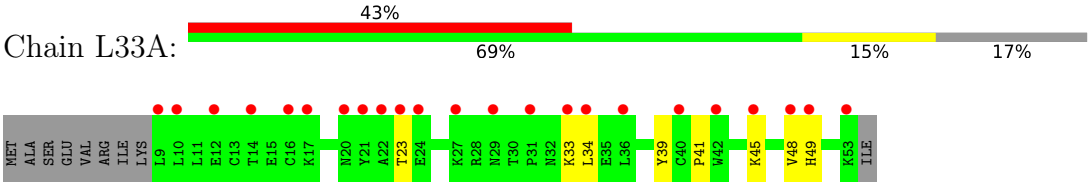

• Molecule 53: 50S ribosomal protein L32

Chain L32B:



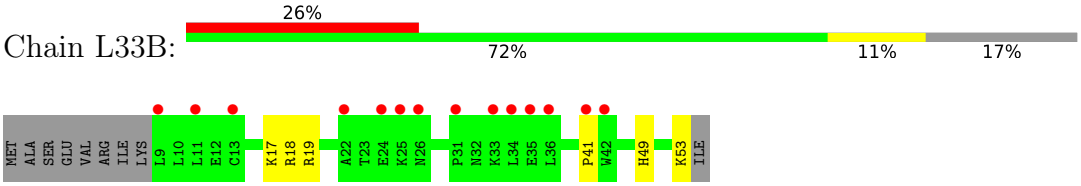

• Molecule 54: 50S ribosomal protein L33

Chain L33A:



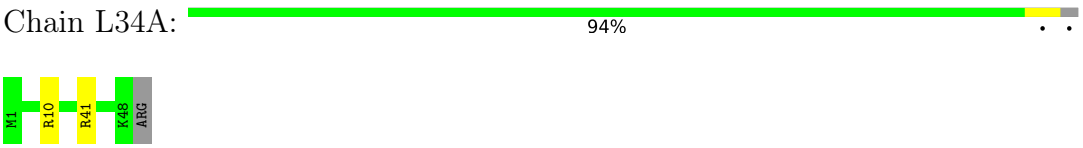

• Molecule 54: 50S ribosomal protein L33

Chain L33B:



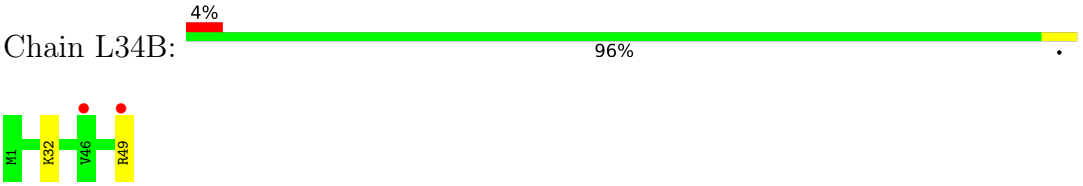

• Molecule 55: 50S ribosomal protein L34

Chain L34A:



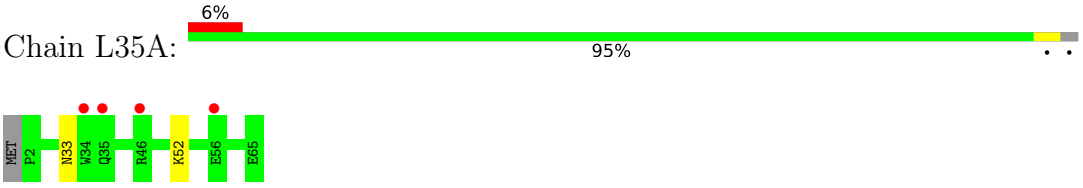

• Molecule 55: 50S ribosomal protein L34

Chain L34B:



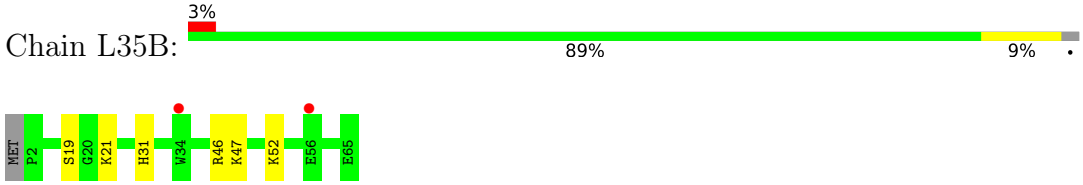

• Molecule 56: 50S ribosomal protein L35

Chain L35A:



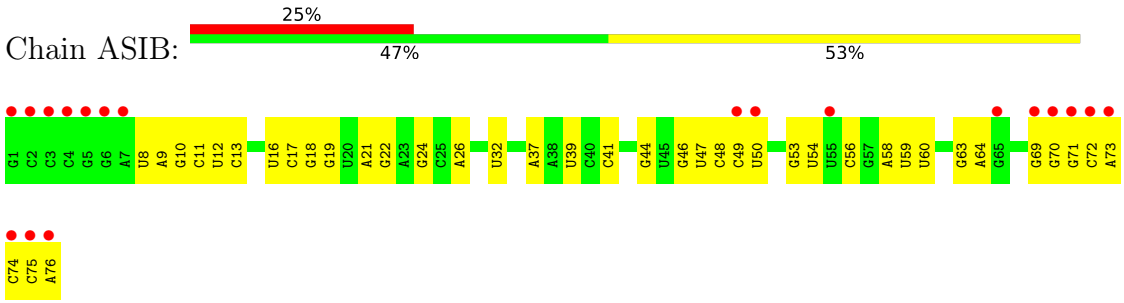
• Molecule 56: 50S ribosomal protein L35

Chain L35B:




• Molecule 57: Phe-tRNA

Chain ASIB:



# 4 Data and refinement statistics (i)

| Property | Value | Source |
|---|---|---|
| Space group | P 21 21 21 | Depositor |
| Cell constants<br>a, b, c, $\alpha$, $\beta$, $\gamma$ | 210.40Å 450.10Å 626.02Å<br>90.00° 90.00° 90.00° | Depositor |
| Resolution (Å) | 256.98 – 3.10<br>256.98 – 3.10 | Depositor<br>EDS |
| % Data completeness<br>(in resolution range) | 100.0 (256.98-3.10)<br>94.2 (256.98-3.10) | Depositor<br>EDS |
| $R_{merge}$ | (Not available) | Depositor |
| $R_{sym}$ | (Not available) | Depositor |
| $< I/\sigma(I) >$ [1] | 1.30 (at 3.07Å) | Xtriage |
| Refinement program | PHENIX 1.18.2_3874 | Depositor |
| R, $R_{free}$ | 0.247 , 0.275<br>0.248 , 0.277 | Depositor<br>DCC |
| $R_{free}$ test set | 31853 reflections (3.00%) | wwPDB-VP |
| Wilson B-factor (Å$^2$) | 79.5 | Xtriage |
| Anisotropy | 0.262 | Xtriage |
| Bulk solvent $k_{sol}$(e/Å$^3$), $B_{sol}$(Å$^2$) | 0.27 , 58.6 | EDS |
| L-test for twinning[2] | $< \|L\| > = 0.46$, $< L^2 > = 0.29$ | Xtriage |
| Estimated twinning fraction | No twinning to report. | Xtriage |
| $F_o$,$F_c$ correlation | 0.93 | EDS |
| Total number of atoms | 306277 | wwPDB-VP |
| Average B, all atoms (Å$^2$) | 93.0 | wwPDB-VP |

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 1.38% 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: OMU, 2MG, M2G, PSU, MG, K, 0TD, 2MA, 4SU, 3AU, 5MU, OMC, OMG, MIA, MA6, SJH, 7MG, UR3, 5MC, 4OC, OHX

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 | 16SA | 0.27 | 1/36066 (0.0%) | 0.58 | 6/56286 (0.0%) |
| 1 | 16SB | 0.27 | 1/35977 (0.0%) | 0.57 | 3/56146 (0.0%) |
| 2 | S2A | 0.28 | 0/1959 | 0.66 | 0/2642 |
| 2 | S2B | 0.28 | 0/1959 | 0.69 | 0/2642 |
| 3 | S3A | 0.27 | 0/1629 | 0.64 | 0/2195 |
| 3 | S3B | 0.25 | 0/1636 | 0.59 | 0/2205 |
| 4 | S4A | 0.31 | 0/1732 | 0.66 | 0/2318 |
| 4 | S4B | 0.26 | 0/1732 | 0.57 | 0/2318 |
| 5 | S5A | 0.34 | 0/1171 | 0.75 | 2/1576 (0.1%) |
| 5 | S5B | 0.25 | 0/1171 | 0.58 | 0/1576 |
| 6 | S6A | 0.23 | 0/855 | 0.57 | 0/1154 |
| 6 | S6B | 0.23 | 0/855 | 0.53 | 0/1154 |
| 7 | S7A | 0.26 | 0/1275 | 0.59 | 0/1709 |
| 7 | S7B | 0.23 | 0/1274 | 0.54 | 0/1706 |
| 8 | S8A | 0.27 | 0/1135 | 0.63 | 0/1527 |
| 8 | S8B | 0.21 | 0/1135 | 0.50 | 0/1527 |
| 9 | S9A | 0.29 | 0/1028 | 0.77 | 2/1379 (0.1%) |
| 9 | S9B | 0.25 | 0/1028 | 0.65 | 0/1379 |
| 10 | S10A | 0.26 | 0/814 | 0.67 | 0/1095 |
| 10 | S10B | 0.26 | 0/814 | 0.63 | 0/1095 |
| 11 | S11A | 0.24 | 0/879 | 0.51 | 0/1187 |
| 11 | S11B | 0.23 | 0/888 | 0.53 | 0/1198 |
| 12 | S12A | 0.29 | 0/982 | 0.77 | 2/1313 (0.2%) |
| 12 | S12B | 0.29 | 0/982 | 0.66 | 2/1313 (0.2%) |
| 13 | S13A | 0.24 | 0/956 | 0.64 | 0/1281 |
| 13 | S13B | 0.23 | 0/974 | 0.58 | 0/1303 |
| 14 | S14A | 0.32 | 0/500 | 0.67 | 1/664 (0.2%) |
| 14 | S14B | 0.27 | 0/495 | 0.67 | 0/657 |
| 15 | S15A | 0.25 | 0/744 | 0.52 | 0/992 |
| 15 | S15B | 0.20 | 0/744 | 0.45 | 0/992 |
| 16 | S16A | 0.26 | 0/716 | 0.63 | 0/963 |

| Mol | Chain | Bond lengths | | Bond angles | |
|---|---|---|---|---|---|
| | | RMSZ | #\|Z\| >5 | RMSZ | #\|Z\| >5 |
| 16 | S16B | 0.26 | 0/721 | 0.54 | 0/970 |
| 17 | S17A | 0.26 | 0/847 | 0.60 | 0/1131 |
| 17 | S17B | 0.21 | 0/847 | 0.52 | 0/1131 |
| 18 | S18A | 0.27 | 0/589 | 0.62 | 0/782 |
| 18 | S18B | 0.25 | 0/578 | 0.62 | 0/768 |
| 19 | S19A | 0.30 | 0/689 | 0.97 | 5/926 (0.5%) |
| 19 | S19B | 0.25 | 0/698 | 0.63 | 0/938 |
| 20 | S20A | 0.28 | 0/764 | 0.66 | 0/1007 |
| 20 | S20B | 0.24 | 0/764 | 0.60 | 0/1007 |
| 21 | THXA | 0.22 | 0/212 | 0.56 | 0/277 |
| 21 | THXB | 0.20 | 0/221 | 0.56 | 0/288 |
| 22 | ASIA | 0.33 | 1/1647 (0.1%) | 0.74 | 0/2565 |
| 23 | PSIA | 0.49 | 3/1624 (0.2%) | 0.70 | 0/2527 |
| 23 | PSIB | 0.41 | 1/1624 (0.1%) | 0.66 | 0/2527 |
| 24 | ESIA | 0.29 | 0/1783 | 0.61 | 0/2776 |
| 24 | ESIB | 0.25 | 0/1783 | 0.58 | 0/2776 |
| 25 | MRNA | 0.25 | 0/689 | 0.61 | 0/1069 |
| 25 | MRNB | 0.28 | 0/689 | 0.65 | 0/1069 |
| 26 | TRNA | 0.47 | 3/1604 (0.2%) | 0.68 | 0/2499 |
| 27 | 23SA | 0.26 | 1/69430 (0.0%) | 0.57 | 12/108380 (0.0%) |
| 27 | 23SB | 0.26 | 0/69097 | 0.57 | 5/107863 (0.0%) |
| 28 | 5SA | 0.28 | 0/2928 | 0.59 | 0/4568 |
| 28 | 5SB | 0.28 | 0/2906 | 0.64 | 1/4533 (0.0%) |
| 29 | L2A | 0.25 | 0/2165 | 0.65 | 0/2919 |
| 29 | L2B | 0.25 | 0/2165 | 0.62 | 0/2919 |
| 30 | L3A | 0.26 | 0/1596 | 0.59 | 0/2153 |
| 30 | L3B | 0.23 | 0/1596 | 0.56 | 0/2153 |
| 31 | L4A | 0.26 | 0/1620 | 0.60 | 0/2194 |
| 31 | L4B | 0.23 | 0/1620 | 0.61 | 0/2194 |
| 32 | L5A | 0.23 | 0/1498 | 0.59 | 0/2016 |
| 32 | L5B | 0.25 | 0/1498 | 0.60 | 2/2016 (0.1%) |
| 33 | L6A | 0.27 | 0/1362 | 0.70 | 0/1841 |
| 33 | L6B | 0.30 | 0/1353 | 0.68 | 0/1830 |
| 34 | L9A | 0.35 | 0/1146 | 0.91 | 3/1551 (0.2%) |
| 34 | L9B | 0.26 | 0/1151 | 0.69 | 0/1558 |
| 35 | L13A | 0.29 | 0/1131 | 0.74 | 2/1525 (0.1%) |
| 35 | L13B | 0.22 | 0/1131 | 0.61 | 0/1525 |
| 36 | L14A | 0.28 | 0/942 | 0.66 | 0/1269 |
| 36 | L14B | 0.25 | 0/942 | 0.59 | 0/1269 |
| 37 | L15A | 0.33 | 0/1161 | 0.92 | 3/1544 (0.2%) |
| 37 | L15B | 0.28 | 0/1161 | 0.88 | 6/1544 (0.4%) |
| 38 | L16A | 0.22 | 0/1142 | 0.60 | 0/1527 |
| 38 | L16B | 0.24 | 0/1142 | 0.60 | 0/1527 |

| Mol | Chain | Bond lengths | | Bond angles | |
|---|---|---|---|---|---|
| | | RMSZ | #\|Z\| >5 | RMSZ | #\|Z\| >5 |
| 39 | L17A | 0.26 | 0/981 | 0.63 | 0/1312 |
| 39 | L17B | 0.24 | 0/981 | 0.57 | 0/1312 |
| 40 | L18A | 0.24 | 0/899 | 0.73 | 0/1197 |
| 40 | L18B | 0.27 | 0/891 | 0.69 | 0/1187 |
| 41 | L19A | 0.28 | 0/1155 | 0.63 | 0/1542 |
| 41 | L19B | 0.25 | 0/1155 | 0.57 | 0/1542 |
| 42 | L20A | 0.25 | 0/981 | 0.63 | 0/1306 |
| 42 | L20B | 0.24 | 0/981 | 0.57 | 0/1306 |
| 43 | L21A | 0.29 | 0/789 | 0.74 | 1/1057 (0.1%) |
| 43 | L21B | 0.29 | 0/789 | 0.81 | 0/1057 |
| 44 | L22A | 0.23 | 0/910 | 0.58 | 0/1220 |
| 44 | L22B | 0.24 | 0/910 | 0.51 | 0/1220 |
| 45 | L23A | 0.26 | 0/761 | 0.61 | 0/1021 |
| 45 | L23B | 0.25 | 0/756 | 0.57 | 0/1014 |
| 46 | L24A | 0.28 | 0/837 | 0.69 | 0/1118 |
| 46 | L24B | 0.33 | 0/787 | 0.80 | 2/1056 (0.2%) |
| 47 | L25A | 0.27 | 0/1460 | 0.67 | 0/1982 |
| 47 | L25B | 0.24 | 0/1435 | 0.66 | 0/1947 |
| 48 | L27A | 0.27 | 0/670 | 0.67 | 0/892 |
| 48 | L27B | 0.26 | 0/670 | 0.58 | 0/892 |
| 49 | L28A | 0.26 | 0/769 | 0.58 | 0/1022 |
| 49 | L28B | 0.26 | 0/769 | 0.67 | 0/1022 |
| 50 | L29A | 0.23 | 0/585 | 0.56 | 0/773 |
| 50 | L29B | 0.23 | 0/577 | 0.58 | 0/763 |
| 51 | L30A | 0.23 | 0/473 | 0.60 | 0/635 |
| 51 | L30B | 0.24 | 0/473 | 0.59 | 0/635 |
| 52 | L31A | 0.29 | 0/593 | 0.84 | 0/795 |
| 52 | L31B | 0.27 | 0/593 | 0.72 | 0/795 |
| 53 | L32A | 0.36 | 0/448 | 0.58 | 0/606 |
| 53 | L32B | 0.38 | 0/448 | 0.72 | 2/606 (0.3%) |
| 54 | L33A | 0.34 | 0/396 | 0.90 | 0/529 |
| 54 | L33B | 0.39 | 0/396 | 0.91 | 0/529 |
| 55 | L34A | 0.23 | 0/426 | 0.55 | 0/561 |
| 55 | L34B | 0.20 | 0/437 | 0.58 | 0/575 |
| 56 | L35A | 0.28 | 0/524 | 0.66 | 1/691 (0.1%) |
| 56 | L35B | 0.27 | 0/524 | 0.67 | 0/691 |
| 57 | ASIB | 0.27 | 0/1717 | 0.70 | 0/2674 |
| All | All | 0.27 | 11/323307 (0.0%) | 0.60 | 63/484025 (0.0%) |

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

| Mol | Chain | #Chirality outliers | #Planarity outliers |
|---|---|---|---|
| 13 | S13A | 0 | 1 |
| 19 | S19B | 0 | 1 |
| 20 | S20A | 0 | 1 |
| 29 | L2A | 0 | 1 |
| 29 | L2B | 0 | 1 |
| 31 | L4A | 0 | 2 |
| 33 | L6A | 0 | 1 |
| 33 | L6B | 0 | 2 |
| 34 | L9A | 0 | 1 |
| 37 | L15A | 0 | 2 |
| 39 | L17A | 0 | 1 |
| 41 | L19A | 0 | 1 |
| 43 | L21A | 0 | 2 |
| 43 | L21B | 0 | 1 |
| 48 | L27A | 0 | 1 |
| 50 | L29A | 0 | 1 |
| All | All | 0 | 20 |

All (11) bond length outliers are listed below:

| Mol | Chain | Res | Type | Atoms | Z | Observed(Å) | Ideal(Å) |
|---|---|---|---|---|---|---|---|
| 26 | TRNA | 20 | U | C5-C6 | 7.94 | 1.50 | 1.34 |
| 23 | PSIB | 16 | U | C5-C6 | 7.87 | 1.49 | 1.34 |
| 23 | PSIA | 16 | U | C5-C6 | 7.76 | 1.49 | 1.34 |
| 23 | PSIA | 20 | U | C5-C6 | 7.74 | 1.49 | 1.34 |
| 26 | TRNA | 16 | U | C5-C6 | 7.73 | 1.49 | 1.34 |
| 1 | 16SB | 2121 | UR3 | O3'-P | 6.24 | 1.62 | 1.56 |
| 1 | 16SA | 2121 | UR3 | O3'-P | 6.05 | 1.62 | 1.56 |
| 26 | TRNA | 8 | 4SU | O3'-P | 5.49 | 1.61 | 1.56 |
| 22 | ASIA | 8 | 4SU | O3'-P | 5.30 | 1.61 | 1.56 |
| 23 | PSIA | 8 | 4SU | O3'-P | 5.14 | 1.61 | 1.56 |
| 27 | 23SA | 2567 | OMU | O3'-P | 5.02 | 1.61 | 1.56 |

All (63) bond angle outliers are listed below:

| Mol | Chain | Res | Type | Atoms | Z | Observed($^o$) | Ideal($^o$) |
|---|---|---|---|---|---|---|---|
| 34 | L9A | 133 | HIS | CA-C-N | 8.53 | 130.50 | 119.84 |
| 34 | L9A | 133 | HIS | C-N-CA | 8.53 | 130.50 | 119.84 |
| 9 | S9A | 89 | ASN | CA-C-N | 8.37 | 128.48 | 119.28 |
| 9 | S9A | 89 | ASN | C-N-CA | 8.37 | 128.48 | 119.28 |
| 19 | S19A | 41 | VAL | C-N-CD | -7.00 | 105.19 | 120.60 |
| 19 | S19A | 41 | VAL | CA-C-N | 6.99 | 143.78 | 127.00 |
| 19 | S19A | 41 | VAL | C-N-CA | 6.99 | 143.78 | 127.00 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed($^o$) | Ideal($^o$) |
|---|---|---|---|---|---|---|---|
| 12 | S12B | 41 | THR | CA-C-N | 6.99 | 128.58 | 119.84 |
| 12 | S12B | 41 | THR | C-N-CA | 6.99 | 128.58 | 119.84 |
| 32 | L5B | 66 | GLN | CA-C-N | 6.79 | 133.85 | 120.94 |
| 32 | L5B | 66 | GLN | C-N-CA | 6.79 | 133.85 | 120.94 |
| 56 | L35A | 33 | ASN | N-CA-C | -6.68 | 103.64 | 112.72 |
| 12 | S12A | 46 | ASN | N-CA-C | 6.66 | 120.04 | 109.65 |
| 27 | 23SA | 895 | C | P-O3'-C3' | 6.32 | 129.67 | 120.20 |
| 19 | S19A | 4 | SER | CA-C-N | 6.31 | 132.67 | 121.75 |
| 19 | S19A | 4 | SER | C-N-CA | 6.31 | 132.67 | 121.75 |
| 27 | 23SA | 2421 | U | C4'-C3'-O3' | 6.26 | 118.80 | 109.40 |
| 27 | 23SA | 1744 | C | C4'-C3'-O3' | 6.25 | 118.78 | 109.40 |
| 12 | S12A | 44 | LYS | N-CA-C | 6.18 | 121.94 | 113.16 |
| 46 | L24B | 55 | TYR | CA-C-N | 6.18 | 127.56 | 119.84 |
| 46 | L24B | 55 | TYR | C-N-CA | 6.18 | 127.56 | 119.84 |
| 27 | 23SA | 1744 | C | P-O3'-C3' | 6.17 | 129.45 | 120.20 |
| 5 | S5A | 51 | VAL | CB-CA-C | -6.06 | 107.94 | 113.70 |
| 27 | 23SB | 2521 | U | C2'-C3'-O3' | -6.04 | 104.64 | 113.70 |
| 37 | L15B | 47 | ASP | CA-C-N | 5.85 | 141.04 | 127.00 |
| 37 | L15B | 47 | ASP | C-N-CA | 5.85 | 141.04 | 127.00 |
| 37 | L15A | 38 | GLN | N-CA-C | -5.83 | 98.38 | 110.80 |
| 1 | 16SA | 1441 | C | C2'-C3'-O3' | 5.72 | 118.08 | 109.50 |
| 27 | 23SA | 2017 | G | C2'-C3'-O3' | 5.63 | 117.94 | 109.50 |
| 1 | 16SA | 1441 | C | P-O3'-C3' | 5.60 | 128.59 | 120.20 |
| 27 | 23SA | 2421 | U | P-O3'-C3' | 5.57 | 128.56 | 120.20 |
| 27 | 23SA | 2696 | C | C2'-C3'-O3' | 5.55 | 117.83 | 109.50 |
| 1 | 16SA | 696 | A | C4'-C3'-O3' | 5.53 | 117.69 | 109.40 |
| 1 | 16SB | 1949 | C | O3'-P-O5' | -5.51 | 95.73 | 104.00 |
| 43 | L21A | 38 | LEU | CA-CB-CG | 5.49 | 135.50 | 116.30 |
| 37 | L15B | 46 | LYS | CA-C-N | -5.48 | 113.75 | 119.83 |
| 37 | L15B | 46 | LYS | C-N-CA | -5.48 | 113.75 | 119.83 |
| 53 | L32B | 32 | PRO | CA-C-N | 5.44 | 132.57 | 121.48 |
| 53 | L32B | 32 | PRO | C-N-CA | 5.44 | 132.57 | 121.48 |
| 1 | 16SA | 1007 | C | C4'-C3'-O3' | 5.38 | 117.48 | 109.40 |
| 27 | 23SA | 2533 | A | N9-C1'-C2' | -5.38 | 105.92 | 114.00 |
| 27 | 23SA | 2696 | C | P-O3'-C3' | 5.37 | 128.26 | 120.20 |
| 27 | 23SB | 2521 | U | C3'-C2'-O2' | 5.35 | 118.72 | 110.70 |
| 27 | 23SB | 1349 | U | P-O3'-C3' | 5.30 | 128.16 | 120.20 |
| 37 | L15A | 56 | SER | CA-C-N | 5.29 | 131.65 | 121.54 |
| 37 | L15A | 56 | SER | C-N-CA | 5.29 | 131.65 | 121.54 |
| 28 | 5SB | 68 | A | P-O3'-C3' | 5.28 | 128.12 | 120.20 |
| 37 | L15B | 53 | GLY | N-CA-C | 5.28 | 125.69 | 113.18 |
| 1 | 16SA | 2121 | UR3 | P-O3'-C3' | 5.23 | 125.98 | 119.70 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed($^o$) | Ideal($^o$) |
|---|---|---|---|---|---|---|---|
| 34 | L9A | 84 | GLY | N-CA-C | -5.22 | 100.80 | 113.18 |
| 35 | L13A | 136 | GLU | CA-C-N | 5.22 | 131.50 | 121.54 |
| 35 | L13A | 136 | GLU | C-N-CA | 5.22 | 131.50 | 121.54 |
| 27 | 23SA | 2441 | A | O3'-P-O5' | -5.21 | 96.19 | 104.00 |
| 27 | 23SB | 2462 | G | P-O3'-C3' | 5.15 | 127.92 | 120.20 |
| 1 | 16SB | 1973 | A | P-O3'-C3' | 5.15 | 127.92 | 120.20 |
| 1 | 16SA | 677 | G | C4'-C3'-O3' | 5.14 | 117.11 | 109.40 |
| 27 | 23SA | 1258 | A | C4'-C3'-O3' | 5.12 | 117.09 | 109.40 |
| 5 | S5A | 51 | VAL | N-CA-C | 5.11 | 119.05 | 112.67 |
| 27 | 23SB | 2017 | G | C2'-C3'-O3' | 5.11 | 117.16 | 109.50 |
| 27 | 23SA | 2441 | A | C4'-C3'-O3' | 5.04 | 116.96 | 109.40 |
| 1 | 16SB | 2121 | UR3 | P-O3'-C3' | 5.03 | 125.74 | 119.70 |
| 14 | S14A | 27 | CYS | CA-CB-SG | 5.02 | 125.94 | 114.40 |
| 37 | L15B | 47 | ASP | C-N-CD | -5.01 | 109.58 | 120.60 |

There are no chirality outliers.

All (20) planarity outliers are listed below:

| Mol | Chain | Res | Type | Group |
|---|---|---|---|---|
| 37 | L15A | 35 | HIS | Peptide |
| 37 | L15A | 9 | ASN | Peptide |
| 39 | L17A | 2 | ARG | Peptide |
| 41 | L19A | 58 | ASN | Peptide |
| 43 | L21A | 43 | GLU | Peptide |
| 43 | L21A | 44 | LYS | Peptide |
| 43 | L21B | 49 | THR | Peptide |
| 48 | L27A | 9 | SER | Peptide |
| 50 | L29A | 15 | LYS | Peptide |
| 29 | L2A | 45 | ASN | Peptide |
| 29 | L2B | 45 | ASN | Peptide |
| 31 | L4A | 132 | VAL | Peptide |
| 31 | L4A | 65 | TRP | Peptide |
| 33 | L6A | 172 | LYS | Peptide |
| 33 | L6B | 100 | GLY | Peptide |
| 33 | L6B | 11 | VAL | Peptide |
| 34 | L9A | 110 | ASP | Peptide |
| 13 | S13A | 105 | THR | Peptide |
| 19 | S19B | 41 | VAL | Peptide |
| 20 | S20A | 95 | ALA | 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 | 16SA | 32489 | 0 | 0 | 0 | 0 |
| 1 | 16SB | 32409 | 0 | 0 | 0 | 9 |
| 2 | S2A | 1924 | 0 | 1975 | 83 | 0 |
| 2 | S2B | 1924 | 0 | 1975 | 101 | 0 |
| 3 | S3A | 1605 | 0 | 1668 | 57 | 0 |
| 3 | S3B | 1612 | 0 | 1677 | 61 | 0 |
| 4 | S4A | 1702 | 0 | 1767 | 63 | 0 |
| 4 | S4B | 1702 | 0 | 1764 | 51 | 0 |
| 5 | S5A | 1155 | 0 | 1213 | 31 | 0 |
| 5 | S5B | 1155 | 0 | 1212 | 33 | 0 |
| 6 | S6A | 842 | 0 | 857 | 26 | 0 |
| 6 | S6B | 842 | 0 | 857 | 23 | 0 |
| 7 | S7A | 1256 | 0 | 1296 | 27 | 0 |
| 7 | S7B | 1256 | 0 | 1295 | 26 | 0 |
| 8 | S8A | 1115 | 0 | 1177 | 46 | 0 |
| 8 | S8B | 1115 | 0 | 1177 | 40 | 0 |
| 9 | S9A | 1009 | 0 | 1037 | 44 | 0 |
| 9 | S9B | 1009 | 0 | 1037 | 53 | 0 |
| 10 | S10A | 801 | 0 | 0 | 0 | 0 |
| 10 | S10B | 801 | 0 | 0 | 0 | 0 |
| 11 | S11A | 864 | 0 | 0 | 0 | 0 |
| 11 | S11B | 873 | 0 | 0 | 0 | 0 |
| 12 | S12A | 977 | 0 | 0 | 0 | 0 |
| 12 | S12B | 977 | 0 | 0 | 0 | 0 |
| 13 | S13A | 946 | 0 | 0 | 0 | 0 |
| 13 | S13B | 964 | 0 | 0 | 0 | 0 |
| 14 | S14A | 491 | 0 | 0 | 0 | 0 |
| 14 | S14B | 486 | 0 | 0 | 0 | 0 |
| 15 | S15A | 733 | 0 | 0 | 0 | 0 |
| 15 | S15B | 733 | 0 | 0 | 0 | 0 |
| 16 | S16A | 700 | 0 | 0 | 0 | 0 |
| 16 | S16B | 705 | 0 | 0 | 0 | 0 |
| 17 | S17A | 834 | 0 | 0 | 0 | 0 |
| 17 | S17B | 834 | 0 | 0 | 0 | 0 |
| 18 | S18A | 584 | 0 | 0 | 0 | 0 |
| 18 | S18B | 573 | 0 | 0 | 0 | 0 |
| 19 | S19A | 674 | 0 | 0 | 0 | 0 |

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| Mol | Chain | Non-H | H(model) | H(added) | Clashes | Symm-Clashes |
|---|---|---|---|---|---|---|
| 19 | S19B | 684 | 0 | 0 | 0 | 0 |
| 20 | S20A | 762 | 0 | 0 | 0 | 0 |
| 20 | S20B | 762 | 0 | 0 | 0 | 0 |
| 21 | THXA | 208 | 0 | 0 | 0 | 0 |
| 21 | THXB | 217 | 0 | 0 | 0 | 0 |
| 22 | ASIA | 1628 | 0 | 0 | 0 | 0 |
| 23 | PSIA | 1635 | 0 | 0 | 0 | 0 |
| 23 | PSIB | 1635 | 0 | 0 | 0 | 0 |
| 24 | ESIA | 1626 | 0 | 0 | 0 | 0 |
| 24 | ESIB | 1626 | 0 | 0 | 0 | 0 |
| 25 | MRNA | 621 | 0 | 0 | 0 | 0 |
| 25 | MRNB | 621 | 0 | 0 | 0 | 0 |
| 26 | TRNA | 1565 | 0 | 0 | 0 | 0 |
| 27 | 23SA | 62225 | 0 | 0 | 0 | 1 |
| 27 | 23SB | 61926 | 0 | 0 | 0 | 0 |
| 28 | 5SA | 2617 | 0 | 1328 | 36 | 0 |
| 28 | 5SB | 2598 | 0 | 1316 | 43 | 0 |
| 29 | L2A | 2115 | 0 | 2195 | 39 | 0 |
| 29 | L2B | 2115 | 0 | 2195 | 49 | 0 |
| 30 | L3A | 1563 | 0 | 1629 | 28 | 0 |
| 30 | L3B | 1563 | 0 | 1629 | 51 | 0 |
| 31 | L4A | 1585 | 0 | 1632 | 47 | 0 |
| 31 | L4B | 1585 | 0 | 1632 | 62 | 0 |
| 32 | L5A | 1473 | 0 | 1535 | 60 | 0 |
| 32 | L5B | 1473 | 0 | 1535 | 60 | 0 |
| 33 | L6A | 1336 | 0 | 1418 | 62 | 0 |
| 33 | L6B | 1327 | 0 | 1405 | 72 | 0 |
| 34 | L9A | 1131 | 0 | 1218 | 81 | 9 |
| 34 | L9B | 1136 | 0 | 1223 | 57 | 0 |
| 35 | L13A | 1104 | 0 | 0 | 0 | 0 |
| 35 | L13B | 1104 | 0 | 0 | 0 | 0 |
| 36 | L14A | 932 | 0 | 0 | 0 | 0 |
| 36 | L14B | 932 | 0 | 0 | 0 | 0 |
| 37 | L15A | 1144 | 0 | 0 | 0 | 0 |
| 37 | L15B | 1144 | 0 | 0 | 0 | 0 |
| 38 | L16A | 1121 | 0 | 0 | 0 | 0 |
| 38 | L16B | 1121 | 0 | 0 | 0 | 0 |
| 39 | L17A | 967 | 0 | 0 | 0 | 0 |
| 39 | L17B | 967 | 0 | 0 | 0 | 0 |
| 40 | L18A | 889 | 0 | 0 | 0 | 0 |
| 40 | L18B | 881 | 0 | 0 | 0 | 0 |
| 41 | L19A | 1141 | 0 | 0 | 0 | 0 |

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| Mol | Chain | Non-H | H(model) | H(added) | Clashes | Symm-Clashes |
|---|---|---|---|---|---|---|
| 41 | L19B | 1141 | 0 | 0 | 0 | 0 |
| 42 | L20A | 963 | 0 | 0 | 0 | 0 |
| 42 | L20B | 963 | 0 | 0 | 0 | 0 |
| 43 | L21A | 778 | 0 | 0 | 0 | 0 |
| 43 | L21B | 778 | 0 | 0 | 0 | 0 |
| 44 | L22A | 899 | 0 | 0 | 0 | 0 |
| 44 | L22B | 899 | 0 | 0 | 0 | 0 |
| 45 | L23A | 747 | 0 | 0 | 0 | 0 |
| 45 | L23B | 742 | 0 | 0 | 0 | 0 |
| 46 | L24A | 824 | 0 | 0 | 0 | 0 |
| 46 | L24B | 775 | 0 | 0 | 0 | 1 |
| 47 | L25A | 1428 | 0 | 0 | 0 | 0 |
| 47 | L25B | 1404 | 0 | 0 | 0 | 0 |
| 48 | L27A | 661 | 0 | 0 | 0 | 0 |
| 48 | L27B | 661 | 0 | 0 | 0 | 0 |
| 49 | L28A | 762 | 0 | 0 | 0 | 0 |
| 49 | L28B | 762 | 0 | 0 | 0 | 0 |
| 50 | L29A | 583 | 0 | 0 | 0 | 0 |
| 50 | L29B | 575 | 0 | 0 | 0 | 0 |
| 51 | L30A | 468 | 0 | 0 | 0 | 0 |
| 51 | L30B | 468 | 0 | 0 | 0 | 0 |
| 52 | L31A | 580 | 0 | 0 | 0 | 0 |
| 52 | L31B | 580 | 0 | 0 | 0 | 0 |
| 53 | L32A | 434 | 0 | 0 | 0 | 0 |
| 53 | L32B | 434 | 0 | 0 | 0 | 0 |
| 54 | L33A | 389 | 0 | 0 | 0 | 0 |
| 54 | L33B | 389 | 0 | 0 | 0 | 0 |
| 55 | L34A | 418 | 0 | 0 | 0 | 0 |
| 55 | L34B | 429 | 0 | 0 | 0 | 0 |
| 56 | L35A | 516 | 0 | 0 | 0 | 0 |
| 56 | L35B | 516 | 0 | 0 | 0 | 0 |
| 57 | ASIB | 1627 | 0 | 0 | 0 | 0 |
| 58 | 16SA | 90 | 0 | 0 | 0 | 0 |
| 58 | 16SB | 86 | 0 | 0 | 0 | 0 |
| 58 | 23SA | 334 | 0 | 0 | 0 | 0 |
| 58 | 23SB | 240 | 0 | 0 | 0 | 0 |
| 58 | 5SA | 6 | 0 | 0 | 0 | 0 |
| 58 | 5SB | 4 | 0 | 0 | 0 | 0 |
| 58 | L15A | 2 | 0 | 0 | 0 | 0 |
| 58 | L17A | 1 | 0 | 0 | 0 | 0 |
| 58 | L23A | 1 | 0 | 0 | 0 | 0 |
| 58 | L27A | 2 | 0 | 0 | 0 | 0 |

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| Mol | Chain | Non-H | H(model) | H(added) | Clashes | Symm-Clashes |
|---|---|---|---|---|---|---|
| 58 | L27B | 1 | 0 | 0 | 0 | 0 |
| 58 | L2B | 1 | 0 | 0 | 0 | 0 |
| 58 | L30A | 1 | 0 | 0 | 0 | 0 |
| 58 | L32A | 1 | 0 | 0 | 0 | 0 |
| 58 | L33A | 1 | 0 | 0 | 0 | 0 |
| 58 | L34A | 1 | 0 | 0 | 0 | 0 |
| 58 | L35A | 1 | 0 | 0 | 0 | 0 |
| 58 | L35B | 2 | 0 | 0 | 0 | 0 |
| 58 | L3A | 2 | 0 | 0 | 0 | 0 |
| 58 | L3B | 2 | 0 | 0 | 0 | 0 |
| 58 | L4A | 2 | 0 | 0 | 0 | 0 |
| 58 | L5A | 1 | 0 | 0 | 0 | 0 |
| 58 | L5B | 1 | 0 | 0 | 0 | 0 |
| 58 | MRNA | 1 | 0 | 0 | 0 | 0 |
| 58 | PSIA | 2 | 0 | 0 | 0 | 0 |
| 58 | PSIB | 3 | 0 | 0 | 0 | 0 |
| 58 | S4A | 1 | 0 | 0 | 0 | 0 |
| 58 | S5B | 2 | 0 | 0 | 0 | 0 |
| 59 | 16SA | 46 | 0 | 0 | 0 | 0 |
| 59 | 16SB | 36 | 0 | 0 | 0 | 0 |
| 59 | 23SA | 101 | 0 | 0 | 0 | 0 |
| 59 | 23SB | 83 | 0 | 0 | 0 | 0 |
| 59 | 5SA | 2 | 0 | 0 | 0 | 0 |
| 59 | 5SB | 1 | 0 | 0 | 0 | 0 |
| 59 | L16A | 1 | 0 | 0 | 0 | 0 |
| 59 | L16B | 1 | 0 | 0 | 0 | 0 |
| 59 | L2A | 1 | 0 | 0 | 0 | 0 |
| 59 | L2B | 1 | 0 | 0 | 0 | 0 |
| 59 | L3A | 1 | 0 | 0 | 0 | 0 |
| 59 | L3B | 1 | 0 | 0 | 0 | 0 |
| 59 | L4A | 1 | 0 | 0 | 0 | 0 |
| 59 | L4B | 1 | 0 | 0 | 0 | 0 |
| 59 | L5A | 1 | 0 | 0 | 0 | 0 |
| 59 | L5B | 1 | 0 | 0 | 0 | 0 |
| 59 | PSIA | 2 | 0 | 0 | 0 | 0 |
| 59 | S13A | 1 | 0 | 0 | 0 | 0 |
| 59 | S13B | 1 | 0 | 0 | 0 | 0 |
| 59 | S20A | 1 | 0 | 0 | 0 | 0 |
| 59 | S20B | 1 | 0 | 0 | 0 | 0 |
| 59 | S4B | 1 | 0 | 0 | 0 | 0 |
| 59 | S6A | 1 | 0 | 0 | 0 | 0 |
| 59 | S6B | 1 | 0 | 0 | 0 | 0 |

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| Mol | Chain | Non-H | H(model) | H(added) | Clashes | Symm-Clashes |
|---|---|---|---|---|---|---|
| 60 | 16SA | 560 | 0 | 0 | 0 | 0 |
| 60 | 16SB | 546 | 0 | 0 | 0 | 0 |
| 60 | 23SA | 1379 | 0 | 0 | 0 | 0 |
| 60 | 23SB | 1344 | 0 | 0 | 0 | 0 |
| 60 | 5SA | 70 | 0 | 0 | 0 | 0 |
| 60 | 5SB | 70 | 0 | 0 | 0 | 0 |
| 60 | ASIA | 21 | 0 | 0 | 0 | 0 |
| 60 | ASIB | 21 | 0 | 0 | 0 | 0 |
| 60 | ESIA | 7 | 0 | 0 | 0 | 0 |
| 60 | ESIB | 7 | 0 | 0 | 0 | 0 |
| 60 | L15A | 7 | 0 | 0 | 0 | 0 |
| 60 | L17A | 7 | 0 | 0 | 0 | 0 |
| 60 | L17B | 7 | 0 | 0 | 0 | 0 |
| 60 | L19A | 7 | 0 | 0 | 0 | 0 |
| 60 | L20B | 7 | 0 | 0 | 0 | 0 |
| 60 | L27A | 14 | 0 | 0 | 0 | 0 |
| 60 | L28A | 7 | 0 | 0 | 0 | 0 |
| 60 | L35A | 7 | 0 | 0 | 0 | 0 |
| 60 | L35B | 7 | 0 | 0 | 0 | 0 |
| 60 | L4A | 7 | 0 | 0 | 0 | 0 |
| 60 | MRNA | 7 | 0 | 0 | 0 | 0 |
| 60 | MRNB | 7 | 0 | 0 | 0 | 0 |
| 60 | PSIA | 7 | 0 | 0 | 0 | 0 |
| 60 | PSIB | 21 | 0 | 0 | 0 | 0 |
| 60 | S14B | 7 | 0 | 0 | 0 | 0 |
| 60 | S19A | 7 | 0 | 0 | 0 | 0 |
| 60 | S4B | 7 | 0 | 0 | 0 | 0 |
| 60 | S8B | 7 | 0 | 0 | 0 | 0 |
| 60 | TRNA | 14 | 0 | 0 | 0 | 0 |
| 61 | 23SA | 83 | 0 | 0 | 0 | 0 |
| 61 | 23SB | 83 | 0 | 0 | 0 | 0 |
| 62 | 16SA | 173 | 0 | 0 | 0 | 0 |
| 62 | 16SB | 158 | 0 | 0 | 0 | 0 |
| 62 | 23SA | 801 | 0 | 0 | 0 | 0 |
| 62 | 23SB | 518 | 0 | 0 | 0 | 0 |
| 62 | 5SA | 14 | 0 | 0 | 4 | 0 |
| 62 | 5SB | 5 | 0 | 0 | 1 | 0 |
| 62 | ESIA | 1 | 0 | 0 | 0 | 0 |
| 62 | L15A | 10 | 0 | 0 | 0 | 0 |
| 62 | L15B | 7 | 0 | 0 | 0 | 0 |
| 62 | L16A | 1 | 0 | 0 | 0 | 0 |
| 62 | L17A | 2 | 0 | 0 | 0 | 0 |

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| Mol | Chain | Non-H | H(model) | H(added) | Clashes | Symm-Clashes |
|---|---|---|---|---|---|---|
| 62 | L18A | 2 | 0 | 0 | 0 | 0 |
| 62 | L19A | 1 | 0 | 0 | 0 | 0 |
| 62 | L23A | 1 | 0 | 0 | 0 | 0 |
| 62 | L27A | 3 | 0 | 0 | 0 | 0 |
| 62 | L27B | 2 | 0 | 0 | 0 | 0 |
| 62 | L28B | 1 | 0 | 0 | 0 | 0 |
| 62 | L2A | 9 | 0 | 0 | 1 | 0 |
| 62 | L2B | 13 | 0 | 0 | 1 | 0 |
| 62 | L30A | 1 | 0 | 0 | 0 | 0 |
| 62 | L30B | 2 | 0 | 0 | 0 | 0 |
| 62 | L34A | 1 | 0 | 0 | 0 | 0 |
| 62 | L35A | 1 | 0 | 0 | 0 | 0 |
| 62 | L35B | 6 | 0 | 0 | 0 | 0 |
| 62 | L3A | 7 | 0 | 0 | 0 | 0 |
| 62 | L3B | 6 | 0 | 0 | 1 | 0 |
| 62 | L4A | 6 | 0 | 0 | 0 | 0 |
| 62 | L4B | 1 | 0 | 0 | 0 | 0 |
| 62 | PSIA | 6 | 0 | 0 | 0 | 0 |
| 62 | S12B | 2 | 0 | 0 | 0 | 0 |
| 62 | S13A | 1 | 0 | 0 | 0 | 0 |
| 62 | S14A | 1 | 0 | 0 | 0 | 0 |
| 62 | S14B | 2 | 0 | 0 | 0 | 0 |
| 62 | S16A | 1 | 0 | 0 | 0 | 0 |
| 62 | S17A | 1 | 0 | 0 | 0 | 0 |
| 62 | S4A | 2 | 0 | 0 | 0 | 0 |
| 62 | S4B | 1 | 0 | 0 | 0 | 0 |
| 62 | S5A | 1 | 0 | 0 | 0 | 0 |
| 62 | S5B | 1 | 0 | 0 | 0 | 0 |
| 62 | S9B | 1 | 0 | 0 | 0 | 0 |
| 62 | THXA | 3 | 0 | 0 | 0 | 0 |
| All | All | 306277 | 0 | 43874 | 1481 | 10 |

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 17.

All (1481) 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) |
|---|---|---|---|
| 34:L9A:115:ALA:CB | 34:L9A:128:LEU:HD21 | 1.50 | 1.39 |
| 2:S2B:55:PHE:CE1 | 2:S2B:221:LEU:HD22 | 1.82 | 1.15 |
| 34:L9A:115:ALA:HB2 | 34:L9A:128:LEU:HD21 | 1.14 | 1.05 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 34:L9A:115:ALA:HB3 | 34:L9A:128:LEU:HD21 | 1.33 | 1.02 |
| 34:L9A:115:ALA:CB | 34:L9A:128:LEU:CD2 | 2.41 | 0.97 |
| 34:L9A:114:LEU:CD1 | 34:L9A:129:THR:O | 2.14 | 0.95 |
| 2:S2B:69:LEU:HD13 | 2:S2B:159:PRO:HG3 | 1.45 | 0.95 |
| 3:S3B:50:ALA:HB2 | 3:S3B:76:VAL:HG11 | 1.46 | 0.94 |
| 34:L9A:114:LEU:HD12 | 34:L9A:129:THR:O | 1.70 | 0.92 |
| 29:L2A:60:ARG:HD3 | 29:L2A:86:PRO:HB2 | 1.51 | 0.91 |
| 29:L2A:242:ARG:O | 62:L2A:401:HOH:O | 1.90 | 0.89 |
| 28:5SB:54:A:O2' | 28:5SB:55:A:N7 | 2.06 | 0.88 |
| 31:L4B:167:ALA:HB1 | 31:L4B:173:VAL:HG11 | 1.56 | 0.88 |
| 34:L9A:115:ALA:HB3 | 34:L9A:128:LEU:CD2 | 2.01 | 0.88 |
| 2:S2B:5:ILE:HG12 | 2:S2B:55:PHE:CD1 | 2.08 | 0.88 |
| 30:L3B:119:ARG:HD3 | 30:L3B:160:TYR:HB2 | 1.54 | 0.88 |
| 4:S4A:13:ARG:HA | 4:S4A:33:MET:HE3 | 1.54 | 0.87 |
| 2:S2B:132:LYS:HA | 2:S2B:135:GLN:HB2 | 1.55 | 0.87 |
| 2:S2B:127:ILE:O | 2:S2B:135:GLN:NE2 | 2.08 | 0.86 |
| 2:S2A:168:THR:HG23 | 2:S2A:169:LYS:N | 1.90 | 0.85 |
| 34:L9A:123:LEU:HD23 | 34:L9A:142:VAL:HG12 | 1.58 | 0.85 |
| 28:5SA:82:U:H2' | 28:5SA:83:G:H21 | 1.40 | 0.84 |
| 28:5SB:17:A:H5' | 28:5SB:18:G:H8 | 1.42 | 0.84 |
| 2:S2A:178:ARG:HH21 | 8:S8A:74:PRO:HG3 | 1.43 | 0.84 |
| 31:L4B:127:GLU:O | 31:L4B:129:PHE:N | 2.09 | 0.84 |
| 31:L4A:103:LYS:HA | 31:L4A:106:ARG:HD3 | 1.60 | 0.83 |
| 30:L3B:9:VAL:HG11 | 30:L3B:27:LEU:HD23 | 1.61 | 0.83 |
| 31:L4A:65:TRP:HB2 | 31:L4A:66:PRO:HD3 | 1.61 | 0.82 |
| 28:5SA:75:A:OP2 | 62:5SA:302:HOH:O | 1.97 | 0.82 |
| 32:L5B:64:THR:HG23 | 32:L5B:66:GLN:H | 1.43 | 0.82 |
| 34:L9A:115:ALA:C | 34:L9A:117:GLU:H | 1.88 | 0.82 |
| 2:S2B:20:GLU:HB3 | 2:S2B:23:ARG:HB2 | 1.61 | 0.81 |
| 28:5SB:17:A:H5' | 28:5SB:18:G:C8 | 2.15 | 0.81 |
| 2:S2A:168:THR:CG2 | 2:S2A:169:LYS:N | 2.43 | 0.81 |
| 33:L6A:41:MET:HG3 | 33:L6A:54:ARG:HA | 1.63 | 0.80 |
| 32:L5B:67:LYS:CD | 32:L5B:67:LYS:H | 1.93 | 0.80 |
| 34:L9A:115:ALA:HB2 | 34:L9A:128:LEU:CD2 | 2.06 | 0.79 |
| 30:L3B:47:VAL:HG11 | 30:L3B:86:PRO:HD2 | 1.65 | 0.79 |
| 28:5SA:27:A:OP1 | 62:5SA:303:HOH:O | 2.01 | 0.79 |
| 5:S5A:152:ARG:NH2 | 8:S8A:107:LEU:O | 2.16 | 0.78 |
| 34:L9A:127:VAL:HG22 | 34:L9A:139:GLN:HB3 | 1.64 | 0.78 |
| 28:5SB:35:G:H5' | 32:L5B:2:PRO:HD3 | 1.64 | 0.78 |
| 4:S4A:96:LEU:HG | 4:S4A:139:ARG:HH22 | 1.48 | 0.77 |
| 2:S2A:82:ARG:NH2 | 2:S2A:92:TYR:OH | 2.17 | 0.77 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 34:L9A:86:THR:H | 34:L9A:123:LEU:HD12 | 1.50 | 0.77 |
| 32:L5B:67:LYS:H | 32:L5B:67:LYS:HD3 | 1.48 | 0.77 |
| 33:L6B:27:LYS:HA | 33:L6B:32:GLU:HB3 | 1.65 | 0.77 |
| 31:L4A:127:GLU:O | 31:L4A:129:PHE:N | 2.17 | 0.77 |
| 9:S9B:19:LEU:HB2 | 9:S9B:59:PHE:HE1 | 1.49 | 0.77 |
| 28:5SA:104:A:OP2 | 62:5SA:304:HOH:O | 2.03 | 0.77 |
| 30:L3A:36:ARG:NH1 | 30:L3A:85:ASN:OD1 | 2.18 | 0.77 |
| 2:S2A:20:GLU:HB3 | 2:S2A:23:ARG:HG3 | 1.66 | 0.76 |
| 7:S7B:5:ARG:C | 7:S7B:7:ALA:HB2 | 2.06 | 0.76 |
| 5:S5B:78:HIS:HB2 | 8:S8B:104:ARG:HD2 | 1.67 | 0.75 |
| 2:S2A:53:ARG:NH2 | 2:S2A:198:ASP:O | 2.20 | 0.75 |
| 33:L6B:86:GLU:HA | 33:L6B:132:ARG:HB2 | 1.66 | 0.75 |
| 3:S3B:9:GLY:HA2 | 3:S3B:12:LEU:HG | 1.69 | 0.75 |
| 28:5SA:54:A:O2' | 28:5SA:55:A:N7 | 2.20 | 0.75 |
| 34:L9B:118:LYS:HG2 | 34:L9B:119:PRO:HD2 | 1.69 | 0.74 |
| 2:S2B:137:ARG:NH1 | 2:S2B:137:ARG:O | 2.20 | 0.74 |
| 2:S2B:224:GLN:HG2 | 2:S2B:229:VAL:HG22 | 1.69 | 0.74 |
| 3:S3B:91:LEU:O | 3:S3B:95:THR:OG1 | 2.04 | 0.74 |
| 28:5SB:104:A:N7 | 62:5SB:301:HOH:O | 2.20 | 0.74 |
| 3:S3B:135:LYS:O | 3:S3B:139:GLN:NE2 | 2.20 | 0.74 |
| 34:L9A:73:GLU:HG3 | 34:L9A:136:VAL:HG23 | 1.68 | 0.74 |
| 30:L3B:11:MET:HG2 | 30:L3B:24:THR:HG22 | 1.70 | 0.73 |
| 33:L6B:73:ALA:O | 33:L6B:77:LYS:N | 2.19 | 0.73 |
| 30:L3A:111:ARG:HG3 | 30:L3A:160:TYR:CD2 | 2.23 | 0.73 |
| 3:S3A:20:SER:HB3 | 3:S3A:40:ARG:HH22 | 1.52 | 0.73 |
| 33:L6B:23:ARG:HG3 | 33:L6B:25:LYS:HE3 | 1.70 | 0.73 |
| 33:L6A:7:LEU:HD22 | 33:L6A:69:ARG:HH21 | 1.51 | 0.73 |
| 9:S9A:83:ARG:HA | 9:S9A:86:VAL:HG12 | 1.70 | 0.72 |
| 2:S2B:55:PHE:CD1 | 2:S2B:221:LEU:HD22 | 2.23 | 0.72 |
| 8:S8A:129:VAL:HG23 | 8:S8A:130:GLY:H | 1.53 | 0.72 |
| 34:L9A:133:HIS:CB | 34:L9A:134:PRO:HD2 | 2.19 | 0.72 |
| 6:S6B:15:ASP:HB2 | 6:S6B:18:GLN:H | 1.52 | 0.72 |
| 30:L3A:119:ARG:HD3 | 30:L3A:160:TYR:HB2 | 1.70 | 0.72 |
| 2:S2B:16:HIS:HB3 | 2:S2B:210:SER:HB2 | 1.72 | 0.72 |
| 32:L5A:161:THR:HG22 | 32:L5A:163:ALA:H | 1.55 | 0.71 |
| 2:S2B:32:ILE:HD11 | 2:S2B:40:HIS:CD2 | 2.25 | 0.71 |
| 34:L9A:64:GLU:HB3 | 34:L9A:67:ARG:HH21 | 1.54 | 0.71 |
| 33:L6B:41:MET:HG2 | 33:L6B:55:PRO:HD3 | 1.71 | 0.71 |
| 5:S5B:102:ALA:HB1 | 5:S5B:106:PRO:HG2 | 1.72 | 0.71 |
| 33:L6A:124:GLU:HG2 | 33:L6A:126:PRO:HD3 | 1.72 | 0.71 |
| 28:5SB:17:A:H1' | 28:5SB:112:G:C5 | 2.25 | 0.71 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 29:L2B:182:LEU:H | 29:L2B:272:ALA:HB3 | 1.56 | 0.71 |
| 3:S3A:36:ASP:HA | 3:S3A:39:ILE:HD12 | 1.72 | 0.71 |
| 4:S4A:26:CYS:HA | 4:S4A:31:CYS:HB2 | 1.73 | 0.70 |
| 34:L9A:133:HIS:HB2 | 34:L9A:134:PRO:HD2 | 1.73 | 0.70 |
| 28:5SA:11:G:O2' | 62:5SA:305:HOH:O | 2.08 | 0.70 |
| 4:S4A:169:LYS:HE2 | 6:S6B:21:LEU:HD12 | 1.73 | 0.70 |
| 4:S4B:162:LEU:HD13 | 4:S4B:181:MET:HE2 | 1.72 | 0.70 |
| 33:L6B:33:LEU:HD21 | 33:L6B:136:ILE:HG22 | 1.74 | 0.70 |
| 34:L9A:85:GLU:OE2 | 34:L9A:86:THR:OG1 | 2.10 | 0.70 |
| 2:S2B:5:ILE:HG12 | 2:S2B:55:PHE:HD1 | 1.52 | 0.70 |
| 9:S9B:28:VAL:HG22 | 9:S9B:63:ILE:HB | 1.73 | 0.70 |
| 5:S5B:142:LEU:O | 5:S5B:143:ARG:NH1 | 2.25 | 0.70 |
| 7:S7A:91:VAL:HG23 | 7:S7A:96:GLN:HG2 | 1.73 | 0.70 |
| 29:L2A:96:HIS:HD2 | 29:L2A:102:LYS:HG2 | 1.57 | 0.70 |
| 29:L2B:5:LYS:H | 29:L2B:5:LYS:HD2 | 1.56 | 0.70 |
| 33:L6B:98:LEU:HD21 | 33:L6B:105:LEU:HB3 | 1.74 | 0.70 |
| 2:S2A:77:ALA:HB2 | 2:S2A:211:ILE:HD13 | 1.74 | 0.70 |
| 31:L4A:117:ARG:NH2 | 31:L4A:189:THR:O | 2.25 | 0.70 |
| 2:S2A:168:THR:CG2 | 2:S2A:169:LYS:H | 2.05 | 0.69 |
| 34:L9A:94:ALA:O | 34:L9A:111:PRO:HG3 | 1.92 | 0.69 |
| 9:S9B:10:ARG:HE | 9:S9B:105:ASP:HB3 | 1.57 | 0.69 |
| 6:S6A:27:GLN:HA | 6:S6A:30:LEU:HD12 | 1.74 | 0.69 |
| 30:L3B:132:HIS:NE2 | 62:L3B:401:HOH:O | 2.26 | 0.69 |
| 9:S9A:16:ARG:O | 9:S9A:63:ILE:HA | 1.93 | 0.69 |
| 29:L2A:142:VAL:HG23 | 29:L2A:193:VAL:HA | 1.72 | 0.69 |
| 33:L6B:121:ILE:HG23 | 33:L6B:133:VAL:HG11 | 1.72 | 0.69 |
| 29:L2B:130:ALA:HB2 | 29:L2B:192:THR:HG22 | 1.75 | 0.69 |
| 4:S4B:187:ARG:NH2 | 4:S4B:193:ASP:OD2 | 2.26 | 0.69 |
| 7:S7B:23:VAL:HG13 | 7:S7B:43:PHE:HE2 | 1.56 | 0.69 |
| 2:S2A:12:GLU:O | 2:S2A:16:HIS:HB2 | 1.92 | 0.69 |
| 9:S9A:61:ALA:HB1 | 9:S9A:63:ILE:HD13 | 1.73 | 0.69 |
| 7:S7B:113:GLU:HB2 | 7:S7B:119:ARG:HG3 | 1.74 | 0.69 |
| 32:L5B:47:LYS:HD2 | 32:L5B:81:LYS:HB2 | 1.73 | 0.69 |
| 30:L3A:47:VAL:HG11 | 30:L3A:86:PRO:HD2 | 1.75 | 0.69 |
| 33:L6B:98:LEU:O | 33:L6B:99:VAL:HG23 | 1.93 | 0.69 |
| 4:S4B:191:ARG:NH1 | 4:S4B:191:ARG:O | 2.24 | 0.69 |
| 34:L9B:54:GLN:HA | 34:L9B:57:ARG:HB2 | 1.74 | 0.69 |
| 29:L2A:166:GLN:HB2 | 29:L2A:174:ILE:HG22 | 1.75 | 0.68 |
| 5:S5B:34:VAL:HG11 | 5:S5B:63:ARG:HG2 | 1.75 | 0.68 |
| 28:5SB:82:U:H2' | 28:5SB:83:G:H21 | 1.58 | 0.68 |
| 8:S8B:100:ILE:O | 8:S8B:125:ARG:NH1 | 2.26 | 0.68 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 34:L9A:72:LEU:HD13 | 34:L9A:107:VAL:HG11 | 1.75 | 0.68 |
| 2:S2B:54:THR:HG23 | 2:S2B:199:TYR:HB3 | 1.76 | 0.68 |
| 3:S3B:152:ILE:HB | 3:S3B:199:LYS:HB2 | 1.76 | 0.68 |
| 34:L9A:94:ALA:HB1 | 34:L9A:111:PRO:HG2 | 1.76 | 0.68 |
| 4:S4A:25:ARG:HG3 | 4:S4A:30:LYS:HG3 | 1.75 | 0.67 |
| 29:L2A:136:ILE:O | 29:L2A:168:ARG:NH2 | 2.27 | 0.67 |
| 28:5SB:15:A:N1 | 28:5SB:71:G:O2' | 2.23 | 0.67 |
| 9:S9B:96:LEU:HD12 | 9:S9B:101:PHE:HB2 | 1.75 | 0.67 |
| 2:S2A:87:ARG:HH11 | 2:S2A:219:VAL:HB | 1.59 | 0.67 |
| 2:S2B:215:LEU:HA | 2:S2B:218:ALA:HB3 | 1.77 | 0.67 |
| 34:L9B:113:ARG:HD2 | 34:L9B:131:LYS:HD2 | 1.76 | 0.67 |
| 34:L9A:144:VAL:HG22 | 34:L9A:145:VAL:HG23 | 1.75 | 0.67 |
| 3:S3B:120:VAL:HG13 | 3:S3B:124:ILE:HD13 | 1.77 | 0.67 |
| 7:S7B:68:ASN:ND2 | 7:S7B:128:ALA:O | 2.27 | 0.67 |
| 5:S5A:48:ALA:HB2 | 5:S5A:57:LYS:HD3 | 1.77 | 0.67 |
| 2:S2B:78:GLN:O | 2:S2B:94:ASN:ND2 | 2.28 | 0.67 |
| 9:S9B:46:ALA:HA | 9:S9B:78:LYS:HE3 | 1.77 | 0.67 |
| 33:L6A:3:ARG:HG3 | 33:L6A:6:ARG:H | 1.60 | 0.67 |
| 31:L4B:197:ASP:HA | 31:L4B:200:GLU:HB2 | 1.77 | 0.67 |
| 3:S3A:84:ILE:HG13 | 3:S3A:101:LEU:HD22 | 1.76 | 0.67 |
| 3:S3A:188:LEU:HD11 | 3:S3A:195:VAL:HG13 | 1.76 | 0.67 |
| 7:S7A:106:GLN:O | 7:S7A:110:GLN:NE2 | 2.21 | 0.67 |
| 33:L6B:157:TYR:HA | 33:L6B:171:LEU:HG | 1.78 | 0.66 |
| 34:L9A:93:THR:HA | 34:L9A:119:PRO:HB3 | 1.75 | 0.66 |
| 7:S7B:16:LEU:HD11 | 9:S9B:42:ARG:HA | 1.78 | 0.66 |
| 29:L2A:71:ASP:OD1 | 29:L2A:103:ARG:NH2 | 2.27 | 0.66 |
| 7:S7A:38:LEU:O | 7:S7A:42:ILE:HG13 | 1.95 | 0.66 |
| 31:L4B:184:TYR:CE2 | 31:L4B:188:ARG:HD2 | 2.30 | 0.66 |
| 28:5SB:47:A:OP2 | 32:L5B:96:ARG:NH1 | 2.28 | 0.66 |
| 29:L2A:182:LEU:H | 29:L2A:272:ALA:HB3 | 1.60 | 0.66 |
| 30:L3B:54:GLN:HG2 | 30:L3B:59:VAL:HG23 | 1.77 | 0.66 |
| 34:L9A:110:ASP:OD1 | 34:L9A:110:ASP:N | 2.17 | 0.66 |
| 9:S9B:110:GLU:HG2 | 9:S9B:119:ALA:HB1 | 1.78 | 0.66 |
| 7:S7B:6:ARG:O | 7:S7B:7:ALA:O | 2.14 | 0.66 |
| 4:S4A:128:VAL:HB | 4:S4A:133:VAL:HG21 | 1.78 | 0.65 |
| 9:S9A:21:PRO:HA | 9:S9A:59:PHE:HA | 1.77 | 0.65 |
| 33:L6B:8:PRO:HG2 | 33:L6B:69:ARG:HG2 | 1.78 | 0.65 |
| 28:5SA:42:U:H3' | 28:5SA:43:U:C5' | 2.27 | 0.65 |
| 2:S2B:55:PHE:CE1 | 2:S2B:221:LEU:CD2 | 2.72 | 0.65 |
| 8:S8A:29:SER:HB3 | 8:S8A:32:LYS:HG3 | 1.79 | 0.65 |
| 29:L2A:72:LYS:NZ | 29:L2A:99:ASP:OD2 | 2.28 | 0.65 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 3:S3B:119:ARG:HH22 | 3:S3B:140:ARG:HG3 | 1.60 | 0.65 |
| 31:L4B:40:GLN:NE2 | 31:L4B:182:ASN:HB2 | 2.12 | 0.65 |
| 31:L4A:101:LEU:HD12 | 31:L4A:102:PRO:HD2 | 1.77 | 0.65 |
| 9:S9B:17:VAL:HG21 | 9:S9B:80:GLY:HA3 | 1.79 | 0.65 |
| 5:S5A:67:VAL:HG21 | 5:S5A:140:ARG:HA | 1.79 | 0.65 |
| 7:S7B:44:TYR:HA | 7:S7B:47:CYS:HB3 | 1.78 | 0.65 |
| 9:S9B:28:VAL:HA | 9:S9B:63:ILE:O | 1.97 | 0.65 |
| 29:L2B:228:PRO:O | 62:L2B:402:HOH:O | 2.14 | 0.65 |
| 4:S4A:109:GLY:HA3 | 4:S4A:165:MET:SD | 2.37 | 0.65 |
| 3:S3B:136:GLN:O | 3:S3B:140:ARG:HG2 | 1.96 | 0.65 |
| 34:L9A:110:ASP:HB2 | 34:L9A:112:LYS:HG3 | 1.79 | 0.64 |
| 28:5SB:44:C:O3' | 32:L5B:67:LYS:HE2 | 1.97 | 0.64 |
| 32:L5A:66:GLN:OE1 | 32:L5A:98:ARG:NH1 | 2.30 | 0.64 |
| 8:S8B:29:SER:HB3 | 8:S8B:32:LYS:HG3 | 1.78 | 0.64 |
| 2:S2A:67:THR:HG21 | 2:S2A:155:LEU:HD11 | 1.78 | 0.64 |
| 6:S6A:62:TRP:CH2 | 6:S6A:64:GLN:HB2 | 2.33 | 0.64 |
| 34:L9B:110:ASP:H | 34:L9B:130:TYR:HH | 1.45 | 0.64 |
| 5:S5A:68:GLU:HG2 | 5:S5A:70:PRO:HD3 | 1.79 | 0.64 |
| 3:S3B:155:GLY:HA2 | 3:S3B:163:ALA:HB1 | 1.78 | 0.64 |
| 8:S8B:69:ARG:NH1 | 8:S8B:75:ARG:O | 2.30 | 0.64 |
| 2:S2A:5:ILE:HD12 | 2:S2A:221:LEU:HD23 | 1.80 | 0.64 |
| 28:5SA:17:A:H5' | 28:5SA:18:G:C8 | 2.32 | 0.64 |
| 33:L6A:130:ARG:HG2 | 33:L6A:130:ARG:HH11 | 1.61 | 0.64 |
| 31:L4B:40:GLN:HE22 | 31:L4B:182:ASN:HB2 | 1.63 | 0.64 |
| 31:L4A:134:GLY:HA2 | 31:L4A:166:ALA:HB2 | 1.78 | 0.64 |
| 5:S5B:31:LEU:HD11 | 5:S5B:43:LEU:HD11 | 1.80 | 0.64 |
| 33:L6B:6:ARG:C | 33:L6B:8:PRO:HD3 | 2.22 | 0.64 |
| 34:L9B:81:VAL:HG13 | 34:L9B:144:VAL:H | 1.63 | 0.64 |
| 28:5SB:16:U:O2' | 28:5SB:110:U:O2' | 2.13 | 0.64 |
| 4:S4A:90:GLY:HA3 | 4:S4A:204:ILE:HD11 | 1.79 | 0.64 |
| 8:S8A:42:GLU:HG3 | 8:S8A:109:ILE:HD12 | 1.79 | 0.64 |
| 9:S9A:46:ALA:HB2 | 9:S9A:74:ILE:HG23 | 1.79 | 0.64 |
| 33:L6A:45:VAL:HA | 33:L6A:50:VAL:HG12 | 1.79 | 0.64 |
| 8:S8B:42:GLU:HG3 | 8:S8B:109:ILE:HD12 | 1.81 | 0.63 |
| 34:L9B:68:LEU:HA | 34:L9B:71:ILE:HG22 | 1.78 | 0.63 |
| 32:L5A:47:LYS:HD3 | 32:L5A:81:LYS:HB2 | 1.79 | 0.63 |
| 5:S5B:76:ILE:HD13 | 5:S5B:118:ILE:HD13 | 1.80 | 0.63 |
| 9:S9B:24:GLY:HA2 | 9:S9B:59:PHE:O | 1.98 | 0.63 |
| 33:L6B:20:ALA:HB1 | 33:L6B:23:ARG:NH1 | 2.14 | 0.63 |
| 33:L6B:77:LYS:HE2 | 33:L6B:138:LYS:HB2 | 1.81 | 0.63 |
| 9:S9A:7:THR:O | 9:S9A:83:ARG:HD2 | 1.98 | 0.63 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 9:S9A:91:ASP:OD1 | 9:S9A:91:ASP:N | 2.31 | 0.63 |
| 28:5SA:17:A:H1' | 28:5SA:112:G:C8 | 2.33 | 0.63 |
| 30:L3A:13:ARG:HD2 | 30:L3A:20:ALA:HB1 | 1.80 | 0.63 |
| 34:L9A:69:LYS:HG3 | 34:L9A:136:VAL:HB | 1.80 | 0.63 |
| 2:S2A:92:TYR:CZ | 2:S2A:151:GLY:HA3 | 2.35 | 0.62 |
| 34:L9A:29:TYR:O | 34:L9A:33:ARG:HG2 | 1.98 | 0.62 |
| 4:S4A:13:ARG:NH1 | 4:S4A:38:TYR:O | 2.31 | 0.62 |
| 31:L4A:133:ASN:HA | 31:L4A:162:LEU:HD22 | 1.81 | 0.62 |
| 2:S2B:223:ILE:HA | 2:S2B:226:ARG:HG2 | 1.80 | 0.62 |
| 4:S4B:100:ARG:HE | 4:S4B:137:SER:HA | 1.63 | 0.62 |
| 7:S7B:54:THR:O | 7:S7B:56:GLN:N | 2.32 | 0.62 |
| 30:L3A:117:MET:O | 30:L3A:118:LYS:HB3 | 1.98 | 0.62 |
| 3:S3B:95:THR:HG22 | 3:S3B:97:LYS:HG2 | 1.81 | 0.62 |
| 8:S8B:17:THR:O | 8:S8B:78:GLN:NE2 | 2.31 | 0.62 |
| 30:L3B:170:LEU:HD23 | 30:L3B:184:VAL:HB | 1.82 | 0.62 |
| 31:L4A:9:ILE:HD11 | 31:L4A:125:LEU:HG | 1.82 | 0.62 |
| 34:L9A:115:ALA:C | 34:L9A:117:GLU:N | 2.54 | 0.62 |
| 29:L2B:8:PRO:HB3 | 29:L2B:14:ARG:HB3 | 1.80 | 0.62 |
| 3:S3A:73:PRO:HA | 3:S3A:76:VAL:HG22 | 1.82 | 0.62 |
| 31:L4B:124:LEU:HB3 | 31:L4B:193:VAL:HG22 | 1.81 | 0.62 |
| 33:L6B:138:LYS:HA | 33:L6B:141:VAL:HG12 | 1.81 | 0.62 |
| 6:S6A:82:ARG:HB2 | 6:S6A:85:VAL:HG23 | 1.82 | 0.62 |
| 8:S8A:10:LEU:HD22 | 8:S8A:83:ILE:HD11 | 1.81 | 0.62 |
| 3:S3A:95:THR:HG23 | 3:S3A:97:LYS:HE2 | 1.81 | 0.62 |
| 2:S2B:178:ARG:NH2 | 8:S8B:68:ARG:HH22 | 1.98 | 0.62 |
| 31:L4B:24:LEU:HD23 | 31:L4B:115:ALA:HA | 1.82 | 0.62 |
| 5:S5A:8:GLU:HG2 | 5:S5A:34:VAL:HG22 | 1.82 | 0.62 |
| 30:L3A:11:MET:HG2 | 30:L3A:24:THR:HB | 1.80 | 0.61 |
| 5:S5B:74:GLY:O | 5:S5B:115:VAL:HG23 | 1.99 | 0.61 |
| 29:L2A:96:HIS:CD2 | 29:L2A:102:LYS:HG2 | 2.35 | 0.61 |
| 9:S9B:19:LEU:HA | 9:S9B:61:ALA:HA | 1.81 | 0.61 |
| 29:L2B:70:TRP:CH2 | 29:L2B:150:LYS:HA | 2.36 | 0.61 |
| 33:L6A:87:LEU:HB2 | 33:L6A:131:VAL:HG12 | 1.82 | 0.61 |
| 9:S9B:44:VAL:O | 9:S9B:51:ARG:NH2 | 2.29 | 0.61 |
| 2:S2B:56:ARG:O | 2:S2B:60:ASP:HB2 | 2.01 | 0.61 |
| 9:S9B:71:SER:HA | 9:S9B:74:ILE:HD12 | 1.82 | 0.61 |
| 2:S2B:153:ARG:O | 2:S2B:155:LEU:N | 2.34 | 0.61 |
| 34:L9B:76:THR:HA | 34:L9B:139:GLN:HB2 | 1.81 | 0.61 |
| 4:S4A:33:MET:HE2 | 4:S4A:33:MET:HA | 1.81 | 0.61 |
| 33:L6B:25:LYS:N | 33:L6B:25:LYS:HD2 | 2.15 | 0.61 |
| 34:L9B:79:ILE:HG12 | 34:L9B:104:GLN:OE1 | 2.01 | 0.61 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 3:S3A:7:PRO:O | 3:S3A:11:ARG:HG2 | 2.00 | 0.61 |
| 31:L4B:117:ARG:NH1 | 31:L4B:120:GLU:OE2 | 2.34 | 0.61 |
| 32:L5B:114:ILE:HD13 | 32:L5B:140:ILE:HG21 | 1.83 | 0.61 |
| 4:S4A:13:ARG:HB2 | 4:S4A:40:PRO:HD3 | 1.83 | 0.61 |
| 3:S3B:36:ASP:HA | 3:S3B:39:ILE:HD12 | 1.83 | 0.61 |
| 8:S8A:83:ILE:HG13 | 8:S8A:137:VAL:HG22 | 1.83 | 0.60 |
| 32:L5B:56:ALA:HB2 | 32:L5B:153:ARG:HE | 1.66 | 0.60 |
| 33:L6B:121:ILE:HG23 | 33:L6B:133:VAL:CG1 | 2.30 | 0.60 |
| 4:S4A:149:ALA:O | 4:S4A:153:ARG:HG2 | 2.01 | 0.60 |
| 32:L5A:37:VAL:HG22 | 32:L5A:159:VAL:HG12 | 1.82 | 0.60 |
| 3:S3A:11:ARG:O | 3:S3A:13:GLY:N | 2.34 | 0.60 |
| 29:L2A:10:THR:HG23 | 29:L2A:13:ARG:HB2 | 1.83 | 0.60 |
| 4:S4A:8:VAL:HG21 | 4:S4A:115:ARG:NH2 | 2.16 | 0.60 |
| 7:S7A:113:GLU:HB2 | 7:S7A:119:ARG:HG2 | 1.83 | 0.60 |
| 8:S8B:100:ILE:HD12 | 8:S8B:125:ARG:HG3 | 1.83 | 0.60 |
| 8:S8A:21:LYS:O | 8:S8A:65:TYR:OH | 2.14 | 0.60 |
| 8:S8A:49:GLU:HG2 | 8:S8A:62:TYR:HE2 | 1.64 | 0.60 |
| 2:S2B:8:LYS:HE3 | 2:S2B:11:LEU:HD22 | 1.84 | 0.60 |
| 2:S2B:223:ILE:O | 2:S2B:227:GLY:N | 2.33 | 0.60 |
| 5:S5B:51:VAL:O | 5:S5B:55:VAL:HG23 | 2.00 | 0.60 |
| 2:S2B:121:LEU:HA | 2:S2B:124:SER:HB3 | 1.83 | 0.60 |
| 6:S6B:20:ALA:HA | 6:S6B:23:LYS:HB2 | 1.84 | 0.60 |
| 7:S7B:27:ILE:HA | 7:S7B:30:ILE:HD12 | 1.82 | 0.60 |
| 9:S9B:18:PHE:O | 9:S9B:62:TYR:N | 2.30 | 0.60 |
| 9:S9A:70:LYS:O | 9:S9A:74:ILE:HG13 | 2.02 | 0.60 |
| 32:L5A:27:ASN:HB3 | 32:L5A:30:GLU:HG3 | 1.82 | 0.60 |
| 31:L4B:23:ASP:OD1 | 31:L4B:203:GLN:NE2 | 2.34 | 0.60 |
| 4:S4A:9:CYS:HB3 | 4:S4A:32:ALA:HB3 | 1.84 | 0.60 |
| 5:S5B:105:VAL:HG21 | 5:S5B:128:PRO:HB3 | 1.82 | 0.60 |
| 5:S5A:102:ALA:HB1 | 5:S5A:106:PRO:HG2 | 1.84 | 0.59 |
| 28:5SA:82:U:H2' | 28:5SA:83:G:N2 | 2.15 | 0.59 |
| 2:S2B:137:ARG:C | 2:S2B:137:ARG:HH11 | 2.10 | 0.59 |
| 30:L3B:34:VAL:HG21 | 30:L3B:78:LEU:HD11 | 1.83 | 0.59 |
| 32:L5B:6:ALA:HB3 | 32:L5B:104:GLU:OE2 | 2.01 | 0.59 |
| 33:L6B:70:THR:HG22 | 33:L6B:74:ASN:ND2 | 2.17 | 0.59 |
| 3:S3B:37:GLN:O | 3:S3B:41:GLY:N | 2.31 | 0.59 |
| 33:L6B:87:LEU:HB3 | 33:L6B:162:ILE:HG22 | 1.84 | 0.59 |
| 29:L2A:70:TRP:O | 29:L2A:73:VAL:HG23 | 2.01 | 0.59 |
| 34:L9A:21:VAL:HG21 | 34:L9A:25:TYR:HD2 | 1.67 | 0.59 |
| 31:L4B:149:ASP:N | 31:L4B:149:ASP:OD1 | 2.35 | 0.59 |
| 4:S4A:187:ARG:NH2 | 4:S4A:190:ASP:H | 1.99 | 0.59 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 28:5SA:43:U:C5 | 32:L5A:69:ALA:HB1 | 2.38 | 0.59 |
| 8:S8B:104:ARG:HB3 | 8:S8B:108:GLY:H | 1.66 | 0.59 |
| 9:S9B:19:LEU:HD21 | 9:S9B:84:ALA:HB1 | 1.84 | 0.59 |
| 30:L3B:87:GLU:H | 30:L3B:87:GLU:CD | 2.11 | 0.59 |
| 3:S3A:57:ILE:HG12 | 3:S3A:66:VAL:HG22 | 1.83 | 0.59 |
| 2:S2B:105:PHE:O | 2:S2B:109:SER:N | 2.35 | 0.59 |
| 2:S2B:224:GLN:HG2 | 2:S2B:229:VAL:CG2 | 2.33 | 0.59 |
| 5:S5A:90:VAL:O | 5:S5A:120:THR:HA | 2.02 | 0.59 |
| 9:S9A:8:GLY:HA3 | 9:S9A:76:ALA:O | 2.02 | 0.59 |
| 29:L2B:206:LEU:O | 29:L2B:211:ARG:HD3 | 2.03 | 0.59 |
| 29:L2B:142:VAL:HG23 | 29:L2B:193:VAL:HA | 1.85 | 0.59 |
| 4:S4A:98:GLU:OE2 | 4:S4A:103:ASN:ND2 | 2.30 | 0.58 |
| 2:S2B:178:ARG:NH2 | 8:S8B:74:PRO:HG3 | 2.17 | 0.58 |
| 28:5SB:2:A:C8 | 28:5SB:3:U:C5 | 2.91 | 0.58 |
| 30:L3B:24:THR:HG23 | 30:L3B:186:GLY:O | 2.03 | 0.58 |
| 3:S3A:122:GLU:O | 3:S3A:126:ARG:HG2 | 2.04 | 0.58 |
| 8:S8B:103:VAL:HG21 | 8:S8B:110:ALA:HB2 | 1.85 | 0.58 |
| 34:L9A:92:VAL:HG13 | 34:L9A:120:ILE:HG23 | 1.85 | 0.58 |
| 33:L6B:87:LEU:HA | 33:L6B:163:TYR:O | 2.02 | 0.58 |
| 3:S3A:150:LYS:HE2 | 3:S3A:152:ILE:HD11 | 1.84 | 0.58 |
| 32:L5A:97:ASP:H | 32:L5A:100:TRP:HD1 | 1.51 | 0.58 |
| 4:S4B:70:ILE:CG1 | 4:S4B:74:GLN:HG3 | 2.33 | 0.58 |
| 29:L2A:70:TRP:CH2 | 29:L2A:150:LYS:HA | 2.38 | 0.58 |
| 32:L5B:86:MET:HA | 32:L5B:86:MET:HE3 | 1.85 | 0.58 |
| 32:L5B:151:ALA:O | 32:L5B:153:ARG:NH1 | 2.36 | 0.58 |
| 33:L6A:172:LYS:O | 33:L6A:174:GLY:N | 2.36 | 0.58 |
| 34:L9A:40:THR:HG22 | 34:L9A:42:SER:H | 1.67 | 0.58 |
| 32:L5B:66:GLN:OE1 | 32:L5B:98:ARG:NH1 | 2.35 | 0.58 |
| 3:S3A:8:ILE:HG23 | 3:S3A:16:ARG:HG2 | 1.86 | 0.58 |
| 8:S8A:9:MET:HG3 | 8:S8A:26:VAL:HG11 | 1.84 | 0.58 |
| 34:L9A:79:ILE:HG22 | 34:L9A:141:LYS:O | 2.03 | 0.58 |
| 32:L5B:37:VAL:HG23 | 32:L5B:99:MET:HE3 | 1.85 | 0.58 |
| 34:L9B:78:THR:HG21 | 34:L9B:140:LEU:HD13 | 1.85 | 0.58 |
| 2:S2A:79:ASP:O | 2:S2A:82:ARG:HB3 | 2.04 | 0.58 |
| 34:L9A:79:ILE:HD12 | 34:L9A:80:PRO:HD2 | 1.85 | 0.58 |
| 2:S2B:167:PRO:O | 2:S2B:171:ALA:HB2 | 2.03 | 0.58 |
| 8:S8A:13:ILE:O | 8:S8A:17:THR:HG23 | 2.04 | 0.58 |
| 28:5SA:16:U:H4' | 28:5SA:17:A:OP2 | 2.04 | 0.58 |
| 33:L6B:33:LEU:HB2 | 33:L6B:75:ALA:HB1 | 1.85 | 0.57 |
| 4:S4B:70:ILE:HG13 | 4:S4B:74:GLN:HG3 | 1.86 | 0.57 |
| 28:5SB:16:U:HO2' | 28:5SB:17:A:P | 2.27 | 0.57 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 32:L5B:64:THR:OG1 | 32:L5B:94:LEU:HD13 | 2.05 | 0.57 |
| 4:S4A:103:ASN:OD1 | 4:S4A:114:ARG:NH2 | 2.33 | 0.57 |
| 9:S9A:77:ILE:O | 9:S9A:81:ILE:HG12 | 2.04 | 0.57 |
| 33:L6A:15:VAL:HG12 | 33:L6A:29:PRO:HD2 | 1.85 | 0.57 |
| 32:L5A:49:ASP:OD1 | 32:L5A:51:ARG:HG3 | 2.04 | 0.57 |
| 8:S8A:1:MET:N | 8:S8A:1:MET:HE3 | 2.19 | 0.57 |
| 9:S9A:25:LYS:HB2 | 9:S9A:60:ASP:OD2 | 2.04 | 0.57 |
| 31:L4A:63:LYS:HE3 | 31:L4A:67:GLN:HB2 | 1.86 | 0.57 |
| 31:L4A:107:LYS:HE3 | 31:L4A:206:ILE:HD12 | 1.86 | 0.57 |
| 3:S3B:44:GLU:HA | 3:S3B:52:LEU:HD11 | 1.86 | 0.57 |
| 31:L4B:185:ASP:HA | 31:L4B:188:ARG:HD3 | 1.86 | 0.57 |
| 32:L5B:106:LEU:HD12 | 32:L5B:110:ALA:HB3 | 1.87 | 0.57 |
| 6:S6A:30:LEU:HD11 | 6:S6A:63:TYR:HE2 | 1.70 | 0.57 |
| 28:5SB:17:A:H3' | 28:5SB:18:G:H5' | 1.86 | 0.57 |
| 30:L3B:176:ILE:HD12 | 30:L3B:181:LEU:HD23 | 1.86 | 0.57 |
| 5:S5A:33:VAL:HG11 | 5:S5A:109:ILE:HA | 1.87 | 0.57 |
| 34:L9A:93:THR:O | 34:L9A:97:ILE:HG13 | 2.05 | 0.57 |
| 30:L3B:40:GLU:HG3 | 30:L3B:41:LYS:N | 2.18 | 0.57 |
| 2:S2A:31:TYR:HB3 | 2:S2A:42:ILE:HD11 | 1.87 | 0.57 |
| 8:S8A:124:ALA:O | 8:S8A:128:GLY:N | 2.38 | 0.57 |
| 2:S2B:7:VAL:HG22 | 2:S2B:8:LYS:H | 1.70 | 0.57 |
| 29:L2A:182:LEU:HB2 | 29:L2A:271:ILE:HG13 | 1.87 | 0.57 |
| 34:L9A:57:ARG:NH1 | 34:L9A:61:ARG:HD2 | 2.19 | 0.57 |
| 34:L9B:110:ASP:N | 34:L9B:130:TYR:OH | 2.29 | 0.57 |
| 29:L2B:35:LYS:HG3 | 29:L2B:36:PRO:HD2 | 1.87 | 0.56 |
| 2:S2A:168:THR:HG22 | 2:S2A:169:LYS:H | 1.70 | 0.56 |
| 9:S9A:8:GLY:HA2 | 9:S9A:79:LEU:HD12 | 1.87 | 0.56 |
| 6:S6B:8:ILE:HB | 6:S6B:61:LEU:HB2 | 1.87 | 0.56 |
| 8:S8B:112:LEU:HB3 | 8:S8B:133:LEU:HA | 1.87 | 0.56 |
| 31:L4B:31:HIS:NE2 | 31:L4B:35:GLU:OE2 | 2.36 | 0.56 |
| 3:S3A:8:ILE:HD12 | 3:S3A:16:ARG:HE | 1.71 | 0.56 |
| 4:S4A:13:ARG:HD3 | 4:S4A:32:ALA:HB1 | 1.87 | 0.56 |
| 4:S4A:61:LYS:HE3 | 4:S4A:65:ARG:HD3 | 1.86 | 0.56 |
| 8:S8A:81:HIS:HB2 | 8:S8A:138:TRP:CZ3 | 2.41 | 0.56 |
| 3:S3B:70:VAL:O | 3:S3B:106:VAL:N | 2.27 | 0.56 |
| 29:L2B:53:PHE:CE2 | 29:L2B:220:HIS:ND1 | 2.73 | 0.56 |
| 5:S5A:45:PHE:CE2 | 5:S5A:47:LYS:HD2 | 2.40 | 0.56 |
| 3:S3A:83:ARG:O | 3:S3A:86:VAL:HG22 | 2.05 | 0.56 |
| 4:S4A:153:ARG:NE | 4:S4A:181:MET:SD | 2.69 | 0.56 |
| 32:L5A:72:ARG:HD3 | 32:L5A:87:PRO:HA | 1.86 | 0.56 |
| 34:L9A:6:LEU:HB2 | 34:L9A:36:ALA:HA | 1.88 | 0.56 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 34:L9B:71:ILE:HG23 | 34:L9B:72:LEU:HG | 1.88 | 0.56 |
| 9:S9A:10:ARG:HG3 | 9:S9A:10:ARG:O | 2.05 | 0.56 |
| 6:S6A:6:VAL:HG22 | 6:S6A:90:VAL:HG22 | 1.86 | 0.56 |
| 6:S6A:16:GLN:HA | 6:S6A:19:LEU:HB3 | 1.87 | 0.56 |
| 28:5SA:50:A:H2' | 28:5SA:51:C:C6 | 2.41 | 0.56 |
| 31:L4A:129:PHE:O | 31:L4A:131:GLY:N | 2.34 | 0.56 |
| 33:L6B:78:GLY:HA3 | 33:L6B:136:ILE:O | 2.06 | 0.56 |
| 33:L6B:154:PRO:HA | 33:L6B:161:GLY:HA3 | 1.87 | 0.56 |
| 31:L4A:66:PRO:O | 31:L4A:67:GLN:HB3 | 2.05 | 0.56 |
| 31:L4A:185:ASP:OD1 | 31:L4A:188:ARG:NH1 | 2.38 | 0.56 |
| 34:L9A:88:ILE:HG12 | 34:L9A:122:GLU:N | 2.21 | 0.56 |
| 4:S4B:172:PRO:HB2 | 4:S4B:187:ARG:HH22 | 1.71 | 0.56 |
| 9:S9B:19:LEU:HD23 | 9:S9B:19:LEU:H | 1.69 | 0.56 |
| 7:S7A:49:ILE:O | 7:S7A:53:LYS:HB3 | 2.05 | 0.56 |
| 8:S8A:4:ASP:OD2 | 8:S8A:85:ARG:NH1 | 2.39 | 0.56 |
| 2:S2B:172:ILE:H | 2:S2B:172:ILE:HD12 | 1.70 | 0.56 |
| 5:S5B:101:ILE:HG13 | 5:S5B:119:LEU:HD23 | 1.88 | 0.56 |
| 6:S6B:17:SER:O | 6:S6B:21:LEU:HD23 | 2.06 | 0.56 |
| 28:5SA:42:U:H3' | 28:5SA:43:U:H5" | 1.88 | 0.56 |
| 30:L3A:24:THR:HG22 | 30:L3A:186:GLY:O | 2.06 | 0.56 |
| 33:L6A:115:VAL:HG11 | 33:L6A:148:ILE:HD11 | 1.87 | 0.56 |
| 31:L4A:127:GLU:C | 31:L4A:129:PHE:H | 2.14 | 0.55 |
| 3:S3B:91:LEU:HB3 | 3:S3B:99:VAL:HG11 | 1.88 | 0.55 |
| 30:L3B:1:MET:N | 30:L3B:200:GLU:HG2 | 2.21 | 0.55 |
| 32:L5B:49:ASP:HB3 | 32:L5B:52:ILE:HG22 | 1.88 | 0.55 |
| 7:S7A:65:ALA:O | 7:S7A:69:VAL:HG23 | 2.06 | 0.55 |
| 7:S7B:79:ARG:HG2 | 7:S7B:84:ASN:HB2 | 1.87 | 0.55 |
| 31:L4B:11:VAL:HG22 | 31:L4B:125:LEU:HB2 | 1.87 | 0.55 |
| 33:L6B:76:VAL:HA | 33:L6B:79:VAL:HG22 | 1.88 | 0.55 |
| 2:S2A:54:THR:HG21 | 2:S2A:201:ILE:HD11 | 1.88 | 0.55 |
| 7:S7A:111:ARG:NH1 | 7:S7A:113:GLU:OE2 | 2.38 | 0.55 |
| 3:S3B:28:GLN:OE1 | 3:S3B:28:GLN:N | 2.39 | 0.55 |
| 30:L3B:77:ILE:HG12 | 30:L3B:195:LEU:HD22 | 1.89 | 0.55 |
| 33:L6B:20:ALA:HB3 | 33:L6B:23:ARG:O | 2.07 | 0.55 |
| 3:S3A:78:GLY:C | 3:S3A:79:ARG:HD3 | 2.31 | 0.55 |
| 34:L9A:115:ALA:O | 34:L9A:117:GLU:N | 2.39 | 0.55 |
| 3:S3B:63:ASN:HB3 | 3:S3B:98:ASN:HB3 | 1.88 | 0.55 |
| 8:S8B:89:PRO:HA | 8:S8B:92:ARG:HH11 | 1.71 | 0.55 |
| 9:S9B:74:ILE:O | 9:S9B:78:LYS:NZ | 2.39 | 0.55 |
| 33:L6A:86:GLU:N | 33:L6A:86:GLU:OE2 | 2.39 | 0.55 |
| 31:L4A:123:LEU:HD12 | 31:L4A:124:LEU:H | 1.70 | 0.55 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 28:5SB:15:A:O2' | 28:5SB:17:A:O5' | 2.24 | 0.55 |
| 9:S9A:57:GLY:C | 9:S9A:59:PHE:H | 2.14 | 0.55 |
| 3:S3B:156:ARG:HD2 | 3:S3B:193:TYR:CD1 | 2.42 | 0.55 |
| 30:L3B:106:GLY:HA3 | 30:L3B:189:PRO:HB2 | 1.88 | 0.55 |
| 31:L4B:63:LYS:HZ1 | 31:L4B:67:GLN:HB2 | 1.71 | 0.55 |
| 31:L4A:28:ILE:HD13 | 31:L4A:30:PRO:HD3 | 1.89 | 0.55 |
| 34:L9A:2:LYS:HE3 | 34:L9A:20:ASP:HB3 | 1.89 | 0.55 |
| 29:L2B:12:SER:HB2 | 29:L2B:208:LYS:HB3 | 1.89 | 0.55 |
| 4:S4A:33:MET:HE1 | 4:S4A:37:PRO:HA | 1.89 | 0.55 |
| 8:S8A:121:ASP:OD1 | 8:S8A:121:ASP:N | 2.38 | 0.55 |
| 9:S9A:3:GLN:HB3 | 9:S9A:20:ARG:HG2 | 1.88 | 0.55 |
| 4:S4B:121:VAL:HG22 | 4:S4B:126:ILE:HG13 | 1.88 | 0.55 |
| 5:S5A:31:LEU:HD22 | 5:S5A:43:LEU:HD11 | 1.89 | 0.55 |
| 6:S6A:69:GLU:O | 6:S6A:72:VAL:HG12 | 2.06 | 0.55 |
| 34:L9A:40:THR:HB | 34:L9A:43:ASN:H | 1.71 | 0.55 |
| 34:L9A:130:TYR:O | 34:L9A:135:GLU:HG3 | 2.06 | 0.55 |
| 9:S9B:19:LEU:CB | 9:S9B:59:PHE:HE1 | 2.17 | 0.55 |
| 34:L9B:109:ILE:HB | 34:L9B:130:TYR:OH | 2.07 | 0.55 |
| 2:S2A:93:VAL:HG11 | 2:S2A:97:TRP:HA | 1.89 | 0.54 |
| 4:S4A:150:GLU:C | 4:S4A:152:SER:H | 2.13 | 0.54 |
| 31:L4A:8:GLN:OE1 | 31:L4A:8:GLN:N | 2.37 | 0.54 |
| 4:S4B:102:ASP:HB3 | 4:S4B:136:PRO:HB3 | 1.87 | 0.54 |
| 9:S9B:19:LEU:HB2 | 9:S9B:59:PHE:CE1 | 2.35 | 0.54 |
| 28:5SB:47:A:C4 | 28:5SB:48:A:C8 | 2.95 | 0.54 |
| 34:L9A:87:LYS:HA | 34:L9A:122:GLU:HA | 1.89 | 0.54 |
| 3:S3B:50:ALA:HB1 | 3:S3B:70:VAL:HG11 | 1.89 | 0.54 |
| 34:L9B:123:LEU:HA | 34:L9B:142:VAL:HG11 | 1.89 | 0.54 |
| 2:S2B:119:GLU:HA | 2:S2B:122:PHE:HB2 | 1.88 | 0.54 |
| 30:L3B:174:ASP:HB3 | 30:L3B:183:LEU:HD22 | 1.90 | 0.54 |
| 4:S4A:15:GLU:OE2 | 4:S4A:59:ARG:NE | 2.35 | 0.54 |
| 7:S7A:26:PHE:O | 7:S7A:30:ILE:HG13 | 2.06 | 0.54 |
| 9:S9A:3:GLN:OE1 | 9:S9A:20:ARG:NH1 | 2.40 | 0.54 |
| 31:L4A:11:VAL:HG22 | 31:L4A:125:LEU:HB2 | 1.89 | 0.54 |
| 33:L6A:88:LEU:HD11 | 33:L6A:130:ARG:HD3 | 1.90 | 0.54 |
| 3:S3B:50:ALA:HB2 | 3:S3B:76:VAL:CG1 | 2.30 | 0.54 |
| 34:L9B:52:ARG:HA | 34:L9B:55:ALA:HB3 | 1.89 | 0.54 |
| 8:S8A:97:VAL:HG23 | 8:S8A:100:ILE:HD12 | 1.87 | 0.54 |
| 3:S3B:58:GLU:HB3 | 3:S3B:65:ALA:HB3 | 1.88 | 0.54 |
| 4:S4B:100:ARG:O | 4:S4B:104:VAL:HG23 | 2.07 | 0.54 |
| 6:S6B:9:VAL:HB | 6:S6B:87:ARG:HB2 | 1.88 | 0.54 |
| 9:S9B:13:ALA:HB2 | 9:S9B:68:GLY:HA3 | 1.89 | 0.54 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 4:S4B:3:ARG:HD2 | 4:S4B:118:ARG:CZ | 2.38 | 0.54 |
| 5:S5B:48:ALA:HB2 | 5:S5B:57:LYS:HD3 | 1.90 | 0.54 |
| 31:L4B:129:PHE:O | 31:L4B:131:GLY:N | 2.37 | 0.54 |
| 2:S2A:10:LEU:O | 2:S2A:13:ALA:N | 2.39 | 0.54 |
| 2:S2A:178:ARG:HH22 | 8:S8A:68:ARG:HH22 | 1.56 | 0.54 |
| 31:L4B:101:LEU:O | 31:L4B:106:ARG:NH1 | 2.41 | 0.54 |
| 34:L9B:31:LEU:HD21 | 34:L9B:38:LEU:HG | 1.88 | 0.54 |
| 34:L9B:78:THR:HB | 34:L9B:80:PRO:HD3 | 1.89 | 0.54 |
| 4:S4A:187:ARG:NH2 | 4:S4A:189:PRO:HA | 2.23 | 0.54 |
| 7:S7A:126:ASP:HB3 | 7:S7A:131:LYS:HG3 | 1.89 | 0.54 |
| 31:L4A:123:LEU:HD13 | 31:L4A:192:LEU:HB3 | 1.90 | 0.54 |
| 34:L9A:6:LEU:H | 34:L9A:36:ALA:HA | 1.73 | 0.54 |
| 4:S4B:152:SER:HA | 4:S4B:155:LEU:HD23 | 1.90 | 0.54 |
| 6:S6B:3:ARG:HG3 | 6:S6B:93:SER:HB3 | 1.90 | 0.54 |
| 9:S9B:3:GLN:HB3 | 9:S9B:20:ARG:HD2 | 1.90 | 0.54 |
| 32:L5B:32:PRO:HB2 | 32:L5B:172:LEU:HD22 | 1.89 | 0.54 |
| 32:L5B:61:ALA:HA | 32:L5B:66:GLN:O | 2.07 | 0.54 |
| 33:L6B:122:THR:HG22 | 33:L6B:123:PHE:H | 1.72 | 0.54 |
| 2:S2A:75:LYS:HA | 2:S2A:78:GLN:HB2 | 1.90 | 0.54 |
| 8:S8A:25:ASP:HA | 8:S8A:59:LEU:O | 2.08 | 0.54 |
| 5:S5A:142:LEU:O | 5:S5A:143:ARG:NH1 | 2.35 | 0.54 |
| 34:L9A:98:ALA:HB2 | 34:L9A:111:PRO:HD3 | 1.90 | 0.54 |
| 3:S3B:6:HIS:HD2 | 3:S3B:8:ILE:H | 1.54 | 0.54 |
| 4:S4B:15:GLU:OE1 | 4:S4B:66:ARG:NH1 | 2.39 | 0.54 |
| 2:S2A:219:VAL:O | 2:S2A:223:ILE:HG13 | 2.07 | 0.53 |
| 28:5SB:91:G:N2 | 28:5SB:92:A:N1 | 2.34 | 0.53 |
| 33:L6B:87:LEU:HD22 | 33:L6B:149:ARG:HG3 | 1.90 | 0.53 |
| 7:S7A:13:GLN:O | 7:S7A:24:THR:HG21 | 2.09 | 0.53 |
| 33:L6A:98:LEU:HD22 | 33:L6A:125:VAL:HB | 1.91 | 0.53 |
| 9:S9B:10:ARG:HH11 | 9:S9B:10:ARG:HG3 | 1.74 | 0.53 |
| 31:L4B:24:LEU:HD21 | 31:L4B:114:VAL:HG12 | 1.89 | 0.53 |
| 31:L4B:143:ALA:HB1 | 31:L4B:148:LEU:HB2 | 1.91 | 0.53 |
| 31:L4B:178:PRO:HB3 | 31:L4B:198:ALA:CB | 2.38 | 0.53 |
| 2:S2A:87:ARG:NH1 | 2:S2A:220:ASP:OD1 | 2.41 | 0.53 |
| 4:S4A:201:GLN:O | 4:S4A:205:GLU:HG3 | 2.07 | 0.53 |
| 34:L9A:4:ILE:HD11 | 34:L9A:44:LEU:HD12 | 1.90 | 0.53 |
| 5:S5B:28:PHE:CD2 | 5:S5B:51:VAL:HG22 | 2.43 | 0.53 |
| 28:5SB:19:C:H2' | 28:5SB:20:G:O4' | 2.07 | 0.53 |
| 31:L4B:66:PRO:O | 31:L4B:67:GLN:HB3 | 2.08 | 0.53 |
| 33:L6B:46:GLU:HB3 | 33:L6B:49:VAL:HG23 | 1.89 | 0.53 |
| 4:S4A:173:TRP:CD2 | 4:S4A:189:PRO:HB3 | 2.44 | 0.53 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 34:L9A:135:GLU:OE1 | 34:L9A:135:GLU:N | 2.40 | 0.53 |
| 7:S7B:50:ILE:HB | 7:S7B:58:PRO:HG3 | 1.90 | 0.53 |
| 8:S8B:120:THR:HG23 | 8:S8B:123:GLU:OE1 | 2.07 | 0.53 |
| 28:5SB:4:C:H2' | 28:5SB:5:C:H6 | 1.74 | 0.53 |
| 9:S9A:65:VAL:HG21 | 9:S9A:77:ILE:HD11 | 1.91 | 0.53 |
| 32:L5B:37:VAL:O | 32:L5B:94:LEU:HD23 | 2.09 | 0.53 |
| 30:L3A:176:ILE:HB | 30:L3A:181:LEU:HB2 | 1.90 | 0.53 |
| 2:S2B:59:GLU:HB2 | 2:S2B:221:LEU:HD21 | 1.90 | 0.53 |
| 3:S3B:74:GLY:O | 3:S3B:79:ARG:NH2 | 2.41 | 0.53 |
| 34:L9B:48:GLU:O | 34:L9B:52:ARG:HG3 | 2.08 | 0.53 |
| 32:L5A:11:TYR:HA | 32:L5A:15:VAL:HB | 1.90 | 0.53 |
| 2:S2B:55:PHE:HE1 | 2:S2B:221:LEU:HD22 | 1.62 | 0.53 |
| 2:S2A:37:ASN:C | 2:S2A:39:ILE:H | 2.17 | 0.53 |
| 3:S3A:150:LYS:HG3 | 3:S3A:169:ALA:HB2 | 1.90 | 0.53 |
| 29:L2B:132:PRO:HD3 | 29:L2B:190:TYR:CE2 | 2.44 | 0.53 |
| 2:S2A:84:GLU:HB3 | 2:S2A:219:VAL:HG21 | 1.91 | 0.53 |
| 32:L5A:55:LYS:HE3 | 32:L5A:59:GLU:OE2 | 2.09 | 0.53 |
| 4:S4B:80:GLU:OE2 | 4:S4B:84:LYS:NZ | 2.40 | 0.53 |
| 9:S9B:45:ALA:HA | 9:S9B:51:ARG:HH12 | 1.74 | 0.53 |
| 28:5SB:45:C:P | 32:L5B:67:LYS:HE2 | 2.49 | 0.53 |
| 30:L3B:28:ALA:HB3 | 30:L3B:93:VAL:HG12 | 1.90 | 0.53 |
| 2:S2A:5:ILE:CD1 | 2:S2A:221:LEU:HD23 | 2.39 | 0.52 |
| 7:S7A:23:VAL:HG13 | 7:S7A:43:PHE:CE2 | 2.43 | 0.52 |
| 29:L2A:60:ARG:HD3 | 29:L2A:86:PRO:CB | 2.33 | 0.52 |
| 30:L3B:21:VAL:HG23 | 30:L3B:185:LYS:HD3 | 1.91 | 0.52 |
| 4:S4A:150:GLU:OE2 | 4:S4A:153:ARG:NH1 | 2.42 | 0.52 |
| 30:L3A:50:GLY:HA3 | 30:L3A:75:VAL:HG21 | 1.91 | 0.52 |
| 28:5SB:4:C:H2' | 28:5SB:5:C:C6 | 2.44 | 0.52 |
| 29:L2B:181:GLU:HA | 29:L2B:272:ALA:HB3 | 1.91 | 0.52 |
| 2:S2A:223:ILE:O | 2:S2A:227:GLY:N | 2.38 | 0.52 |
| 3:S3A:39:ILE:O | 3:S3A:43:LEU:HG | 2.08 | 0.52 |
| 6:S6A:62:TRP:C | 6:S6A:63:TYR:HD1 | 2.17 | 0.52 |
| 4:S4B:106:TYR:HE1 | 4:S4B:112:VAL:O | 1.92 | 0.52 |
| 28:5SB:4:C:C2 | 28:5SB:5:C:C5 | 2.97 | 0.52 |
| 3:S3A:20:SER:HB3 | 3:S3A:40:ARG:NH2 | 2.22 | 0.52 |
| 8:S8A:1:MET:HE3 | 8:S8A:1:MET:H3 | 1.74 | 0.52 |
| 28:5SA:17:A:H5' | 28:5SA:18:G:H8 | 1.73 | 0.52 |
| 29:L2A:17:THR:HB | 29:L2A:205:VAL:H | 1.73 | 0.52 |
| 33:L6A:26:VAL:HG21 | 33:L6A:75:ALA:HB1 | 1.90 | 0.52 |
| 33:L6A:113:VAL:HG11 | 33:L6A:151:ILE:HD13 | 1.90 | 0.52 |
| 5:S5B:33:VAL:HG11 | 5:S5B:109:ILE:HA | 1.91 | 0.52 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 28:5SA:42:U:H1' | 28:5SA:47:A:H61 | 1.74 | 0.52 |
| 32:L5A:146:TYR:O | 32:L5A:149:VAL:HG22 | 2.10 | 0.52 |
| 2:S2B:21:ARG:HA | 2:S2B:39:ILE:HA | 1.91 | 0.52 |
| 5:S5A:18:ARG:CZ | 5:S5A:27:ARG:HH21 | 2.22 | 0.52 |
| 8:S8A:6:ILE:HB | 8:S8A:85:ARG:NH1 | 2.25 | 0.52 |
| 32:L5A:43:LEU:HD21 | 32:L5A:153:ARG:HD2 | 1.90 | 0.52 |
| 29:L2B:242:ARG:H | 29:L2B:242:ARG:HD2 | 1.75 | 0.52 |
| 5:S5A:31:LEU:HD11 | 5:S5A:129:ILE:HA | 1.90 | 0.52 |
| 34:L9A:11:ASN:O | 34:L9A:12:LEU:HB2 | 2.10 | 0.52 |
| 34:L9A:48:GLU:O | 34:L9A:52:ARG:HG2 | 2.10 | 0.52 |
| 29:L2B:145:VAL:HG13 | 29:L2B:191:ALA:HB2 | 1.92 | 0.52 |
| 30:L3B:179:GLU:HB3 | 30:L3B:181:LEU:HB2 | 1.92 | 0.52 |
| 9:S9A:10:ARG:HD3 | 9:S9A:75:ASP:HB2 | 1.91 | 0.52 |
| 9:S9A:97:LYS:HB2 | 9:S9A:102:LEU:HD12 | 1.91 | 0.52 |
| 3:S3B:44:GLU:HA | 3:S3B:52:LEU:HD21 | 1.91 | 0.52 |
| 3:S3B:156:ARG:NH1 | 3:S3B:193:TYR:O | 2.42 | 0.52 |
| 4:S4B:26:CYS:HA | 4:S4B:31:CYS:HB2 | 1.92 | 0.52 |
| 4:S4B:101:LEU:CB | 4:S4B:138:TYR:HB3 | 2.40 | 0.52 |
| 2:S2A:209:ARG:O | 2:S2A:213:LEU:HG | 2.10 | 0.52 |
| 3:S3B:14:ILE:O | 3:S3B:15:THR:HG22 | 2.09 | 0.52 |
| 3:S3A:87:LEU:O | 3:S3A:91:LEU:HG | 2.10 | 0.52 |
| 2:S2B:83:MET:HE1 | 2:S2B:233:SER:OG | 2.10 | 0.52 |
| 8:S8B:38:ILE:HD11 | 8:S8B:118:VAL:O | 2.09 | 0.52 |
| 28:5SB:16:U:O2' | 28:5SB:17:A:OP1 | 2.27 | 0.52 |
| 33:L6B:92:ILE:HG13 | 33:L6B:160:LYS:HD3 | 1.92 | 0.52 |
| 34:L9B:75:LEU:O | 34:L9B:77:LEU:N | 2.43 | 0.52 |
| 3:S3A:188:LEU:CD1 | 3:S3A:195:VAL:HG13 | 2.38 | 0.51 |
| 33:L6A:30:LYS:HD2 | 33:L6A:81:GLU:H | 1.75 | 0.51 |
| 34:L9A:86:THR:N | 34:L9A:123:LEU:HD12 | 2.21 | 0.51 |
| 3:S3B:47:LEU:HB3 | 3:S3B:52:LEU:HD13 | 1.92 | 0.51 |
| 8:S8B:13:ILE:O | 8:S8B:17:THR:HG23 | 2.10 | 0.51 |
| 29:L2B:238:GLY:O | 29:L2B:240:ALA:N | 2.43 | 0.51 |
| 6:S6A:15:ASP:OD2 | 6:S6A:17:SER:HB2 | 2.09 | 0.51 |
| 6:S6A:30:LEU:HD11 | 6:S6A:63:TYR:CE2 | 2.45 | 0.51 |
| 7:S7A:27:ILE:HA | 7:S7A:30:ILE:HD12 | 1.93 | 0.51 |
| 30:L3B:101:ARG:CZ | 30:L3B:171:GLU:HB2 | 2.41 | 0.51 |
| 31:L4B:135:LYS:HB3 | 31:L4B:138:GLU:HG3 | 1.93 | 0.51 |
| 33:L6B:69:ARG:NH1 | 33:L6B:73:ALA:HB2 | 2.25 | 0.51 |
| 31:L4A:65:TRP:HB2 | 31:L4A:66:PRO:CD | 2.38 | 0.51 |
| 31:L4A:107:LYS:HG2 | 31:L4A:206:ILE:HA | 1.92 | 0.51 |
| 2:S2A:47:THR:O | 2:S2A:51:LEU:HG | 2.11 | 0.51 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 2:S2A:55:PHE:HD1 | 2:S2A:221:LEU:HG | 1.75 | 0.51 |
| 4:S4A:190:ASP:HB2 | 4:S4A:193:ASP:OD1 | 2.11 | 0.51 |
| 28:5SA:89:G:C2 | 28:5SA:91:G:H5" | 2.45 | 0.51 |
| 8:S8B:124:ALA:O | 8:S8B:128:GLY:N | 2.44 | 0.51 |
| 9:S9B:125:TYR:HD1 | 9:S9B:126:SER:N | 2.09 | 0.51 |
| 33:L6B:74:ASN:HA | 33:L6B:77:LYS:HB3 | 1.92 | 0.51 |
| 33:L6B:89:ILE:HG22 | 33:L6B:94:TYR:CD2 | 2.46 | 0.51 |
| 32:L5A:4:ASP:OD2 | 32:L5A:9:ARG:NH1 | 2.43 | 0.51 |
| 32:L5A:55:LYS:O | 32:L5A:58:GLN:HG3 | 2.10 | 0.51 |
| 33:L6A:18:GLU:HB2 | 33:L6A:25:LYS:HB2 | 1.93 | 0.51 |
| 33:L6A:169:VAL:HG22 | 33:L6A:171:LEU:HD11 | 1.92 | 0.51 |
| 29:L2B:79:VAL:HG12 | 29:L2B:113:VAL:HA | 1.92 | 0.51 |
| 30:L3B:9:VAL:HG22 | 30:L3B:25:VAL:O | 2.10 | 0.51 |
| 34:L9B:118:LYS:HG2 | 34:L9B:119:PRO:CD | 2.39 | 0.51 |
| 5:S5A:18:ARG:NH2 | 5:S5A:27:ARG:HE | 2.07 | 0.51 |
| 2:S2B:56:ARG:NH1 | 2:S2B:56:ARG:HB3 | 2.26 | 0.51 |
| 4:S4B:81:GLU:CD | 4:S4B:139:ARG:HH22 | 2.19 | 0.51 |
| 3:S3A:134:ILE:HG22 | 3:S3A:168:ALA:HB3 | 1.92 | 0.51 |
| 4:S4A:12:CYS:HB3 | 4:S4A:33:MET:CG | 2.41 | 0.51 |
| 31:L4A:178:PRO:HG2 | 31:L4A:179:GLU:OE2 | 2.10 | 0.51 |
| 3:S3B:138:VAL:HG11 | 3:S3B:170:GLN:HG3 | 1.92 | 0.51 |
| 30:L3B:119:ARG:CD | 30:L3B:160:TYR:HB2 | 2.32 | 0.51 |
| 2:S2A:71:VAL:HG23 | 2:S2A:164:VAL:HA | 1.93 | 0.51 |
| 33:L6A:131:VAL:HG22 | 33:L6A:132:ARG:H | 1.76 | 0.51 |
| 3:S3B:36:ASP:OD1 | 3:S3B:57:ILE:HD13 | 2.11 | 0.51 |
| 9:S9B:24:GLY:N | 9:S9B:60:ASP:OD1 | 2.37 | 0.51 |
| 30:L3B:5:LEU:HD22 | 30:L3B:197:ILE:HG12 | 1.93 | 0.51 |
| 4:S4A:98:GLU:OE1 | 4:S4A:194:LEU:HD11 | 2.12 | 0.51 |
| 31:L4A:110:LEU:HG | 31:L4A:202:PHE:HE1 | 1.76 | 0.51 |
| 3:S3A:108:ASN:OD1 | 3:S3A:110:ASN:HB2 | 2.11 | 0.50 |
| 3:S3A:123:GLN:O | 3:S3A:128:PHE:HB2 | 2.11 | 0.50 |
| 3:S3A:136:GLN:HG2 | 3:S3A:140:ARG:NH2 | 2.26 | 0.50 |
| 4:S4A:8:VAL:HG21 | 4:S4A:115:ARG:CZ | 2.40 | 0.50 |
| 2:S2B:187:LEU:HD11 | 2:S2B:204:ASN:N | 2.26 | 0.50 |
| 29:L2B:17:THR:HG22 | 29:L2B:205:VAL:H | 1.76 | 0.50 |
| 31:L4A:167:ALA:HB1 | 31:L4A:173:VAL:HG11 | 1.94 | 0.50 |
| 31:L4A:181:LEU:HD22 | 31:L4A:186:ILE:HD11 | 1.93 | 0.50 |
| 33:L6A:9:ILE:HG22 | 33:L6A:69:ARG:NE | 2.26 | 0.50 |
| 31:L4B:75:HIS:HD2 | 31:L4B:82:ILE:HD11 | 1.75 | 0.50 |
| 32:L5B:6:ALA:O | 32:L5B:10:LYS:N | 2.25 | 0.50 |
| 4:S4A:12:CYS:HB3 | 4:S4A:33:MET:HG2 | 1.91 | 0.50 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 5:S5A:28:PHE:O | 5:S5A:47:LYS:HA | 2.12 | 0.50 |
| 6:S6A:46:ARG:HB3 | 6:S6A:60:PHE:CE1 | 2.47 | 0.50 |
| 7:S7A:20:ASP:OD2 | 7:S7A:23:VAL:N | 2.42 | 0.50 |
| 7:S7A:115:ARG:O | 7:S7A:119:ARG:HG3 | 2.11 | 0.50 |
| 8:S8A:82:HIS:HE1 | 8:S8A:136:GLU:HG3 | 1.76 | 0.50 |
| 33:L6A:4:ILE:O | 33:L6A:69:ARG:HG2 | 2.11 | 0.50 |
| 33:L6A:127:GLU:O | 33:L6A:129:THR:N | 2.44 | 0.50 |
| 34:L9A:4:ILE:HG12 | 34:L9A:18:VAL:HG22 | 1.93 | 0.50 |
| 8:S8B:11:THR:HG23 | 8:S8B:14:ARG:NH1 | 2.27 | 0.50 |
| 9:S9B:19:LEU:HD21 | 9:S9B:84:ALA:CB | 2.40 | 0.50 |
| 29:L2B:71:ASP:N | 29:L2B:71:ASP:OD1 | 2.43 | 0.50 |
| 31:L4B:123:LEU:HD12 | 31:L4B:124:LEU:H | 1.76 | 0.50 |
| 32:L5B:129:GLY:HA2 | 32:L5B:166:ASP:HA | 1.93 | 0.50 |
| 34:L9B:42:SER:HA | 34:L9B:45:LYS:HE3 | 1.92 | 0.50 |
| 4:S4A:33:MET:CE | 4:S4A:37:PRO:HA | 2.42 | 0.50 |
| 4:S4A:88:VAL:O | 4:S4A:89:THR:HB | 2.12 | 0.50 |
| 8:S8A:51:VAL:HG21 | 8:S8A:60:ARG:HG2 | 1.94 | 0.50 |
| 28:5SA:17:A:H1' | 28:5SA:112:G:N9 | 2.26 | 0.50 |
| 2:S2B:73:THR:HB | 2:S2B:96:ARG:H | 1.76 | 0.50 |
| 4:S4B:61:LYS:HD2 | 4:S4B:206:PHE:CE2 | 2.46 | 0.50 |
| 4:S4B:63:LYS:O | 4:S4B:67:ILE:HG13 | 2.12 | 0.50 |
| 4:S4B:176:LEU:HG | 4:S4B:178:VAL:HG22 | 1.93 | 0.50 |
| 8:S8B:122:ARG:HA | 8:S8B:125:ARG:HB2 | 1.92 | 0.50 |
| 30:L3B:11:MET:CG | 30:L3B:24:THR:HG22 | 2.39 | 0.50 |
| 31:L4B:197:ASP:N | 31:L4B:197:ASP:OD1 | 2.43 | 0.50 |
| 7:S7A:5:ARG:HB3 | 7:S7A:7:ALA:H | 1.77 | 0.50 |
| 7:S7A:91:VAL:CG2 | 7:S7A:96:GLN:HG2 | 2.41 | 0.50 |
| 28:5SA:98:U:H2' | 28:5SA:99:G:H8 | 1.77 | 0.50 |
| 33:L6A:24:VAL:HG22 | 33:L6A:35:VAL:HB | 1.92 | 0.50 |
| 34:L9A:110:ASP:HB2 | 34:L9A:112:LYS:H | 1.76 | 0.50 |
| 28:5SB:89:G:N2 | 28:5SB:92:A:OP2 | 2.44 | 0.50 |
| 29:L2A:10:THR:CG2 | 29:L2A:13:ARG:HB2 | 2.42 | 0.50 |
| 31:L4A:178:PRO:HB3 | 31:L4A:198:ALA:CB | 2.41 | 0.50 |
| 32:L5A:106:LEU:HD12 | 32:L5A:110:ALA:HB3 | 1.93 | 0.50 |
| 32:L5A:131:TYR:HB3 | 32:L5A:159:VAL:HG22 | 1.93 | 0.50 |
| 2:S2B:76:GLN:O | 2:S2B:208:ILE:HG12 | 2.12 | 0.50 |
| 4:S4B:3:ARG:O | 4:S4B:5:ILE:HD12 | 2.12 | 0.50 |
| 3:S3A:64:VAL:HG12 | 3:S3A:66:VAL:HG23 | 1.94 | 0.50 |
| 9:S9A:46:ALA:HA | 9:S9A:78:LYS:HB2 | 1.94 | 0.50 |
| 5:S5B:67:VAL:HG21 | 5:S5B:140:ARG:HA | 1.94 | 0.50 |
| 32:L5B:7:LEU:HA | 32:L5B:10:LYS:HB3 | 1.93 | 0.50 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 2:S2A:158:LEU:HD12 | 2:S2A:158:LEU:O | 2.12 | 0.50 |
| 4:S4A:166:LYS:HG3 | 4:S4A:178:VAL:HG11 | 1.94 | 0.50 |
| 6:S6A:16:GLN:H | 6:S6A:16:GLN:CD | 2.19 | 0.50 |
| 5:S5A:148:VAL:HG21 | 8:S8A:107:LEU:HD22 | 1.94 | 0.50 |
| 9:S9A:43:ALA:HA | 9:S9A:74:ILE:HD13 | 1.94 | 0.50 |
| 30:L3A:28:ALA:HB3 | 30:L3A:93:VAL:HG12 | 1.93 | 0.50 |
| 33:L6A:27:LYS:HA | 33:L6A:32:GLU:HB3 | 1.94 | 0.50 |
| 34:L9A:94:ALA:O | 34:L9A:111:PRO:CG | 2.60 | 0.50 |
| 8:S8B:116:LYS:HD2 | 8:S8B:129:VAL:HG11 | 1.94 | 0.50 |
| 32:L5B:60:LEU:HD12 | 32:L5B:63:ILE:HD11 | 1.93 | 0.50 |
| 34:L9B:1:MET:HB3 | 34:L9B:21:VAL:O | 2.12 | 0.50 |
| 2:S2A:17:PHE:HB3 | 2:S2A:44:LEU:HD21 | 1.93 | 0.49 |
| 2:S2A:80:ILE:HD11 | 2:S2A:208:ILE:HG23 | 1.93 | 0.49 |
| 5:S5A:96:PRO:HA | 5:S5A:117:ASP:OD2 | 2.12 | 0.49 |
| 34:L9B:75:LEU:HD21 | 34:L9B:105:HIS:CE1 | 2.47 | 0.49 |
| 29:L2A:130:ALA:HB2 | 29:L2A:192:THR:HG22 | 1.93 | 0.49 |
| 28:5SB:17:A:H3' | 28:5SB:18:G:C5' | 2.43 | 0.49 |
| 34:L9B:144:VAL:HG22 | 34:L9B:145:VAL:H | 1.77 | 0.49 |
| 4:S4A:19:LEU:HD12 | 4:S4A:67:ILE:CG1 | 2.41 | 0.49 |
| 9:S9A:17:VAL:HG11 | 9:S9A:81:ILE:HA | 1.94 | 0.49 |
| 28:5SA:31:A:H2' | 28:5SA:32:C:O4' | 2.13 | 0.49 |
| 32:L5A:18:GLU:CD | 32:L5A:21:ARG:HH21 | 2.21 | 0.49 |
| 33:L6A:74:ASN:HA | 33:L6A:77:LYS:HB3 | 1.93 | 0.49 |
| 30:L3B:6:GLY:N | 30:L3B:196:VAL:O | 2.42 | 0.49 |
| 31:L4B:6:VAL:HG21 | 31:L4B:119:ARG:HG3 | 1.94 | 0.49 |
| 32:L5B:80:PHE:O | 32:L5B:82:LEU:HB2 | 2.11 | 0.49 |
| 7:S7A:99:LEU:HD22 | 7:S7A:103:TRP:CZ2 | 2.47 | 0.49 |
| 31:L4A:184:TYR:O | 31:L4A:188:ARG:HB2 | 2.12 | 0.49 |
| 31:L4A:197:ASP:O | 31:L4A:198:ALA:HB3 | 2.11 | 0.49 |
| 34:L9A:88:ILE:O | 34:L9A:121:LYS:HE3 | 2.12 | 0.49 |
| 28:5SB:60:A:H5' | 28:5SB:61:A:OP2 | 2.12 | 0.49 |
| 29:L2B:17:THR:HG22 | 29:L2B:205:VAL:HB | 1.94 | 0.49 |
| 32:L5B:43:LEU:HD21 | 32:L5B:153:ARG:HD2 | 1.95 | 0.49 |
| 33:L6B:30:LYS:HB3 | 33:L6B:79:VAL:HA | 1.93 | 0.49 |
| 3:S3A:9:GLY:HA2 | 3:S3A:12:LEU:HG | 1.95 | 0.49 |
| 9:S9A:26:VAL:HB | 9:S9A:33:PHE:HB2 | 1.94 | 0.49 |
| 32:L5A:133:LEU:CD2 | 32:L5A:157:ILE:HB | 2.43 | 0.49 |
| 5:S5B:70:PRO:HB3 | 5:S5B:144:THR:CG2 | 2.42 | 0.49 |
| 8:S8B:20:TYR:HA | 8:S8B:65:TYR:CZ | 2.48 | 0.49 |
| 9:S9B:99:LEU:HB3 | 9:S9B:101:PHE:CE2 | 2.48 | 0.49 |
| 33:L6B:7:LEU:HB3 | 33:L6B:65:HIS:HE1 | 1.77 | 0.49 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 3:S3A:20:SER:HB2 | 3:S3A:57:ILE:HB | 1.93 | 0.49 |
| 30:L3A:73:GLU:OE1 | 30:L3A:73:GLU:N | 2.43 | 0.49 |
| 2:S2B:165:VAL:HA | 2:S2B:187:LEU:HB3 | 1.93 | 0.49 |
| 5:S5B:144:THR:N | 5:S5B:147:ASP:OD1 | 2.45 | 0.49 |
| 34:L9B:82:ARG:NH2 | 34:L9B:96:ASP:OD2 | 2.45 | 0.49 |
| 3:S3A:119:ARG:O | 3:S3A:123:GLN:HG3 | 2.13 | 0.49 |
| 5:S5A:147:ASP:HA | 5:S5A:150:ARG:NH1 | 2.28 | 0.49 |
| 8:S8A:97:VAL:HA | 8:S8A:100:ILE:HG13 | 1.94 | 0.49 |
| 33:L6A:15:VAL:HG12 | 33:L6A:29:PRO:CD | 2.41 | 0.49 |
| 33:L6A:20:ALA:HB3 | 33:L6A:23:ARG:HG3 | 1.94 | 0.49 |
| 3:S3B:179:ARG:HD2 | 3:S3B:207:VAL:H | 1.78 | 0.49 |
| 5:S5B:42:GLY:HA3 | 5:S5B:65:ASN:O | 2.13 | 0.49 |
| 9:S9B:10:ARG:NH2 | 9:S9B:105:ASP:OD2 | 2.41 | 0.49 |
| 31:L4B:116:ASP:OD1 | 31:L4B:119:ARG:NH2 | 2.39 | 0.49 |
| 33:L6B:124:GLU:O | 33:L6B:125:VAL:HB | 2.13 | 0.49 |
| 2:S2A:24:TRP:HB2 | 2:S2A:190:THR:HB | 1.95 | 0.49 |
| 3:S3A:182:ILE:HG13 | 3:S3A:203:PHE:HD1 | 1.76 | 0.49 |
| 4:S4A:83:SER:HA | 4:S4A:89:THR:HG23 | 1.95 | 0.49 |
| 7:S7A:73:MET:HG2 | 7:S7A:90:GLU:HA | 1.95 | 0.49 |
| 32:L5A:97:ASP:H | 32:L5A:100:TRP:CD1 | 2.31 | 0.49 |
| 2:S2B:91:PRO:HA | 2:S2B:154:LEU:HD12 | 1.94 | 0.49 |
| 8:S8B:17:THR:HG22 | 8:S8B:63:LEU:HD23 | 1.93 | 0.49 |
| 5:S5A:81:GLU:CG | 5:S5A:90:VAL:HG22 | 2.42 | 0.49 |
| 9:S9A:50:LEU:HD22 | 9:S9A:55:ALA:HB3 | 1.95 | 0.49 |
| 32:L5A:126:ASP:CG | 32:L5A:127:GLY:H | 2.21 | 0.49 |
| 32:L5A:133:LEU:HD21 | 32:L5A:157:ILE:HB | 1.95 | 0.49 |
| 9:S9B:10:ARG:NE | 9:S9B:105:ASP:HB3 | 2.26 | 0.49 |
| 6:S6B:33:TYR:OH | 6:S6B:78:GLU:HG3 | 2.12 | 0.49 |
| 32:L5B:135:LEU:HD11 | 32:L5B:155:MET:HG2 | 1.94 | 0.49 |
| 33:L6B:60:ARG:O | 33:L6B:64:LEU:HG | 2.13 | 0.49 |
| 9:S9A:29:ASN:OD1 | 9:S9A:64:THR:HA | 2.12 | 0.48 |
| 9:S9A:42:ARG:HH12 | 9:S9A:75:ASP:CG | 2.20 | 0.48 |
| 34:L9A:1:MET:HE3 | 34:L9A:23:PRO:HA | 1.94 | 0.48 |
| 30:L3B:120:TRP:CG | 30:L3B:155:LYS:HB3 | 2.48 | 0.48 |
| 32:L5B:102:PHE:HE1 | 32:L5B:141:PHE:HE1 | 1.59 | 0.48 |
| 34:L9B:80:PRO:O | 34:L9B:143:SER:HB2 | 2.12 | 0.48 |
| 3:S3A:70:VAL:HG12 | 3:S3A:72:LYS:H | 1.78 | 0.48 |
| 31:L4A:125:LEU:HD11 | 31:L4A:199:TRP:CD2 | 2.47 | 0.48 |
| 33:L6A:157:TYR:CE1 | 33:L6A:172:LYS:HB2 | 2.47 | 0.48 |
| 5:S5B:72:GLN:O | 5:S5B:75:THR:HG22 | 2.13 | 0.48 |
| 34:L9B:89:TYR:N | 34:L9B:89:TYR:CD1 | 2.81 | 0.48 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 34:L9B:143:SER:OG | 34:L9B:144:VAL:N | 2.46 | 0.48 |
| 4:S4A:65:ARG:HG2 | 4:S4A:75:PHE:CE2 | 2.49 | 0.48 |
| 6:S6A:53:ALA:O | 6:S6A:54:LYS:HG2 | 2.12 | 0.48 |
| 32:L5A:16:ARG:HB3 | 32:L5A:17:PRO:HD3 | 1.96 | 0.48 |
| 2:S2B:200:ILE:O | 2:S2B:201:ILE:HD13 | 2.12 | 0.48 |
| 9:S9B:49:PRO:O | 9:S9B:53:VAL:HG22 | 2.13 | 0.48 |
| 33:L6B:101:ARG:O | 33:L6B:101:ARG:HD3 | 2.12 | 0.48 |
| 5:S5A:52:PRO:O | 5:S5A:55:VAL:HG12 | 2.13 | 0.48 |
| 6:S6A:20:ALA:HA | 6:S6A:23:LYS:HB2 | 1.94 | 0.48 |
| 31:L4A:143:ALA:HB1 | 31:L4A:148:LEU:HB2 | 1.95 | 0.48 |
| 34:L9A:81:VAL:HG21 | 34:L9A:88:ILE:HD12 | 1.95 | 0.48 |
| 34:L9B:127:VAL:HA | 34:L9B:138:ILE:O | 2.13 | 0.48 |
| 5:S5A:81:GLU:HG3 | 5:S5A:90:VAL:HG22 | 1.95 | 0.48 |
| 33:L6A:15:VAL:HG12 | 33:L6A:28:GLY:HA3 | 1.95 | 0.48 |
| 34:L9A:129:THR:HA | 34:L9A:137:PRO:HA | 1.94 | 0.48 |
| 2:S2B:92:TYR:CE2 | 2:S2B:151:GLY:HA3 | 2.49 | 0.48 |
| 3:S3B:129:ALA:HB3 | 3:S3B:132:ARG:HB3 | 1.94 | 0.48 |
| 9:S9B:63:ILE:HD11 | 9:S9B:81:ILE:HD11 | 1.96 | 0.48 |
| 28:5SB:26:G:H2' | 28:5SB:58:G:N7 | 2.28 | 0.48 |
| 29:L2B:71:ASP:CG | 29:L2B:103:ARG:HH22 | 2.22 | 0.48 |
| 2:S2A:170:GLU:O | 2:S2A:174:VAL:HG23 | 2.13 | 0.48 |
| 2:S2B:221:LEU:HG | 2:S2B:221:LEU:O | 2.12 | 0.48 |
| 4:S4B:81:GLU:HG2 | 4:S4B:96:LEU:HD21 | 1.95 | 0.48 |
| 29:L2B:105:ILE:HD11 | 29:L2B:192:THR:HG21 | 1.95 | 0.48 |
| 30:L3B:59:VAL:HG21 | 30:L3B:74:PRO:HB2 | 1.96 | 0.48 |
| 33:L6B:35:VAL:HG11 | 33:L6B:71:LEU:HB3 | 1.95 | 0.48 |
| 34:L9B:38:LEU:H | 34:L9B:38:LEU:HD12 | 1.79 | 0.48 |
| 3:S3A:12:LEU:C | 3:S3A:14:ILE:H | 2.21 | 0.48 |
| 3:S3A:155:GLY:HA3 | 3:S3A:196:LEU:HD13 | 1.96 | 0.48 |
| 7:S7B:113:GLU:HG3 | 7:S7B:119:ARG:HA | 1.94 | 0.48 |
| 29:L2B:58:HIS:ND1 | 29:L2B:59:LYS:O | 2.37 | 0.48 |
| 29:L2B:148:GLU:HB2 | 29:L2B:151:LYS:HD2 | 1.96 | 0.48 |
| 32:L5B:111:LEU:HB2 | 32:L5B:112:PRO:HD3 | 1.94 | 0.48 |
| 33:L6B:144:VAL:O | 33:L6B:147:ASN:HB2 | 2.13 | 0.48 |
| 2:S2A:36:ARG:HD3 | 2:S2A:36:ARG:HA | 1.71 | 0.48 |
| 2:S2A:69:LEU:HB3 | 2:S2A:162:ILE:HG22 | 1.96 | 0.48 |
| 6:S6A:44:GLY:HA2 | 6:S6A:59:TYR:CE1 | 2.48 | 0.48 |
| 32:L5A:124:SER:HB2 | 32:L5A:131:TYR:CE1 | 2.49 | 0.48 |
| 2:S2B:158:LEU:H | 2:S2B:158:LEU:HD12 | 1.78 | 0.48 |
| 7:S7B:13:GLN:HG2 | 7:S7B:14:PRO:HD2 | 1.95 | 0.48 |
| 33:L6B:139:GLN:O | 33:L6B:139:GLN:NE2 | 2.47 | 0.48 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 3:S3B:182:ILE:HA | 3:S3B:202:ILE:O | 2.13 | 0.48 |
| 6:S6B:76:ALA:HB1 | 6:S6B:80:ARG:HH21 | 1.79 | 0.48 |
| 8:S8B:97:VAL:HA | 8:S8B:100:ILE:HD11 | 1.95 | 0.48 |
| 33:L6B:130:ARG:O | 33:L6B:131:VAL:HG23 | 2.13 | 0.48 |
| 34:L9B:29:TYR:O | 34:L9B:32:PRO:HD2 | 2.14 | 0.48 |
| 9:S9A:48:GLU:N | 9:S9A:49:PRO:HD2 | 2.29 | 0.48 |
| 2:S2B:51:LEU:HG | 2:S2B:201:ILE:HG23 | 1.96 | 0.48 |
| 2:S2B:54:THR:O | 2:S2B:58:ILE:HG12 | 2.14 | 0.48 |
| 2:S2B:69:LEU:HG | 2:S2B:91:PRO:HB2 | 1.94 | 0.48 |
| 3:S3B:6:HIS:CD2 | 3:S3B:7:PRO:HD2 | 2.49 | 0.48 |
| 29:L2B:183:ARG:HG3 | 29:L2B:184:LYS:N | 2.28 | 0.48 |
| 33:L6B:76:VAL:O | 33:L6B:79:VAL:HG22 | 2.14 | 0.48 |
| 31:L4A:179:GLU:CD | 31:L4A:179:GLU:H | 2.22 | 0.47 |
| 33:L6A:7:LEU:HB3 | 33:L6A:69:ARG:HE | 1.77 | 0.47 |
| 33:L6A:91:GLY:C | 33:L6A:93:GLY:H | 2.22 | 0.47 |
| 9:S9B:4:TYR:HB2 | 9:S9B:19:LEU:CD2 | 2.44 | 0.47 |
| 9:S9B:17:VAL:HA | 9:S9B:63:ILE:HG23 | 1.96 | 0.47 |
| 31:L4B:129:PHE:C | 31:L4B:131:GLY:H | 2.20 | 0.47 |
| 34:L9B:97:ILE:HG22 | 34:L9B:101:LEU:HD23 | 1.96 | 0.47 |
| 3:S3A:76:VAL:O | 3:S3A:83:ARG:HG2 | 2.14 | 0.47 |
| 7:S7A:15:ASP:OD1 | 7:S7A:44:TYR:OH | 2.31 | 0.47 |
| 9:S9A:42:ARG:NH1 | 9:S9A:75:ASP:OD2 | 2.46 | 0.47 |
| 28:5SA:33:C:O2' | 28:5SA:55:A:N1 | 2.46 | 0.47 |
| 29:L2A:33:LEU:O | 29:L2A:64:ILE:HG22 | 2.14 | 0.47 |
| 34:L9B:75:LEU:C | 34:L9B:77:LEU:H | 2.22 | 0.47 |
| 2:S2A:9:GLU:N | 2:S2A:9:GLU:OE1 | 2.47 | 0.47 |
| 2:S2B:68:ILE:HA | 2:S2B:161:ALA:O | 2.13 | 0.47 |
| 5:S5B:152:ARG:O | 8:S8B:64:LYS:NZ | 2.46 | 0.47 |
| 31:L4B:39:TRP:O | 31:L4B:43:LYS:HG2 | 2.14 | 0.47 |
| 31:L4B:47:GLY:HA3 | 31:L4B:95:ARG:O | 2.14 | 0.47 |
| 2:S2A:212:GLN:OE1 | 2:S2A:216:SER:HB2 | 2.13 | 0.47 |
| 3:S3A:70:VAL:O | 3:S3A:106:VAL:N | 2.45 | 0.47 |
| 5:S5A:31:LEU:HG | 5:S5A:45:PHE:CD1 | 2.49 | 0.47 |
| 6:S6A:30:LEU:HB3 | 6:S6A:35:ALA:HB3 | 1.95 | 0.47 |
| 2:S2B:91:PRO:HG3 | 2:S2B:154:LEU:HB2 | 1.97 | 0.47 |
| 2:S2B:143:GLU:O | 2:S2B:147:LYS:HB2 | 2.13 | 0.47 |
| 4:S4B:173:TRP:O | 4:S4B:186:LEU:HB2 | 2.15 | 0.47 |
| 34:L9B:29:TYR:C | 34:L9B:32:PRO:HD2 | 2.39 | 0.47 |
| 3:S3A:56:ASP:O | 3:S3A:66:VAL:HA | 2.15 | 0.47 |
| 32:L5A:170:ARG:HE | 32:L5A:174:GLU:HG2 | 1.79 | 0.47 |
| 33:L6A:126:PRO:O | 33:L6A:127:GLU:C | 2.57 | 0.47 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 2:S2B:60:ASP:O | 2:S2B:64:ARG:HD3 | 2.14 | 0.47 |
| 2:S2A:92:TYR:CE1 | 2:S2A:151:GLY:HA3 | 2.49 | 0.47 |
| 4:S4A:170:VAL:HG11 | 4:S4A:176:LEU:HD23 | 1.95 | 0.47 |
| 7:S7B:6:ARG:O | 7:S7B:7:ALA:C | 2.48 | 0.47 |
| 8:S8B:39:LEU:HD12 | 8:S8B:44:PHE:CB | 2.44 | 0.47 |
| 28:5SB:39:C:N3 | 28:5SB:50:A:O2' | 2.44 | 0.47 |
| 30:L3B:144:ARG:HB3 | 30:L3B:145:LYS:H | 1.57 | 0.47 |
| 34:L9B:2:LYS:HG3 | 34:L9B:39:ALA:HB3 | 1.97 | 0.47 |
| 7:S7A:155:ARG:HD3 | 7:S7A:155:ARG:N | 2.29 | 0.47 |
| 30:L3A:174:ASP:HB3 | 30:L3A:183:LEU:HD22 | 1.95 | 0.47 |
| 3:S3B:73:PRO:O | 3:S3B:77:ILE:HG22 | 2.14 | 0.47 |
| 3:S3B:82:GLU:H | 3:S3B:85:ARG:NH1 | 2.13 | 0.47 |
| 4:S4B:156:GLU:O | 4:S4B:159:ARG:HG2 | 2.14 | 0.47 |
| 4:S4B:177:ASP:HB3 | 4:S4B:182:LYS:HG3 | 1.95 | 0.47 |
| 7:S7B:15:ASP:OD1 | 7:S7B:16:LEU:N | 2.44 | 0.47 |
| 9:S9B:4:TYR:O | 9:S9B:18:PHE:HA | 2.15 | 0.47 |
| 31:L4B:181:LEU:HD23 | 31:L4B:181:LEU:HA | 1.76 | 0.47 |
| 32:L5B:84:LYS:HE2 | 32:L5B:84:LYS:HB3 | 1.74 | 0.47 |
| 33:L6B:91:GLY:HA3 | 33:L6B:94:TYR:CD2 | 2.50 | 0.47 |
| 33:L6A:46:GLU:CD | 33:L6A:51:ARG:HH12 | 2.23 | 0.47 |
| 33:L6A:86:GLU:N | 33:L6A:86:GLU:CD | 2.73 | 0.47 |
| 2:S2B:32:ILE:HD11 | 2:S2B:40:HIS:NE2 | 2.29 | 0.47 |
| 2:S2B:83:MET:CE | 2:S2B:84:GLU:HG2 | 2.44 | 0.47 |
| 4:S4B:8:VAL:CG1 | 4:S4B:21:LEU:HB2 | 2.45 | 0.47 |
| 6:S6B:82:ARG:HB2 | 6:S6B:85:VAL:HG23 | 1.96 | 0.47 |
| 28:5SB:44:C:C4 | 32:L5B:91:ARG:NH2 | 2.82 | 0.47 |
| 30:L3B:77:ILE:HD11 | 30:L3B:79:ARG:NH2 | 2.29 | 0.47 |
| 2:S2A:209:ARG:HE | 2:S2A:209:ARG:HB3 | 1.27 | 0.47 |
| 4:S4A:170:VAL:HG13 | 4:S4A:174:LEU:HB2 | 1.97 | 0.47 |
| 2:S2B:17:PHE:CE2 | 2:S2B:44:LEU:HB3 | 2.50 | 0.47 |
| 3:S3B:8:ILE:HG23 | 3:S3B:16:ARG:HG2 | 1.96 | 0.47 |
| 3:S3B:88:ARG:HA | 3:S3B:91:LEU:HD12 | 1.97 | 0.47 |
| 5:S5B:79:GLU:HG3 | 5:S5B:93:PRO:HD2 | 1.97 | 0.47 |
| 6:S6B:79:LEU:O | 6:S6B:85:VAL:HG11 | 2.14 | 0.47 |
| 9:S9B:9:ARG:O | 9:S9B:104:ARG:HG2 | 2.15 | 0.47 |
| 9:S9B:53:VAL:HG13 | 9:S9B:95:LYS:HD3 | 1.95 | 0.47 |
| 30:L3B:117:MET:O | 30:L3B:118:LYS:HG2 | 2.15 | 0.47 |
| 31:L4B:129:PHE:CD2 | 31:L4B:163:VAL:HG21 | 2.50 | 0.47 |
| 32:L5B:60:LEU:O | 32:L5B:64:THR:HG22 | 2.15 | 0.47 |
| 2:S2A:108:ILE:O | 2:S2A:112:VAL:HG23 | 2.15 | 0.47 |
| 5:S5A:92:LYS:O | 5:S5A:118:ILE:HD12 | 2.14 | 0.47 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 28:5SA:34:C:C2 | 28:5SA:53:G:N2 | 2.83 | 0.47 |
| 33:L6A:30:LYS:O | 33:L6A:136:ILE:HG21 | 2.15 | 0.47 |
| 2:S2B:17:PHE:HB3 | 2:S2B:42:ILE:HG23 | 1.97 | 0.47 |
| 7:S7B:15:ASP:HB3 | 7:S7B:20:ASP:H | 1.79 | 0.47 |
| 7:S7B:76:ARG:N | 7:S7B:87:VAL:O | 2.48 | 0.47 |
| 29:L2B:218:ARG:HB3 | 29:L2B:219:PRO:HD2 | 1.96 | 0.47 |
| 2:S2A:165:VAL:HG23 | 2:S2A:166:ASP:H | 1.80 | 0.46 |
| 8:S8A:37:ARG:O | 8:S8A:41:ARG:HB2 | 2.14 | 0.46 |
| 29:L2A:16:MET:HG3 | 29:L2A:207:GLY:HA3 | 1.97 | 0.46 |
| 29:L2A:175:LEU:HD23 | 29:L2A:175:LEU:HA | 1.79 | 0.46 |
| 2:S2B:205:ASP:OD1 | 2:S2B:206:ASP:N | 2.48 | 0.46 |
| 3:S3B:58:GLU:O | 3:S3B:65:ALA:N | 2.41 | 0.46 |
| 29:L2B:62:TYR:HA | 29:L2B:87:ASN:OD1 | 2.15 | 0.46 |
| 31:L4B:110:LEU:HD11 | 31:L4B:181:LEU:HB3 | 1.97 | 0.46 |
| 32:L5B:59:GLU:HG3 | 32:L5B:144:ILE:HD11 | 1.97 | 0.46 |
| 33:L6B:87:LEU:N | 33:L6B:131:VAL:O | 2.44 | 0.46 |
| 2:S2A:132:LYS:HA | 2:S2A:135:GLN:HB2 | 1.96 | 0.46 |
| 34:L9A:39:ALA:HB1 | 34:L9A:44:LEU:HD11 | 1.97 | 0.46 |
| 3:S3B:119:ARG:NH2 | 3:S3B:140:ARG:HG3 | 2.30 | 0.46 |
| 7:S7B:156:TRP:H | 7:S7B:156:TRP:CD1 | 2.32 | 0.46 |
| 30:L3B:32:PRO:HA | 30:L3B:90:THR:HA | 1.97 | 0.46 |
| 30:L3B:169:ASN:HD22 | 30:L3B:203:LYS:HB2 | 1.81 | 0.46 |
| 31:L4B:185:ASP:OD1 | 31:L4B:188:ARG:NH1 | 2.43 | 0.46 |
| 5:S5A:34:VAL:O | 5:S5A:41:VAL:HA | 2.14 | 0.46 |
| 28:5SA:47:A:OP1 | 32:L5A:96:ARG:NH1 | 2.49 | 0.46 |
| 29:L2A:111:LEU:HA | 29:L2A:115:GLN:NE2 | 2.30 | 0.46 |
| 34:L9B:69:LYS:HG2 | 34:L9B:136:VAL:HB | 1.97 | 0.46 |
| 34:L9B:79:ILE:N | 34:L9B:80:PRO:HD3 | 2.29 | 0.46 |
| 2:S2A:24:TRP:CZ3 | 2:S2A:26:PRO:HA | 2.51 | 0.46 |
| 4:S4A:150:GLU:C | 4:S4A:152:SER:N | 2.73 | 0.46 |
| 9:S9A:5:TYR:OH | 9:S9A:16:ARG:HD3 | 2.14 | 0.46 |
| 2:S2B:22:LYS:HA | 2:S2B:24:TRP:HD1 | 1.81 | 0.46 |
| 3:S3B:123:GLN:HG2 | 3:S3B:128:PHE:CD2 | 2.50 | 0.46 |
| 32:L5B:11:TYR:HE1 | 32:L5B:172:LEU:HD11 | 1.80 | 0.46 |
| 33:L6B:46:GLU:OE1 | 33:L6B:51:ARG:NH1 | 2.47 | 0.46 |
| 4:S4A:175:SER:HB3 | 4:S4A:184:LYS:HB2 | 1.98 | 0.46 |
| 9:S9A:18:PHE:HB2 | 9:S9A:62:TYR:O | 2.16 | 0.46 |
| 30:L3A:179:GLU:HB3 | 30:L3A:181:LEU:HD13 | 1.98 | 0.46 |
| 3:S3B:153:VAL:HG22 | 3:S3B:198:VAL:HG13 | 1.96 | 0.46 |
| 28:5SB:119:G:H2' | 28:5SB:120:G:O4' | 2.15 | 0.46 |
| 29:L2B:70:TRP:O | 29:L2B:73:VAL:HG23 | 2.16 | 0.46 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 2:S2A:97:TRP:HH2 | 2:S2A:176:GLU:CD | 2.23 | 0.46 |
| 6:S6A:54:LYS:HE2 | 6:S6A:54:LYS:HB3 | 1.57 | 0.46 |
| 31:L4A:11:VAL:HB | 31:L4A:18:ARG:HG3 | 1.97 | 0.46 |
| 31:L4A:24:LEU:HD23 | 31:L4A:115:ALA:HA | 1.97 | 0.46 |
| 29:L2B:182:LEU:HB3 | 29:L2B:271:ILE:HG13 | 1.97 | 0.46 |
| 3:S3A:19:GLU:O | 3:S3A:56:ASP:HA | 2.16 | 0.46 |
| 3:S3A:130:VAL:O | 3:S3A:134:ILE:HG12 | 2.16 | 0.46 |
| 8:S8A:121:ASP:HB2 | 8:S8A:125:ARG:NH2 | 2.30 | 0.46 |
| 28:5SA:98:U:H2' | 28:5SA:99:G:C8 | 2.49 | 0.46 |
| 30:L3A:9:VAL:HG22 | 30:L3A:25:VAL:O | 2.15 | 0.46 |
| 33:L6A:9:ILE:HD13 | 33:L6A:9:ILE:HG21 | 1.70 | 0.46 |
| 4:S4B:173:TRP:CD2 | 4:S4B:189:PRO:HB3 | 2.51 | 0.46 |
| 7:S7B:31:MET:HA | 7:S7B:39:ALA:HB2 | 1.97 | 0.46 |
| 8:S8B:49:GLU:HG2 | 8:S8B:62:TYR:HE2 | 1.81 | 0.46 |
| 30:L3B:2:LYS:NZ | 30:L3B:95:ILE:O | 2.39 | 0.46 |
| 30:L3B:181:LEU:HD12 | 30:L3B:181:LEU:HA | 1.72 | 0.46 |
| 31:L4B:153:SER:OG | 31:L4B:190:GLU:HG3 | 2.15 | 0.46 |
| 34:L9B:93:THR:O | 34:L9B:97:ILE:HG13 | 2.16 | 0.46 |
| 2:S2A:189:ASP:C | 2:S2A:191:ASP:H | 2.24 | 0.46 |
| 3:S3A:77:ILE:HG12 | 3:S3A:84:ILE:HB | 1.98 | 0.46 |
| 4:S4A:27:TYR:CE1 | 6:S6B:15:ASP:OD1 | 2.68 | 0.46 |
| 4:S4A:93:PHE:O | 4:S4A:96:LEU:HB2 | 2.16 | 0.46 |
| 5:S5A:52:PRO:HA | 5:S5A:55:VAL:HG12 | 1.97 | 0.46 |
| 9:S9A:10:ARG:NH2 | 9:S9A:11:LYS:HE3 | 2.31 | 0.46 |
| 30:L3A:1:MET:O | 30:L3A:84:PHE:HB2 | 2.16 | 0.46 |
| 31:L4A:101:LEU:HD23 | 31:L4A:106:ARG:HG3 | 1.98 | 0.46 |
| 32:L5A:64:THR:HB | 32:L5A:94:LEU:HD11 | 1.97 | 0.46 |
| 33:L6A:154:PRO:HD3 | 33:L6A:162:ILE:O | 2.16 | 0.46 |
| 2:S2B:82:ARG:O | 2:S2B:86:GLU:HG3 | 2.15 | 0.46 |
| 2:S2B:113:HIS:O | 2:S2B:116:GLU:HG2 | 2.16 | 0.46 |
| 2:S2B:239:VAL:HG12 | 2:S2B:240:GLN:HG3 | 1.98 | 0.46 |
| 3:S3B:131:ARG:HD3 | 3:S3B:135:LYS:HZ1 | 1.81 | 0.46 |
| 29:L2B:26:LYS:HB3 | 29:L2B:83:GLU:HG2 | 1.98 | 0.46 |
| 34:L9B:81:VAL:HA | 34:L9B:143:SER:CB | 2.45 | 0.46 |
| 2:S2A:44:LEU:O | 2:S2A:47:THR:HB | 2.16 | 0.46 |
| 2:S2A:70:PHE:HB2 | 2:S2A:92:TYR:HB3 | 1.97 | 0.46 |
| 4:S4A:194:LEU:HD12 | 4:S4A:194:LEU:HA | 1.65 | 0.46 |
| 7:S7A:29:LYS:HG3 | 7:S7A:101:LEU:HD13 | 1.98 | 0.46 |
| 32:L5A:102:PHE:HA | 32:L5A:105:LYS:HE2 | 1.98 | 0.46 |
| 32:L5A:107:LEU:HD22 | 32:L5A:178:PHE:HA | 1.98 | 0.46 |
| 33:L6A:16:SER:O | 33:L6A:26:VAL:O | 2.33 | 0.46 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 34:L9A:7:GLU:HA | 34:L9A:15:VAL:HG12 | 1.97 | 0.46 |
| 2:S2B:30:ARG:H | 2:S2B:30:ARG:HG3 | 1.42 | 0.46 |
| 2:S2B:56:ARG:HB3 | 2:S2B:56:ARG:CZ | 2.46 | 0.46 |
| 4:S4B:13:ARG:HD2 | 4:S4B:36:ARG:O | 2.16 | 0.46 |
| 5:S5B:12:LEU:O | 5:S5B:30:ALA:HA | 2.16 | 0.46 |
| 28:5SB:111:C:H5' | 28:5SB:112:G:H5' | 1.98 | 0.46 |
| 32:L5B:135:LEU:HD11 | 32:L5B:155:MET:HE3 | 1.98 | 0.46 |
| 2:S2A:51:LEU:HA | 2:S2A:54:THR:HB | 1.98 | 0.46 |
| 3:S3A:16:ARG:NH2 | 3:S3A:183:ASP:HA | 2.31 | 0.46 |
| 4:S4A:163:GLU:O | 4:S4A:166:LYS:HB2 | 2.16 | 0.46 |
| 28:5SA:15:A:O2' | 28:5SA:17:A:O5' | 2.34 | 0.46 |
| 32:L5A:47:LYS:HG2 | 32:L5A:86:MET:HE2 | 1.98 | 0.46 |
| 32:L5A:60:LEU:O | 32:L5A:64:THR:HG23 | 2.16 | 0.46 |
| 33:L6A:41:MET:HA | 33:L6A:53:GLU:O | 2.15 | 0.46 |
| 33:L6A:68:THR:O | 33:L6A:72:ILE:HG12 | 2.16 | 0.46 |
| 2:S2B:7:VAL:HG13 | 2:S2B:8:LYS:N | 2.31 | 0.46 |
| 2:S2B:34:ALA:HB1 | 2:S2B:36:ARG:HG3 | 1.98 | 0.46 |
| 2:S2B:34:ALA:O | 2:S2B:41:ILE:HB | 2.16 | 0.46 |
| 2:S2A:17:PHE:HD2 | 2:S2A:44:LEU:HD11 | 1.81 | 0.45 |
| 7:S7A:16:LEU:HD11 | 9:S9A:45:ALA:HB2 | 1.98 | 0.45 |
| 9:S9A:50:LEU:HA | 9:S9A:53:VAL:HG12 | 1.98 | 0.45 |
| 30:L3A:200:GLU:HG2 | 30:L3A:201:THR:N | 2.30 | 0.45 |
| 3:S3B:23:TYR:CG | 3:S3B:24:ALA:N | 2.84 | 0.45 |
| 4:S4B:108:LEU:HD21 | 4:S4B:183:GLY:HA3 | 1.97 | 0.45 |
| 31:L4B:157:VAL:HB | 31:L4B:194:MET:HG2 | 1.99 | 0.45 |
| 33:L6B:88:LEU:HG | 33:L6B:163:TYR:HB2 | 1.97 | 0.45 |
| 3:S3A:50:ALA:HB1 | 3:S3A:76:VAL:HG11 | 1.98 | 0.45 |
| 4:S4A:173:TRP:HB2 | 4:S4A:187:ARG:O | 2.15 | 0.45 |
| 31:L4A:29:ASN:HB3 | 31:L4A:32:LEU:HB3 | 1.98 | 0.45 |
| 2:S2B:43:ASP:OD1 | 2:S2B:44:LEU:N | 2.49 | 0.45 |
| 6:S6B:1:MET:HE2 | 6:S6B:68:PRO:HD3 | 1.98 | 0.45 |
| 3:S3A:34:LEU:O | 3:S3A:38:ARG:HG3 | 2.15 | 0.45 |
| 6:S6A:98:LEU:HB2 | 6:S6A:101:ALA:HB2 | 1.98 | 0.45 |
| 34:L9A:21:VAL:HG22 | 34:L9A:22:LYS:H | 1.80 | 0.45 |
| 5:S5B:41:VAL:HG13 | 5:S5B:113:ALA:HA | 1.97 | 0.45 |
| 5:S5B:81:GLU:HB3 | 5:S5B:90:VAL:HG12 | 1.99 | 0.45 |
| 5:S5B:147:ASP:HA | 5:S5B:150:ARG:HD2 | 1.97 | 0.45 |
| 28:5SB:44:C:H4' | 32:L5B:67:LYS:HG2 | 1.99 | 0.45 |
| 29:L2B:182:LEU:HD23 | 29:L2B:182:LEU:HA | 1.77 | 0.45 |
| 34:L9B:142:VAL:HG23 | 34:L9B:143:SER:H | 1.81 | 0.45 |
| 2:S2A:9:GLU:HA | 2:S2A:12:GLU:OE2 | 2.16 | 0.45 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 2:S2A:195:ASP:O | 8:S8A:68:ARG:NH2 | 2.49 | 0.45 |
| 4:S4A:6:GLY:O | 4:S4A:8:VAL:HG23 | 2.16 | 0.45 |
| 8:S8A:97:VAL:HB | 8:S8A:129:VAL:O | 2.17 | 0.45 |
| 28:5SA:35:G:H5' | 32:L5A:2:PRO:HD3 | 1.97 | 0.45 |
| 32:L5A:63:ILE:O | 32:L5A:105:LYS:NZ | 2.38 | 0.45 |
| 2:S2B:97:TRP:HZ3 | 2:S2B:99:GLY:HA2 | 1.81 | 0.45 |
| 3:S3B:36:ASP:OD1 | 3:S3B:57:ILE:HG21 | 2.16 | 0.45 |
| 6:S6B:3:ARG:HB3 | 6:S6B:3:ARG:CZ | 2.46 | 0.45 |
| 7:S7B:52:GLU:H | 7:S7B:52:GLU:HG2 | 1.61 | 0.45 |
| 31:L4B:29:ASN:H | 31:L4B:112:MET:HE1 | 1.81 | 0.45 |
| 31:L4B:37:VAL:O | 31:L4B:41:LEU:HG | 2.17 | 0.45 |
| 31:L4B:152:GLU:HA | 31:L4B:190:GLU:OE2 | 2.17 | 0.45 |
| 34:L9B:4:ILE:HG12 | 34:L9B:18:VAL:HG22 | 1.98 | 0.45 |
| 28:5SA:3:U:H2' | 28:5SA:4:C:C6 | 2.51 | 0.45 |
| 29:L2A:78:LYS:HB2 | 29:L2A:78:LYS:HE3 | 1.65 | 0.45 |
| 31:L4A:178:PRO:HB3 | 31:L4A:198:ALA:HB1 | 1.98 | 0.45 |
| 33:L6A:59:ARG:HA | 33:L6A:62:LYS:HE2 | 1.98 | 0.45 |
| 2:S2B:47:THR:HG23 | 2:S2B:202:PRO:HG2 | 1.98 | 0.45 |
| 2:S2B:166:ASP:C | 2:S2B:168:THR:H | 2.25 | 0.45 |
| 9:S9B:95:LYS:HA | 9:S9B:98:PRO:HG2 | 1.99 | 0.45 |
| 31:L4B:32:LEU:O | 31:L4B:36:VAL:HG23 | 2.16 | 0.45 |
| 32:L5B:80:PHE:O | 32:L5B:81:LYS:C | 2.59 | 0.45 |
| 29:L2A:148:GLU:HB2 | 29:L2A:151:LYS:HD2 | 1.98 | 0.45 |
| 32:L5A:56:ALA:HB2 | 32:L5A:153:ARG:CZ | 2.47 | 0.45 |
| 32:L5A:145:THR:C | 32:L5A:147:ASP:H | 2.25 | 0.45 |
| 2:S2B:83:MET:HE2 | 2:S2B:83:MET:HB3 | 1.57 | 0.45 |
| 4:S4B:88:VAL:O | 4:S4B:90:GLY:N | 2.41 | 0.45 |
| 7:S7B:44:TYR:O | 7:S7B:48:LYS:HG2 | 2.17 | 0.45 |
| 29:L2B:10:THR:OG1 | 29:L2B:13:ARG:HB2 | 2.17 | 0.45 |
| 31:L4B:157:VAL:O | 31:L4B:194:MET:HA | 2.16 | 0.45 |
| 6:S6A:3:ARG:HD3 | 6:S6A:38:GLU:OE1 | 2.17 | 0.45 |
| 31:L4A:16:GLY:O | 31:L4A:18:ARG:N | 2.47 | 0.45 |
| 33:L6A:27:LYS:HE3 | 33:L6A:27:LYS:HB2 | 1.77 | 0.45 |
| 33:L6A:103:LEU:HB3 | 33:L6A:115:VAL:HB | 1.98 | 0.45 |
| 3:S3B:166:GLU:HG3 | 3:S3B:167:TRP:H | 1.81 | 0.45 |
| 6:S6B:12:PRO:HG3 | 6:S6B:57:GLN:O | 2.17 | 0.45 |
| 29:L2B:130:ALA:HA | 29:L2B:192:THR:HA | 1.99 | 0.45 |
| 33:L6B:137:ASP:HB3 | 33:L6B:140:LYS:HB2 | 1.99 | 0.45 |
| 31:L4A:63:LYS:CE | 31:L4A:67:GLN:HB2 | 2.47 | 0.45 |
| 32:L5A:28:VAL:O | 32:L5A:31:VAL:HG12 | 2.16 | 0.45 |
| 32:L5A:118:ARG:HA | 32:L5A:118:ARG:HE | 1.81 | 0.45 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 3:S3B:22:TRP:HB3 | 3:S3B:59:ARG:HB2 | 1.99 | 0.45 |
| 8:S8B:1:MET:SD | 8:S8B:1:MET:N | 2.89 | 0.45 |
| 28:5SB:6:C:H2' | 28:5SB:7:C:O4' | 2.16 | 0.45 |
| 33:L6B:21:PRO:HD2 | 33:L6B:23:ARG:HH12 | 1.81 | 0.45 |
| 33:L6B:91:GLY:HA3 | 33:L6B:94:TYR:CG | 2.52 | 0.45 |
| 34:L9B:133:HIS:ND1 | 34:L9B:134:PRO:HD3 | 2.31 | 0.45 |
| 2:S2A:189:ASP:OD1 | 2:S2A:191:ASP:HB2 | 2.17 | 0.45 |
| 33:L6A:85:LYS:HE3 | 33:L6A:142:GLY:HA2 | 1.99 | 0.45 |
| 34:L9A:97:ILE:O | 34:L9A:101:LEU:N | 2.48 | 0.45 |
| 2:S2B:12:GLU:HG2 | 2:S2B:12:GLU:O | 2.15 | 0.45 |
| 29:L2B:65:ILE:HD11 | 29:L2B:67:PHE:CZ | 2.52 | 0.45 |
| 31:L4B:123:LEU:HD12 | 31:L4B:124:LEU:N | 2.32 | 0.45 |
| 6:S6A:2:ARG:HD3 | 6:S6A:4:TYR:OH | 2.17 | 0.45 |
| 9:S9A:45:ALA:O | 9:S9A:78:LYS:HE3 | 2.16 | 0.45 |
| 33:L6A:15:VAL:HG11 | 33:L6A:79:VAL:HG23 | 1.98 | 0.45 |
| 8:S8B:87:SER:HB2 | 8:S8B:93:VAL:HB | 1.98 | 0.45 |
| 28:5SB:47:A:H8 | 28:5SB:47:A:OP1 | 2.00 | 0.45 |
| 32:L5B:94:LEU:HD23 | 32:L5B:94:LEU:H | 1.81 | 0.45 |
| 33:L6B:72:ILE:O | 33:L6B:76:VAL:HG23 | 2.17 | 0.45 |
| 33:L6B:148:ILE:H | 33:L6B:148:ILE:HD12 | 1.82 | 0.45 |
| 34:L9B:111:PRO:C | 34:L9B:113:ARG:H | 2.24 | 0.45 |
| 2:S2A:77:ALA:HA | 2:S2A:80:ILE:HD12 | 1.99 | 0.44 |
| 8:S8A:103:VAL:HG21 | 8:S8A:110:ALA:HB2 | 1.99 | 0.44 |
| 33:L6A:41:MET:HB3 | 33:L6A:52:VAL:HG23 | 1.99 | 0.44 |
| 3:S3B:19:GLU:HA | 3:S3B:54:ARG:HH12 | 1.82 | 0.44 |
| 4:S4B:13:ARG:NH1 | 4:S4B:38:TYR:O | 2.50 | 0.44 |
| 6:S6B:67:MET:HB2 | 6:S6B:68:PRO:HD2 | 1.99 | 0.44 |
| 7:S7B:43:PHE:O | 7:S7B:47:CYS:N | 2.35 | 0.44 |
| 33:L6B:125:VAL:H | 33:L6B:126:PRO:HD3 | 1.82 | 0.44 |
| 34:L9B:138:ILE:HG12 | 34:L9B:139:GLN:H | 1.82 | 0.44 |
| 29:L2A:17:THR:HG22 | 29:L2A:204:ILE:HA | 1.99 | 0.44 |
| 29:L2A:221:VAL:HG13 | 29:L2A:226:MET:HE3 | 1.99 | 0.44 |
| 30:L3A:188:VAL:HG13 | 30:L3A:189:PRO:HD2 | 1.99 | 0.44 |
| 33:L6A:41:MET:HE2 | 33:L6A:41:MET:HB2 | 1.81 | 0.44 |
| 30:L3B:61:ARG:HB2 | 30:L3B:62:PRO:HD3 | 1.98 | 0.44 |
| 30:L3B:101:ARG:NH1 | 30:L3B:171:GLU:HB2 | 2.33 | 0.44 |
| 32:L5B:43:LEU:HD12 | 32:L5B:43:LEU:HA | 1.79 | 0.44 |
| 33:L6B:5:GLY:O | 33:L6B:8:PRO:HG3 | 2.18 | 0.44 |
| 2:S2A:178:ARG:NH2 | 8:S8A:74:PRO:HG3 | 2.22 | 0.44 |
| 9:S9A:5:TYR:HA | 9:S9A:17:VAL:O | 2.17 | 0.44 |
| 29:L2A:46:GLN:H | 29:L2A:46:GLN:HG3 | 1.64 | 0.44 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 31:L4A:183:VAL:O | 31:L4A:187:VAL:HG23 | 2.17 | 0.44 |
| 34:L9A:24:GLY:O | 34:L9A:28:ASN:HB2 | 2.18 | 0.44 |
| 3:S3B:153:VAL:HG12 | 3:S3B:196:LEU:HD12 | 1.98 | 0.44 |
| 31:L4B:128:ALA:C | 31:L4B:130:ALA:H | 2.24 | 0.44 |
| 33:L6B:149:ARG:HD2 | 33:L6B:164:TYR:HE1 | 1.81 | 0.44 |
| 34:L9B:128:LEU:HD12 | 34:L9B:128:LEU:HA | 1.80 | 0.44 |
| 8:S8A:104:ARG:O | 8:S8A:107:LEU:HB2 | 2.16 | 0.44 |
| 30:L3A:108:SER:O | 30:L3A:162:ALA:HA | 2.17 | 0.44 |
| 4:S4B:119:GLN:HG3 | 4:S4B:123:HIS:CE1 | 2.52 | 0.44 |
| 9:S9B:53:VAL:HG11 | 9:S9B:92:TYR:CZ | 2.52 | 0.44 |
| 32:L5B:135:LEU:HD22 | 32:L5B:140:ILE:HD11 | 1.98 | 0.44 |
| 33:L6B:156:ALA:O | 33:L6B:171:LEU:HA | 2.17 | 0.44 |
| 4:S4A:108:LEU:HB3 | 4:S4A:110:PHE:CE1 | 2.53 | 0.44 |
| 5:S5A:31:LEU:HG | 5:S5A:45:PHE:HD1 | 1.82 | 0.44 |
| 6:S6A:20:ALA:HA | 6:S6A:23:LYS:HD3 | 2.00 | 0.44 |
| 9:S9A:48:GLU:HB2 | 9:S9A:78:LYS:HE2 | 1.99 | 0.44 |
| 31:L4B:8:GLN:HA | 31:L4B:20:LEU:O | 2.17 | 0.44 |
| 28:5SA:44:C:O5' | 32:L5A:67:LYS:NZ | 2.47 | 0.44 |
| 30:L3A:54:GLN:CD | 30:L3A:76:ARG:HG2 | 2.42 | 0.44 |
| 34:L9A:46:ALA:O | 34:L9A:50:ARG:HD3 | 2.18 | 0.44 |
| 34:L9A:64:GLU:HA | 34:L9A:67:ARG:HE | 1.83 | 0.44 |
| 28:5SB:20:G:H1 | 28:5SB:67:C:H42 | 1.65 | 0.44 |
| 32:L5B:146:TYR:O | 32:L5B:149:VAL:HG22 | 2.17 | 0.44 |
| 34:L9B:81:VAL:HA | 34:L9B:143:SER:HB2 | 2.00 | 0.44 |
| 4:S4A:155:LEU:O | 4:S4A:159:ARG:HG2 | 2.18 | 0.44 |
| 6:S6A:21:LEU:O | 6:S6A:25:ILE:HG12 | 2.18 | 0.44 |
| 31:L4A:129:PHE:C | 31:L4A:131:GLY:H | 2.22 | 0.44 |
| 32:L5A:64:THR:HG21 | 32:L5A:92:VAL:HG11 | 2.00 | 0.44 |
| 2:S2B:187:LEU:HD22 | 2:S2B:201:ILE:O | 2.18 | 0.44 |
| 4:S4B:101:LEU:HB2 | 4:S4B:138:TYR:HB3 | 1.99 | 0.44 |
| 5:S5B:129:ILE:H | 5:S5B:129:ILE:HD12 | 1.82 | 0.44 |
| 5:S5B:135:THR:O | 5:S5B:139:LEU:HG | 2.17 | 0.44 |
| 30:L3B:54:GLN:HB2 | 30:L3B:76:ARG:HG2 | 1.99 | 0.44 |
| 2:S2A:87:ARG:NH1 | 2:S2A:216:SER:O | 2.42 | 0.44 |
| 5:S5A:123:LEU:HD23 | 5:S5A:123:LEU:HA | 1.79 | 0.44 |
| 2:S2B:44:LEU:HD12 | 2:S2B:45:GLN:N | 2.31 | 0.44 |
| 29:L2B:9:TYR:CD1 | 29:L2B:10:THR:HG23 | 2.53 | 0.44 |
| 30:L3B:151:TYR:CE1 | 30:L3B:154:LYS:HD3 | 2.53 | 0.44 |
| 31:L4B:116:ASP:O | 31:L4B:120:GLU:HG2 | 2.18 | 0.44 |
| 31:L4B:161:GLU:OE2 | 31:L4B:164:ARG:NH2 | 2.50 | 0.44 |
| 32:L5B:106:LEU:HA | 32:L5B:110:ALA:HB3 | 2.00 | 0.44 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 7:S7A:121:ALA:O | 7:S7A:125:MET:HG3 | 2.18 | 0.44 |
| 8:S8A:51:VAL:HG11 | 8:S8A:60:ARG:HG3 | 1.99 | 0.44 |
| 30:L3A:119:ARG:CD | 30:L3A:160:TYR:HB2 | 2.44 | 0.44 |
| 31:L4A:198:ALA:HA | 31:L4A:201:VAL:HB | 2.00 | 0.44 |
| 6:S6B:15:ASP:O | 6:S6B:19:LEU:N | 2.29 | 0.44 |
| 33:L6B:125:VAL:O | 33:L6B:125:VAL:HG13 | 2.18 | 0.44 |
| 2:S2A:46:LYS:HA | 2:S2A:49:GLU:HB2 | 2.00 | 0.43 |
| 5:S5A:99:GLY:O | 5:S5A:117:ASP:HA | 2.18 | 0.43 |
| 6:S6A:67:MET:HB2 | 6:S6A:68:PRO:HD2 | 2.00 | 0.43 |
| 29:L2A:70:TRP:CZ2 | 29:L2A:150:LYS:HD3 | 2.53 | 0.43 |
| 30:L3A:77:ILE:HD12 | 30:L3A:77:ILE:HA | 1.86 | 0.43 |
| 30:L3A:195:LEU:HD12 | 30:L3A:196:VAL:H | 1.83 | 0.43 |
| 34:L9A:57:ARG:O | 34:L9A:61:ARG:HG2 | 2.18 | 0.43 |
| 9:S9B:19:LEU:HD23 | 9:S9B:19:LEU:N | 2.32 | 0.43 |
| 30:L3B:14:ILE:HD11 | 30:L3B:173:VAL:HG11 | 1.99 | 0.43 |
| 32:L5B:173:LEU:HD23 | 32:L5B:173:LEU:HA | 1.80 | 0.43 |
| 34:L9B:2:LYS:HA | 34:L9B:20:ASP:HA | 1.99 | 0.43 |
| 28:5SA:1:A:H2' | 28:5SA:1:A:N3 | 2.33 | 0.43 |
| 29:L2A:105:ILE:HD12 | 29:L2A:105:ILE:HA | 1.84 | 0.43 |
| 30:L3A:120:TRP:CD1 | 30:L3A:155:LYS:HB3 | 2.52 | 0.43 |
| 32:L5B:129:GLY:HA3 | 32:L5B:163:ALA:HB3 | 2.00 | 0.43 |
| 3:S3A:79:ARG:O | 3:S3A:79:ARG:HG2 | 2.18 | 0.43 |
| 7:S7A:108:ALA:O | 7:S7A:111:ARG:HG3 | 2.18 | 0.43 |
| 8:S8A:100:ILE:HG22 | 8:S8A:125:ARG:NH1 | 2.32 | 0.43 |
| 31:L4A:170:LEU:HD13 | 31:L4A:170:LEU:HA | 1.87 | 0.43 |
| 32:L5A:60:LEU:HD23 | 32:L5A:60:LEU:HA | 1.81 | 0.43 |
| 2:S2B:82:ARG:HB2 | 2:S2B:94:ASN:HD22 | 1.83 | 0.43 |
| 2:S2B:91:PRO:HD3 | 2:S2B:155:LEU:HD23 | 1.99 | 0.43 |
| 2:S2B:178:ARG:NH2 | 8:S8B:68:ARG:NH2 | 2.65 | 0.43 |
| 4:S4B:94:LEU:O | 4:S4B:98:GLU:N | 2.39 | 0.43 |
| 4:S4B:129:ASN:OD1 | 4:S4B:145:GLU:N | 2.45 | 0.43 |
| 3:S3A:16:ARG:HH22 | 3:S3A:183:ASP:HA | 1.84 | 0.43 |
| 6:S6A:1:MET:HG2 | 6:S6A:68:PRO:HA | 2.00 | 0.43 |
| 29:L2A:122:ASP:CG | 29:L2A:123:ALA:H | 2.25 | 0.43 |
| 2:S2B:112:VAL:O | 2:S2B:115:LEU:HB3 | 2.18 | 0.43 |
| 2:S2B:215:LEU:HA | 2:S2B:215:LEU:HD13 | 1.89 | 0.43 |
| 4:S4B:145:GLU:OE2 | 4:S4B:182:LYS:HD2 | 2.19 | 0.43 |
| 28:5SB:13:C:H3' | 28:5SB:14:C:C5 | 2.53 | 0.43 |
| 28:5SB:82:U:H2' | 28:5SB:83:G:N2 | 2.30 | 0.43 |
| 30:L3B:120:TRP:CD1 | 30:L3B:155:LYS:HB3 | 2.53 | 0.43 |
| 31:L4B:178:PRO:HB3 | 31:L4B:198:ALA:HB2 | 2.00 | 0.43 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 32:L5B:16:ARG:NH2 | 32:L5B:31:VAL:HB | 2.33 | 0.43 |
| 33:L6B:58:GLU:O | 33:L6B:62:LYS:HG3 | 2.19 | 0.43 |
| 3:S3A:91:LEU:HD11 | 3:S3A:101:LEU:HD12 | 2.00 | 0.43 |
| 3:S3A:181:ASN:OD1 | 3:S3A:204:LEU:HD12 | 2.18 | 0.43 |
| 32:L5A:33:ARG:O | 32:L5A:162:THR:HG23 | 2.18 | 0.43 |
| 2:S2B:67:THR:HA | 2:S2B:90:MET:SD | 2.59 | 0.43 |
| 4:S4B:13:ARG:HB3 | 4:S4B:38:TYR:O | 2.18 | 0.43 |
| 5:S5B:60:TYR:HB3 | 5:S5B:64:ARG:NH2 | 2.33 | 0.43 |
| 29:L2B:17:THR:HG23 | 29:L2B:204:ILE:HA | 2.00 | 0.43 |
| 30:L3B:51:PHE:O | 30:L3B:75:VAL:HB | 2.18 | 0.43 |
| 31:L4B:57:VAL:HG22 | 31:L4B:58:ALA:H | 1.83 | 0.43 |
| 31:L4B:117:ARG:HD3 | 31:L4B:117:ARG:HA | 1.78 | 0.43 |
| 32:L5B:124:SER:HB2 | 32:L5B:131:TYR:CE1 | 2.54 | 0.43 |
| 4:S4A:196:LEU:O | 4:S4A:198:VAL:N | 2.47 | 0.43 |
| 5:S5A:42:GLY:HA2 | 5:S5A:65:ASN:O | 2.18 | 0.43 |
| 28:5SA:30:C:H2' | 28:5SA:31:A:C8 | 2.54 | 0.43 |
| 32:L5A:120:LEU:O | 32:L5A:181:ARG:HB2 | 2.18 | 0.43 |
| 33:L6A:121:ILE:HG12 | 33:L6A:140:LYS:HD3 | 1.99 | 0.43 |
| 34:L9A:49:ALA:O | 34:L9A:53:ALA:N | 2.44 | 0.43 |
| 34:L9A:78:THR:HA | 34:L9A:141:LYS:HB2 | 2.00 | 0.43 |
| 34:L9A:79:ILE:HG23 | 34:L9A:81:VAL:HG13 | 2.01 | 0.43 |
| 3:S3B:50:ALA:CB | 3:S3B:76:VAL:HG11 | 2.34 | 0.43 |
| 8:S8B:104:ARG:HB3 | 8:S8B:108:GLY:N | 2.32 | 0.43 |
| 30:L3B:21:VAL:CG2 | 30:L3B:185:LYS:HD3 | 2.48 | 0.43 |
| 32:L5B:75:LYS:HA | 32:L5B:84:LYS:HG2 | 1.99 | 0.43 |
| 2:S2A:87:ARG:O | 2:S2A:87:ARG:HG2 | 2.17 | 0.43 |
| 8:S8A:83:ILE:HA | 8:S8A:136:GLU:O | 2.18 | 0.43 |
| 28:5SA:47:A:C4 | 28:5SA:48:A:C8 | 3.07 | 0.43 |
| 33:L6A:54:ARG:NE | 33:L6A:57:ASP:OD1 | 2.45 | 0.43 |
| 33:L6A:117:PRO:HB3 | 33:L6A:123:PHE:CE2 | 2.53 | 0.43 |
| 34:L9A:1:MET:C | 34:L9A:20:ASP:HB2 | 2.44 | 0.43 |
| 2:S2B:88:ALA:O | 2:S2B:226:ARG:NH1 | 2.51 | 0.43 |
| 8:S8B:121:ASP:OD1 | 8:S8B:121:ASP:N | 2.52 | 0.43 |
| 31:L4B:64:ILE:HD12 | 31:L4B:64:ILE:HA | 1.88 | 0.43 |
| 8:S8A:122:ARG:HG2 | 8:S8A:126:LYS:NZ | 2.33 | 0.43 |
| 28:5SA:3:U:H2' | 28:5SA:4:C:H6 | 1.84 | 0.43 |
| 32:L5A:97:ASP:HA | 32:L5A:100:TRP:HB2 | 2.01 | 0.43 |
| 34:L9A:5:LEU:HD12 | 34:L9A:17:GLN:HB3 | 2.00 | 0.43 |
| 34:L9A:47:LEU:O | 34:L9A:51:ILE:HG13 | 2.19 | 0.43 |
| 2:S2B:185:ILE:HG22 | 2:S2B:199:TYR:HB2 | 2.00 | 0.43 |
| 2:S2B:208:ILE:HA | 2:S2B:211:ILE:HD12 | 2.01 | 0.43 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 5:S5B:71:LEU:HD23 | 5:S5B:71:LEU:HA | 1.77 | 0.43 |
| 8:S8B:112:LEU:HA | 8:S8B:134:ILE:H | 1.84 | 0.43 |
| 30:L3B:37:ARG:HA | 30:L3B:42:ASP:OD2 | 2.18 | 0.43 |
| 31:L4A:125:LEU:HA | 31:L4A:194:MET:O | 2.19 | 0.43 |
| 33:L6A:12:PRO:C | 33:L6A:14:GLY:H | 2.26 | 0.43 |
| 33:L6A:125:VAL:HG22 | 33:L6A:131:VAL:HG23 | 1.99 | 0.43 |
| 2:S2B:60:ASP:HA | 2:S2B:63:MET:HE2 | 2.00 | 0.43 |
| 3:S3B:123:GLN:HG2 | 3:S3B:128:PHE:HD2 | 1.83 | 0.43 |
| 4:S4B:101:LEU:HB3 | 4:S4B:138:TYR:HB3 | 2.00 | 0.43 |
| 9:S9B:31:GLN:HG2 | 9:S9B:36:TYR:HB2 | 2.01 | 0.43 |
| 28:5SB:30:C:H2' | 28:5SB:31:A:C8 | 2.54 | 0.43 |
| 33:L6B:10:PRO:HB2 | 33:L6B:50:VAL:HG13 | 2.00 | 0.43 |
| 2:S2A:69:LEU:HA | 2:S2A:91:PRO:HG2 | 2.01 | 0.43 |
| 29:L2A:232:PRO:HB3 | 29:L2A:244:ARG:NH1 | 2.34 | 0.43 |
| 33:L6A:98:LEU:HD12 | 33:L6A:98:LEU:HA | 1.90 | 0.43 |
| 2:S2B:111:ARG:HD3 | 2:S2B:111:ARG:HA | 1.76 | 0.43 |
| 4:S4B:63:LYS:HE3 | 4:S4B:63:LYS:HB2 | 1.80 | 0.43 |
| 4:S4B:74:GLN:H | 4:S4B:74:GLN:HG2 | 1.59 | 0.43 |
| 8:S8B:12:ARG:NH1 | 8:S8B:27:PRO:HD3 | 2.34 | 0.43 |
| 9:S9B:96:LEU:HB3 | 9:S9B:102:LEU:HG | 2.00 | 0.43 |
| 30:L3B:9:VAL:CG1 | 30:L3B:27:LEU:HD23 | 2.42 | 0.43 |
| 2:S2A:101:MET:HA | 2:S2A:108:ILE:HG13 | 2.01 | 0.42 |
| 2:S2A:165:VAL:O | 2:S2A:187:LEU:O | 2.37 | 0.42 |
| 9:S9A:9:ARG:HG2 | 9:S9A:104:ARG:CZ | 2.49 | 0.42 |
| 9:S9A:50:LEU:HB3 | 9:S9A:55:ALA:O | 2.19 | 0.42 |
| 28:5SA:33:C:C2 | 28:5SA:34:C:C5 | 3.07 | 0.42 |
| 28:5SA:94:C:H2' | 28:5SA:95:G:H8 | 1.84 | 0.42 |
| 33:L6A:77:LYS:HE2 | 33:L6A:138:LYS:HD2 | 2.00 | 0.42 |
| 3:S3B:56:ASP:O | 3:S3B:66:VAL:HA | 2.18 | 0.42 |
| 4:S4B:4:TYR:O | 4:S4B:115:ARG:NH1 | 2.51 | 0.42 |
| 9:S9B:3:GLN:CB | 9:S9B:20:ARG:HD2 | 2.49 | 0.42 |
| 32:L5B:95:ARG:HE | 32:L5B:95:ARG:HB3 | 1.69 | 0.42 |
| 2:S2A:55:PHE:CD1 | 2:S2A:221:LEU:HG | 2.54 | 0.42 |
| 4:S4A:117:ALA:O | 4:S4A:121:VAL:HG23 | 2.20 | 0.42 |
| 4:S4A:163:GLU:HG3 | 4:S4A:166:LYS:HE3 | 2.00 | 0.42 |
| 8:S8A:11:THR:HG23 | 8:S8A:14:ARG:NH1 | 2.34 | 0.42 |
| 33:L6A:30:LYS:HE3 | 33:L6A:80:SER:HA | 2.01 | 0.42 |
| 33:L6A:41:MET:H | 33:L6A:55:PRO:HG3 | 1.84 | 0.42 |
| 34:L9A:38:LEU:HD12 | 34:L9A:40:THR:OG1 | 2.18 | 0.42 |
| 2:S2B:83:MET:HE2 | 2:S2B:84:GLU:HG2 | 2.00 | 0.42 |
| 2:S2B:178:ARG:HH21 | 8:S8B:74:PRO:HG3 | 1.83 | 0.42 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 3:S3B:127:ARG:HH21 | 3:S3B:191:THR:HB | 1.84 | 0.42 |
| 6:S6B:7:ASN:OD1 | 6:S6B:62:TRP:HD1 | 2.02 | 0.42 |
| 28:5SB:57:U:O3' | 32:L5B:27:ASN:ND2 | 2.51 | 0.42 |
| 34:L9B:89:TYR:N | 34:L9B:89:TYR:HD1 | 2.15 | 0.42 |
| 33:L6A:9:ILE:HG22 | 33:L6A:69:ARG:CZ | 2.48 | 0.42 |
| 34:L9A:66:GLU:HA | 34:L9A:69:LYS:HB3 | 2.02 | 0.42 |
| 3:S3B:130:VAL:O | 3:S3B:134:ILE:HG12 | 2.19 | 0.42 |
| 3:S3B:175:LEU:HD11 | 3:S3B:201:TYR:CE2 | 2.53 | 0.42 |
| 4:S4B:160:GLN:O | 4:S4B:163:GLU:HB3 | 2.19 | 0.42 |
| 29:L2B:61:LEU:HD12 | 29:L2B:61:LEU:HA | 1.90 | 0.42 |
| 30:L3B:64:LYS:HB2 | 30:L3B:64:LYS:HE2 | 1.95 | 0.42 |
| 31:L4B:20:LEU:HD12 | 31:L4B:20:LEU:HA | 1.90 | 0.42 |
| 33:L6B:89:ILE:HG12 | 33:L6B:162:ILE:HG23 | 2.01 | 0.42 |
| 3:S3A:72:LYS:O | 3:S3A:76:VAL:HG13 | 2.19 | 0.42 |
| 4:S4A:209:ARG:HE | 4:S4A:209:ARG:HB3 | 1.67 | 0.42 |
| 6:S6A:86:ARG:O | 6:S6A:87:ARG:HG2 | 2.19 | 0.42 |
| 29:L2A:133:LEU:HG | 29:L2A:189:CYS:O | 2.20 | 0.42 |
| 34:L9A:138:ILE:HG12 | 34:L9A:139:GLN:H | 1.85 | 0.42 |
| 2:S2B:73:THR:HB | 2:S2B:96:ARG:N | 2.34 | 0.42 |
| 4:S4B:121:VAL:HG12 | 4:S4B:134:ASP:HA | 2.01 | 0.42 |
| 6:S6B:61:LEU:HB3 | 6:S6B:63:TYR:HE1 | 1.83 | 0.42 |
| 29:L2B:43:ARG:HA | 29:L2B:48:ARG:O | 2.19 | 0.42 |
| 31:L4B:16:GLY:O | 31:L4B:18:ARG:N | 2.45 | 0.42 |
| 31:L4B:196:LEU:HD23 | 31:L4B:196:LEU:HA | 1.71 | 0.42 |
| 33:L6B:18:GLU:O | 33:L6B:24:VAL:HG23 | 2.19 | 0.42 |
| 33:L6B:46:GLU:HG2 | 33:L6B:47:GLU:H | 1.82 | 0.42 |
| 2:S2A:8:LYS:HD3 | 2:S2A:10:LEU:HB2 | 2.02 | 0.42 |
| 4:S4A:27:TYR:HE1 | 6:S6B:15:ASP:OD1 | 2.01 | 0.42 |
| 29:L2A:46:GLN:C | 29:L2A:48:ARG:H | 2.28 | 0.42 |
| 34:L9A:97:ILE:HA | 34:L9A:100:ALA:HB3 | 2.01 | 0.42 |
| 2:S2B:137:ARG:HH12 | 2:S2B:141:GLU:H | 1.68 | 0.42 |
| 4:S4B:12:CYS:C | 4:S4B:33:MET:HE2 | 2.44 | 0.42 |
| 32:L5B:34:LEU:HD23 | 32:L5B:34:LEU:HA | 1.89 | 0.42 |
| 2:S2A:149:LEU:HD22 | 2:S2A:152:PHE:HB3 | 2.02 | 0.42 |
| 3:S3A:11:ARG:HH22 | 3:S3A:175:LEU:HA | 1.85 | 0.42 |
| 3:S3A:77:ILE:HG23 | 3:S3A:84:ILE:HG22 | 2.01 | 0.42 |
| 3:S3A:186:PHE:HD1 | 3:S3A:198:VAL:O | 2.03 | 0.42 |
| 32:L5A:62:LEU:HD12 | 32:L5A:62:LEU:HA | 1.88 | 0.42 |
| 2:S2B:137:ARG:HH12 | 2:S2B:141:GLU:N | 2.16 | 0.42 |
| 2:S2B:145:LEU:O | 2:S2B:149:LEU:HB2 | 2.20 | 0.42 |
| 28:5SB:47:A:C5 | 28:5SB:48:A:N7 | 2.88 | 0.42 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 31:L4B:196:LEU:O | 31:L4B:199:TRP:HB3 | 2.20 | 0.42 |
| 3:S3A:14:ILE:HG12 | 3:S3A:15:THR:OG1 | 2.20 | 0.42 |
| 4:S4A:152:SER:HA | 4:S4A:155:LEU:HG | 2.01 | 0.42 |
| 2:S2B:166:ASP:CG | 2:S2B:169:LYS:HB2 | 2.45 | 0.42 |
| 9:S9B:128:ARG:HD3 | 9:S9B:128:ARG:HA | 1.72 | 0.42 |
| 30:L3B:11:MET:O | 30:L3B:12:THR:HG23 | 2.20 | 0.42 |
| 34:L9B:2:LYS:HE2 | 34:L9B:2:LYS:HB3 | 1.91 | 0.42 |
| 2:S2A:162:ILE:O | 2:S2A:185:ILE:HD12 | 2.20 | 0.42 |
| 3:S3A:116:VAL:HG21 | 3:S3A:202:ILE:HD11 | 2.01 | 0.42 |
| 4:S4A:187:ARG:HH21 | 4:S4A:190:ASP:H | 1.64 | 0.42 |
| 5:S5A:53:LEU:O | 5:S5A:57:LYS:HG2 | 2.20 | 0.42 |
| 8:S8A:103:VAL:CG2 | 8:S8A:110:ALA:HB2 | 2.50 | 0.42 |
| 9:S9A:22:GLY:O | 9:S9A:23:ASN:ND2 | 2.53 | 0.42 |
| 34:L9A:92:VAL:CG1 | 34:L9A:120:ILE:HG23 | 2.49 | 0.42 |
| 2:S2B:187:LEU:HD11 | 2:S2B:204:ASN:H | 1.85 | 0.42 |
| 4:S4B:201:GLN:HE21 | 5:S5B:99:GLY:HA2 | 1.84 | 0.42 |
| 9:S9B:4:TYR:HB2 | 9:S9B:19:LEU:HD23 | 2.02 | 0.42 |
| 29:L2B:78:LYS:HB2 | 29:L2B:78:LYS:HE3 | 1.87 | 0.42 |
| 31:L4B:46:ARG:HA | 31:L4B:46:ARG:HD2 | 1.90 | 0.42 |
| 32:L5B:41:GLN:O | 32:L5B:89:GLY:HA2 | 2.20 | 0.42 |
| 34:L9B:11:ASN:ND2 | 34:L9B:11:ASN:O | 2.52 | 0.42 |
| 2:S2A:91:PRO:HG3 | 2:S2A:155:LEU:HG | 2.01 | 0.42 |
| 4:S4A:108:LEU:HD11 | 4:S4A:174:LEU:HD22 | 2.02 | 0.42 |
| 29:L2A:181:GLU:HA | 29:L2A:272:ALA:HB3 | 2.01 | 0.42 |
| 32:L5A:16:ARG:NH1 | 32:L5A:31:VAL:HG11 | 2.35 | 0.42 |
| 32:L5A:43:LEU:HD11 | 32:L5A:153:ARG:HD2 | 2.02 | 0.42 |
| 32:L5A:96:ARG:O | 32:L5A:98:ARG:N | 2.50 | 0.42 |
| 34:L9A:85:GLU:C | 34:L9A:87:LYS:H | 2.28 | 0.42 |
| 31:L4B:182:ASN:O | 31:L4B:186:ILE:HG13 | 2.20 | 0.42 |
| 29:L2A:70:TRP:CE2 | 29:L2A:150:LYS:HD3 | 2.55 | 0.42 |
| 29:L2A:111:LEU:HD22 | 29:L2A:115:GLN:CD | 2.45 | 0.42 |
| 2:S2B:15:VAL:HG23 | 2:S2B:16:HIS:CE1 | 2.54 | 0.42 |
| 3:S3B:92:ALA:HB2 | 3:S3B:99:VAL:HG22 | 2.01 | 0.42 |
| 4:S4B:6:GLY:O | 4:S4B:8:VAL:HG23 | 2.20 | 0.42 |
| 7:S7B:93:PRO:HA | 7:S7B:96:GLN:HB2 | 2.01 | 0.42 |
| 28:5SB:24:U:H3 | 28:5SB:63:G:H1 | 1.67 | 0.42 |
| 29:L2B:255:LYS:HA | 29:L2B:255:LYS:HD2 | 1.77 | 0.42 |
| 33:L6B:12:PRO:HG3 | 33:L6B:48:GLY:O | 2.18 | 0.42 |
| 4:S4A:25:ARG:NH2 | 4:S4A:30:LYS:HB2 | 2.34 | 0.41 |
| 8:S8A:20:TYR:HD1 | 8:S8A:65:TYR:CD2 | 2.38 | 0.41 |
| 32:L5A:67:LYS:HG3 | 32:L5A:67:LYS:H | 1.76 | 0.41 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 6:S6B:67:MET:SD | 6:S6B:72:VAL:HG12 | 2.60 | 0.41 |
| 31:L4B:23:ASP:OD1 | 31:L4B:23:ASP:N | 2.41 | 0.41 |
| 2:S2A:87:ARG:HD3 | 2:S2A:223:ILE:HD11 | 2.01 | 0.41 |
| 3:S3A:12:LEU:C | 3:S3A:14:ILE:N | 2.77 | 0.41 |
| 8:S8A:6:ILE:O | 8:S8A:10:LEU:HG | 2.19 | 0.41 |
| 9:S9A:118:LYS:C | 9:S9A:120:ARG:H | 2.28 | 0.41 |
| 2:S2B:114:ARG:O | 2:S2B:118:LEU:HG | 2.20 | 0.41 |
| 28:5SB:60:A:H3' | 28:5SB:61:A:H8 | 1.84 | 0.41 |
| 32:L5B:75:LYS:HE2 | 32:L5B:75:LYS:HB3 | 1.86 | 0.41 |
| 2:S2A:111:ARG:NH2 | 2:S2A:114:ARG:HG2 | 2.35 | 0.41 |
| 2:S2A:176:GLU:O | 2:S2A:180:LEU:HD12 | 2.21 | 0.41 |
| 8:S8A:82:HIS:O | 8:S8A:137:VAL:HA | 2.21 | 0.41 |
| 31:L4A:7:TYR:O | 31:L4A:21:ALA:HA | 2.19 | 0.41 |
| 32:L5A:28:VAL:HG23 | 32:L5A:29:TRP:CD1 | 2.55 | 0.41 |
| 4:S4B:52:SER:O | 4:S4B:56:VAL:HG23 | 2.20 | 0.41 |
| 30:L3B:89:ASP:OD1 | 30:L3B:89:ASP:N | 2.49 | 0.41 |
| 9:S9A:20:ARG:HH21 | 9:S9A:62:TYR:CB | 2.33 | 0.41 |
| 33:L6A:83:TYR:HD2 | 33:L6A:132:ARG:HH12 | 1.69 | 0.41 |
| 3:S3B:62:ASP:O | 3:S3B:97:LYS:HB2 | 2.20 | 0.41 |
| 3:S3B:120:VAL:HA | 3:S3B:123:GLN:HB2 | 2.02 | 0.41 |
| 9:S9B:28:VAL:HG11 | 9:S9B:65:VAL:HG12 | 2.02 | 0.41 |
| 31:L4B:63:LYS:NZ | 31:L4B:67:GLN:HB2 | 2.34 | 0.41 |
| 31:L4B:158:THR:HA | 31:L4B:195:ASP:OD1 | 2.21 | 0.41 |
| 33:L6B:118:PRO:HB2 | 33:L6B:119:GLU:H | 1.70 | 0.41 |
| 2:S2A:28:PHE:HE2 | 2:S2A:42:ILE:HD12 | 1.85 | 0.41 |
| 28:5SA:82:U:C2 | 28:5SA:83:G:N2 | 2.89 | 0.41 |
| 29:L2A:77:ALA:HB2 | 29:L2A:97:TYR:CD1 | 2.55 | 0.41 |
| 32:L5A:82:LEU:HD23 | 32:L5A:82:LEU:HA | 1.90 | 0.41 |
| 34:L9A:120:ILE:HG13 | 34:L9A:121:LYS:O | 2.21 | 0.41 |
| 4:S4B:103:ASN:OD1 | 4:S4B:114:ARG:NH2 | 2.53 | 0.41 |
| 9:S9B:49:PRO:HB2 | 9:S9B:85:LEU:HD21 | 2.02 | 0.41 |
| 32:L5B:103:LEU:O | 32:L5B:107:LEU:HG | 2.20 | 0.41 |
| 32:L5B:135:LEU:CD1 | 32:L5B:155:MET:HG2 | 2.51 | 0.41 |
| 33:L6B:30:LYS:HB3 | 33:L6B:79:VAL:CA | 2.50 | 0.41 |
| 34:L9B:76:THR:HG22 | 34:L9B:139:GLN:OE1 | 2.20 | 0.41 |
| 8:S8A:109:ILE:CG2 | 8:S8A:137:VAL:HB | 2.50 | 0.41 |
| 9:S9A:22:GLY:O | 9:S9A:24:GLY:N | 2.49 | 0.41 |
| 30:L3A:114:ALA:HB3 | 30:L3A:119:ARG:HG2 | 2.02 | 0.41 |
| 2:S2B:215:LEU:HD13 | 2:S2B:218:ALA:HB3 | 2.03 | 0.41 |
| 3:S3B:101:LEU:HD23 | 3:S3B:101:LEU:HA | 1.95 | 0.41 |
| 5:S5B:79:GLU:OE2 | 8:S8B:105:ARG:HG2 | 2.21 | 0.41 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 30:L3B:11:MET:SD | 30:L3B:24:THR:HG22 | 2.61 | 0.41 |
| 32:L5B:13:GLU:O | 32:L5B:17:PRO:HG3 | 2.21 | 0.41 |
| 5:S5A:152:ARG:HD3 | 8:S8A:44:PHE:CZ | 2.55 | 0.41 |
| 7:S7A:72:ARG:HA | 7:S7A:72:ARG:HD3 | 1.88 | 0.41 |
| 9:S9A:56:LEU:HB3 | 9:S9A:57:GLY:H | 1.31 | 0.41 |
| 29:L2A:268:ARG:HE | 29:L2A:268:ARG:HB3 | 1.68 | 0.41 |
| 30:L3A:117:MET:HE2 | 30:L3A:136:ARG:NH1 | 2.36 | 0.41 |
| 31:L4A:63:LYS:NZ | 31:L4A:67:GLN:HB2 | 2.36 | 0.41 |
| 32:L5A:81:LYS:HD3 | 32:L5A:81:LYS:N | 2.35 | 0.41 |
| 32:L5A:101:ILE:O | 32:L5A:105:LYS:HG3 | 2.20 | 0.41 |
| 32:L5A:111:LEU:HB2 | 32:L5A:112:PRO:HD3 | 2.02 | 0.41 |
| 4:S4B:4:TYR:CE2 | 4:S4B:11:LEU:HD11 | 2.54 | 0.41 |
| 5:S5B:100:VAL:HG12 | 5:S5B:118:ILE:HG22 | 2.03 | 0.41 |
| 9:S9B:19:LEU:HD12 | 9:S9B:59:PHE:CE1 | 2.56 | 0.41 |
| 9:S9B:96:LEU:O | 9:S9B:100:GLY:N | 2.53 | 0.41 |
| 29:L2B:11:PRO:O | 29:L2B:12:SER:OG | 2.28 | 0.41 |
| 32:L5B:102:PHE:HE1 | 32:L5B:141:PHE:CE1 | 2.38 | 0.41 |
| 2:S2A:96:ARG:HD2 | 2:S2A:96:ARG:N | 2.36 | 0.41 |
| 4:S4A:49:ARG:H | 4:S4A:49:ARG:HD3 | 1.85 | 0.41 |
| 32:L5A:118:ARG:HA | 32:L5A:118:ARG:NE | 2.35 | 0.41 |
| 34:L9A:23:PRO:O | 34:L9A:27:ARG:HG2 | 2.21 | 0.41 |
| 34:L9A:94:ALA:CB | 34:L9A:111:PRO:HG2 | 2.48 | 0.41 |
| 6:S6B:81:ILE:H | 6:S6B:81:ILE:HG13 | 1.67 | 0.41 |
| 9:S9B:46:ALA:HA | 9:S9B:78:LYS:HB3 | 2.03 | 0.41 |
| 33:L6B:90:LYS:O | 33:L6B:160:LYS:HA | 2.20 | 0.41 |
| 33:L6B:153:LYS:HB2 | 33:L6B:154:PRO:HD2 | 2.03 | 0.41 |
| 34:L9B:6:LEU:H | 34:L9B:36:ALA:HA | 1.86 | 0.41 |
| 2:S2A:31:TYR:C | 2:S2A:42:ILE:HG13 | 2.46 | 0.41 |
| 2:S2A:100:GLY:O | 2:S2A:101:MET:C | 2.63 | 0.41 |
| 4:S4A:95:GLY:HA3 | 4:S4A:188:LEU:HD11 | 2.03 | 0.41 |
| 9:S9A:95:LYS:HA | 9:S9A:98:PRO:HG2 | 2.02 | 0.41 |
| 28:5SA:96:C:H2' | 28:5SA:97:C:H6 | 1.85 | 0.41 |
| 29:L2A:79:VAL:HG12 | 29:L2A:113:VAL:HA | 2.03 | 0.41 |
| 32:L5A:3:LEU:HA | 32:L5A:3:LEU:HD23 | 1.74 | 0.41 |
| 32:L5A:99:MET:HG3 | 32:L5A:100:TRP:N | 2.34 | 0.41 |
| 2:S2B:53:ARG:HA | 2:S2B:56:ARG:HE | 1.86 | 0.41 |
| 3:S3B:180:ALA:HB1 | 3:S3B:182:ILE:HG13 | 2.02 | 0.41 |
| 4:S4B:120:LEU:HD23 | 4:S4B:120:LEU:HA | 1.88 | 0.41 |
| 9:S9B:26:VAL:HG13 | 9:S9B:61:ALA:HB3 | 2.03 | 0.41 |
| 9:S9B:121:ARG:HD3 | 9:S9B:122:ALA:O | 2.21 | 0.41 |
| 29:L2B:37:LEU:HD13 | 29:L2B:62:TYR:HB2 | 2.01 | 0.41 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 29:L2B:68:LYS:HB2 | 29:L2B:70:TRP:CH2 | 2.56 | 0.41 |
| 29:L2B:121:PRO:HB3 | 29:L2B:135:PHE:CE2 | 2.56 | 0.41 |
| 29:L2B:242:ARG:HD2 | 29:L2B:242:ARG:N | 2.36 | 0.41 |
| 30:L3B:195:LEU:HG | 30:L3B:196:VAL:N | 2.36 | 0.41 |
| 33:L6B:164:TYR:HB2 | 33:L6B:167:GLU:HG3 | 2.03 | 0.41 |
| 34:L9B:130:TYR:HB3 | 34:L9B:136:VAL:HG13 | 2.02 | 0.41 |
| 2:S2A:114:ARG:NH2 | 2:S2A:141:GLU:OE1 | 2.54 | 0.41 |
| 3:S3A:47:LEU:HB2 | 3:S3A:52:LEU:HD13 | 2.01 | 0.41 |
| 4:S4A:105:VAL:HG13 | 4:S4A:110:PHE:HB2 | 2.02 | 0.41 |
| 6:S6A:62:TRP:O | 6:S6A:63:TYR:HD1 | 2.04 | 0.41 |
| 8:S8A:11:THR:HG23 | 8:S8A:14:ARG:HH12 | 1.85 | 0.41 |
| 31:L4A:64:ILE:CD1 | 31:L4A:78:ILE:HD11 | 2.51 | 0.41 |
| 32:L5A:109:VAL:C | 32:L5A:112:PRO:HD2 | 2.45 | 0.41 |
| 34:L9A:121:LYS:HB3 | 34:L9A:122:GLU:HG3 | 2.03 | 0.41 |
| 2:S2B:118:LEU:HB2 | 2:S2B:142:LEU:HD12 | 2.03 | 0.41 |
| 2:S2B:154:LEU:O | 2:S2B:155:LEU:HD22 | 2.21 | 0.41 |
| 7:S7B:76:ARG:HD3 | 7:S7B:89:MET:HG3 | 2.02 | 0.41 |
| 8:S8B:4:ASP:HB3 | 8:S8B:7:ALA:HB3 | 2.03 | 0.41 |
| 8:S8B:10:LEU:HD22 | 8:S8B:83:ILE:HD11 | 2.03 | 0.41 |
| 28:5SB:116:C:H2' | 28:5SB:117:G:C8 | 2.56 | 0.41 |
| 29:L2B:108:PRO:HG3 | 29:L2B:143:HIS:CE1 | 2.55 | 0.41 |
| 31:L4B:66:PRO:HD2 | 31:L4B:70:THR:HG21 | 2.02 | 0.41 |
| 32:L5B:173:LEU:HD13 | 32:L5B:178:PHE:CD2 | 2.56 | 0.41 |
| 34:L9B:77:LEU:HD12 | 34:L9B:104:GLN:HE22 | 1.86 | 0.41 |
| 2:S2A:48:MET:HE2 | 2:S2A:48:MET:HB3 | 1.90 | 0.40 |
| 2:S2A:97:TRP:HZ2 | 2:S2A:102:LEU:HD13 | 1.87 | 0.40 |
| 3:S3A:79:ARG:NH2 | 3:S3A:82:GLU:HG3 | 2.35 | 0.40 |
| 7:S7A:26:PHE:CE2 | 7:S7A:30:ILE:HD11 | 2.57 | 0.40 |
| 8:S8A:49:GLU:HG2 | 8:S8A:62:TYR:CE2 | 2.51 | 0.40 |
| 32:L5A:97:ASP:O | 32:L5A:101:ILE:N | 2.31 | 0.40 |
| 33:L6A:7:LEU:HD23 | 33:L6A:8:PRO:HD2 | 2.03 | 0.40 |
| 33:L6A:55:PRO:HD2 | 33:L6A:61:HIS:ND1 | 2.36 | 0.40 |
| 33:L6A:149:ARG:O | 33:L6A:149:ARG:HG2 | 2.22 | 0.40 |
| 34:L9A:78:THR:HG22 | 34:L9A:141:LYS:HB2 | 2.01 | 0.40 |
| 3:S3B:59:ARG:HG2 | 3:S3B:64:VAL:HG23 | 2.03 | 0.40 |
| 8:S8B:111:ILE:HB | 8:S8B:135:CYS:SG | 2.60 | 0.40 |
| 29:L2B:5:LYS:HD2 | 29:L2B:5:LYS:N | 2.30 | 0.40 |
| 31:L4B:128:ALA:O | 31:L4B:130:ALA:N | 2.51 | 0.40 |
| 33:L6B:151:ILE:H | 33:L6B:151:ILE:HG13 | 1.64 | 0.40 |
| 4:S4A:192:GLU:HG2 | 4:S4A:193:ASP:H | 1.87 | 0.40 |
| 30:L3A:14:ILE:HG13 | 30:L3A:21:VAL:HG13 | 2.01 | 0.40 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 32:L5A:170:ARG:HE | 32:L5A:174:GLU:CG | 2.34 | 0.40 |
| 33:L6A:3:ARG:HD3 | 33:L6A:5:GLY:H | 1.85 | 0.40 |
| 8:S8B:25:ASP:N | 8:S8B:25:ASP:OD1 | 2.54 | 0.40 |
| 30:L3B:171:GLU:O | 30:L3B:184:VAL:HA | 2.21 | 0.40 |
| 31:L4B:197:ASP:O | 31:L4B:198:ALA:HB3 | 2.21 | 0.40 |
| 32:L5B:47:LYS:HD2 | 32:L5B:81:LYS:CB | 2.49 | 0.40 |
| 34:L9B:56:LYS:O | 34:L9B:60:GLU:N | 2.36 | 0.40 |
| 2:S2A:100:GLY:O | 2:S2A:104:ASN:N | 2.42 | 0.40 |
| 2:S2A:112:VAL:HG22 | 2:S2A:149:LEU:HD13 | 2.04 | 0.40 |
| 3:S3A:59:ARG:HG2 | 3:S3A:64:VAL:HG22 | 2.03 | 0.40 |
| 30:L3A:111:ARG:HG2 | 30:L3A:160:TYR:O | 2.21 | 0.40 |
| 3:S3B:50:ALA:HB1 | 3:S3B:70:VAL:CG1 | 2.51 | 0.40 |
| 5:S5B:127:ASN:HA | 5:S5B:128:PRO:HD3 | 1.94 | 0.40 |
| 9:S9B:69:GLY:O | 9:S9B:73:GLN:HG3 | 2.21 | 0.40 |
| 33:L6B:149:ARG:HD2 | 33:L6B:164:TYR:CE1 | 2.56 | 0.40 |
| 33:L6B:172:LYS:N | 33:L6B:173:PRO:HA | 2.37 | 0.40 |
| 34:L9B:144:VAL:HG13 | 34:L9B:145:VAL:N | 2.37 | 0.40 |
| 2:S2A:156:LYS:H | 2:S2A:156:LYS:HD2 | 1.86 | 0.40 |
| 7:S7A:24:THR:HA | 7:S7A:27:ILE:HD12 | 2.03 | 0.40 |
| 31:L4A:128:ALA:C | 31:L4A:130:ALA:H | 2.29 | 0.40 |
| 32:L5A:173:LEU:O | 32:L5A:178:PHE:HB2 | 2.21 | 0.40 |
| 34:L9A:61:ARG:NH2 | 34:L9A:64:GLU:OE2 | 2.55 | 0.40 |
| 2:S2B:44:LEU:O | 2:S2B:47:THR:HB | 2.22 | 0.40 |
| 6:S6B:15:ASP:HB2 | 6:S6B:18:GLN:HB2 | 2.04 | 0.40 |
| 8:S8B:44:PHE:CD1 | 8:S8B:80:ILE:HG12 | 2.57 | 0.40 |
| 9:S9B:42:ARG:NH1 | 9:S9B:75:ASP:OD1 | 2.43 | 0.40 |
| 29:L2B:67:PHE:HD1 | 29:L2B:67:PHE:HA | 1.81 | 0.40 |
| 30:L3B:16:ARG:O | 30:L3B:19:ARG:HB3 | 2.22 | 0.40 |
| 33:L6B:83:TYR:HD2 | 33:L6B:132:ARG:HH22 | 1.69 | 0.40 |
| 2:S2A:70:PHE:H | 2:S2A:92:TYR:HA | 1.87 | 0.40 |
| 2:S2A:77:ALA:O | 2:S2A:81:VAL:HG23 | 2.22 | 0.40 |
| 3:S3A:83:ARG:O | 3:S3A:83:ARG:HG3 | 2.20 | 0.40 |
| 3:S3A:137:ALA:O | 3:S3A:141:VAL:HG23 | 2.21 | 0.40 |
| 8:S8A:20:TYR:HA | 8:S8A:65:TYR:CE2 | 2.56 | 0.40 |
| 2:S2B:26:PRO:O | 2:S2B:29:ALA:HB2 | 2.22 | 0.40 |
| 5:S5B:110:LEU:HD23 | 5:S5B:110:LEU:HA | 1.86 | 0.40 |
| 7:S7B:74:GLU:O | 7:S7B:88:PRO:HA | 2.21 | 0.40 |
| 7:S7B:126:ASP:O | 7:S7B:131:LYS:N | 2.54 | 0.40 |
| 29:L2B:11:PRO:C | 29:L2B:13:ARG:H | 2.29 | 0.40 |
| 32:L5B:133:LEU:HD11 | 32:L5B:157:ILE:HD12 | 2.04 | 0.40 |
| 33:L6B:4:ILE:HG21 | 33:L6B:6:ARG:CZ | 2.52 | 0.40 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 34:L9B:124:GLY:H | 34:L9B:142:VAL:CG2 | 2.35 | 0.40 |
| 34:L9B:132:PRO:HB2 | 34:L9B:133:HIS:H | 1.68 | 0.40 |

All (10) 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) |
|---|---|---|---|
| 34:L9A:112:LYS:NZ | 1:16SB:1115:G:C1'[4_555] | 0.88 | 1.32 |
| 34:L9A:112:LYS:CE | 1:16SB:1115:G:N3[4_555] | 1.44 | 0.76 |
| 34:L9A:112:LYS:CE | 1:16SB:1115:G:C4[4_555] | 1.53 | 0.67 |
| 34:L9A:112:LYS:NZ | 1:16SB:1115:G:O4'[4_555] | 1.54 | 0.66 |
| 34:L9A:112:LYS:NZ | 1:16SB:1115:G:N9[4_555] | 1.66 | 0.54 |
| 34:L9A:82:ARG:NH1 | 1:16SB:702:U:O2'[4_555] | 1.79 | 0.41 |
| 34:L9A:112:LYS:CE | 1:16SB:1115:G:N9[4_555] | 1.99 | 0.21 |
| 27:23SA:314:A:OP1 | 46:L24B:57:GLN:NE2[2_564] | 2.07 | 0.13 |
| 34:L9A:112:LYS:NZ | 1:16SB:1115:G:C4[4_555] | 2.10 | 0.10 |
| 34:L9A:112:LYS:NZ | 1:16SB:1115:G:N3[4_555] | 2.16 | 0.04 |

## 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 | S2A | 235/256 (92%) | 194 (83%) | 37 (16%) | 4 (2%) | 7 30 |
| 2 | S2B | 235/256 (92%) | 196 (83%) | 33 (14%) | 6 (3%) | 4 21 |
| 3 | S3A | 203/239 (85%) | 177 (87%) | 23 (11%) | 3 (2%) | 8 32 |
| 3 | S3B | 204/239 (85%) | 184 (90%) | 19 (9%) | 1 (0%) | 24 57 |
| 4 | S4A | 206/209 (99%) | 188 (91%) | 18 (9%) | 0 | 100 100 |
| 4 | S4B | 206/209 (99%) | 189 (92%) | 17 (8%) | 0 | 100 100 |
| 5 | S5A | 149/162 (92%) | 140 (94%) | 8 (5%) | 1 (1%) | 18 49 |

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| Mol | Chain | Analysed | Favoured | Allowed | Outliers | Percentiles |
|---|---|---|---|---|---|---|
| 5 | S5B | 149/162 (92%) | 140 (94%) | 9 (6%) | 0 | 100 100 |
| 6 | S6A | 99/101 (98%) | 92 (93%) | 7 (7%) | 0 | 100 100 |
| 6 | S6B | 99/101 (98%) | 93 (94%) | 6 (6%) | 0 | 100 100 |
| 7 | S7A | 153/156 (98%) | 142 (93%) | 11 (7%) | 0 | 100 100 |
| 7 | S7B | 151/156 (97%) | 140 (93%) | 10 (7%) | 1 (1%) | 18 49 |
| 8 | S8A | 136/138 (99%) | 122 (90%) | 13 (10%) | 1 (1%) | 18 49 |
| 8 | S8B | 136/138 (99%) | 124 (91%) | 12 (9%) | 0 | 100 100 |
| 9 | S9A | 125/128 (98%) | 104 (83%) | 20 (16%) | 1 (1%) | 16 47 |
| 9 | S9B | 125/128 (98%) | 107 (86%) | 18 (14%) | 0 | 100 100 |
| 10 | S10A | 97/105 (92%) | 87 (90%) | 10 (10%) | 0 | 100 100 |
| 10 | S10B | 97/105 (92%) | 81 (84%) | 14 (14%) | 2 (2%) | 5 25 |
| 11 | S11A | 114/129 (88%) | 104 (91%) | 10 (9%) | 0 | 100 100 |
| 11 | S11B | 115/129 (89%) | 104 (90%) | 11 (10%) | 0 | 100 100 |
| 12 | S12A | 122/132 (92%) | 105 (86%) | 16 (13%) | 1 (1%) | 16 47 |
| 12 | S12B | 122/132 (92%) | 109 (89%) | 11 (9%) | 2 (2%) | 7 30 |
| 13 | S13A | 117/126 (93%) | 100 (86%) | 13 (11%) | 4 (3%) | 3 16 |
| 13 | S13B | 119/126 (94%) | 95 (80%) | 20 (17%) | 4 (3%) | 3 16 |
| 14 | S14A | 58/61 (95%) | 51 (88%) | 6 (10%) | 1 (2%) | 7 30 |
| 14 | S14B | 57/61 (93%) | 48 (84%) | 6 (10%) | 3 (5%) | 1 10 |
| 15 | S15A | 86/89 (97%) | 81 (94%) | 3 (4%) | 2 (2%) | 5 23 |
| 15 | S15B | 86/89 (97%) | 82 (95%) | 3 (4%) | 1 (1%) | 10 37 |
| 16 | S16A | 81/88 (92%) | 77 (95%) | 4 (5%) | 0 | 100 100 |
| 16 | S16B | 82/88 (93%) | 79 (96%) | 3 (4%) | 0 | 100 100 |
| 17 | S17A | 98/105 (93%) | 91 (93%) | 7 (7%) | 0 | 100 100 |
| 17 | S17B | 98/105 (93%) | 91 (93%) | 7 (7%) | 0 | 100 100 |
| 18 | S18A | 69/88 (78%) | 63 (91%) | 4 (6%) | 2 (3%) | 3 19 |
| 18 | S18B | 68/88 (77%) | 62 (91%) | 6 (9%) | 0 | 100 100 |
| 19 | S19A | 82/93 (88%) | 61 (74%) | 19 (23%) | 2 (2%) | 4 22 |
| 19 | S19B | 84/93 (90%) | 66 (79%) | 17 (20%) | 1 (1%) | 10 37 |
| 20 | S20A | 97/106 (92%) | 83 (86%) | 11 (11%) | 3 (3%) | 3 18 |
| 20 | S20B | 97/106 (92%) | 83 (86%) | 11 (11%) | 3 (3%) | 3 18 |

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| Mol | Chain | Analysed | Favoured | Allowed | Outliers | Percentiles |
|---|---|---|---|---|---|---|
| 21 | THXA | 22/27 (82%) | 20 (91%) | 2 (9%) | 0 | 100 100 |
| 21 | THXB | 23/27 (85%) | 20 (87%) | 2 (9%) | 1 (4%) | 2 12 |
| 29 | L2A | 270/276 (98%) | 244 (90%) | 21 (8%) | 5 (2%) | 6 27 |
| 29 | L2B | 270/276 (98%) | 246 (91%) | 21 (8%) | 3 (1%) | 11 39 |
| 30 | L3A | 202/206 (98%) | 187 (93%) | 13 (6%) | 2 (1%) | 12 41 |
| 30 | L3B | 202/206 (98%) | 187 (93%) | 13 (6%) | 2 (1%) | 12 41 |
| 31 | L4A | 200/210 (95%) | 183 (92%) | 16 (8%) | 1 (0%) | 24 57 |
| 31 | L4B | 200/210 (95%) | 179 (90%) | 20 (10%) | 1 (0%) | 24 57 |
| 32 | L5A | 179/182 (98%) | 153 (86%) | 20 (11%) | 6 (3%) | 3 16 |
| 32 | L5B | 179/182 (98%) | 155 (87%) | 19 (11%) | 5 (3%) | 4 20 |
| 33 | L6A | 172/180 (96%) | 141 (82%) | 25 (14%) | 6 (4%) | 3 16 |
| 33 | L6B | 171/180 (95%) | 126 (74%) | 36 (21%) | 9 (5%) | 1 10 |
| 34 | L9A | 143/148 (97%) | 116 (81%) | 18 (13%) | 9 (6%) | 1 6 |
| 34 | L9B | 144/148 (97%) | 121 (84%) | 20 (14%) | 3 (2%) | 5 25 |
| 35 | L13A | 136/140 (97%) | 115 (85%) | 17 (12%) | 4 (3%) | 3 19 |
| 35 | L13B | 136/140 (97%) | 118 (87%) | 17 (12%) | 1 (1%) | 18 49 |
| 36 | L14A | 120/122 (98%) | 111 (92%) | 8 (7%) | 1 (1%) | 16 47 |
| 36 | L14B | 120/122 (98%) | 107 (89%) | 11 (9%) | 2 (2%) | 7 30 |
| 37 | L15A | 148/150 (99%) | 115 (78%) | 25 (17%) | 8 (5%) | 1 9 |
| 37 | L15B | 148/150 (99%) | 115 (78%) | 23 (16%) | 10 (7%) | 1 5 |
| 38 | L16A | 139/141 (99%) | 115 (83%) | 18 (13%) | 6 (4%) | 2 12 |
| 38 | L16B | 139/141 (99%) | 115 (83%) | 19 (14%) | 5 (4%) | 2 16 |
| 39 | L17A | 116/118 (98%) | 103 (89%) | 13 (11%) | 0 | 100 100 |
| 39 | L17B | 116/118 (98%) | 106 (91%) | 10 (9%) | 0 | 100 100 |
| 40 | L18A | 110/112 (98%) | 90 (82%) | 18 (16%) | 2 (2%) | 6 28 |
| 40 | L18B | 109/112 (97%) | 88 (81%) | 21 (19%) | 0 | 100 100 |
| 41 | L19A | 135/146 (92%) | 118 (87%) | 15 (11%) | 2 (2%) | 8 32 |
| 41 | L19B | 135/146 (92%) | 118 (87%) | 17 (13%) | 0 | 100 100 |
| 42 | L20A | 115/118 (98%) | 109 (95%) | 6 (5%) | 0 | 100 100 |
| 42 | L20B | 115/118 (98%) | 105 (91%) | 7 (6%) | 3 (3%) | 4 21 |
| 43 | L21A | 99/101 (98%) | 86 (87%) | 9 (9%) | 4 (4%) | 2 13 |

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| Mol | Chain | Analysed | Favoured | Allowed | Outliers | Percentiles |
|---|---|---|---|---|---|---|
| 43 | L21B | 99/101 (98%) | 78 (79%) | 16 (16%) | 5 (5%) | 1 10 |
| 44 | L22A | 111/113 (98%) | 103 (93%) | 8 (7%) | 0 | 100 100 |
| 44 | L22B | 111/113 (98%) | 100 (90%) | 10 (9%) | 1 (1%) | 14 44 |
| 45 | L23A | 93/96 (97%) | 89 (96%) | 4 (4%) | 0 | 100 100 |
| 45 | L23B | 92/96 (96%) | 85 (92%) | 7 (8%) | 0 | 100 100 |
| 46 | L24A | 106/110 (96%) | 83 (78%) | 16 (15%) | 7 (7%) | 1 6 |
| 46 | L24B | 104/110 (94%) | 83 (80%) | 16 (15%) | 5 (5%) | 2 11 |
| 47 | L25A | 177/206 (86%) | 136 (77%) | 32 (18%) | 9 (5%) | 1 10 |
| 47 | L25B | 174/206 (84%) | 136 (78%) | 32 (18%) | 6 (3%) | 3 16 |
| 48 | L27A | 82/85 (96%) | 72 (88%) | 10 (12%) | 0 | 100 100 |
| 48 | L27B | 82/85 (96%) | 70 (85%) | 11 (13%) | 1 (1%) | 10 37 |
| 49 | L28A | 95/98 (97%) | 83 (87%) | 10 (10%) | 2 (2%) | 5 25 |
| 49 | L28B | 95/98 (97%) | 79 (83%) | 14 (15%) | 2 (2%) | 5 25 |
| 50 | L29A | 67/72 (93%) | 61 (91%) | 6 (9%) | 0 | 100 100 |
| 50 | L29B | 66/72 (92%) | 61 (92%) | 5 (8%) | 0 | 100 100 |
| 51 | L30A | 57/60 (95%) | 54 (95%) | 3 (5%) | 0 | 100 100 |
| 51 | L30B | 57/60 (95%) | 55 (96%) | 2 (4%) | 0 | 100 100 |
| 52 | L31A | 69/71 (97%) | 43 (62%) | 22 (32%) | 4 (6%) | 1 8 |
| 52 | L31B | 69/71 (97%) | 46 (67%) | 18 (26%) | 5 (7%) | 1 5 |
| 53 | L32A | 54/60 (90%) | 43 (80%) | 11 (20%) | 0 | 100 100 |
| 53 | L32B | 54/60 (90%) | 47 (87%) | 6 (11%) | 1 (2%) | 6 27 |
| 54 | L33A | 43/54 (80%) | 27 (63%) | 11 (26%) | 5 (12%) | 0 1 |
| 54 | L33B | 43/54 (80%) | 30 (70%) | 10 (23%) | 3 (7%) | 1 5 |
| 55 | L34A | 46/49 (94%) | 43 (94%) | 3 (6%) | 0 | 100 100 |
| 55 | L34B | 47/49 (96%) | 45 (96%) | 2 (4%) | 0 | 100 100 |
| 56 | L35A | 62/65 (95%) | 55 (89%) | 7 (11%) | 0 | 100 100 |
| 56 | L35B | 62/65 (95%) | 56 (90%) | 6 (10%) | 0 | 100 100 |
| All | All | 11387/12054 (94%) | 9910 (87%) | 1271 (11%) | 206 (2%) | 6 28 |

All (206) Ramachandran outliers are listed below:

| Mol | Chain | Res | Type |
|---|---|---|---|
| 3 | S3A | 12 | LEU |

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| Mol | Chain | Res | Type |
|---|---|---|---|
| 12 | S12A | 62 | GLU |
| 13 | S13A | 67 | GLU |
| 13 | S13A | 101 | GLN |
| 14 | S14A | 24 | CYS |
| 19 | S19A | 41 | VAL |
| 20 | S20A | 48 | LYS |
| 29 | L2A | 122 | ASP |
| 29 | L2A | 123 | ALA |
| 30 | L3A | 118 | LYS |
| 31 | L4A | 128 | ALA |
| 32 | L5A | 96 | ARG |
| 33 | L6A | 81 | GLU |
| 33 | L6A | 173 | PRO |
| 34 | L9A | 134 | PRO |
| 35 | L13A | 97 | ARG |
| 35 | L13A | 137 | LYS |
| 36 | L14A | 97 | ARG |
| 37 | L15A | 7 | ARG |
| 37 | L15A | 15 | ARG |
| 37 | L15A | 29 | LYS |
| 37 | L15A | 38 | GLN |
| 37 | L15A | 57 | THR |
| 37 | L15A | 106 | LEU |
| 38 | L16A | 105 | GLU |
| 38 | L16A | 139 | GLU |
| 40 | L18A | 3 | ARG |
| 41 | L19A | 18 | ASP |
| 43 | L21A | 45 | THR |
| 43 | L21A | 50 | PRO |
| 46 | L24A | 81 | LYS |
| 46 | L24A | 90 | LEU |
| 46 | L24A | 92 | ASN |
| 47 | L25A | 13 | GLU |
| 47 | L25A | 111 | VAL |
| 54 | L33A | 45 | LYS |
| 54 | L33A | 48 | VAL |
| 54 | L33A | 49 | HIS |
| 2 | S2B | 20 | GLU |
| 2 | S2B | 154 | LEU |
| 7 | S7B | 55 | GLY |
| 10 | S10B | 17 | ASP |
| 12 | S12B | 62 | GLU |

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| Mol | Chain | Res | Type |
|---|---|---|---|
| 13 | S13B | 83 | ASP |
| 13 | S13B | 106 | ASN |
| 14 | S14B | 14 | PRO |
| 14 | S14B | 17 | LYS |
| 20 | S20B | 70 | SER |
| 20 | S20B | 74 | LYS |
| 21 | THXB | 3 | LYS |
| 29 | L2B | 239 | ARG |
| 31 | L4B | 128 | ALA |
| 32 | L5B | 5 | VAL |
| 32 | L5B | 81 | LYS |
| 32 | L5B | 96 | ARG |
| 33 | L6B | 99 | VAL |
| 34 | L9B | 76 | THR |
| 34 | L9B | 142 | VAL |
| 35 | L13B | 77 | GLY |
| 37 | L15B | 15 | ARG |
| 37 | L15B | 19 | VAL |
| 37 | L15B | 36 | LYS |
| 37 | L15B | 46 | LYS |
| 37 | L15B | 53 | GLY |
| 37 | L15B | 110 | TYR |
| 38 | L16B | 105 | GLU |
| 38 | L16B | 139 | GLU |
| 42 | L20B | 93 | LYS |
| 43 | L21B | 44 | LYS |
| 46 | L24B | 81 | LYS |
| 47 | L25B | 60 | GLU |
| 47 | L25B | 63 | ASP |
| 49 | L28B | 91 | LYS |
| 52 | L31B | 67 | TYR |
| 54 | L33B | 19 | ARG |
| 2 | S2A | 10 | LEU |
| 2 | S2A | 207 | ALA |
| 13 | S13A | 14 | ARG |
| 20 | S20A | 102 | GLY |
| 32 | L5A | 49 | ASP |
| 33 | L6A | 92 | ILE |
| 34 | L9A | 13 | GLY |
| 34 | L9A | 122 | GLU |
| 35 | L13A | 22 | THR |
| 37 | L15A | 19 | VAL |

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| Mol | Chain | Res | Type |
|---|---|---|---|
| 47 | L25A | 59 | LEU |
| 47 | L25A | 63 | ASP |
| 47 | L25A | 109 | ALA |
| 47 | L25A | 159 | PRO |
| 10 | S10B | 54 | PHE |
| 14 | S14B | 29 | ARG |
| 15 | S15B | 88 | ARG |
| 30 | L3B | 118 | LYS |
| 32 | L5B | 117 | PHE |
| 33 | L6B | 118 | PRO |
| 37 | L15B | 29 | LYS |
| 38 | L16B | 90 | VAL |
| 42 | L20B | 101 | ARG |
| 43 | L21B | 50 | PRO |
| 43 | L21B | 79 | VAL |
| 53 | L32B | 50 | GLY |
| 54 | L33B | 49 | HIS |
| 2 | S2A | 5 | ILE |
| 3 | S3A | 82 | GLU |
| 9 | S9A | 56 | LEU |
| 29 | L2A | 239 | ARG |
| 32 | L5A | 127 | GLY |
| 33 | L6A | 127 | GLU |
| 34 | L9A | 116 | LEU |
| 37 | L15A | 148 | LEU |
| 38 | L16A | 6 | ARG |
| 38 | L16A | 79 | LEU |
| 38 | L16A | 90 | VAL |
| 41 | L19A | 124 | ASP |
| 43 | L21A | 30 | GLY |
| 49 | L28A | 91 | LYS |
| 2 | S2B | 191 | ASP |
| 3 | S3B | 3 | ASN |
| 19 | S19B | 42 | PRO |
| 33 | L6B | 12 | PRO |
| 33 | L6B | 21 | PRO |
| 33 | L6B | 125 | VAL |
| 36 | L14B | 48 | PRO |
| 37 | L15B | 16 | ARG |
| 37 | L15B | 57 | THR |
| 2 | S2A | 155 | LEU |
| 15 | S15A | 23 | GLY |

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| Mol | Chain | Res | Type |
|---|---|---|---|
| 15 | S15A | 87 | ILE |
| 18 | S18A | 19 | LYS |
| 30 | L3A | 52 | LEU |
| 32 | L5A | 126 | ASP |
| 34 | L9A | 82 | ARG |
| 46 | L24A | 91 | GLU |
| 52 | L31A | 40 | HIS |
| 54 | L33A | 41 | PRO |
| 13 | S13B | 120 | LYS |
| 30 | L3B | 52 | LEU |
| 33 | L6B | 108 | GLY |
| 37 | L15B | 119 | GLU |
| 43 | L21B | 30 | GLY |
| 43 | L21B | 49 | THR |
| 44 | L22B | 67 | ASP |
| 46 | L24B | 76 | CYS |
| 47 | L25B | 6 | LYS |
| 47 | L25B | 61 | LEU |
| 52 | L31B | 41 | PRO |
| 52 | L31B | 49 | PHE |
| 8 | S8A | 129 | VAL |
| 20 | S20A | 97 | ALA |
| 29 | L2A | 240 | ALA |
| 32 | L5A | 82 | LEU |
| 32 | L5A | 86 | MET |
| 40 | L18A | 94 | TYR |
| 43 | L21A | 38 | LEU |
| 46 | L24A | 52 | SER |
| 47 | L25A | 52 | SER |
| 49 | L28A | 97 | LEU |
| 52 | L31A | 43 | TYR |
| 54 | L33A | 23 | THR |
| 2 | S2B | 96 | ARG |
| 2 | S2B | 130 | ARG |
| 12 | S12B | 42 | PRO |
| 20 | S20B | 68 | LYS |
| 29 | L2B | 240 | ALA |
| 33 | L6B | 127 | GLU |
| 38 | L16B | 6 | ARG |
| 38 | L16B | 79 | LEU |
| 48 | L27B | 3 | HIS |
| 3 | S3A | 4 | LYS |

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| Mol | Chain | Res | Type |
|---|---|---|---|
| 13 | S13A | 4 | ILE |
| 18 | S18A | 87 | ARG |
| 33 | L6A | 93 | GLY |
| 34 | L9A | 11 | ASN |
| 38 | L16A | 11 | LYS |
| 46 | L24A | 76 | CYS |
| 52 | L31A | 34 | GLU |
| 52 | L31A | 46 | GLN |
| 2 | S2B | 7 | VAL |
| 13 | S13B | 5 | ALA |
| 29 | L2B | 271 | ILE |
| 32 | L5B | 36 | LYS |
| 36 | L14B | 5 | GLN |
| 42 | L20B | 116 | ALA |
| 46 | L24B | 52 | SER |
| 46 | L24B | 54 | LYS |
| 47 | L25B | 13 | GLU |
| 52 | L31B | 42 | PHE |
| 5 | S5A | 22 | GLY |
| 19 | S19A | 40 | ILE |
| 33 | L6A | 126 | PRO |
| 34 | L9A | 132 | PRO |
| 46 | L24A | 51 | VAL |
| 34 | L9A | 133 | HIS |
| 47 | L25A | 61 | LEU |
| 33 | L6B | 120 | GLY |
| 46 | L24B | 96 | ILE |
| 54 | L33B | 41 | PRO |
| 29 | L2A | 271 | ILE |
| 49 | L28B | 55 | GLY |
| 52 | L31B | 29 | PRO |
| 34 | L9A | 118 | LYS |
| 35 | L13A | 126 | PRO |
| 47 | L25A | 114 | GLY |
| 33 | L6B | 151 | ILE |
| 47 | L25B | 159 | PRO |
| 34 | L9B | 132 | 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 | S2A | 205/220 (93%) | 187 (91%) | 18 (9%) | 9 33 |
| 2 | S2B | 205/220 (93%) | 198 (97%) | 7 (3%) | 32 63 |
| 3 | S3A | 159/188 (85%) | 152 (96%) | 7 (4%) | 25 56 |
| 3 | S3B | 160/188 (85%) | 143 (89%) | 17 (11%) | 6 26 |
| 4 | S4A | 180/181 (99%) | 171 (95%) | 9 (5%) | 22 53 |
| 4 | S4B | 180/181 (99%) | 174 (97%) | 6 (3%) | 33 63 |
| 5 | S5A | 116/123 (94%) | 112 (97%) | 4 (3%) | 32 63 |
| 5 | S5B | 116/123 (94%) | 112 (97%) | 4 (3%) | 32 63 |
| 6 | S6A | 90/90 (100%) | 86 (96%) | 4 (4%) | 25 56 |
| 6 | S6B | 90/90 (100%) | 87 (97%) | 3 (3%) | 33 63 |
| 7 | S7A | 126/127 (99%) | 120 (95%) | 6 (5%) | 23 54 |
| 7 | S7B | 126/127 (99%) | 118 (94%) | 8 (6%) | 16 45 |
| 8 | S8A | 119/119 (100%) | 111 (93%) | 8 (7%) | 15 43 |
| 8 | S8B | 119/119 (100%) | 113 (95%) | 6 (5%) | 22 53 |
| 9 | S9A | 98/99 (99%) | 91 (93%) | 7 (7%) | 13 41 |
| 9 | S9B | 98/99 (99%) | 89 (91%) | 9 (9%) | 8 31 |
| 10 | S10A | 89/92 (97%) | 86 (97%) | 3 (3%) | 32 63 |
| 10 | S10B | 89/92 (97%) | 83 (93%) | 6 (7%) | 15 43 |
| 11 | S11A | 88/99 (89%) | 85 (97%) | 3 (3%) | 32 63 |
| 11 | S11B | 89/99 (90%) | 88 (99%) | 1 (1%) | 65 78 |
| 12 | S12A | 103/108 (95%) | 98 (95%) | 5 (5%) | 22 53 |
| 12 | S12B | 103/108 (95%) | 100 (97%) | 3 (3%) | 37 66 |
| 13 | S13A | 95/101 (94%) | 91 (96%) | 4 (4%) | 26 58 |
| 13 | S13B | 97/101 (96%) | 93 (96%) | 4 (4%) | 27 59 |
| 14 | S14A | 49/50 (98%) | 44 (90%) | 5 (10%) | 7 28 |
| 14 | S14B | 49/50 (98%) | 46 (94%) | 3 (6%) | 17 46 |
| 15 | S15A | 79/80 (99%) | 77 (98%) | 2 (2%) | 42 69 |
| 15 | S15B | 79/80 (99%) | 77 (98%) | 2 (2%) | 42 69 |
| 16 | S16A | 72/74 (97%) | 68 (94%) | 4 (6%) | 19 49 |

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| Mol | Chain | Analysed | Rotameric | Outliers | Percentiles | |
|---|---|---|---|---|---|---|
| 16 | S16B | 72/74 (97%) | 70 (97%) | 2 (3%) | 38 | 66 |
| 17 | S17A | 95/97 (98%) | 91 (96%) | 4 (4%) | 26 | 58 |
| 17 | S17B | 95/97 (98%) | 91 (96%) | 4 (4%) | 26 | 58 |
| 18 | S18A | 62/77 (80%) | 60 (97%) | 2 (3%) | 34 | 64 |
| 18 | S18B | 61/77 (79%) | 58 (95%) | 3 (5%) | 22 | 53 |
| 19 | S19A | 73/80 (91%) | 68 (93%) | 5 (7%) | 14 | 42 |
| 19 | S19B | 73/80 (91%) | 69 (94%) | 4 (6%) | 19 | 50 |
| 20 | S20A | 76/82 (93%) | 74 (97%) | 2 (3%) | 40 | 68 |
| 20 | S20B | 76/82 (93%) | 73 (96%) | 3 (4%) | 28 | 60 |
| 21 | THXA | 19/22 (86%) | 19 (100%) | 0 | 100 | 100 |
| 21 | THXB | 20/22 (91%) | 19 (95%) | 1 (5%) | 22 | 53 |
| 29 | L2A | 214/218 (98%) | 209 (98%) | 5 (2%) | 44 | 70 |
| 29 | L2B | 214/218 (98%) | 209 (98%) | 5 (2%) | 44 | 70 |
| 30 | L3A | 165/166 (99%) | 161 (98%) | 4 (2%) | 43 | 69 |
| 30 | L3B | 165/166 (99%) | 163 (99%) | 2 (1%) | 63 | 78 |
| 31 | L4A | 161/166 (97%) | 156 (97%) | 5 (3%) | 35 | 64 |
| 31 | L4B | 161/166 (97%) | 158 (98%) | 3 (2%) | 50 | 73 |
| 32 | L5A | 155/156 (99%) | 148 (96%) | 7 (4%) | 24 | 56 |
| 32 | L5B | 155/156 (99%) | 143 (92%) | 12 (8%) | 12 | 38 |
| 33 | L6A | 145/148 (98%) | 140 (97%) | 5 (3%) | 32 | 63 |
| 33 | L6B | 144/148 (97%) | 128 (89%) | 16 (11%) | 6 | 24 |
| 34 | L9A | 122/124 (98%) | 116 (95%) | 6 (5%) | 22 | 53 |
| 34 | L9B | 122/124 (98%) | 114 (93%) | 8 (7%) | 15 | 43 |
| 35 | L13A | 117/119 (98%) | 112 (96%) | 5 (4%) | 26 | 57 |
| 35 | L13B | 117/119 (98%) | 115 (98%) | 2 (2%) | 53 | 74 |
| 36 | L14A | 100/100 (100%) | 98 (98%) | 2 (2%) | 48 | 72 |
| 36 | L14B | 100/100 (100%) | 97 (97%) | 3 (3%) | 36 | 65 |
| 37 | L15A | 116/116 (100%) | 105 (90%) | 11 (10%) | 8 | 30 |
| 37 | L15B | 116/116 (100%) | 109 (94%) | 7 (6%) | 17 | 47 |
| 38 | L16A | 111/111 (100%) | 104 (94%) | 7 (6%) | 16 | 45 |
| 38 | L16B | 111/111 (100%) | 105 (95%) | 6 (5%) | 20 | 50 |

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| Mol | Chain | Analysed | Rotameric | Outliers | Percentiles | |
|---|---|---|---|---|---|---|
| 39 | L17A | 101/101 (100%) | 98 (97%) | 3 (3%) | 36 | 65 |
| 39 | L17B | 101/101 (100%) | 97 (96%) | 4 (4%) | 28 | 60 |
| 40 | L18A | 88/88 (100%) | 85 (97%) | 3 (3%) | 32 | 63 |
| 40 | L18B | 87/88 (99%) | 79 (91%) | 8 (9%) | 8 | 31 |
| 41 | L19A | 120/127 (94%) | 114 (95%) | 6 (5%) | 22 | 53 |
| 41 | L19B | 120/127 (94%) | 116 (97%) | 4 (3%) | 33 | 63 |
| 42 | L20A | 93/94 (99%) | 90 (97%) | 3 (3%) | 34 | 64 |
| 42 | L20B | 93/94 (99%) | 84 (90%) | 9 (10%) | 8 | 30 |
| 43 | L21A | 82/82 (100%) | 76 (93%) | 6 (7%) | 13 | 40 |
| 43 | L21B | 82/82 (100%) | 73 (89%) | 9 (11%) | 6 | 24 |
| 44 | L22A | 92/92 (100%) | 87 (95%) | 5 (5%) | 20 | 50 |
| 44 | L22B | 92/92 (100%) | 87 (95%) | 5 (5%) | 20 | 50 |
| 45 | L23A | 76/78 (97%) | 75 (99%) | 1 (1%) | 61 | 77 |
| 45 | L23B | 76/78 (97%) | 71 (93%) | 5 (7%) | 15 | 43 |
| 46 | L24A | 89/91 (98%) | 85 (96%) | 4 (4%) | 24 | 56 |
| 46 | L24B | 79/91 (87%) | 75 (95%) | 4 (5%) | 21 | 52 |
| 47 | L25A | 158/179 (88%) | 153 (97%) | 5 (3%) | 34 | 64 |
| 47 | L25B | 155/179 (87%) | 143 (92%) | 12 (8%) | 12 | 38 |
| 48 | L27A | 66/67 (98%) | 63 (96%) | 3 (4%) | 24 | 56 |
| 48 | L27B | 66/67 (98%) | 63 (96%) | 3 (4%) | 24 | 56 |
| 49 | L28A | 82/83 (99%) | 79 (96%) | 3 (4%) | 30 | 61 |
| 49 | L28B | 82/83 (99%) | 81 (99%) | 1 (1%) | 63 | 78 |
| 50 | L29A | 65/67 (97%) | 64 (98%) | 1 (2%) | 57 | 75 |
| 50 | L29B | 64/67 (96%) | 62 (97%) | 2 (3%) | 35 | 64 |
| 51 | L30A | 51/52 (98%) | 50 (98%) | 1 (2%) | 48 | 72 |
| 51 | L30B | 51/52 (98%) | 50 (98%) | 1 (2%) | 48 | 72 |
| 52 | L31A | 63/63 (100%) | 57 (90%) | 6 (10%) | 8 | 30 |
| 52 | L31B | 63/63 (100%) | 56 (89%) | 7 (11%) | 6 | 24 |
| 53 | L32A | 48/52 (92%) | 45 (94%) | 3 (6%) | 16 | 45 |
| 53 | L32B | 48/52 (92%) | 43 (90%) | 5 (10%) | 7 | 27 |
| 54 | L33A | 44/52 (85%) | 41 (93%) | 3 (7%) | 14 | 42 |

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| Mol | Chain | Analysed | Rotameric | Outliers | Percentiles |
|---|---|---|---|---|---|
| 54 | L33B | 44/52 (85%) | 41 (93%) | 3 (7%) | 14 42 |
| 55 | L34A | 41/42 (98%) | 39 (95%) | 2 (5%) | 22 53 |
| 55 | L34B | 42/42 (100%) | 40 (95%) | 2 (5%) | 23 54 |
| 56 | L35A | 54/55 (98%) | 53 (98%) | 1 (2%) | 50 73 |
| 56 | L35B | 54/55 (98%) | 48 (89%) | 6 (11%) | 6 24 |
| All | All | 9613/9996 (96%) | 9145 (95%) | 468 (5%) | 22 53 |

All (468) residues with a non-rotameric sidechain are listed below:

| Mol | Chain | Res | Type |
|---|---|---|---|
| 2 | S2A | 9 | GLU |
| 2 | S2A | 12 | GLU |
| 2 | S2A | 17 | PHE |
| 2 | S2A | 28 | PHE |
| 2 | S2A | 30 | ARG |
| 2 | S2A | 74 | LYS |
| 2 | S2A | 75 | LYS |
| 2 | S2A | 96 | ARG |
| 2 | S2A | 111 | ARG |
| 2 | S2A | 124 | SER |
| 2 | S2A | 137 | ARG |
| 2 | S2A | 163 | PHE |
| 2 | S2A | 192 | SER |
| 2 | S2A | 196 | LEU |
| 2 | S2A | 209 | ARG |
| 2 | S2A | 210 | SER |
| 2 | S2A | 212 | GLN |
| 2 | S2A | 215 | LEU |
| 3 | S3A | 17 | ASP |
| 3 | S3A | 29 | TYR |
| 3 | S3A | 79 | ARG |
| 3 | S3A | 98 | ASN |
| 3 | S3A | 112 | SER |
| 3 | S3A | 128 | PHE |
| 3 | S3A | 167 | TRP |
| 4 | S4A | 3 | ARG |
| 4 | S4A | 10 | ARG |
| 4 | S4A | 49 | ARG |
| 4 | S4A | 84 | LYS |
| 4 | S4A | 134 | ASP |

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| Mol | Chain | Res | Type |
|---|---|---|---|
| 4 | S4A | 150 | GLU |
| 4 | S4A | 187 | ARG |
| 4 | S4A | 193 | ASP |
| 4 | S4A | 209 | ARG |
| 5 | S5A | 10 | MET |
| 5 | S5A | 73 | ASN |
| 5 | S5A | 79 | GLU |
| 5 | S5A | 155 | GLU |
| 6 | S6A | 7 | ASN |
| 6 | S6A | 15 | ASP |
| 6 | S6A | 19 | LEU |
| 6 | S6A | 54 | LYS |
| 7 | S7A | 6 | ARG |
| 7 | S7A | 78 | ARG |
| 7 | S7A | 94 | ARG |
| 7 | S7A | 114 | ARG |
| 7 | S7A | 137 | LYS |
| 7 | S7A | 155 | ARG |
| 8 | S8A | 1 | MET |
| 8 | S8A | 41 | ARG |
| 8 | S8A | 56 | LYS |
| 8 | S8A | 88 | LYS |
| 8 | S8A | 91 | ARG |
| 8 | S8A | 104 | ARG |
| 8 | S8A | 112 | LEU |
| 8 | S8A | 121 | ASP |
| 9 | S9A | 91 | ASP |
| 9 | S9A | 95 | LYS |
| 9 | S9A | 105 | ASP |
| 9 | S9A | 111 | ARG |
| 9 | S9A | 112 | LYS |
| 9 | S9A | 114 | TYR |
| 9 | S9A | 121 | ARG |
| 10 | S10A | 3 | LYS |
| 10 | S10A | 60 | ARG |
| 10 | S10A | 78 | ASN |
| 11 | S11A | 13 | GLN |
| 11 | S11A | 51 | LYS |
| 11 | S11A | 77 | MET |
| 12 | S12A | 16 | ARG |
| 12 | S12A | 17 | LYS |
| 12 | S12A | 25 | LYS |

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| Mol | Chain | Res | Type |
|---|---|---|---|
| 12 | S12A | 30 | ARG |
| 12 | S12A | 95 | TYR |
| 13 | S13A | 48 | LEU |
| 13 | S13A | 64 | TRP |
| 13 | S13A | 65 | LYS |
| 13 | S13A | 69 | GLU |
| 14 | S14A | 16 | PHE |
| 14 | S14A | 23 | ARG |
| 14 | S14A | 24 | CYS |
| 14 | S14A | 35 | ARG |
| 14 | S14A | 41 | ARG |
| 15 | S15A | 21 | ASP |
| 15 | S15A | 64 | ARG |
| 16 | S16A | 8 | ARG |
| 16 | S16A | 43 | LYS |
| 16 | S16A | 72 | ARG |
| 16 | S16A | 75 | ARG |
| 17 | S17A | 52 | LYS |
| 17 | S17A | 68 | ARG |
| 17 | S17A | 91 | ARG |
| 17 | S17A | 101 | ARG |
| 18 | S18A | 19 | LYS |
| 18 | S18A | 26 | LEU |
| 19 | S19A | 27 | GLU |
| 19 | S19A | 37 | ARG |
| 19 | S19A | 44 | MET |
| 19 | S19A | 78 | ARG |
| 19 | S19A | 81 | ARG |
| 20 | S20A | 45 | GLN |
| 20 | S20A | 92 | LEU |
| 29 | L2A | 13 | ARG |
| 29 | L2A | 14 | ARG |
| 29 | L2A | 38 | LYS |
| 29 | L2A | 212 | SER |
| 29 | L2A | 237 | GLU |
| 30 | L3A | 64 | LYS |
| 30 | L3A | 111 | ARG |
| 30 | L3A | 113 | PHE |
| 30 | L3A | 154 | LYS |
| 31 | L4A | 17 | ARG |
| 31 | L4A | 95 | ARG |
| 31 | L4A | 98 | SER |

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| Mol | Chain | Res | Type |
|---|---|---|---|
| 31 | L4A | 108 | LYS |
| 31 | L4A | 117 | ARG |
| 32 | L5A | 18 | GLU |
| 32 | L5A | 51 | ARG |
| 32 | L5A | 58 | GLN |
| 32 | L5A | 67 | LYS |
| 32 | L5A | 80 | PHE |
| 32 | L5A | 86 | MET |
| 32 | L5A | 174 | GLU |
| 33 | L6A | 77 | LYS |
| 33 | L6A | 86 | GLU |
| 33 | L6A | 104 | GLU |
| 33 | L6A | 149 | ARG |
| 33 | L6A | 155 | SER |
| 34 | L9A | 25 | TYR |
| 34 | L9A | 57 | ARG |
| 34 | L9A | 110 | ASP |
| 34 | L9A | 126 | TYR |
| 34 | L9A | 133 | HIS |
| 34 | L9A | 139 | GLN |
| 35 | L13A | 7 | LYS |
| 35 | L13A | 39 | ARG |
| 35 | L13A | 90 | MET |
| 35 | L13A | 97 | ARG |
| 35 | L13A | 115 | ARG |
| 36 | L14A | 7 | TYR |
| 36 | L14A | 28 | SER |
| 37 | L15A | 13 | ASN |
| 37 | L15A | 15 | ARG |
| 37 | L15A | 19 | VAL |
| 37 | L15A | 21 | ARG |
| 37 | L15A | 27 | HIS |
| 37 | L15A | 50 | ARG |
| 37 | L15A | 55 | ARG |
| 37 | L15A | 108 | LYS |
| 37 | L15A | 133 | SER |
| 37 | L15A | 144 | GLU |
| 37 | L15A | 148 | LEU |
| 38 | L16A | 10 | ARG |
| 38 | L16A | 14 | ARG |
| 38 | L16A | 25 | ASP |
| 38 | L16A | 45 | GLN |

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| Mol | Chain | Res | Type |
|---|---|---|---|
| 38 | L16A | 59 | ARG |
| 38 | L16A | 89 | ASN |
| 38 | L16A | 101 | ARG |
| 39 | L17A | 44 | LEU |
| 39 | L17A | 64 | ARG |
| 39 | L17A | 105 | ARG |
| 40 | L18A | 15 | ARG |
| 40 | L18A | 58 | LEU |
| 40 | L18A | 89 | ARG |
| 41 | L19A | 1 | MET |
| 41 | L19A | 51 | ARG |
| 41 | L19A | 78 | LEU |
| 41 | L19A | 96 | ARG |
| 41 | L19A | 111 | ARG |
| 41 | L19A | 112 | ARG |
| 42 | L20A | 5 | LYS |
| 42 | L20A | 92 | ARG |
| 42 | L20A | 104 | GLN |
| 43 | L21A | 10 | LYS |
| 43 | L21A | 12 | TYR |
| 43 | L21A | 21 | ARG |
| 43 | L21A | 38 | LEU |
| 43 | L21A | 44 | LYS |
| 43 | L21A | 52 | VAL |
| 44 | L22A | 11 | ARG |
| 44 | L22A | 37 | ARG |
| 44 | L22A | 67 | ASP |
| 44 | L22A | 70 | TYR |
| 44 | L22A | 92 | ARG |
| 45 | L23A | 64 | LYS |
| 46 | L24A | 6 | HIS |
| 46 | L24A | 57 | GLN |
| 46 | L24A | 81 | LYS |
| 46 | L24A | 102 | CYS |
| 47 | L25A | 1 | MET |
| 47 | L25A | 49 | ARG |
| 47 | L25A | 72 | ARG |
| 47 | L25A | 81 | ARG |
| 47 | L25A | 132 | ASN |
| 48 | L27A | 14 | ARG |
| 48 | L27A | 44 | ARG |
| 48 | L27A | 64 | ASP |

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| Mol | Chain | Res | Type |
|---|---|---|---|
| 49 | L28A | 69 | LYS |
| 49 | L28A | 78 | LYS |
| 49 | L28A | 81 | LYS |
| 50 | L29A | 8 | LYS |
| 51 | L30A | 33 | GLN |
| 52 | L31A | 18 | CYS |
| 52 | L31A | 38 | LYS |
| 52 | L31A | 55 | ARG |
| 52 | L31A | 61 | ARG |
| 52 | L31A | 63 | TYR |
| 52 | L31A | 67 | TYR |
| 53 | L32A | 16 | ARG |
| 53 | L32A | 23 | HIS |
| 53 | L32A | 51 | TYR |
| 54 | L33A | 33 | LYS |
| 54 | L33A | 34 | LEU |
| 54 | L33A | 39 | TYR |
| 55 | L34A | 10 | ARG |
| 55 | L34A | 41 | ARG |
| 56 | L35A | 52 | LYS |
| 2 | S2B | 21 | ARG |
| 2 | S2B | 56 | ARG |
| 2 | S2B | 64 | ARG |
| 2 | S2B | 137 | ARG |
| 2 | S2B | 163 | PHE |
| 2 | S2B | 217 | ARG |
| 2 | S2B | 233 | SER |
| 3 | S3B | 16 | ARG |
| 3 | S3B | 26 | LYS |
| 3 | S3B | 29 | TYR |
| 3 | S3B | 36 | ASP |
| 3 | S3B | 45 | LYS |
| 3 | S3B | 48 | TYR |
| 3 | S3B | 52 | LEU |
| 3 | S3B | 54 | ARG |
| 3 | S3B | 56 | ASP |
| 3 | S3B | 62 | ASP |
| 3 | S3B | 72 | LYS |
| 3 | S3B | 79 | ARG |
| 3 | S3B | 83 | ARG |
| 3 | S3B | 101 | LEU |
| 3 | S3B | 119 | ARG |

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| Mol | Chain | Res | Type |
|---|---|---|---|
| 3 | S3B | 131 | ARG |
| 3 | S3B | 196 | LEU |
| 4 | S4B | 10 | ARG |
| 4 | S4B | 33 | MET |
| 4 | S4B | 49 | ARG |
| 4 | S4B | 118 | ARG |
| 4 | S4B | 162 | LEU |
| 4 | S4B | 181 | MET |
| 5 | S5B | 10 | MET |
| 5 | S5B | 26 | PHE |
| 5 | S5B | 126 | ARG |
| 5 | S5B | 137 | GLU |
| 6 | S6B | 3 | ARG |
| 6 | S6B | 82 | ARG |
| 6 | S6B | 93 | SER |
| 7 | S7B | 41 | ARG |
| 7 | S7B | 54 | THR |
| 7 | S7B | 56 | GLN |
| 7 | S7B | 72 | ARG |
| 7 | S7B | 85 | TYR |
| 7 | S7B | 114 | ARG |
| 7 | S7B | 140 | ASP |
| 7 | S7B | 156 | TRP |
| 8 | S8B | 1 | MET |
| 8 | S8B | 25 | ASP |
| 8 | S8B | 77 | GLU |
| 8 | S8B | 84 | ARG |
| 8 | S8B | 102 | ARG |
| 8 | S8B | 112 | LEU |
| 9 | S9B | 4 | TYR |
| 9 | S9B | 20 | ARG |
| 9 | S9B | 71 | SER |
| 9 | S9B | 95 | LYS |
| 9 | S9B | 97 | LYS |
| 9 | S9B | 107 | ARG |
| 9 | S9B | 113 | LYS |
| 9 | S9B | 121 | ARG |
| 9 | S9B | 125 | TYR |
| 10 | S10B | 21 | GLN |
| 10 | S10B | 22 | LYS |
| 10 | S10B | 45 | ARG |
| 10 | S10B | 69 | ASN |

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| Mol | Chain | Res | Type |
|---|---|---|---|
| 10 | S10B | 70 | ARG |
| 10 | S10B | 79 | ARG |
| 11 | S11B | 116 | HIS |
| 12 | S12B | 61 | TYR |
| 12 | S12B | 72 | HIS |
| 12 | S12B | 99 | ARG |
| 13 | S13B | 47 | ASP |
| 13 | S13B | 64 | TRP |
| 13 | S13B | 88 | ARG |
| 13 | S13B | 94 | ARG |
| 14 | S14B | 29 | ARG |
| 14 | S14B | 35 | ARG |
| 14 | S14B | 58 | LYS |
| 15 | S15B | 10 | LYS |
| 15 | S15B | 63 | ARG |
| 16 | S16B | 43 | LYS |
| 16 | S16B | 82 | GLN |
| 17 | S17B | 63 | ARG |
| 17 | S17B | 68 | ARG |
| 17 | S17B | 79 | SER |
| 17 | S17B | 101 | ARG |
| 18 | S18B | 28 | GLU |
| 18 | S18B | 54 | ARG |
| 18 | S18B | 87 | ARG |
| 19 | S19B | 29 | ARG |
| 19 | S19B | 32 | LYS |
| 19 | S19B | 80 | TYR |
| 19 | S19B | 83 | HIS |
| 20 | S20B | 11 | SER |
| 20 | S20B | 23 | ARG |
| 20 | S20B | 74 | LYS |
| 21 | THXB | 15 | ARG |
| 29 | L2B | 5 | LYS |
| 29 | L2B | 38 | LYS |
| 29 | L2B | 88 | ARG |
| 29 | L2B | 262 | ARG |
| 29 | L2B | 273 | ARG |
| 30 | L3B | 79 | ARG |
| 30 | L3B | 111 | ARG |
| 31 | L4B | 29 | ASN |
| 31 | L4B | 50 | SER |
| 31 | L4B | 205 | ARG |

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| Mol | Chain | Res | Type |
|---|---|---|---|
| 32 | L5B | 4 | ASP |
| 32 | L5B | 10 | LYS |
| 32 | L5B | 21 | ARG |
| 32 | L5B | 33 | ARG |
| 32 | L5B | 47 | LYS |
| 32 | L5B | 51 | ARG |
| 32 | L5B | 67 | LYS |
| 32 | L5B | 80 | PHE |
| 32 | L5B | 91 | ARG |
| 32 | L5B | 95 | ARG |
| 32 | L5B | 118 | ARG |
| 32 | L5B | 153 | ARG |
| 33 | L6B | 23 | ARG |
| 33 | L6B | 25 | LYS |
| 33 | L6B | 59 | ARG |
| 33 | L6B | 67 | LEU |
| 33 | L6B | 77 | LYS |
| 33 | L6B | 83 | TYR |
| 33 | L6B | 86 | GLU |
| 33 | L6B | 88 | LEU |
| 33 | L6B | 97 | ARG |
| 33 | L6B | 101 | ARG |
| 33 | L6B | 111 | HIS |
| 33 | L6B | 147 | ASN |
| 33 | L6B | 152 | ARG |
| 33 | L6B | 153 | LYS |
| 33 | L6B | 155 | SER |
| 33 | L6B | 167 | GLU |
| 34 | L9B | 38 | LEU |
| 34 | L9B | 56 | LYS |
| 34 | L9B | 69 | LYS |
| 34 | L9B | 89 | TYR |
| 34 | L9B | 103 | ARG |
| 34 | L9B | 104 | GLN |
| 34 | L9B | 121 | LYS |
| 34 | L9B | 133 | HIS |
| 35 | L13B | 76 | SER |
| 35 | L13B | 114 | ARG |
| 36 | L14B | 13 | ASN |
| 36 | L14B | 23 | ARG |
| 36 | L14B | 104 | ARG |
| 37 | L15B | 21 | ARG |

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| Mol | Chain | Res | Type |
|---|---|---|---|
| 37 | L15B | 35 | HIS |
| 37 | L15B | 85 | LEU |
| 37 | L15B | 110 | TYR |
| 37 | L15B | 115 | LEU |
| 37 | L15B | 117 | GLU |
| 37 | L15B | 124 | LYS |
| 38 | L16B | 10 | ARG |
| 38 | L16B | 14 | ARG |
| 38 | L16B | 45 | GLN |
| 38 | L16B | 59 | ARG |
| 38 | L16B | 89 | ASN |
| 38 | L16B | 101 | ARG |
| 39 | L17B | 1 | MET |
| 39 | L17B | 2 | ARG |
| 39 | L17B | 88 | ARG |
| 39 | L17B | 91 | GLN |
| 40 | L18B | 15 | ARG |
| 40 | L18B | 25 | ARG |
| 40 | L18B | 30 | ARG |
| 40 | L18B | 34 | HIS |
| 40 | L18B | 56 | LEU |
| 40 | L18B | 75 | GLU |
| 40 | L18B | 89 | ARG |
| 40 | L18B | 110 | LEU |
| 41 | L19B | 1 | MET |
| 41 | L19B | 98 | LYS |
| 41 | L19B | 112 | ARG |
| 41 | L19B | 125 | ARG |
| 42 | L20B | 15 | LYS |
| 42 | L20B | 19 | LYS |
| 42 | L20B | 25 | TRP |
| 42 | L20B | 57 | PHE |
| 42 | L20B | 60 | LEU |
| 42 | L20B | 69 | CYS |
| 42 | L20B | 79 | PHE |
| 42 | L20B | 97 | ASP |
| 42 | L20B | 114 | LYS |
| 43 | L21B | 10 | LYS |
| 43 | L21B | 44 | LYS |
| 43 | L21B | 60 | GLU |
| 43 | L21B | 73 | SER |
| 43 | L21B | 74 | LYS |

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| Mol | Chain | Res | Type |
|---|---|---|---|
| 43 | L21B | 75 | PHE |
| 43 | L21B | 78 | LYS |
| 43 | L21B | 82 | ARG |
| 43 | L21B | 98 | GLU |
| 44 | L22B | 11 | ARG |
| 44 | L22B | 67 | ASP |
| 44 | L22B | 70 | TYR |
| 44 | L22B | 111 | HIS |
| 44 | L22B | 113 | LYS |
| 45 | L23B | 14 | SER |
| 45 | L23B | 53 | LYS |
| 45 | L23B | 62 | LYS |
| 45 | L23B | 64 | LYS |
| 45 | L23B | 76 | ARG |
| 46 | L24B | 43 | ASN |
| 46 | L24B | 55 | TYR |
| 46 | L24B | 101 | LYS |
| 46 | L24B | 102 | CYS |
| 47 | L25B | 2 | GLU |
| 47 | L25B | 31 | ARG |
| 47 | L25B | 34 | ASN |
| 47 | L25B | 76 | LEU |
| 47 | L25B | 82 | ARG |
| 47 | L25B | 87 | ASP |
| 47 | L25B | 94 | GLU |
| 47 | L25B | 119 | GLU |
| 47 | L25B | 131 | ARG |
| 47 | L25B | 136 | PHE |
| 47 | L25B | 154 | ASP |
| 47 | L25B | 169 | GLU |
| 48 | L27B | 5 | LYS |
| 48 | L27B | 25 | ARG |
| 48 | L27B | 35 | ASN |
| 49 | L28B | 88 | LYS |
| 50 | L29B | 3 | LEU |
| 50 | L29B | 67 | LYS |
| 51 | L30B | 30 | ARG |
| 52 | L31B | 40 | HIS |
| 52 | L31B | 49 | PHE |
| 52 | L31B | 53 | GLU |
| 52 | L31B | 58 | ARG |
| 52 | L31B | 61 | ARG |

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| Mol | Chain | Res | Type |
|---|---|---|---|
| 52 | L31B | 62 | ARG |
| 52 | L31B | 69 | LYS |
| 53 | L32B | 21 | SER |
| 53 | L32B | 33 | CYS |
| 53 | L32B | 40 | LYS |
| 53 | L32B | 52 | TYR |
| 53 | L32B | 55 | ARG |
| 54 | L33B | 17 | LYS |
| 54 | L33B | 18 | ARG |
| 54 | L33B | 53 | LYS |
| 55 | L34B | 32 | LYS |
| 55 | L34B | 49 | ARG |
| 56 | L35B | 19 | SER |
| 56 | L35B | 21 | LYS |
| 56 | L35B | 31 | HIS |
| 56 | L35B | 46 | ARG |
| 56 | L35B | 47 | LYS |
| 56 | L35B | 52 | LYS |

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. There are no such sidechains identified.

### 5.3.3 RNA

| Mol | Chain | Analysed | Backbone Outliers | Pucker Outliers |
|---|---|---|---|---|
| 1 | 16SA | 1510/1512 (99%) | 335 (22%) | 52 (3%) |
| 1 | 16SB | 1506/1512 (99%) | 338 (22%) | 48 (3%) |
| 22 | ASIA | 75/76 (98%) | 44 (58%) | 2 (2%) |
| 23 | PSIA | 75/76 (98%) | 23 (30%) | 2 (2%) |
| 23 | PSIB | 75/76 (98%) | 31 (41%) | 2 (2%) |
| 24 | ESIA | 75/76 (98%) | 33 (44%) | 1 (1%) |
| 24 | ESIB | 75/76 (98%) | 24 (32%) | 3 (4%) |
| 25 | MRNA | 29/30 (96%) | 7 (24%) | 2 (6%) |
| 25 | MRNB | 29/30 (96%) | 11 (37%) | 2 (6%) |
| 26 | TRNA | 72/76 (94%) | 34 (47%) | 3 (4%) |
| 27 | 23SA | 2884/2911 (99%) | 652 (22%) | 66 (2%) |
| 27 | 23SB | 2871/2911 (98%) | 670 (23%) | 67 (2%) |
| 28 | 5SA | 121/124 (97%) | 25 (20%) | 1 (0%) |
| 28 | 5SB | 120/124 (96%) | 33 (27%) | 5 (4%) |
| 57 | ASIB | 75/76 (98%) | 36 (48%) | 2 (2%) |
| All | All | 9592/9686 (99%) | 2296 (23%) | 258 (2%) |

All (2296) RNA backbone outliers are listed below:

| Mol | Chain | Res | Type |
|---|---|---|---|
| 1 | 16SA | 654 | A |
| 1 | 16SA | 655 | G |
| 1 | 16SA | 656 | A |
| 1 | 16SA | 678 | A |
| 1 | 16SA | 685 | G |
| 1 | 16SA | 687 | G |
| 1 | 16SA | 693 | C |
| 1 | 16SA | 694 | C |
| 1 | 16SA | 697 | A |
| 1 | 16SA | 707 | G |
| 1 | 16SA | 711 | U |
| 1 | 16SA | 712 | G |
| 1 | 16SA | 719 | G |
| 1 | 16SA | 724 | G |
| 1 | 16SA | 725 | U |
| 1 | 16SA | 726 | U |
| 1 | 16SA | 727 | U |
| 1 | 16SA | 728 | U |
| 1 | 16SA | 729 | A |
| 1 | 16SA | 732 | C |
| 1 | 16SA | 733 | C |
| 1 | 16SA | 740 | A |
| 1 | 16SA | 747 | G |
| 1 | 16SA | 758 | A |
| 1 | 16SA | 759 | A |
| 1 | 16SA | 760 | C |
| 1 | 16SA | 773 | U |
| 1 | 16SA | 777 | C |
| 1 | 16SA | 782 | G |
| 1 | 16SA | 784 | G |
| 1 | 16SA | 800 | A |
| 1 | 16SA | 802 | A |
| 1 | 16SA | 803 | C |
| 1 | 16SA | 809 | C |
| 1 | 16SA | 810 | U |
| 1 | 16SA | 812 | A |
| 1 | 16SA | 813 | U |
| 1 | 16SA | 821 | G |
| 1 | 16SA | 832 | C |
| 1 | 16SA | 835 | U |
| 1 | 16SA | 836 | G |
| 1 | 16SA | 837 | G |

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| Mol | Chain | Res | Type |
|---|---|---|---|
| 1 | 16SA | 847 | A |
| 1 | 16SA | 848 | A |
| 1 | 16SA | 849 | A |
| 1 | 16SA | 853 | C |
| 1 | 16SA | 855 | U |
| 1 | 16SA | 856 | U |
| 1 | 16SA | 857 | G |
| 1 | 16SA | 867 | G |
| 1 | 16SA | 872 | G |
| 1 | 16SA | 885 | U |
| 1 | 16SA | 888 | G |
| 1 | 16SA | 892 | G |
| 1 | 16SA | 907 | G |
| 1 | 16SA | 908 | C |
| 1 | 16SA | 911 | A |
| 1 | 16SA | 922 | G |
| 1 | 16SA | 930 | G |
| 1 | 16SA | 962 | A |
| 1 | 16SA | 969 | C |
| 1 | 16SA | 970 | A |
| 1 | 16SA | 973 | G |
| 1 | 16SA | 985 | A |
| 1 | 16SA | 986 | C |
| 1 | 16SA | 987 | G |
| 1 | 16SA | 988 | G |
| 1 | 16SA | 990 | A |
| 1 | 16SA | 992 | G |
| 1 | 16SA | 993 | C |
| 1 | 16SA | 994 | A |
| 1 | 16SA | 995 | G |
| 1 | 16SA | 1008 | U |
| 1 | 16SA | 1014 | A |
| 1 | 16SA | 1029 | G |
| 1 | 16SA | 1038 | A |
| 1 | 16SA | 1039 | C |
| 1 | 16SA | 1047 | G |
| 1 | 16SA | 1050 | G |
| 1 | 16SA | 1053 | A |
| 1 | 16SA | 1054 | G |
| 1 | 16SA | 1055 | A |
| 1 | 16SA | 1062 | U |
| 1 | 16SA | 1063 | C |

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| Mol | Chain | Res | Type |
|---|---|---|---|
| 1 | 16SA | 1064 | G |
| 1 | 16SA | 1065 | G |
| 1 | 16SA | 1070 | U |
| 1 | 16SA | 1071 | A |
| 1 | 16SA | 1075 | U |
| 1 | 16SA | 1080 | A |
| 1 | 16SA | 1081 | A |
| 1 | 16SA | 1100 | A |
| 1 | 16SA | 1101 | C |
| 1 | 16SA | 1102 | G |
| 1 | 16SA | 1105 | G |
| 1 | 16SA | 1112 | A |
| 1 | 16SA | 1115 | G |
| 1 | 16SA | 1116 | U |
| 1 | 16SA | 1126 | A |
| 1 | 16SA | 1127 | U |
| 1 | 16SA | 1134 | G |
| 1 | 16SA | 1138 | A |
| 1 | 16SA | 1139 | A |
| 1 | 16SA | 1140 | C |
| 1 | 16SA | 1147 | C |
| 1 | 16SA | 1156 | 7MG |
| 1 | 16SA | 1159 | G |
| 1 | 16SA | 1160 | U |
| 1 | 16SA | 1161 | A |
| 1 | 16SA | 1162 | A |
| 1 | 16SA | 1165 | C |
| 1 | 16SA | 1174 | C |
| 1 | 16SA | 1176 | A |
| 1 | 16SA | 1178 | C |
| 1 | 16SA | 1188 | A |
| 1 | 16SA | 1190 | U |
| 1 | 16SA | 1191 | C |
| 1 | 16SA | 1193 | C |
| 1 | 16SA | 1197 | G |
| 1 | 16SA | 1201 | A |
| 1 | 16SA | 1202 | A |
| 1 | 16SA | 1205 | G |
| 1 | 16SA | 1206 | G |
| 1 | 16SA | 1236 | A |
| 1 | 16SA | 1243 | A |
| 1 | 16SA | 1252 | C |

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| Mol | Chain | Res | Type |
|---|---|---|---|
| 1 | 16SA | 1256 | G |
| 1 | 16SA | 1260 | G |
| 1 | 16SA | 1279 | G |
| 1 | 16SA | 1282 | A |
| 1 | 16SA | 1290 | G |
| 1 | 16SA | 1291 | G |
| 1 | 16SA | 1294 | A |
| 1 | 16SA | 1295 | G |
| 1 | 16SA | 1300 | G |
| 1 | 16SA | 1316 | A |
| 1 | 16SA | 1330 | C |
| 1 | 16SA | 1331 | A |
| 1 | 16SA | 1332 | G |
| 1 | 16SA | 1333 | A |
| 1 | 16SA | 1350 | G |
| 1 | 16SA | 1352 | U |
| 1 | 16SA | 1353 | G |
| 1 | 16SA | 1360 | G |
| 1 | 16SA | 1377 | C |
| 1 | 16SA | 1378 | C |
| 1 | 16SA | 1382 | A |
| 1 | 16SA | 1384 | G |
| 1 | 16SA | 1395 | A |
| 1 | 16SA | 1406 | A |
| 1 | 16SA | 1407 | G |
| 1 | 16SA | 1421 | A |
| 1 | 16SA | 1422 | U |
| 1 | 16SA | 1423 | A |
| 1 | 16SA | 1442 | U |
| 1 | 16SA | 1444 | A |
| 1 | 16SA | 1446 | C |
| 1 | 16SA | 1447 | G |
| 1 | 16SA | 1449 | U |
| 1 | 16SA | 1450 | G |
| 1 | 16SA | 1457 | A |
| 1 | 16SA | 1468 | U |
| 1 | 16SA | 1469 | C |
| 1 | 16SA | 1470 | U |
| 1 | 16SA | 1471 | C |
| 1 | 16SA | 1476 | G |
| 1 | 16SA | 1482 | A |
| 1 | 16SA | 1493 | U |

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| Mol | Chain | Res | Type |
|---|---|---|---|
| 1 | 16SA | 1496 | A |
| 1 | 16SA | 1497 | G |
| 1 | 16SA | 1525 | G |
| 1 | 16SA | 1536 | A |
| 1 | 16SA | 1537 | A |
| 1 | 16SA | 1539 | G |
| 1 | 16SA | 1549 | G |
| 1 | 16SA | 1550 | G |
| 1 | 16SA | 1557 | C |
| 1 | 16SA | 1558 | A |
| 1 | 16SA | 1559 | C |
| 1 | 16SA | 1583 | U |
| 1 | 16SA | 1589 | M2G |
| 1 | 16SA | 1591 | A |
| 1 | 16SA | 1592 | A |
| 1 | 16SA | 1594 | G |
| 1 | 16SA | 1595 | C |
| 1 | 16SA | 1597 | A |
| 1 | 16SA | 1598 | A |
| 1 | 16SA | 1599 | G |
| 1 | 16SA | 1600 | A |
| 1 | 16SA | 1603 | C |
| 1 | 16SA | 1604 | U |
| 1 | 16SA | 1605 | U |
| 1 | 16SA | 1609 | A |
| 1 | 16SA | 1614 | U |
| 1 | 16SA | 1615 | U |
| 1 | 16SA | 1616 | G |
| 1 | 16SA | 1625 | G |
| 1 | 16SA | 1628 | A |
| 1 | 16SA | 1629 | A |
| 1 | 16SA | 1630 | C |
| 1 | 16SA | 1633 | G |
| 1 | 16SA | 1640 | A |
| 1 | 16SA | 1641 | G |
| 1 | 16SA | 1645 | G |
| 1 | 16SA | 1648 | G |
| 1 | 16SA | 1649 | U |
| 1 | 16SA | 1650 | G |
| 1 | 16SA | 1652 | C |
| 1 | 16SA | 1653 | C |
| 1 | 16SA | 1655 | G |

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| Mol | Chain | Res | Type |
|---|---|---|---|
| 1 | 16SA | 1657 | G |
| 1 | 16SA | 1659 | G |
| 1 | 16SA | 1661 | G |
| 1 | 16SA | 1664 | G |
| 1 | 16SA | 1666 | C |
| 1 | 16SA | 1668 | U |
| 1 | 16SA | 1674 | A |
| 1 | 16SA | 1681 | G |
| 1 | 16SA | 1682 | C |
| 1 | 16SA | 1683 | A |
| 1 | 16SA | 1694 | C |
| 1 | 16SA | 1709 | G |
| 1 | 16SA | 1710 | G |
| 1 | 16SA | 1722 | G |
| 1 | 16SA | 1723 | U |
| 1 | 16SA | 1729 | A |
| 1 | 16SA | 1750 | U |
| 1 | 16SA | 1753 | U |
| 1 | 16SA | 1754 | U |
| 1 | 16SA | 1755 | G |
| 1 | 16SA | 1756 | C |
| 1 | 16SA | 1757 | C |
| 1 | 16SA | 1758 | A |
| 1 | 16SA | 1759 | G |
| 1 | 16SA | 1760 | C |
| 1 | 16SA | 1761 | G |
| 1 | 16SA | 1764 | U |
| 1 | 16SA | 1765 | C |
| 1 | 16SA | 1766 | G |
| 1 | 16SA | 1767 | G |
| 1 | 16SA | 1768 | C |
| 1 | 16SA | 1774 | A |
| 1 | 16SA | 1780 | A |
| 1 | 16SA | 1785 | A |
| 1 | 16SA | 1786 | C |
| 1 | 16SA | 1787 | U |
| 1 | 16SA | 1789 | C |
| 1 | 16SA | 1798 | G |
| 1 | 16SA | 1808 | G |
| 1 | 16SA | 1809 | G |
| 1 | 16SA | 1810 | A |
| 1 | 16SA | 1811 | G |

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| Mol | Chain | Res | Type |
|---|---|---|---|
| 1 | 16SA | 1812 | G |
| 1 | 16SA | 1814 | G |
| 1 | 16SA | 1815 | A |
| 1 | 16SA | 1823 | U |
| 1 | 16SA | 1825 | G |
| 1 | 16SA | 1827 | C |
| 1 | 16SA | 1828 | A |
| 1 | 16SA | 1829 | G |
| 1 | 16SA | 1839 | U |
| 1 | 16SA | 1845 | C |
| 1 | 16SA | 1852 | A |
| 1 | 16SA | 1854 | A |
| 1 | 16SA | 1865 | A |
| 1 | 16SA | 1877 | A |
| 1 | 16SA | 1883 | A |
| 1 | 16SA | 1884 | U |
| 1 | 16SA | 1885 | G |
| 1 | 16SA | 1889 | C |
| 1 | 16SA | 1890 | C |
| 1 | 16SA | 1896 | A |
| 1 | 16SA | 1899 | G |
| 1 | 16SA | 1900 | G |
| 1 | 16SA | 1902 | A |
| 1 | 16SA | 1905 | U |
| 1 | 16SA | 1907 | A |
| 1 | 16SA | 1908 | U |
| 1 | 16SA | 1909 | C |
| 1 | 16SA | 1912 | A |
| 1 | 16SA | 1913 | A |
| 1 | 16SA | 1914 | A |
| 1 | 16SA | 1916 | A |
| 1 | 16SA | 1919 | U |
| 1 | 16SA | 1924 | C |
| 1 | 16SA | 1926 | A |
| 1 | 16SA | 1927 | G |
| 1 | 16SA | 1928 | U |
| 1 | 16SA | 1929 | U |
| 1 | 16SA | 1932 | G |
| 1 | 16SA | 1933 | A |
| 1 | 16SA | 1941 | C |
| 1 | 16SA | 1945 | A |
| 1 | 16SA | 1946 | A |

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| Mol | Chain | Res | Type |
|---|---|---|---|
| 1 | 16SA | 1947 | C |
| 1 | 16SA | 1948 | C |
| 1 | 16SA | 1949 | C |
| 1 | 16SA | 1950 | G |
| 1 | 16SA | 1954 | C |
| 1 | 16SA | 1962 | C |
| 1 | 16SA | 1963 | C |
| 1 | 16SA | 1965 | G |
| 1 | 16SA | 1973 | A |
| 1 | 16SA | 1980 | G |
| 1 | 16SA | 1990 | C |
| 1 | 16SA | 1991 | A |
| 1 | 16SA | 1992 | U |
| 1 | 16SA | 1996 | G |
| 1 | 16SA | 1998 | G |
| 1 | 16SA | 2026 | A |
| 1 | 16SA | 2030 | 4OC |
| 1 | 16SA | 2047 | G |
| 1 | 16SA | 2070 | G |
| 1 | 16SA | 2071 | G |
| 1 | 16SA | 2072 | A |
| 1 | 16SA | 2073 | G |
| 1 | 16SA | 2077 | A |
| 1 | 16SA | 2078 | C |
| 1 | 16SA | 2079 | G |
| 1 | 16SA | 2080 | G |
| 1 | 16SA | 2092 | G |
| 1 | 16SA | 2110 | G |
| 1 | 16SA | 2115 | A |
| 1 | 16SA | 2120 | G |
| 1 | 16SA | 2121 | UR3 |
| 1 | 16SA | 2122 | A |
| 1 | 16SA | 2125 | A |
| 1 | 16SA | 2127 | G |
| 1 | 16SA | 2129 | U |
| 1 | 16SA | 2140 | G |
| 1 | 16SA | 2142 | MA6 |
| 1 | 16SA | 2143 | G |
| 1 | 16SA | 2152 | G |
| 1 | 16SA | 2153 | G |
| 1 | 16SA | 2154 | A |
| 22 | ASIA | 2 | C |

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| Mol | Chain | Res | Type |
|---|---|---|---|
| 22 | ASIA | 3 | C |
| 22 | ASIA | 5 | G |
| 22 | ASIA | 7 | A |
| 22 | ASIA | 8 | 4SU |
| 22 | ASIA | 9 | A |
| 22 | ASIA | 10 | G |
| 22 | ASIA | 11 | C |
| 22 | ASIA | 14 | A |
| 22 | ASIA | 15 | G |
| 22 | ASIA | 16 | U |
| 22 | ASIA | 17 | C |
| 22 | ASIA | 18 | G |
| 22 | ASIA | 19 | G |
| 22 | ASIA | 20 | U |
| 22 | ASIA | 21 | A |
| 22 | ASIA | 22 | G |
| 22 | ASIA | 24 | G |
| 22 | ASIA | 30 | G |
| 22 | ASIA | 36 | A |
| 22 | ASIA | 37 | MIA |
| 22 | ASIA | 42 | C |
| 22 | ASIA | 44 | G |
| 22 | ASIA | 45 | U |
| 22 | ASIA | 46 | 7MG |
| 22 | ASIA | 47 | U |
| 22 | ASIA | 48 | C |
| 22 | ASIA | 49 | C |
| 22 | ASIA | 52 | G |
| 22 | ASIA | 53 | G |
| 22 | ASIA | 55 | PSU |
| 22 | ASIA | 58 | A |
| 22 | ASIA | 59 | U |
| 22 | ASIA | 60 | U |
| 22 | ASIA | 61 | C |
| 22 | ASIA | 63 | G |
| 22 | ASIA | 64 | A |
| 22 | ASIA | 66 | U |
| 22 | ASIA | 70 | G |
| 22 | ASIA | 72 | C |
| 22 | ASIA | 73 | A |
| 22 | ASIA | 74 | C |
| 22 | ASIA | 75 | C |

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| Mol | Chain | Res | Type |
|---|---|---|---|
| 22 | ASIA | 76 | A |
| 23 | PSIA | 2 | C |
| 23 | PSIA | 3 | C |
| 23 | PSIA | 8 | 4SU |
| 23 | PSIA | 11 | C |
| 23 | PSIA | 13 | C |
| 23 | PSIA | 17 | C |
| 23 | PSIA | 18 | G |
| 23 | PSIA | 20 | U |
| 23 | PSIA | 21 | A |
| 23 | PSIA | 22 | G |
| 23 | PSIA | 25 | C |
| 23 | PSIA | 30 | G |
| 23 | PSIA | 37 | MIA |
| 23 | PSIA | 44 | G |
| 23 | PSIA | 45 | U |
| 23 | PSIA | 46 | 7MG |
| 23 | PSIA | 47 | 3AU |
| 23 | PSIA | 48 | C |
| 23 | PSIA | 55 | PSU |
| 23 | PSIA | 56 | C |
| 23 | PSIA | 58 | A |
| 23 | PSIA | 63 | G |
| 23 | PSIA | 69 | G |
| 24 | ESIA | 2 | C |
| 24 | ESIA | 3 | C |
| 24 | ESIA | 8 | U |
| 24 | ESIA | 9 | A |
| 24 | ESIA | 10 | G |
| 24 | ESIA | 14 | A |
| 24 | ESIA | 15 | G |
| 24 | ESIA | 16 | U |
| 24 | ESIA | 17 | C |
| 24 | ESIA | 18 | G |
| 24 | ESIA | 19 | G |
| 24 | ESIA | 20 | U |
| 24 | ESIA | 21 | A |
| 24 | ESIA | 22 | G |
| 24 | ESIA | 30 | G |
| 24 | ESIA | 38 | A |
| 24 | ESIA | 42 | C |
| 24 | ESIA | 45 | U |

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| Mol | Chain | Res | Type |
|---|---|---|---|
| 24 | ESIA | 46 | G |
| 24 | ESIA | 47 | U |
| 24 | ESIA | 48 | C |
| 24 | ESIA | 49 | C |
| 24 | ESIA | 53 | G |
| 24 | ESIA | 55 | U |
| 24 | ESIA | 56 | C |
| 24 | ESIA | 58 | A |
| 24 | ESIA | 59 | U |
| 24 | ESIA | 63 | G |
| 24 | ESIA | 65 | G |
| 24 | ESIA | 66 | U |
| 24 | ESIA | 72 | C |
| 24 | ESIA | 73 | A |
| 24 | ESIA | 76 | A |
| 25 | MRNA | 33 | G |
| 25 | MRNA | 43 | U |
| 25 | MRNA | 45 | U |
| 25 | MRNA | 46 | U |
| 25 | MRNA | 54 | U |
| 25 | MRNA | 56 | U |
| 25 | MRNA | 57 | U |
| 26 | TRNA | 2 | C |
| 26 | TRNA | 3 | C |
| 26 | TRNA | 6 | G |
| 26 | TRNA | 8 | 4SU |
| 26 | TRNA | 10 | G |
| 26 | TRNA | 11 | C |
| 26 | TRNA | 12 | U |
| 26 | TRNA | 13 | C |
| 26 | TRNA | 15 | G |
| 26 | TRNA | 16 | U |
| 26 | TRNA | 19 | G |
| 26 | TRNA | 20 | U |
| 26 | TRNA | 21 | A |
| 26 | TRNA | 22 | G |
| 26 | TRNA | 23 | A |
| 26 | TRNA | 27 | G |
| 26 | TRNA | 35 | A |
| 26 | TRNA | 37 | MIA |
| 26 | TRNA | 38 | A |
| 26 | TRNA | 40 | C |

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| Mol | Chain | Res | Type |
|---|---|---|---|
| 26 | TRNA | 43 | C |
| 26 | TRNA | 44 | G |
| 26 | TRNA | 45 | U |
| 26 | TRNA | 46 | G |
| 26 | TRNA | 47 | U |
| 26 | TRNA | 48 | C |
| 26 | TRNA | 49 | C |
| 26 | TRNA | 50 | U |
| 26 | TRNA | 52 | G |
| 26 | TRNA | 53 | G |
| 26 | TRNA | 54 | 5MU |
| 26 | TRNA | 58 | A |
| 26 | TRNA | 63 | G |
| 26 | TRNA | 66 | U |
| 27 | 23SA | 3 | U |
| 27 | 23SA | 4 | C |
| 27 | 23SA | 5 | A |
| 27 | 23SA | 10 | G |
| 27 | 23SA | 15 | G |
| 27 | 23SA | 34 | C |
| 27 | 23SA | 35 | G |
| 27 | 23SA | 45 | C |
| 27 | 23SA | 48 | A |
| 27 | 23SA | 57 | G |
| 27 | 23SA | 59 | G |
| 27 | 23SA | 60 | G |
| 27 | 23SA | 62 | U |
| 27 | 23SA | 70 | A |
| 27 | 23SA | 71 | U |
| 27 | 23SA | 73 | A |
| 27 | 23SA | 74 | G |
| 27 | 23SA | 77 | A |
| 27 | 23SA | 82 | G |
| 27 | 23SA | 83 | A |
| 27 | 23SA | 89 | U |
| 27 | 23SA | 100 | G |
| 27 | 23SA | 116 | A |
| 27 | 23SA | 117 | A |
| 27 | 23SA | 118 | U |
| 27 | 23SA | 129 | G |
| 27 | 23SA | 137 | G |
| 27 | 23SA | 155 | C |

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| Mol | Chain | Res | Type |
|---|---|---|---|
| 27 | 23SA | 157 | U |
| 27 | 23SA | 158 | U |
| 27 | 23SA | 160 | U |
| 27 | 23SA | 186 | A |
| 27 | 23SA | 187 | A |
| 27 | 23SA | 189 | A |
| 27 | 23SA | 204 | G |
| 27 | 23SA | 205 | G |
| 27 | 23SA | 206 | A |
| 27 | 23SA | 207 | G |
| 27 | 23SA | 211 | A |
| 27 | 23SA | 212 | A |
| 27 | 23SA | 213 | A |
| 27 | 23SA | 217 | A |
| 27 | 23SA | 218 | A |
| 27 | 23SA | 219 | A |
| 27 | 23SA | 220 | U |
| 27 | 23SA | 222 | G |
| 27 | 23SA | 223 | A |
| 27 | 23SA | 229 | U |
| 27 | 23SA | 238 | G |
| 27 | 23SA | 239 | C |
| 27 | 23SA | 242 | G |
| 27 | 23SA | 255 | A |
| 27 | 23SA | 256 | G |
| 27 | 23SA | 272 | U |
| 27 | 23SA | 273 | U |
| 27 | 23SA | 274 | G |
| 27 | 23SA | 276 | C |
| 27 | 23SA | 289 | U |
| 27 | 23SA | 290 | G |
| 27 | 23SA | 297 | U |
| 27 | 23SA | 298 | C |
| 27 | 23SA | 304 | C |
| 27 | 23SA | 324 | A |
| 27 | 23SA | 336 | A |
| 27 | 23SA | 340 | G |
| 27 | 23SA | 349 | A |
| 27 | 23SA | 354 | G |
| 27 | 23SA | 355 | A |
| 27 | 23SA | 367 | G |
| 27 | 23SA | 377 | G |

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| Mol | Chain | Res | Type |
|---|---|---|---|
| 27 | 23SA | 388 | G |
| 27 | 23SA | 393 | U |
| 27 | 23SA | 395 | C |
| 27 | 23SA | 400 | G |
| 27 | 23SA | 401 | U |
| 27 | 23SA | 414 | G |
| 27 | 23SA | 423 | U |
| 27 | 23SA | 424 | G |
| 27 | 23SA | 432 | C |
| 27 | 23SA | 433 | U |
| 27 | 23SA | 435 | G |
| 27 | 23SA | 439 | G |
| 27 | 23SA | 449 | C |
| 27 | 23SA | 457 | A |
| 27 | 23SA | 472 | C |
| 27 | 23SA | 476 | U |
| 27 | 23SA | 479 | C |
| 27 | 23SA | 482 | A |
| 27 | 23SA | 483 | C |
| 27 | 23SA | 485 | A |
| 27 | 23SA | 492 | U |
| 27 | 23SA | 498 | A |
| 27 | 23SA | 499 | A |
| 27 | 23SA | 507 | A |
| 27 | 23SA | 509 | G |
| 27 | 23SA | 523 | G |
| 27 | 23SA | 530 | A |
| 27 | 23SA | 531 | U |
| 27 | 23SA | 532 | A |
| 27 | 23SA | 535 | G |
| 27 | 23SA | 536 | C |
| 27 | 23SA | 537 | C |
| 27 | 23SA | 555 | A |
| 27 | 23SA | 556 | A |
| 27 | 23SA | 557 | G |
| 27 | 23SA | 558 | C |
| 27 | 23SA | 559 | A |
| 27 | 23SA | 560 | G |
| 27 | 23SA | 563 | A |
| 27 | 23SA | 564 | C |
| 27 | 23SA | 565 | G |
| 27 | 23SA | 572 | C |

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| Mol | Chain | Res | Type |
|---|---|---|---|
| 27 | 23SA | 575 | G |
| 27 | 23SA | 580 | U |
| 27 | 23SA | 581 | G |
| 27 | 23SA | 588 | G |
| 27 | 23SA | 589 | C |
| 27 | 23SA | 595 | G |
| 27 | 23SA | 598 | G |
| 27 | 23SA | 600 | A |
| 27 | 23SA | 608 | G |
| 27 | 23SA | 613 | U |
| 27 | 23SA | 617 | G |
| 27 | 23SA | 618 | G |
| 27 | 23SA | 627 | G |
| 27 | 23SA | 628 | A |
| 27 | 23SA | 632 | U |
| 27 | 23SA | 635 | G |
| 27 | 23SA | 639 | U |
| 27 | 23SA | 640 | U |
| 27 | 23SA | 641 | G |
| 27 | 23SA | 643 | G |
| 27 | 23SA | 644 | G |
| 27 | 23SA | 647 | G |
| 27 | 23SA | 648 | A |
| 27 | 23SA | 649 | G |
| 27 | 23SA | 654 | A |
| 27 | 23SA | 656 | G |
| 27 | 23SA | 664 | A |
| 27 | 23SA | 672 | C |
| 27 | 23SA | 673 | A |
| 27 | 23SA | 681 | A |
| 27 | 23SA | 682 | A |
| 27 | 23SA | 684 | G |
| 27 | 23SA | 699 | C |
| 27 | 23SA | 700 | G |
| 27 | 23SA | 701 | A |
| 27 | 23SA | 706 | U |
| 27 | 23SA | 719 | A |
| 27 | 23SA | 726 | A |
| 27 | 23SA | 735 | G |
| 27 | 23SA | 750 | G |
| 27 | 23SA | 758 | U |
| 27 | 23SA | 779 | C |

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| Mol | Chain | Res | Type |
|---|---|---|---|
| 27 | 23SA | 789 | U |
| 27 | 23SA | 811 | U |
| 27 | 23SA | 824 | G |
| 27 | 23SA | 825 | G |
| 27 | 23SA | 831 | A |
| 27 | 23SA | 833 | A |
| 27 | 23SA | 834 | G |
| 27 | 23SA | 839 | C |
| 27 | 23SA | 841 | G |
| 27 | 23SA | 842 | A |
| 27 | 23SA | 854 | G |
| 27 | 23SA | 861 | C |
| 27 | 23SA | 868 | A |
| 27 | 23SA | 876 | U |
| 27 | 23SA | 877 | U |
| 27 | 23SA | 881 | G |
| 27 | 23SA | 895 | C |
| 27 | 23SA | 896 | U |
| 27 | 23SA | 908 | G |
| 27 | 23SA | 926 | U |
| 27 | 23SA | 927 | A |
| 27 | 23SA | 929 | G |
| 27 | 23SA | 930 | G |
| 27 | 23SA | 931 | G |
| 27 | 23SA | 932 | G |
| 27 | 23SA | 933 | C |
| 27 | 23SA | 934 | C |
| 27 | 23SA | 935 | C |
| 27 | 23SA | 936 | A |
| 27 | 23SA | 937 | C |
| 27 | 23SA | 938 | C |
| 27 | 23SA | 939 | A |
| 27 | 23SA | 940 | G |
| 27 | 23SA | 941 | C |
| 27 | 23SA | 944 | A |
| 27 | 23SA | 945 | C |
| 27 | 23SA | 946 | C |
| 27 | 23SA | 947 | A |
| 27 | 23SA | 948 | A |
| 27 | 23SA | 952 | C |
| 27 | 23SA | 954 | G |
| 27 | 23SA | 958 | A |

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| Mol | Chain | Res | Type |
|---|---|---|---|
| 27 | 23SA | 959 | A |
| 27 | 23SA | 963 | C |
| 27 | 23SA | 965 | A |
| 27 | 23SA | 967 | G |
| 27 | 23SA | 978 | G |
| 27 | 23SA | 979 | G |
| 27 | 23SA | 985 | G |
| 27 | 23SA | 988 | A |
| 27 | 23SA | 992 | A |
| 27 | 23SA | 993 | G |
| 27 | 23SA | 1000 | A |
| 27 | 23SA | 1006 | A |
| 27 | 23SA | 1008 | C |
| 27 | 23SA | 1021 | G |
| 27 | 23SA | 1028 | A |
| 27 | 23SA | 1031 | A |
| 27 | 23SA | 1038 | A |
| 27 | 23SA | 1039 | C |
| 27 | 23SA | 1044 | A |
| 27 | 23SA | 1058 | A |
| 27 | 23SA | 1059 | G |
| 27 | 23SA | 1060 | U |
| 27 | 23SA | 1061 | C |
| 27 | 23SA | 1070 | G |
| 27 | 23SA | 1071 | U |
| 27 | 23SA | 1073 | G |
| 27 | 23SA | 1074 | U |
| 27 | 23SA | 1075 | A |
| 27 | 23SA | 1081 | U |
| 27 | 23SA | 1086 | C |
| 27 | 23SA | 1093 | A |
| 27 | 23SA | 1095 | G |
| 27 | 23SA | 1098 | A |
| 27 | 23SA | 1106 | U |
| 27 | 23SA | 1108 | U |
| 27 | 23SA | 1110 | G |
| 27 | 23SA | 1119 | G |
| 27 | 23SA | 1122 | G |
| 27 | 23SA | 1124 | C |
| 27 | 23SA | 1125 | A |
| 27 | 23SA | 1126 | U |
| 27 | 23SA | 1127 | C |

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| Mol | Chain | Res | Type |
|---|---|---|---|
| 27 | 23SA | 1130 | U |
| 27 | 23SA | 1131 | U |
| 27 | 23SA | 1132 | A |
| 27 | 23SA | 1133 | A |
| 27 | 23SA | 1134 | A |
| 27 | 23SA | 1135 | G |
| 27 | 23SA | 1136 | A |
| 27 | 23SA | 1138 | U |
| 27 | 23SA | 1139 | G |
| 27 | 23SA | 1158 | G |
| 27 | 23SA | 1159 | A |
| 27 | 23SA | 1160 | G |
| 27 | 23SA | 1170 | G |
| 27 | 23SA | 1177 | A |
| 27 | 23SA | 1178 | U |
| 27 | 23SA | 1179 | G |
| 27 | 23SA | 1183 | C |
| 27 | 23SA | 1184 | G |
| 27 | 23SA | 1186 | G |
| 27 | 23SA | 1187 | G |
| 27 | 23SA | 1189 | U |
| 27 | 23SA | 1190 | U |
| 27 | 23SA | 1191 | A |
| 27 | 23SA | 1192 | A |
| 27 | 23SA | 1198 | G |
| 27 | 23SA | 1205 | A |
| 27 | 23SA | 1206 | G |
| 27 | 23SA | 1208 | U |
| 27 | 23SA | 1217 | G |
| 27 | 23SA | 1221 | G |
| 27 | 23SA | 1223 | U |
| 27 | 23SA | 1224 | G |
| 27 | 23SA | 1225 | A |
| 27 | 23SA | 1227 | C |
| 27 | 23SA | 1228 | C |
| 27 | 23SA | 1243 | G |
| 27 | 23SA | 1245 | G |
| 27 | 23SA | 1252 | A |
| 27 | 23SA | 1253 | U |
| 27 | 23SA | 1254 | G |
| 27 | 23SA | 1259 | U |
| 27 | 23SA | 1268 | A |

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| Mol | Chain | Res | Type |
|---|---|---|---|
| 27 | 23SA | 1269 | C |
| 27 | 23SA | 1276 | G |
| 27 | 23SA | 1293 | G |
| 27 | 23SA | 1302 | A |
| 27 | 23SA | 1305 | G |
| 27 | 23SA | 1314 | A |
| 27 | 23SA | 1318 | A |
| 27 | 23SA | 1320 | G |
| 27 | 23SA | 1321 | A |
| 27 | 23SA | 1322 | U |
| 27 | 23SA | 1335 | A |
| 27 | 23SA | 1349 | U |
| 27 | 23SA | 1350 | A |
| 27 | 23SA | 1358 | G |
| 27 | 23SA | 1362 | U |
| 27 | 23SA | 1363 | C |
| 27 | 23SA | 1368 | G |
| 27 | 23SA | 1378 | U |
| 27 | 23SA | 1390 | U |
| 27 | 23SA | 1394 | C |
| 27 | 23SA | 1398 | A |
| 27 | 23SA | 1401 | U |
| 27 | 23SA | 1408 | A |
| 27 | 23SA | 1409 | A |
| 27 | 23SA | 1414 | A |
| 27 | 23SA | 1419 | C |
| 27 | 23SA | 1428 | A |
| 27 | 23SA | 1433 | A |
| 27 | 23SA | 1434 | G |
| 27 | 23SA | 1435 | C |
| 27 | 23SA | 1437 | G |
| 27 | 23SA | 1460 | C |
| 27 | 23SA | 1465 | G |
| 27 | 23SA | 1466 | C |
| 27 | 23SA | 1468 | A |
| 27 | 23SA | 1469 | U |
| 27 | 23SA | 1470 | G |
| 27 | 23SA | 1477 | C |
| 27 | 23SA | 1486 | C |
| 27 | 23SA | 1492 | G |
| 27 | 23SA | 1494 | A |
| 27 | 23SA | 1499 | A |

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| Mol | Chain | Res | Type |
|---|---|---|---|
| 27 | 23SA | 1500 | G |
| 27 | 23SA | 1502 | C |
| 27 | 23SA | 1505 | G |
| 27 | 23SA | 1508 | C |
| 27 | 23SA | 1509 | G |
| 27 | 23SA | 1511 | G |
| 27 | 23SA | 1517 | C |
| 27 | 23SA | 1521 | A |
| 27 | 23SA | 1524 | C |
| 27 | 23SA | 1525 | G |
| 27 | 23SA | 1526 | C |
| 27 | 23SA | 1528 | G |
| 27 | 23SA | 1531 | U |
| 27 | 23SA | 1532 | G |
| 27 | 23SA | 1534 | G |
| 27 | 23SA | 1535 | A |
| 27 | 23SA | 1536 | G |
| 27 | 23SA | 1539 | A |
| 27 | 23SA | 1542 | C |
| 27 | 23SA | 1546 | U |
| 27 | 23SA | 1554 | C |
| 27 | 23SA | 1555 | C |
| 27 | 23SA | 1557 | A |
| 27 | 23SA | 1558 | C |
| 27 | 23SA | 1559 | A |
| 27 | 23SA | 1563 | U |
| 27 | 23SA | 1564 | C |
| 27 | 23SA | 1565 | U |
| 27 | 23SA | 1574 | G |
| 27 | 23SA | 1577 | A |
| 27 | 23SA | 1582 | C |
| 27 | 23SA | 1583 | G |
| 27 | 23SA | 1584 | U |
| 27 | 23SA | 1586 | C |
| 27 | 23SA | 1587 | G |
| 27 | 23SA | 1592 | A |
| 27 | 23SA | 1593 | C |
| 27 | 23SA | 1594 | A |
| 27 | 23SA | 1604 | A |
| 27 | 23SA | 1605 | G |
| 27 | 23SA | 1608 | A |
| 27 | 23SA | 1609 | G |

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| Mol | Chain | Res | Type |
|---|---|---|---|
| 27 | 23SA | 1610 | G |
| 27 | 23SA | 1616 | A |
| 27 | 23SA | 1619 | A |
| 27 | 23SA | 1628 | U |
| 27 | 23SA | 1629 | A |
| 27 | 23SA | 1635 | A |
| 27 | 23SA | 1642 | G |
| 27 | 23SA | 1644 | G |
| 27 | 23SA | 1647 | C |
| 27 | 23SA | 1657 | A |
| 27 | 23SA | 1659 | A |
| 27 | 23SA | 1660 | C |
| 27 | 23SA | 1666 | C |
| 27 | 23SA | 1667 | A |
| 27 | 23SA | 1671 | G |
| 27 | 23SA | 1696 | C |
| 27 | 23SA | 1698 | C |
| 27 | 23SA | 1703 | G |
| 27 | 23SA | 1704 | A |
| 27 | 23SA | 1724 | G |
| 27 | 23SA | 1745 | G |
| 27 | 23SA | 1753 | G |
| 27 | 23SA | 1766 | G |
| 27 | 23SA | 1769 | G |
| 27 | 23SA | 1770 | A |
| 27 | 23SA | 1771 | U |
| 27 | 23SA | 1772 | G |
| 27 | 23SA | 1773 | A |
| 27 | 23SA | 1776 | C |
| 27 | 23SA | 1784 | G |
| 27 | 23SA | 1792 | G |
| 27 | 23SA | 1796 | A |
| 27 | 23SA | 1797 | G |
| 27 | 23SA | 1798 | G |
| 27 | 23SA | 1807 | A |
| 27 | 23SA | 1814 | A |
| 27 | 23SA | 1816 | C |
| 27 | 23SA | 1825 | A |
| 27 | 23SA | 1832 | U |
| 27 | 23SA | 1833 | G |
| 27 | 23SA | 1834 | C |
| 27 | 23SA | 1835 | G |

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| Mol | Chain | Res | Type |
|---|---|---|---|
| 27 | 23SA | 1850 | G |
| 27 | 23SA | 1854 | U |
| 27 | 23SA | 1863 | A |
| 27 | 23SA | 1873 | G |
| 27 | 23SA | 1880 | G |
| 27 | 23SA | 1881 | A |
| 27 | 23SA | 1882 | A |
| 27 | 23SA | 1883 | G |
| 27 | 23SA | 1892 | G |
| 27 | 23SA | 1899 | G |
| 27 | 23SA | 1902 | A |
| 27 | 23SA | 1903 | G |
| 27 | 23SA | 1907 | C |
| 27 | 23SA | 1913 | G |
| 27 | 23SA | 1914 | A |
| 27 | 23SA | 1924 | G |
| 27 | 23SA | 1925 | A |
| 27 | 23SA | 1931 | G |
| 27 | 23SA | 1939 | C |
| 27 | 23SA | 1954 | G |
| 27 | 23SA | 1955 | G |
| 27 | 23SA | 1961 | A |
| 27 | 23SA | 1962 | A |
| 27 | 23SA | 1963 | A |
| 27 | 23SA | 1964 | 5MU |
| 27 | 23SA | 1965 | U |
| 27 | 23SA | 1980 | U |
| 27 | 23SA | 1985 | A |
| 27 | 23SA | 1988 | U |
| 27 | 23SA | 1989 | G |
| 27 | 23SA | 1992 | C |
| 27 | 23SA | 1994 | A |
| 27 | 23SA | 1995 | A |
| 27 | 23SA | 1996 | A |
| 27 | 23SA | 1997 | A |
| 27 | 23SA | 2007 | C |
| 27 | 23SA | 2016 | U |
| 27 | 23SA | 2018 | U |
| 27 | 23SA | 2045 | A |
| 27 | 23SA | 2048 | G |
| 27 | 23SA | 2052 | G |
| 27 | 23SA | 2056 | A |

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| Mol | Chain | Res | Type |
|---|---|---|---|
| 27 | 23SA | 2057 | G |
| 27 | 23SA | 2058 | A |
| 27 | 23SA | 2068 | C |
| 27 | 23SA | 2076 | A |
| 27 | 23SA | 2079 | A |
| 27 | 23SA | 2080 | C |
| 27 | 23SA | 2081 | G |
| 27 | 23SA | 2084 | A |
| 27 | 23SA | 2085 | A |
| 27 | 23SA | 2086 | G |
| 27 | 23SA | 2094 | G |
| 27 | 23SA | 2118 | G |
| 27 | 23SA | 2124 | U |
| 27 | 23SA | 2125 | G |
| 27 | 23SA | 2126 | G |
| 27 | 23SA | 2136 | C |
| 27 | 23SA | 2138 | U |
| 27 | 23SA | 2139 | A |
| 27 | 23SA | 2140 | G |
| 27 | 23SA | 2141 | G |
| 27 | 23SA | 2142 | A |
| 27 | 23SA | 2143 | U |
| 27 | 23SA | 2144 | A |
| 27 | 23SA | 2145 | G |
| 27 | 23SA | 2150 | G |
| 27 | 23SA | 2152 | G |
| 27 | 23SA | 2153 | C |
| 27 | 23SA | 2154 | C |
| 27 | 23SA | 2157 | U |
| 27 | 23SA | 2158 | G |
| 27 | 23SA | 2161 | C |
| 27 | 23SA | 2170 | C |
| 27 | 23SA | 2171 | C |
| 27 | 23SA | 2172 | G |
| 27 | 23SA | 2173 | G |
| 27 | 23SA | 2183 | A |
| 27 | 23SA | 2185 | G |
| 27 | 23SA | 2188 | C |
| 27 | 23SA | 2191 | G |
| 27 | 23SA | 2193 | G |
| 27 | 23SA | 2194 | A |
| 27 | 23SA | 2195 | A |

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| Mol | Chain | Res | Type |
|---|---|---|---|
| 27 | 23SA | 2196 | A |
| 27 | 23SA | 2197 | U |
| 27 | 23SA | 2198 | A |
| 27 | 23SA | 2199 | C |
| 27 | 23SA | 2201 | A |
| 27 | 23SA | 2203 | C |
| 27 | 23SA | 2206 | G |
| 27 | 23SA | 2214 | U |
| 27 | 23SA | 2215 | G |
| 27 | 23SA | 2217 | G |
| 27 | 23SA | 2223 | A |
| 27 | 23SA | 2230 | G |
| 27 | 23SA | 2231 | G |
| 27 | 23SA | 2232 | A |
| 27 | 23SA | 2233 | U |
| 27 | 23SA | 2234 | G |
| 27 | 23SA | 2240 | A |
| 27 | 23SA | 2253 | G |
| 27 | 23SA | 2254 | G |
| 27 | 23SA | 2261 | G |
| 27 | 23SA | 2267 | G |
| 27 | 23SA | 2282 | A |
| 27 | 23SA | 2288 | A |
| 27 | 23SA | 2290 | C |
| 27 | 23SA | 2293 | A |
| 27 | 23SA | 2295 | G |
| 27 | 23SA | 2298 | C |
| 27 | 23SA | 2302 | A |
| 27 | 23SA | 2303 | A |
| 27 | 23SA | 2304 | G |
| 27 | 23SA | 2319 | G |
| 27 | 23SA | 2320 | A |
| 27 | 23SA | 2322 | G |
| 27 | 23SA | 2323 | G |
| 27 | 23SA | 2327 | U |
| 27 | 23SA | 2329 | C |
| 27 | 23SA | 2334 | G |
| 27 | 23SA | 2335 | A |
| 27 | 23SA | 2336 | G |
| 27 | 23SA | 2340 | G |
| 27 | 23SA | 2341 | C |
| 27 | 23SA | 2349 | G |

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| Mol | Chain | Res | Type |
|---|---|---|---|
| 27 | 23SA | 2351 | A |
| 27 | 23SA | 2361 | A |
| 27 | 23SA | 2362 | C |
| 27 | 23SA | 2365 | C |
| 27 | 23SA | 2394 | G |
| 27 | 23SA | 2398 | G |
| 27 | 23SA | 2400 | C |
| 27 | 23SA | 2406 | G |
| 27 | 23SA | 2407 | A |
| 27 | 23SA | 2421 | U |
| 27 | 23SA | 2422 | G |
| 27 | 23SA | 2426 | A |
| 27 | 23SA | 2437 | A |
| 27 | 23SA | 2438 | U |
| 27 | 23SA | 2439 | C |
| 27 | 23SA | 2440 | A |
| 27 | 23SA | 2441 | A |
| 27 | 23SA | 2442 | C |
| 27 | 23SA | 2443 | G |
| 27 | 23SA | 2444 | G |
| 27 | 23SA | 2445 | A |
| 27 | 23SA | 2450 | A |
| 27 | 23SA | 2454 | A |
| 27 | 23SA | 2455 | C |
| 27 | 23SA | 2456 | C |
| 27 | 23SA | 2463 | A |
| 27 | 23SA | 2475 | U |
| 27 | 23SA | 2484 | A |
| 27 | 23SA | 2485 | G |
| 27 | 23SA | 2488 | U |
| 27 | 23SA | 2489 | C |
| 27 | 23SA | 2490 | C |
| 27 | 23SA | 2491 | A |
| 27 | 23SA | 2497 | G |
| 27 | 23SA | 2509 | G |
| 27 | 23SA | 2517 | G |
| 27 | 23SA | 2518 | 2MA |
| 27 | 23SA | 2519 | U |
| 27 | 23SA | 2520 | G |
| 27 | 23SA | 2522 | C |
| 27 | 23SA | 2533 | A |
| 27 | 23SA | 2534 | U |

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| Mol | Chain | Res | Type |
|---|---|---|---|
| 27 | 23SA | 2540 | G |
| 27 | 23SA | 2544 | G |
| 27 | 23SA | 2558 | G |
| 27 | 23SA | 2569 | U |
| 27 | 23SA | 2581 | A |
| 27 | 23SA | 2582 | G |
| 27 | 23SA | 2588 | C |
| 27 | 23SA | 2597 | G |
| 27 | 23SA | 2600 | U |
| 27 | 23SA | 2614 | G |
| 27 | 23SA | 2617 | A |
| 27 | 23SA | 2624 | U |
| 27 | 23SA | 2625 | C |
| 27 | 23SA | 2626 | U |
| 27 | 23SA | 2627 | C |
| 27 | 23SA | 2644 | A |
| 27 | 23SA | 2645 | G |
| 27 | 23SA | 2660 | G |
| 27 | 23SA | 2661 | C |
| 27 | 23SA | 2669 | A |
| 27 | 23SA | 2670 | G |
| 27 | 23SA | 2680 | A |
| 27 | 23SA | 2681 | C |
| 27 | 23SA | 2688 | G |
| 27 | 23SA | 2694 | A |
| 27 | 23SA | 2697 | U |
| 27 | 23SA | 2701 | G |
| 27 | 23SA | 2704 | U |
| 27 | 23SA | 2706 | C |
| 27 | 23SA | 2717 | U |
| 27 | 23SA | 2718 | C |
| 27 | 23SA | 2722 | G |
| 27 | 23SA | 2727 | U |
| 27 | 23SA | 2728 | A |
| 27 | 23SA | 2729 | A |
| 27 | 23SA | 2730 | G |
| 27 | 23SA | 2742 | U |
| 27 | 23SA | 2743 | G |
| 27 | 23SA | 2749 | A |
| 27 | 23SA | 2750 | A |
| 27 | 23SA | 2760 | G |
| 27 | 23SA | 2764 | A |

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| Mol | Chain | Res | Type |
|---|---|---|---|
| 27 | 23SA | 2767 | G |
| 27 | 23SA | 2768 | C |
| 27 | 23SA | 2773 | A |
| 27 | 23SA | 2777 | G |
| 27 | 23SA | 2778 | G |
| 27 | 23SA | 2780 | A |
| 27 | 23SA | 2781 | A |
| 27 | 23SA | 2782 | G |
| 27 | 23SA | 2786 | G |
| 27 | 23SA | 2794 | A |
| 27 | 23SA | 2795 | U |
| 27 | 23SA | 2806 | A |
| 27 | 23SA | 2807 | C |
| 27 | 23SA | 2809 | G |
| 27 | 23SA | 2810 | C |
| 27 | 23SA | 2812 | U |
| 27 | 23SA | 2815 | A |
| 27 | 23SA | 2821 | U |
| 27 | 23SA | 2826 | A |
| 27 | 23SA | 2831 | G |
| 27 | 23SA | 2833 | A |
| 27 | 23SA | 2834 | A |
| 27 | 23SA | 2836 | A |
| 27 | 23SA | 2843 | G |
| 27 | 23SA | 2845 | U |
| 27 | 23SA | 2846 | G |
| 27 | 23SA | 2847 | G |
| 27 | 23SA | 2848 | A |
| 27 | 23SA | 2885 | G |
| 27 | 23SA | 2886 | A |
| 27 | 23SA | 2892 | C |
| 27 | 23SA | 2893 | C |
| 27 | 23SA | 2899 | G |
| 27 | 23SA | 2903 | G |
| 27 | 23SA | 2904 | A |
| 27 | 23SA | 2906 | G |
| 28 | 5SA | 9 | G |
| 28 | 5SA | 13 | C |
| 28 | 5SA | 14 | C |
| 28 | 5SA | 15 | A |
| 28 | 5SA | 17 | A |
| 28 | 5SA | 18 | G |

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| Mol | Chain | Res | Type |
|---|---|---|---|
| 28 | 5SA | 21 | G |
| 28 | 5SA | 27 | A |
| 28 | 5SA | 29 | C |
| 28 | 5SA | 33 | C |
| 28 | 5SA | 42 | U |
| 28 | 5SA | 43 | U |
| 28 | 5SA | 44 | C |
| 28 | 5SA | 54 | A |
| 28 | 5SA | 55 | A |
| 28 | 5SA | 58 | G |
| 28 | 5SA | 68 | A |
| 28 | 5SA | 69 | G |
| 28 | 5SA | 75 | A |
| 28 | 5SA | 83 | G |
| 28 | 5SA | 87 | G |
| 28 | 5SA | 91 | G |
| 28 | 5SA | 98 | U |
| 28 | 5SA | 104 | A |
| 28 | 5SA | 112 | G |
| 1 | 16SB | 654 | A |
| 1 | 16SB | 655 | G |
| 1 | 16SB | 656 | A |
| 1 | 16SB | 678 | A |
| 1 | 16SB | 685 | G |
| 1 | 16SB | 687 | G |
| 1 | 16SB | 693 | C |
| 1 | 16SB | 694 | C |
| 1 | 16SB | 697 | A |
| 1 | 16SB | 700 | C |
| 1 | 16SB | 711 | U |
| 1 | 16SB | 712 | G |
| 1 | 16SB | 719 | G |
| 1 | 16SB | 723 | G |
| 1 | 16SB | 729 | A |
| 1 | 16SB | 730 | C |
| 1 | 16SB | 732 | C |
| 1 | 16SB | 733 | C |
| 1 | 16SB | 735 | U |
| 1 | 16SB | 740 | A |
| 1 | 16SB | 747 | G |
| 1 | 16SB | 755 | A |
| 1 | 16SB | 758 | A |

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| Mol | Chain | Res | Type |
|---|---|---|---|
| 1 | 16SB | 759 | A |
| 1 | 16SB | 760 | C |
| 1 | 16SB | 771 | C |
| 1 | 16SB | 777 | C |
| 1 | 16SB | 803 | C |
| 1 | 16SB | 809 | C |
| 1 | 16SB | 814 | C |
| 1 | 16SB | 821 | G |
| 1 | 16SB | 822 | U |
| 1 | 16SB | 823 | G |
| 1 | 16SB | 826 | C |
| 1 | 16SB | 832 | C |
| 1 | 16SB | 834 | U |
| 1 | 16SB | 835 | U |
| 1 | 16SB | 836 | G |
| 1 | 16SB | 837 | G |
| 1 | 16SB | 840 | U |
| 1 | 16SB | 841 | G |
| 1 | 16SB | 847 | A |
| 1 | 16SB | 848 | A |
| 1 | 16SB | 849 | A |
| 1 | 16SB | 854 | U |
| 1 | 16SB | 855 | U |
| 1 | 16SB | 856 | U |
| 1 | 16SB | 857 | G |
| 1 | 16SB | 872 | G |
| 1 | 16SB | 885 | U |
| 1 | 16SB | 888 | G |
| 1 | 16SB | 892 | G |
| 1 | 16SB | 903 | A |
| 1 | 16SB | 907 | G |
| 1 | 16SB | 908 | C |
| 1 | 16SB | 921 | C |
| 1 | 16SB | 922 | G |
| 1 | 16SB | 930 | G |
| 1 | 16SB | 962 | A |
| 1 | 16SB | 969 | C |
| 1 | 16SB | 970 | A |
| 1 | 16SB | 973 | G |
| 1 | 16SB | 982 | C |
| 1 | 16SB | 986 | C |
| 1 | 16SB | 987 | G |

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| Mol | Chain | Res | Type |
|---|---|---|---|
| 1 | 16SB | 988 | G |
| 1 | 16SB | 991 | G |
| 1 | 16SB | 992 | G |
| 1 | 16SB | 993 | C |
| 1 | 16SB | 994 | A |
| 1 | 16SB | 995 | G |
| 1 | 16SB | 1008 | U |
| 1 | 16SB | 1013 | C |
| 1 | 16SB | 1014 | A |
| 1 | 16SB | 1029 | G |
| 1 | 16SB | 1038 | A |
| 1 | 16SB | 1039 | C |
| 1 | 16SB | 1047 | G |
| 1 | 16SB | 1050 | G |
| 1 | 16SB | 1053 | A |
| 1 | 16SB | 1054 | G |
| 1 | 16SB | 1055 | A |
| 1 | 16SB | 1060 | C |
| 1 | 16SB | 1063 | C |
| 1 | 16SB | 1064 | G |
| 1 | 16SB | 1065 | G |
| 1 | 16SB | 1070 | U |
| 1 | 16SB | 1071 | A |
| 1 | 16SB | 1075 | U |
| 1 | 16SB | 1080 | A |
| 1 | 16SB | 1082 | C |
| 1 | 16SB | 1092 | A |
| 1 | 16SB | 1100 | A |
| 1 | 16SB | 1101 | C |
| 1 | 16SB | 1102 | G |
| 1 | 16SB | 1105 | G |
| 1 | 16SB | 1112 | A |
| 1 | 16SB | 1115 | G |
| 1 | 16SB | 1116 | U |
| 1 | 16SB | 1126 | A |
| 1 | 16SB | 1127 | U |
| 1 | 16SB | 1134 | G |
| 1 | 16SB | 1138 | A |
| 1 | 16SB | 1139 | A |
| 1 | 16SB | 1140 | C |
| 1 | 16SB | 1147 | C |
| 1 | 16SB | 1156 | 7MG |

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| Mol | Chain | Res | Type |
|---|---|---|---|
| 1 | 16SB | 1159 | G |
| 1 | 16SB | 1160 | U |
| 1 | 16SB | 1161 | A |
| 1 | 16SB | 1162 | A |
| 1 | 16SB | 1165 | C |
| 1 | 16SB | 1174 | C |
| 1 | 16SB | 1176 | A |
| 1 | 16SB | 1188 | A |
| 1 | 16SB | 1190 | U |
| 1 | 16SB | 1191 | C |
| 1 | 16SB | 1193 | C |
| 1 | 16SB | 1197 | G |
| 1 | 16SB | 1201 | A |
| 1 | 16SB | 1202 | A |
| 1 | 16SB | 1205 | G |
| 1 | 16SB | 1236 | A |
| 1 | 16SB | 1243 | A |
| 1 | 16SB | 1252 | C |
| 1 | 16SB | 1256 | G |
| 1 | 16SB | 1260 | G |
| 1 | 16SB | 1279 | G |
| 1 | 16SB | 1282 | A |
| 1 | 16SB | 1290 | G |
| 1 | 16SB | 1291 | G |
| 1 | 16SB | 1294 | A |
| 1 | 16SB | 1300 | G |
| 1 | 16SB | 1315 | U |
| 1 | 16SB | 1316 | A |
| 1 | 16SB | 1317 | G |
| 1 | 16SB | 1330 | C |
| 1 | 16SB | 1331 | A |
| 1 | 16SB | 1332 | G |
| 1 | 16SB | 1333 | A |
| 1 | 16SB | 1350 | G |
| 1 | 16SB | 1352 | U |
| 1 | 16SB | 1353 | G |
| 1 | 16SB | 1360 | G |
| 1 | 16SB | 1363 | G |
| 1 | 16SB | 1377 | C |
| 1 | 16SB | 1378 | C |
| 1 | 16SB | 1381 | G |
| 1 | 16SB | 1382 | A |

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| Mol | Chain | Res | Type |
|---|---|---|---|
| 1 | 16SB | 1384 | G |
| 1 | 16SB | 1395 | A |
| 1 | 16SB | 1406 | A |
| 1 | 16SB | 1407 | G |
| 1 | 16SB | 1422 | U |
| 1 | 16SB | 1423 | A |
| 1 | 16SB | 1431 | A |
| 1 | 16SB | 1444 | A |
| 1 | 16SB | 1446 | C |
| 1 | 16SB | 1450 | G |
| 1 | 16SB | 1457 | A |
| 1 | 16SB | 1468 | U |
| 1 | 16SB | 1470 | U |
| 1 | 16SB | 1471 | C |
| 1 | 16SB | 1476 | G |
| 1 | 16SB | 1495 | A |
| 1 | 16SB | 1496 | A |
| 1 | 16SB | 1497 | G |
| 1 | 16SB | 1536 | A |
| 1 | 16SB | 1537 | A |
| 1 | 16SB | 1549 | G |
| 1 | 16SB | 1550 | G |
| 1 | 16SB | 1557 | C |
| 1 | 16SB | 1558 | A |
| 1 | 16SB | 1559 | C |
| 1 | 16SB | 1583 | U |
| 1 | 16SB | 1584 | U |
| 1 | 16SB | 1589 | M2G |
| 1 | 16SB | 1591 | A |
| 1 | 16SB | 1592 | A |
| 1 | 16SB | 1594 | G |
| 1 | 16SB | 1595 | C |
| 1 | 16SB | 1597 | A |
| 1 | 16SB | 1598 | A |
| 1 | 16SB | 1599 | G |
| 1 | 16SB | 1600 | A |
| 1 | 16SB | 1601 | A |
| 1 | 16SB | 1602 | C |
| 1 | 16SB | 1603 | C |
| 1 | 16SB | 1604 | U |
| 1 | 16SB | 1609 | A |
| 1 | 16SB | 1614 | U |

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| Mol | Chain | Res | Type |
|---|---|---|---|
| 1 | 16SB | 1615 | U |
| 1 | 16SB | 1616 | G |
| 1 | 16SB | 1621 | G |
| 1 | 16SB | 1629 | A |
| 1 | 16SB | 1630 | C |
| 1 | 16SB | 1633 | G |
| 1 | 16SB | 1640 | A |
| 1 | 16SB | 1641 | G |
| 1 | 16SB | 1645 | G |
| 1 | 16SB | 1647 | G |
| 1 | 16SB | 1648 | G |
| 1 | 16SB | 1649 | U |
| 1 | 16SB | 1650 | G |
| 1 | 16SB | 1652 | C |
| 1 | 16SB | 1653 | C |
| 1 | 16SB | 1654 | C |
| 1 | 16SB | 1655 | G |
| 1 | 16SB | 1657 | G |
| 1 | 16SB | 1659 | G |
| 1 | 16SB | 1661 | G |
| 1 | 16SB | 1663 | A |
| 1 | 16SB | 1664 | G |
| 1 | 16SB | 1668 | U |
| 1 | 16SB | 1674 | A |
| 1 | 16SB | 1678 | G |
| 1 | 16SB | 1681 | G |
| 1 | 16SB | 1682 | C |
| 1 | 16SB | 1683 | A |
| 1 | 16SB | 1694 | C |
| 1 | 16SB | 1709 | G |
| 1 | 16SB | 1710 | G |
| 1 | 16SB | 1722 | G |
| 1 | 16SB | 1723 | U |
| 1 | 16SB | 1727 | G |
| 1 | 16SB | 1729 | A |
| 1 | 16SB | 1745 | G |
| 1 | 16SB | 1750 | U |
| 1 | 16SB | 1752 | G |
| 1 | 16SB | 1753 | U |
| 1 | 16SB | 1755 | G |
| 1 | 16SB | 1756 | C |
| 1 | 16SB | 1757 | C |

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| Mol | Chain | Res | Type |
|---|---|---|---|
| 1 | 16SB | 1758 | A |
| 1 | 16SB | 1759 | G |
| 1 | 16SB | 1764 | U |
| 1 | 16SB | 1765 | C |
| 1 | 16SB | 1766 | G |
| 1 | 16SB | 1767 | G |
| 1 | 16SB | 1768 | C |
| 1 | 16SB | 1774 | A |
| 1 | 16SB | 1775 | C |
| 1 | 16SB | 1782 | G |
| 1 | 16SB | 1785 | A |
| 1 | 16SB | 1786 | C |
| 1 | 16SB | 1787 | U |
| 1 | 16SB | 1788 | G |
| 1 | 16SB | 1789 | C |
| 1 | 16SB | 1798 | G |
| 1 | 16SB | 1808 | G |
| 1 | 16SB | 1810 | A |
| 1 | 16SB | 1811 | G |
| 1 | 16SB | 1812 | G |
| 1 | 16SB | 1814 | G |
| 1 | 16SB | 1815 | A |
| 1 | 16SB | 1817 | G |
| 1 | 16SB | 1820 | G |
| 1 | 16SB | 1823 | U |
| 1 | 16SB | 1825 | G |
| 1 | 16SB | 1827 | C |
| 1 | 16SB | 1828 | A |
| 1 | 16SB | 1829 | G |
| 1 | 16SB | 1834 | 2MG |
| 1 | 16SB | 1838 | U |
| 1 | 16SB | 1839 | U |
| 1 | 16SB | 1840 | A |
| 1 | 16SB | 1841 | C |
| 1 | 16SB | 1845 | C |
| 1 | 16SB | 1852 | A |
| 1 | 16SB | 1854 | A |
| 1 | 16SB | 1865 | A |
| 1 | 16SB | 1868 | G |
| 1 | 16SB | 1883 | A |
| 1 | 16SB | 1884 | U |
| 1 | 16SB | 1885 | G |

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| Mol | Chain | Res | Type |
|---|---|---|---|
| 1 | 16SB | 1887 | C |
| 1 | 16SB | 1891 | C |
| 1 | 16SB | 1899 | G |
| 1 | 16SB | 1900 | G |
| 1 | 16SB | 1905 | U |
| 1 | 16SB | 1907 | A |
| 1 | 16SB | 1908 | U |
| 1 | 16SB | 1909 | C |
| 1 | 16SB | 1912 | A |
| 1 | 16SB | 1913 | A |
| 1 | 16SB | 1914 | A |
| 1 | 16SB | 1916 | A |
| 1 | 16SB | 1919 | U |
| 1 | 16SB | 1924 | C |
| 1 | 16SB | 1925 | C |
| 1 | 16SB | 1926 | A |
| 1 | 16SB | 1928 | U |
| 1 | 16SB | 1932 | G |
| 1 | 16SB | 1933 | A |
| 1 | 16SB | 1941 | C |
| 1 | 16SB | 1945 | A |
| 1 | 16SB | 1946 | A |
| 1 | 16SB | 1947 | C |
| 1 | 16SB | 1948 | C |
| 1 | 16SB | 1949 | C |
| 1 | 16SB | 1950 | G |
| 1 | 16SB | 1954 | C |
| 1 | 16SB | 1958 | G |
| 1 | 16SB | 1962 | C |
| 1 | 16SB | 1963 | C |
| 1 | 16SB | 1964 | G |
| 1 | 16SB | 1965 | G |
| 1 | 16SB | 1973 | A |
| 1 | 16SB | 1974 | G |
| 1 | 16SB | 1980 | G |
| 1 | 16SB | 1990 | C |
| 1 | 16SB | 1991 | A |
| 1 | 16SB | 1992 | U |
| 1 | 16SB | 1996 | G |
| 1 | 16SB | 1998 | G |
| 1 | 16SB | 2015 | G |
| 1 | 16SB | 2025 | C |

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| Mol | Chain | Res | Type |
|---|---|---|---|
| 1 | 16SB | 2026 | A |
| 1 | 16SB | 2030 | 4OC |
| 1 | 16SB | 2047 | G |
| 1 | 16SB | 2070 | G |
| 1 | 16SB | 2071 | G |
| 1 | 16SB | 2072 | A |
| 1 | 16SB | 2076 | U |
| 1 | 16SB | 2077 | A |
| 1 | 16SB | 2078 | C |
| 1 | 16SB | 2079 | G |
| 1 | 16SB | 2110 | G |
| 1 | 16SB | 2115 | A |
| 1 | 16SB | 2122 | A |
| 1 | 16SB | 2129 | U |
| 1 | 16SB | 2140 | G |
| 1 | 16SB | 2142 | MA6 |
| 1 | 16SB | 2143 | G |
| 1 | 16SB | 2152 | G |
| 1 | 16SB | 2153 | G |
| 1 | 16SB | 2160 | U |
| 1 | 16SB | 2161 | C |
| 57 | ASIB | 8 | U |
| 57 | ASIB | 9 | A |
| 57 | ASIB | 10 | G |
| 57 | ASIB | 11 | C |
| 57 | ASIB | 12 | U |
| 57 | ASIB | 13 | C |
| 57 | ASIB | 16 | U |
| 57 | ASIB | 17 | C |
| 57 | ASIB | 18 | G |
| 57 | ASIB | 19 | G |
| 57 | ASIB | 21 | A |
| 57 | ASIB | 22 | G |
| 57 | ASIB | 24 | G |
| 57 | ASIB | 26 | A |
| 57 | ASIB | 41 | C |
| 57 | ASIB | 44 | G |
| 57 | ASIB | 46 | G |
| 57 | ASIB | 47 | U |
| 57 | ASIB | 48 | C |
| 57 | ASIB | 49 | C |
| 57 | ASIB | 50 | U |

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| Mol | Chain | Res | Type |
|---|---|---|---|
| 57 | ASIB | 53 | G |
| 57 | ASIB | 56 | C |
| 57 | ASIB | 58 | A |
| 57 | ASIB | 59 | U |
| 57 | ASIB | 60 | U |
| 57 | ASIB | 63 | G |
| 57 | ASIB | 64 | A |
| 57 | ASIB | 69 | G |
| 57 | ASIB | 70 | G |
| 57 | ASIB | 71 | G |
| 57 | ASIB | 72 | C |
| 57 | ASIB | 73 | A |
| 57 | ASIB | 74 | C |
| 57 | ASIB | 75 | C |
| 57 | ASIB | 76 | A |
| 23 | PSIB | 2 | C |
| 23 | PSIB | 3 | C |
| 23 | PSIB | 8 | 4SU |
| 23 | PSIB | 9 | A |
| 23 | PSIB | 11 | C |
| 23 | PSIB | 15 | G |
| 23 | PSIB | 16 | U |
| 23 | PSIB | 17 | C |
| 23 | PSIB | 18 | G |
| 23 | PSIB | 19 | G |
| 23 | PSIB | 20 | U |
| 23 | PSIB | 21 | A |
| 23 | PSIB | 22 | G |
| 23 | PSIB | 25 | C |
| 23 | PSIB | 30 | G |
| 23 | PSIB | 42 | C |
| 23 | PSIB | 43 | C |
| 23 | PSIB | 44 | G |
| 23 | PSIB | 45 | U |
| 23 | PSIB | 47 | 3AU |
| 23 | PSIB | 48 | C |
| 23 | PSIB | 52 | G |
| 23 | PSIB | 54 | 5MU |
| 23 | PSIB | 56 | C |
| 23 | PSIB | 58 | A |
| 23 | PSIB | 60 | U |
| 23 | PSIB | 61 | C |

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| Mol | Chain | Res | Type |
|---|---|---|---|
| 23 | PSIB | 67 | C |
| 23 | PSIB | 70 | G |
| 23 | PSIB | 74 | C |
| 23 | PSIB | 76 | A |
| 24 | ESIB | 2 | C |
| 24 | ESIB | 9 | A |
| 24 | ESIB | 13 | C |
| 24 | ESIB | 14 | A |
| 24 | ESIB | 16 | U |
| 24 | ESIB | 17 | C |
| 24 | ESIB | 18 | G |
| 24 | ESIB | 19 | G |
| 24 | ESIB | 20 | U |
| 24 | ESIB | 21 | A |
| 24 | ESIB | 22 | G |
| 24 | ESIB | 34 | G |
| 24 | ESIB | 36 | A |
| 24 | ESIB | 37 | MIA |
| 24 | ESIB | 38 | A |
| 24 | ESIB | 40 | C |
| 24 | ESIB | 46 | G |
| 24 | ESIB | 48 | C |
| 24 | ESIB | 58 | A |
| 24 | ESIB | 59 | U |
| 24 | ESIB | 65 | G |
| 24 | ESIB | 72 | C |
| 24 | ESIB | 73 | A |
| 24 | ESIB | 76 | A |
| 25 | MRNB | 29 | G |
| 25 | MRNB | 37 | G |
| 25 | MRNB | 43 | U |
| 25 | MRNB | 46 | U |
| 25 | MRNB | 49 | U |
| 25 | MRNB | 51 | U |
| 25 | MRNB | 52 | U |
| 25 | MRNB | 54 | U |
| 25 | MRNB | 55 | U |
| 25 | MRNB | 56 | U |
| 25 | MRNB | 57 | U |
| 27 | 23SB | 3 | U |
| 27 | 23SB | 4 | C |
| 27 | 23SB | 5 | A |

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| Mol | Chain | Res | Type |
|---|---|---|---|
| 27 | 23SB | 10 | G |
| 27 | 23SB | 13 | A |
| 27 | 23SB | 15 | G |
| 27 | 23SB | 34 | C |
| 27 | 23SB | 35 | G |
| 27 | 23SB | 45 | C |
| 27 | 23SB | 48 | A |
| 27 | 23SB | 49 | U |
| 27 | 23SB | 50 | G |
| 27 | 23SB | 57 | G |
| 27 | 23SB | 59 | G |
| 27 | 23SB | 60 | G |
| 27 | 23SB | 62 | U |
| 27 | 23SB | 68 | C |
| 27 | 23SB | 70 | A |
| 27 | 23SB | 73 | A |
| 27 | 23SB | 74 | G |
| 27 | 23SB | 77 | A |
| 27 | 23SB | 82 | G |
| 27 | 23SB | 83 | A |
| 27 | 23SB | 84 | G |
| 27 | 23SB | 85 | C |
| 27 | 23SB | 89 | U |
| 27 | 23SB | 94 | G |
| 27 | 23SB | 100 | G |
| 27 | 23SB | 116 | A |
| 27 | 23SB | 117 | A |
| 27 | 23SB | 118 | U |
| 27 | 23SB | 119 | G |
| 27 | 23SB | 127 | C |
| 27 | 23SB | 137 | G |
| 27 | 23SB | 140 | A |
| 27 | 23SB | 155 | C |
| 27 | 23SB | 156 | U |
| 27 | 23SB | 157 | U |
| 27 | 23SB | 162 | C |
| 27 | 23SB | 163 | G |
| 27 | 23SB | 164 | C |
| 27 | 23SB | 186 | A |
| 27 | 23SB | 189 | A |
| 27 | 23SB | 196 | U |
| 27 | 23SB | 204 | G |

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| Mol | Chain | Res | Type |
|---|---|---|---|
| 27 | 23SB | 205 | G |
| 27 | 23SB | 206 | A |
| 27 | 23SB | 207 | G |
| 27 | 23SB | 211 | A |
| 27 | 23SB | 212 | A |
| 27 | 23SB | 217 | A |
| 27 | 23SB | 219 | A |
| 27 | 23SB | 223 | A |
| 27 | 23SB | 238 | G |
| 27 | 23SB | 239 | C |
| 27 | 23SB | 242 | G |
| 27 | 23SB | 255 | A |
| 27 | 23SB | 256 | G |
| 27 | 23SB | 271 | C |
| 27 | 23SB | 272 | U |
| 27 | 23SB | 273 | U |
| 27 | 23SB | 274 | G |
| 27 | 23SB | 275 | U |
| 27 | 23SB | 276 | C |
| 27 | 23SB | 282 | G |
| 27 | 23SB | 289 | U |
| 27 | 23SB | 290 | G |
| 27 | 23SB | 296 | C |
| 27 | 23SB | 298 | C |
| 27 | 23SB | 301 | A |
| 27 | 23SB | 302 | C |
| 27 | 23SB | 303 | A |
| 27 | 23SB | 304 | C |
| 27 | 23SB | 308 | A |
| 27 | 23SB | 311 | C |
| 27 | 23SB | 313 | C |
| 27 | 23SB | 314 | A |
| 27 | 23SB | 315 | G |
| 27 | 23SB | 320 | G |
| 27 | 23SB | 336 | A |
| 27 | 23SB | 340 | G |
| 27 | 23SB | 342 | G |
| 27 | 23SB | 354 | G |
| 27 | 23SB | 355 | A |
| 27 | 23SB | 356 | A |
| 27 | 23SB | 370 | A |
| 27 | 23SB | 377 | G |

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| Mol | Chain | Res | Type |
|---|---|---|---|
| 27 | 23SB | 381 | G |
| 27 | 23SB | 387 | U |
| 27 | 23SB | 389 | A |
| 27 | 23SB | 390 | G |
| 27 | 23SB | 392 | G |
| 27 | 23SB | 393 | U |
| 27 | 23SB | 394 | A |
| 27 | 23SB | 395 | C |
| 27 | 23SB | 414 | G |
| 27 | 23SB | 424 | G |
| 27 | 23SB | 432 | C |
| 27 | 23SB | 433 | U |
| 27 | 23SB | 434 | G |
| 27 | 23SB | 435 | G |
| 27 | 23SB | 439 | G |
| 27 | 23SB | 457 | A |
| 27 | 23SB | 472 | C |
| 27 | 23SB | 476 | U |
| 27 | 23SB | 479 | C |
| 27 | 23SB | 482 | A |
| 27 | 23SB | 483 | C |
| 27 | 23SB | 485 | A |
| 27 | 23SB | 492 | U |
| 27 | 23SB | 498 | A |
| 27 | 23SB | 499 | A |
| 27 | 23SB | 503 | U |
| 27 | 23SB | 507 | A |
| 27 | 23SB | 509 | G |
| 27 | 23SB | 521 | G |
| 27 | 23SB | 532 | A |
| 27 | 23SB | 535 | G |
| 27 | 23SB | 536 | C |
| 27 | 23SB | 539 | G |
| 27 | 23SB | 556 | A |
| 27 | 23SB | 557 | G |
| 27 | 23SB | 558 | C |
| 27 | 23SB | 559 | A |
| 27 | 23SB | 560 | G |
| 27 | 23SB | 564 | C |
| 27 | 23SB | 575 | G |
| 27 | 23SB | 588 | G |
| 27 | 23SB | 589 | C |

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| Mol | Chain | Res | Type |
|---|---|---|---|
| 27 | 23SB | 595 | G |
| 27 | 23SB | 598 | G |
| 27 | 23SB | 600 | A |
| 27 | 23SB | 608 | G |
| 27 | 23SB | 613 | U |
| 27 | 23SB | 618 | G |
| 27 | 23SB | 628 | A |
| 27 | 23SB | 629 | G |
| 27 | 23SB | 632 | U |
| 27 | 23SB | 635 | G |
| 27 | 23SB | 638 | G |
| 27 | 23SB | 639 | U |
| 27 | 23SB | 640 | U |
| 27 | 23SB | 641 | G |
| 27 | 23SB | 643 | G |
| 27 | 23SB | 644 | G |
| 27 | 23SB | 648 | A |
| 27 | 23SB | 649 | G |
| 27 | 23SB | 653 | U |
| 27 | 23SB | 654 | A |
| 27 | 23SB | 656 | G |
| 27 | 23SB | 664 | A |
| 27 | 23SB | 672 | C |
| 27 | 23SB | 673 | A |
| 27 | 23SB | 678 | G |
| 27 | 23SB | 679 | C |
| 27 | 23SB | 680 | A |
| 27 | 23SB | 681 | A |
| 27 | 23SB | 682 | A |
| 27 | 23SB | 686 | C |
| 27 | 23SB | 699 | C |
| 27 | 23SB | 700 | G |
| 27 | 23SB | 701 | A |
| 27 | 23SB | 706 | U |
| 27 | 23SB | 719 | A |
| 27 | 23SB | 726 | A |
| 27 | 23SB | 735 | G |
| 27 | 23SB | 758 | U |
| 27 | 23SB | 779 | C |
| 27 | 23SB | 807 | C |
| 27 | 23SB | 811 | U |
| 27 | 23SB | 824 | G |

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| Mol | Chain | Res | Type |
|---|---|---|---|
| 27 | 23SB | 825 | G |
| 27 | 23SB | 831 | A |
| 27 | 23SB | 833 | A |
| 27 | 23SB | 834 | G |
| 27 | 23SB | 838 | A |
| 27 | 23SB | 839 | C |
| 27 | 23SB | 841 | G |
| 27 | 23SB | 842 | A |
| 27 | 23SB | 854 | G |
| 27 | 23SB | 861 | C |
| 27 | 23SB | 868 | A |
| 27 | 23SB | 876 | U |
| 27 | 23SB | 877 | U |
| 27 | 23SB | 881 | G |
| 27 | 23SB | 895 | C |
| 27 | 23SB | 896 | U |
| 27 | 23SB | 908 | G |
| 27 | 23SB | 914 | C |
| 27 | 23SB | 920 | U |
| 27 | 23SB | 927 | A |
| 27 | 23SB | 932 | G |
| 27 | 23SB | 934 | C |
| 27 | 23SB | 935 | C |
| 27 | 23SB | 936 | A |
| 27 | 23SB | 937 | C |
| 27 | 23SB | 938 | C |
| 27 | 23SB | 942 | C |
| 27 | 23SB | 944 | A |
| 27 | 23SB | 945 | C |
| 27 | 23SB | 947 | A |
| 27 | 23SB | 948 | A |
| 27 | 23SB | 949 | A |
| 27 | 23SB | 952 | C |
| 27 | 23SB | 954 | G |
| 27 | 23SB | 955 | U |
| 27 | 23SB | 958 | A |
| 27 | 23SB | 963 | C |
| 27 | 23SB | 965 | A |
| 27 | 23SB | 967 | G |
| 27 | 23SB | 978 | G |
| 27 | 23SB | 979 | G |
| 27 | 23SB | 985 | G |

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| Mol | Chain | Res | Type |
|---|---|---|---|
| 27 | 23SB | 988 | A |
| 27 | 23SB | 992 | A |
| 27 | 23SB | 993 | G |
| 27 | 23SB | 1000 | A |
| 27 | 23SB | 1005 | U |
| 27 | 23SB | 1006 | A |
| 27 | 23SB | 1008 | C |
| 27 | 23SB | 1021 | G |
| 27 | 23SB | 1028 | A |
| 27 | 23SB | 1031 | A |
| 27 | 23SB | 1038 | A |
| 27 | 23SB | 1039 | C |
| 27 | 23SB | 1044 | A |
| 27 | 23SB | 1058 | A |
| 27 | 23SB | 1059 | G |
| 27 | 23SB | 1060 | U |
| 27 | 23SB | 1061 | C |
| 27 | 23SB | 1070 | G |
| 27 | 23SB | 1071 | U |
| 27 | 23SB | 1073 | G |
| 27 | 23SB | 1074 | U |
| 27 | 23SB | 1075 | A |
| 27 | 23SB | 1081 | U |
| 27 | 23SB | 1085 | G |
| 27 | 23SB | 1086 | C |
| 27 | 23SB | 1092 | G |
| 27 | 23SB | 1093 | A |
| 27 | 23SB | 1094 | A |
| 27 | 23SB | 1095 | G |
| 27 | 23SB | 1096 | A |
| 27 | 23SB | 1102 | A |
| 27 | 23SB | 1104 | G |
| 27 | 23SB | 1108 | U |
| 27 | 23SB | 1110 | G |
| 27 | 23SB | 1128 | A |
| 27 | 23SB | 1133 | A |
| 27 | 23SB | 1134 | A |
| 27 | 23SB | 1135 | G |
| 27 | 23SB | 1136 | A |
| 27 | 23SB | 1138 | U |
| 27 | 23SB | 1139 | G |
| 27 | 23SB | 1153 | U |

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| Mol | Chain | Res | Type |
|---|---|---|---|
| 27 | 23SB | 1159 | A |
| 27 | 23SB | 1160 | G |
| 27 | 23SB | 1161 | U |
| 27 | 23SB | 1170 | G |
| 27 | 23SB | 1176 | A |
| 27 | 23SB | 1177 | A |
| 27 | 23SB | 1178 | U |
| 27 | 23SB | 1179 | G |
| 27 | 23SB | 1183 | C |
| 27 | 23SB | 1184 | G |
| 27 | 23SB | 1187 | G |
| 27 | 23SB | 1191 | A |
| 27 | 23SB | 1192 | A |
| 27 | 23SB | 1205 | A |
| 27 | 23SB | 1218 | G |
| 27 | 23SB | 1221 | G |
| 27 | 23SB | 1222 | A |
| 27 | 23SB | 1223 | U |
| 27 | 23SB | 1224 | G |
| 27 | 23SB | 1225 | A |
| 27 | 23SB | 1226 | C |
| 27 | 23SB | 1228 | C |
| 27 | 23SB | 1243 | G |
| 27 | 23SB | 1245 | G |
| 27 | 23SB | 1252 | A |
| 27 | 23SB | 1253 | U |
| 27 | 23SB | 1254 | G |
| 27 | 23SB | 1258 | A |
| 27 | 23SB | 1259 | U |
| 27 | 23SB | 1260 | G |
| 27 | 23SB | 1268 | A |
| 27 | 23SB | 1269 | C |
| 27 | 23SB | 1302 | A |
| 27 | 23SB | 1304 | U |
| 27 | 23SB | 1305 | G |
| 27 | 23SB | 1314 | A |
| 27 | 23SB | 1318 | A |
| 27 | 23SB | 1320 | G |
| 27 | 23SB | 1321 | A |
| 27 | 23SB | 1322 | U |
| 27 | 23SB | 1335 | A |
| 27 | 23SB | 1349 | U |

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| Mol | Chain | Res | Type |
|---|---|---|---|
| 27 | 23SB | 1350 | A |
| 27 | 23SB | 1358 | G |
| 27 | 23SB | 1362 | U |
| 27 | 23SB | 1363 | C |
| 27 | 23SB | 1367 | C |
| 27 | 23SB | 1368 | G |
| 27 | 23SB | 1378 | U |
| 27 | 23SB | 1390 | U |
| 27 | 23SB | 1394 | C |
| 27 | 23SB | 1398 | A |
| 27 | 23SB | 1401 | U |
| 27 | 23SB | 1408 | A |
| 27 | 23SB | 1409 | A |
| 27 | 23SB | 1414 | A |
| 27 | 23SB | 1417 | G |
| 27 | 23SB | 1428 | A |
| 27 | 23SB | 1433 | A |
| 27 | 23SB | 1434 | G |
| 27 | 23SB | 1435 | C |
| 27 | 23SB | 1437 | G |
| 27 | 23SB | 1456 | C |
| 27 | 23SB | 1465 | G |
| 27 | 23SB | 1466 | C |
| 27 | 23SB | 1469 | U |
| 27 | 23SB | 1470 | G |
| 27 | 23SB | 1477 | C |
| 27 | 23SB | 1486 | C |
| 27 | 23SB | 1492 | G |
| 27 | 23SB | 1494 | A |
| 27 | 23SB | 1499 | A |
| 27 | 23SB | 1500 | G |
| 27 | 23SB | 1502 | C |
| 27 | 23SB | 1508 | C |
| 27 | 23SB | 1510 | A |
| 27 | 23SB | 1511 | G |
| 27 | 23SB | 1516 | G |
| 27 | 23SB | 1521 | A |
| 27 | 23SB | 1524 | C |
| 27 | 23SB | 1525 | G |
| 27 | 23SB | 1526 | C |
| 27 | 23SB | 1528 | G |
| 27 | 23SB | 1529 | G |

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| Mol | Chain | Res | Type |
|---|---|---|---|
| 27 | 23SB | 1530 | G |
| 27 | 23SB | 1531 | U |
| 27 | 23SB | 1532 | G |
| 27 | 23SB | 1535 | A |
| 27 | 23SB | 1536 | G |
| 27 | 23SB | 1537 | G |
| 27 | 23SB | 1539 | A |
| 27 | 23SB | 1542 | C |
| 27 | 23SB | 1548 | C |
| 27 | 23SB | 1551 | C |
| 27 | 23SB | 1554 | C |
| 27 | 23SB | 1557 | A |
| 27 | 23SB | 1558 | C |
| 27 | 23SB | 1559 | A |
| 27 | 23SB | 1564 | C |
| 27 | 23SB | 1565 | U |
| 27 | 23SB | 1575 | G |
| 27 | 23SB | 1576 | G |
| 27 | 23SB | 1577 | A |
| 27 | 23SB | 1583 | G |
| 27 | 23SB | 1584 | U |
| 27 | 23SB | 1586 | C |
| 27 | 23SB | 1587 | G |
| 27 | 23SB | 1592 | A |
| 27 | 23SB | 1593 | C |
| 27 | 23SB | 1594 | A |
| 27 | 23SB | 1604 | A |
| 27 | 23SB | 1605 | G |
| 27 | 23SB | 1608 | A |
| 27 | 23SB | 1609 | G |
| 27 | 23SB | 1610 | G |
| 27 | 23SB | 1616 | A |
| 27 | 23SB | 1619 | A |
| 27 | 23SB | 1625 | C |
| 27 | 23SB | 1628 | U |
| 27 | 23SB | 1629 | A |
| 27 | 23SB | 1631 | G |
| 27 | 23SB | 1635 | A |
| 27 | 23SB | 1637 | C |
| 27 | 23SB | 1647 | C |
| 27 | 23SB | 1657 | A |
| 27 | 23SB | 1659 | A |

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| Mol | Chain | Res | Type |
|---|---|---|---|
| 27 | 23SB | 1660 | C |
| 27 | 23SB | 1667 | A |
| 27 | 23SB | 1690 | C |
| 27 | 23SB | 1698 | C |
| 27 | 23SB | 1703 | G |
| 27 | 23SB | 1704 | A |
| 27 | 23SB | 1714 | A |
| 27 | 23SB | 1724 | G |
| 27 | 23SB | 1746 | G |
| 27 | 23SB | 1750 | A |
| 27 | 23SB | 1751 | A |
| 27 | 23SB | 1766 | G |
| 27 | 23SB | 1769 | G |
| 27 | 23SB | 1770 | A |
| 27 | 23SB | 1771 | U |
| 27 | 23SB | 1772 | G |
| 27 | 23SB | 1776 | C |
| 27 | 23SB | 1790 | G |
| 27 | 23SB | 1792 | G |
| 27 | 23SB | 1796 | A |
| 27 | 23SB | 1797 | G |
| 27 | 23SB | 1798 | G |
| 27 | 23SB | 1807 | A |
| 27 | 23SB | 1814 | A |
| 27 | 23SB | 1815 | C |
| 27 | 23SB | 1816 | C |
| 27 | 23SB | 1825 | A |
| 27 | 23SB | 1832 | U |
| 27 | 23SB | 1834 | C |
| 27 | 23SB | 1835 | G |
| 27 | 23SB | 1850 | G |
| 27 | 23SB | 1854 | U |
| 27 | 23SB | 1863 | A |
| 27 | 23SB | 1873 | G |
| 27 | 23SB | 1880 | G |
| 27 | 23SB | 1881 | A |
| 27 | 23SB | 1882 | A |
| 27 | 23SB | 1883 | G |
| 27 | 23SB | 1892 | G |
| 27 | 23SB | 1902 | A |
| 27 | 23SB | 1903 | G |
| 27 | 23SB | 1907 | C |

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| Mol | Chain | Res | Type |
|---|---|---|---|
| 27 | 23SB | 1913 | G |
| 27 | 23SB | 1914 | A |
| 27 | 23SB | 1924 | G |
| 27 | 23SB | 1925 | A |
| 27 | 23SB | 1931 | G |
| 27 | 23SB | 1939 | C |
| 27 | 23SB | 1941 | A |
| 27 | 23SB | 1954 | G |
| 27 | 23SB | 1955 | G |
| 27 | 23SB | 1956 | U |
| 27 | 23SB | 1959 | C |
| 27 | 23SB | 1961 | A |
| 27 | 23SB | 1962 | A |
| 27 | 23SB | 1963 | A |
| 27 | 23SB | 1964 | 5MU |
| 27 | 23SB | 1972 | C |
| 27 | 23SB | 1973 | G |
| 27 | 23SB | 1980 | U |
| 27 | 23SB | 1985 | A |
| 27 | 23SB | 1988 | U |
| 27 | 23SB | 1989 | G |
| 27 | 23SB | 1992 | C |
| 27 | 23SB | 1995 | A |
| 27 | 23SB | 1996 | A |
| 27 | 23SB | 1997 | A |
| 27 | 23SB | 2007 | C |
| 27 | 23SB | 2018 | U |
| 27 | 23SB | 2045 | A |
| 27 | 23SB | 2048 | G |
| 27 | 23SB | 2052 | G |
| 27 | 23SB | 2056 | A |
| 27 | 23SB | 2057 | G |
| 27 | 23SB | 2058 | A |
| 27 | 23SB | 2068 | C |
| 27 | 23SB | 2076 | A |
| 27 | 23SB | 2079 | A |
| 27 | 23SB | 2080 | C |
| 27 | 23SB | 2081 | G |
| 27 | 23SB | 2084 | A |
| 27 | 23SB | 2085 | A |
| 27 | 23SB | 2086 | G |
| 27 | 23SB | 2087 | A |

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| Mol | Chain | Res | Type |
|---|---|---|---|
| 27 | 23SB | 2094 | G |
| 27 | 23SB | 2118 | G |
| 27 | 23SB | 2124 | U |
| 27 | 23SB | 2125 | G |
| 27 | 23SB | 2126 | G |
| 27 | 23SB | 2133 | C |
| 27 | 23SB | 2135 | G |
| 27 | 23SB | 2136 | C |
| 27 | 23SB | 2138 | U |
| 27 | 23SB | 2139 | A |
| 27 | 23SB | 2140 | G |
| 27 | 23SB | 2141 | G |
| 27 | 23SB | 2142 | A |
| 27 | 23SB | 2143 | U |
| 27 | 23SB | 2148 | G |
| 27 | 23SB | 2151 | A |
| 27 | 23SB | 2152 | G |
| 27 | 23SB | 2153 | C |
| 27 | 23SB | 2156 | G |
| 27 | 23SB | 2157 | U |
| 27 | 23SB | 2158 | G |
| 27 | 23SB | 2161 | C |
| 27 | 23SB | 2166 | G |
| 27 | 23SB | 2172 | G |
| 27 | 23SB | 2173 | G |
| 27 | 23SB | 2174 | G |
| 27 | 23SB | 2188 | C |
| 27 | 23SB | 2191 | G |
| 27 | 23SB | 2194 | A |
| 27 | 23SB | 2196 | A |
| 27 | 23SB | 2197 | U |
| 27 | 23SB | 2198 | A |
| 27 | 23SB | 2199 | C |
| 27 | 23SB | 2203 | C |
| 27 | 23SB | 2214 | U |
| 27 | 23SB | 2215 | G |
| 27 | 23SB | 2217 | G |
| 27 | 23SB | 2219 | G |
| 27 | 23SB | 2223 | A |
| 27 | 23SB | 2230 | G |
| 27 | 23SB | 2231 | G |
| 27 | 23SB | 2232 | A |

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| Mol | Chain | Res | Type |
|---|---|---|---|
| 27 | 23SB | 2233 | U |
| 27 | 23SB | 2234 | G |
| 27 | 23SB | 2240 | A |
| 27 | 23SB | 2253 | G |
| 27 | 23SB | 2254 | G |
| 27 | 23SB | 2260 | U |
| 27 | 23SB | 2261 | G |
| 27 | 23SB | 2267 | G |
| 27 | 23SB | 2288 | A |
| 27 | 23SB | 2290 | C |
| 27 | 23SB | 2295 | G |
| 27 | 23SB | 2298 | C |
| 27 | 23SB | 2302 | A |
| 27 | 23SB | 2303 | A |
| 27 | 23SB | 2304 | G |
| 27 | 23SB | 2309 | C |
| 27 | 23SB | 2319 | G |
| 27 | 23SB | 2320 | A |
| 27 | 23SB | 2322 | G |
| 27 | 23SB | 2323 | G |
| 27 | 23SB | 2325 | A |
| 27 | 23SB | 2327 | U |
| 27 | 23SB | 2329 | C |
| 27 | 23SB | 2334 | G |
| 27 | 23SB | 2335 | A |
| 27 | 23SB | 2336 | G |
| 27 | 23SB | 2340 | G |
| 27 | 23SB | 2341 | C |
| 27 | 23SB | 2349 | G |
| 27 | 23SB | 2351 | A |
| 27 | 23SB | 2361 | A |
| 27 | 23SB | 2362 | C |
| 27 | 23SB | 2364 | G |
| 27 | 23SB | 2365 | C |
| 27 | 23SB | 2387 | G |
| 27 | 23SB | 2394 | G |
| 27 | 23SB | 2398 | G |
| 27 | 23SB | 2400 | C |
| 27 | 23SB | 2406 | G |
| 27 | 23SB | 2407 | A |
| 27 | 23SB | 2417 | C |
| 27 | 23SB | 2418 | C |

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| Mol | Chain | Res | Type |
|---|---|---|---|
| 27 | 23SB | 2421 | U |
| 27 | 23SB | 2426 | A |
| 27 | 23SB | 2429 | G |
| 27 | 23SB | 2438 | U |
| 27 | 23SB | 2439 | C |
| 27 | 23SB | 2440 | A |
| 27 | 23SB | 2441 | A |
| 27 | 23SB | 2443 | G |
| 27 | 23SB | 2444 | G |
| 27 | 23SB | 2445 | A |
| 27 | 23SB | 2449 | A |
| 27 | 23SB | 2450 | A |
| 27 | 23SB | 2454 | A |
| 27 | 23SB | 2455 | C |
| 27 | 23SB | 2456 | C |
| 27 | 23SB | 2463 | A |
| 27 | 23SB | 2475 | U |
| 27 | 23SB | 2484 | A |
| 27 | 23SB | 2485 | G |
| 27 | 23SB | 2487 | G |
| 27 | 23SB | 2489 | C |
| 27 | 23SB | 2490 | C |
| 27 | 23SB | 2491 | A |
| 27 | 23SB | 2493 | A |
| 27 | 23SB | 2497 | G |
| 27 | 23SB | 2509 | G |
| 27 | 23SB | 2517 | G |
| 27 | 23SB | 2520 | G |
| 27 | 23SB | 2521 | U |
| 27 | 23SB | 2522 | C |
| 27 | 23SB | 2533 | A |
| 27 | 23SB | 2534 | U |
| 27 | 23SB | 2539 | G |
| 27 | 23SB | 2540 | G |
| 27 | 23SB | 2544 | G |
| 27 | 23SB | 2557 | A |
| 27 | 23SB | 2558 | G |
| 27 | 23SB | 2569 | U |
| 27 | 23SB | 2581 | A |
| 27 | 23SB | 2582 | G |
| 27 | 23SB | 2584 | G |
| 27 | 23SB | 2586 | C |

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| Mol | Chain | Res | Type |
|---|---|---|---|
| 27 | 23SB | 2588 | C |
| 27 | 23SB | 2600 | U |
| 27 | 23SB | 2617 | A |
| 27 | 23SB | 2618 | G |
| 27 | 23SB | 2624 | U |
| 27 | 23SB | 2625 | C |
| 27 | 23SB | 2626 | U |
| 27 | 23SB | 2627 | C |
| 27 | 23SB | 2644 | A |
| 27 | 23SB | 2645 | G |
| 27 | 23SB | 2660 | G |
| 27 | 23SB | 2661 | C |
| 27 | 23SB | 2669 | A |
| 27 | 23SB | 2670 | G |
| 27 | 23SB | 2680 | A |
| 27 | 23SB | 2681 | C |
| 27 | 23SB | 2687 | G |
| 27 | 23SB | 2688 | G |
| 27 | 23SB | 2694 | A |
| 27 | 23SB | 2701 | G |
| 27 | 23SB | 2704 | U |
| 27 | 23SB | 2705 | C |
| 27 | 23SB | 2706 | C |
| 27 | 23SB | 2717 | U |
| 27 | 23SB | 2718 | C |
| 27 | 23SB | 2722 | G |
| 27 | 23SB | 2727 | U |
| 27 | 23SB | 2728 | A |
| 27 | 23SB | 2729 | A |
| 27 | 23SB | 2730 | G |
| 27 | 23SB | 2742 | U |
| 27 | 23SB | 2743 | G |
| 27 | 23SB | 2748 | G |
| 27 | 23SB | 2749 | A |
| 27 | 23SB | 2750 | A |
| 27 | 23SB | 2752 | G |
| 27 | 23SB | 2757 | A |
| 27 | 23SB | 2760 | G |
| 27 | 23SB | 2764 | A |
| 27 | 23SB | 2766 | A |
| 27 | 23SB | 2767 | G |
| 27 | 23SB | 2768 | C |

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| Mol | Chain | Res | Type |
|---|---|---|---|
| 27 | 23SB | 2770 | U |
| 27 | 23SB | 2773 | A |
| 27 | 23SB | 2777 | G |
| 27 | 23SB | 2778 | G |
| 27 | 23SB | 2781 | A |
| 27 | 23SB | 2786 | G |
| 27 | 23SB | 2793 | G |
| 27 | 23SB | 2794 | A |
| 27 | 23SB | 2795 | U |
| 27 | 23SB | 2806 | A |
| 27 | 23SB | 2807 | C |
| 27 | 23SB | 2810 | C |
| 27 | 23SB | 2811 | G |
| 27 | 23SB | 2812 | U |
| 27 | 23SB | 2821 | U |
| 27 | 23SB | 2826 | A |
| 27 | 23SB | 2831 | G |
| 27 | 23SB | 2833 | A |
| 27 | 23SB | 2834 | A |
| 27 | 23SB | 2836 | A |
| 27 | 23SB | 2839 | A |
| 27 | 23SB | 2840 | C |
| 27 | 23SB | 2846 | G |
| 27 | 23SB | 2847 | G |
| 27 | 23SB | 2848 | A |
| 27 | 23SB | 2873 | A |
| 27 | 23SB | 2879 | U |
| 27 | 23SB | 2885 | G |
| 27 | 23SB | 2886 | A |
| 27 | 23SB | 2892 | C |
| 27 | 23SB | 2893 | C |
| 27 | 23SB | 2904 | A |
| 27 | 23SB | 2906 | G |
| 27 | 23SB | 2907 | U |
| 27 | 23SB | 2908 | C |
| 27 | 23SB | 2909 | U |
| 27 | 23SB | 2914 | C |
| 28 | 5SB | 9 | G |
| 28 | 5SB | 10 | U |
| 28 | 5SB | 14 | C |
| 28 | 5SB | 15 | A |
| 28 | 5SB | 16 | U |

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| Mol | Chain | Res | Type |
|---|---|---|---|
| 28 | 5SB | 17 | A |
| 28 | 5SB | 18 | G |
| 28 | 5SB | 24 | U |
| 28 | 5SB | 26 | G |
| 28 | 5SB | 27 | A |
| 28 | 5SB | 29 | C |
| 28 | 5SB | 33 | C |
| 28 | 5SB | 37 | U |
| 28 | 5SB | 43 | U |
| 28 | 5SB | 44 | C |
| 28 | 5SB | 47 | A |
| 28 | 5SB | 55 | A |
| 28 | 5SB | 58 | G |
| 28 | 5SB | 68 | A |
| 28 | 5SB | 69 | G |
| 28 | 5SB | 75 | A |
| 28 | 5SB | 83 | G |
| 28 | 5SB | 87 | G |
| 28 | 5SB | 90 | C |
| 28 | 5SB | 91 | G |
| 28 | 5SB | 92 | A |
| 28 | 5SB | 93 | C |
| 28 | 5SB | 98 | U |
| 28 | 5SB | 99 | G |
| 28 | 5SB | 104 | A |
| 28 | 5SB | 112 | G |
| 28 | 5SB | 115 | G |
| 28 | 5SB | 121 | G |

All (258) RNA pucker outliers are listed below:

| Mol | Chain | Res | Type |
|---|---|---|---|
| 1 | 16SA | 677 | G |
| 1 | 16SA | 696 | A |
| 1 | 16SA | 706 | A |
| 1 | 16SA | 731 | U |
| 1 | 16SA | 758 | A |
| 1 | 16SA | 813 | U |
| 1 | 16SA | 836 | G |
| 1 | 16SA | 891 | A |
| 1 | 16SA | 907 | G |
| 1 | 16SA | 969 | C |

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| Mol | Chain | Res | Type |
|---|---|---|---|
| 1 | 16SA | 1007 | C |
| 1 | 16SA | 1053 | A |
| 1 | 16SA | 1063 | C |
| 1 | 16SA | 1069 | G |
| 1 | 16SA | 1070 | U |
| 1 | 16SA | 1111 | G |
| 1 | 16SA | 1114 | G |
| 1 | 16SA | 1115 | G |
| 1 | 16SA | 1138 | A |
| 1 | 16SA | 1159 | G |
| 1 | 16SA | 1161 | A |
| 1 | 16SA | 1189 | U |
| 1 | 16SA | 1315 | U |
| 1 | 16SA | 1330 | C |
| 1 | 16SA | 1332 | G |
| 1 | 16SA | 1377 | C |
| 1 | 16SA | 1381 | G |
| 1 | 16SA | 1422 | U |
| 1 | 16SA | 1441 | C |
| 1 | 16SA | 1536 | A |
| 1 | 16SA | 1614 | U |
| 1 | 16SA | 1615 | U |
| 1 | 16SA | 1649 | U |
| 1 | 16SA | 1651 | C |
| 1 | 16SA | 1753 | U |
| 1 | 16SA | 1757 | C |
| 1 | 16SA | 1767 | G |
| 1 | 16SA | 1773 | C |
| 1 | 16SA | 1785 | A |
| 1 | 16SA | 1810 | A |
| 1 | 16SA | 1817 | G |
| 1 | 16SA | 1827 | C |
| 1 | 16SA | 1838 | U |
| 1 | 16SA | 1907 | A |
| 1 | 16SA | 1912 | A |
| 1 | 16SA | 1927 | G |
| 1 | 16SA | 1928 | U |
| 1 | 16SA | 1932 | G |
| 1 | 16SA | 1946 | A |
| 1 | 16SA | 1949 | C |
| 1 | 16SA | 2078 | C |
| 1 | 16SA | 2126 | A |

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| Mol | Chain | Res | Type |
|---|---|---|---|
| 22 | ASIA | 10 | G |
| 22 | ASIA | 19 | G |
| 23 | PSIA | 20 | U |
| 23 | PSIA | 45 | U |
| 24 | ESIA | 45 | U |
| 25 | MRNA | 44 | U |
| 25 | MRNA | 56 | U |
| 26 | TRNA | 20 | U |
| 26 | TRNA | 34 | G |
| 26 | TRNA | 65 | G |
| 27 | 23SA | 34 | C |
| 27 | 23SA | 186 | A |
| 27 | 23SA | 218 | A |
| 27 | 23SA | 219 | A |
| 27 | 23SA | 400 | G |
| 27 | 23SA | 423 | U |
| 27 | 23SA | 432 | C |
| 27 | 23SA | 530 | A |
| 27 | 23SA | 555 | A |
| 27 | 23SA | 557 | G |
| 27 | 23SA | 580 | U |
| 27 | 23SA | 612 | C |
| 27 | 23SA | 672 | C |
| 27 | 23SA | 680 | A |
| 27 | 23SA | 700 | G |
| 27 | 23SA | 813 | A |
| 27 | 23SA | 823 | A |
| 27 | 23SA | 895 | C |
| 27 | 23SA | 929 | G |
| 27 | 23SA | 992 | A |
| 27 | 23SA | 1070 | G |
| 27 | 23SA | 1074 | U |
| 27 | 23SA | 1105 | A |
| 27 | 23SA | 1133 | A |
| 27 | 23SA | 1157 | C |
| 27 | 23SA | 1189 | U |
| 27 | 23SA | 1226 | C |
| 27 | 23SA | 1252 | A |
| 27 | 23SA | 1258 | A |
| 27 | 23SA | 1469 | U |
| 27 | 23SA | 1476 | A |
| 27 | 23SA | 1608 | A |

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| Mol | Chain | Res | Type |
|---|---|---|---|
| 27 | 23SA | 1657 | A |
| 27 | 23SA | 1695 | G |
| 27 | 23SA | 1702 | A |
| 27 | 23SA | 1703 | G |
| 27 | 23SA | 1744 | C |
| 27 | 23SA | 1770 | A |
| 27 | 23SA | 1833 | G |
| 27 | 23SA | 1853 | A |
| 27 | 23SA | 1924 | G |
| 27 | 23SA | 1964 | 5MU |
| 27 | 23SA | 2017 | G |
| 27 | 23SA | 2085 | A |
| 27 | 23SA | 2192 | U |
| 27 | 23SA | 2231 | G |
| 27 | 23SA | 2322 | G |
| 27 | 23SA | 2335 | A |
| 27 | 23SA | 2361 | A |
| 27 | 23SA | 2420 | G |
| 27 | 23SA | 2421 | U |
| 27 | 23SA | 2437 | A |
| 27 | 23SA | 2441 | A |
| 27 | 23SA | 2454 | A |
| 27 | 23SA | 2496 | G |
| 27 | 23SA | 2533 | A |
| 27 | 23SA | 2581 | A |
| 27 | 23SA | 2653 | G |
| 27 | 23SA | 2660 | G |
| 27 | 23SA | 2696 | C |
| 27 | 23SA | 2727 | U |
| 27 | 23SA | 2742 | U |
| 27 | 23SA | 2767 | G |
| 27 | 23SA | 2772 | U |
| 27 | 23SA | 2806 | A |
| 27 | 23SA | 2845 | U |
| 28 | 5SA | 68 | A |
| 1 | 16SB | 728 | U |
| 1 | 16SB | 729 | A |
| 1 | 16SB | 754 | G |
| 1 | 16SB | 758 | A |
| 1 | 16SB | 813 | U |
| 1 | 16SB | 821 | G |
| 1 | 16SB | 853 | C |

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| Mol | Chain | Res | Type |
|---|---|---|---|
| 1 | 16SB | 855 | U |
| 1 | 16SB | 891 | A |
| 1 | 16SB | 920 | A |
| 1 | 16SB | 969 | C |
| 1 | 16SB | 1053 | A |
| 1 | 16SB | 1063 | C |
| 1 | 16SB | 1070 | U |
| 1 | 16SB | 1138 | A |
| 1 | 16SB | 1161 | A |
| 1 | 16SB | 1189 | U |
| 1 | 16SB | 1315 | U |
| 1 | 16SB | 1316 | A |
| 1 | 16SB | 1330 | C |
| 1 | 16SB | 1332 | G |
| 1 | 16SB | 1377 | C |
| 1 | 16SB | 1381 | G |
| 1 | 16SB | 1422 | U |
| 1 | 16SB | 1495 | A |
| 1 | 16SB | 1536 | A |
| 1 | 16SB | 1583 | U |
| 1 | 16SB | 1615 | U |
| 1 | 16SB | 1651 | C |
| 1 | 16SB | 1677 | U |
| 1 | 16SB | 1754 | U |
| 1 | 16SB | 1765 | C |
| 1 | 16SB | 1773 | C |
| 1 | 16SB | 1785 | A |
| 1 | 16SB | 1827 | C |
| 1 | 16SB | 1867 | U |
| 1 | 16SB | 1883 | A |
| 1 | 16SB | 1908 | U |
| 1 | 16SB | 1912 | A |
| 1 | 16SB | 1924 | C |
| 1 | 16SB | 1927 | G |
| 1 | 16SB | 1932 | G |
| 1 | 16SB | 1946 | A |
| 1 | 16SB | 1949 | C |
| 1 | 16SB | 1957 | U |
| 1 | 16SB | 1963 | C |
| 1 | 16SB | 1973 | A |
| 1 | 16SB | 2078 | C |
| 57 | ASIB | 10 | G |

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| Mol | Chain | Res | Type |
|---|---|---|---|
| 57 | ASIB | 69 | G |
| 23 | PSIB | 8 | 4SU |
| 23 | PSIB | 60 | U |
| 24 | ESIB | 9 | A |
| 24 | ESIB | 47 | U |
| 24 | ESIB | 58 | A |
| 25 | MRNB | 53 | U |
| 25 | MRNB | 56 | U |
| 27 | 23SB | 34 | C |
| 27 | 23SB | 48 | A |
| 27 | 23SB | 49 | U |
| 27 | 23SB | 126 | C |
| 27 | 23SB | 186 | A |
| 27 | 23SB | 195 | G |
| 27 | 23SB | 301 | A |
| 27 | 23SB | 302 | C |
| 27 | 23SB | 303 | A |
| 27 | 23SB | 319 | A |
| 27 | 23SB | 355 | A |
| 27 | 23SB | 431 | U |
| 27 | 23SB | 557 | G |
| 27 | 23SB | 580 | U |
| 27 | 23SB | 612 | C |
| 27 | 23SB | 680 | A |
| 27 | 23SB | 700 | G |
| 27 | 23SB | 813 | A |
| 27 | 23SB | 823 | A |
| 27 | 23SB | 876 | U |
| 27 | 23SB | 895 | C |
| 27 | 23SB | 926 | U |
| 27 | 23SB | 935 | C |
| 27 | 23SB | 937 | C |
| 27 | 23SB | 941 | C |
| 27 | 23SB | 1133 | A |
| 27 | 23SB | 1191 | A |
| 27 | 23SB | 1220 | G |
| 27 | 23SB | 1252 | A |
| 27 | 23SB | 1258 | A |
| 27 | 23SB | 1349 | U |
| 27 | 23SB | 1350 | A |
| 27 | 23SB | 1469 | U |
| 27 | 23SB | 1476 | A |

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| Mol | Chain | Res | Type |
|---|---|---|---|
| 27 | 23SB | 1510 | A |
| 27 | 23SB | 1575 | G |
| 27 | 23SB | 1608 | A |
| 27 | 23SB | 1657 | A |
| 27 | 23SB | 1702 | A |
| 27 | 23SB | 1703 | G |
| 27 | 23SB | 1770 | A |
| 27 | 23SB | 1853 | A |
| 27 | 23SB | 1924 | G |
| 27 | 23SB | 1940 | 5MU |
| 27 | 23SB | 1955 | G |
| 27 | 23SB | 2017 | G |
| 27 | 23SB | 2135 | G |
| 27 | 23SB | 2170 | C |
| 27 | 23SB | 2216 | G |
| 27 | 23SB | 2230 | G |
| 27 | 23SB | 2231 | G |
| 27 | 23SB | 2335 | A |
| 27 | 23SB | 2350 | A |
| 27 | 23SB | 2437 | A |
| 27 | 23SB | 2454 | A |
| 27 | 23SB | 2462 | G |
| 27 | 23SB | 2496 | G |
| 27 | 23SB | 2617 | A |
| 27 | 23SB | 2660 | G |
| 27 | 23SB | 2704 | U |
| 27 | 23SB | 2741 | A |
| 27 | 23SB | 2742 | U |
| 27 | 23SB | 2748 | G |
| 27 | 23SB | 2772 | U |
| 27 | 23SB | 2792 | A |
| 27 | 23SB | 2806 | A |
| 27 | 23SB | 2872 | G |
| 28 | 5SB | 13 | C |
| 28 | 5SB | 16 | U |
| 28 | 5SB | 17 | A |
| 28 | 5SB | 26 | G |
| 28 | 5SB | 68 | A |

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

83 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 | $\#\|Z\| > 2$ |
| 27 | OMU | 23SB | 2567 | 58,27 | 19,22,23 | 2.99 | 8 (42%) | 25,31,34 | 1.88 | 4 (16%) |
| 22 | PSU | ASIA | 55 | 22 | 18,21,22 | 1.17 | 1 (5%) | 21,30,33 | 1.68 | 4 (19%) |
| 23 | 5MU | PSIB | 54 | 23 | 19,22,23 | 3.97 | 5 (26%) | 27,32,35 | 3.01 | 10 (37%) |
| 23 | PSU | PSIA | 32 | 23 | 18,21,22 | 1.04 | 1 (5%) | 21,30,33 | 1.64 | 4 (19%) |
| 27 | OMG | 23SB | 2266 | 59,23,27 | 23,26,27 | 5.03 | 11 (47%) | 32,38,41 | 4.79 | 18 (56%) |
| 22 | 4SU | ASIA | 8 | 22 | 18,21,22 | 1.90 | 5 (27%) | 25,30,33 | 2.42 | 5 (20%) |
| 22 | PSU | ASIA | 32 | 22 | 18,21,22 | 1.22 | 1 (5%) | 21,30,33 | 1.72 | 4 (19%) |
| 22 | MIA | ASIA | 37 | 22 | 28,31,32 | 2.29 | 3 (10%) | 38,44,47 | 3.57 | 16 (42%) |
| 27 | OMU | 23SA | 2567 | 58,27 | 19,22,23 | 2.99 | 8 (42%) | 25,31,34 | 1.75 | 4 (16%) |
| 1 | PSU | 16SB | 1145 | 58,1 | 18,21,22 | 1.19 | 1 (5%) | 21,30,33 | 1.81 | 4 (19%) |
| 1 | 5MC | 16SA | 2032 | 1 | 19,22,23 | 4.09 | 8 (42%) | 26,32,35 | 0.98 | 2 (7%) |
| 27 | 5MC | 23SA | 1987 | 59,27 | 19,22,23 | 4.07 | 8 (42%) | 26,32,35 | 0.88 | 1 (3%) |
| 1 | UR3 | 16SA | 2121 | 1 | 19,22,23 | 2.96 | 8 (42%) | 26,32,35 | 1.87 | 3 (11%) |
| 24 | MIA | ESIB | 37 | 24 | 28,31,32 | 2.38 | 4 (14%) | 38,44,47 | 3.88 | 13 (34%) |
| 1 | 5MC | 16SB | 2035 | 1 | 19,22,23 | 4.05 | 8 (42%) | 26,32,35 | 1.12 | 2 (7%) |
| 27 | 2MA | 23SB | 2518 | 59,58,27 | 22,25,26 | 3.63 | 7 (31%) | 32,37,40 | 2.49 | 12 (37%) |
| 27 | 5MC | 23SB | 1967 | 27 | 19,22,23 | 4.09 | 8 (42%) | 26,32,35 | 1.01 | 3 (11%) |
| 1 | MA6 | 16SB | 2141 | 1 | 23,26,27 | 1.44 | 5 (21%) | 33,38,41 | 2.63 | 11 (33%) |
| 57 | 5MU | ASIB | 54 | 57 | 19,22,23 | 3.98 | 5 (26%) | 27,32,35 | 3.13 | 8 (29%) |
| 23 | PSU | PSIB | 39 | 23 | 18,21,22 | 1.18 | 1 (5%) | 21,30,33 | 1.70 | 4 (19%) |
| 24 | MIA | ESIA | 37 | 24 | 28,31,32 | 2.32 | 3 (10%) | 38,44,47 | 3.17 | 14 (36%) |
| 27 | 5MU | 23SB | 1964 | 59,27 | 19,22,23 | 3.98 | 5 (26%) | 27,32,35 | 3.28 | 9 (33%) |
| 1 | 4OC | 16SB | 2030 | 58,1 | 20,23,24 | 2.92 | 8 (40%) | 25,32,35 | 1.62 | 3 (12%) |
| 27 | PSU | 23SA | 1936 | 27 | 18,21,22 | 1.06 | 1 (5%) | 21,30,33 | 1.95 | 4 (19%) |
| 23 | PSU | PSIB | 55 | 23 | 18,21,22 | 1.16 | 1 (5%) | 21,30,33 | 1.74 | 3 (14%) |
| 27 | OMC | 23SA | 1945 | 27 | 19,22,23 | 1.82 | 4 (21%) | 25,31,34 | 1.07 | 1 (4%) |
| 23 | PSU | PSIA | 39 | 23 | 18,21,22 | 1.08 | 1 (5%) | 21,30,33 | 1.94 | 4 (19%) |
| 1 | 4OC | 16SA | 2030 | 58,1 | 20,23,24 | 3.17 | 8 (40%) | 25,32,35 | 1.00 | 3 (12%) |
| 1 | MA6 | 16SB | 2142 | 1 | 23,26,27 | 1.42 | 5 (21%) | 33,38,41 | 2.74 | 12 (36%) |

| Mol | Type | Chain | Res | Link | Bond lengths | | | Bond angles | | |
|---|---|---|---|---|---|---|---|---|---|---|
| | | | | | Counts | RMSZ | $\#\|Z\|>2$ | Counts | RMSZ | $\#\|Z\|>2$ |
| 27 | PSU | 23SA | 1942 | 27 | 18,21,22 | 1.12 | 1 (5%) | 21,30,33 | 1.82 | 4 (19%) |
| 1 | 5MC | 16SA | 1590 | 1 | 19,22,23 | 4.14 | 8 (42%) | 26,32,35 | 1.03 | 1 (3%) |
| 23 | 7MG | PSIB | 46 | 23 | 23,26,27 | 3.15 | 8 (34%) | 27,39,42 | 2.76 | 9 (33%) |
| 12 | 0TD | S12B | 89 | 12 | 8,9,10 | 1.68 | 2 (25%) | 6,11,13 | 2.00 | 2 (33%) |
| 27 | 5MU | 23SA | 1940 | 27 | 19,22,23 | 4.03 | 5 (26%) | 27,32,35 | 3.26 | 10 (37%) |
| 1 | 5MC | 16SB | 2028 | 1 | 19,22,23 | 4.03 | 8 (42%) | 26,32,35 | 1.33 | 4 (15%) |
| 23 | PSU | PSIA | 55 | 23 | 18,21,22 | 1.22 | 1 (5%) | 21,30,33 | 1.82 | 4 (19%) |
| 1 | 5MC | 16SA | 2028 | 1 | 19,22,23 | 4.02 | 8 (42%) | 26,32,35 | 1.23 | 2 (7%) |
| 26 | PSU | TRNA | 39 | 26 | 18,21,22 | 1.16 | 1 (5%) | 21,30,33 | 1.89 | 4 (19%) |
| 23 | 7MG | PSIA | 46 | 23 | 23,26,27 | 2.95 | 8 (34%) | 27,39,42 | 2.85 | 10 (37%) |
| 1 | 7MG | 16SA | 1156 | 59,1 | 23,26,27 | 3.06 | 8 (34%) | 27,39,42 | 2.90 | 10 (37%) |
| 27 | PSU | 23SB | 1936 | 27 | 18,21,22 | 1.14 | 1 (5%) | 21,30,33 | 1.73 | 3 (14%) |
| 27 | OMG | 23SA | 2266 | 59,23,27 | 23,26,27 | 4.98 | 11 (47%) | 32,38,41 | 4.57 | 18 (56%) |
| 27 | 5MC | 23SA | 1967 | 27 | 19,22,23 | 4.01 | 8 (42%) | 26,32,35 | 1.26 | 2 (7%) |
| 23 | PSU | PSIB | 32 | 23 | 18,21,22 | 1.03 | 1 (5%) | 21,30,33 | 2.03 | 5 (23%) |
| 22 | 5MU | ASIA | 54 | 22 | 19,22,23 | 3.91 | 5 (26%) | 27,32,35 | 3.10 | 9 (33%) |
| 26 | PSU | TRNA | 32 | 26 | 18,21,22 | 1.18 | 1 (5%) | 21,30,33 | 1.77 | 4 (19%) |
| 27 | 5MU | 23SB | 1940 | 27 | 19,22,23 | 4.05 | 5 (26%) | 27,32,35 | 3.52 | 9 (33%) |
| 22 | 7MG | ASIA | 46 | 22 | 23,26,27 | 3.11 | 7 (30%) | 27,39,42 | 2.84 | 9 (33%) |
| 23 | 3AU | PSIA | 47 | 23 | 24,28,29 | 2.77 | 8 (33%) | 30,40,43 | 1.74 | 5 (16%) |
| 12 | 0TD | S12A | 89 | 12 | 8,9,10 | 1.37 | 1 (12%) | 6,11,13 | 1.92 | 1 (16%) |
| 57 | MIA | ASIB | 37 | 57 | 28,31,32 | 2.32 | 5 (17%) | 38,44,47 | 3.31 | 15 (39%) |
| 27 | PSU | 23SA | 2620 | 27 | 18,21,22 | 1.13 | 1 (5%) | 21,30,33 | 1.90 | 4 (19%) |
| 23 | 3AU | PSIB | 47 | 23 | 24,28,29 | 2.87 | 8 (33%) | 30,40,43 | 2.17 | 7 (23%) |
| 27 | 5MC | 23SB | 1987 | 59,27 | 19,22,23 | 4.15 | 8 (42%) | 26,32,35 | 0.91 | 2 (7%) |
| 1 | 5MC | 16SB | 1590 | 1 | 19,22,23 | 4.24 | 8 (42%) | 26,32,35 | 1.01 | 2 (7%) |
| 23 | 4SU | PSIB | 8 | 23,58 | 18,21,22 | 1.75 | 5 (27%) | 25,30,33 | 2.93 | 6 (24%) |
| 26 | PSU | TRNA | 55 | 26 | 18,21,22 | 1.14 | 1 (5%) | 21,30,33 | 1.91 | 4 (19%) |
| 57 | PSU | ASIB | 32 | 57 | 18,21,22 | 1.10 | 1 (5%) | 21,30,33 | 2.03 | 5 (23%) |
| 1 | MA6 | 16SA | 2142 | 1 | 23,26,27 | 1.43 | 5 (21%) | 33,38,41 | 2.76 | 11 (33%) |
| 1 | M2G | 16SA | 1589 | 1 | 24,27,28 | 2.92 | 8 (33%) | 33,40,43 | 1.63 | 7 (21%) |
| 23 | 4SU | PSIA | 8 | 23 | 18,21,22 | 1.91 | 3 (16%) | 25,30,33 | 2.30 | 4 (16%) |
| 1 | 2MG | 16SB | 1834 | 1 | 23,26,27 | 3.12 | 8 (34%) | 33,38,41 | 2.32 | 12 (36%) |
| 1 | 5MC | 16SB | 2032 | 1 | 19,22,23 | 4.13 | 8 (42%) | 26,32,35 | 0.98 | 2 (7%) |
| 1 | 5MC | 16SA | 2035 | 1 | 19,22,23 | 3.95 | 8 (42%) | 26,32,35 | 1.07 | 2 (7%) |

| Mol | Type | Chain | Res | Link | Bond lengths | | | Bond angles | | |
|---|---|---|---|---|---|---|---|---|---|---|
| | | | | | Counts | RMSZ | $\#\|Z\|>2$ | Counts | RMSZ | $\#\|Z\|>2$ |
| 1 | M2G | 16SB | 1589 | 1 | 24,27,28 | 2.94 | 8 (33%) | 33,40,43 | 1.80 | 6 (18%) |
| 1 | UR3 | 16SB | 2121 | 1 | 19,22,23 | 2.91 | 8 (42%) | 26,32,35 | 1.70 | 3 (11%) |
| 1 | 7MG | 16SB | 1156 | 59,1 | 23,26,27 | 3.22 | 6 (26%) | 27,39,42 | 2.85 | 10 (37%) |
| 27 | 2MA | 23SA | 2518 | 59,27 | 22,25,26 | 3.58 | 7 (31%) | 32,37,40 | 2.37 | 11 (34%) |
| 23 | 5MU | PSIA | 54 | 23 | 19,22,23 | 3.86 | 5 (26%) | 27,32,35 | 3.03 | 7 (25%) |
| 23 | MIA | PSIB | 37 | 23 | 28,31,32 | 2.15 | 4 (14%) | 38,44,47 | 3.03 | 13 (34%) |
| 26 | MIA | TRNA | 37 | 26 | 28,31,32 | 2.48 | 5 (17%) | 38,44,47 | 3.85 | 17 (44%) |
| 1 | 2MG | 16SA | 1834 | 59,1 | 23,26,27 | 3.10 | 8 (34%) | 33,38,41 | 2.41 | 12 (36%) |
| 1 | PSU | 16SA | 1145 | 59,58,1 | 18,21,22 | 1.16 | 1 (5%) | 21,30,33 | 2.21 | 6 (28%) |
| 1 | MA6 | 16SA | 2141 | 1 | 23,26,27 | 1.43 | 5 (21%) | 33,38,41 | 2.76 | 13 (39%) |
| 27 | PSU | 23SB | 1942 | 27 | 18,21,22 | 1.16 | 1 (5%) | 21,30,33 | 1.99 | 5 (23%) |
| 27 | 5MU | 23SA | 1964 | 59,27 | 19,22,23 | 3.86 | 5 (26%) | 27,32,35 | 3.40 | 11 (40%) |
| 22 | PSU | ASIA | 39 | 22 | 18,21,22 | 1.17 | 1 (5%) | 21,30,33 | 1.75 | 4 (19%) |
| 23 | MIA | PSIA | 37 | 23 | 28,31,32 | 2.29 | 4 (14%) | 38,44,47 | 3.15 | 14 (36%) |
| 57 | PSU | ASIB | 39 | 57 | 18,21,22 | 1.21 | 1 (5%) | 21,30,33 | 1.87 | 5 (23%) |
| 27 | OMC | 23SB | 1945 | 27 | 19,22,23 | 1.85 | 4 (21%) | 25,31,34 | 0.98 | 1 (4%) |
| 26 | 4SU | TRNA | 8 | 26 | 18,21,22 | 1.90 | 3 (16%) | 25,30,33 | 2.29 | 5 (20%) |
| 26 | 5MU | TRNA | 54 | 26 | 19,22,23 | 3.98 | 5 (26%) | 27,32,35 | 3.10 | 8 (29%) |
| 27 | PSU | 23SB | 2620 | 27 | 18,21,22 | 1.20 | 1 (5%) | 21,30,33 | 1.89 | 3 (14%) |

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 |
|---|---|---|---|---|---|---|---|
| 27 | OMU | 23SB | 2567 | 58,27 | - | 2/9/27/28 | 0/2/2/2 |
| 22 | PSU | ASIA | 55 | 22 | - | 3/7/25/26 | 0/2/2/2 |
| 23 | 5MU | PSIB | 54 | 23 | - | 2/7/25/26 | 0/2/2/2 |
| 23 | PSU | PSIA | 32 | 23 | - | 0/7/25/26 | 0/2/2/2 |
| 27 | OMG | 23SB | 2266 | 59,23,27 | - | 0/9/27/28 | 0/3/3/3 |
| 22 | 4SU | ASIA | 8 | 22 | - | 1/7/25/26 | 0/2/2/2 |
| 22 | PSU | ASIA | 32 | 22 | - | 0/7/25/26 | 0/2/2/2 |
| 22 | MIA | ASIA | 37 | 22 | - | 4/15/33/34 | 0/3/3/3 |
| 27 | OMU | 23SA | 2567 | 58,27 | - | 0/9/27/28 | 0/2/2/2 |
| 1 | PSU | 16SB | 1145 | 58,1 | - | 0/7/25/26 | 0/2/2/2 |
| 1 | 5MC | 16SA | 2032 | 1 | - | 0/7/25/26 | 0/2/2/2 |

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| Mol | Type | Chain | Res | Link | Chirals | Torsions | Rings |
|---|---|---|---|---|---|---|---|
| 27 | 5MC | 23SA | 1987 | 59,27 | - | 0/7/25/26 | 0/2/2/2 |
| 1 | UR3 | 16SA | 2121 | 1 | - | 0/7/25/26 | 0/2/2/2 |
| 24 | MIA | ESIB | 37 | 24 | - | 6/15/33/34 | 0/3/3/3 |
| 1 | 5MC | 16SB | 2035 | 1 | - | 0/7/25/26 | 0/2/2/2 |
| 27 | 2MA | 23SB | 2518 | 59,58,27 | - | 3/7/25/26 | 0/3/3/3 |
| 27 | 5MC | 23SB | 1967 | 27 | - | 0/7/25/26 | 0/2/2/2 |
| 1 | MA6 | 16SB | 2141 | 1 | - | 1/11/29/30 | 0/3/3/3 |
| 57 | 5MU | ASIB | 54 | 57 | - | 2/7/25/26 | 0/2/2/2 |
| 23 | PSU | PSIB | 39 | 23 | - | 0/7/25/26 | 0/2/2/2 |
| 24 | MIA | ESIA | 37 | 24 | - | 6/15/33/34 | 0/3/3/3 |
| 27 | 5MU | 23SB | 1964 | 59,27 | - | 2/7/25/26 | 0/2/2/2 |
| 1 | 4OC | 16SB | 2030 | 58,1 | - | 2/9/29/30 | 0/2/2/2 |
| 27 | PSU | 23SA | 1936 | 27 | - | 2/7/25/26 | 0/2/2/2 |
| 23 | PSU | PSIB | 55 | 23 | - | 0/7/25/26 | 0/2/2/2 |
| 27 | OMC | 23SA | 1945 | 27 | - | 0/9/27/28 | 0/2/2/2 |
| 23 | PSU | PSIA | 39 | 23 | - | 0/7/25/26 | 0/2/2/2 |
| 1 | 4OC | 16SA | 2030 | 58,1 | - | 2/9/29/30 | 0/2/2/2 |
| 1 | MA6 | 16SB | 2142 | 1 | - | 3/11/29/30 | 0/3/3/3 |
| 27 | PSU | 23SA | 1942 | 27 | - | 0/7/25/26 | 0/2/2/2 |
| 1 | 5MC | 16SA | 1590 | 1 | - | 0/7/25/26 | 0/2/2/2 |
| 23 | 7MG | PSIB | 46 | 23 | - | 1/7/37/38 | 0/3/3/3 |
| 12 | 0TD | S12B | 89 | 12 | - | 3/7/12/14 | - |
| 27 | 5MU | 23SA | 1940 | 27 | - | 2/7/25/26 | 0/2/2/2 |
| 1 | 5MC | 16SB | 2028 | 1 | - | 0/7/25/26 | 0/2/2/2 |
| 23 | PSU | PSIA | 55 | 23 | - | 3/7/25/26 | 0/2/2/2 |
| 1 | 5MC | 16SA | 2028 | 1 | - | 0/7/25/26 | 0/2/2/2 |
| 26 | PSU | TRNA | 39 | 26 | - | 0/7/25/26 | 0/2/2/2 |
| 23 | 7MG | PSIA | 46 | 23 | - | 1/7/37/38 | 0/3/3/3 |
| 1 | 7MG | 16SA | 1156 | 59,1 | - | 2/7/37/38 | 0/3/3/3 |
| 27 | PSU | 23SB | 1936 | 27 | - | 0/7/25/26 | 0/2/2/2 |
| 27 | OMG | 23SA | 2266 | 59,23,27 | - | 0/9/27/28 | 0/3/3/3 |
| 27 | 5MC | 23SA | 1967 | 27 | - | 0/7/25/26 | 0/2/2/2 |
| 23 | PSU | PSIB | 32 | 23 | - | 0/7/25/26 | 0/2/2/2 |
| 22 | 5MU | ASIA | 54 | 22 | - | 0/7/25/26 | 0/2/2/2 |
| 26 | PSU | TRNA | 32 | 26 | - | 0/7/25/26 | 0/2/2/2 |
| 27 | 5MU | 23SB | 1940 | 27 | - | 0/7/25/26 | 0/2/2/2 |
| 22 | 7MG | ASIA | 46 | 22 | - | 2/7/37/38 | 0/3/3/3 |
| 23 | 3AU | PSIA | 47 | 23 | - | 7/16/34/35 | 0/2/2/2 |

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| Mol | Type | Chain | Res | Link | Chirals | Torsions | Rings |
|---|---|---|---|---|---|---|---|
| 12 | 0TD | S12A | 89 | 12 | - | 4/7/12/14 | - |
| 57 | MIA | ASIB | 37 | 57 | - | 2/15/33/34 | 0/3/3/3 |
| 27 | PSU | 23SA | 2620 | 27 | - | 0/7/25/26 | 0/2/2/2 |
| 23 | 3AU | PSIB | 47 | 23 | - | 8/16/34/35 | 0/2/2/2 |
| 27 | 5MC | 23SB | 1987 | 59,27 | - | 0/7/25/26 | 0/2/2/2 |
| 1 | 5MC | 16SB | 1590 | 1 | - | 0/7/25/26 | 0/2/2/2 |
| 23 | 4SU | PSIB | 8 | 23,58 | - | 2/7/25/26 | 0/2/2/2 |
| 26 | PSU | TRNA | 55 | 26 | - | 0/7/25/26 | 0/2/2/2 |
| 57 | PSU | ASIB | 32 | 57 | - | 0/7/25/26 | 0/2/2/2 |
| 1 | MA6 | 16SA | 2142 | 1 | - | 3/11/29/30 | 0/3/3/3 |
| 1 | M2G | 16SA | 1589 | 1 | - | 2/11/29/30 | 0/3/3/3 |
| 23 | 4SU | PSIA | 8 | 23 | - | 0/7/25/26 | 0/2/2/2 |
| 1 | 2MG | 16SB | 1834 | 1 | - | 2/9/27/28 | 0/3/3/3 |
| 1 | 5MC | 16SB | 2032 | 1 | - | 0/7/25/26 | 0/2/2/2 |
| 1 | 5MC | 16SA | 2035 | 1 | - | 0/7/25/26 | 0/2/2/2 |
| 1 | M2G | 16SB | 1589 | 1 | - | 0/11/29/30 | 0/3/3/3 |
| 1 | UR3 | 16SB | 2121 | 1 | - | 0/7/25/26 | 0/2/2/2 |
| 1 | 7MG | 16SB | 1156 | 59,1 | - | 2/7/37/38 | 0/3/3/3 |
| 27 | 2MA | 23SA | 2518 | 59,27 | - | 1/7/25/26 | 0/3/3/3 |
| 23 | 5MU | PSIA | 54 | 23 | - | 0/7/25/26 | 0/2/2/2 |
| 23 | MIA | PSIB | 37 | 23 | - | 2/15/33/34 | 0/3/3/3 |
| 26 | MIA | TRNA | 37 | 26 | - | 6/15/33/34 | 0/3/3/3 |
| 1 | 2MG | 16SA | 1834 | 59,1 | - | 0/9/27/28 | 0/3/3/3 |
| 1 | PSU | 16SA | 1145 | 59,58,1 | - | 0/7/25/26 | 0/2/2/2 |
| 1 | MA6 | 16SA | 2141 | 1 | - | 0/11/29/30 | 0/3/3/3 |
| 27 | PSU | 23SB | 1942 | 27 | - | 0/7/25/26 | 0/2/2/2 |
| 27 | 5MU | 23SA | 1964 | 59,27 | - | 1/7/25/26 | 0/2/2/2 |
| 22 | PSU | ASIA | 39 | 22 | - | 0/7/25/26 | 0/2/2/2 |
| 23 | MIA | PSIA | 37 | 23 | - | 5/15/33/34 | 0/3/3/3 |
| 57 | PSU | ASIB | 39 | 57 | - | 0/7/25/26 | 0/2/2/2 |
| 27 | OMC | 23SB | 1945 | 27 | - | 0/9/27/28 | 0/2/2/2 |
| 26 | 4SU | TRNA | 8 | 26 | - | 2/7/25/26 | 0/2/2/2 |
| 26 | 5MU | TRNA | 54 | 26 | - | 2/7/25/26 | 0/2/2/2 |
| 27 | PSU | 23SB | 2620 | 27 | - | 0/7/25/26 | 0/2/2/2 |

All (407) bond length outliers are listed below:

| Mol | Chain | Res | Type | Atoms | Z | Observed(Å) | Ideal(Å) |
|---|---|---|---|---|---|---|---|
| 27 | 23SB | 1940 | 5MU | C2-N1 | 13.22 | 1.59 | 1.38 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(Å) | Ideal(Å) |
|---|---|---|---|---|---|---|---|
| 23 | PSIB | 54 | 5MU | C2-N1 | 13.10 | 1.59 | 1.38 |
| 27 | 23SA | 1940 | 5MU | C2-N1 | 13.09 | 1.59 | 1.38 |
| 57 | ASIB | 54 | 5MU | C2-N1 | 12.96 | 1.58 | 1.38 |
| 26 | TRNA | 54 | 5MU | C2-N1 | 12.83 | 1.58 | 1.38 |
| 27 | 23SB | 1964 | 5MU | C2-N1 | 12.83 | 1.58 | 1.38 |
| 23 | PSIA | 54 | 5MU | C2-N1 | 12.48 | 1.58 | 1.38 |
| 22 | ASIA | 54 | 5MU | C2-N1 | 12.44 | 1.57 | 1.38 |
| 27 | 23SA | 1964 | 5MU | C2-N1 | 12.27 | 1.57 | 1.38 |
| 27 | 23SB | 2266 | OMG | C4-N3 | 11.78 | 1.61 | 1.34 |
| 27 | 23SA | 2266 | OMG | C4-N3 | 11.64 | 1.60 | 1.34 |
| 27 | 23SB | 2518 | 2MA | C4-N3 | 11.51 | 1.49 | 1.34 |
| 27 | 23SA | 2518 | 2MA | C4-N3 | 11.47 | 1.49 | 1.34 |
| 27 | 23SB | 2266 | OMG | C5-N7 | -11.25 | 1.16 | 1.39 |
| 27 | 23SA | 2266 | OMG | C5-N7 | -11.21 | 1.16 | 1.39 |
| 27 | 23SB | 1987 | 5MC | C6-C5 | 9.77 | 1.50 | 1.34 |
| 1 | 16SA | 1590 | 5MC | C6-C5 | 9.66 | 1.50 | 1.34 |
| 27 | 23SA | 1987 | 5MC | C6-C5 | 9.65 | 1.50 | 1.34 |
| 1 | 16SB | 1590 | 5MC | C6-C5 | 9.63 | 1.50 | 1.34 |
| 1 | 16SA | 2028 | 5MC | C6-C5 | 9.54 | 1.50 | 1.34 |
| 27 | 23SB | 1967 | 5MC | C6-C5 | 9.51 | 1.50 | 1.34 |
| 1 | 16SB | 2035 | 5MC | C6-C5 | 9.44 | 1.50 | 1.34 |
| 1 | 16SB | 2032 | 5MC | C6-C5 | 9.33 | 1.49 | 1.34 |
| 23 | PSIB | 47 | 3AU | C2-N1 | 9.22 | 1.51 | 1.38 |
| 1 | 16SB | 2028 | 5MC | C6-C5 | 9.19 | 1.49 | 1.34 |
| 27 | 23SA | 1967 | 5MC | C6-C5 | 9.19 | 1.49 | 1.34 |
| 1 | 16SA | 2032 | 5MC | C6-C5 | 9.18 | 1.49 | 1.34 |
| 27 | 23SB | 2266 | OMG | C4-N9 | 9.13 | 1.61 | 1.38 |
| 1 | 16SA | 2035 | 5MC | C6-C5 | 9.11 | 1.49 | 1.34 |
| 27 | 23SA | 2266 | OMG | C4-N9 | 8.57 | 1.59 | 1.38 |
| 23 | PSIA | 47 | 3AU | C2-N1 | 8.46 | 1.50 | 1.38 |
| 1 | 16SB | 1156 | 7MG | C5-N7 | 8.33 | 1.46 | 1.35 |
| 22 | ASIA | 46 | 7MG | C5-N7 | 8.26 | 1.46 | 1.35 |
| 23 | PSIB | 46 | 7MG | C5-N7 | 8.19 | 1.46 | 1.35 |
| 57 | ASIB | 37 | MIA | C13-C14 | 8.18 | 1.56 | 1.32 |
| 27 | 23SB | 2266 | OMG | C8-N7 | -8.12 | 1.09 | 1.32 |
| 23 | PSIA | 37 | MIA | C13-C14 | 8.12 | 1.56 | 1.32 |
| 27 | 23SA | 2266 | OMG | C5-C4 | 8.12 | 1.61 | 1.38 |
| 27 | 23SB | 2266 | OMG | C5-C4 | 8.11 | 1.61 | 1.38 |
| 24 | ESIB | 37 | MIA | C13-C14 | 8.09 | 1.56 | 1.32 |
| 1 | 16SA | 2032 | 5MC | C4-N3 | 8.05 | 1.47 | 1.34 |
| 27 | 23SA | 2266 | OMG | C8-N7 | -8.05 | 1.10 | 1.32 |
| 1 | 16SB | 1590 | 5MC | C4-N3 | 8.04 | 1.47 | 1.34 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(Å) | Ideal(Å) |
|---|---|---|---|---|---|---|---|
| 24 | ESIA | 37 | MIA | C13-C14 | 8.04 | 1.56 | 1.32 |
| 22 | ASIA | 37 | MIA | C13-C14 | 8.03 | 1.56 | 1.32 |
| 1 | 16SB | 1156 | 7MG | C4-N9 | -8.01 | 1.28 | 1.37 |
| 1 | 16SA | 2121 | UR3 | C2-N1 | 7.98 | 1.49 | 1.38 |
| 26 | TRNA | 37 | MIA | C13-C14 | 7.95 | 1.56 | 1.32 |
| 1 | 16SA | 1156 | 7MG | C5-N7 | 7.92 | 1.45 | 1.35 |
| 23 | PSIB | 37 | MIA | C13-C14 | 7.90 | 1.56 | 1.32 |
| 23 | PSIB | 46 | 7MG | C4-N9 | -7.88 | 1.28 | 1.37 |
| 1 | 16SB | 2032 | 5MC | C4-N3 | 7.79 | 1.46 | 1.34 |
| 1 | 16SA | 1589 | M2G | C2-N2 | 7.75 | 1.49 | 1.35 |
| 27 | 23SB | 1987 | 5MC | C4-N3 | 7.73 | 1.46 | 1.34 |
| 1 | 16SB | 1834 | 2MG | C2-N3 | 7.71 | 1.46 | 1.32 |
| 1 | 16SB | 2121 | UR3 | C2-N1 | 7.68 | 1.49 | 1.38 |
| 1 | 16SA | 1834 | 2MG | C2-N3 | 7.63 | 1.46 | 1.32 |
| 1 | 16SB | 1589 | M2G | C2-N2 | 7.60 | 1.49 | 1.35 |
| 1 | 16SB | 1589 | M2G | C4-N3 | 7.55 | 1.51 | 1.34 |
| 27 | 23SA | 1987 | 5MC | C4-N3 | 7.54 | 1.46 | 1.34 |
| 27 | 23SA | 2266 | OMG | C6-N1 | -7.54 | 1.24 | 1.38 |
| 23 | PSIA | 46 | 7MG | C5-N7 | 7.48 | 1.45 | 1.35 |
| 1 | 16SA | 1590 | 5MC | C5-C4 | 7.46 | 1.49 | 1.44 |
| 1 | 16SB | 1590 | 5MC | C5-C4 | 7.44 | 1.49 | 1.44 |
| 27 | 23SB | 1967 | 5MC | C4-N3 | 7.42 | 1.46 | 1.34 |
| 1 | 16SA | 1590 | 5MC | C4-N3 | 7.41 | 1.46 | 1.34 |
| 27 | 23SA | 1967 | 5MC | C4-N3 | 7.39 | 1.46 | 1.34 |
| 1 | 16SB | 2035 | 5MC | C4-N3 | 7.33 | 1.45 | 1.34 |
| 1 | 16SB | 2028 | 5MC | C4-N3 | 7.31 | 1.45 | 1.34 |
| 1 | 16SA | 2028 | 5MC | C4-N3 | 7.28 | 1.45 | 1.34 |
| 1 | 16SA | 2035 | 5MC | C4-N3 | 7.28 | 1.45 | 1.34 |
| 26 | TRNA | 37 | MIA | C6-N6 | 7.26 | 1.45 | 1.34 |
| 22 | ASIA | 46 | 7MG | C4-N9 | -7.23 | 1.29 | 1.37 |
| 1 | 16SB | 2032 | 5MC | C5-C4 | 7.22 | 1.49 | 1.44 |
| 1 | 16SB | 2028 | 5MC | C5-C4 | 7.21 | 1.49 | 1.44 |
| 1 | 16SA | 2030 | 4OC | C4-N3 | 7.21 | 1.44 | 1.32 |
| 27 | 23SB | 2266 | OMG | C6-N1 | -7.21 | 1.25 | 1.38 |
| 1 | 16SA | 2028 | 5MC | C5-C4 | 7.08 | 1.49 | 1.44 |
| 1 | 16SA | 1589 | M2G | C4-N3 | 7.08 | 1.50 | 1.34 |
| 1 | 16SA | 1834 | 2MG | C4-N3 | 7.07 | 1.50 | 1.34 |
| 1 | 16SA | 1834 | 2MG | C2-N2 | 7.00 | 1.48 | 1.33 |
| 27 | 23SA | 2567 | OMU | C2-N1 | 7.00 | 1.49 | 1.38 |
| 1 | 16SB | 1834 | 2MG | C2-N2 | 6.99 | 1.48 | 1.33 |
| 27 | 23SB | 1967 | 5MC | C5-C4 | 6.90 | 1.49 | 1.44 |
| 1 | 16SB | 2035 | 5MC | C5-C4 | 6.89 | 1.49 | 1.44 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(Å) | Ideal(Å) |
|---|---|---|---|---|---|---|---|
| 1 | 16SB | 1590 | 5MC | C2-N3 | 6.88 | 1.50 | 1.36 |
| 27 | 23SA | 1967 | 5MC | C5-C4 | 6.84 | 1.49 | 1.44 |
| 1 | 16SB | 1834 | 2MG | C4-N3 | 6.82 | 1.49 | 1.34 |
| 27 | 23SB | 2567 | OMU | C2-N1 | 6.82 | 1.49 | 1.38 |
| 24 | ESIB | 37 | MIA | C6-N6 | 6.80 | 1.45 | 1.34 |
| 27 | 23SB | 1987 | 5MC | C2-N3 | 6.77 | 1.49 | 1.36 |
| 23 | PSIA | 46 | 7MG | C4-N9 | -6.76 | 1.29 | 1.37 |
| 1 | 16SB | 2032 | 5MC | C2-N3 | 6.73 | 1.49 | 1.36 |
| 27 | 23SB | 1987 | 5MC | C5-C4 | 6.72 | 1.49 | 1.44 |
| 27 | 23SB | 1967 | 5MC | C2-N3 | 6.67 | 1.49 | 1.36 |
| 27 | 23SB | 2567 | OMU | C2-N3 | 6.66 | 1.49 | 1.38 |
| 24 | ESIA | 37 | MIA | C6-N6 | 6.66 | 1.44 | 1.34 |
| 27 | 23SA | 2567 | OMU | C2-N3 | 6.63 | 1.49 | 1.38 |
| 1 | 16SA | 2032 | 5MC | C5-C4 | 6.63 | 1.49 | 1.44 |
| 1 | 16SA | 2032 | 5MC | C2-N3 | 6.62 | 1.49 | 1.36 |
| 57 | ASIB | 37 | MIA | C6-N6 | 6.58 | 1.44 | 1.34 |
| 27 | 23SA | 1987 | 5MC | C5-C4 | 6.57 | 1.49 | 1.44 |
| 27 | 23SB | 1940 | 5MU | C4-N3 | -6.54 | 1.26 | 1.38 |
| 1 | 16SA | 1156 | 7MG | C4-N9 | -6.51 | 1.29 | 1.37 |
| 1 | 16SA | 2035 | 5MC | C5-C4 | 6.50 | 1.49 | 1.44 |
| 1 | 16SB | 2035 | 5MC | C2-N3 | 6.47 | 1.49 | 1.36 |
| 1 | 16SA | 2035 | 5MC | C2-N3 | 6.46 | 1.49 | 1.36 |
| 1 | 16SB | 2028 | 5MC | C2-N3 | 6.44 | 1.49 | 1.36 |
| 27 | 23SA | 1987 | 5MC | C2-N3 | 6.44 | 1.49 | 1.36 |
| 1 | 16SB | 2121 | UR3 | C6-C5 | 6.44 | 1.50 | 1.35 |
| 1 | 16SA | 1590 | 5MC | C2-N3 | 6.44 | 1.49 | 1.36 |
| 1 | 16SA | 2121 | UR3 | C6-C5 | 6.42 | 1.50 | 1.35 |
| 1 | 16SB | 2030 | 4OC | C4-N3 | 6.39 | 1.43 | 1.32 |
| 1 | 16SA | 2030 | 4OC | C2-N3 | 6.38 | 1.49 | 1.36 |
| 27 | 23SB | 2518 | 2MA | C2-N1 | 6.35 | 1.44 | 1.34 |
| 27 | 23SA | 1967 | 5MC | C2-N3 | 6.33 | 1.48 | 1.36 |
| 1 | 16SA | 1156 | 7MG | C4-N3 | 6.33 | 1.48 | 1.34 |
| 23 | PSIA | 54 | 5MU | C4-N3 | -6.31 | 1.27 | 1.38 |
| 27 | 23SB | 1964 | 5MU | C2-N3 | 6.29 | 1.48 | 1.38 |
| 1 | 16SA | 2028 | 5MC | C2-N3 | 6.29 | 1.48 | 1.36 |
| 27 | 23SA | 1964 | 5MU | C4-N3 | -6.29 | 1.27 | 1.38 |
| 23 | PSIA | 47 | 3AU | C6-C5 | 6.27 | 1.49 | 1.35 |
| 27 | 23SA | 1940 | 5MU | C2-N3 | 6.27 | 1.48 | 1.38 |
| 27 | 23SB | 1964 | 5MU | C4-N3 | -6.25 | 1.27 | 1.38 |
| 27 | 23SB | 2518 | 2MA | C6-N1 | 6.24 | 1.43 | 1.35 |
| 22 | ASIA | 46 | 7MG | C4-N3 | 6.20 | 1.48 | 1.34 |
| 23 | PSIB | 47 | 3AU | C6-C5 | 6.19 | 1.49 | 1.35 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(Å) | Ideal(Å) |
|---|---|---|---|---|---|---|---|
| 1 | 16SA | 2030 | 4OC | C6-C5 | 6.16 | 1.49 | 1.35 |
| 27 | 23SA | 2518 | 2MA | C2-N1 | 6.15 | 1.44 | 1.34 |
| 22 | ASIA | 37 | MIA | C6-N6 | 6.15 | 1.44 | 1.34 |
| 23 | PSIB | 37 | MIA | C6-N6 | 6.12 | 1.44 | 1.34 |
| 26 | TRNA | 54 | 5MU | C2-N3 | 6.11 | 1.48 | 1.38 |
| 57 | ASIB | 54 | 5MU | C4-N3 | -6.08 | 1.27 | 1.38 |
| 23 | PSIB | 54 | 5MU | C4-N3 | -6.07 | 1.27 | 1.38 |
| 22 | ASIA | 54 | 5MU | C4-N3 | -6.07 | 1.27 | 1.38 |
| 1 | 16SB | 1156 | 7MG | C4-N3 | 6.04 | 1.48 | 1.34 |
| 26 | TRNA | 54 | 5MU | C6-N1 | 6.01 | 1.48 | 1.38 |
| 27 | 23SA | 2518 | 2MA | C6-N1 | 6.00 | 1.43 | 1.35 |
| 1 | 16SB | 1589 | M2G | C2-N3 | 5.98 | 1.46 | 1.32 |
| 23 | PSIA | 37 | MIA | C6-N6 | 5.96 | 1.43 | 1.34 |
| 23 | PSIA | 46 | 7MG | C4-N3 | 5.95 | 1.47 | 1.34 |
| 26 | TRNA | 54 | 5MU | C4-N3 | -5.94 | 1.27 | 1.38 |
| 1 | 16SB | 2030 | 4OC | C6-C5 | 5.94 | 1.48 | 1.35 |
| 27 | 23SA | 1940 | 5MU | C6-N1 | 5.91 | 1.48 | 1.38 |
| 22 | ASIA | 54 | 5MU | C2-N3 | 5.91 | 1.48 | 1.38 |
| 57 | ASIB | 54 | 5MU | C6-N1 | 5.90 | 1.48 | 1.38 |
| 27 | 23SA | 1964 | 5MU | C2-N3 | 5.89 | 1.48 | 1.38 |
| 57 | ASIB | 54 | 5MU | C2-N3 | 5.88 | 1.48 | 1.38 |
| 27 | 23SA | 1940 | 5MU | C4-N3 | -5.87 | 1.27 | 1.38 |
| 22 | ASIA | 54 | 5MU | C6-N1 | 5.86 | 1.48 | 1.38 |
| 23 | PSIB | 54 | 5MU | C2-N3 | 5.84 | 1.48 | 1.38 |
| 23 | PSIB | 46 | 7MG | C4-N3 | 5.81 | 1.47 | 1.34 |
| 23 | PSIB | 47 | 3AU | C2-N3 | 5.77 | 1.48 | 1.38 |
| 26 | TRNA | 8 | 4SU | C5-C4 | 5.77 | 1.49 | 1.42 |
| 23 | PSIA | 8 | 4SU | C5-C4 | 5.73 | 1.49 | 1.42 |
| 23 | PSIB | 54 | 5MU | C6-N1 | 5.73 | 1.47 | 1.38 |
| 23 | PSIA | 54 | 5MU | C6-N1 | 5.72 | 1.47 | 1.38 |
| 27 | 23SB | 1940 | 5MU | C6-N1 | 5.71 | 1.47 | 1.38 |
| 23 | PSIA | 47 | 3AU | C2-N3 | 5.71 | 1.48 | 1.38 |
| 27 | 23SA | 2518 | 2MA | C2-N3 | 5.70 | 1.43 | 1.34 |
| 26 | TRNA | 37 | MIA | C2-S10 | 5.67 | 1.80 | 1.75 |
| 27 | 23SB | 1940 | 5MU | C2-N3 | 5.66 | 1.47 | 1.38 |
| 23 | PSIA | 54 | 5MU | C2-N3 | 5.64 | 1.47 | 1.38 |
| 27 | 23SB | 2567 | OMU | C6-C5 | 5.63 | 1.48 | 1.35 |
| 27 | 23SB | 1964 | 5MU | C6-N1 | 5.62 | 1.47 | 1.38 |
| 27 | 23SA | 2567 | OMU | C6-C5 | 5.60 | 1.48 | 1.35 |
| 22 | ASIA | 8 | 4SU | C5-C4 | 5.58 | 1.49 | 1.42 |
| 27 | 23SB | 2518 | 2MA | C2-N3 | 5.57 | 1.43 | 1.34 |
| 1 | 16SA | 1589 | M2G | C2-N3 | 5.56 | 1.45 | 1.32 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(Å) | Ideal(Å) |
|---|---|---|---|---|---|---|---|
| 1 | 16SB | 2030 | 4OC | C2-N3 | 5.39 | 1.47 | 1.36 |
| 1 | 16SB | 1834 | 2MG | C2-N1 | 5.32 | 1.45 | 1.36 |
| 22 | ASIA | 37 | MIA | C2-S10 | 5.29 | 1.80 | 1.75 |
| 1 | 16SA | 2121 | UR3 | C2-N3 | 5.27 | 1.49 | 1.39 |
| 27 | 23SA | 1964 | 5MU | C6-N1 | 5.22 | 1.46 | 1.38 |
| 1 | 16SB | 2121 | UR3 | C2-N3 | 5.15 | 1.49 | 1.39 |
| 24 | ESIB | 37 | MIA | C2-S10 | 5.13 | 1.79 | 1.75 |
| 23 | PSIA | 37 | MIA | C2-S10 | 5.13 | 1.79 | 1.75 |
| 27 | 23SA | 1964 | 5MU | C4-C5 | 5.11 | 1.53 | 1.44 |
| 1 | 16SB | 1590 | 5MC | C4-N4 | 5.11 | 1.47 | 1.34 |
| 27 | 23SB | 1987 | 5MC | C4-N4 | 5.06 | 1.47 | 1.34 |
| 1 | 16SA | 2032 | 5MC | C4-N4 | 5.01 | 1.46 | 1.34 |
| 1 | 16SB | 2032 | 5MC | C4-N4 | 5.01 | 1.46 | 1.34 |
| 27 | 23SA | 1967 | 5MC | C2-N1 | 5.00 | 1.50 | 1.40 |
| 27 | 23SA | 1987 | 5MC | C6-N1 | 4.99 | 1.46 | 1.38 |
| 22 | ASIA | 54 | 5MU | C4-C5 | 4.97 | 1.52 | 1.44 |
| 27 | 23SB | 1967 | 5MC | C4-N4 | 4.96 | 1.46 | 1.34 |
| 1 | 16SA | 1590 | 5MC | C4-N4 | 4.93 | 1.46 | 1.34 |
| 1 | 16SA | 1834 | 2MG | C2-N1 | 4.92 | 1.44 | 1.36 |
| 27 | 23SB | 1987 | 5MC | C6-N1 | 4.92 | 1.46 | 1.38 |
| 1 | 16SB | 2035 | 5MC | C4-N4 | 4.88 | 1.46 | 1.34 |
| 1 | 16SB | 1590 | 5MC | C6-N1 | 4.87 | 1.46 | 1.38 |
| 1 | 16SA | 1590 | 5MC | C6-N1 | 4.87 | 1.46 | 1.38 |
| 27 | 23SA | 1967 | 5MC | C4-N4 | 4.85 | 1.46 | 1.34 |
| 27 | 23SA | 1987 | 5MC | C4-N4 | 4.83 | 1.46 | 1.34 |
| 1 | 16SA | 2032 | 5MC | C6-N1 | 4.82 | 1.46 | 1.38 |
| 1 | 16SB | 2028 | 5MC | C4-N4 | 4.82 | 1.46 | 1.34 |
| 23 | PSIB | 8 | 4SU | C5-C4 | 4.82 | 1.48 | 1.42 |
| 26 | TRNA | 54 | 5MU | C4-C5 | 4.80 | 1.52 | 1.44 |
| 1 | 16SA | 2028 | 5MC | C4-N4 | 4.80 | 1.46 | 1.34 |
| 27 | 23SB | 1967 | 5MC | C6-N1 | 4.80 | 1.46 | 1.38 |
| 1 | 16SB | 2032 | 5MC | C6-N1 | 4.77 | 1.46 | 1.38 |
| 24 | ESIA | 37 | MIA | C2-S10 | 4.76 | 1.79 | 1.75 |
| 1 | 16SA | 2035 | 5MC | C4-N4 | 4.76 | 1.46 | 1.34 |
| 27 | 23SB | 1940 | 5MU | C4-C5 | 4.75 | 1.52 | 1.44 |
| 23 | PSIB | 46 | 7MG | C8-N7 | 4.74 | 1.65 | 1.42 |
| 1 | 16SB | 1156 | 7MG | C8-N7 | 4.71 | 1.65 | 1.42 |
| 27 | 23SB | 1945 | OMC | C2-N3 | 4.71 | 1.45 | 1.36 |
| 57 | ASIB | 54 | 5MU | C4-C5 | 4.71 | 1.52 | 1.44 |
| 1 | 16SA | 2032 | 5MC | C2-N1 | 4.70 | 1.49 | 1.40 |
| 27 | 23SA | 1987 | 5MC | C2-N1 | 4.70 | 1.49 | 1.40 |
| 23 | PSIB | 46 | 7MG | C5-C4 | -4.70 | 1.23 | 1.37 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(Å) | Ideal(Å) |
|---|---|---|---|---|---|---|---|
| 1 | 16SB | 2035 | 5MC | C6-N1 | 4.70 | 1.46 | 1.38 |
| 27 | 23SA | 1940 | 5MU | C4-C5 | 4.68 | 1.52 | 1.44 |
| 1 | 16SB | 1156 | 7MG | C5-C4 | -4.67 | 1.23 | 1.37 |
| 1 | 16SB | 2028 | 5MC | C2-N1 | 4.66 | 1.49 | 1.40 |
| 1 | 16SA | 2035 | 5MC | C6-N1 | 4.65 | 1.45 | 1.38 |
| 1 | 16SA | 2030 | 4OC | C2-N1 | 4.63 | 1.49 | 1.40 |
| 27 | 23SB | 1967 | 5MC | C2-N1 | 4.63 | 1.49 | 1.40 |
| 1 | 16SA | 1156 | 7MG | C8-N7 | 4.63 | 1.64 | 1.42 |
| 22 | ASIA | 46 | 7MG | C5-C4 | -4.61 | 1.23 | 1.37 |
| 22 | ASIA | 46 | 7MG | C8-N7 | 4.60 | 1.64 | 1.42 |
| 57 | ASIB | 37 | MIA | C2-S10 | 4.58 | 1.79 | 1.75 |
| 1 | 16SA | 1156 | 7MG | C5-C4 | -4.57 | 1.24 | 1.37 |
| 1 | 16SB | 2030 | 4OC | C2-N1 | 4.55 | 1.49 | 1.40 |
| 1 | 16SA | 2028 | 5MC | C6-N1 | 4.54 | 1.45 | 1.38 |
| 23 | PSIA | 46 | 7MG | C8-N7 | 4.53 | 1.64 | 1.42 |
| 1 | 16SA | 1589 | M2G | C2-N1 | 4.53 | 1.47 | 1.36 |
| 1 | 16SB | 2035 | 5MC | C2-N1 | 4.52 | 1.49 | 1.40 |
| 27 | 23SA | 1967 | 5MC | C6-N1 | 4.48 | 1.45 | 1.38 |
| 1 | 16SA | 1590 | 5MC | C2-N1 | 4.48 | 1.49 | 1.40 |
| 1 | 16SB | 1590 | 5MC | C2-N1 | 4.47 | 1.49 | 1.40 |
| 23 | PSIA | 46 | 7MG | C5-C4 | -4.47 | 1.24 | 1.37 |
| 27 | 23SB | 1964 | 5MU | C4-C5 | 4.46 | 1.52 | 1.44 |
| 1 | 16SB | 2028 | 5MC | C6-N1 | 4.43 | 1.45 | 1.38 |
| 1 | 16SB | 1589 | M2G | C2-N1 | 4.43 | 1.46 | 1.36 |
| 1 | 16SB | 2032 | 5MC | C2-N1 | 4.42 | 1.49 | 1.40 |
| 23 | PSIA | 54 | 5MU | C4-C5 | 4.40 | 1.52 | 1.44 |
| 27 | 23SB | 1987 | 5MC | C2-N1 | 4.38 | 1.49 | 1.40 |
| 27 | 23SA | 1945 | OMC | C2-N3 | 4.38 | 1.45 | 1.36 |
| 1 | 16SA | 2035 | 5MC | C2-N1 | 4.35 | 1.49 | 1.40 |
| 27 | 23SB | 1945 | OMC | C4-N4 | 4.35 | 1.44 | 1.33 |
| 23 | PSIB | 54 | 5MU | C4-C5 | 4.34 | 1.51 | 1.44 |
| 1 | 16SA | 2030 | 4OC | C4-N4 | 4.33 | 1.45 | 1.36 |
| 22 | ASIA | 32 | PSU | C6-C5 | 4.27 | 1.40 | 1.35 |
| 27 | 23SB | 2266 | OMG | C8-N9 | -4.26 | 1.28 | 1.37 |
| 27 | 23SA | 1945 | OMC | C4-N4 | 4.23 | 1.44 | 1.33 |
| 27 | 23SA | 2266 | OMG | C8-N9 | -4.22 | 1.28 | 1.37 |
| 1 | 16SA | 2028 | 5MC | C2-N1 | 4.13 | 1.48 | 1.40 |
| 27 | 23SA | 2567 | OMU | C4-N3 | 4.13 | 1.45 | 1.38 |
| 1 | 16SB | 1145 | PSU | C6-C5 | 4.08 | 1.39 | 1.35 |
| 26 | TRNA | 8 | 4SU | C2-N1 | 4.04 | 1.44 | 1.38 |
| 23 | PSIA | 55 | PSU | C6-C5 | 4.03 | 1.39 | 1.35 |
| 23 | PSIB | 39 | PSU | C6-C5 | 4.03 | 1.39 | 1.35 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(Å) | Ideal(Å) |
|---|---|---|---|---|---|---|---|
| 22 | ASIA | 39 | PSU | C6-C5 | 4.02 | 1.39 | 1.35 |
| 27 | 23SB | 2620 | PSU | C6-C5 | 4.02 | 1.39 | 1.35 |
| 22 | ASIA | 55 | PSU | C6-C5 | 4.01 | 1.39 | 1.35 |
| 26 | TRNA | 32 | PSU | C6-C5 | 4.00 | 1.39 | 1.35 |
| 27 | 23SB | 2567 | OMU | C4-N3 | 3.98 | 1.45 | 1.38 |
| 26 | TRNA | 39 | PSU | C6-C5 | 3.98 | 1.39 | 1.35 |
| 22 | ASIA | 8 | 4SU | C2-N1 | 3.96 | 1.44 | 1.38 |
| 57 | ASIB | 39 | PSU | C6-C5 | 3.96 | 1.39 | 1.35 |
| 23 | PSIB | 55 | PSU | C6-C5 | 3.95 | 1.39 | 1.35 |
| 27 | 23SB | 1942 | PSU | C6-C5 | 3.91 | 1.39 | 1.35 |
| 1 | 16SA | 1145 | PSU | C6-C5 | 3.91 | 1.39 | 1.35 |
| 23 | PSIA | 8 | 4SU | C2-N1 | 3.87 | 1.44 | 1.38 |
| 1 | 16SB | 2030 | 4OC | C5-C4 | 3.82 | 1.49 | 1.41 |
| 27 | 23SB | 2518 | 2MA | C5-C6 | 3.80 | 1.51 | 1.41 |
| 26 | TRNA | 55 | PSU | C6-C5 | 3.76 | 1.39 | 1.35 |
| 27 | 23SA | 2518 | 2MA | C5-C6 | 3.76 | 1.51 | 1.41 |
| 27 | 23SA | 2620 | PSU | C6-C5 | 3.76 | 1.39 | 1.35 |
| 27 | 23SA | 1945 | OMC | C5-C4 | 3.75 | 1.51 | 1.42 |
| 27 | 23SB | 1936 | PSU | C6-C5 | 3.74 | 1.39 | 1.35 |
| 27 | 23SB | 1945 | OMC | C5-C4 | 3.72 | 1.51 | 1.42 |
| 1 | 16SA | 2141 | MA6 | C6-N6 | 3.70 | 1.47 | 1.36 |
| 23 | PSIB | 37 | MIA | C2-S10 | 3.69 | 1.78 | 1.75 |
| 27 | 23SA | 1942 | PSU | C6-C5 | 3.67 | 1.39 | 1.35 |
| 57 | ASIB | 32 | PSU | C6-C5 | 3.61 | 1.39 | 1.35 |
| 1 | 16SA | 2030 | 4OC | C5-C4 | 3.57 | 1.48 | 1.41 |
| 1 | 16SB | 1589 | M2G | C5-N7 | -3.54 | 1.32 | 1.39 |
| 23 | PSIB | 8 | 4SU | C2-N1 | 3.52 | 1.44 | 1.38 |
| 23 | PSIA | 39 | PSU | C6-C5 | 3.48 | 1.39 | 1.35 |
| 1 | 16SA | 2142 | MA6 | C6-N6 | 3.48 | 1.46 | 1.36 |
| 1 | 16SB | 2141 | MA6 | C6-N6 | 3.48 | 1.46 | 1.36 |
| 23 | PSIA | 32 | PSU | C6-C5 | 3.45 | 1.39 | 1.35 |
| 1 | 16SA | 1589 | M2G | C5-N7 | -3.41 | 1.32 | 1.39 |
| 1 | 16SB | 2142 | MA6 | C6-N6 | 3.40 | 1.46 | 1.36 |
| 1 | 16SA | 2121 | UR3 | C6-N1 | 3.39 | 1.46 | 1.38 |
| 1 | 16SB | 2121 | UR3 | C6-N1 | 3.38 | 1.46 | 1.38 |
| 27 | 23SA | 1936 | PSU | C6-C5 | 3.36 | 1.39 | 1.35 |
| 23 | PSIB | 32 | PSU | C6-C5 | 3.32 | 1.39 | 1.35 |
| 27 | 23SB | 2518 | 2MA | C5-N7 | -3.31 | 1.33 | 1.39 |
| 27 | 23SA | 2518 | 2MA | C5-N7 | -3.29 | 1.33 | 1.39 |
| 27 | 23SA | 2567 | OMU | O4-C4 | -3.20 | 1.18 | 1.24 |
| 1 | 16SA | 2030 | 4OC | C6-N1 | 3.19 | 1.45 | 1.38 |
| 1 | 16SB | 1834 | 2MG | C5-N7 | -3.19 | 1.32 | 1.39 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(Å) | Ideal(Å) |
|---|---|---|---|---|---|---|---|
| 1 | 16SA | 2035 | 5MC | O2-C2 | -3.18 | 1.17 | 1.23 |
| 1 | 16SB | 1156 | 7MG | C2-N2 | 3.17 | 1.41 | 1.34 |
| 1 | 16SA | 1834 | 2MG | O6-C6 | -3.16 | 1.17 | 1.23 |
| 1 | 16SA | 1590 | 5MC | O2-C2 | -3.16 | 1.17 | 1.23 |
| 1 | 16SB | 2035 | 5MC | O2-C2 | -3.15 | 1.17 | 1.23 |
| 1 | 16SA | 1156 | 7MG | C2-N2 | 3.14 | 1.41 | 1.34 |
| 1 | 16SA | 2028 | 5MC | O2-C2 | -3.13 | 1.17 | 1.23 |
| 1 | 16SB | 2028 | 5MC | O2-C2 | -3.11 | 1.17 | 1.23 |
| 27 | 23SB | 2567 | OMU | O4-C4 | -3.09 | 1.18 | 1.24 |
| 22 | ASIA | 46 | 7MG | C2-N2 | 3.09 | 1.41 | 1.34 |
| 1 | 16SB | 2030 | 4OC | C6-N1 | 3.04 | 1.45 | 1.38 |
| 1 | 16SA | 1834 | 2MG | C5-N7 | -3.04 | 1.33 | 1.39 |
| 23 | PSIB | 46 | 7MG | C2-N2 | 3.03 | 1.41 | 1.34 |
| 27 | 23SB | 1967 | 5MC | O2-C2 | -3.03 | 1.18 | 1.23 |
| 23 | PSIA | 46 | 7MG | C2-N2 | 3.03 | 1.41 | 1.34 |
| 1 | 16SA | 1589 | M2G | C5-C6 | 3.03 | 1.55 | 1.44 |
| 1 | 16SA | 1589 | M2G | C4-N9 | -3.01 | 1.30 | 1.38 |
| 23 | PSIB | 47 | 3AU | C4-N3 | 3.01 | 1.45 | 1.40 |
| 1 | 16SB | 1589 | M2G | C5-C6 | 2.99 | 1.55 | 1.44 |
| 27 | 23SB | 1987 | 5MC | O2-C2 | -2.97 | 1.18 | 1.23 |
| 1 | 16SB | 2032 | 5MC | O2-C2 | -2.97 | 1.18 | 1.23 |
| 23 | PSIA | 47 | 3AU | C4-N3 | 2.95 | 1.45 | 1.40 |
| 1 | 16SB | 2030 | 4OC | C4-N4 | 2.94 | 1.42 | 1.36 |
| 27 | 23SA | 1967 | 5MC | O2-C2 | -2.93 | 1.18 | 1.23 |
| 1 | 16SB | 1590 | 5MC | O2-C2 | -2.91 | 1.18 | 1.23 |
| 27 | 23SA | 2266 | OMG | O6-C6 | -2.90 | 1.18 | 1.23 |
| 1 | 16SB | 1834 | 2MG | O6-C6 | -2.87 | 1.18 | 1.23 |
| 23 | PSIA | 47 | 3AU | C6-N1 | 2.86 | 1.44 | 1.38 |
| 23 | PSIA | 8 | 4SU | C6-N1 | 2.83 | 1.44 | 1.38 |
| 27 | 23SB | 2266 | OMG | C2-N2 | 2.83 | 1.40 | 1.34 |
| 1 | 16SB | 2141 | MA6 | C5-N7 | -2.83 | 1.33 | 1.39 |
| 1 | 16SB | 2141 | MA6 | C8-N9 | -2.82 | 1.32 | 1.37 |
| 27 | 23SA | 2567 | OMU | C6-N1 | 2.81 | 1.44 | 1.38 |
| 27 | 23SA | 2266 | OMG | C2-N2 | 2.80 | 1.40 | 1.34 |
| 27 | 23SB | 2266 | OMG | O6-C6 | -2.78 | 1.18 | 1.23 |
| 27 | 23SB | 2567 | OMU | C6-N1 | 2.76 | 1.44 | 1.38 |
| 27 | 23SA | 1987 | 5MC | O2-C2 | -2.73 | 1.18 | 1.23 |
| 1 | 16SA | 1589 | M2G | C6-N1 | 2.73 | 1.44 | 1.38 |
| 23 | PSIB | 47 | 3AU | C6-N1 | 2.72 | 1.44 | 1.38 |
| 1 | 16SA | 2141 | MA6 | C5-N7 | -2.71 | 1.34 | 1.39 |
| 22 | ASIA | 8 | 4SU | C6-N1 | 2.70 | 1.44 | 1.38 |
| 27 | 23SB | 2266 | OMG | C2-N3 | 2.70 | 1.39 | 1.33 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(Å) | Ideal(Å) |
|---|---|---|---|---|---|---|---|
| 1 | 16SA | 2032 | 5MC | O2-C2 | -2.69 | 1.18 | 1.23 |
| 26 | TRNA | 37 | MIA | C5-N7 | -2.67 | 1.34 | 1.39 |
| 1 | 16SB | 1834 | 2MG | C6-N1 | 2.65 | 1.43 | 1.38 |
| 27 | 23SB | 2518 | 2MA | C8-N7 | 2.64 | 1.36 | 1.31 |
| 1 | 16SA | 1834 | 2MG | C6-N1 | 2.64 | 1.43 | 1.38 |
| 1 | 16SB | 2142 | MA6 | C5-C4 | -2.63 | 1.34 | 1.39 |
| 1 | 16SA | 2142 | MA6 | C8-N9 | -2.63 | 1.33 | 1.37 |
| 1 | 16SA | 2142 | MA6 | C5-N7 | -2.62 | 1.34 | 1.39 |
| 26 | TRNA | 8 | 4SU | C6-N1 | 2.62 | 1.44 | 1.38 |
| 1 | 16SB | 2030 | 4OC | O2-C2 | -2.62 | 1.18 | 1.23 |
| 1 | 16SB | 2142 | MA6 | C5-N7 | -2.60 | 1.34 | 1.39 |
| 1 | 16SA | 2030 | 4OC | O2-C2 | -2.60 | 1.18 | 1.23 |
| 1 | 16SB | 2142 | MA6 | C8-N9 | -2.60 | 1.33 | 1.37 |
| 1 | 16SB | 1834 | 2MG | C5-C6 | 2.59 | 1.54 | 1.44 |
| 1 | 16SA | 2142 | MA6 | C5-C4 | -2.58 | 1.34 | 1.39 |
| 23 | PSIB | 8 | 4SU | C4-N3 | 2.56 | 1.40 | 1.37 |
| 27 | 23SA | 2266 | OMG | C2-N3 | 2.54 | 1.39 | 1.33 |
| 1 | 16SA | 1834 | 2MG | C5-C6 | 2.54 | 1.53 | 1.44 |
| 1 | 16SB | 2141 | MA6 | C5-C4 | -2.53 | 1.34 | 1.39 |
| 1 | 16SA | 2141 | MA6 | C5-C4 | -2.52 | 1.34 | 1.39 |
| 1 | 16SA | 2142 | MA6 | C8-N7 | 2.51 | 1.36 | 1.31 |
| 1 | 16SB | 2142 | MA6 | C8-N7 | 2.50 | 1.36 | 1.31 |
| 23 | PSIA | 46 | 7MG | C6-N1 | -2.49 | 1.34 | 1.38 |
| 1 | 16SA | 2141 | MA6 | C8-N9 | -2.49 | 1.33 | 1.37 |
| 23 | PSIA | 47 | 3AU | O4-C4 | -2.47 | 1.18 | 1.23 |
| 27 | 23SB | 2567 | OMU | O2-C2 | -2.46 | 1.18 | 1.23 |
| 1 | 16SB | 1589 | M2G | C6-N1 | 2.45 | 1.43 | 1.38 |
| 23 | PSIA | 47 | 3AU | C5-C4 | 2.44 | 1.49 | 1.43 |
| 27 | 23SA | 2518 | 2MA | C8-N7 | 2.43 | 1.36 | 1.31 |
| 1 | 16SA | 2141 | MA6 | C8-N7 | 2.42 | 1.36 | 1.31 |
| 23 | PSIB | 47 | 3AU | O4-C4 | -2.42 | 1.18 | 1.23 |
| 27 | 23SB | 2567 | OMU | C5-C4 | 2.42 | 1.49 | 1.43 |
| 57 | ASIB | 37 | MIA | C5-N7 | -2.39 | 1.34 | 1.39 |
| 1 | 16SA | 1156 | 7MG | C6-N1 | -2.36 | 1.34 | 1.38 |
| 12 | S12B | 89 | 0TD | OD1-CG | 2.35 | 1.29 | 1.22 |
| 1 | 16SA | 2121 | UR3 | C5-C4 | 2.35 | 1.49 | 1.43 |
| 23 | PSIB | 47 | 3AU | C5-C4 | 2.34 | 1.49 | 1.43 |
| 1 | 16SB | 2121 | UR3 | C4-N3 | 2.32 | 1.45 | 1.40 |
| 27 | 23SA | 1945 | OMC | C6-N1 | 2.30 | 1.43 | 1.38 |
| 1 | 16SB | 2121 | UR3 | C5-C4 | 2.29 | 1.49 | 1.43 |
| 23 | PSIB | 8 | 4SU | C6-N1 | 2.27 | 1.43 | 1.38 |
| 1 | 16SA | 2121 | UR3 | O4-C4 | -2.27 | 1.18 | 1.23 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(Å) | Ideal(Å) |
|---|---|---|---|---|---|---|---|
| 27 | 23SA | 2567 | OMU | C5-C4 | 2.26 | 1.48 | 1.43 |
| 1 | 16SA | 2121 | UR3 | C4-N3 | 2.24 | 1.45 | 1.40 |
| 23 | PSIA | 47 | 3AU | O2-C2 | -2.23 | 1.18 | 1.22 |
| 23 | PSIB | 47 | 3AU | O2-C2 | -2.22 | 1.18 | 1.22 |
| 27 | 23SB | 1945 | OMC | C6-N1 | 2.19 | 1.43 | 1.38 |
| 27 | 23SA | 2266 | OMG | C2-N1 | -2.19 | 1.32 | 1.37 |
| 23 | PSIA | 37 | MIA | C5-N7 | -2.18 | 1.35 | 1.39 |
| 1 | 16SB | 2121 | UR3 | O4-C4 | -2.16 | 1.19 | 1.23 |
| 27 | 23SA | 2567 | OMU | O2-C2 | -2.16 | 1.19 | 1.23 |
| 1 | 16SB | 2121 | UR3 | O2-C2 | -2.15 | 1.18 | 1.22 |
| 23 | PSIB | 8 | 4SU | C2-N3 | 2.15 | 1.41 | 1.38 |
| 1 | 16SB | 1589 | M2G | C4-N9 | -2.15 | 1.32 | 1.38 |
| 1 | 16SB | 2141 | MA6 | C8-N7 | 2.14 | 1.35 | 1.31 |
| 23 | PSIB | 46 | 7MG | C5-C6 | 2.13 | 1.48 | 1.43 |
| 27 | 23SB | 2266 | OMG | C2-N1 | -2.11 | 1.32 | 1.37 |
| 12 | S12A | 89 | 0TD | CSB-SB | -2.11 | 1.75 | 1.79 |
| 22 | ASIA | 8 | 4SU | C2-N3 | 2.10 | 1.41 | 1.38 |
| 1 | 16SA | 1156 | 7MG | C5-C6 | 2.10 | 1.48 | 1.43 |
| 22 | ASIA | 8 | 4SU | C4-N3 | 2.10 | 1.39 | 1.37 |
| 24 | ESIB | 37 | MIA | C5-N7 | -2.07 | 1.35 | 1.39 |
| 23 | PSIB | 37 | MIA | C5-N7 | -2.07 | 1.35 | 1.39 |
| 57 | ASIB | 37 | MIA | C5-C4 | 2.06 | 1.42 | 1.39 |
| 22 | ASIA | 46 | 7MG | C6-N1 | -2.05 | 1.35 | 1.38 |
| 12 | S12B | 89 | 0TD | CB-CG | 2.05 | 1.55 | 1.52 |
| 1 | 16SA | 2121 | UR3 | O2-C2 | -2.05 | 1.18 | 1.22 |
| 23 | PSIB | 46 | 7MG | C6-N1 | -2.04 | 1.35 | 1.38 |
| 23 | PSIA | 46 | 7MG | C5-C6 | 2.03 | 1.48 | 1.43 |
| 26 | TRNA | 37 | MIA | C5-C4 | 2.02 | 1.42 | 1.39 |

All (547) bond angle outliers are listed below:

| Mol | Chain | Res | Type | Atoms | Z | Observed($^o$) | Ideal($^o$) |
|---|---|---|---|---|---|---|---|
| 24 | ESIB | 37 | MIA | C12-C13-C14 | -13.34 | 103.08 | 127.01 |
| 24 | ESIB | 37 | MIA | C11-S10-C2 | 12.96 | 111.97 | 102.25 |
| 22 | ASIA | 37 | MIA | C11-S10-C2 | 12.48 | 111.61 | 102.25 |
| 27 | 23SB | 2266 | OMG | C6-C5-N7 | 11.72 | 151.62 | 130.29 |
| 27 | 23SA | 2266 | OMG | C6-C5-N7 | 11.62 | 151.43 | 130.29 |
| 23 | PSIB | 37 | MIA | C12-C13-C14 | -10.71 | 107.78 | 127.01 |
| 27 | 23SB | 1940 | 5MU | C5-C4-N3 | 10.66 | 124.59 | 115.32 |
| 24 | ESIA | 37 | MIA | C11-S10-C2 | 10.54 | 110.16 | 102.25 |
| 27 | 23SB | 2266 | OMG | C8-N7-C5 | 10.50 | 122.97 | 104.26 |
| 57 | ASIB | 54 | 5MU | C5-C4-N3 | 10.37 | 124.33 | 115.32 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed($^o$) | Ideal($^o$) |
|---|---|---|---|---|---|---|---|
| 27 | 23SA | 1940 | 5MU | C5-C4-N3 | 10.36 | 124.33 | 115.32 |
| 22 | ASIA | 54 | 5MU | C5-C4-N3 | 10.33 | 124.30 | 115.32 |
| 27 | 23SA | 1964 | 5MU | C5-C4-N3 | 10.30 | 124.28 | 115.32 |
| 26 | TRNA | 54 | 5MU | C5-C4-N3 | 10.18 | 124.17 | 115.32 |
| 23 | PSIB | 54 | 5MU | C5-C4-N3 | 10.16 | 124.15 | 115.32 |
| 23 | PSIA | 54 | 5MU | C5-C4-N3 | 10.13 | 124.12 | 115.32 |
| 22 | ASIA | 37 | MIA | C12-C13-C14 | -10.08 | 108.92 | 127.01 |
| 57 | ASIB | 37 | MIA | C11-S10-C2 | 10.06 | 109.80 | 102.25 |
| 26 | TRNA | 37 | MIA | C11-S10-C2 | 9.97 | 109.73 | 102.25 |
| 27 | 23SA | 2266 | OMG | C8-N7-C5 | 9.85 | 121.81 | 104.26 |
| 57 | ASIB | 37 | MIA | C12-C13-C14 | -9.84 | 109.35 | 127.01 |
| 27 | 23SB | 1964 | 5MU | C5-C4-N3 | 9.48 | 123.56 | 115.32 |
| 27 | 23SB | 2266 | OMG | N9-C4-N3 | 9.44 | 144.82 | 125.95 |
| 26 | TRNA | 37 | MIA | C5-C4-N3 | -9.41 | 117.27 | 127.18 |
| 26 | TRNA | 37 | MIA | C12-C13-C14 | -9.38 | 110.17 | 127.01 |
| 23 | PSIA | 37 | MIA | C11-S10-C2 | 9.10 | 109.08 | 102.25 |
| 1 | 16SB | 2142 | MA6 | N1-C6-N6 | -9.03 | 105.85 | 116.86 |
| 27 | 23SA | 2266 | OMG | N9-C4-N3 | 9.00 | 143.95 | 125.95 |
| 1 | 16SA | 2142 | MA6 | N1-C6-N6 | -8.90 | 106.02 | 116.86 |
| 23 | PSIB | 8 | 4SU | C4-N3-C2 | -8.74 | 118.94 | 127.31 |
| 1 | 16SA | 2141 | MA6 | N1-C6-N6 | -8.51 | 106.48 | 116.86 |
| 23 | PSIA | 37 | MIA | C5-C4-N3 | -8.49 | 118.24 | 127.18 |
| 24 | ESIA | 37 | MIA | C12-C13-C14 | -8.48 | 111.79 | 127.01 |
| 26 | TRNA | 37 | MIA | N3-C4-N9 | 8.44 | 137.70 | 126.99 |
| 27 | 23SA | 2266 | OMG | C6-C5-C4 | -8.28 | 106.38 | 118.83 |
| 1 | 16SB | 1156 | 7MG | C4-C5-N7 | 8.22 | 115.09 | 105.38 |
| 1 | 16SB | 2141 | MA6 | N1-C6-N6 | -8.11 | 106.97 | 116.86 |
| 22 | ASIA | 46 | 7MG | C4-C5-N7 | 8.08 | 114.92 | 105.38 |
| 23 | PSIA | 46 | 7MG | C4-C5-N7 | 8.04 | 114.88 | 105.38 |
| 1 | 16SA | 1156 | 7MG | C4-C5-N7 | 7.81 | 114.61 | 105.38 |
| 57 | ASIB | 37 | MIA | C5-C4-N3 | -7.69 | 119.08 | 127.18 |
| 22 | ASIA | 8 | 4SU | C4-N3-C2 | -7.68 | 119.95 | 127.31 |
| 23 | PSIB | 46 | 7MG | C4-C5-N7 | 7.60 | 114.35 | 105.38 |
| 27 | 23SB | 2266 | OMG | C6-C5-C4 | -7.54 | 107.48 | 118.83 |
| 24 | ESIB | 37 | MIA | C5-C4-N3 | -7.53 | 119.25 | 127.18 |
| 26 | TRNA | 8 | 4SU | C4-N3-C2 | -7.52 | 120.10 | 127.31 |
| 27 | 23SB | 2266 | OMG | C1'-N9-C4 | 7.45 | 148.49 | 126.49 |
| 27 | 23SA | 2518 | 2MA | C5-C4-N3 | -7.39 | 119.39 | 127.18 |
| 23 | PSIA | 8 | 4SU | C4-N3-C2 | -7.38 | 120.24 | 127.31 |
| 23 | PSIA | 37 | MIA | C12-C13-C14 | -7.27 | 113.97 | 127.01 |
| 1 | 16SA | 1834 | 2MG | C2-N3-C4 | 7.20 | 121.01 | 112.00 |
| 27 | 23SB | 2518 | 2MA | C5-C4-N3 | -7.18 | 119.61 | 127.18 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed($^o$) | Ideal($^o$) |
|---|---|---|---|---|---|---|---|
| 23 | PSIB | 8 | 4SU | C5-C4-S4 | -7.09 | 116.21 | 124.31 |
| 22 | ASIA | 37 | MIA | C5-C4-N3 | -7.03 | 119.77 | 127.18 |
| 23 | PSIA | 37 | MIA | N3-C4-N9 | 6.93 | 135.78 | 126.99 |
| 23 | PSIB | 37 | MIA | C11-S10-C2 | 6.80 | 107.35 | 102.25 |
| 27 | 23SB | 1940 | 5MU | C4-N3-C2 | -6.79 | 118.44 | 127.34 |
| 24 | ESIA | 37 | MIA | C5-C4-N3 | -6.69 | 120.13 | 127.18 |
| 23 | PSIB | 8 | 4SU | C5-C4-N3 | 6.66 | 120.94 | 114.75 |
| 27 | 23SB | 2266 | OMG | C5-C6-N1 | 6.63 | 130.11 | 113.25 |
| 1 | 16SB | 1834 | 2MG | C2-N3-C4 | 6.61 | 120.27 | 112.00 |
| 27 | 23SA | 1964 | 5MU | C4-N3-C2 | -6.58 | 118.72 | 127.34 |
| 27 | 23SA | 2266 | OMG | C5-C6-N1 | 6.57 | 129.98 | 113.25 |
| 23 | PSIB | 37 | MIA | C5-C4-N3 | -6.52 | 120.31 | 127.18 |
| 27 | 23SB | 2266 | OMG | C5-C4-N3 | -6.48 | 118.08 | 128.39 |
| 27 | 23SB | 1940 | 5MU | C6-C5-C4 | 6.44 | 123.32 | 118.02 |
| 27 | 23SB | 1964 | 5MU | C6-C5-C4 | 6.42 | 123.31 | 118.02 |
| 27 | 23SA | 1940 | 5MU | O4-C4-C5 | -6.41 | 117.58 | 124.92 |
| 57 | ASIB | 37 | MIA | N3-C4-N9 | 6.37 | 135.07 | 126.99 |
| 27 | 23SB | 1964 | 5MU | C4-N3-C2 | -6.21 | 119.19 | 127.34 |
| 23 | PSIB | 46 | 7MG | C5-C4-N9 | 6.20 | 114.28 | 106.33 |
| 27 | 23SA | 2266 | OMG | C1'-N9-C4 | 6.19 | 144.78 | 126.49 |
| 27 | 23SA | 1940 | 5MU | C4-N3-C2 | -6.17 | 119.25 | 127.34 |
| 27 | 23SB | 2266 | OMG | C4-C5-N7 | -6.17 | 100.90 | 110.67 |
| 1 | 16SB | 1156 | 7MG | C5-C4-N9 | 6.12 | 114.17 | 106.33 |
| 22 | ASIA | 37 | MIA | N3-C4-N9 | 6.07 | 134.70 | 126.99 |
| 1 | 16SA | 1156 | 7MG | C5-C4-N9 | 6.07 | 114.11 | 106.33 |
| 26 | TRNA | 37 | MIA | N6-C6-N1 | 6.07 | 126.46 | 118.33 |
| 23 | PSIB | 47 | 3AU | O2-C2-N3 | -6.04 | 113.84 | 121.98 |
| 1 | 16SB | 2142 | MA6 | N1-C2-N3 | -6.04 | 119.44 | 128.58 |
| 26 | TRNA | 37 | MIA | C15-C14-C13 | -6.04 | 104.53 | 122.66 |
| 23 | PSIB | 47 | 3AU | C1'-N1-C2 | 6.04 | 126.93 | 117.04 |
| 27 | 23SB | 2567 | OMU | C4-N3-C2 | -5.98 | 119.19 | 126.61 |
| 23 | PSIA | 8 | 4SU | C5-C4-N3 | 5.96 | 120.30 | 114.75 |
| 1 | 16SA | 1145 | PSU | N1-C2-N3 | 5.95 | 121.45 | 115.17 |
| 27 | 23SA | 1964 | 5MU | C6-C5-C4 | 5.90 | 122.88 | 118.02 |
| 27 | 23SB | 1940 | 5MU | C5-C6-N1 | -5.90 | 116.91 | 123.31 |
| 22 | ASIA | 8 | 4SU | C5-C4-N3 | 5.89 | 120.23 | 114.75 |
| 1 | 16SA | 2142 | MA6 | N1-C2-N3 | -5.87 | 119.70 | 128.58 |
| 26 | TRNA | 8 | 4SU | C5-C4-N3 | 5.86 | 120.20 | 114.75 |
| 1 | 16SA | 2141 | MA6 | N1-C2-N3 | -5.84 | 119.74 | 128.58 |
| 1 | 16SB | 2141 | MA6 | N1-C2-N3 | -5.83 | 119.76 | 128.58 |
| 24 | ESIB | 37 | MIA | N3-C4-N9 | 5.82 | 134.38 | 126.99 |
| 27 | 23SA | 1964 | 5MU | C5-C6-N1 | -5.81 | 117.00 | 123.31 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed($^o$) | Ideal($^o$) |
|---|---|---|---|---|---|---|---|
| 1 | 16SB | 1589 | M2G | C5-C4-N3 | -5.77 | 119.21 | 128.39 |
| 57 | ASIB | 54 | 5MU | C4-N3-C2 | -5.76 | 119.78 | 127.34 |
| 22 | ASIA | 54 | 5MU | C4-N3-C2 | -5.76 | 119.79 | 127.34 |
| 27 | 23SB | 1964 | 5MU | O4-C4-C5 | -5.75 | 118.34 | 124.92 |
| 26 | TRNA | 54 | 5MU | C4-N3-C2 | -5.71 | 119.85 | 127.34 |
| 1 | 16SB | 1834 | 2MG | C5-C4-N3 | -5.66 | 119.39 | 128.39 |
| 23 | PSIB | 54 | 5MU | O4-C4-C5 | -5.63 | 118.47 | 124.92 |
| 23 | PSIA | 54 | 5MU | C5-C6-N1 | -5.63 | 117.20 | 123.31 |
| 1 | 16SA | 2121 | UR3 | C4-N3-C2 | -5.59 | 120.08 | 124.58 |
| 23 | PSIA | 54 | 5MU | O4-C4-C5 | -5.53 | 118.59 | 124.92 |
| 1 | 16SA | 1834 | 2MG | C5-C4-N3 | -5.53 | 119.59 | 128.39 |
| 27 | 23SA | 2567 | OMU | C4-N3-C2 | -5.49 | 119.80 | 126.61 |
| 24 | ESIB | 37 | MIA | C16-C14-C13 | -5.48 | 106.20 | 122.66 |
| 22 | ASIA | 46 | 7MG | C5-C4-N9 | 5.47 | 113.35 | 106.33 |
| 23 | PSIA | 46 | 7MG | C5-C4-N9 | 5.47 | 113.34 | 106.33 |
| 1 | 16SB | 2030 | 4OC | CM4-N4-C4 | -5.45 | 111.80 | 122.45 |
| 1 | 16SA | 1156 | 7MG | C5-C6-N1 | 5.44 | 120.52 | 110.94 |
| 24 | ESIA | 37 | MIA | N3-C4-N9 | 5.44 | 133.89 | 126.99 |
| 27 | 23SA | 1964 | 5MU | C5M-C5-C6 | -5.41 | 115.53 | 122.85 |
| 23 | PSIB | 32 | PSU | N1-C2-N3 | 5.38 | 120.84 | 115.17 |
| 26 | TRNA | 54 | 5MU | O4-C4-C5 | -5.36 | 118.78 | 124.92 |
| 27 | 23SA | 2266 | OMG | C4-C5-N7 | -5.35 | 102.19 | 110.67 |
| 27 | 23SA | 2266 | OMG | C5-C4-N3 | -5.34 | 119.88 | 128.39 |
| 27 | 23SB | 1940 | 5MU | O4-C4-C5 | -5.34 | 118.81 | 124.92 |
| 23 | PSIA | 54 | 5MU | C6-C5-C4 | 5.31 | 122.39 | 118.02 |
| 27 | 23SA | 2266 | OMG | C5-C4-N9 | -5.30 | 96.16 | 105.66 |
| 57 | ASIB | 54 | 5MU | O4-C4-C5 | -5.30 | 118.86 | 124.92 |
| 23 | PSIA | 46 | 7MG | C6-C5-N7 | -5.29 | 123.74 | 131.93 |
| 23 | PSIA | 54 | 5MU | C4-N3-C2 | -5.27 | 120.43 | 127.34 |
| 27 | 23SA | 1940 | 5MU | C6-C5-C4 | 5.25 | 122.34 | 118.02 |
| 22 | ASIA | 37 | MIA | C16-C14-C13 | -5.21 | 107.02 | 122.66 |
| 1 | 16SB | 1156 | 7MG | C5-C6-N1 | 5.19 | 120.08 | 110.94 |
| 57 | ASIB | 32 | PSU | N1-C2-N3 | 5.17 | 120.63 | 115.17 |
| 23 | PSIB | 54 | 5MU | C4-N3-C2 | -5.16 | 120.57 | 127.34 |
| 22 | ASIA | 54 | 5MU | O4-C4-C5 | -5.15 | 119.03 | 124.92 |
| 1 | 16SA | 2142 | MA6 | C5-C6-N6 | 5.14 | 133.47 | 125.33 |
| 22 | ASIA | 46 | 7MG | C5-C6-N1 | 5.14 | 119.98 | 110.94 |
| 1 | 16SA | 2141 | MA6 | C5-C6-N6 | 5.14 | 133.46 | 125.33 |
| 1 | 16SB | 2142 | MA6 | C5-C6-N6 | 5.13 | 133.45 | 125.33 |
| 27 | 23SB | 2266 | OMG | C8-N9-C4 | -5.07 | 96.53 | 106.03 |
| 24 | ESIA | 37 | MIA | C16-C14-C13 | -5.04 | 107.52 | 122.66 |
| 1 | 16SA | 1156 | 7MG | C2-N3-C4 | 5.02 | 120.95 | 112.30 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed($^o$) | Ideal($^o$) |
|---|---|---|---|---|---|---|---|
| 1 | 16SA | 2141 | MA6 | C5-C4-N3 | -5.00 | 119.83 | 126.72 |
| 27 | 23SB | 1964 | 5MU | C5-C6-N1 | -5.00 | 117.88 | 123.31 |
| 23 | PSIB | 54 | 5MU | C6-N1-C2 | -4.97 | 116.36 | 121.30 |
| 23 | PSIB | 37 | MIA | C15-C14-C13 | -4.93 | 107.85 | 122.66 |
| 57 | ASIB | 54 | 5MU | C6-C5-C4 | 4.93 | 122.08 | 118.02 |
| 22 | ASIA | 8 | 4SU | C5-C4-S4 | -4.92 | 118.69 | 124.31 |
| 26 | TRNA | 55 | PSU | C4-N3-C2 | -4.92 | 119.60 | 126.37 |
| 27 | 23SB | 2266 | OMG | N9-C8-N7 | 4.91 | 122.51 | 113.40 |
| 27 | 23SB | 1942 | PSU | N1-C2-N3 | 4.91 | 120.35 | 115.17 |
| 26 | TRNA | 54 | 5MU | C6-C5-C4 | 4.90 | 122.06 | 118.02 |
| 23 | PSIB | 37 | MIA | C16-C14-C13 | -4.90 | 107.97 | 122.66 |
| 27 | 23SB | 1942 | PSU | C4-N3-C2 | -4.88 | 119.64 | 126.37 |
| 26 | TRNA | 37 | MIA | C1'-N9-C8 | -4.88 | 116.27 | 127.09 |
| 27 | 23SB | 2620 | PSU | C4-N3-C2 | -4.87 | 119.66 | 126.37 |
| 27 | 23SA | 1936 | PSU | C4-N3-C2 | -4.87 | 119.67 | 126.37 |
| 27 | 23SA | 2620 | PSU | N1-C2-N3 | 4.83 | 120.26 | 115.17 |
| 23 | PSIB | 46 | 7MG | C5-C6-N1 | 4.80 | 119.40 | 110.94 |
| 1 | 16SB | 2141 | MA6 | C5-C4-N3 | -4.80 | 120.11 | 126.72 |
| 22 | ASIA | 54 | 5MU | C5-C6-N1 | -4.80 | 118.10 | 123.31 |
| 23 | PSIA | 39 | PSU | N1-C2-N3 | 4.80 | 120.23 | 115.17 |
| 27 | 23SA | 2518 | 2MA | N3-C4-N9 | 4.79 | 133.07 | 126.99 |
| 57 | ASIB | 32 | PSU | C4-N3-C2 | -4.79 | 119.78 | 126.37 |
| 1 | 16SA | 1145 | PSU | C4-N3-C2 | -4.78 | 119.79 | 126.37 |
| 27 | 23SB | 2266 | OMG | C5-C4-N9 | -4.78 | 97.10 | 105.66 |
| 27 | 23SB | 1936 | PSU | C4-N3-C2 | -4.75 | 119.83 | 126.37 |
| 23 | PSIA | 39 | PSU | C4-N3-C2 | -4.73 | 119.85 | 126.37 |
| 27 | 23SB | 2518 | 2MA | N9-C8-N7 | -4.72 | 107.24 | 113.94 |
| 57 | ASIB | 54 | 5MU | C5-C6-N1 | -4.71 | 118.19 | 123.31 |
| 27 | 23SB | 2620 | PSU | N1-C2-N3 | 4.71 | 120.13 | 115.17 |
| 26 | TRNA | 39 | PSU | C4-N3-C2 | -4.68 | 119.92 | 126.37 |
| 27 | 23SB | 2518 | 2MA | C4-N9-C1' | -4.68 | 115.70 | 126.63 |
| 27 | 23SA | 2620 | PSU | C4-N3-C2 | -4.67 | 119.94 | 126.37 |
| 57 | ASIB | 39 | PSU | C4-N3-C2 | -4.66 | 119.95 | 126.37 |
| 1 | 16SA | 2028 | 5MC | C5-C6-N1 | -4.66 | 118.25 | 123.31 |
| 1 | 16SB | 1145 | PSU | C4-N3-C2 | -4.66 | 119.96 | 126.37 |
| 1 | 16SA | 2142 | MA6 | C5-C4-N3 | -4.65 | 120.32 | 126.72 |
| 1 | 16SB | 2121 | UR3 | C4-N3-C2 | -4.64 | 120.84 | 124.58 |
| 27 | 23SA | 1940 | 5MU | C5-C6-N1 | -4.63 | 118.29 | 123.31 |
| 23 | PSIA | 46 | 7MG | C5-C6-N1 | 4.63 | 119.08 | 110.94 |
| 1 | 16SB | 1145 | PSU | N1-C2-N3 | 4.62 | 120.04 | 115.17 |
| 1 | 16SA | 1156 | 7MG | C5-C4-N3 | -4.62 | 119.47 | 128.13 |
| 23 | PSIA | 46 | 7MG | C5-C4-N3 | -4.61 | 119.47 | 128.13 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed($^o$) | Ideal($^o$) |
|---|---|---|---|---|---|---|---|
| 22 | ASIA | 54 | 5MU | C6-C5-C4 | 4.60 | 121.81 | 118.02 |
| 27 | 23SB | 1964 | 5MU | C6-N1-C2 | -4.60 | 116.72 | 121.30 |
| 27 | 23SA | 2266 | OMG | N9-C8-N7 | 4.59 | 121.92 | 113.40 |
| 23 | PSIB | 55 | PSU | C4-N3-C2 | -4.59 | 120.05 | 126.37 |
| 1 | 16SB | 2141 | MA6 | C5-C6-N6 | 4.59 | 132.59 | 125.33 |
| 57 | ASIB | 39 | PSU | N1-C2-N3 | 4.59 | 120.00 | 115.17 |
| 26 | TRNA | 39 | PSU | N1-C2-N3 | 4.58 | 120.00 | 115.17 |
| 26 | TRNA | 54 | 5MU | C5-C6-N1 | -4.57 | 118.34 | 123.31 |
| 27 | 23SA | 1936 | PSU | N1-C2-N3 | 4.57 | 119.99 | 115.17 |
| 23 | PSIA | 55 | PSU | N1-C2-N3 | 4.55 | 119.97 | 115.17 |
| 27 | 23SA | 1964 | 5MU | O4-C4-C5 | -4.55 | 119.71 | 124.92 |
| 26 | TRNA | 55 | PSU | N1-C2-N3 | 4.55 | 119.96 | 115.17 |
| 27 | 23SB | 2518 | 2MA | N3-C4-N9 | 4.52 | 132.73 | 126.99 |
| 1 | 16SB | 1834 | 2MG | N1-C2-N2 | 4.51 | 121.16 | 116.56 |
| 23 | PSIB | 32 | PSU | C4-N3-C2 | -4.51 | 120.16 | 126.37 |
| 23 | PSIB | 47 | 3AU | C6-N1-C2 | -4.51 | 118.12 | 121.80 |
| 26 | TRNA | 37 | MIA | C4-C5-C6 | 4.50 | 120.52 | 116.78 |
| 22 | ASIA | 46 | 7MG | C2-N3-C4 | 4.49 | 120.04 | 112.30 |
| 26 | TRNA | 32 | PSU | C4-N3-C2 | -4.48 | 120.20 | 126.37 |
| 23 | PSIA | 47 | 3AU | O2-C2-N3 | -4.44 | 116.00 | 121.98 |
| 1 | 16SB | 1156 | 7MG | C2-N3-C4 | 4.43 | 119.92 | 112.30 |
| 22 | ASIA | 32 | PSU | N1-C2-N3 | 4.42 | 119.83 | 115.17 |
| 1 | 16SA | 2142 | MA6 | N9-C8-N7 | -4.41 | 107.68 | 113.94 |
| 27 | 23SA | 1942 | PSU | N1-C2-N3 | 4.40 | 119.81 | 115.17 |
| 1 | 16SA | 1589 | M2G | C5-C4-N3 | -4.40 | 121.39 | 128.39 |
| 1 | 16SB | 1589 | M2G | C2-N3-C4 | 4.39 | 120.63 | 112.51 |
| 23 | PSIB | 39 | PSU | C4-N3-C2 | -4.39 | 120.33 | 126.37 |
| 1 | 16SB | 2142 | MA6 | N9-C8-N7 | -4.38 | 107.72 | 113.94 |
| 57 | ASIB | 37 | MIA | C15-C14-C13 | -4.36 | 109.56 | 122.66 |
| 22 | ASIA | 39 | PSU | C4-N3-C2 | -4.35 | 120.38 | 126.37 |
| 27 | 23SA | 2266 | OMG | O6-C6-C5 | -4.35 | 115.05 | 126.53 |
| 27 | 23SA | 2518 | 2MA | N9-C8-N7 | -4.34 | 107.77 | 113.94 |
| 24 | ESIB | 37 | MIA | C15-C14-C13 | -4.34 | 109.62 | 122.66 |
| 27 | 23SA | 2266 | OMG | C8-N9-C4 | -4.33 | 97.91 | 106.03 |
| 27 | 23SB | 2266 | OMG | O6-C6-C5 | -4.32 | 115.12 | 126.53 |
| 1 | 16SA | 2121 | UR3 | C6-N1-C2 | -4.32 | 118.27 | 121.80 |
| 23 | PSIA | 32 | PSU | C4-N3-C2 | -4.30 | 120.44 | 126.37 |
| 1 | 16SB | 2142 | MA6 | C5-C4-N3 | -4.30 | 120.80 | 126.72 |
| 1 | 16SA | 2141 | MA6 | N9-C8-N7 | -4.30 | 107.84 | 113.94 |
| 22 | ASIA | 46 | 7MG | C6-C5-N7 | -4.28 | 125.29 | 131.93 |
| 26 | TRNA | 37 | MIA | C4-N9-C1' | 4.27 | 136.62 | 126.63 |
| 1 | 16SA | 1589 | M2G | C2-N3-C4 | 4.24 | 120.35 | 112.51 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed($^o$) | Ideal($^o$) |
|---|---|---|---|---|---|---|---|
| 27 | 23SA | 1942 | PSU | C4-N3-C2 | -4.24 | 120.53 | 126.37 |
| 1 | 16SA | 1834 | 2MG | N1-C2-N2 | 4.22 | 120.87 | 116.56 |
| 22 | ASIA | 39 | PSU | N1-C2-N3 | 4.22 | 119.61 | 115.17 |
| 27 | 23SA | 2567 | OMU | C5-C4-N3 | 4.21 | 120.70 | 114.80 |
| 1 | 16SB | 2121 | UR3 | C6-N1-C2 | -4.16 | 118.40 | 121.80 |
| 23 | PSIA | 55 | PSU | C4-N3-C2 | -4.16 | 120.65 | 126.37 |
| 23 | PSIB | 46 | 7MG | C2-N3-C4 | 4.15 | 119.44 | 112.30 |
| 23 | PSIA | 37 | MIA | C15-C14-C13 | -4.15 | 110.22 | 122.66 |
| 27 | 23SB | 2266 | OMG | C1'-N9-C8 | -4.13 | 114.98 | 126.73 |
| 26 | TRNA | 32 | PSU | N1-C2-N3 | 4.13 | 119.53 | 115.17 |
| 26 | TRNA | 54 | 5MU | C5M-C5-C6 | -4.13 | 117.26 | 122.85 |
| 23 | PSIA | 8 | 4SU | C5-C4-S4 | -4.12 | 119.61 | 124.31 |
| 27 | 23SB | 2567 | OMU | C5-C4-N3 | 4.10 | 120.55 | 114.80 |
| 23 | PSIA | 46 | 7MG | C2-N3-C4 | 4.10 | 119.36 | 112.30 |
| 23 | PSIB | 37 | MIA | N3-C4-N9 | 4.10 | 132.19 | 126.99 |
| 1 | 16SA | 1156 | 7MG | C6-C5-N7 | -4.09 | 125.59 | 131.93 |
| 1 | 16SB | 1834 | 2MG | C2-N1-C6 | -4.08 | 119.61 | 124.55 |
| 22 | ASIA | 46 | 7MG | C5-C4-N3 | -4.08 | 120.46 | 128.13 |
| 27 | 23SA | 1940 | 5MU | C6-N1-C2 | -4.04 | 117.28 | 121.30 |
| 23 | PSIB | 37 | MIA | C6-C5-N7 | 4.03 | 136.83 | 132.43 |
| 27 | 23SA | 1967 | 5MC | C5-C6-N1 | -4.00 | 118.97 | 123.31 |
| 22 | ASIA | 32 | PSU | C4-N3-C2 | -4.00 | 120.86 | 126.37 |
| 1 | 16SB | 2028 | 5MC | C5-C6-N1 | -3.96 | 119.01 | 123.31 |
| 23 | PSIB | 55 | PSU | N1-C2-N3 | 3.96 | 119.35 | 115.17 |
| 22 | ASIA | 55 | PSU | N1-C2-N3 | 3.96 | 119.34 | 115.17 |
| 23 | PSIB | 39 | PSU | N1-C2-N3 | 3.94 | 119.33 | 115.17 |
| 23 | PSIA | 32 | PSU | N1-C2-N3 | 3.94 | 119.32 | 115.17 |
| 22 | ASIA | 55 | PSU | C4-N3-C2 | -3.93 | 120.95 | 126.37 |
| 57 | ASIB | 54 | 5MU | C5M-C5-C6 | -3.92 | 117.54 | 122.85 |
| 23 | PSIA | 37 | MIA | C5-N7-C8 | 3.92 | 109.61 | 103.45 |
| 1 | 16SB | 1156 | 7MG | C6-C5-N7 | -3.92 | 125.86 | 131.93 |
| 23 | PSIB | 8 | 4SU | N3-C2-N1 | 3.92 | 120.00 | 114.89 |
| 23 | PSIA | 47 | 3AU | C1'-N1-C2 | 3.91 | 123.44 | 117.04 |
| 27 | 23SB | 1936 | PSU | N1-C2-N3 | 3.89 | 119.27 | 115.17 |
| 23 | PSIB | 46 | 7MG | C6-C5-N7 | -3.89 | 125.90 | 131.93 |
| 27 | 23SB | 2518 | 2MA | C1'-N9-C8 | 3.89 | 135.73 | 127.09 |
| 1 | 16SB | 2141 | MA6 | N9-C8-N7 | -3.89 | 108.42 | 113.94 |
| 27 | 23SB | 1940 | 5MU | C6-N1-C2 | -3.88 | 117.44 | 121.30 |
| 27 | 23SB | 1940 | 5MU | C5M-C5-C6 | -3.88 | 117.60 | 122.85 |
| 22 | ASIA | 54 | 5MU | C5M-C5-C6 | -3.88 | 117.60 | 122.85 |
| 27 | 23SB | 2567 | OMU | N3-C2-N1 | 3.86 | 119.92 | 114.89 |
| 1 | 16SA | 1834 | 2MG | C2-N1-C6 | -3.85 | 119.89 | 124.55 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed($^o$) | Ideal($^o$) |
|---|---|---|---|---|---|---|---|
| 23 | PSIB | 47 | 3AU | C4-N3-C2 | -3.85 | 120.14 | 124.66 |
| 26 | TRNA | 8 | 4SU | C5-C4-S4 | -3.80 | 119.96 | 124.31 |
| 23 | PSIA | 37 | MIA | C2-N3-C4 | 3.78 | 122.20 | 112.29 |
| 23 | PSIA | 37 | MIA | C16-C14-C13 | -3.75 | 111.40 | 122.66 |
| 27 | 23SA | 1936 | PSU | O2-C2-N1 | -3.74 | 118.93 | 122.79 |
| 12 | S12B | 89 | 0TD | OD2-CG-CB | 3.73 | 121.20 | 113.15 |
| 24 | ESIA | 37 | MIA | C15-C14-C13 | -3.72 | 111.49 | 122.66 |
| 23 | PSIB | 46 | 7MG | C5-C4-N3 | -3.72 | 121.15 | 128.13 |
| 22 | ASIA | 37 | MIA | C15-C14-C13 | -3.72 | 111.50 | 122.66 |
| 23 | PSIB | 54 | 5MU | C5M-C5-C6 | -3.70 | 117.85 | 122.85 |
| 22 | ASIA | 37 | MIA | C5-N7-C8 | 3.68 | 109.23 | 103.45 |
| 23 | PSIB | 32 | PSU | C6-N1-C2 | -3.68 | 119.28 | 122.69 |
| 26 | TRNA | 54 | 5MU | C6-N1-C2 | -3.66 | 117.66 | 121.30 |
| 1 | 16SB | 1156 | 7MG | C5-C4-N3 | -3.65 | 121.28 | 128.13 |
| 22 | ASIA | 37 | MIA | C2-N3-C4 | 3.64 | 121.82 | 112.29 |
| 27 | 23SB | 1964 | 5MU | C5M-C5-C6 | -3.64 | 117.93 | 122.85 |
| 23 | PSIB | 37 | MIA | C4-C5-N7 | -3.63 | 106.43 | 110.58 |
| 27 | 23SB | 2266 | OMG | N2-C2-N1 | 3.63 | 124.42 | 116.76 |
| 22 | ASIA | 37 | MIA | N3-C2-N1 | -3.63 | 120.37 | 127.00 |
| 26 | TRNA | 8 | 4SU | N3-C2-N1 | 3.63 | 119.61 | 114.89 |
| 24 | ESIA | 37 | MIA | C5-N7-C8 | 3.62 | 109.14 | 103.45 |
| 24 | ESIB | 37 | MIA | C5-N7-C8 | 3.62 | 109.14 | 103.45 |
| 22 | ASIA | 8 | 4SU | N3-C2-N1 | 3.62 | 119.60 | 114.89 |
| 23 | PSIB | 37 | MIA | C5-N7-C8 | 3.61 | 109.12 | 103.45 |
| 1 | 16SA | 2141 | MA6 | C2-N3-C4 | 3.61 | 120.64 | 111.83 |
| 1 | 16SA | 1145 | PSU | C6-N1-C2 | -3.60 | 119.35 | 122.69 |
| 57 | ASIB | 54 | 5MU | C6-N1-C2 | -3.59 | 117.72 | 121.30 |
| 57 | ASIB | 37 | MIA | C5-N7-C8 | 3.58 | 109.07 | 103.45 |
| 1 | 16SA | 2121 | UR3 | C5-C4-N3 | 3.57 | 119.74 | 115.04 |
| 23 | PSIA | 47 | 3AU | C4-N3-C2 | -3.57 | 120.47 | 124.66 |
| 57 | ASIB | 37 | MIA | C16-C14-C13 | -3.54 | 112.03 | 122.66 |
| 26 | TRNA | 37 | MIA | C5-N7-C8 | 3.52 | 108.98 | 103.45 |
| 27 | 23SB | 2518 | 2MA | N3-C2-N1 | -3.51 | 119.57 | 125.77 |
| 1 | 16SB | 2121 | UR3 | C5-C4-N3 | 3.51 | 119.67 | 115.04 |
| 23 | PSIB | 54 | 5MU | C6-C5-C4 | 3.51 | 120.91 | 118.02 |
| 24 | ESIB | 37 | MIA | C2-N3-C4 | 3.48 | 121.41 | 112.29 |
| 23 | PSIA | 8 | 4SU | N3-C2-N1 | 3.48 | 119.42 | 114.89 |
| 23 | PSIA | 47 | 3AU | C6-N1-C2 | -3.47 | 118.96 | 121.80 |
| 1 | 16SA | 1834 | 2MG | N9-C4-N3 | 3.47 | 132.89 | 125.95 |
| 1 | 16SB | 2142 | MA6 | C2-N3-C4 | 3.47 | 120.31 | 111.83 |
| 1 | 16SB | 2142 | MA6 | C2-N1-C6 | 3.46 | 120.29 | 111.83 |
| 1 | 16SA | 2141 | MA6 | C4-C5-C6 | 3.46 | 119.49 | 115.91 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed($^o$) | Ideal($^o$) |
|---|---|---|---|---|---|---|---|
| 27 | 23SA | 2518 | 2MA | C4-N9-C1' | -3.46 | 118.54 | 126.63 |
| 1 | 16SB | 2141 | MA6 | C2-N3-C4 | 3.46 | 120.28 | 111.83 |
| 1 | 16SA | 2141 | MA6 | C2-N1-C6 | 3.46 | 120.27 | 111.83 |
| 1 | 16SB | 1589 | M2G | N9-C4-N3 | 3.45 | 132.86 | 125.95 |
| 26 | TRNA | 37 | MIA | C5-C6-N6 | -3.45 | 115.37 | 122.03 |
| 27 | 23SA | 1942 | PSU | O2-C2-N1 | -3.45 | 119.23 | 122.79 |
| 23 | PSIA | 39 | PSU | O2-C2-N1 | -3.45 | 119.23 | 122.79 |
| 23 | PSIA | 55 | PSU | C6-N1-C2 | -3.45 | 119.49 | 122.69 |
| 1 | 16SA | 2142 | MA6 | C2-N3-C4 | 3.44 | 120.23 | 111.83 |
| 23 | PSIA | 54 | 5MU | C5M-C5-C6 | -3.42 | 118.23 | 122.85 |
| 27 | 23SB | 1964 | 5MU | N3-C2-N1 | 3.41 | 119.33 | 114.89 |
| 23 | PSIA | 37 | MIA | N3-C2-N1 | -3.40 | 120.80 | 127.00 |
| 1 | 16SA | 2142 | MA6 | C2-N1-C6 | 3.37 | 120.07 | 111.83 |
| 26 | TRNA | 37 | MIA | C16-C14-C13 | -3.37 | 112.54 | 122.66 |
| 1 | 16SB | 2141 | MA6 | C2-N1-C6 | 3.37 | 120.06 | 111.83 |
| 26 | TRNA | 37 | MIA | C2-N3-C4 | 3.37 | 121.11 | 112.29 |
| 27 | 23SB | 1940 | 5MU | N3-C2-N1 | 3.36 | 119.27 | 114.89 |
| 23 | PSIA | 55 | PSU | O2-C2-N1 | -3.35 | 119.34 | 122.79 |
| 23 | PSIB | 46 | 7MG | N9-C8-N7 | -3.34 | 98.64 | 103.37 |
| 1 | 16SB | 2141 | MA6 | C4-C5-C6 | 3.34 | 119.36 | 115.91 |
| 27 | 23SA | 2266 | OMG | C1'-N9-C8 | -3.34 | 117.25 | 126.73 |
| 1 | 16SA | 1589 | M2G | N9-C8-N7 | -3.31 | 107.27 | 113.40 |
| 1 | 16SB | 1834 | 2MG | N9-C4-N3 | 3.29 | 132.53 | 125.95 |
| 26 | TRNA | 39 | PSU | O2-C2-N1 | -3.28 | 119.40 | 122.79 |
| 23 | PSIB | 8 | 4SU | O2-C2-N1 | -3.28 | 118.53 | 122.80 |
| 27 | 23SB | 2518 | 2MA | C5-N7-C8 | 3.27 | 108.60 | 103.45 |
| 27 | 23SA | 2567 | OMU | N3-C2-N1 | 3.27 | 119.15 | 114.89 |
| 22 | ASIA | 54 | 5MU | C6-N1-C2 | -3.27 | 118.05 | 121.30 |
| 1 | 16SA | 1590 | 5MC | C5-C6-N1 | -3.25 | 119.78 | 123.31 |
| 12 | S12A | 89 | 0TD | OD2-CG-CB | 3.23 | 120.12 | 113.15 |
| 27 | 23SA | 1940 | 5MU | C5M-C5-C6 | -3.21 | 118.51 | 122.85 |
| 27 | 23SA | 2266 | OMG | N2-C2-N1 | 3.21 | 123.54 | 116.76 |
| 22 | ASIA | 46 | 7MG | O6-C6-C5 | -3.20 | 119.78 | 127.62 |
| 27 | 23SA | 2518 | 2MA | N3-C2-N1 | -3.20 | 120.13 | 125.77 |
| 22 | ASIA | 39 | PSU | O2-C2-N1 | -3.17 | 119.52 | 122.79 |
| 27 | 23SA | 2518 | 2MA | C5-N7-C8 | 3.16 | 108.42 | 103.45 |
| 1 | 16SA | 2142 | MA6 | C4-C5-C6 | 3.16 | 119.17 | 115.91 |
| 27 | 23SB | 1942 | PSU | O2-C2-N1 | -3.16 | 119.53 | 122.79 |
| 22 | ASIA | 46 | 7MG | N9-C8-N7 | -3.14 | 98.92 | 103.37 |
| 1 | 16SB | 1156 | 7MG | O6-C6-C5 | -3.14 | 119.92 | 127.62 |
| 24 | ESIA | 37 | MIA | C2-N3-C4 | 3.12 | 120.46 | 112.29 |
| 1 | 16SA | 1834 | 2MG | N9-C8-N7 | -3.12 | 107.62 | 113.40 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed($^o$) | Ideal($^o$) |
|---|---|---|---|---|---|---|---|
| 26 | TRNA | 32 | PSU | O2-C2-N1 | -3.08 | 119.61 | 122.79 |
| 22 | ASIA | 32 | PSU | C6-N1-C2 | -3.08 | 119.83 | 122.69 |
| 23 | PSIB | 37 | MIA | C2-N3-C4 | 3.08 | 120.35 | 112.29 |
| 27 | 23SA | 1945 | OMC | O2-C2-N3 | -3.07 | 117.49 | 122.33 |
| 1 | 16SB | 2141 | MA6 | N3-C4-N9 | 3.07 | 132.39 | 127.17 |
| 57 | ASIB | 37 | MIA | C1'-N9-C8 | -3.05 | 120.33 | 127.09 |
| 57 | ASIB | 37 | MIA | C2-N3-C4 | 3.04 | 120.26 | 112.29 |
| 57 | ASIB | 37 | MIA | C4-C5-N7 | -3.04 | 107.11 | 110.58 |
| 22 | ASIA | 37 | MIA | N9-C8-N7 | -3.03 | 109.63 | 113.94 |
| 24 | ESIB | 37 | MIA | C4-C5-N7 | -3.03 | 107.12 | 110.58 |
| 22 | ASIA | 37 | MIA | C6-C5-N7 | 3.02 | 135.72 | 132.43 |
| 24 | ESIA | 37 | MIA | N3-C2-N1 | -3.02 | 121.49 | 127.00 |
| 24 | ESIB | 37 | MIA | C16-C14-C15 | -3.02 | 107.64 | 114.59 |
| 22 | ASIA | 55 | PSU | O2-C2-N1 | -3.02 | 119.68 | 122.79 |
| 27 | 23SA | 1964 | 5MU | O2-C2-N1 | -3.02 | 118.87 | 122.80 |
| 23 | PSIA | 46 | 7MG | C2-N1-C6 | -3.01 | 119.65 | 125.11 |
| 23 | PSIA | 37 | MIA | C4-C5-N7 | -3.01 | 107.14 | 110.58 |
| 23 | PSIB | 54 | 5MU | C1'-N1-C2 | 3.01 | 123.00 | 117.59 |
| 24 | ESIB | 37 | MIA | N3-C2-N1 | -3.01 | 121.51 | 127.00 |
| 1 | 16SB | 2032 | 5MC | C5-C6-N1 | -2.99 | 120.06 | 123.31 |
| 1 | 16SA | 1145 | PSU | C6-C5-C4 | 2.98 | 120.19 | 118.17 |
| 1 | 16SA | 2035 | 5MC | C5-C6-N1 | -2.98 | 120.08 | 123.31 |
| 1 | 16SA | 2141 | MA6 | C5-N7-C8 | 2.97 | 108.12 | 103.45 |
| 1 | 16SB | 2030 | 4OC | O2-C2-N3 | -2.95 | 117.67 | 122.33 |
| 1 | 16SB | 2035 | 5MC | C5-C6-N1 | -2.94 | 120.12 | 123.31 |
| 24 | ESIA | 37 | MIA | N9-C8-N7 | -2.94 | 109.77 | 113.94 |
| 23 | PSIA | 46 | 7MG | N9-C8-N7 | -2.94 | 99.22 | 103.37 |
| 1 | 16SA | 2142 | MA6 | N3-C4-N9 | 2.93 | 132.16 | 127.17 |
| 26 | TRNA | 55 | PSU | O2-C2-N1 | -2.93 | 119.77 | 122.79 |
| 27 | 23SA | 2266 | OMG | C2-N1-C6 | 2.92 | 130.41 | 125.11 |
| 24 | ESIA | 37 | MIA | C4-C5-N7 | -2.92 | 107.25 | 110.58 |
| 23 | PSIB | 39 | PSU | O2-C2-N1 | -2.92 | 119.78 | 122.79 |
| 1 | 16SB | 2030 | 4OC | C2'-C1'-N1 | -2.89 | 108.75 | 114.24 |
| 23 | PSIB | 46 | 7MG | C2-N1-C6 | -2.88 | 119.88 | 125.11 |
| 57 | ASIB | 32 | PSU | C6-N1-C2 | -2.88 | 120.02 | 122.69 |
| 1 | 16SA | 1156 | 7MG | C2-N1-C6 | -2.88 | 119.89 | 125.11 |
| 1 | 16SA | 1156 | 7MG | N9-C8-N7 | -2.88 | 99.30 | 103.37 |
| 27 | 23SA | 2567 | OMU | O4-C4-C5 | -2.87 | 120.20 | 125.16 |
| 1 | 16SB | 1589 | M2G | C5-C6-N1 | 2.86 | 120.54 | 113.25 |
| 1 | 16SA | 1834 | 2MG | C1'-N9-C4 | -2.86 | 118.03 | 126.49 |
| 27 | 23SA | 1964 | 5MU | N3-C2-N1 | 2.86 | 118.61 | 114.89 |
| 57 | ASIB | 32 | PSU | O2-C2-N1 | -2.84 | 119.86 | 122.79 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed($^o$) | Ideal($^o$) |
|---|---|---|---|---|---|---|---|
| 27 | 23SB | 2266 | OMG | O6-C6-N1 | -2.84 | 114.77 | 120.11 |
| 22 | ASIA | 46 | 7MG | C2-N1-C6 | -2.82 | 119.99 | 125.11 |
| 27 | 23SA | 1964 | 5MU | C6-N1-C2 | -2.81 | 118.51 | 121.30 |
| 23 | PSIB | 55 | PSU | O2-C2-N1 | -2.81 | 119.89 | 122.79 |
| 1 | 16SB | 1156 | 7MG | N9-C8-N7 | -2.79 | 99.42 | 103.37 |
| 1 | 16SA | 2142 | MA6 | C4-N9-C8 | 2.79 | 108.66 | 105.74 |
| 24 | ESIA | 37 | MIA | C6-C5-N7 | 2.78 | 135.46 | 132.43 |
| 1 | 16SA | 2141 | MA6 | N3-C4-N9 | 2.78 | 131.89 | 127.17 |
| 23 | PSIB | 46 | 7MG | O6-C6-C5 | -2.78 | 120.80 | 127.62 |
| 23 | PSIA | 37 | MIA | N9-C8-N7 | -2.78 | 109.99 | 113.94 |
| 27 | 23SA | 1940 | 5MU | N3-C2-N1 | 2.77 | 118.50 | 114.89 |
| 27 | 23SB | 2266 | OMG | N1-C2-N3 | -2.77 | 118.25 | 123.32 |
| 1 | 16SB | 1156 | 7MG | C2-N1-C6 | -2.76 | 120.10 | 125.11 |
| 27 | 23SB | 2518 | 2MA | CM2-C2-N1 | 2.76 | 121.26 | 117.13 |
| 1 | 16SA | 1156 | 7MG | O6-C6-C5 | -2.76 | 120.85 | 127.62 |
| 1 | 16SA | 2142 | MA6 | C5-N7-C8 | 2.75 | 107.77 | 103.45 |
| 22 | ASIA | 55 | PSU | C6-N1-C2 | -2.74 | 120.14 | 122.69 |
| 27 | 23SA | 2266 | OMG | O6-C6-N1 | -2.74 | 114.97 | 120.11 |
| 27 | 23SA | 2518 | 2MA | C1'-N9-C8 | 2.73 | 133.16 | 127.09 |
| 23 | PSIA | 47 | 3AU | C5-C4-N3 | 2.73 | 119.42 | 115.64 |
| 23 | PSIB | 47 | 3AU | C1'-N1-C6 | -2.73 | 114.94 | 120.78 |
| 27 | 23SB | 1936 | PSU | O2-C2-N1 | -2.73 | 119.97 | 122.79 |
| 27 | 23SA | 2620 | PSU | C6-N1-C2 | -2.73 | 120.16 | 122.69 |
| 27 | 23SA | 1967 | 5MC | CM5-C5-C6 | -2.72 | 119.16 | 122.85 |
| 23 | PSIB | 54 | 5MU | C5-C6-N1 | -2.72 | 120.36 | 123.31 |
| 27 | 23SA | 1942 | PSU | C6-N1-C2 | -2.72 | 120.17 | 122.69 |
| 22 | ASIA | 37 | MIA | C4-C5-N7 | -2.72 | 107.47 | 110.58 |
| 1 | 16SB | 2142 | MA6 | C4-N9-C8 | 2.72 | 108.59 | 105.74 |
| 1 | 16SB | 1589 | M2G | N9-C8-N7 | -2.71 | 108.37 | 113.40 |
| 27 | 23SA | 1940 | 5MU | C1'-N1-C2 | 2.71 | 122.47 | 117.59 |
| 1 | 16SB | 2028 | 5MC | CM5-C5-C6 | -2.71 | 119.18 | 122.85 |
| 27 | 23SB | 2518 | 2MA | C4-N9-C8 | 2.70 | 108.58 | 105.74 |
| 22 | ASIA | 54 | 5MU | O2-C2-N1 | -2.70 | 119.28 | 122.80 |
| 1 | 16SA | 1834 | 2MG | C5-C6-N1 | 2.70 | 120.12 | 113.25 |
| 1 | 16SA | 1589 | M2G | C5-C6-N1 | 2.68 | 120.08 | 113.25 |
| 1 | 16SA | 1834 | 2MG | N1-C2-N3 | -2.67 | 119.18 | 123.68 |
| 1 | 16SB | 2142 | MA6 | C5-N7-C8 | 2.66 | 107.63 | 103.45 |
| 27 | 23SB | 1964 | 5MU | O2-C2-N1 | -2.64 | 119.36 | 122.80 |
| 23 | PSIA | 39 | PSU | C6-N1-C2 | -2.64 | 120.24 | 122.69 |
| 27 | 23SB | 1967 | 5MC | C5-C6-N1 | -2.64 | 120.45 | 123.31 |
| 27 | 23SB | 2567 | OMU | O4-C4-C5 | -2.64 | 120.61 | 125.16 |
| 27 | 23SA | 1964 | 5MU | C5M-C5-C4 | 2.63 | 121.59 | 118.78 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed($^o$) | Ideal($^o$) |
|---|---|---|---|---|---|---|---|
| 24 | ESIB | 37 | MIA | C6-C5-N7 | 2.62 | 135.28 | 132.43 |
| 1 | 16SA | 1834 | 2MG | O6-C6-C5 | -2.61 | 119.64 | 126.53 |
| 27 | 23SA | 2266 | OMG | N1-C2-N3 | -2.60 | 118.56 | 123.32 |
| 1 | 16SB | 1834 | 2MG | N9-C8-N7 | -2.60 | 108.58 | 113.40 |
| 1 | 16SA | 2032 | 5MC | C5-C6-N1 | -2.60 | 120.49 | 123.31 |
| 23 | PSIA | 46 | 7MG | O6-C6-C5 | -2.59 | 121.27 | 127.62 |
| 1 | 16SB | 1589 | M2G | O6-C6-C5 | -2.58 | 119.72 | 126.53 |
| 1 | 16SA | 2035 | 5MC | CM5-C5-C6 | -2.58 | 119.36 | 122.85 |
| 23 | PSIA | 37 | MIA | C6-C5-N7 | 2.57 | 135.23 | 132.43 |
| 27 | 23SB | 1967 | 5MC | CM5-C5-C6 | -2.57 | 119.38 | 122.85 |
| 22 | ASIA | 37 | MIA | C1'-N9-C8 | -2.56 | 121.41 | 127.09 |
| 57 | ASIB | 32 | PSU | C6-C5-C4 | 2.56 | 119.90 | 118.17 |
| 23 | PSIB | 47 | 3AU | C5-C4-N3 | 2.56 | 119.17 | 115.64 |
| 23 | PSIB | 37 | MIA | N9-C8-N7 | -2.55 | 110.32 | 113.94 |
| 1 | 16SB | 1834 | 2MG | O6-C6-C5 | -2.55 | 119.81 | 126.53 |
| 23 | PSIA | 32 | PSU | O2-C2-N1 | -2.55 | 120.16 | 122.79 |
| 24 | ESIB | 37 | MIA | N9-C8-N7 | -2.55 | 110.32 | 113.94 |
| 27 | 23SB | 1942 | PSU | C6-C5-C4 | 2.54 | 119.89 | 118.17 |
| 57 | ASIB | 39 | PSU | O2-C2-N1 | -2.53 | 120.18 | 122.79 |
| 22 | ASIA | 37 | MIA | C16-C14-C15 | -2.53 | 108.77 | 114.59 |
| 23 | PSIB | 8 | 4SU | S4-C4-N3 | 2.52 | 122.84 | 120.20 |
| 1 | 16SA | 2028 | 5MC | CM5-C5-C6 | -2.52 | 119.44 | 122.85 |
| 1 | 16SB | 2141 | MA6 | C5-N7-C8 | 2.52 | 107.41 | 103.45 |
| 1 | 16SA | 1145 | PSU | O2-C2-N1 | -2.50 | 120.21 | 122.79 |
| 1 | 16SA | 2141 | MA6 | C4-C5-N7 | -2.50 | 107.73 | 110.58 |
| 1 | 16SB | 2142 | MA6 | C4-C5-C6 | 2.49 | 118.48 | 115.91 |
| 57 | ASIB | 37 | MIA | C16-C14-C15 | -2.49 | 108.86 | 114.59 |
| 1 | 16SB | 2142 | MA6 | N3-C4-N9 | 2.48 | 131.38 | 127.17 |
| 23 | PSIB | 32 | PSU | O2-C2-N1 | -2.46 | 120.25 | 122.79 |
| 57 | ASIB | 37 | MIA | C4-N9-C1' | 2.45 | 132.37 | 126.63 |
| 1 | 16SB | 1834 | 2MG | C1'-N9-C4 | -2.45 | 119.24 | 126.49 |
| 27 | 23SB | 2266 | OMG | C2-N1-C6 | 2.45 | 129.56 | 125.11 |
| 27 | 23SB | 2266 | OMG | C2-N3-C4 | 2.44 | 116.50 | 112.30 |
| 23 | PSIB | 37 | MIA | N3-C2-N1 | -2.44 | 122.55 | 127.00 |
| 1 | 16SB | 2028 | 5MC | C1'-N1-C6 | -2.43 | 117.14 | 121.15 |
| 27 | 23SA | 2518 | 2MA | C4-N9-C8 | 2.42 | 108.28 | 105.74 |
| 27 | 23SB | 1945 | OMC | O2-C2-N3 | -2.41 | 118.52 | 122.33 |
| 1 | 16SA | 1834 | 2MG | C1'-N9-C8 | 2.41 | 133.58 | 126.73 |
| 26 | TRNA | 37 | MIA | C16-C14-C15 | -2.41 | 109.04 | 114.59 |
| 1 | 16SA | 1834 | 2MG | C8-N7-C5 | 2.40 | 108.54 | 104.26 |
| 27 | 23SA | 1987 | 5MC | C5-C6-N1 | -2.40 | 120.71 | 123.31 |
| 27 | 23SB | 1940 | 5MU | O3'-C3'-C2' | 2.38 | 119.46 | 111.82 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed($^o$) | Ideal($^o$) |
|---|---|---|---|---|---|---|---|
| 26 | TRNA | 37 | MIA | N3-C2-N1 | -2.38 | 122.65 | 127.00 |
| 57 | ASIB | 37 | MIA | C4-C5-C6 | 2.38 | 118.75 | 116.78 |
| 57 | ASIB | 39 | PSU | C6-N1-C2 | -2.38 | 120.49 | 122.69 |
| 1 | 16SB | 1834 | 2MG | C5-C6-N1 | 2.38 | 119.30 | 113.25 |
| 27 | 23SA | 1940 | 5MU | O2-C2-N1 | -2.36 | 119.72 | 122.80 |
| 1 | 16SB | 2032 | 5MC | CM5-C5-C6 | -2.35 | 119.67 | 122.85 |
| 27 | 23SA | 2518 | 2MA | C6-C5-C4 | 2.35 | 120.39 | 117.18 |
| 57 | ASIB | 37 | MIA | N3-C2-N1 | -2.35 | 122.71 | 127.00 |
| 27 | 23SA | 2620 | PSU | O2-C2-N1 | -2.35 | 120.37 | 122.79 |
| 22 | ASIA | 39 | PSU | C6-N1-C2 | -2.34 | 120.52 | 122.69 |
| 22 | ASIA | 54 | 5MU | N3-C2-N1 | 2.34 | 117.94 | 114.89 |
| 1 | 16SB | 2035 | 5MC | CM5-C5-C6 | -2.34 | 119.69 | 122.85 |
| 23 | PSIA | 54 | 5MU | C6-N1-C2 | -2.34 | 118.97 | 121.30 |
| 27 | 23SB | 1987 | 5MC | C5-C4-N3 | -2.32 | 119.38 | 121.75 |
| 27 | 23SB | 2518 | 2MA | N6-C6-N1 | 2.32 | 120.16 | 117.03 |
| 26 | TRNA | 54 | 5MU | N3-C2-N1 | 2.32 | 117.91 | 114.89 |
| 27 | 23SB | 2518 | 2MA | C4-C5-N7 | -2.32 | 107.93 | 110.58 |
| 23 | PSIB | 39 | PSU | C6-N1-C2 | -2.31 | 120.54 | 122.69 |
| 1 | 16SB | 1834 | 2MG | C1'-N9-C8 | 2.31 | 133.31 | 126.73 |
| 27 | 23SB | 2620 | PSU | C6-N1-C2 | -2.31 | 120.55 | 122.69 |
| 57 | ASIB | 37 | MIA | N9-C8-N7 | -2.30 | 110.67 | 113.94 |
| 23 | PSIB | 54 | 5MU | C5M-C5-C4 | 2.30 | 121.24 | 118.78 |
| 1 | 16SB | 2141 | MA6 | C4-N9-C8 | 2.30 | 108.15 | 105.74 |
| 24 | ESIA | 37 | MIA | C2-N1-C6 | 2.30 | 121.90 | 117.54 |
| 12 | S12B | 89 | 0TD | OD1-CG-CB | -2.29 | 117.64 | 122.44 |
| 26 | TRNA | 37 | MIA | C4-C5-N7 | -2.29 | 107.96 | 110.58 |
| 57 | ASIB | 54 | 5MU | N3-C2-N1 | 2.29 | 117.88 | 114.89 |
| 27 | 23SA | 2518 | 2MA | C4-C5-N7 | -2.28 | 107.98 | 110.58 |
| 22 | ASIA | 37 | MIA | C4-N9-C8 | 2.28 | 108.13 | 105.74 |
| 1 | 16SA | 1145 | PSU | O4'-C1'-C2' | 2.27 | 108.29 | 105.15 |
| 26 | TRNA | 8 | 4SU | C1'-N1-C2 | 2.27 | 121.67 | 117.59 |
| 22 | ASIA | 37 | MIA | C2-N1-C6 | 2.27 | 121.85 | 117.54 |
| 27 | 23SB | 1967 | 5MC | C5-C4-N3 | -2.27 | 119.43 | 121.75 |
| 23 | PSIB | 32 | PSU | C6-C5-C4 | 2.27 | 119.70 | 118.17 |
| 23 | PSIB | 47 | 3AU | C10-N3-C4 | 2.26 | 121.47 | 117.10 |
| 1 | 16SA | 2141 | MA6 | C5-C4-N9 | 2.26 | 108.27 | 105.81 |
| 22 | ASIA | 8 | 4SU | C1'-N1-C2 | 2.25 | 121.64 | 117.59 |
| 27 | 23SA | 1936 | PSU | C6-N1-C2 | -2.25 | 120.60 | 122.69 |
| 26 | TRNA | 32 | PSU | C6-N1-C2 | -2.24 | 120.61 | 122.69 |
| 22 | ASIA | 32 | PSU | O2-C2-N1 | -2.23 | 120.49 | 122.79 |
| 23 | PSIB | 37 | MIA | C16-C14-C15 | -2.22 | 109.48 | 114.59 |
| 1 | 16SB | 1590 | 5MC | CM5-C5-C6 | -2.21 | 119.86 | 122.85 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed($^o$) | Ideal($^o$) |
|---|---|---|---|---|---|---|---|
| 27 | 23SA | 2266 | OMG | C2'-C1'-N9 | -2.19 | 110.08 | 114.24 |
| 1 | 16SA | 2141 | MA6 | C4-N9-C8 | 2.19 | 108.03 | 105.74 |
| 27 | 23SA | 1964 | 5MU | O4-C4-N3 | -2.18 | 116.01 | 120.11 |
| 1 | 16SA | 1589 | M2G | O6-C6-C5 | -2.18 | 120.78 | 126.53 |
| 26 | TRNA | 39 | PSU | C6-N1-C2 | -2.17 | 120.67 | 122.69 |
| 27 | 23SB | 1942 | PSU | C6-N1-C2 | -2.17 | 120.68 | 122.69 |
| 1 | 16SA | 2030 | 4OC | C6-C5-C4 | 2.17 | 119.61 | 117.00 |
| 23 | PSIA | 32 | PSU | C6-N1-C2 | -2.16 | 120.69 | 122.69 |
| 1 | 16SA | 1156 | 7MG | N1-C2-N3 | -2.16 | 119.37 | 123.32 |
| 1 | 16SB | 1145 | PSU | O4'-C1'-C2' | 2.15 | 108.12 | 105.15 |
| 1 | 16SA | 1589 | M2G | C4-C5-N7 | -2.13 | 107.29 | 110.67 |
| 1 | 16SA | 2030 | 4OC | C5-C4-N3 | -2.13 | 119.27 | 122.60 |
| 1 | 16SB | 1834 | 2MG | C8-N7-C5 | 2.12 | 108.04 | 104.26 |
| 27 | 23SB | 1987 | 5MC | C5-C6-N1 | -2.12 | 121.01 | 123.31 |
| 57 | ASIB | 39 | PSU | C6-C5-C4 | 2.12 | 119.60 | 118.17 |
| 1 | 16SA | 1589 | M2G | C8-N7-C5 | 2.11 | 108.02 | 104.26 |
| 26 | TRNA | 37 | MIA | N9-C8-N7 | -2.11 | 110.95 | 113.94 |
| 27 | 23SA | 2518 | 2MA | N6-C6-N1 | 2.10 | 119.86 | 117.03 |
| 23 | PSIB | 54 | 5MU | N3-C2-N1 | 2.10 | 117.62 | 114.89 |
| 1 | 16SB | 2028 | 5MC | O2-C2-N3 | -2.10 | 119.03 | 122.33 |
| 27 | 23SB | 2518 | 2MA | C6-C5-C4 | 2.09 | 120.03 | 117.18 |
| 26 | TRNA | 55 | PSU | C6-N1-C2 | -2.09 | 120.76 | 122.69 |
| 1 | 16SA | 2030 | 4OC | O2-C2-N3 | -2.08 | 119.04 | 122.33 |
| 1 | 16SB | 1156 | 7MG | N1-C2-N3 | -2.05 | 119.56 | 123.32 |
| 1 | 16SB | 2142 | MA6 | C4-C5-N7 | -2.05 | 108.23 | 110.58 |
| 1 | 16SB | 1145 | PSU | C6-N1-C2 | -2.05 | 120.79 | 122.69 |
| 1 | 16SB | 1590 | 5MC | C1'-N1-C6 | -2.04 | 117.80 | 121.15 |
| 1 | 16SB | 1834 | 2MG | N1-C2-N3 | -2.03 | 120.26 | 123.68 |
| 24 | ESIA | 37 | MIA | C4-N9-C8 | 2.02 | 107.86 | 105.74 |
| 23 | PSIA | 37 | MIA | C2-N1-C6 | 2.02 | 121.38 | 117.54 |
| 1 | 16SA | 2032 | 5MC | C5-C4-N4 | -2.02 | 118.55 | 121.39 |
| 23 | PSIA | 46 | 7MG | O4'-C1'-N9 | -2.02 | 106.55 | 109.30 |
| 23 | PSIA | 37 | MIA | C16-C14-C15 | -2.01 | 109.97 | 114.59 |

There are no chirality outliers.

All (106) torsion outliers are listed below:

| Mol | Chain | Res | Type | Atoms |
|---|---|---|---|---|
| 12 | S12A | 89 | 0TD | SB-CB-CG-OD2 |
| 12 | S12A | 89 | 0TD | SB-CB-CG-OD1 |
| 12 | S12B | 89 | 0TD | CA-CB-SB-CSB |
| 1 | 16SA | 1156 | 7MG | O4'-C4'-C5'-O5' |

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| Mol | Chain | Res | Type | Atoms |
|---|---|---|---|---|
| 1 | 16SB | 1834 | 2MG | O4'-C4'-C5'-O5' |
| 1 | 16SB | 1834 | 2MG | C3'-C4'-C5'-O5' |
| 1 | 16SA | 2142 | MA6 | O4'-C4'-C5'-O5' |
| 1 | 16SB | 2142 | MA6 | O4'-C4'-C5'-O5' |
| 22 | ASIA | 37 | MIA | O4'-C4'-C5'-O5' |
| 22 | ASIA | 37 | MIA | C12-C13-C14-C15 |
| 22 | ASIA | 37 | MIA | C12-C13-C14-C16 |
| 23 | PSIA | 37 | MIA | C3'-C4'-C5'-O5' |
| 23 | PSIA | 37 | MIA | C12-C13-C14-C15 |
| 23 | PSIB | 37 | MIA | C12-C13-C14-C15 |
| 23 | PSIB | 37 | MIA | C12-C13-C14-C16 |
| 23 | PSIA | 47 | 3AU | N3-C10-C11-C12 |
| 23 | PSIA | 47 | 3AU | C10-C11-C12-C13 |
| 23 | PSIA | 47 | 3AU | C10-C11-C12-N40 |
| 23 | PSIB | 47 | 3AU | C2'-C1'-N1-C2 |
| 23 | PSIB | 54 | 5MU | C3'-C4'-C5'-O5' |
| 23 | PSIB | 54 | 5MU | O4'-C4'-C5'-O5' |
| 24 | ESIA | 37 | MIA | N1-C2-S10-C11 |
| 24 | ESIA | 37 | MIA | N3-C2-S10-C11 |
| 24 | ESIA | 37 | MIA | C12-C13-C14-C16 |
| 24 | ESIB | 37 | MIA | N1-C2-S10-C11 |
| 24 | ESIB | 37 | MIA | N3-C2-S10-C11 |
| 24 | ESIB | 37 | MIA | C12-C13-C14-C16 |
| 26 | TRNA | 8 | 4SU | C3'-C4'-C5'-O5' |
| 26 | TRNA | 8 | 4SU | O4'-C4'-C5'-O5' |
| 26 | TRNA | 37 | MIA | N1-C2-S10-C11 |
| 26 | TRNA | 37 | MIA | N3-C2-S10-C11 |
| 26 | TRNA | 37 | MIA | C12-C13-C14-C15 |
| 26 | TRNA | 37 | MIA | C12-C13-C14-C16 |
| 26 | TRNA | 54 | 5MU | C3'-C4'-C5'-O5' |
| 26 | TRNA | 54 | 5MU | O4'-C4'-C5'-O5' |
| 27 | 23SB | 1964 | 5MU | O4'-C4'-C5'-O5' |
| 57 | ASIB | 37 | MIA | C12-C13-C14-C15 |
| 1 | 16SA | 1156 | 7MG | C3'-C4'-C5'-O5' |
| 1 | 16SB | 1156 | 7MG | O4'-C4'-C5'-O5' |
| 1 | 16SB | 1156 | 7MG | C3'-C4'-C5'-O5' |
| 1 | 16SA | 2030 | 4OC | O4'-C4'-C5'-O5' |
| 1 | 16SB | 2030 | 4OC | O4'-C4'-C5'-O5' |
| 1 | 16SA | 2142 | MA6 | C3'-C4'-C5'-O5' |
| 23 | PSIB | 8 | 4SU | O4'-C4'-C5'-O5' |
| 23 | PSIA | 47 | 3AU | C3'-C4'-C5'-O5' |
| 23 | PSIA | 47 | 3AU | O4'-C4'-C5'-O5' |

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| Mol | Chain | Res | Type | Atoms |
|---|---|---|---|---|
| 23 | PSIA | 55 | PSU | C3'-C4'-C5'-O5' |
| 24 | ESIB | 37 | MIA | O4'-C4'-C5'-O5' |
| 24 | ESIB | 37 | MIA | C3'-C4'-C5'-O5' |
| 23 | PSIB | 47 | 3AU | C2'-C1'-N1-C6 |
| 1 | 16SB | 2142 | MA6 | C3'-C4'-C5'-O5' |
| 23 | PSIA | 37 | MIA | O4'-C4'-C5'-O5' |
| 23 | PSIB | 47 | 3AU | O4'-C4'-C5'-O5' |
| 27 | 23SA | 1940 | 5MU | C3'-C4'-C5'-O5' |
| 27 | 23SA | 1940 | 5MU | O4'-C4'-C5'-O5' |
| 27 | 23SB | 2567 | OMU | C3'-C4'-C5'-O5' |
| 22 | ASIA | 37 | MIA | C3'-C4'-C5'-O5' |
| 23 | PSIB | 8 | 4SU | C3'-C4'-C5'-O5' |
| 23 | PSIB | 47 | 3AU | C3'-C4'-C5'-O5' |
| 1 | 16SB | 2030 | 4OC | C3'-C4'-C5'-O5' |
| 22 | ASIA | 46 | 7MG | C3'-C4'-C5'-O5' |
| 22 | ASIA | 55 | PSU | C3'-C4'-C5'-O5' |
| 27 | 23SB | 1964 | 5MU | C3'-C4'-C5'-O5' |
| 1 | 16SA | 2030 | 4OC | C3'-C4'-C5'-O5' |
| 22 | ASIA | 55 | PSU | O4'-C4'-C5'-O5' |
| 27 | 23SB | 2567 | OMU | O4'-C4'-C5'-O5' |
| 23 | PSIA | 55 | PSU | O4'-C4'-C5'-O5' |
| 26 | TRNA | 37 | MIA | C4'-C5'-O5'-P |
| 24 | ESIA | 37 | MIA | C12-C13-C14-C15 |
| 23 | PSIB | 47 | 3AU | C11-C12-C13-O31 |
| 24 | ESIA | 37 | MIA | C3'-C4'-C5'-O5' |
| 12 | S12A | 89 | 0TD | CG-CB-SB-CSB |
| 23 | PSIB | 47 | 3AU | C11-C12-C13-O30 |
| 12 | S12B | 89 | 0TD | SB-CB-CG-OD1 |
| 27 | 23SB | 2518 | 2MA | O4'-C4'-C5'-O5' |
| 23 | PSIB | 47 | 3AU | C4'-C5'-O5'-P |
| 23 | PSIA | 55 | PSU | C4'-C5'-O5'-P |
| 22 | ASIA | 55 | PSU | O4'-C1'-C5-C4 |
| 27 | 23SA | 1936 | PSU | O4'-C1'-C5-C4 |
| 57 | ASIB | 54 | 5MU | C3'-C4'-C5'-O5' |
| 24 | ESIA | 37 | MIA | N6-C12-C13-C14 |
| 26 | TRNA | 37 | MIA | N6-C12-C13-C14 |
| 1 | 16SB | 2141 | MA6 | C5-C6-N6-C9 |
| 1 | 16SB | 2142 | MA6 | C4'-C5'-O5'-P |
| 22 | ASIA | 8 | 4SU | C4'-C5'-O5'-P |
| 22 | ASIA | 46 | 7MG | O4'-C4'-C5'-O5' |
| 1 | 16SA | 2142 | MA6 | C4'-C5'-O5'-P |
| 27 | 23SA | 2518 | 2MA | C4'-C5'-O5'-P |

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| Mol | Chain | Res | Type | Atoms |
|---|---|---|---|---|
| 12 | S12A | 89 | 0TD | CA-CB-SB-CSB |
| 23 | PSIA | 46 | 7MG | O4'-C4'-C5'-O5' |
| 27 | 23SA | 1936 | PSU | O4'-C1'-C5-C6 |
| 23 | PSIA | 47 | 3AU | C2'-C1'-N1-C6 |
| 23 | PSIB | 46 | 7MG | C2'-C1'-N9-C8 |
| 1 | 16SA | 1589 | M2G | C3'-C4'-C5'-O5' |
| 23 | PSIA | 47 | 3AU | C2'-C1'-N1-C2 |
| 12 | S12B | 89 | 0TD | CG-CB-SB-CSB |
| 24 | ESIB | 37 | MIA | C4'-C5'-O5'-P |
| 23 | PSIA | 37 | MIA | N1-C2-S10-C11 |
| 23 | PSIA | 37 | MIA | N3-C2-S10-C11 |
| 57 | ASIB | 37 | MIA | N3-C2-S10-C11 |
| 1 | 16SA | 1589 | M2G | O4'-C4'-C5'-O5' |
| 27 | 23SB | 2518 | 2MA | C3'-C4'-C5'-O5' |
| 57 | ASIB | 54 | 5MU | O4'-C4'-C5'-O5' |
| 23 | PSIB | 47 | 3AU | N40-C12-C13-O31 |
| 27 | 23SB | 2518 | 2MA | C4'-C5'-O5'-P |
| 27 | 23SA | 1964 | 5MU | O4'-C4'-C5'-O5' |

There are no ring outliers.

No monomer is involved in short contacts.

## 5.5 Carbohydrates (i)

There are no oligosaccharides in this entry.

## 5.6 Ligand geometry (i)

Of 1680 ligands modelled in this entry, 1080 are monoatomic - leaving 600 for Mogul analysis.

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

| Mol | Type | Chain | Res | Link | Bond lengths | | | Bond angles | | |
|---|---|---|---|---|---|---|---|---|---|---|
| | | | | | Counts | RMSZ | $\#\|Z\| > 2$ | Counts | RMSZ | $\#\|Z\| > 2$ |
| 60 | OHX | 5SA | 217 | - | 0,6,6 | - | - | - | | |
| 60 | OHX | 23SB | 3344 | - | 0,6,6 | - | - | - | | |

| Mol | Type | Chain | Res | Link | Bond lengths | | | Bond angles | | |
|---|---|---|---|---|---|---|---|---|---|---|
| | | | | | Counts | RMSZ | $\#\|Z\|>2$ | Counts | RMSZ | $\#\|Z\|>2$ |
| 60 | OHX | 23SA | 3479 | - | 0,6,6 | - | - | - | | |
| 60 | OHX | 23SA | 3603 | - | 0,6,6 | - | - | - | | |
| 60 | OHX | 23SB | 3461 | - | 0,6,6 | - | - | - | | |
| 60 | OHX | 23SB | 3402 | - | 0,6,6 | - | - | - | | |
| 60 | OHX | 16SB | 2363 | - | 0,6,6 | - | - | - | | |
| 60 | OHX | 23SB | 3508 | - | 0,6,6 | - | - | - | | |
| 60 | OHX | 23SA | 3465 | - | 0,6,6 | - | - | - | | |
| 60 | OHX | 16SA | 2381 | - | 0,6,6 | - | - | - | | |
| 60 | OHX | 23SA | 3477 | - | 0,6,6 | - | - | - | | |
| 60 | OHX | 23SA | 3528 | - | 0,6,6 | - | - | - | | |
| 60 | OHX | 23SB | 3496 | - | 0,6,6 | - | - | - | | |
| 60 | OHX | 23SB | 3468 | - | 0,6,6 | - | - | - | | |
| 60 | OHX | 16SB | 2324 | - | 0,6,6 | - | - | - | | |
| 60 | OHX | 16SA | 2415 | - | 0,6,6 | - | - | - | | |
| 60 | OHX | 16SB | 2377 | - | 0,6,6 | - | - | - | | |
| 60 | OHX | 23SA | 3553 | - | 0,6,6 | - | - | - | | |
| 60 | OHX | 23SA | 3537 | - | 0,6,6 | - | - | - | | |
| 60 | OHX | 23SB | 3446 | - | 0,6,6 | - | - | - | | |
| 60 | OHX | 5SB | 206 | - | 0,6,6 | - | - | - | | |
| 60 | OHX | 16SB | 2345 | - | 0,6,6 | - | - | - | | |
| 60 | OHX | 23SB | 3340 | - | 0,6,6 | - | - | - | | |
| 60 | OHX | 23SB | 3440 | - | 0,6,6 | - | - | - | | |
| 60 | OHX | 23SB | 3480 | - | 0,6,6 | - | - | - | | |
| 60 | OHX | 5SA | 218 | - | 0,6,6 | - | - | - | | |
| 60 | OHX | 16SB | 2335 | 1 | 0,6,6 | - | - | - | | |
| 60 | OHX | 23SA | 3570 | 27 | 0,6,6 | - | - | - | | |
| 60 | OHX | L4A | 304 | - | 0,6,6 | - | - | - | | |
| 60 | OHX | 23SB | 3438 | - | 0,6,6 | - | - | - | | |
| 60 | OHX | 23SB | 3430 | - | 0,6,6 | - | - | - | | |
| 60 | OHX | 16SA | 2394 | - | 0,6,6 | - | - | - | | |
| 60 | OHX | 23SA | 3444 | - | 0,6,6 | - | - | - | | |
| 60 | OHX | 23SB | 3361 | - | 0,6,6 | - | - | - | | |
| 60 | OHX | 23SB | 3351 | - | 0,6,6 | - | - | - | | |
| 60 | OHX | 16SB | 2336 | - | 0,6,6 | - | - | - | | |
| 60 | OHX | 5SB | 215 | - | 0,6,6 | - | - | - | | |
| 60 | OHX | 23SA | 3540 | - | 0,6,6 | - | - | - | | |
| 60 | OHX | 23SA | 3542 | - | 0,6,6 | - | - | - | | |
| 60 | OHX | 23SA | 3633 | - | 0,6,6 | - | - | - | | |
| 60 | OHX | 23SB | 3384 | - | 0,6,6 | - | - | - | | |
| 60 | OHX | 23SB | 3450 | - | 0,6,6 | - | - | - | | |
| 60 | OHX | 16SB | 2380 | - | 0,6,6 | - | - | - | | |
| 60 | OHX | 23SB | 3485 | - | 0,6,6 | - | - | - | | |
| 60 | OHX | 16SA | 2364 | - | 0,6,6 | - | - | - | | |

| Mol | Type | Chain | Res | Link | Bond lengths | | | Bond angles | | |
|---|---|---|---|---|---|---|---|---|---|---|
| | | | | | Counts | RMSZ | $\#\|Z\| > 2$ | Counts | RMSZ | $\#\|Z\| > 2$ |
| 60 | OHX | 23SA | 3549 | - | 0,6,6 | - | - | - | | |
| 60 | OHX | 16SB | 2389 | - | 0,6,6 | - | - | - | | |
| 60 | OHX | 23SA | 3474 | - | 0,6,6 | - | - | - | | |
| 60 | OHX | 16SA | 2342 | - | 0,6,6 | - | - | - | | |
| 60 | OHX | 16SB | 2355 | 1 | 0,6,6 | - | - | - | | |
| 60 | OHX | 16SB | 2396 | - | 0,6,6 | - | - | - | | |
| 60 | OHX | 23SB | 3405 | - | 0,6,6 | - | - | - | | |
| 60 | OHX | 23SB | 3369 | - | 0,6,6 | - | - | - | | |
| 60 | OHX | 5SB | 209 | 28 | 0,6,6 | - | - | - | | |
| 60 | OHX | 16SB | 2352 | - | 0,6,6 | - | - | - | | |
| 60 | OHX | 23SB | 3436 | - | 0,6,6 | - | - | - | | |
| 60 | OHX | 23SA | 3614 | - | 0,6,6 | - | - | - | | |
| 60 | OHX | MRNA | 102 | - | 0,6,6 | - | - | - | | |
| 60 | OHX | 23SA | 3601 | - | 0,6,6 | - | - | - | | |
| 60 | OHX | 23SA | 3470 | - | 0,6,6 | - | - | - | | |
| 60 | OHX | 23SA | 3530 | - | 0,6,6 | - | - | - | | |
| 60 | OHX | L17A | 202 | - | 0,6,6 | - | - | - | | |
| 60 | OHX | 23SA | 3450 | 27 | 0,6,6 | - | - | - | | |
| 60 | OHX | 16SB | 2375 | - | 0,6,6 | - | - | - | | |
| 60 | OHX | 23SB | 3466 | - | 0,6,6 | - | - | - | | |
| 60 | OHX | 23SA | 3531 | - | 0,6,6 | - | - | - | | |
| 60 | OHX | 16SA | 2351 | - | 0,6,6 | - | - | - | | |
| 60 | OHX | 23SB | 3426 | - | 0,6,6 | - | - | - | | |
| 60 | OHX | 23SB | 3347 | - | 0,6,6 | - | - | - | | |
| 60 | OHX | 23SA | 3620 | - | 0,6,6 | - | - | - | | |
| 60 | OHX | 23SA | 3582 | - | 0,6,6 | - | - | - | | |
| 60 | OHX | 23SA | 3482 | - | 0,6,6 | - | - | - | | |
| 60 | OHX | 23SB | 3481 | - | 0,6,6 | - | - | - | | |
| 60 | OHX | 23SA | 3452 | - | 0,6,6 | - | - | - | | |
| 60 | OHX | 16SA | 2349 | - | 0,6,6 | - | - | - | | |
| 60 | OHX | 23SA | 3575 | - | 0,6,6 | - | - | - | | |
| 60 | OHX | 16SA | 2357 | - | 0,6,6 | - | - | - | | |
| 60 | OHX | 23SA | 3606 | - | 0,6,6 | - | - | - | | |
| 60 | OHX | 23SA | 3497 | - | 0,6,6 | - | - | - | | |
| 60 | OHX | 23SB | 3412 | - | 0,6,6 | - | - | - | | |
| 60 | OHX | 23SA | 3489 | - | 0,6,6 | - | - | - | | |
| 60 | OHX | 23SA | 3597 | - | 0,6,6 | - | - | - | | |
| 60 | OHX | 5SB | 211 | - | 0,6,6 | - | - | - | | |
| 60 | OHX | 16SA | 2403 | - | 0,6,6 | - | - | - | | |
| 60 | OHX | 23SB | 3437 | - | 0,6,6 | - | - | - | | |
| 60 | OHX | 16SB | 2340 | - | 0,6,6 | - | - | - | | |
| 60 | OHX | 16SA | 2398 | - | 0,6,6 | - | - | - | | |
| 60 | OHX | 16SB | 2391 | - | 0,6,6 | - | - | - | | |

| Mol | Type | Chain | Res | Link | Bond lengths | | | Bond angles | | |
|---|---|---|---|---|---|---|---|---|---|---|
| | | | | | Counts | RMSZ | $\#\|Z\|>2$ | Counts | RMSZ | $\#\|Z\|>2$ |
| 60 | OHX | 23SA | 3627 | - | 0,6,6 | - | - | - | | |
| 60 | OHX | 5SA | 211 | - | 0,6,6 | - | - | - | | |
| 60 | OHX | 16SA | 2341 | - | 0,6,6 | - | - | - | | |
| 60 | OHX | 16SA | 2384 | - | 0,6,6 | - | - | - | | |
| 60 | OHX | 23SA | 3589 | - | 0,6,6 | - | - | - | | |
| 60 | OHX | 16SB | 2362 | - | 0,6,6 | - | - | - | | |
| 60 | OHX | 23SA | 3631 | - | 0,6,6 | - | - | - | | |
| 60 | OHX | 23SA | 3602 | - | 0,6,6 | - | - | - | | |
| 60 | OHX | 23SA | 3567 | - | 0,6,6 | - | - | - | | |
| 60 | OHX | 16SA | 2385 | - | 0,6,6 | - | - | - | | |
| 60 | OHX | 16SA | 2391 | - | 0,6,6 | - | - | - | | |
| 60 | OHX | 23SA | 3566 | - | 0,6,6 | - | - | - | | |
| 60 | OHX | 16SA | 2402 | - | 0,6,6 | - | - | - | | |
| 60 | OHX | 23SA | 3617 | - | 0,6,6 | - | - | - | | |
| 60 | OHX | 16SB | 2394 | - | 0,6,6 | - | - | - | | |
| 60 | OHX | 23SA | 3599 | - | 0,6,6 | - | - | - | | |
| 60 | OHX | 16SA | 2378 | - | 0,6,6 | - | - | - | | |
| 60 | OHX | 23SB | 3354 | - | 0,6,6 | - | - | - | | |
| 60 | OHX | 23SA | 3475 | - | 0,6,6 | - | - | - | | |
| 60 | OHX | 16SA | 2386 | - | 0,6,6 | - | - | - | | |
| 60 | OHX | 16SA | 2406 | - | 0,6,6 | - | - | - | | |
| 60 | OHX | 23SA | 3443 | - | 0,6,6 | - | - | - | | |
| 60 | OHX | 16SA | 2359 | - | 0,6,6 | - | - | - | | |
| 60 | OHX | 23SB | 3375 | - | 0,6,6 | - | - | - | | |
| 60 | OHX | 16SA | 2399 | - | 0,6,6 | - | - | - | | |
| 60 | OHX | 16SA | 2408 | - | 0,6,6 | - | - | - | | |
| 60 | OHX | 16SB | 2327 | - | 0,6,6 | - | - | - | | |
| 60 | OHX | 23SB | 3332 | - | 0,6,6 | - | - | - | | |
| 60 | OHX | 23SB | 3429 | - | 0,6,6 | - | - | - | | |
| 60 | OHX | 23SA | 3487 | - | 0,6,6 | - | - | - | | |
| 60 | OHX | 16SB | 2353 | - | 0,6,6 | - | - | - | | |
| 60 | OHX | 23SB | 3374 | - | 0,6,6 | - | - | - | | |
| 60 | OHX | 23SB | 3364 | - | 0,6,6 | - | - | - | | |
| 60 | OHX | 23SB | 3495 | - | 0,6,6 | - | - | - | | |
| 60 | OHX | 23SA | 3517 | - | 0,6,6 | - | - | - | | |
| 60 | OHX | 23SB | 3434 | - | 0,6,6 | - | - | - | | |
| 60 | OHX | 23SA | 3568 | - | 0,6,6 | - | - | - | | |
| 60 | OHX | 16SA | 2382 | 1 | 0,6,6 | - | - | - | | |
| 60 | OHX | 23SB | 3366 | - | 0,6,6 | - | - | - | | |
| 60 | OHX | 16SA | 2393 | - | 0,6,6 | - | - | - | | |
| 60 | OHX | 23SA | 3454 | - | 0,6,6 | - | - | - | | |
| 60 | OHX | 16SB | 2338 | - | 0,6,6 | - | - | - | | |
| 60 | OHX | 23SB | 3493 | - | 0,6,6 | - | - | - | | |

| Mol | Type | Chain | Res | Link | Bond lengths | | | Bond angles | | |
|---|---|---|---|---|---|---|---|---|---|---|
| | | | | | Counts | RMSZ | $\#\|Z\| > 2$ | Counts | RMSZ | $\#\|Z\| > 2$ |
| 60 | OHX | 16SB | 2323 | - | 0,6,6 | - | - | - | | |
| 60 | OHX | 23SB | 3360 | - | 0,6,6 | - | - | - | | |
| 60 | OHX | 23SB | 3400 | - | 0,6,6 | - | - | - | | |
| 60 | OHX | 23SA | 3591 | - | 0,6,6 | - | - | - | | |
| 60 | OHX | 23SB | 3382 | - | 0,6,6 | - | - | - | | |
| 60 | OHX | 23SB | 3376 | - | 0,6,6 | - | - | - | | |
| 60 | OHX | 16SB | 2339 | - | 0,6,6 | - | - | - | | |
| 60 | OHX | 23SA | 3539 | - | 0,6,6 | - | - | - | | |
| 60 | OHX | 23SA | 3480 | - | 0,6,6 | - | - | - | | |
| 60 | OHX | L15A | 203 | - | 0,6,6 | - | - | - | | |
| 60 | OHX | 23SA | 3625 | - | 0,6,6 | - | - | - | | |
| 60 | OHX | 16SB | 2334 | - | 0,6,6 | - | - | - | | |
| 60 | OHX | 23SB | 3449 | - | 0,6,6 | - | - | - | | |
| 60 | OHX | 16SB | 2372 | - | 0,6,6 | - | - | - | | |
| 60 | OHX | L20B | 201 | - | 0,6,6 | - | - | - | | |
| 60 | OHX | L27A | 103 | - | 0,6,6 | - | - | - | | |
| 60 | OHX | 23SA | 3532 | - | 0,6,6 | - | - | - | | |
| 60 | OHX | 23SB | 3448 | - | 0,6,6 | - | - | - | | |
| 60 | OHX | 23SB | 3475 | - | 0,6,6 | - | - | - | | |
| 60 | OHX | 23SA | 3472 | - | 0,6,6 | - | - | - | | |
| 60 | OHX | 23SB | 3505 | - | 0,6,6 | - | - | - | | |
| 60 | OHX | 23SB | 3455 | - | 0,6,6 | - | - | - | | |
| 60 | OHX | 23SB | 3503 | - | 0,6,6 | - | - | - | | |
| 60 | OHX | 23SA | 3459 | - | 0,6,6 | - | - | - | | |
| 60 | OHX | 23SA | 3462 | - | 0,6,6 | - | - | - | | |
| 60 | OHX | 23SA | 3485 | - | 0,6,6 | - | - | - | | |
| 60 | OHX | 16SB | 2374 | - | 0,6,6 | - | - | - | | |
| 60 | OHX | 23SB | 3365 | - | 0,6,6 | - | - | - | | |
| 60 | OHX | 23SA | 3457 | - | 0,6,6 | - | - | - | | |
| 60 | OHX | 23SA | 3580 | - | 0,6,6 | - | - | - | | |
| 60 | OHX | 23SA | 3538 | - | 0,6,6 | - | - | - | | |
| 60 | OHX | 23SB | 3377 | - | 0,6,6 | - | - | - | | |
| 60 | OHX | 23SB | 3339 | 27 | 0,6,6 | - | - | - | | |
| 60 | OHX | 23SA | 3558 | - | 0,6,6 | - | - | - | | |
| 60 | OHX | 23SA | 3536 | - | 0,6,6 | - | - | - | | |
| 60 | OHX | 23SA | 3488 | - | 0,6,6 | - | - | - | | |
| 60 | OHX | 23SA | 3605 | - | 0,6,6 | - | - | - | | |
| 60 | OHX | 23SB | 3324 | - | 0,6,6 | - | - | - | | |
| 60 | OHX | 23SB | 3482 | - | 0,6,6 | - | - | - | | |
| 60 | OHX | 23SA | 3632 | - | 0,6,6 | - | - | - | | |
| 60 | OHX | 23SB | 3342 | - | 0,6,6 | - | - | - | | |
| 60 | OHX | 23SA | 3473 | - | 0,6,6 | - | - | - | | |
| 60 | OHX | 23SA | 3469 | - | 0,6,6 | - | - | - | | |

| Mol | Type | Chain | Res | Link | Bond lengths | | | Bond angles | | |
|---|---|---|---|---|---|---|---|---|---|---|
| | | | | | Counts | RMSZ | $\#\|Z\|>2$ | Counts | RMSZ | $\#\|Z\|>2$ |
| 60 | OHX | 23SB | 3478 | - | 0,6,6 | - | - | - | | |
| 60 | OHX | S19A | 101 | - | 0,6,6 | - | - | - | | |
| 60 | OHX | 23SB | 3509 | - | 0,6,6 | - | - | - | | |
| 60 | OHX | 5SA | 210 | - | 0,6,6 | - | - | - | | |
| 60 | OHX | 23SA | 3629 | - | 0,6,6 | - | - | - | | |
| 60 | OHX | 23SB | 3424 | - | 0,6,6 | - | - | - | | |
| 60 | OHX | 16SB | 2367 | 1 | 0,6,6 | - | - | - | | |
| 60 | OHX | 23SA | 3534 | - | 0,6,6 | - | - | - | | |
| 60 | OHX | 23SA | 3592 | - | 0,6,6 | - | - | - | | |
| 60 | OHX | 23SB | 3395 | - | 0,6,6 | - | - | - | | |
| 60 | OHX | ESIB | 101 | - | 0,6,6 | - | - | - | | |
| 60 | OHX | 23SB | 3413 | - | 0,6,6 | - | - | - | | |
| 60 | OHX | 16SA | 2363 | - | 0,6,6 | - | - | - | | |
| 60 | OHX | 16SA | 2376 | - | 0,6,6 | - | - | - | | |
| 60 | OHX | 23SA | 3624 | - | 0,6,6 | - | - | - | | |
| 60 | OHX | 23SA | 3484 | - | 0,6,6 | - | - | - | | |
| 60 | OHX | 23SB | 3349 | - | 0,6,6 | - | - | - | | |
| 60 | OHX | 16SA | 2389 | - | 0,6,6 | - | - | - | | |
| 60 | OHX | 23SB | 3444 | - | 0,6,6 | - | - | - | | |
| 60 | OHX | 23SA | 3630 | - | 0,6,6 | - | - | - | | |
| 60 | OHX | 23SB | 3443 | - | 0,6,6 | - | - | - | | |
| 60 | OHX | 16SA | 2407 | - | 0,6,6 | - | - | - | | |
| 60 | OHX | L35B | 103 | - | 0,6,6 | - | - | - | | |
| 60 | OHX | 16SA | 2392 | - | 0,6,6 | - | - | - | | |
| 60 | OHX | 5SA | 216 | - | 0,6,6 | - | - | - | | |
| 60 | OHX | 16SA | 2355 | - | 0,6,6 | - | - | - | | |
| 60 | OHX | 16SA | 2344 | - | 0,6,6 | - | - | - | | |
| 60 | OHX | 23SA | 3573 | - | 0,6,6 | - | - | - | | |
| 60 | OHX | 23SB | 3487 | - | 0,6,6 | - | - | - | | |
| 60 | OHX | 23SA | 3496 | - | 0,6,6 | - | - | - | | |
| 60 | OHX | 5SB | 207 | - | 0,6,6 | - | - | - | | |
| 60 | OHX | 23SB | 3416 | - | 0,6,6 | - | - | - | | |
| 60 | OHX | 16SA | 2414 | - | 0,6,6 | - | - | - | | |
| 60 | OHX | 16SB | 2330 | 1 | 0,6,6 | - | - | - | | |
| 60 | OHX | 23SB | 3454 | - | 0,6,6 | - | - | - | | |
| 60 | OHX | 23SB | 3393 | - | 0,6,6 | - | - | - | | |
| 60 | OHX | 23SA | 3492 | - | 0,6,6 | - | - | - | | |
| 60 | OHX | 23SA | 3577 | - | 0,6,6 | - | - | - | | |
| 60 | OHX | 16SB | 2383 | - | 0,6,6 | - | - | - | | |
| 60 | OHX | 23SA | 3611 | - | 0,6,6 | - | - | - | | |
| 60 | OHX | 23SA | 3545 | - | 0,6,6 | - | - | - | | |
| 60 | OHX | 16SB | 2399 | - | 0,6,6 | - | - | - | | |
| 60 | OHX | 23SA | 3519 | - | 0,6,6 | - | - | - | | |

| Mol | Type | Chain | Res | Link | Bond lengths | | | Bond angles | | |
|---|---|---|---|---|---|---|---|---|---|---|
| | | | | | Counts | RMSZ | $\#\|Z\|>2$ | Counts | RMSZ | $\#\|Z\|>2$ |
| 60 | OHX | 23SA | 3560 | - | 0,6,6 | - | - | - | | |
| 60 | OHX | 5SA | 209 | - | 0,6,6 | - | - | - | | |
| 60 | OHX | 16SB | 2354 | - | 0,6,6 | - | - | - | | |
| 60 | OHX | 16SB | 2357 | - | 0,6,6 | - | - | - | | |
| 60 | OHX | 23SA | 3529 | - | 0,6,6 | - | - | - | | |
| 60 | OHX | 16SB | 2370 | - | 0,6,6 | - | - | - | | |
| 60 | OHX | 23SB | 3378 | - | 0,6,6 | - | - | - | | |
| 60 | OHX | 16SB | 2351 | - | 0,6,6 | - | - | - | | |
| 60 | OHX | 23SA | 3613 | - | 0,6,6 | - | - | - | | |
| 60 | OHX | 23SA | 3619 | - | 0,6,6 | - | - | - | | |
| 60 | OHX | 16SB | 2343 | - | 0,6,6 | - | - | - | | |
| 60 | OHX | 23SA | 3466 | - | 0,6,6 | - | - | - | | |
| 60 | OHX | 16SB | 2384 | - | 0,6,6 | - | - | - | | |
| 60 | OHX | 16SB | 2356 | - | 0,6,6 | - | - | - | | |
| 60 | OHX | 23SB | 3341 | - | 0,6,6 | - | - | - | | |
| 60 | OHX | 23SB | 3510 | - | 0,6,6 | - | - | - | | |
| 60 | OHX | 16SB | 2371 | - | 0,6,6 | - | - | - | | |
| 60 | OHX | 23SA | 3446 | - | 0,6,6 | - | - | - | | |
| 60 | OHX | 16SA | 2354 | - | 0,6,6 | - | - | - | | |
| 60 | OHX | 5SA | 215 | - | 0,6,6 | - | - | - | | |
| 60 | OHX | 16SB | 2349 | - | 0,6,6 | - | - | - | | |
| 60 | OHX | ASIA | 101 | - | 0,6,6 | - | - | - | | |
| 60 | OHX | 23SB | 3500 | - | 0,6,6 | - | - | - | | |
| 60 | OHX | 16SA | 2383 | - | 0,6,6 | - | - | - | | |
| 60 | OHX | 16SB | 2341 | - | 0,6,6 | - | - | - | | |
| 60 | OHX | 23SA | 3516 | - | 0,6,6 | - | - | - | | |
| 60 | OHX | 16SB | 2326 | - | 0,6,6 | - | - | - | | |
| 60 | OHX | 23SA | 3449 | 27 | 0,6,6 | - | - | - | | |
| 60 | OHX | 23SB | 3337 | - | 0,6,6 | - | - | - | | |
| 60 | OHX | 16SA | 2343 | - | 0,6,6 | - | - | - | | |
| 60 | OHX | 23SB | 3346 | - | 0,6,6 | - | - | - | | |
| 60 | OHX | 23SA | 3524 | - | 0,6,6 | - | - | - | | |
| 60 | OHX | 23SB | 3355 | - | 0,6,6 | - | - | - | | |
| 60 | OHX | 23SA | 3622 | - | 0,6,6 | - | - | - | | |
| 60 | OHX | 23SB | 3447 | - | 0,6,6 | - | - | - | | |
| 60 | OHX | 23SA | 3563 | - | 0,6,6 | - | - | - | | |
| 60 | OHX | 16SA | 2379 | - | 0,6,6 | - | - | - | | |
| 60 | OHX | 16SA | 2396 | - | 0,6,6 | - | - | - | | |
| 60 | OHX | 23SB | 3499 | - | 0,6,6 | - | - | - | | |
| 60 | OHX | 23SB | 3386 | - | 0,6,6 | - | - | - | | |
| 60 | OHX | 23SB | 3452 | - | 0,6,6 | - | - | - | | |
| 60 | OHX | 23SB | 3512 | - | 0,6,6 | - | - | - | | |
| 60 | OHX | 16SA | 2345 | - | 0,6,6 | - | - | - | | |

| Mol | Type | Chain | Res | Link | Bond lengths | | | Bond angles | | |
|---|---|---|---|---|---|---|---|---|---|---|
| | | | | | Counts | RMSZ | $\#\|Z\| > 2$ | Counts | RMSZ | $\#\|Z\| > 2$ |
| 60 | OHX | 23SB | 3514 | - | 0,6,6 | - | - | - | | |
| 60 | OHX | 23SB | 3390 | - | 0,6,6 | - | - | - | | |
| 60 | OHX | 5SB | 208 | - | 0,6,6 | - | - | - | | |
| 60 | OHX | 23SA | 3628 | - | 0,6,6 | - | - | - | | |
| 60 | OHX | 16SB | 2381 | - | 0,6,6 | - | - | - | | |
| 60 | OHX | 23SA | 3440 | - | 0,6,6 | - | - | - | | |
| 60 | OHX | 23SA | 3437 | - | 0,6,6 | - | - | - | | |
| 60 | OHX | 16SB | 2386 | - | 0,6,6 | - | - | - | | |
| 60 | OHX | 16SB | 2322 | - | 0,6,6 | - | - | - | | |
| 60 | OHX | 23SA | 3559 | - | 0,6,6 | - | - | - | | |
| 60 | OHX | 23SB | 3435 | - | 0,6,6 | - | - | - | | |
| 60 | OHX | 5SB | 213 | - | 0,6,6 | - | - | - | | |
| 60 | OHX | 23SB | 3441 | - | 0,6,6 | - | - | - | | |
| 60 | OHX | 23SA | 3494 | - | 0,6,6 | - | - | - | | |
| 60 | OHX | ESIA | 101 | - | 0,6,6 | - | - | - | | |
| 60 | OHX | 23SB | 3345 | - | 0,6,6 | - | - | - | | |
| 60 | OHX | 23SA | 3598 | - | 0,6,6 | - | - | - | | |
| 60 | OHX | 23SB | 3330 | - | 0,6,6 | - | - | - | | |
| 60 | OHX | 23SB | 3498 | - | 0,6,6 | - | - | - | | |
| 60 | OHX | 16SA | 2371 | - | 0,6,6 | - | - | - | | |
| 60 | OHX | 23SB | 3370 | - | 0,6,6 | - | - | - | | |
| 60 | OHX | 23SA | 3442 | 27 | 0,6,6 | - | - | - | | |
| 60 | OHX | 23SA | 3547 | - | 0,6,6 | - | - | - | | |
| 60 | OHX | 23SA | 3618 | - | 0,6,6 | - | - | - | | |
| 60 | OHX | MRNB | 101 | - | 0,6,6 | - | - | - | | |
| 60 | OHX | 23SB | 3327 | 27 | 0,6,6 | - | - | - | | |
| 60 | OHX | 23SA | 3505 | - | 0,6,6 | - | - | - | | |
| 60 | OHX | 23SA | 3518 | - | 0,6,6 | - | - | - | | |
| 60 | OHX | 23SB | 3398 | - | 0,6,6 | - | - | - | | |
| 60 | OHX | 23SB | 3385 | - | 0,6,6 | - | - | - | | |
| 60 | OHX | 23SB | 3474 | - | 0,6,6 | - | - | - | | |
| 60 | OHX | 16SB | 2378 | - | 0,6,6 | - | - | - | | |
| 60 | OHX | L35A | 102 | 56 | 0,6,6 | - | - | - | | |
| 60 | OHX | 5SB | 214 | - | 0,6,6 | - | - | - | | |
| 60 | OHX | 23SA | 3467 | - | 0,6,6 | - | - | - | | |
| 60 | OHX | 16SA | 2366 | - | 0,6,6 | - | - | - | | |
| 60 | OHX | S4B | 302 | 4 | 0,6,6 | - | - | - | | |
| 60 | OHX | 23SA | 3507 | - | 0,6,6 | - | - | - | | |
| 60 | OHX | 23SB | 3379 | - | 0,6,6 | - | - | - | | |
| 60 | OHX | 23SB | 3406 | - | 0,6,6 | - | - | - | | |
| 60 | OHX | 23SA | 3495 | - | 0,6,6 | - | - | - | | |
| 60 | OHX | 23SB | 3439 | - | 0,6,6 | - | - | - | | |
| 60 | OHX | 23SB | 3407 | - | 0,6,6 | - | - | - | | |

| Mol | Type | Chain | Res | Link | Bond lengths | | | Bond angles | | |
|---|---|---|---|---|---|---|---|---|---|---|
| | | | | | Counts | RMSZ | $\#\|Z\|>2$ | Counts | RMSZ | $\#\|Z\|>2$ |
| 60 | OHX | 16SB | 2369 | - | 0,6,6 | - | - | - | | |
| 60 | OHX | 23SB | 3431 | - | 0,6,6 | - | - | - | | |
| 60 | OHX | 23SB | 3399 | - | 0,6,6 | - | - | - | | |
| 60 | OHX | 23SA | 3579 | - | 0,6,6 | - | - | - | | |
| 60 | OHX | 23SA | 3569 | - | 0,6,6 | - | - | - | | |
| 60 | OHX | 23SA | 3453 | - | 0,6,6 | - | - | - | | |
| 60 | OHX | 23SB | 3488 | - | 0,6,6 | - | - | - | | |
| 60 | OHX | 23SB | 3357 | - | 0,6,6 | - | - | - | | |
| 60 | OHX | 23SA | 3587 | - | 0,6,6 | - | - | - | | |
| 60 | OHX | 16SB | 2376 | - | 0,6,6 | - | - | - | | |
| 60 | OHX | 5SB | 210 | - | 0,6,6 | - | - | - | | |
| 60 | OHX | 23SA | 3572 | - | 0,6,6 | - | - | - | | |
| 60 | OHX | 23SA | 3439 | - | 0,6,6 | - | - | - | | |
| 60 | OHX | 16SB | 2368 | - | 0,6,6 | - | - | - | | |
| 60 | OHX | 23SA | 3508 | - | 0,6,6 | - | - | - | | |
| 60 | OHX | 16SB | 2395 | - | 0,6,6 | - | - | - | | |
| 60 | OHX | 23SB | 3336 | - | 0,6,6 | - | - | - | | |
| 60 | OHX | 23SA | 3581 | - | 0,6,6 | - | - | - | | |
| 60 | OHX | 16SB | 2390 | - | 0,6,6 | - | - | - | | |
| 60 | OHX | 23SB | 3411 | - | 0,6,6 | - | - | - | | |
| 60 | OHX | 23SB | 3506 | - | 0,6,6 | - | - | - | | |
| 60 | OHX | 23SB | 3362 | - | 0,6,6 | - | - | - | | |
| 60 | OHX | 23SB | 3388 | 27 | 0,6,6 | - | - | - | | |
| 60 | OHX | 16SA | 2356 | - | 0,6,6 | - | - | - | | |
| 60 | OHX | 23SB | 3352 | - | 0,6,6 | - | - | - | | |
| 60 | OHX | 16SA | 2338 | - | 0,6,6 | - | - | - | | |
| 60 | OHX | 23SB | 3489 | - | 0,6,6 | - | - | - | | |
| 60 | OHX | 23SB | 3471 | - | 0,6,6 | - | - | - | | |
| 60 | OHX | 16SB | 2392 | - | 0,6,6 | - | - | - | | |
| 60 | OHX | 23SB | 3418 | - | 0,6,6 | - | - | - | | |
| 60 | OHX | 23SB | 3476 | - | 0,6,6 | - | - | - | | |
| 60 | OHX | 16SA | 2373 | - | 0,6,6 | - | - | - | | |
| 60 | OHX | 23SB | 3427 | - | 0,6,6 | - | - | - | | |
| 60 | OHX | 23SA | 3490 | - | 0,6,6 | - | - | - | | |
| 60 | OHX | 23SB | 3417 | - | 0,6,6 | - | - | - | | |
| 60 | OHX | 16SB | 2385 | - | 0,6,6 | - | - | - | | |
| 60 | OHX | 16SB | 2331 | - | 0,6,6 | - | - | - | | |
| 60 | OHX | 23SA | 3546 | - | 0,6,6 | - | - | - | | |
| 60 | OHX | 23SA | 3555 | - | 0,6,6 | - | - | - | | |
| 60 | OHX | 23SA | 3502 | - | 0,6,6 | - | - | - | | |
| 60 | OHX | 23SA | 3564 | - | 0,6,6 | - | - | - | | |
| 60 | OHX | 23SB | 3415 | - | 0,6,6 | - | - | - | | |
| 60 | OHX | 23SA | 3607 | - | 0,6,6 | - | - | - | | |

| Mol | Type | Chain | Res | Link | Bond lengths | | | Bond angles | | |
|---|---|---|---|---|---|---|---|---|---|---|
| | | | | | Counts | RMSZ | $\#\|Z\|>2$ | Counts | RMSZ | $\#\|Z\|>2$ |
| 60 | OHX | 23SB | 3414 | - | 0,6,6 | - | - | - | | |
| 60 | OHX | 23SA | 3463 | - | 0,6,6 | - | - | - | | |
| 60 | OHX | 23SB | 3371 | 27 | 0,6,6 | - | - | - | | |
| 60 | OHX | 23SA | 3493 | - | 0,6,6 | - | - | - | | |
| 60 | OHX | S14B | 101 | - | 0,6,6 | - | - | - | | |
| 60 | OHX | 23SA | 3522 | - | 0,6,6 | - | - | - | | |
| 60 | OHX | L28A | 101 | - | 0,6,6 | - | - | - | | |
| 60 | OHX | 16SA | 2353 | - | 0,6,6 | - | - | - | | |
| 60 | OHX | 23SB | 3333 | - | 0,6,6 | - | - | - | | |
| 60 | OHX | 23SB | 3456 | - | 0,6,6 | - | - | - | | |
| 60 | OHX | 23SA | 3527 | - | 0,6,6 | - | - | - | | |
| 60 | OHX | 23SA | 3562 | - | 0,6,6 | - | - | - | | |
| 60 | OHX | 23SA | 3456 | - | 0,6,6 | - | - | - | | |
| 60 | OHX | 23SA | 3583 | - | 0,6,6 | - | - | - | | |
| 60 | OHX | 23SA | 3458 | - | 0,6,6 | - | - | - | | |
| 60 | OHX | 16SB | 2348 | - | 0,6,6 | - | - | - | | |
| 60 | OHX | 16SA | 2339 | - | 0,6,6 | - | - | - | | |
| 60 | OHX | 16SB | 2398 | - | 0,6,6 | - | - | - | | |
| 60 | OHX | 23SB | 3465 | - | 0,6,6 | - | - | - | | |
| 60 | OHX | 23SA | 3483 | - | 0,6,6 | - | - | - | | |
| 60 | OHX | 23SA | 3621 | - | 0,6,6 | - | - | - | | |
| 60 | OHX | 23SB | 3420 | - | 0,6,6 | - | - | - | | |
| 60 | OHX | 23SA | 3556 | - | 0,6,6 | - | - | - | | |
| 60 | OHX | 23SB | 3479 | - | 0,6,6 | - | - | - | | |
| 60 | OHX | 23SB | 3470 | - | 0,6,6 | - | - | - | | |
| 60 | OHX | 23SB | 3325 | - | 0,6,6 | - | - | - | | |
| 60 | OHX | 23SA | 3486 | - | 0,6,6 | - | - | - | | |
| 60 | OHX | 23SA | 3544 | - | 0,6,6 | - | - | - | | |
| 60 | OHX | 16SA | 2413 | - | 0,6,6 | - | - | - | | |
| 60 | OHX | 23SB | 3419 | - | 0,6,6 | - | - | - | | |
| 61 | SJH | 23SB | 3323 | - | 83,87,87 | 2.34 | 20 (24%) | 108,128,128 | 1.85 | 20 (18%) |
| 60 | OHX | 16SA | 2360 | - | 0,6,6 | - | - | - | | |
| 60 | OHX | 23SA | 3455 | - | 0,6,6 | - | - | - | | |
| 60 | OHX | 23SA | 3445 | - | 0,6,6 | - | - | - | | |
| 60 | OHX | 23SA | 3476 | - | 0,6,6 | - | - | - | | |
| 60 | OHX | 23SA | 3498 | - | 0,6,6 | - | - | - | | |
| 60 | OHX | 23SA | 3526 | - | 0,6,6 | - | - | - | | |
| 60 | OHX | 16SA | 2367 | - | 0,6,6 | - | - | - | | |
| 60 | OHX | 23SB | 3403 | - | 0,6,6 | - | - | - | | |
| 60 | OHX | 23SB | 3491 | - | 0,6,6 | - | - | - | | |
| 60 | OHX | 23SB | 3457 | - | 0,6,6 | - | - | - | | |
| 60 | OHX | 23SA | 3586 | - | 0,6,6 | - | - | - | | |
| 60 | OHX | 23SB | 3387 | 62 | 0,6,6 | - | - | - | | |

| Mol | Type | Chain | Res | Link | Bond lengths | | | Bond angles | | |
|---|---|---|---|---|---|---|---|---|---|---|
| | | | | | Counts | RMSZ | $\#\|Z\|>2$ | Counts | RMSZ | $\#\|Z\|>2$ |
| 60 | OHX | 23SB | 3404 | - | 0,6,6 | - | - | - | | |
| 60 | OHX | 16SA | 2401 | - | 0,6,6 | - | - | - | | |
| 60 | OHX | 16SB | 2329 | - | 0,6,6 | - | - | - | | |
| 60 | OHX | 23SA | 3557 | - | 0,6,6 | - | - | - | | |
| 60 | OHX | 23SB | 3343 | - | 0,6,6 | - | - | - | | |
| 60 | OHX | 23SA | 3588 | - | 0,6,6 | - | - | - | | |
| 60 | OHX | 23SB | 3353 | - | 0,6,6 | - | - | - | | |
| 60 | OHX | 16SA | 2374 | - | 0,6,6 | - | - | - | | |
| 60 | OHX | 23SB | 3380 | - | 0,6,6 | - | - | - | | |
| 60 | OHX | 16SA | 2388 | - | 0,6,6 | - | - | - | | |
| 60 | OHX | ASIA | 103 | - | 0,6,6 | - | - | - | | |
| 60 | OHX | 23SA | 3468 | - | 0,6,6 | - | - | - | | |
| 60 | OHX | 23SA | 3541 | - | 0,6,6 | - | - | - | | |
| 60 | OHX | 16SB | 2359 | - | 0,6,6 | - | - | - | | |
| 60 | OHX | 23SB | 3515 | - | 0,6,6 | - | - | - | | |
| 60 | OHX | 23SB | 3356 | - | 0,6,6 | - | - | - | | |
| 60 | OHX | ASIA | 102 | - | 0,6,6 | - | - | - | | |
| 60 | OHX | 23SA | 3512 | - | 0,6,6 | - | - | - | | |
| 60 | OHX | 16SB | 2393 | - | 0,6,6 | - | - | - | | |
| 60 | OHX | 23SB | 3350 | - | 0,6,6 | - | - | - | | |
| 60 | OHX | 23SB | 3425 | - | 0,6,6 | - | - | - | | |
| 60 | OHX | 16SA | 2358 | - | 0,6,6 | - | - | - | | |
| 60 | OHX | 16SB | 2382 | - | 0,6,6 | - | - | - | | |
| 60 | OHX | 23SA | 3535 | - | 0,6,6 | - | - | - | | |
| 60 | OHX | 16SA | 2397 | - | 0,6,6 | - | - | - | | |
| 60 | OHX | 16SA | 2411 | - | 0,6,6 | - | - | - | | |
| 60 | OHX | 23SA | 3514 | - | 0,6,6 | - | - | - | | |
| 60 | OHX | 23SB | 3483 | - | 0,6,6 | - | - | - | | |
| 60 | OHX | 23SA | 3565 | - | 0,6,6 | - | - | - | | |
| 60 | OHX | 23SA | 3509 | - | 0,6,6 | - | - | - | | |
| 60 | OHX | 23SA | 3491 | - | 0,6,6 | - | - | - | | |
| 60 | OHX | 23SA | 3460 | - | 0,6,6 | - | - | - | | |
| 60 | OHX | TRNA | 102 | - | 0,6,6 | - | - | - | | |
| 60 | OHX | 16SA | 2346 | - | 0,6,6 | - | - | - | | |
| 60 | OHX | 23SB | 3422 | - | 0,6,6 | - | - | - | | |
| 60 | OHX | 23SA | 3506 | - | 0,6,6 | - | - | - | | |
| 60 | OHX | 23SA | 3551 | - | 0,6,6 | - | - | - | | |
| 60 | OHX | 23SB | 3373 | - | 0,6,6 | - | - | - | | |
| 60 | OHX | 23SA | 3441 | 27 | 0,6,6 | - | - | - | | |
| 60 | OHX | 23SA | 3585 | - | 0,6,6 | - | - | - | | |
| 60 | OHX | 5SA | 214 | - | 0,6,6 | - | - | - | | |
| 60 | OHX | 16SB | 2347 | - | 0,6,6 | - | - | - | | |
| 60 | OHX | 16SA | 2416 | 1 | 0,6,6 | - | - | - | | |

| Mol | Type | Chain | Res | Link | Bond lengths | | | Bond angles | | |
|---|---|---|---|---|---|---|---|---|---|---|
| | | | | | Counts | RMSZ | $\#\|Z\|>2$ | Counts | RMSZ | $\#\|Z\|>2$ |
| 60 | OHX | 16SA | 2400 | - | 0,6,6 | - | - | - | | |
| 60 | OHX | 16SA | 2337 | - | 0,6,6 | - | - | - | | |
| 60 | OHX | 23SA | 3513 | - | 0,6,6 | - | - | - | | |
| 60 | OHX | 23SA | 3554 | - | 0,6,6 | - | - | - | | |
| 60 | OHX | 16SA | 2369 | - | 0,6,6 | - | - | - | | |
| 60 | OHX | 23SB | 3397 | - | 0,6,6 | - | - | - | | |
| 60 | OHX | L19A | 201 | 41 | 0,6,6 | - | - | - | | |
| 60 | OHX | 5SA | 213 | - | 0,6,6 | - | - | - | | |
| 60 | OHX | 23SB | 3408 | - | 0,6,6 | - | - | - | | |
| 60 | OHX | PSIB | 106 | - | 0,6,6 | - | - | - | | |
| 60 | OHX | 16SA | 2380 | - | 0,6,6 | - | - | - | | |
| 60 | OHX | 23SA | 3600 | - | 0,6,6 | - | - | - | | |
| 60 | OHX | 23SA | 3521 | - | 0,6,6 | - | - | - | | |
| 60 | OHX | 23SA | 3447 | - | 0,6,6 | - | - | - | | |
| 60 | OHX | 23SA | 3515 | - | 0,6,6 | - | - | - | | |
| 60 | OHX | ASIB | 103 | - | 0,6,6 | - | - | - | | |
| 60 | OHX | 23SA | 3578 | - | 0,6,6 | - | - | - | | |
| 60 | OHX | 23SB | 3458 | - | 0,6,6 | - | - | - | | |
| 60 | OHX | 23SA | 3571 | - | 0,6,6 | - | - | - | | |
| 60 | OHX | 23SA | 3448 | - | 0,6,6 | - | - | - | | |
| 60 | OHX | 16SB | 2388 | - | 0,6,6 | - | - | - | | |
| 60 | OHX | 23SB | 3368 | - | 0,6,6 | - | - | - | | |
| 60 | OHX | 16SA | 2404 | - | 0,6,6 | - | - | - | | |
| 60 | OHX | 23SB | 3391 | - | 0,6,6 | - | - | - | | |
| 60 | OHX | 23SB | 3477 | - | 0,6,6 | - | - | - | | |
| 60 | OHX | PSIB | 104 | - | 0,6,6 | - | - | - | | |
| 60 | OHX | 23SA | 3609 | - | 0,6,6 | - | - | - | | |
| 60 | OHX | 16SB | 2365 | - | 0,6,6 | - | - | - | | |
| 60 | OHX | 23SA | 3574 | - | 0,6,6 | - | - | - | | |
| 60 | OHX | 23SB | 3428 | - | 0,6,6 | - | - | - | | |
| 60 | OHX | 16SA | 2370 | - | 0,6,6 | - | - | - | | |
| 60 | OHX | 16SB | 2328 | - | 0,6,6 | - | - | - | | |
| 60 | OHX | ASIB | 101 | - | 0,6,6 | - | - | - | | |
| 60 | OHX | 16SA | 2387 | - | 0,6,6 | - | - | - | | |
| 60 | OHX | 16SA | 2409 | - | 0,6,6 | - | - | - | | |
| 60 | OHX | 23SB | 3445 | - | 0,6,6 | - | - | - | | |
| 60 | OHX | 16SB | 2333 | - | 0,6,6 | - | - | - | | |
| 60 | OHX | 23SA | 3550 | - | 0,6,6 | - | - | - | | |
| 60 | OHX | 23SA | 3501 | - | 0,6,6 | - | - | - | | |
| 60 | OHX | 23SA | 3594 | - | 0,6,6 | - | - | - | | |
| 60 | OHX | 23SA | 3604 | - | 0,6,6 | - | - | - | | |
| 60 | OHX | 16SA | 2340 | - | 0,6,6 | - | - | - | | |
| 60 | OHX | 23SA | 3612 | - | 0,6,6 | - | - | - | | |

| Mol | Type | Chain | Res | Link | Bond lengths | | | Bond angles | | |
|---|---|---|---|---|---|---|---|---|---|---|
| | | | | | Counts | RMSZ | $\#\|Z\| > 2$ | Counts | RMSZ | $\#\|Z\| > 2$ |
| 60 | OHX | 23SA | 3520 | - | 0,6,6 | - | - | - | | |
| 60 | OHX | 23SB | 3511 | - | 0,6,6 | - | - | - | | |
| 60 | OHX | 23SB | 3494 | - | 0,6,6 | - | - | - | | |
| 60 | OHX | 23SB | 3497 | - | 0,6,6 | - | - | - | | |
| 60 | OHX | 23SB | 3392 | - | 0,6,6 | - | - | - | | |
| 60 | OHX | 23SA | 3464 | - | 0,6,6 | - | - | - | | |
| 60 | OHX | 23SA | 3616 | - | 0,6,6 | - | - | - | | |
| 60 | OHX | 23SB | 3410 | - | 0,6,6 | - | - | - | | |
| 60 | OHX | 23SB | 3453 | - | 0,6,6 | - | - | - | | |
| 60 | OHX | 16SB | 2373 | - | 0,6,6 | - | - | - | | |
| 60 | OHX | S8B | 201 | - | 0,6,6 | - | - | - | | |
| 60 | OHX | 16SB | 2360 | 1 | 0,6,6 | - | - | - | | |
| 60 | OHX | 23SA | 3499 | - | 0,6,6 | - | - | - | | |
| 60 | OHX | 16SB | 2361 | - | 0,6,6 | - | - | - | | |
| 60 | OHX | 16SB | 2397 | - | 0,6,6 | - | - | - | | |
| 60 | OHX | 23SB | 3442 | - | 0,6,6 | - | - | - | | |
| 60 | OHX | 23SB | 3451 | - | 0,6,6 | - | - | - | | |
| 60 | OHX | 16SA | 2365 | - | 0,6,6 | - | - | - | | |
| 60 | OHX | 16SA | 2405 | - | 0,6,6 | - | - | - | | |
| 60 | OHX | 23SB | 3367 | - | 0,6,6 | - | - | - | | |
| 60 | OHX | 23SA | 3511 | - | 0,6,6 | - | - | - | | |
| 60 | OHX | 16SB | 2332 | - | 0,6,6 | - | - | - | | |
| 60 | OHX | 23SB | 3513 | - | 0,6,6 | - | - | - | | |
| 60 | OHX | 23SB | 3433 | - | 0,6,6 | - | - | - | | |
| 60 | OHX | 16SA | 2362 | - | 0,6,6 | - | - | - | | |
| 60 | OHX | 23SB | 3331 | - | 0,6,6 | - | - | - | | |
| 60 | OHX | 23SB | 3396 | - | 0,6,6 | - | - | - | | |
| 60 | OHX | 23SB | 3329 | - | 0,6,6 | - | - | - | | |
| 60 | OHX | 23SB | 3490 | - | 0,6,6 | - | - | - | | |
| 60 | OHX | 23SA | 3608 | 27 | 0,6,6 | - | - | - | | |
| 60 | OHX | 23SA | 3503 | - | 0,6,6 | - | - | - | | |
| 60 | OHX | 23SA | 3451 | - | 0,6,6 | - | - | - | | |
| 60 | OHX | 16SA | 2347 | - | 0,6,6 | - | - | - | | |
| 60 | OHX | 23SB | 3358 | - | 0,6,6 | - | - | - | | |
| 60 | OHX | 23SB | 3504 | - | 0,6,6 | - | - | - | | |
| 60 | OHX | 16SA | 2412 | - | 0,6,6 | - | - | - | | |
| 60 | OHX | 23SA | 3593 | - | 0,6,6 | - | - | - | | |
| 60 | OHX | L17B | 201 | - | 0,6,6 | - | - | - | | |
| 60 | OHX | 16SA | 2352 | - | 0,6,6 | - | - | - | | |
| 60 | OHX | 23SA | 3590 | - | 0,6,6 | - | - | - | | |
| 60 | OHX | 23SA | 3478 | - | 0,6,6 | - | - | - | | |
| 60 | OHX | 23SB | 3423 | - | 0,6,6 | - | - | - | | |
| 60 | OHX | 16SA | 2375 | - | 0,6,6 | - | - | - | | |

| Mol | Type | Chain | Res | Link | Bond lengths | | | Bond angles | | |
|---|---|---|---|---|---|---|---|---|---|---|
| | | | | | Counts | RMSZ | $\#\|Z\|>2$ | Counts | RMSZ | $\#\|Z\|>2$ |
| 60 | OHX | 23SB | 3473 | - | 0,6,6 | - | - | - | | |
| 60 | OHX | 23SA | 3610 | - | 0,6,6 | - | - | - | | |
| 60 | OHX | 23SA | 3461 | - | 0,6,6 | - | - | - | | |
| 60 | OHX | 23SA | 3510 | - | 0,6,6 | - | - | - | | |
| 60 | OHX | 23SB | 3335 | - | 0,6,6 | - | - | - | | |
| 60 | OHX | 23SB | 3372 | - | 0,6,6 | - | - | - | | |
| 61 | SJH | 23SA | 3436 | - | 83,87,87 | 2.34 | 21 (25%) | 108,128,128 | 1.85 | 20 (18%) |
| 60 | OHX | 16SB | 2325 | - | 0,6,6 | - | - | - | | |
| 60 | OHX | 23SA | 3533 | - | 0,6,6 | - | - | - | | |
| 60 | OHX | 23SA | 3626 | - | 0,6,6 | - | - | - | | |
| 60 | OHX | 23SA | 3500 | - | 0,6,6 | - | - | - | | |
| 60 | OHX | 16SB | 2346 | - | 0,6,6 | - | - | - | | |
| 60 | OHX | 23SB | 3459 | 27 | 0,6,6 | - | - | - | | |
| 60 | OHX | 23SA | 3561 | - | 0,6,6 | - | - | - | | |
| 60 | OHX | 23SA | 3576 | - | 0,6,6 | - | - | - | | |
| 60 | OHX | 16SB | 2379 | - | 0,6,6 | - | - | - | | |
| 60 | OHX | 23SB | 3328 | - | 0,6,6 | - | - | - | | |
| 60 | OHX | 23SB | 3501 | - | 0,6,6 | - | - | - | | |
| 60 | OHX | 23SB | 3463 | - | 0,6,6 | - | - | - | | |
| 60 | OHX | 23SB | 3381 | - | 0,6,6 | - | - | - | | |
| 60 | OHX | 23SA | 3504 | - | 0,6,6 | - | - | - | | |
| 60 | OHX | 23SB | 3326 | - | 0,6,6 | - | - | - | | |
| 60 | OHX | PSIA | 105 | - | 0,6,6 | - | - | - | | |
| 60 | OHX | 16SB | 2337 | - | 0,6,6 | - | - | - | | |
| 60 | OHX | 16SA | 2368 | - | 0,6,6 | - | - | - | | |
| 60 | OHX | 16SA | 2395 | - | 0,6,6 | - | - | - | | |
| 60 | OHX | 23SB | 3484 | - | 0,6,6 | - | - | - | | |
| 60 | OHX | 23SA | 3548 | - | 0,6,6 | - | - | - | | |
| 60 | OHX | 23SB | 3432 | - | 0,6,6 | - | - | - | | |
| 60 | OHX | 16SA | 2390 | - | 0,6,6 | - | - | - | | |
| 60 | OHX | 23SB | 3467 | - | 0,6,6 | - | - | - | | |
| 60 | OHX | 23SA | 3543 | - | 0,6,6 | - | - | - | | |
| 60 | OHX | 16SB | 2344 | - | 0,6,6 | - | - | - | | |
| 60 | OHX | 23SA | 3552 | - | 0,6,6 | - | - | - | | |
| 60 | OHX | 23SB | 3472 | - | 0,6,6 | - | - | - | | |
| 60 | OHX | 23SB | 3486 | - | 0,6,6 | - | - | - | | |
| 60 | OHX | 23SB | 3462 | - | 0,6,6 | - | - | - | | |
| 60 | OHX | 16SA | 2377 | - | 0,6,6 | - | - | - | | |
| 60 | OHX | 23SB | 3363 | - | 0,6,6 | - | - | - | | |
| 60 | OHX | 23SA | 3525 | - | 0,6,6 | - | - | - | | |
| 60 | OHX | 23SB | 3409 | - | 0,6,6 | - | - | - | | |
| 60 | OHX | 16SA | 2410 | - | 0,6,6 | - | - | - | | |
| 60 | OHX | 16SB | 2366 | 1 | 0,6,6 | - | - | - | | |

| Mol | Type | Chain | Res | Link | Bond lengths | | | Bond angles | | |
|---|---|---|---|---|---|---|---|---|---|---|
| | | | | | Counts | RMSZ | $\#\|Z\|>2$ | Counts | RMSZ | $\#\|Z\|>2$ |
| 60 | OHX | 23SB | 3334 | - | 0,6,6 | - | - | - | | |
| 60 | OHX | 23SB | 3502 | - | 0,6,6 | - | - | - | | |
| 60 | OHX | 5SA | 212 | - | 0,6,6 | - | - | - | | |
| 60 | OHX | PSIB | 105 | - | 0,6,6 | - | - | - | | |
| 60 | OHX | 23SB | 3464 | - | 0,6,6 | - | - | - | | |
| 60 | OHX | 23SB | 3383 | - | 0,6,6 | - | - | - | | |
| 60 | OHX | 23SB | 3338 | - | 0,6,6 | - | - | - | | |
| 60 | OHX | 23SB | 3401 | - | 0,6,6 | - | - | - | | |
| 60 | OHX | 23SB | 3469 | - | 0,6,6 | - | - | - | | |
| 60 | OHX | 23SB | 3359 | - | 0,6,6 | - | - | - | | |
| 60 | OHX | 23SB | 3492 | - | 0,6,6 | - | - | - | | |
| 60 | OHX | 23SA | 3471 | - | 0,6,6 | - | - | - | | |
| 60 | OHX | 16SA | 2361 | - | 0,6,6 | - | - | - | | |
| 60 | OHX | 16SB | 2387 | - | 0,6,6 | - | - | - | | |
| 60 | OHX | 23SB | 3460 | - | 0,6,6 | - | - | - | | |
| 60 | OHX | 16SB | 2350 | - | 0,6,6 | - | - | - | | |
| 60 | OHX | 23SA | 3481 | - | 0,6,6 | - | - | - | | |
| 60 | OHX | 23SB | 3389 | - | 0,6,6 | - | - | - | | |
| 60 | OHX | 23SB | 3507 | - | 0,6,6 | - | - | - | | |
| 60 | OHX | 16SB | 2342 | - | 0,6,6 | - | - | - | | |
| 60 | OHX | 16SA | 2348 | - | 0,6,6 | - | - | - | | |
| 60 | OHX | 23SB | 3394 | - | 0,6,6 | - | - | - | | |
| 60 | OHX | 23SA | 3596 | - | 0,6,6 | - | - | - | | |
| 60 | OHX | 16SB | 2358 | 1 | 0,6,6 | - | - | - | | |
| 60 | OHX | TRNA | 101 | - | 0,6,6 | - | - | - | | |
| 60 | OHX | 23SA | 3595 | - | 0,6,6 | - | - | - | | |
| 60 | OHX | 23SA | 3584 | - | 0,6,6 | - | - | - | | |
| 60 | OHX | 23SA | 3438 | - | 0,6,6 | - | - | - | | |
| 60 | OHX | 16SB | 2364 | - | 0,6,6 | - | - | - | | |
| 60 | OHX | 23SA | 3523 | - | 0,6,6 | - | - | - | | |
| 60 | OHX | L27A | 104 | - | 0,6,6 | - | - | - | | |
| 60 | OHX | 23SB | 3421 | - | 0,6,6 | - | - | - | | |
| 60 | OHX | 16SA | 2372 | - | 0,6,6 | - | - | - | | |
| 60 | OHX | ASIB | 102 | - | 0,6,6 | - | - | - | | |
| 60 | OHX | 23SB | 3348 | - | 0,6,6 | - | - | - | | |
| 60 | OHX | 5SB | 212 | - | 0,6,6 | - | - | - | | |
| 60 | OHX | 23SA | 3623 | - | 0,6,6 | - | - | - | | |
| 60 | OHX | 16SA | 2350 | - | 0,6,6 | - | - | - | | |
| 60 | OHX | 23SA | 3615 | - | 0,6,6 | - | - | - | | |

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 |
|---|---|---|---|---|---|---|---|
| 61 | SJH | 23SA | 3436 | - | - | 36/95/153/153 | 0/5/5/5 |
| 61 | SJH | 23SB | 3323 | - | - | 36/95/153/153 | 0/5/5/5 |

All (41) bond length outliers are listed below:

| Mol | Chain | Res | Type | Atoms | Z | Observed(Å) | Ideal(Å) |
|---|---|---|---|---|---|---|---|
| 61 | 23SB | 3323 | SJH | C18-N20 | 7.38 | 1.49 | 1.34 |
| 61 | 23SA | 3436 | SJH | C18-N20 | 7.37 | 1.49 | 1.34 |
| 61 | 23SA | 3436 | SJH | C14-C15 | 6.51 | 1.64 | 1.53 |
| 61 | 23SB | 3323 | SJH | C14-C15 | 6.49 | 1.64 | 1.53 |
| 61 | 23SB | 3323 | SJH | C25-C24 | 6.30 | 1.59 | 1.49 |
| 61 | 23SA | 3436 | SJH | C25-C24 | 6.28 | 1.59 | 1.49 |
| 61 | 23SA | 3436 | SJH | O47-C48 | 6.25 | 1.48 | 1.34 |
| 61 | 23SB | 3323 | SJH | O47-C48 | 6.24 | 1.48 | 1.34 |
| 61 | 23SA | 3436 | SJH | O17-C18 | 6.23 | 1.46 | 1.34 |
| 61 | 23SB | 3323 | SJH | O17-C18 | 6.23 | 1.46 | 1.34 |
| 61 | 23SB | 3323 | SJH | C28-N23 | -6.15 | 1.33 | 1.38 |
| 61 | 23SA | 3436 | SJH | C28-N23 | -6.10 | 1.33 | 1.38 |
| 61 | 23SA | 3436 | SJH | O17-C15 | -4.69 | 1.39 | 1.46 |
| 61 | 23SB | 3323 | SJH | O17-C15 | -4.68 | 1.39 | 1.46 |
| 61 | 23SB | 3323 | SJH | C40-C38 | 4.42 | 1.59 | 1.50 |
| 61 | 23SA | 3436 | SJH | C40-C38 | 4.40 | 1.59 | 1.50 |
| 61 | 23SB | 3323 | SJH | O37-C38 | 3.54 | 1.44 | 1.34 |
| 61 | 23SA | 3436 | SJH | O37-C38 | 3.54 | 1.44 | 1.34 |
| 61 | 23SA | 3436 | SJH | O71-C70 | 3.28 | 1.50 | 1.41 |
| 61 | 23SB | 3323 | SJH | O71-C70 | 3.26 | 1.50 | 1.41 |
| 61 | 23SB | 3323 | SJH | C56-C59 | -3.06 | 1.47 | 1.53 |
| 61 | 23SA | 3436 | SJH | C56-C59 | -3.05 | 1.47 | 1.53 |
| 61 | 23SA | 3436 | SJH | C24-N23 | -3.01 | 1.32 | 1.37 |
| 61 | 23SB | 3323 | SJH | C24-N23 | -3.00 | 1.32 | 1.37 |
| 61 | 23SB | 3323 | SJH | O69-C68 | 2.95 | 1.48 | 1.43 |
| 61 | 23SA | 3436 | SJH | O69-C68 | 2.92 | 1.48 | 1.43 |
| 61 | 23SA | 3436 | SJH | O37-C36 | -2.72 | 1.40 | 1.44 |
| 61 | 23SB | 3323 | SJH | O37-C36 | -2.68 | 1.40 | 1.44 |
| 61 | 23SA | 3436 | SJH | O30-N29 | -2.53 | 1.18 | 1.22 |
| 61 | 23SB | 3323 | SJH | O30-N29 | -2.52 | 1.18 | 1.22 |
| 61 | 23SB | 3323 | SJH | O10-C11 | -2.23 | 1.38 | 1.43 |
| 61 | 23SA | 3436 | SJH | O10-C11 | -2.22 | 1.38 | 1.43 |
| 61 | 23SA | 3436 | SJH | O63-C61 | 2.21 | 1.49 | 1.44 |
| 61 | 23SB | 3323 | SJH | O63-C61 | 2.21 | 1.49 | 1.44 |
| 61 | 23SA | 3436 | SJH | C50-C48 | 2.16 | 1.56 | 1.51 |

*Continued on next page...*

*Continued from previous page...*

| Mol | Chain | Res | Type | Atoms | Z | Observed(Å) | Ideal(Å) |
|---|---|---|---|---|---|---|---|
| 61 | 23SB | 3323 | SJH | C50-C48 | 2.14 | 1.56 | 1.51 |
| 61 | 23SA | 3436 | SJH | C55-C56 | -2.08 | 1.49 | 1.53 |
| 61 | 23SB | 3323 | SJH | C55-C56 | -2.08 | 1.49 | 1.53 |
| 61 | 23SB | 3323 | SJH | C14-C12 | 2.07 | 1.57 | 1.54 |
| 61 | 23SA | 3436 | SJH | C14-C12 | 2.03 | 1.56 | 1.54 |
| 61 | 23SA | 3436 | SJH | C27-C28 | 2.01 | 1.38 | 1.36 |

All (40) bond angle outliers are listed below:

| Mol | Chain | Res | Type | Atoms | Z | Observed($^o$) | Ideal($^o$) |
|---|---|---|---|---|---|---|---|
| 61 | 23SB | 3323 | SJH | O17-C18-N20 | 7.58 | 120.75 | 110.00 |
| 61 | 23SA | 3436 | SJH | O17-C18-N20 | 7.57 | 120.75 | 110.00 |
| 61 | 23SB | 3323 | SJH | C05-C04-N03 | -5.79 | 120.17 | 126.93 |
| 61 | 23SA | 3436 | SJH | C05-C04-N03 | -5.78 | 120.19 | 126.93 |
| 61 | 23SA | 3436 | SJH | O37-C38-C40 | 5.49 | 121.28 | 111.43 |
| 61 | 23SB | 3323 | SJH | O37-C38-C40 | 5.49 | 121.26 | 111.43 |
| 61 | 23SA | 3436 | SJH | C28-N23-C24 | 5.39 | 107.97 | 105.25 |
| 61 | 23SB | 3323 | SJH | C28-N23-C24 | 5.36 | 107.95 | 105.25 |
| 61 | 23SA | 3436 | SJH | C22-N23-C28 | -4.66 | 124.94 | 128.94 |
| 61 | 23SB | 3323 | SJH | C22-N23-C28 | -4.61 | 124.98 | 128.94 |
| 61 | 23SB | 3323 | SJH | O47-C48-C50 | 4.18 | 120.46 | 111.53 |
| 61 | 23SA | 3436 | SJH | O47-C48-C50 | 4.18 | 120.46 | 111.53 |
| 61 | 23SA | 3436 | SJH | O19-C18-N20 | -4.05 | 118.84 | 124.93 |
| 61 | 23SB | 3323 | SJH | O19-C18-N20 | -4.04 | 118.84 | 124.93 |
| 61 | 23SB | 3323 | SJH | O08-C06-C05 | 3.20 | 113.08 | 108.62 |
| 61 | 23SA | 3436 | SJH | O08-C06-C05 | 3.18 | 113.05 | 108.62 |
| 61 | 23SB | 3323 | SJH | N23-C24-N26 | -3.10 | 109.41 | 111.72 |
| 61 | 23SA | 3436 | SJH | N23-C24-N26 | -3.10 | 109.42 | 111.72 |
| 61 | 23SB | 3323 | SJH | O17-C18-O19 | -2.95 | 120.40 | 125.64 |
| 61 | 23SA | 3436 | SJH | O17-C18-O19 | -2.94 | 120.41 | 125.64 |
| 61 | 23SA | 3436 | SJH | C28-C27-N26 | -2.67 | 106.59 | 109.66 |
| 61 | 23SB | 3323 | SJH | C28-C27-N26 | -2.66 | 106.60 | 109.66 |
| 61 | 23SB | 3323 | SJH | C07-C06-C05 | -2.64 | 108.52 | 113.27 |
| 61 | 23SA | 3436 | SJH | C07-C06-C05 | -2.64 | 108.52 | 113.27 |
| 61 | 23SA | 3436 | SJH | C27-N26-C24 | 2.55 | 108.42 | 106.03 |
| 61 | 23SB | 3323 | SJH | C27-N26-C24 | 2.55 | 108.41 | 106.03 |
| 61 | 23SA | 3436 | SJH | C73-C72-C74 | -2.45 | 108.60 | 113.08 |
| 61 | 23SB | 3323 | SJH | O39-C38-C40 | -2.45 | 118.97 | 124.65 |
| 61 | 23SA | 3436 | SJH | O39-C38-C40 | -2.44 | 118.97 | 124.65 |
| 61 | 23SB | 3323 | SJH | C73-C72-C74 | -2.44 | 108.62 | 113.08 |
| 61 | 23SA | 3436 | SJH | C62-C61-C59 | -2.40 | 108.61 | 112.58 |
| 61 | 23SB | 3323 | SJH | C62-C61-C59 | -2.40 | 108.61 | 112.58 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed($^o$) | Ideal($^o$) |
|---|---|---|---|---|---|---|---|
| 61 | 23SA | 3436 | SJH | O47-C48-O49 | -2.27 | 119.86 | 123.95 |
| 61 | 23SB | 3323 | SJH | O47-C48-O49 | -2.26 | 119.87 | 123.95 |
| 61 | 23SB | 3323 | SJH | C46-O47-C48 | -2.14 | 114.22 | 117.76 |
| 61 | 23SA | 3436 | SJH | C46-O47-C48 | -2.13 | 114.22 | 117.76 |
| 61 | 23SB | 3323 | SJH | C55-C56-C59 | 2.09 | 113.40 | 107.90 |
| 61 | 23SA | 3436 | SJH | C55-C56-C59 | 2.09 | 113.39 | 107.90 |
| 61 | 23SA | 3436 | SJH | C66-C46-C44 | -2.08 | 108.73 | 114.29 |
| 61 | 23SB | 3323 | SJH | C66-C46-C44 | -2.08 | 108.73 | 114.29 |

There are no chirality outliers.

All (72) torsion outliers are listed below:

| Mol | Chain | Res | Type | Atoms |
|---|---|---|---|---|
| 61 | 23SA | 3436 | SJH | C12-C14-C15-C16 |
| 61 | 23SA | 3436 | SJH | C12-C14-C15-O17 |
| 61 | 23SA | 3436 | SJH | C16-C15-C32-C34 |
| 61 | 23SA | 3436 | SJH | O17-C15-C32-O33 |
| 61 | 23SA | 3436 | SJH | O17-C18-N20-C21 |
| 61 | 23SA | 3436 | SJH | O19-C18-N20-C21 |
| 61 | 23SA | 3436 | SJH | C05-C04-N03-O02 |
| 61 | 23SA | 3436 | SJH | C21-C22-N23-C24 |
| 61 | 23SA | 3436 | SJH | C21-C22-N23-C28 |
| 61 | 23SA | 3436 | SJH | C27-C28-N29-O30 |
| 61 | 23SA | 3436 | SJH | N23-C28-N29-O30 |
| 61 | 23SA | 3436 | SJH | C32-C34-C36-O37 |
| 61 | 23SA | 3436 | SJH | C35-C34-C36-O37 |
| 61 | 23SA | 3436 | SJH | C34-C36-C44-C45 |
| 61 | 23SA | 3436 | SJH | O37-C36-C44-C45 |
| 61 | 23SA | 3436 | SJH | O37-C36-C44-C46 |
| 61 | 23SA | 3436 | SJH | C40-C38-O37-C36 |
| 61 | 23SA | 3436 | SJH | O39-C38-O37-C36 |
| 61 | 23SA | 3436 | SJH | C04-N03-O02-C01 |
| 61 | 23SB | 3323 | SJH | C12-C14-C15-C16 |
| 61 | 23SB | 3323 | SJH | C12-C14-C15-O17 |
| 61 | 23SB | 3323 | SJH | C16-C15-C32-C34 |
| 61 | 23SB | 3323 | SJH | O17-C15-C32-O33 |
| 61 | 23SB | 3323 | SJH | O17-C18-N20-C21 |
| 61 | 23SB | 3323 | SJH | O19-C18-N20-C21 |
| 61 | 23SB | 3323 | SJH | C05-C04-N03-O02 |
| 61 | 23SB | 3323 | SJH | C21-C22-N23-C24 |
| 61 | 23SB | 3323 | SJH | C21-C22-N23-C28 |
| 61 | 23SB | 3323 | SJH | C27-C28-N29-O30 |

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| Mol | Chain | Res | Type | Atoms |
|---|---|---|---|---|
| 61 | 23SB | 3323 | SJH | N23-C28-N29-O30 |
| 61 | 23SB | 3323 | SJH | C32-C34-C36-O37 |
| 61 | 23SB | 3323 | SJH | C35-C34-C36-O37 |
| 61 | 23SB | 3323 | SJH | C34-C36-C44-C45 |
| 61 | 23SB | 3323 | SJH | O37-C36-C44-C45 |
| 61 | 23SB | 3323 | SJH | O37-C36-C44-C46 |
| 61 | 23SB | 3323 | SJH | C40-C38-O37-C36 |
| 61 | 23SB | 3323 | SJH | O39-C38-O37-C36 |
| 61 | 23SB | 3323 | SJH | C04-N03-O02-C01 |
| 61 | 23SA | 3436 | SJH | N20-C21-C22-N23 |
| 61 | 23SB | 3323 | SJH | N20-C21-C22-N23 |
| 61 | 23SA | 3436 | SJH | O10-C11-C64-C52 |
| 61 | 23SB | 3323 | SJH | O10-C11-C64-C52 |
| 61 | 23SA | 3436 | SJH | C12-C11-C64-C52 |
| 61 | 23SB | 3323 | SJH | C12-C11-C64-C52 |
| 61 | 23SA | 3436 | SJH | C12-C11-C64-C65 |
| 61 | 23SB | 3323 | SJH | C12-C11-C64-C65 |
| 61 | 23SA | 3436 | SJH | C74-C76-O77-C78 |
| 61 | 23SB | 3323 | SJH | C74-C76-O77-C78 |
| 61 | 23SA | 3436 | SJH | C34-C36-C44-C46 |
| 61 | 23SB | 3323 | SJH | C34-C36-C44-C46 |
| 61 | 23SA | 3436 | SJH | C38-C40-C41-C42 |
| 61 | 23SB | 3323 | SJH | C38-C40-C41-C42 |
| 61 | 23SA | 3436 | SJH | O10-C11-C64-C65 |
| 61 | 23SB | 3323 | SJH | O10-C11-C64-C65 |
| 61 | 23SA | 3436 | SJH | C32-C34-C36-C44 |
| 61 | 23SB | 3323 | SJH | C32-C34-C36-C44 |
| 61 | 23SA | 3436 | SJH | C12-C14-C15-C32 |
| 61 | 23SA | 3436 | SJH | C14-C15-C32-C34 |
| 61 | 23SB | 3323 | SJH | C12-C14-C15-C32 |
| 61 | 23SB | 3323 | SJH | C14-C15-C32-C34 |
| 61 | 23SA | 3436 | SJH | O08-C09-O10-C11 |
| 61 | 23SA | 3436 | SJH | C35-C34-C36-C44 |
| 61 | 23SB | 3323 | SJH | C35-C34-C36-C44 |
| 61 | 23SB | 3323 | SJH | O08-C09-O10-C11 |
| 61 | 23SA | 3436 | SJH | C82-C09-O10-C11 |
| 61 | 23SB | 3323 | SJH | C82-C09-O10-C11 |
| 61 | 23SA | 3436 | SJH | O10-C11-C12-C14 |
| 61 | 23SB | 3323 | SJH | O10-C11-C12-C14 |
| 61 | 23SA | 3436 | SJH | C16-C15-C32-O33 |
| 61 | 23SB | 3323 | SJH | C16-C15-C32-O33 |
| 61 | 23SA | 3436 | SJH | O47-C46-C66-C68 |

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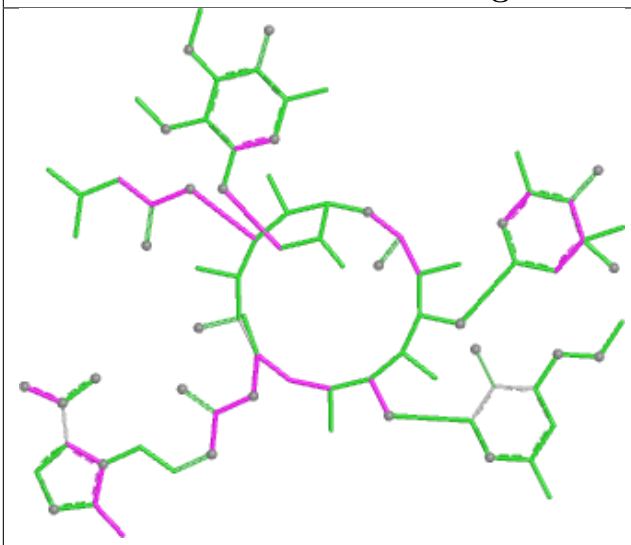
| Mol | Chain | Res | Type | Atoms |
|---|---|---|---|---|
| 61 | 23SB | 3323 | SJH | O47-C46-C66-C68 |

There are no ring outliers.

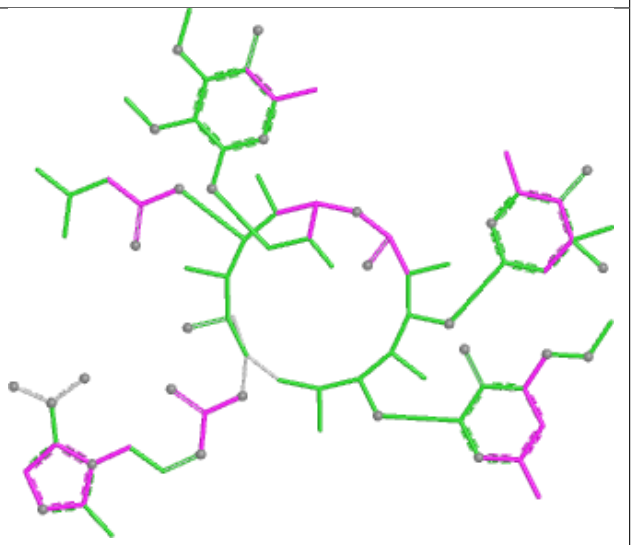
No monomer is involved in short contacts.

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

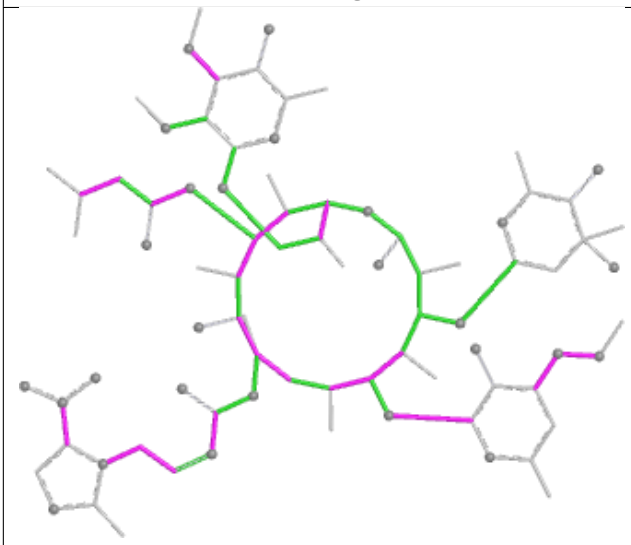
**Ligand SJH 23SB 3323**



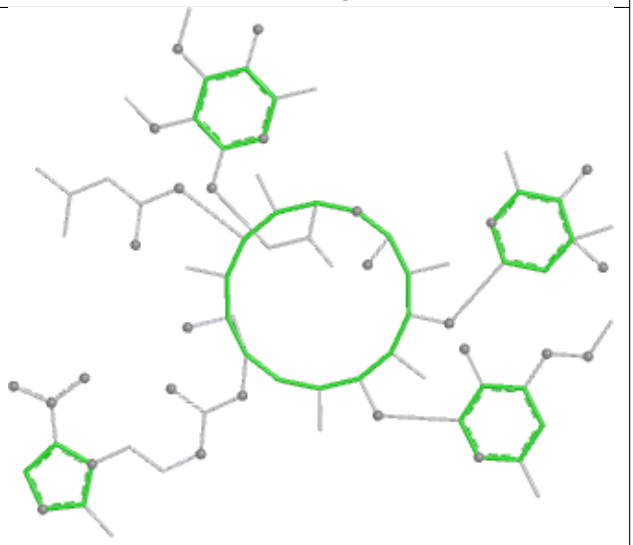
**Bond lengths**



**Bond angles**

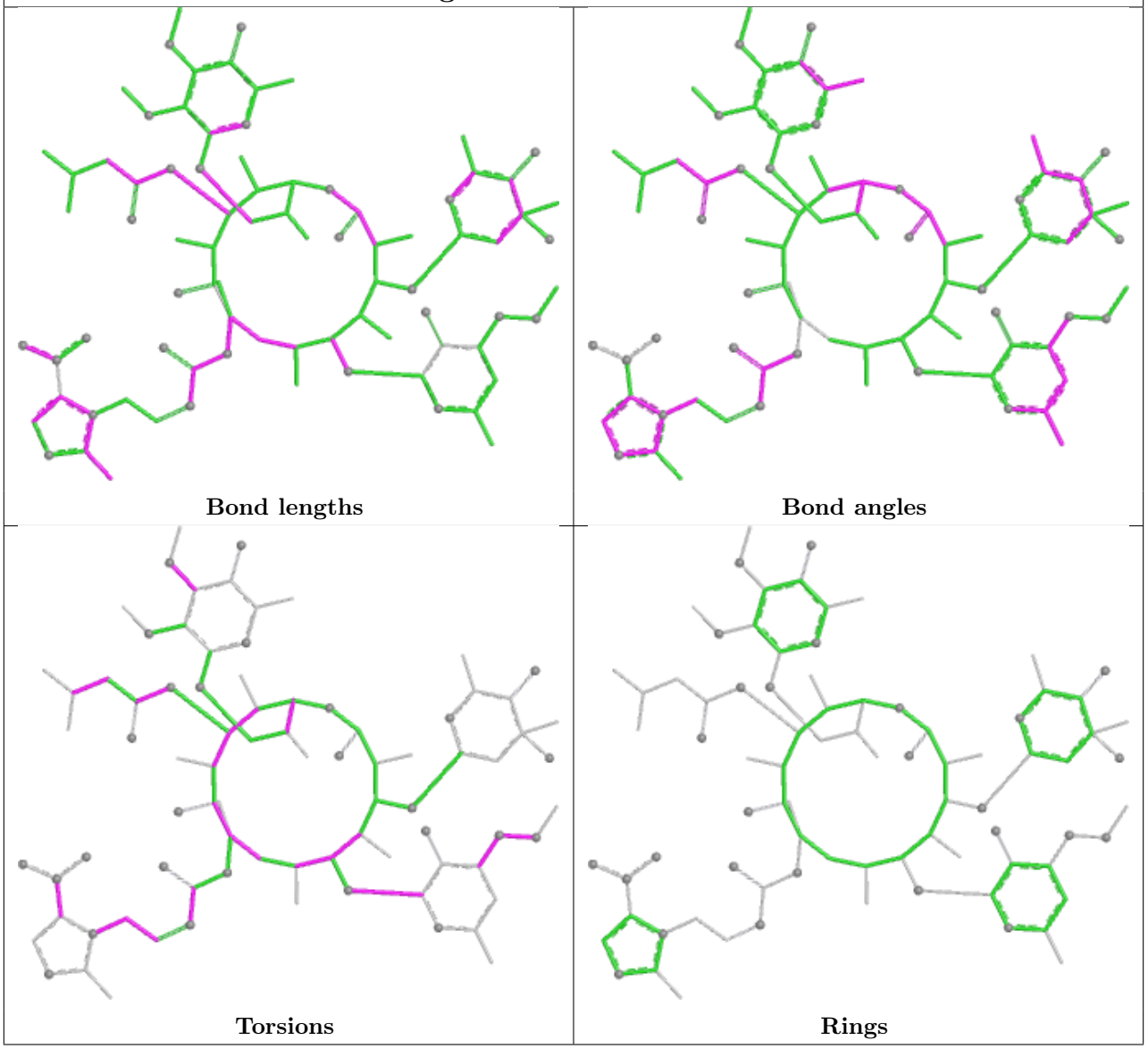


**Torsions**



**Rings**

**Ligand SJH 23SA 3436**




## 5.7 Other polymers (i)

There are no such residues in this entry.

## 5.8 Polymer linkage issues (i)

The following chains have linkage breaks:

| Mol | Chain | Number of breaks |
|---|---|---|
| 7 | S7B | 1 |

All chain breaks are listed below:

| Model | Chain | Residue-1 | Atom-1 | Residue-2 | Atom-2 | Distance (Å) |
|---|---|---|---|---|---|---|
| 1 | S7B | 6:ARG | C | 7:ALA | N | 3.28 |

# 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 | 16SA | 1499/1512 (99%) | 0.56 | 54 (3%) 46 26 | 42, 89, 169, 259 | 0 |
| 1 | 16SB | 1495/1512 (98%) | 0.62 | 30 (2%) 65 44 | 55, 100, 163, 267 | 0 |
| 2 | S2A | 237/256 (92%) | 1.77 | 88 (37%) 1 0 | 90, 125, 163, 177 | 0 |
| 2 | S2B | 237/256 (92%) | 1.91 | 93 (39%) 1 0 | 104, 154, 184, 204 | 0 |
| 3 | S3A | 205/239 (85%) | 2.04 | 97 (47%) 0 0 | 81, 102, 141, 169 | 0 |
| 3 | S3B | 206/239 (86%) | 2.05 | 98 (47%) 0 0 | 104, 129, 156, 162 | 0 |
| 4 | S4A | 208/209 (99%) | 2.55 | 140 (67%) 0 0 | 77, 100, 120, 125 | 0 |
| 4 | S4B | 208/209 (99%) | 2.52 | 134 (64%) 0 0 | 78, 98, 117, 140 | 0 |
| 5 | S5A | 151/162 (93%) | 1.75 | 55 (36%) 1 0 | 66, 88, 109, 135 | 0 |
| 5 | S5B | 151/162 (93%) | 1.81 | 58 (38%) 1 0 | 86, 105, 124, 151 | 0 |
| 6 | S6A | 101/101 (100%) | 1.12 | 6 (5%) 28 15 | 70, 92, 108, 125 | 0 |
| 6 | S6B | 101/101 (100%) | 1.61 | 36 (35%) 1 0 | 72, 93, 110, 132 | 0 |
| 7 | S7A | 155/156 (99%) | 1.38 | 35 (22%) 2 1 | 88, 104, 129, 137 | 0 |
| 7 | S7B | 155/156 (99%) | 1.22 | 32 (20%) 2 1 | 98, 115, 150, 173 | 0 |
| 8 | S8A | 138/138 (100%) | 1.27 | 22 (15%) 5 2 | 77, 92, 105, 112 | 0 |
| 8 | S8B | 138/138 (100%) | 1.65 | 42 (30%) 1 1 | 84, 107, 117, 125 | 0 |
| 9 | S9A | 127/128 (99%) | 1.23 | 23 (18%) 3 1 | 73, 122, 139, 144 | 0 |
| 9 | S9B | 127/128 (99%) | 0.80 | 5 (3%) 43 24 | 97, 136, 153, 155 | 0 |
| 10 | S10A | 99/105 (94%) | 1.57 | 25 (25%) 1 1 | 71, 125, 149, 156 | 0 |
| 10 | S10B | 99/105 (94%) | 1.79 | 33 (33%) 1 0 | 105, 143, 161, 164 | 0 |
| 11 | S11A | 116/129 (89%) | 1.31 | 23 (19%) 3 1 | 58, 89, 112, 143 | 0 |
| 11 | S11B | 117/129 (90%) | 1.63 | 37 (31%) 1 1 | 71, 98, 123, 157 | 0 |
| 12 | S12A | 124/132 (93%) | 1.79 | 45 (36%) 1 0 | 58, 67, 99, 158 | 0 |
| 12 | S12B | 124/132 (93%) | 1.78 | 50 (40%) 0 0 | 69, 87, 114, 167 | 0 |

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| Mol | Chain | Analysed | <RSRZ> | #RSRZ>2 | OWAB(Å$^2$) | Q<0.9 |
|---|---|---|---|---|---|---|
| 13 | S13A | 119/126 (94%) | 1.31 | 22 (18%) 3 1 | 74, 111, 128, 136 | 0 |
| 13 | S13B | 121/126 (96%) | 1.02 | 14 (11%) 9 5 | 98, 138, 149, 159 | 0 |
| 14 | S14A | 60/61 (98%) | 1.48 | 15 (25%) 2 1 | 78, 91, 102, 115 | 0 |
| 14 | S14B | 59/61 (96%) | 1.41 | 13 (22%) 2 1 | 99, 120, 139, 144 | 0 |
| 15 | S15A | 88/89 (98%) | 0.65 | 6 (6%) 23 12 | 62, 83, 108, 117 | 0 |
| 15 | S15B | 88/89 (98%) | 0.97 | 8 (9%) 15 8 | 71, 93, 111, 118 | 0 |
| 16 | S16A | 83/88 (94%) | 1.65 | 22 (26%) 1 1 | 88, 99, 120, 147 | 0 |
| 16 | S16B | 84/88 (95%) | 1.92 | 38 (45%) 0 0 | 78, 89, 108, 143 | 0 |
| 17 | S17A | 100/105 (95%) | 0.93 | 4 (4%) 42 23 | 73, 91, 102, 107 | 0 |
| 17 | S17B | 100/105 (95%) | 1.05 | 13 (13%) 7 4 | 78, 96, 113, 126 | 0 |
| 18 | S18A | 71/88 (80%) | 1.14 | 7 (9%) 13 7 | 70, 86, 121, 148 | 0 |
| 18 | S18B | 70/88 (79%) | 1.73 | 26 (37%) 1 0 | 78, 97, 125, 146 | 0 |
| 19 | S19A | 84/93 (90%) | 1.97 | 34 (40%) 0 0 | 86, 114, 133, 137 | 0 |
| 19 | S19B | 86/93 (92%) | 1.12 | 10 (11%) 9 5 | 127, 150, 175, 187 | 0 |
| 20 | S20A | 99/106 (93%) | 1.47 | 23 (23%) 2 1 | 88, 105, 133, 138 | 0 |
| 20 | S20B | 99/106 (93%) | 1.02 | 10 (10%) 12 6 | 81, 102, 127, 132 | 0 |
| 21 | THXA | 24/27 (88%) | 1.00 | 3 (12%) 8 5 | 88, 100, 111, 129 | 0 |
| 21 | THXB | 25/27 (92%) | 0.51 | 0 100 100 | 111, 126, 141, 146 | 0 |
| 22 | ASIA | 69/76 (90%) | 2.96 | 47 (68%) 0 0 | 70, 184, 222, 237 | 0 |
| 23 | PSIA | 68/76 (89%) | 0.97 | 14 (20%) 2 1 | 60, 86, 105, 153 | 0 |
| 23 | PSIB | 68/76 (89%) | 0.65 | 5 (7%) 20 11 | 73, 101, 133, 166 | 0 |
| 24 | ESIA | 75/76 (98%) | 1.79 | 25 (33%) 1 0 | 62, 190, 215, 221 | 0 |
| 24 | ESIB | 75/76 (98%) | 1.31 | 12 (16%) 5 2 | 71, 195, 220, 233 | 0 |
| 25 | MRNA | 30/30 (100%) | 1.73 | 10 (33%) 1 0 | 60, 151, 237, 249 | 0 |
| 25 | MRNB | 30/30 (100%) | 1.11 | 5 (16%) 4 2 | 79, 167, 236, 242 | 0 |
| 26 | TRNA | 67/76 (88%) | 1.17 | 5 (7%) 20 11 | 106, 174, 201, 215 | 0 |
| 27 | 23SA | 2878/2911 (98%) | -0.29 | 47 (1%) 70 49 | 31, 58, 189, 261 | 0 |
| 27 | 23SB | 2864/2911 (98%) | 0.01 | 50 (1%) 69 48 | 41, 75, 213, 268 | 0 |
| 28 | 5SA | 122/124 (98%) | -0.27 | 1 (0%) 82 65 | 55, 74, 90, 166 | 0 |
| 28 | 5SB | 121/124 (97%) | 0.14 | 4 (3%) 49 29 | 77, 103, 137, 191 | 0 |
| 29 | L2A | 272/276 (98%) | 0.16 | 3 (1%) 78 59 | 30, 50, 67, 83 | 0 |

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| Mol | Chain | Analysed | <RSRZ> | #RSRZ>2 | OWAB(Å$^2$) | Q<0.9 |
|---|---|---|---|---|---|---|
| 29 | L2B | 272/276 (98%) | 0.48 | 7 (2%) 57 36 | 39, 61, 79, 89 | 0 |
| 30 | L3A | 204/206 (99%) | 0.79 | 19 (9%) 14 8 | 39, 69, 96, 111 | 0 |
| 30 | L3B | 204/206 (99%) | 1.27 | 43 (21%) 2 1 | 52, 86, 116, 127 | 0 |
| 31 | L4A | 202/210 (96%) | 0.27 | 8 (3%) 42 23 | 35, 63, 93, 118 | 0 |
| 31 | L4B | 202/210 (96%) | 1.01 | 27 (13%) 7 4 | 44, 82, 113, 129 | 0 |
| 32 | L5A | 181/182 (99%) | 0.98 | 18 (9%) 13 7 | 68, 84, 115, 128 | 0 |
| 32 | L5B | 181/182 (99%) | 0.87 | 10 (5%) 30 16 | 97, 117, 141, 150 | 0 |
| 33 | L6A | 174/180 (96%) | 1.82 | 66 (37%) 1 0 | 73, 95, 114, 138 | 0 |
| 33 | L6B | 173/180 (96%) | 2.64 | 107 (61%) 0 0 | 154, 199, 241, 259 | 0 |
| 34 | L9A | 145/148 (97%) | 1.87 | 57 (39%) 1 0 | 61, 116, 131, 144 | 0 |
| 34 | L9B | 146/148 (98%) | 1.71 | 51 (34%) 1 0 | 73, 114, 136, 151 | 0 |
| 35 | L13A | 138/140 (98%) | 0.84 | 15 (10%) 10 5 | 50, 68, 100, 111 | 0 |
| 35 | L13B | 138/140 (98%) | 1.97 | 66 (47%) 0 0 | 69, 102, 129, 136 | 0 |
| 36 | L14A | 122/122 (100%) | 1.08 | 18 (14%) 5 3 | 43, 62, 76, 83 | 0 |
| 36 | L14B | 122/122 (100%) | 1.21 | 23 (18%) 3 1 | 59, 81, 101, 114 | 0 |
| 37 | L15A | 150/150 (100%) | 0.39 | 5 (3%) 49 29 | 38, 69, 102, 141 | 0 |
| 37 | L15B | 150/150 (100%) | 0.75 | 11 (7%) 21 11 | 50, 94, 128, 143 | 0 |
| 38 | L16A | 141/141 (100%) | 0.74 | 9 (6%) 25 14 | 43, 64, 90, 122 | 0 |
| 38 | L16B | 141/141 (100%) | 0.69 | 9 (6%) 25 14 | 54, 73, 94, 123 | 0 |
| 39 | L17A | 118/118 (100%) | 0.32 | 1 (0%) 82 65 | 46, 65, 86, 94 | 0 |
| 39 | L17B | 118/118 (100%) | 0.50 | 3 (2%) 58 37 | 55, 74, 94, 111 | 0 |
| 40 | L18A | 112/112 (100%) | 0.68 | 10 (8%) 15 8 | 54, 71, 97, 114 | 0 |
| 40 | L18B | 111/112 (99%) | 0.49 | 5 (4%) 38 20 | 74, 103, 140, 150 | 0 |
| 41 | L19A | 137/146 (93%) | 1.23 | 26 (18%) 3 1 | 57, 74, 125, 158 | 0 |
| 41 | L19B | 137/146 (93%) | 1.14 | 20 (14%) 6 3 | 70, 89, 164, 184 | 0 |
| 42 | L20A | 117/118 (99%) | 0.10 | 3 (2%) 57 36 | 39, 57, 85, 115 | 0 |
| 42 | L20B | 117/118 (99%) | 1.57 | 37 (31%) 1 1 | 54, 94, 135, 148 | 0 |
| 43 | L21A | 101/101 (100%) | 0.48 | 2 (1%) 65 44 | 41, 80, 98, 107 | 0 |
| 43 | L21B | 101/101 (100%) | 2.22 | 51 (50%) 0 0 | 55, 113, 129, 141 | 0 |
| 44 | L22A | 113/113 (100%) | 0.00 | 2 (1%) 67 47 | 45, 56, 85, 127 | 0 |
| 44 | L22B | 113/113 (100%) | 0.96 | 11 (9%) 13 7 | 51, 66, 112, 149 | 0 |

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| Mol | Chain | Analysed | <RSRZ> | #RSRZ>2 | OWAB(Å$^2$) | Q<0.9 |
|---|---|---|---|---|---|---|
| 45 | L23A | 95/96 (98%) | 0.05 | 0 100 100 | 41, 56, 76, 95 | 0 |
| 45 | L23B | 94/96 (97%) | 0.37 | 3 (3%) 50 30 | 54, 72, 98, 121 | 0 |
| 46 | L24A | 108/110 (98%) | 0.72 | 9 (8%) 17 9 | 58, 89, 137, 151 | 0 |
| 46 | L24B | 106/110 (96%) | 1.46 | 28 (26%) 1 1 | 67, 97, 146, 152 | 0 |
| 47 | L25A | 179/206 (86%) | 1.36 | 37 (20%) 2 1 | 68, 104, 181, 189 | 0 |
| 47 | L25B | 176/206 (85%) | 1.50 | 49 (27%) 1 1 | 105, 144, 222, 227 | 0 |
| 48 | L27A | 84/85 (98%) | 0.41 | 6 (7%) 22 12 | 43, 57, 84, 105 | 0 |
| 48 | L27B | 84/85 (98%) | 0.47 | 9 (10%) 11 6 | 61, 78, 106, 126 | 0 |
| 49 | L28A | 97/98 (98%) | 0.66 | 10 (10%) 12 6 | 41, 62, 108, 132 | 0 |
| 49 | L28B | 97/98 (98%) | 0.78 | 11 (11%) 10 5 | 51, 73, 116, 132 | 0 |
| 50 | L29A | 69/72 (95%) | 0.57 | 2 (2%) 53 32 | 47, 65, 81, 103 | 0 |
| 50 | L29B | 68/72 (94%) | 0.40 | 1 (1%) 72 52 | 66, 87, 106, 114 | 0 |
| 51 | L30A | 59/60 (98%) | 0.20 | 2 (3%) 48 28 | 47, 63, 93, 114 | 0 |
| 51 | L30B | 59/60 (98%) | 1.23 | 11 (18%) 3 1 | 67, 91, 130, 144 | 0 |
| 52 | L31A | 71/71 (100%) | 1.76 | 22 (30%) 1 1 | 88, 134, 169, 174 | 0 |
| 52 | L31B | 71/71 (100%) | 0.87 | 4 (5%) 30 16 | 119, 160, 187, 195 | 0 |
| 53 | L32A | 56/60 (93%) | 0.37 | 4 (7%) 22 12 | 31, 68, 128, 133 | 0 |
| 53 | L32B | 56/60 (93%) | 1.15 | 12 (21%) 2 1 | 51, 79, 138, 149 | 0 |
| 54 | L33A | 45/54 (83%) | 2.29 | 23 (51%) 0 0 | 104, 128, 157, 161 | 0 |
| 54 | L33B | 45/54 (83%) | 1.60 | 14 (31%) 1 1 | 129, 155, 181, 187 | 0 |
| 55 | L34A | 48/49 (97%) | -0.21 | 0 100 100 | 31, 41, 68, 98 | 0 |
| 55 | L34B | 49/49 (100%) | 0.10 | 2 (4%) 41 23 | 44, 51, 95, 109 | 0 |
| 56 | L35A | 64/65 (98%) | 0.10 | 4 (6%) 26 14 | 39, 53, 68, 94 | 0 |
| 56 | L35B | 64/65 (98%) | 0.55 | 2 (3%) 51 30 | 44, 69, 92, 116 | 0 |
| 57 | ASIB | 72/76 (94%) | 1.60 | 19 (26%) 1 1 | 100, 215, 252, 257 | 0 |
| All | All | 21114/21740 (97%) | 0.74 | 2781 (13%) 7 4 | 30, 87, 175, 268 | 0 |

All (2781) RSRZ outliers are listed below:

| Mol | Chain | Res | Type | RSRZ |
|---|---|---|---|---|
| 4 | S4A | 26 | CYS | 9.6 |
| 4 | S4B | 26 | CYS | 9.4 |
| 43 | L21B | 36 | PRO | 9.2 |

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| Mol | Chain | Res | Type | RSRZ |
|---|---|---|---|---|
| 22 | ASIA | 1 | G | 8.0 |
| 4 | S4B | 31 | CYS | 7.7 |
| 22 | ASIA | 3 | C | 7.5 |
| 34 | L9A | 140 | LEU | 7.3 |
| 2 | S2A | 118 | LEU | 7.3 |
| 42 | L20B | 113 | ALA | 7.2 |
| 33 | L6B | 38 | SER | 7.1 |
| 4 | S4A | 32 | ALA | 7.0 |
| 13 | S13A | 117 | VAL | 6.9 |
| 47 | L25A | 97 | GLU | 6.7 |
| 22 | ASIA | 70 | G | 6.6 |
| 4 | S4A | 31 | CYS | 6.6 |
| 4 | S4A | 115 | ARG | 6.5 |
| 2 | S2B | 218 | ALA | 6.5 |
| 19 | S19A | 85 | LYS | 6.5 |
| 42 | L20B | 109 | LEU | 6.4 |
| 19 | S19A | 61 | TYR | 6.4 |
| 22 | ASIA | 17 | C | 6.4 |
| 4 | S4A | 89 | THR | 6.3 |
| 4 | S4B | 158 | ILE | 6.3 |
| 27 | 23SB | 2911 | G | 6.2 |
| 33 | L6B | 16 | SER | 6.2 |
| 34 | L9B | 80 | PRO | 6.2 |
| 2 | S2B | 222 | ILE | 6.2 |
| 33 | L6B | 113 | VAL | 6.2 |
| 2 | S2B | 215 | LEU | 6.1 |
| 4 | S4A | 9 | CYS | 6.1 |
| 30 | L3B | 57 | LYS | 6.1 |
| 4 | S4B | 19 | LEU | 6.0 |
| 10 | S10B | 85 | LEU | 6.0 |
| 33 | L6B | 72 | ILE | 6.0 |
| 32 | L5A | 75 | LYS | 5.9 |
| 34 | L9B | 86 | THR | 5.9 |
| 52 | L31A | 33 | VAL | 5.9 |
| 22 | ASIA | 73 | A | 5.9 |
| 34 | L9B | 85 | GLU | 5.9 |
| 27 | 23SB | 4 | C | 5.8 |
| 27 | 23SB | 2913 | C | 5.8 |
| 28 | 5SB | 90 | C | 5.8 |
| 57 | ASIB | 1 | G | 5.7 |
| 4 | S4B | 128 | VAL | 5.6 |
| 33 | L6B | 150 | ALA | 5.6 |

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| Mol | Chain | Res | Type | RSRZ |
|---|---|---|---|---|
| 27 | 23SB | 2912 | A | 5.6 |
| 2 | S2B | 230 | VAL | 5.6 |
| 2 | S2B | 186 | ALA | 5.5 |
| 22 | ASIA | 72 | C | 5.5 |
| 33 | L6B | 174 | GLY | 5.5 |
| 2 | S2B | 164 | VAL | 5.4 |
| 3 | S3B | 182 | ILE | 5.4 |
| 10 | S10B | 23 | ILE | 5.4 |
| 19 | S19A | 81 | ARG | 5.4 |
| 43 | L21B | 45 | THR | 5.4 |
| 34 | L9B | 84 | GLY | 5.4 |
| 4 | S4B | 32 | ALA | 5.4 |
| 4 | S4A | 58 | LEU | 5.3 |
| 33 | L6B | 103 | LEU | 5.3 |
| 34 | L9A | 129 | THR | 5.3 |
| 33 | L6B | 36 | PRO | 5.3 |
| 33 | L6B | 115 | VAL | 5.3 |
| 54 | L33A | 22 | ALA | 5.3 |
| 3 | S3B | 205 | GLY | 5.3 |
| 24 | ESIA | 6 | G | 5.3 |
| 33 | L6B | 105 | LEU | 5.3 |
| 33 | L6B | 35 | VAL | 5.3 |
| 33 | L6B | 24 | VAL | 5.2 |
| 33 | L6B | 148 | ILE | 5.2 |
| 4 | S4A | 178 | VAL | 5.2 |
| 43 | L21B | 71 | LEU | 5.2 |
| 5 | S5A | 51 | VAL | 5.2 |
| 33 | L6A | 119 | GLU | 5.2 |
| 5 | S5B | 13 | ILE | 5.1 |
| 4 | S4B | 86 | LYS | 5.1 |
| 24 | ESIA | 14 | A | 5.1 |
| 33 | L6B | 17 | VAL | 5.1 |
| 4 | S4A | 86 | LYS | 5.1 |
| 33 | L6B | 26 | VAL | 5.1 |
| 33 | L6B | 131 | VAL | 5.1 |
| 33 | L6B | 146 | ALA | 5.1 |
| 26 | TRNA | 73 | A | 5.1 |
| 3 | S3A | 193 | TYR | 5.1 |
| 3 | S3B | 203 | PHE | 5.0 |
| 33 | L6B | 152 | ARG | 5.0 |
| 12 | S12A | 92 | GLY | 5.0 |
| 25 | MRNA | 53 | U | 5.0 |

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| Mol | Chain | Res | Type | RSRZ |
|---|---|---|---|---|
| 7 | S7A | 147 | ALA | 5.0 |
| 12 | S12A | 117 | TYR | 5.0 |
| 43 | L21B | 35 | LEU | 5.0 |
| 22 | ASIA | 71 | G | 4.9 |
| 3 | S3B | 117 | ALA | 4.9 |
| 4 | S4B | 88 | VAL | 4.9 |
| 4 | S4B | 110 | PHE | 4.9 |
| 43 | L21B | 91 | TYR | 4.9 |
| 4 | S4A | 114 | ARG | 4.9 |
| 27 | 23SB | 1110 | G | 4.9 |
| 35 | L13A | 96 | GLU | 4.9 |
| 4 | S4A | 21 | LEU | 4.9 |
| 2 | S2B | 32 | ILE | 4.9 |
| 2 | S2B | 214 | ILE | 4.9 |
| 24 | ESIA | 1 | G | 4.9 |
| 4 | S4A | 110 | PHE | 4.9 |
| 34 | L9B | 122 | GLU | 4.9 |
| 34 | L9A | 79 | ILE | 4.9 |
| 4 | S4B | 9 | CYS | 4.9 |
| 34 | L9A | 130 | TYR | 4.8 |
| 4 | S4B | 103 | ASN | 4.8 |
| 12 | S12A | 60 | GLY | 4.8 |
| 2 | S2A | 145 | LEU | 4.8 |
| 33 | L6B | 114 | VAL | 4.8 |
| 22 | ASIA | 4 | C | 4.8 |
| 42 | L20B | 88 | ILE | 4.8 |
| 24 | ESIA | 12 | U | 4.7 |
| 22 | ASIA | 49 | C | 4.7 |
| 34 | L9B | 140 | LEU | 4.7 |
| 3 | S3B | 37 | GLN | 4.7 |
| 33 | L6B | 37 | VAL | 4.7 |
| 3 | S3A | 167 | TRP | 4.7 |
| 46 | L24B | 40 | GLU | 4.7 |
| 4 | S4B | 7 | PRO | 4.7 |
| 3 | S3A | 80 | GLY | 4.7 |
| 47 | L25A | 177 | PRO | 4.7 |
| 4 | S4B | 178 | VAL | 4.7 |
| 20 | S20A | 63 | ILE | 4.6 |
| 36 | L14B | 91 | LEU | 4.6 |
| 3 | S3B | 66 | VAL | 4.6 |
| 2 | S2A | 188 | ALA | 4.6 |
| 43 | L21B | 93 | GLU | 4.6 |

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| Mol | Chain | Res | Type | RSRZ |
|---|---|---|---|---|
| 35 | L13A | 134 | ARG | 4.6 |
| 54 | L33A | 9 | LEU | 4.6 |
| 39 | L17B | 69 | ASP | 4.6 |
| 2 | S2B | 162 | ILE | 4.6 |
| 54 | L33B | 9 | LEU | 4.6 |
| 33 | L6B | 133 | VAL | 4.6 |
| 35 | L13B | 10 | GLU | 4.5 |
| 12 | S12A | 126 | ALA | 4.5 |
| 2 | S2A | 171 | ALA | 4.5 |
| 3 | S3B | 157 | ILE | 4.5 |
| 47 | L25A | 116 | VAL | 4.5 |
| 2 | S2B | 47 | THR | 4.5 |
| 30 | L3B | 53 | PRO | 4.5 |
| 42 | L20B | 91 | ASP | 4.5 |
| 42 | L20B | 117 | GLN | 4.5 |
| 12 | S12B | 82 | ILE | 4.5 |
| 34 | L9B | 138 | ILE | 4.5 |
| 34 | L9B | 92 | VAL | 4.5 |
| 22 | ASIA | 12 | U | 4.4 |
| 47 | L25B | 176 | PRO | 4.4 |
| 3 | S3B | 207 | VAL | 4.4 |
| 35 | L13B | 133 | GLN | 4.4 |
| 10 | S10B | 82 | ILE | 4.4 |
| 18 | S18B | 82 | THR | 4.4 |
| 31 | L4B | 133 | ASN | 4.4 |
| 7 | S7A | 85 | TYR | 4.4 |
| 34 | L9A | 132 | PRO | 4.4 |
| 33 | L6A | 116 | GLU | 4.4 |
| 38 | L16A | 1 | MET | 4.4 |
| 4 | S4B | 126 | ILE | 4.4 |
| 5 | S5B | 125 | SER | 4.4 |
| 24 | ESIA | 11 | C | 4.4 |
| 3 | S3A | 94 | LEU | 4.4 |
| 5 | S5B | 76 | ILE | 4.4 |
| 27 | 23SB | 1139 | G | 4.4 |
| 42 | L20B | 106 | PHE | 4.4 |
| 3 | S3B | 100 | ALA | 4.4 |
| 4 | S4B | 101 | LEU | 4.4 |
| 34 | L9A | 77 | LEU | 4.4 |
| 27 | 23SA | 2913 | C | 4.4 |
| 12 | S12B | 59 | SER | 4.4 |
| 13 | S13A | 120 | LYS | 4.3 |

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| Mol | Chain | Res | Type | RSRZ |
|---|---|---|---|---|
| 52 | L31A | 63 | TYR | 4.3 |
| 35 | L13B | 57 | ALA | 4.3 |
| 2 | S2A | 162 | ILE | 4.3 |
| 12 | S12A | 59 | SER | 4.3 |
| 31 | L4B | 12 | LEU | 4.3 |
| 34 | L9A | 116 | LEU | 4.3 |
| 4 | S4A | 88 | VAL | 4.3 |
| 22 | ASIA | 5 | G | 4.3 |
| 2 | S2B | 93 | VAL | 4.3 |
| 6 | S6B | 45 | LEU | 4.3 |
| 43 | L21B | 86 | GLY | 4.3 |
| 33 | L6A | 34 | GLU | 4.3 |
| 5 | S5A | 148 | VAL | 4.3 |
| 22 | ASIA | 6 | G | 4.2 |
| 2 | S2B | 202 | PRO | 4.2 |
| 4 | S4A | 189 | PRO | 4.2 |
| 11 | S11B | 81 | ASP | 4.2 |
| 18 | S18A | 88 | LYS | 4.2 |
| 2 | S2B | 145 | LEU | 4.2 |
| 33 | L6B | 151 | ILE | 4.2 |
| 5 | S5A | 124 | GLY | 4.2 |
| 16 | S16B | 39 | TYR | 4.2 |
| 4 | S4B | 12 | CYS | 4.2 |
| 18 | S18B | 26 | LEU | 4.2 |
| 4 | S4A | 126 | ILE | 4.2 |
| 14 | S14B | 38 | GLY | 4.2 |
| 41 | L19B | 4 | GLY | 4.2 |
| 32 | L5A | 35 | GLU | 4.2 |
| 33 | L6B | 34 | GLU | 4.2 |
| 5 | S5A | 50 | GLU | 4.2 |
| 4 | S4A | 96 | LEU | 4.2 |
| 7 | S7B | 86 | GLN | 4.2 |
| 33 | L6B | 55 | PRO | 4.2 |
| 47 | L25B | 76 | LEU | 4.1 |
| 8 | S8A | 113 | SER | 4.1 |
| 27 | 23SB | 2910 | U | 4.1 |
| 5 | S5B | 28 | PHE | 4.1 |
| 33 | L6B | 121 | ILE | 4.1 |
| 10 | S10A | 93 | GLY | 4.1 |
| 33 | L6B | 48 | GLY | 4.1 |
| 2 | S2B | 211 | ILE | 4.1 |
| 10 | S10B | 6 | ILE | 4.1 |

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| Mol | Chain | Res | Type | RSRZ |
|---|---|---|---|---|
| 4 | S4A | 152 | SER | 4.1 |
| 20 | S20A | 59 | ALA | 4.1 |
| 47 | L25A | 173 | ALA | 4.1 |
| 5 | S5B | 124 | GLY | 4.1 |
| 27 | 23SB | 2914 | C | 4.1 |
| 2 | S2B | 174 | VAL | 4.1 |
| 4 | S4B | 150 | GLU | 4.1 |
| 20 | S20B | 63 | ILE | 4.1 |
| 34 | L9B | 88 | ILE | 4.1 |
| 10 | S10B | 27 | ALA | 4.1 |
| 4 | S4A | 136 | PRO | 4.0 |
| 2 | S2A | 61 | LEU | 4.0 |
| 4 | S4B | 96 | LEU | 4.0 |
| 54 | L33A | 48 | VAL | 4.0 |
| 33 | L6A | 175 | LYS | 4.0 |
| 33 | L6B | 84 | SER | 4.0 |
| 36 | L14B | 37 | ASP | 4.0 |
| 10 | S10A | 23 | ILE | 4.0 |
| 52 | L31A | 43 | TYR | 4.0 |
| 27 | 23SB | 5 | A | 4.0 |
| 4 | S4B | 162 | LEU | 4.0 |
| 19 | S19B | 76 | PRO | 4.0 |
| 47 | L25B | 67 | LEU | 4.0 |
| 43 | L21B | 12 | TYR | 4.0 |
| 22 | ASIA | 27 | G | 4.0 |
| 13 | S13A | 119 | GLY | 4.0 |
| 33 | L6B | 15 | VAL | 4.0 |
| 55 | L34B | 49 | ARG | 4.0 |
| 3 | S3A | 203 | PHE | 4.0 |
| 3 | S3A | 184 | TYR | 4.0 |
| 3 | S3B | 62 | ASP | 4.0 |
| 14 | S14A | 59 | ALA | 4.0 |
| 33 | L6B | 85 | LYS | 4.0 |
| 47 | L25A | 144 | LEU | 4.0 |
| 3 | S3B | 64 | VAL | 4.0 |
| 4 | S4B | 91 | SER | 4.0 |
| 54 | L33A | 23 | THR | 4.0 |
| 39 | L17A | 5 | LYS | 4.0 |
| 48 | L27B | 7 | LEU | 4.0 |
| 2 | S2A | 71 | VAL | 3.9 |
| 30 | L3B | 48 | GLN | 3.9 |
| 4 | S4A | 146 | ILE | 3.9 |

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| Mol | Chain | Res | Type | RSRZ |
|---|---|---|---|---|
| 33 | L6A | 89 | ILE | 3.9 |
| 34 | L9B | 109 | ILE | 3.9 |
| 44 | L22B | 113 | LYS | 3.9 |
| 3 | S3B | 90 | GLU | 3.9 |
| 12 | S12A | 64 | THR | 3.9 |
| 20 | S20A | 84 | LEU | 3.9 |
| 23 | PSIA | 1 | G | 3.9 |
| 33 | L6B | 43 | VAL | 3.9 |
| 34 | L9A | 138 | ILE | 3.9 |
| 4 | S4A | 19 | LEU | 3.9 |
| 30 | L3B | 27 | LEU | 3.9 |
| 47 | L25A | 59 | LEU | 3.9 |
| 33 | L6B | 147 | ASN | 3.9 |
| 30 | L3B | 47 | VAL | 3.9 |
| 3 | S3A | 128 | PHE | 3.9 |
| 57 | ASIB | 70 | G | 3.9 |
| 40 | L18B | 55 | ALA | 3.9 |
| 4 | S4B | 24 | GLU | 3.9 |
| 5 | S5A | 55 | VAL | 3.9 |
| 34 | L9B | 125 | GLU | 3.9 |
| 4 | S4B | 99 | SER | 3.9 |
| 33 | L6B | 39 | PRO | 3.9 |
| 3 | S3B | 171 | GLY | 3.9 |
| 4 | S4B | 134 | ASP | 3.9 |
| 34 | L9A | 139 | GLN | 3.9 |
| 45 | L23B | 92 | LEU | 3.9 |
| 35 | L13B | 93 | THR | 3.8 |
| 35 | L13B | 7 | LYS | 3.8 |
| 10 | S10B | 35 | SER | 3.8 |
| 26 | TRNA | 1 | G | 3.8 |
| 27 | 23SA | 931 | G | 3.8 |
| 27 | 23SA | 2911 | G | 3.8 |
| 27 | 23SB | 2909 | U | 3.8 |
| 57 | ASIB | 6 | G | 3.8 |
| 2 | S2B | 196 | LEU | 3.8 |
| 9 | S9A | 82 | ALA | 3.8 |
| 4 | S4B | 92 | VAL | 3.8 |
| 33 | L6B | 11 | VAL | 3.8 |
| 36 | L14A | 108 | GLU | 3.8 |
| 41 | L19B | 1 | MET | 3.8 |
| 33 | L6B | 14 | GLY | 3.8 |
| 35 | L13B | 32 | THR | 3.8 |

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| Mol | Chain | Res | Type | RSRZ |
|---|---|---|---|---|
| 47 | L25A | 107 | THR | 3.8 |
| 2 | S2B | 172 | ILE | 3.8 |
| 43 | L21B | 38 | LEU | 3.8 |
| 27 | 23SA | 1121 | A | 3.8 |
| 30 | L3B | 204 | ALA | 3.8 |
| 4 | S4B | 170 | VAL | 3.8 |
| 34 | L9A | 144 | VAL | 3.8 |
| 46 | L24B | 49 | VAL | 3.8 |
| 35 | L13B | 1 | MET | 3.8 |
| 2 | S2B | 80 | ILE | 3.8 |
| 3 | S3A | 95 | THR | 3.8 |
| 13 | S13B | 6 | GLY | 3.8 |
| 30 | L3A | 52 | LEU | 3.8 |
| 4 | S4B | 111 | ALA | 3.8 |
| 7 | S7B | 147 | ALA | 3.8 |
| 53 | L32B | 53 | ALA | 3.8 |
| 10 | S10B | 73 | ASP | 3.8 |
| 5 | S5B | 69 | VAL | 3.8 |
| 33 | L6A | 115 | VAL | 3.8 |
| 22 | ASIA | 45 | U | 3.8 |
| 1 | 16SA | 1063 | C | 3.8 |
| 3 | S3A | 161 | GLU | 3.8 |
| 9 | S9A | 115 | GLY | 3.8 |
| 33 | L6A | 168 | PRO | 3.8 |
| 33 | L6B | 112 | PRO | 3.8 |
| 38 | L16B | 104 | PHE | 3.8 |
| 14 | S14B | 52 | GLN | 3.8 |
| 34 | L9B | 87 | LYS | 3.8 |
| 3 | S3B | 41 | GLY | 3.8 |
| 42 | L20B | 83 | LEU | 3.8 |
| 22 | ASIA | 14 | A | 3.8 |
| 27 | 23SA | 1118 | A | 3.8 |
| 27 | 23SB | 3 | U | 3.8 |
| 21 | THXA | 14 | TRP | 3.7 |
| 25 | MRNA | 55 | U | 3.7 |
| 3 | S3A | 182 | ILE | 3.7 |
| 43 | L21B | 40 | LEU | 3.7 |
| 12 | S12A | 35 | THR | 3.7 |
| 2 | S2B | 13 | ALA | 3.7 |
| 33 | L6A | 170 | ARG | 3.7 |
| 10 | S10B | 75 | ILE | 3.7 |
| 8 | S8A | 39 | LEU | 3.7 |

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| Mol | Chain | Res | Type | RSRZ |
|---|---|---|---|---|
| 41 | L19A | 19 | LEU | 3.7 |
| 35 | L13B | 127 | ASP | 3.7 |
| 2 | S2B | 167 | PRO | 3.7 |
| 5 | S5B | 77 | PRO | 3.7 |
| 22 | ASIA | 11 | C | 3.7 |
| 33 | L6B | 102 | ALA | 3.7 |
| 33 | L6B | 19 | VAL | 3.7 |
| 34 | L9A | 92 | VAL | 3.7 |
| 12 | S12B | 16 | ARG | 3.7 |
| 1 | 16SA | 1054 | G | 3.7 |
| 2 | S2A | 115 | LEU | 3.7 |
| 3 | S3A | 87 | LEU | 3.7 |
| 4 | S4A | 135 | LEU | 3.7 |
| 41 | L19A | 78 | LEU | 3.7 |
| 54 | L33A | 34 | LEU | 3.7 |
| 12 | S12A | 44 | LYS | 3.7 |
| 31 | L4B | 131 | GLY | 3.7 |
| 46 | L24B | 101 | LYS | 3.7 |
| 11 | S11A | 67 | ASP | 3.7 |
| 34 | L9A | 110 | ASP | 3.7 |
| 48 | L27A | 85 | ALA | 3.7 |
| 3 | S3A | 195 | VAL | 3.7 |
| 3 | S3B | 75 | VAL | 3.7 |
| 4 | S4A | 128 | VAL | 3.7 |
| 5 | S5B | 55 | VAL | 3.7 |
| 19 | S19A | 45 | VAL | 3.7 |
| 37 | L15B | 71 | VAL | 3.7 |
| 22 | ASIA | 62 | C | 3.7 |
| 57 | ASIB | 74 | C | 3.7 |
| 13 | S13B | 84 | ILE | 3.7 |
| 13 | S13B | 121 | LYS | 3.7 |
| 4 | S4A | 87 | GLY | 3.7 |
| 16 | S16B | 80 | PHE | 3.7 |
| 8 | S8B | 101 | PRO | 3.6 |
| 3 | S3B | 138 | VAL | 3.6 |
| 17 | S17A | 35 | VAL | 3.6 |
| 27 | 23SA | 1111 | G | 3.6 |
| 33 | L6B | 96 | ALA | 3.6 |
| 34 | L9B | 126 | TYR | 3.6 |
| 43 | L21B | 46 | VAL | 3.6 |
| 22 | ASIA | 47 | U | 3.6 |
| 4 | S4A | 11 | LEU | 3.6 |

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| Mol | Chain | Res | Type | RSRZ |
|---|---|---|---|---|
| 22 | ASIA | 26 | A | 3.6 |
| 12 | S12B | 20 | LYS | 3.6 |
| 22 | ASIA | 2 | C | 3.6 |
| 24 | ESIB | 11 | C | 3.6 |
| 30 | L3A | 88 | GLY | 3.6 |
| 33 | L6B | 56 | SER | 3.6 |
| 47 | L25A | 175 | VAL | 3.6 |
| 19 | S19A | 79 | THR | 3.6 |
| 8 | S8B | 112 | LEU | 3.6 |
| 25 | MRNA | 56 | U | 3.6 |
| 22 | ASIA | 76 | A | 3.6 |
| 4 | S4A | 39 | PRO | 3.6 |
| 34 | L9A | 80 | PRO | 3.6 |
| 6 | S6B | 99 | ALA | 3.6 |
| 33 | L6A | 114 | VAL | 3.6 |
| 47 | L25A | 174 | VAL | 3.6 |
| 57 | ASIB | 3 | C | 3.6 |
| 4 | S4A | 91 | SER | 3.6 |
| 4 | S4B | 144 | ASP | 3.6 |
| 4 | S4A | 158 | ILE | 3.6 |
| 34 | L9A | 72 | LEU | 3.6 |
| 40 | L18A | 110 | LEU | 3.6 |
| 44 | L22B | 111 | HIS | 3.6 |
| 4 | S4B | 87 | GLY | 3.6 |
| 22 | ASIA | 16 | U | 3.6 |
| 46 | L24B | 58 | GLY | 3.6 |
| 2 | S2A | 159 | PRO | 3.6 |
| 4 | S4A | 197 | PRO | 3.6 |
| 16 | S16B | 46 | PRO | 3.6 |
| 30 | L3B | 56 | PRO | 3.6 |
| 33 | L6B | 118 | PRO | 3.6 |
| 4 | S4B | 133 | VAL | 3.6 |
| 4 | S4A | 12 | CYS | 3.6 |
| 23 | PSIB | 1 | G | 3.6 |
| 4 | S4B | 108 | LEU | 3.6 |
| 1 | 16SA | 986 | C | 3.6 |
| 34 | L9A | 108 | THR | 3.6 |
| 4 | S4A | 195 | ALA | 3.6 |
| 3 | S3A | 44 | GLU | 3.6 |
| 3 | S3A | 188 | LEU | 3.6 |
| 5 | S5A | 31 | LEU | 3.6 |
| 3 | S3A | 134 | ILE | 3.6 |

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| Mol | Chain | Res | Type | RSRZ |
|---|---|---|---|---|
| 3 | S3B | 77 | ILE | 3.6 |
| 43 | L21B | 99 | ILE | 3.6 |
| 53 | L32B | 51 | TYR | 3.6 |
| 4 | S4A | 52 | SER | 3.6 |
| 9 | S9A | 126 | SER | 3.6 |
| 31 | L4B | 175 | THR | 3.6 |
| 38 | L16A | 21 | THR | 3.6 |
| 7 | S7A | 78 | ARG | 3.5 |
| 24 | ESIA | 27 | G | 3.5 |
| 24 | ESIB | 1 | G | 3.5 |
| 27 | 23SA | 2846 | G | 3.5 |
| 19 | S19A | 83 | HIS | 3.5 |
| 4 | S4B | 95 | GLY | 3.5 |
| 27 | 23SA | 937 | C | 3.5 |
| 33 | L6B | 76 | VAL | 3.5 |
| 4 | S4B | 195 | ALA | 3.5 |
| 16 | S16B | 56 | ALA | 3.5 |
| 35 | L13B | 31 | ALA | 3.5 |
| 4 | S4B | 181 | MET | 3.5 |
| 8 | S8B | 59 | LEU | 3.5 |
| 34 | L9B | 135 | GLU | 3.5 |
| 12 | S12A | 113 | SER | 3.5 |
| 42 | L20B | 104 | GLN | 3.5 |
| 7 | S7A | 82 | GLY | 3.5 |
| 31 | L4B | 6 | VAL | 3.5 |
| 1 | 16SA | 1053 | A | 3.5 |
| 33 | L6B | 21 | PRO | 3.5 |
| 3 | S3A | 47 | LEU | 3.5 |
| 18 | S18A | 31 | LEU | 3.5 |
| 54 | L33A | 36 | LEU | 3.5 |
| 2 | S2B | 42 | ILE | 3.5 |
| 4 | S4B | 115 | ARG | 3.5 |
| 42 | L20A | 106 | PHE | 3.5 |
| 34 | L9A | 102 | SER | 3.5 |
| 19 | S19A | 82 | GLY | 3.5 |
| 33 | L6B | 107 | VAL | 3.5 |
| 19 | S19B | 89 | ALA | 3.5 |
| 4 | S4A | 172 | PRO | 3.5 |
| 35 | L13B | 90 | MET | 3.5 |
| 33 | L6A | 86 | GLU | 3.5 |
| 24 | ESIA | 7 | A | 3.5 |
| 33 | L6A | 147 | ASN | 3.5 |

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| Mol | Chain | Res | Type | RSRZ |
|---|---|---|---|---|
| 4 | S4B | 127 | THR | 3.5 |
| 35 | L13B | 37 | LYS | 3.5 |
| 5 | S5A | 105 | VAL | 3.5 |
| 10 | S10A | 59 | SER | 3.5 |
| 46 | L24B | 45 | VAL | 3.5 |
| 49 | L28A | 86 | SER | 3.5 |
| 4 | S4A | 176 | LEU | 3.5 |
| 34 | L9A | 68 | LEU | 3.5 |
| 35 | L13B | 138 | LEU | 3.5 |
| 3 | S3A | 152 | ILE | 3.5 |
| 14 | S14A | 12 | ARG | 3.5 |
| 13 | S13B | 8 | GLU | 3.5 |
| 4 | S4B | 185 | PHE | 3.5 |
| 34 | L9B | 141 | LYS | 3.5 |
| 2 | S2B | 184 | VAL | 3.5 |
| 4 | S4B | 17 | VAL | 3.5 |
| 10 | S10B | 67 | THR | 3.5 |
| 12 | S12B | 41 | THR | 3.5 |
| 5 | S5A | 22 | GLY | 3.5 |
| 5 | S5B | 33 | VAL | 3.5 |
| 16 | S16B | 79 | VAL | 3.5 |
| 19 | S19A | 84 | GLY | 3.5 |
| 33 | L6B | 45 | VAL | 3.5 |
| 42 | L20A | 118 | GLY | 3.5 |
| 7 | S7B | 150 | ALA | 3.5 |
| 3 | S3B | 73 | PRO | 3.5 |
| 11 | S11B | 77 | MET | 3.5 |
| 27 | 23SA | 4 | C | 3.5 |
| 2 | S2A | 114 | ARG | 3.5 |
| 2 | S2B | 200 | ILE | 3.5 |
| 3 | S3A | 19 | GLU | 3.4 |
| 4 | S4B | 34 | GLU | 3.4 |
| 33 | L6A | 133 | VAL | 3.4 |
| 51 | L30B | 58 | VAL | 3.4 |
| 3 | S3A | 78 | GLY | 3.4 |
| 2 | S2A | 186 | ALA | 3.4 |
| 4 | S4B | 157 | LEU | 3.4 |
| 5 | S5B | 30 | ALA | 3.4 |
| 8 | S8A | 133 | LEU | 3.4 |
| 33 | L6B | 33 | LEU | 3.4 |
| 34 | L9A | 94 | ALA | 3.4 |
| 2 | S2B | 192 | SER | 3.4 |

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| Mol | Chain | Res | Type | RSRZ |
|---|---|---|---|---|
| 10 | S10A | 46 | ARG | 3.4 |
| 11 | S11A | 101 | SER | 3.4 |
| 17 | S17B | 91 | ARG | 3.4 |
| 19 | S19B | 42 | PRO | 3.4 |
| 27 | 23SB | 1125 | A | 3.4 |
| 35 | L13B | 41 | ASP | 3.4 |
| 6 | S6B | 39 | LYS | 3.4 |
| 32 | L5A | 80 | PHE | 3.4 |
| 11 | S11A | 25 | TYR | 3.4 |
| 2 | S2A | 15 | VAL | 3.4 |
| 2 | S2A | 81 | VAL | 3.4 |
| 23 | PSIA | 5 | G | 3.4 |
| 4 | S4A | 108 | LEU | 3.4 |
| 19 | S19A | 5 | LEU | 3.4 |
| 33 | L6B | 120 | GLY | 3.4 |
| 34 | L9A | 124 | GLY | 3.4 |
| 40 | L18B | 56 | LEU | 3.4 |
| 9 | S9A | 52 | ALA | 3.4 |
| 33 | L6A | 129 | THR | 3.4 |
| 40 | L18B | 2 | ALA | 3.4 |
| 5 | S5A | 10 | MET | 3.4 |
| 4 | S4B | 172 | PRO | 3.4 |
| 4 | S4A | 85 | LYS | 3.4 |
| 52 | L31A | 59 | PHE | 3.4 |
| 27 | 23SA | 1125 | A | 3.4 |
| 4 | S4A | 121 | VAL | 3.4 |
| 32 | L5B | 127 | GLY | 3.4 |
| 57 | ASIB | 75 | C | 3.4 |
| 3 | S3B | 65 | ALA | 3.4 |
| 34 | L9A | 115 | ALA | 3.4 |
| 10 | S10A | 48 | THR | 3.4 |
| 42 | L20B | 94 | ASN | 3.4 |
| 20 | S20A | 55 | ILE | 3.4 |
| 54 | L33A | 31 | PRO | 3.4 |
| 4 | S4A | 194 | LEU | 3.4 |
| 13 | S13B | 117 | VAL | 3.4 |
| 38 | L16A | 79 | LEU | 3.4 |
| 3 | S3A | 190 | ARG | 3.4 |
| 22 | ASIA | 7 | A | 3.4 |
| 5 | S5A | 49 | PRO | 3.4 |
| 33 | L6B | 117 | PRO | 3.4 |
| 24 | ESIA | 13 | C | 3.4 |

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| Mol | Chain | Res | Type | RSRZ |
|---|---|---|---|---|
| 33 | L6B | 80 | SER | 3.4 |
| 2 | S2A | 187 | LEU | 3.4 |
| 3 | S3B | 196 | LEU | 3.4 |
| 4 | S4A | 150 | GLU | 3.4 |
| 4 | S4A | 118 | ARG | 3.4 |
| 9 | S9B | 19 | LEU | 3.4 |
| 13 | S13A | 83 | ASP | 3.4 |
| 33 | L6A | 99 | VAL | 3.4 |
| 37 | L15B | 18 | ARG | 3.4 |
| 12 | S12B | 61 | TYR | 3.4 |
| 4 | S4A | 48 | ALA | 3.4 |
| 33 | L6A | 165 | ALA | 3.4 |
| 4 | S4B | 146 | ILE | 3.4 |
| 34 | L9B | 79 | ILE | 3.4 |
| 41 | L19B | 88 | ILE | 3.4 |
| 2 | S2A | 110 | GLN | 3.4 |
| 1 | 16SA | 1841 | C | 3.3 |
| 3 | S3A | 66 | VAL | 3.3 |
| 22 | ASIA | 68 | C | 3.3 |
| 47 | L25B | 116 | VAL | 3.3 |
| 8 | S8B | 54 | ASP | 3.3 |
| 3 | S3A | 121 | ALA | 3.3 |
| 4 | S4B | 48 | ALA | 3.3 |
| 7 | S7A | 150 | ALA | 3.3 |
| 41 | L19A | 1 | MET | 3.3 |
| 22 | ASIA | 69 | G | 3.3 |
| 2 | S2A | 152 | PHE | 3.3 |
| 20 | S20B | 10 | LEU | 3.3 |
| 47 | L25B | 161 | VAL | 3.3 |
| 43 | L21B | 15 | GLU | 3.3 |
| 8 | S8B | 113 | SER | 3.3 |
| 22 | ASIA | 23 | A | 3.3 |
| 27 | 23SA | 2912 | A | 3.3 |
| 2 | S2A | 222 | ILE | 3.3 |
| 4 | S4B | 5 | ILE | 3.3 |
| 7 | S7B | 152 | ALA | 3.3 |
| 11 | S11B | 64 | ALA | 3.3 |
| 12 | S12B | 65 | ALA | 3.3 |
| 12 | S12B | 84 | GLY | 3.3 |
| 34 | L9B | 83 | ALA | 3.3 |
| 38 | L16B | 40 | ALA | 3.3 |
| 47 | L25A | 7 | ALA | 3.3 |

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| Mol | Chain | Res | Type | RSRZ |
|---|---|---|---|---|
| 53 | L32B | 2 | ALA | 3.3 |
| 8 | S8B | 72 | PRO | 3.3 |
| 9 | S9A | 49 | PRO | 3.3 |
| 12 | S12A | 56 | ARG | 3.3 |
| 8 | S8B | 133 | LEU | 3.3 |
| 9 | S9A | 19 | LEU | 3.3 |
| 33 | L6B | 44 | VAL | 3.3 |
| 36 | L14B | 9 | GLU | 3.3 |
| 8 | S8B | 131 | GLY | 3.3 |
| 13 | S13B | 18 | ALA | 3.3 |
| 29 | L2A | 251 | GLY | 3.3 |
| 35 | L13A | 18 | ALA | 3.3 |
| 40 | L18A | 108 | GLY | 3.3 |
| 47 | L25A | 146 | ILE | 3.3 |
| 4 | S4A | 102 | ASP | 3.3 |
| 53 | L32B | 34 | PRO | 3.3 |
| 17 | S17A | 101 | ARG | 3.3 |
| 33 | L6B | 111 | HIS | 3.3 |
| 52 | L31A | 52 | THR | 3.3 |
| 4 | S4B | 94 | LEU | 3.3 |
| 22 | ASIA | 13 | C | 3.3 |
| 27 | 23SB | 2908 | C | 3.3 |
| 33 | L6B | 50 | VAL | 3.3 |
| 30 | L3B | 55 | ASN | 3.3 |
| 48 | L27B | 4 | LYS | 3.3 |
| 54 | L33B | 42 | TRP | 3.3 |
| 3 | S3A | 189 | ALA | 3.3 |
| 4 | S4A | 82 | ALA | 3.3 |
| 45 | L23B | 91 | ALA | 3.3 |
| 34 | L9A | 119 | PRO | 3.3 |
| 2 | S2A | 54 | THR | 3.3 |
| 4 | S4B | 135 | LEU | 3.3 |
| 27 | 23SA | 929 | G | 3.3 |
| 48 | L27B | 3 | HIS | 3.3 |
| 54 | L33B | 36 | LEU | 3.3 |
| 3 | S3B | 141 | VAL | 3.3 |
| 4 | S4A | 105 | VAL | 3.3 |
| 28 | 5SA | 1 | A | 3.3 |
| 57 | ASIB | 73 | A | 3.3 |
| 4 | S4A | 33 | MET | 3.3 |
| 3 | S3B | 206 | GLU | 3.3 |
| 8 | S8B | 45 | ILE | 3.3 |

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| Mol | Chain | Res | Type | RSRZ |
|---|---|---|---|---|
| 27 | 23SB | 2817 | C | 3.3 |
| 38 | L16A | 20 | ALA | 3.3 |
| 57 | ASIB | 2 | C | 3.3 |
| 31 | L4B | 207 | GLY | 3.3 |
| 52 | L31B | 54 | GLY | 3.3 |
| 3 | S3A | 48 | TYR | 3.2 |
| 42 | L20B | 101 | ARG | 3.2 |
| 10 | S10B | 77 | PRO | 3.2 |
| 4 | S4B | 64 | LEU | 3.2 |
| 4 | S4B | 97 | LEU | 3.2 |
| 49 | L28B | 95 | LEU | 3.2 |
| 4 | S4A | 160 | GLN | 3.2 |
| 4 | S4A | 206 | PHE | 3.2 |
| 33 | L6B | 123 | PHE | 3.2 |
| 4 | S4B | 198 | VAL | 3.2 |
| 4 | S4B | 203 | VAL | 3.2 |
| 42 | L20B | 110 | VAL | 3.2 |
| 43 | L21B | 14 | VAL | 3.2 |
| 3 | S3B | 53 | ALA | 3.2 |
| 6 | S6B | 81 | ILE | 3.2 |
| 34 | L9B | 11 | ASN | 3.2 |
| 3 | S3B | 80 | GLY | 3.2 |
| 19 | S19A | 68 | GLY | 3.2 |
| 3 | S3A | 131 | ARG | 3.2 |
| 3 | S3A | 101 | LEU | 3.2 |
| 3 | S3B | 94 | LEU | 3.2 |
| 12 | S12B | 44 | LYS | 3.2 |
| 17 | S17A | 6 | LEU | 3.2 |
| 52 | L31B | 37 | SER | 3.2 |
| 2 | S2B | 15 | VAL | 3.2 |
| 9 | S9A | 86 | VAL | 3.2 |
| 34 | L9B | 78 | THR | 3.2 |
| 2 | S2B | 185 | ILE | 3.2 |
| 5 | S5B | 109 | ILE | 3.2 |
| 8 | S8A | 111 | ILE | 3.2 |
| 2 | S2B | 18 | GLY | 3.2 |
| 5 | S5A | 23 | GLY | 3.2 |
| 3 | S3A | 135 | LYS | 3.2 |
| 34 | L9A | 87 | LYS | 3.2 |
| 3 | S3A | 103 | VAL | 3.2 |
| 4 | S4A | 133 | VAL | 3.2 |
| 12 | S12B | 29 | PHE | 3.2 |

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| Mol | Chain | Res | Type | RSRZ |
|---|---|---|---|---|
| 24 | ESIA | 10 | G | 3.2 |
| 33 | L6B | 49 | VAL | 3.2 |
| 3 | S3B | 57 | ILE | 3.2 |
| 8 | S8B | 111 | ILE | 3.2 |
| 35 | L13B | 16 | ILE | 3.2 |
| 12 | S12A | 30 | ARG | 3.2 |
| 10 | S10B | 10 | GLY | 3.2 |
| 34 | L9A | 131 | LYS | 3.2 |
| 4 | S4A | 162 | LEU | 3.2 |
| 20 | S20A | 99 | LEU | 3.2 |
| 47 | L25A | 117 | LEU | 3.2 |
| 4 | S4B | 27 | TYR | 3.2 |
| 33 | L6B | 154 | PRO | 3.2 |
| 3 | S3B | 151 | VAL | 3.2 |
| 12 | S12B | 19 | SER | 3.2 |
| 2 | S2A | 68 | ILE | 3.2 |
| 4 | S4B | 165 | MET | 3.2 |
| 33 | L6B | 129 | THR | 3.2 |
| 27 | 23SA | 936 | A | 3.2 |
| 47 | L25B | 113 | ALA | 3.2 |
| 53 | L32A | 53 | ALA | 3.2 |
| 2 | S2A | 149 | LEU | 3.2 |
| 34 | L9B | 72 | LEU | 3.2 |
| 4 | S4B | 4 | TYR | 3.2 |
| 8 | S8B | 26 | VAL | 3.2 |
| 12 | S12A | 107 | VAL | 3.2 |
| 14 | S14B | 37 | PHE | 3.2 |
| 19 | S19A | 41 | VAL | 3.2 |
| 52 | L31A | 11 | PRO | 3.2 |
| 35 | L13B | 130 | HIS | 3.2 |
| 3 | S3B | 202 | ILE | 3.2 |
| 16 | S16B | 4 | ILE | 3.2 |
| 2 | S2A | 173 | ALA | 3.2 |
| 3 | S3A | 169 | ALA | 3.2 |
| 3 | S3B | 169 | ALA | 3.2 |
| 42 | L20B | 84 | LYS | 3.1 |
| 46 | L24A | 107 | ASP | 3.1 |
| 2 | S2B | 228 | GLY | 3.1 |
| 20 | S20A | 103 | GLY | 3.1 |
| 31 | L4B | 147 | GLY | 3.1 |
| 8 | S8B | 119 | LEU | 3.1 |
| 12 | S12B | 90 | LEU | 3.1 |

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| Mol | Chain | Res | Type | RSRZ |
|---|---|---|---|---|
| 54 | L33A | 42 | TRP | 3.1 |
| 3 | S3A | 90 | GLU | 3.1 |
| 4 | S4A | 15 | GLU | 3.1 |
| 44 | L22B | 30 | GLU | 3.1 |
| 2 | S2A | 148 | TYR | 3.1 |
| 4 | S4B | 93 | PHE | 3.1 |
| 12 | S12B | 52 | VAL | 3.1 |
| 47 | L25A | 111 | VAL | 3.1 |
| 1 | 16SB | 1115 | G | 3.1 |
| 22 | ASIA | 10 | G | 3.1 |
| 23 | PSIA | 70 | G | 3.1 |
| 4 | S4A | 49 | ARG | 3.1 |
| 54 | L33A | 53 | LYS | 3.1 |
| 33 | L6A | 80 | SER | 3.1 |
| 8 | S8A | 66 | GLY | 3.1 |
| 47 | L25A | 179 | ASP | 3.1 |
| 33 | L6A | 81 | GLU | 3.1 |
| 33 | L6B | 47 | GLU | 3.1 |
| 25 | MRNB | 45 | U | 3.1 |
| 4 | S4A | 199 | ASN | 3.1 |
| 8 | S8B | 27 | PRO | 3.1 |
| 2 | S2A | 214 | ILE | 3.1 |
| 33 | L6B | 162 | ILE | 3.1 |
| 34 | L9A | 120 | ILE | 3.1 |
| 7 | S7B | 153 | HIS | 3.1 |
| 54 | L33A | 49 | HIS | 3.1 |
| 10 | S10A | 26 | ALA | 3.1 |
| 14 | S14A | 30 | ALA | 3.1 |
| 23 | PSIA | 17 | C | 3.1 |
| 23 | PSIA | 67 | C | 3.1 |
| 33 | L6B | 88 | LEU | 3.1 |
| 38 | L16B | 21 | THR | 3.1 |
| 4 | S4A | 99 | SER | 3.1 |
| 22 | ASIA | 24 | G | 3.1 |
| 7 | S7A | 156 | TRP | 3.1 |
| 4 | S4B | 156 | GLU | 3.1 |
| 5 | S5A | 68 | GLU | 3.1 |
| 5 | S5B | 68 | GLU | 3.1 |
| 3 | S3A | 198 | VAL | 3.1 |
| 4 | S4B | 75 | PHE | 3.1 |
| 10 | S10B | 72 | VAL | 3.1 |
| 7 | S7A | 155 | ARG | 3.1 |

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| Mol | Chain | Res | Type | RSRZ |
|---|---|---|---|---|
| 53 | L32A | 52 | TYR | 3.1 |
| 34 | L9A | 133 | HIS | 3.1 |
| 47 | L25B | 164 | ALA | 3.1 |
| 34 | L9B | 9 | LEU | 3.1 |
| 33 | L6A | 120 | GLY | 3.1 |
| 4 | S4A | 144 | ASP | 3.1 |
| 4 | S4B | 72 | GLU | 3.1 |
| 42 | L20B | 89 | GLU | 3.1 |
| 49 | L28A | 93 | GLU | 3.1 |
| 20 | S20A | 87 | LYS | 3.1 |
| 33 | L6A | 126 | PRO | 3.1 |
| 35 | L13B | 44 | PRO | 3.1 |
| 1 | 16SB | 1104 | G | 3.1 |
| 2 | S2A | 108 | ILE | 3.1 |
| 2 | S2A | 182 | ILE | 3.1 |
| 14 | S14A | 34 | TYR | 3.1 |
| 4 | S4B | 199 | ASN | 3.1 |
| 42 | L20B | 66 | ASN | 3.1 |
| 11 | S11A | 68 | ALA | 3.1 |
| 12 | S12B | 23 | ALA | 3.1 |
| 18 | S18A | 20 | ALA | 3.1 |
| 34 | L9A | 83 | ALA | 3.1 |
| 34 | L9B | 123 | LEU | 3.1 |
| 42 | L20B | 72 | HIS | 3.1 |
| 33 | L6A | 174 | GLY | 3.1 |
| 12 | S12B | 80 | VAL | 3.1 |
| 33 | L6B | 109 | PHE | 3.1 |
| 11 | S11A | 36 | ASP | 3.1 |
| 35 | L13B | 17 | ASP | 3.1 |
| 16 | S16B | 66 | PRO | 3.1 |
| 4 | S4A | 106 | TYR | 3.1 |
| 12 | S12A | 61 | TYR | 3.1 |
| 10 | S10B | 71 | LEU | 3.0 |
| 11 | S11A | 60 | ALA | 3.0 |
| 44 | L22B | 65 | LEU | 3.0 |
| 54 | L33B | 34 | LEU | 3.0 |
| 12 | S12B | 77 | HIS | 3.0 |
| 13 | S13A | 100 | GLY | 3.0 |
| 22 | ASIA | 63 | G | 3.0 |
| 27 | 23SA | 1221 | G | 3.0 |
| 27 | 23SA | 2166 | G | 3.0 |
| 2 | S2A | 136 | VAL | 3.0 |

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| Mol | Chain | Res | Type | RSRZ |
|---|---|---|---|---|
| 33 | L6B | 99 | VAL | 3.0 |
| 3 | S3B | 49 | SER | 3.0 |
| 4 | S4A | 137 | SER | 3.0 |
| 4 | S4B | 152 | SER | 3.0 |
| 34 | L9A | 117 | GLU | 3.0 |
| 2 | S2A | 26 | PRO | 3.0 |
| 14 | S14A | 7 | ILE | 3.0 |
| 40 | L18A | 1 | MET | 3.0 |
| 46 | L24A | 56 | PRO | 3.0 |
| 2 | S2B | 98 | LEU | 3.0 |
| 2 | S2B | 173 | ALA | 3.0 |
| 4 | S4A | 111 | ALA | 3.0 |
| 33 | L6A | 71 | LEU | 3.0 |
| 33 | L6B | 64 | LEU | 3.0 |
| 4 | S4B | 153 | ARG | 3.0 |
| 47 | L25B | 79 | ARG | 3.0 |
| 1 | 16SB | 986 | C | 3.0 |
| 12 | S12A | 84 | GLY | 3.0 |
| 23 | PSIA | 4 | C | 3.0 |
| 23 | PSIB | 67 | C | 3.0 |
| 27 | 23SB | 572 | C | 3.0 |
| 27 | 23SB | 2771 | C | 3.0 |
| 3 | S3A | 165 | THR | 3.0 |
| 3 | S3B | 165 | THR | 3.0 |
| 32 | L5B | 75 | LYS | 3.0 |
| 33 | L6A | 131 | VAL | 3.0 |
| 34 | L9A | 141 | LYS | 3.0 |
| 5 | S5B | 50 | GLU | 3.0 |
| 10 | S10B | 96 | ILE | 3.0 |
| 4 | S4A | 51 | PRO | 3.0 |
| 25 | MRNA | 54 | U | 3.0 |
| 53 | L32B | 30 | LEU | 3.0 |
| 2 | S2B | 34 | ALA | 3.0 |
| 4 | S4A | 4 | TYR | 3.0 |
| 6 | S6B | 101 | ALA | 3.0 |
| 12 | S12B | 30 | ARG | 3.0 |
| 41 | L19B | 3 | ARG | 3.0 |
| 4 | S4B | 161 | ASN | 3.0 |
| 32 | L5A | 67 | LYS | 3.0 |
| 36 | L14B | 113 | LYS | 3.0 |
| 44 | L22B | 112 | GLY | 3.0 |
| 54 | L33A | 29 | ASN | 3.0 |

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| Mol | Chain | Res | Type | RSRZ |
|---|---|---|---|---|
| 3 | S3B | 68 | VAL | 3.0 |
| 4 | S4B | 112 | VAL | 3.0 |
| 43 | L21B | 5 | VAL | 3.0 |
| 33 | L6A | 123 | PHE | 3.0 |
| 22 | ASIA | 25 | C | 3.0 |
| 35 | L13B | 60 | ILE | 3.0 |
| 29 | L2B | 162 | SER | 3.0 |
| 34 | L9B | 35 | LEU | 3.0 |
| 41 | L19B | 106 | SER | 3.0 |
| 43 | L21B | 20 | LEU | 3.0 |
| 2 | S2A | 85 | ALA | 3.0 |
| 3 | S3A | 132 | ARG | 3.0 |
| 4 | S4A | 207 | TYR | 3.0 |
| 4 | S4B | 20 | TYR | 3.0 |
| 4 | S4B | 35 | ARG | 3.0 |
| 13 | S13B | 87 | TYR | 3.0 |
| 20 | S20A | 97 | ALA | 3.0 |
| 33 | L6B | 20 | ALA | 3.0 |
| 47 | L25A | 172 | ALA | 3.0 |
| 49 | L28B | 63 | ALA | 3.0 |
| 27 | 23SA | 1142 | U | 3.0 |
| 11 | S11B | 11 | LYS | 3.0 |
| 37 | L15A | 121 | LYS | 3.0 |
| 42 | L20A | 117 | GLN | 3.0 |
| 43 | L21B | 41 | GLY | 3.0 |
| 43 | L21B | 37 | VAL | 3.0 |
| 6 | S6B | 32 | ASN | 3.0 |
| 5 | S5B | 111 | GLU | 3.0 |
| 2 | S2B | 159 | PRO | 3.0 |
| 3 | S3A | 34 | LEU | 3.0 |
| 56 | L35B | 56 | GLU | 3.0 |
| 4 | S4A | 29 | PRO | 3.0 |
| 12 | S12B | 45 | PRO | 3.0 |
| 19 | S19A | 42 | PRO | 3.0 |
| 27 | 23SB | 8 | A | 3.0 |
| 33 | L6A | 128 | PRO | 3.0 |
| 12 | S12A | 38 | ARG | 3.0 |
| 47 | L25B | 81 | ARG | 3.0 |
| 5 | S5B | 86 | ALA | 3.0 |
| 12 | S12B | 126 | ALA | 3.0 |
| 16 | S16A | 7 | ALA | 3.0 |
| 30 | L3B | 20 | ALA | 3.0 |

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| Mol | Chain | Res | Type | RSRZ |
|---|---|---|---|---|
| 6 | S6B | 4 | TYR | 3.0 |
| 4 | S4B | 148 | VAL | 3.0 |
| 7 | S7A | 80 | VAL | 3.0 |
| 7 | S7B | 9 | VAL | 3.0 |
| 7 | S7B | 87 | VAL | 3.0 |
| 8 | S8B | 61 | VAL | 3.0 |
| 10 | S10B | 36 | GLY | 3.0 |
| 42 | L20B | 87 | GLY | 3.0 |
| 4 | S4B | 119 | GLN | 3.0 |
| 24 | ESIB | 12 | U | 3.0 |
| 3 | S3B | 102 | ASN | 3.0 |
| 8 | S8B | 35 | ILE | 3.0 |
| 10 | S10A | 50 | ILE | 3.0 |
| 19 | S19A | 31 | ILE | 3.0 |
| 3 | S3A | 42 | LEU | 2.9 |
| 3 | S3A | 52 | LEU | 2.9 |
| 4 | S4A | 101 | LEU | 2.9 |
| 46 | L24B | 106 | LEU | 2.9 |
| 5 | S5A | 7 | GLU | 2.9 |
| 7 | S7A | 5 | ARG | 2.9 |
| 8 | S8A | 42 | GLU | 2.9 |
| 36 | L14A | 105 | GLU | 2.9 |
| 53 | L32B | 32 | PRO | 2.9 |
| 7 | S7A | 127 | ALA | 2.9 |
| 12 | S12A | 17 | LYS | 2.9 |
| 43 | L21B | 85 | LYS | 2.9 |
| 1 | 16SB | 1053 | A | 2.9 |
| 57 | ASIB | 76 | A | 2.9 |
| 2 | S2A | 122 | PHE | 2.9 |
| 5 | S5A | 72 | GLN | 2.9 |
| 7 | S7B | 43 | PHE | 2.9 |
| 23 | PSIA | 72 | C | 2.9 |
| 57 | ASIB | 4 | C | 2.9 |
| 4 | S4A | 181 | MET | 2.9 |
| 2 | S2B | 6 | THR | 2.9 |
| 2 | S2B | 102 | LEU | 2.9 |
| 5 | S5B | 12 | LEU | 2.9 |
| 10 | S10B | 90 | LEU | 2.9 |
| 35 | L13A | 138 | LEU | 2.9 |
| 47 | L25A | 163 | LEU | 2.9 |
| 54 | L33A | 16 | CYS | 2.9 |
| 35 | L13B | 12 | ARG | 2.9 |

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| Mol | Chain | Res | Type | RSRZ |
|---|---|---|---|---|
| 16 | S16A | 59 | TRP | 2.9 |
| 35 | L13B | 109 | LYS | 2.9 |
| 42 | L20B | 111 | GLU | 2.9 |
| 47 | L25B | 25 | PRO | 2.9 |
| 51 | L30B | 20 | LYS | 2.9 |
| 2 | S2A | 165 | VAL | 2.9 |
| 2 | S2B | 165 | VAL | 2.9 |
| 8 | S8B | 97 | VAL | 2.9 |
| 41 | L19B | 30 | VAL | 2.9 |
| 3 | S3A | 81 | GLY | 2.9 |
| 35 | L13A | 77 | GLY | 2.9 |
| 1 | 16SA | 1065 | G | 2.9 |
| 1 | 16SB | 1817 | G | 2.9 |
| 3 | S3A | 186 | PHE | 2.9 |
| 10 | S10B | 63 | PHE | 2.9 |
| 22 | ASIA | 22 | G | 2.9 |
| 35 | L13B | 38 | HIS | 2.9 |
| 3 | S3B | 124 | ILE | 2.9 |
| 36 | L14B | 1 | MET | 2.9 |
| 3 | S3B | 43 | LEU | 2.9 |
| 17 | S17B | 53 | LEU | 2.9 |
| 42 | L20B | 59 | ARG | 2.9 |
| 2 | S2B | 190 | THR | 2.9 |
| 4 | S4B | 18 | LYS | 2.9 |
| 7 | S7B | 148 | ASN | 2.9 |
| 1 | 16SA | 790 | C | 2.9 |
| 4 | S4B | 189 | PRO | 2.9 |
| 23 | PSIA | 68 | C | 2.9 |
| 31 | L4B | 14 | PRO | 2.9 |
| 2 | S2A | 218 | ALA | 2.9 |
| 4 | S4B | 147 | ALA | 2.9 |
| 10 | S10B | 20 | ALA | 2.9 |
| 33 | L6B | 32 | GLU | 2.9 |
| 34 | L9A | 7 | GLU | 2.9 |
| 40 | L18A | 2 | ALA | 2.9 |
| 51 | L30B | 60 | GLU | 2.9 |
| 3 | S3B | 184 | TYR | 2.9 |
| 34 | L9A | 81 | VAL | 2.9 |
| 34 | L9A | 145 | VAL | 2.9 |
| 43 | L21B | 51 | VAL | 2.9 |
| 4 | S4B | 171 | GLY | 2.9 |
| 15 | S15A | 89 | GLY | 2.9 |

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| Mol | Chain | Res | Type | RSRZ |
|---|---|---|---|---|
| 30 | L3B | 3 | GLY | 2.9 |
| 35 | L13B | 51 | PHE | 2.9 |
| 2 | S2A | 11 | LEU | 2.9 |
| 4 | S4B | 114 | ARG | 2.9 |
| 18 | S18B | 31 | LEU | 2.9 |
| 19 | S19A | 3 | ARG | 2.9 |
| 35 | L13A | 85 | ILE | 2.9 |
| 10 | S10A | 90 | LEU | 2.9 |
| 16 | S16B | 49 | LEU | 2.9 |
| 35 | L13B | 87 | LEU | 2.9 |
| 43 | L21B | 39 | LEU | 2.9 |
| 31 | L4A | 23 | ASP | 2.9 |
| 33 | L6B | 27 | LYS | 2.9 |
| 46 | L24B | 34 | LYS | 2.9 |
| 3 | S3B | 19 | GLU | 2.9 |
| 4 | S4B | 149 | ALA | 2.9 |
| 5 | S5B | 54 | ALA | 2.9 |
| 16 | S16A | 41 | PRO | 2.9 |
| 27 | 23SB | 11 | G | 2.9 |
| 31 | L4B | 130 | ALA | 2.9 |
| 33 | L6B | 18 | GLU | 2.9 |
| 34 | L9A | 65 | ALA | 2.9 |
| 41 | L19A | 21 | GLU | 2.9 |
| 24 | ESIB | 36 | A | 2.9 |
| 2 | S2A | 164 | VAL | 2.9 |
| 4 | S4B | 105 | VAL | 2.9 |
| 5 | S5B | 82 | VAL | 2.9 |
| 16 | S16B | 53 | VAL | 2.9 |
| 33 | L6B | 169 | VAL | 2.9 |
| 47 | L25B | 96 | VAL | 2.9 |
| 7 | S7A | 151 | TYR | 2.9 |
| 18 | S18B | 27 | GLY | 2.9 |
| 22 | ASIA | 74 | C | 2.9 |
| 2 | S2B | 163 | PHE | 2.9 |
| 25 | MRNB | 56 | U | 2.9 |
| 38 | L16A | 104 | PHE | 2.9 |
| 2 | S2A | 172 | ILE | 2.9 |
| 4 | S4B | 155 | LEU | 2.9 |
| 33 | L6A | 30 | LYS | 2.9 |
| 33 | L6A | 103 | LEU | 2.9 |
| 33 | L6B | 98 | LEU | 2.9 |
| 37 | L15B | 106 | LEU | 2.9 |

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| Mol | Chain | Res | Type | RSRZ |
|---|---|---|---|---|
| 46 | L24A | 101 | LYS | 2.9 |
| 48 | L27B | 5 | LYS | 2.9 |
| 3 | S3A | 65 | ALA | 2.9 |
| 4 | S4B | 136 | PRO | 2.9 |
| 16 | S16A | 56 | ALA | 2.9 |
| 40 | L18A | 86 | ALA | 2.9 |
| 46 | L24B | 53 | PRO | 2.9 |
| 12 | S12A | 15 | VAL | 2.9 |
| 14 | S14A | 43 | CYS | 2.9 |
| 14 | S14B | 56 | VAL | 2.9 |
| 32 | L5A | 160 | VAL | 2.9 |
| 4 | S4A | 167 | GLY | 2.9 |
| 7 | S7B | 81 | GLY | 2.9 |
| 11 | S11A | 49 | GLY | 2.9 |
| 47 | L25A | 115 | GLY | 2.9 |
| 2 | S2A | 155 | LEU | 2.9 |
| 3 | S3A | 5 | ILE | 2.9 |
| 34 | L9A | 95 | LYS | 2.9 |
| 41 | L19A | 137 | LYS | 2.9 |
| 24 | ESIA | 8 | U | 2.8 |
| 36 | L14A | 116 | SER | 2.8 |
| 1 | 16SA | 1060 | C | 2.8 |
| 3 | S3B | 129 | ALA | 2.8 |
| 3 | S3B | 183 | ASP | 2.8 |
| 16 | S16B | 47 | ASP | 2.8 |
| 35 | L13B | 92 | ALA | 2.8 |
| 2 | S2B | 168 | THR | 2.8 |
| 35 | L13B | 129 | PRO | 2.8 |
| 4 | S4A | 170 | VAL | 2.8 |
| 4 | S4A | 209 | ARG | 2.8 |
| 2 | S2A | 181 | PHE | 2.8 |
| 3 | S3B | 45 | LYS | 2.8 |
| 3 | S3B | 186 | PHE | 2.8 |
| 4 | S4A | 2 | GLY | 2.8 |
| 2 | S2A | 42 | ILE | 2.8 |
| 2 | S2B | 149 | LEU | 2.8 |
| 2 | S2B | 201 | ILE | 2.8 |
| 3 | S3B | 29 | TYR | 2.8 |
| 4 | S4A | 64 | LEU | 2.8 |
| 6 | S6A | 43 | LEU | 2.8 |
| 4 | S4B | 33 | MET | 2.8 |
| 12 | S12B | 67 | ILE | 2.8 |

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| Mol | Chain | Res | Type | RSRZ |
|---|---|---|---|---|
| 18 | S18B | 85 | LEU | 2.8 |
| 19 | S19A | 15 | LEU | 2.8 |
| 33 | L6B | 89 | ILE | 2.8 |
| 5 | S5A | 21 | ALA | 2.8 |
| 11 | S11B | 60 | ALA | 2.8 |
| 31 | L4A | 198 | ALA | 2.8 |
| 1 | 16SA | 1062 | U | 2.8 |
| 22 | ASIA | 51 | U | 2.8 |
| 24 | ESIA | 15 | G | 2.8 |
| 47 | L25B | 130 | PRO | 2.8 |
| 2 | S2A | 190 | THR | 2.8 |
| 3 | S3A | 75 | VAL | 2.8 |
| 4 | S4A | 14 | ARG | 2.8 |
| 7 | S7A | 79 | ARG | 2.8 |
| 34 | L9A | 113 | ARG | 2.8 |
| 49 | L28A | 53 | VAL | 2.8 |
| 11 | S11B | 42 | TRP | 2.8 |
| 12 | S12B | 51 | LYS | 2.8 |
| 18 | S18B | 84 | LYS | 2.8 |
| 43 | L21B | 19 | LYS | 2.8 |
| 48 | L27B | 12 | ASN | 2.8 |
| 3 | S3A | 124 | ILE | 2.8 |
| 3 | S3B | 101 | LEU | 2.8 |
| 5 | S5B | 151 | LEU | 2.8 |
| 8 | S8A | 45 | ILE | 2.8 |
| 19 | S19A | 30 | LEU | 2.8 |
| 19 | S19A | 71 | LEU | 2.8 |
| 30 | L3A | 176 | ILE | 2.8 |
| 30 | L3B | 49 | LEU | 2.8 |
| 30 | L3B | 52 | LEU | 2.8 |
| 32 | L5B | 173 | LEU | 2.8 |
| 34 | L9A | 128 | LEU | 2.8 |
| 34 | L9B | 120 | ILE | 2.8 |
| 54 | L33A | 40 | CYS | 2.8 |
| 49 | L28B | 38 | SER | 2.8 |
| 12 | S12A | 31 | ARG | 2.8 |
| 38 | L16A | 6 | ARG | 2.8 |
| 53 | L32B | 28 | PRO | 2.8 |
| 34 | L9B | 129 | THR | 2.8 |
| 52 | L31A | 10 | VAL | 2.8 |
| 2 | S2A | 193 | ASP | 2.8 |
| 7 | S7A | 90 | GLU | 2.8 |

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| Mol | Chain | Res | Type | RSRZ |
|---|---|---|---|---|
| 12 | S12A | 62 | GLU | 2.8 |
| 44 | L22B | 66 | GLU | 2.8 |
| 47 | L25B | 117 | LEU | 2.8 |
| 2 | S2B | 37 | ASN | 2.8 |
| 4 | S4B | 2 | GLY | 2.8 |
| 11 | S11A | 29 | ILE | 2.8 |
| 33 | L6B | 9 | ILE | 2.8 |
| 1 | 16SB | 1132 | C | 2.8 |
| 7 | S7B | 85 | TYR | 2.8 |
| 22 | ASIA | 15 | G | 2.8 |
| 23 | PSIA | 71 | G | 2.8 |
| 27 | 23SB | 10 | G | 2.8 |
| 27 | 23SB | 2166 | G | 2.8 |
| 2 | S2B | 171 | ALA | 2.8 |
| 3 | S3B | 189 | ALA | 2.8 |
| 20 | S20B | 106 | ALA | 2.8 |
| 34 | L9B | 146 | ALA | 2.8 |
| 43 | L21B | 80 | GLN | 2.8 |
| 4 | S4B | 40 | PRO | 2.8 |
| 6 | S6B | 96 | PRO | 2.8 |
| 9 | S9A | 41 | VAL | 2.8 |
| 13 | S13A | 98 | VAL | 2.8 |
| 34 | L9B | 144 | VAL | 2.8 |
| 37 | L15A | 125 | VAL | 2.8 |
| 43 | L21B | 72 | VAL | 2.8 |
| 2 | S2A | 73 | THR | 2.8 |
| 12 | S12B | 62 | GLU | 2.8 |
| 19 | S19B | 79 | THR | 2.8 |
| 43 | L21B | 18 | LEU | 2.8 |
| 47 | L25A | 138 | GLU | 2.8 |
| 52 | L31B | 52 | THR | 2.8 |
| 10 | S10A | 96 | ILE | 2.8 |
| 11 | S11A | 42 | TRP | 2.8 |
| 16 | S16A | 80 | PHE | 2.8 |
| 52 | L31A | 31 | ILE | 2.8 |
| 4 | S4A | 129 | ASN | 2.8 |
| 4 | S4A | 27 | TYR | 2.8 |
| 22 | ASIA | 20 | U | 2.8 |
| 27 | 23SB | 2521 | U | 2.8 |
| 34 | L9B | 133 | HIS | 2.8 |
| 3 | S3B | 30 | ARG | 2.8 |
| 3 | S3B | 168 | ALA | 2.8 |

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| Mol | Chain | Res | Type | RSRZ |
|---|---|---|---|---|
| 4 | S4A | 119 | GLN | 2.8 |
| 7 | S7A | 86 | GLN | 2.8 |
| 7 | S7A | 108 | ALA | 2.8 |
| 8 | S8A | 70 | GLN | 2.8 |
| 11 | S11A | 64 | ALA | 2.8 |
| 16 | S16B | 7 | ALA | 2.8 |
| 29 | L2B | 144 | ALA | 2.8 |
| 34 | L9A | 98 | ALA | 2.8 |
| 1 | 16SA | 797 | G | 2.8 |
| 2 | S2B | 71 | VAL | 2.8 |
| 5 | S5B | 70 | PRO | 2.8 |
| 27 | 23SB | 2 | G | 2.8 |
| 57 | ASIB | 71 | G | 2.8 |
| 4 | S4B | 196 | LEU | 2.8 |
| 48 | L27A | 84 | LEU | 2.8 |
| 2 | S2A | 231 | GLU | 2.8 |
| 2 | S2B | 9 | GLU | 2.8 |
| 33 | L6B | 119 | GLU | 2.8 |
| 35 | L13B | 3 | THR | 2.8 |
| 43 | L21B | 28 | GLU | 2.8 |
| 3 | S3B | 128 | PHE | 2.7 |
| 5 | S5A | 6 | PHE | 2.7 |
| 6 | S6B | 60 | PHE | 2.7 |
| 9 | S9A | 37 | PHE | 2.7 |
| 4 | S4A | 193 | ASP | 2.7 |
| 8 | S8A | 90 | GLY | 2.7 |
| 35 | L13B | 45 | ASN | 2.7 |
| 34 | L9A | 126 | TYR | 2.7 |
| 3 | S3A | 21 | ARG | 2.7 |
| 4 | S4A | 36 | ARG | 2.7 |
| 4 | S4A | 164 | ALA | 2.7 |
| 7 | S7A | 83 | ALA | 2.7 |
| 16 | S16B | 84 | ALA | 2.7 |
| 30 | L3B | 70 | ALA | 2.7 |
| 34 | L9B | 94 | ALA | 2.7 |
| 35 | L13B | 84 | LYS | 2.7 |
| 2 | S2A | 93 | VAL | 2.7 |
| 3 | S3B | 120 | VAL | 2.7 |
| 14 | S14A | 52 | GLN | 2.7 |
| 27 | 23SA | 681 | A | 2.7 |
| 41 | L19A | 15 | VAL | 2.7 |
| 47 | L25A | 126 | VAL | 2.7 |

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| Mol | Chain | Res | Type | RSRZ |
|---|---|---|---|---|
| 30 | L3B | 74 | PRO | 2.7 |
| 32 | L5B | 111 | LEU | 2.7 |
| 47 | L25B | 125 | LEU | 2.7 |
| 49 | L28B | 97 | LEU | 2.7 |
| 4 | S4A | 75 | PHE | 2.7 |
| 4 | S4A | 185 | PHE | 2.7 |
| 27 | 23SA | 1123 | C | 2.7 |
| 34 | L9A | 109 | ILE | 2.7 |
| 34 | L9B | 91 | SER | 2.7 |
| 11 | S11A | 87 | THR | 2.7 |
| 38 | L16B | 1 | MET | 2.7 |
| 7 | S7B | 156 | TRP | 2.7 |
| 56 | L35A | 34 | TRP | 2.7 |
| 1 | 16SB | 1054 | G | 2.7 |
| 17 | S17B | 101 | ARG | 2.7 |
| 20 | S20B | 8 | ARG | 2.7 |
| 33 | L6A | 101 | ARG | 2.7 |
| 4 | S4B | 138 | TYR | 2.7 |
| 7 | S7B | 154 | TYR | 2.7 |
| 41 | L19B | 100 | TYR | 2.7 |
| 6 | S6B | 29 | ALA | 2.7 |
| 16 | S16B | 77 | ALA | 2.7 |
| 2 | S2A | 7 | VAL | 2.7 |
| 35 | L13B | 8 | GLN | 2.7 |
| 35 | L13B | 54 | VAL | 2.7 |
| 3 | S3B | 178 | LEU | 2.7 |
| 4 | S4B | 58 | LEU | 2.7 |
| 4 | S4B | 188 | LEU | 2.7 |
| 12 | S12A | 45 | PRO | 2.7 |
| 19 | S19A | 59 | PRO | 2.7 |
| 34 | L9A | 111 | PRO | 2.7 |
| 36 | L14B | 106 | LEU | 2.7 |
| 8 | S8B | 80 | ILE | 2.7 |
| 24 | ESIA | 47 | U | 2.7 |
| 25 | MRNB | 39 | U | 2.7 |
| 2 | S2A | 72 | GLY | 2.7 |
| 3 | S3A | 41 | GLY | 2.7 |
| 3 | S3A | 67 | THR | 2.7 |
| 5 | S5A | 98 | THR | 2.7 |
| 9 | S9A | 100 | GLY | 2.7 |
| 11 | S11B | 87 | THR | 2.7 |
| 16 | S16B | 10 | GLY | 2.7 |

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| Mol | Chain | Res | Type | RSRZ |
|---|---|---|---|---|
| 33 | L6B | 108 | GLY | 2.7 |
| 4 | S4B | 139 | ARG | 2.7 |
| 9 | S9A | 113 | LYS | 2.7 |
| 12 | S12A | 123 | LYS | 2.7 |
| 34 | L9A | 118 | LYS | 2.7 |
| 1 | 16SA | 1699 | C | 2.7 |
| 30 | L3A | 174 | ASP | 2.7 |
| 57 | ASIB | 49 | C | 2.7 |
| 4 | S4B | 82 | ALA | 2.7 |
| 7 | S7A | 134 | ALA | 2.7 |
| 33 | L6A | 96 | ALA | 2.7 |
| 36 | L14B | 51 | ALA | 2.7 |
| 5 | S5B | 105 | VAL | 2.7 |
| 5 | S5B | 115 | VAL | 2.7 |
| 16 | S16A | 51 | VAL | 2.7 |
| 3 | S3B | 87 | LEU | 2.7 |
| 10 | S10B | 65 | LEU | 2.7 |
| 18 | S18B | 40 | LEU | 2.7 |
| 22 | ASIA | 52 | G | 2.7 |
| 24 | ESIA | 34 | G | 2.7 |
| 30 | L3B | 39 | PRO | 2.7 |
| 4 | S4A | 165 | MET | 2.7 |
| 2 | S2B | 141 | GLU | 2.7 |
| 33 | L6B | 81 | GLU | 2.7 |
| 42 | L20B | 108 | GLU | 2.7 |
| 46 | L24A | 109 | GLU | 2.7 |
| 13 | S13A | 94 | ARG | 2.7 |
| 4 | S4B | 85 | LYS | 2.7 |
| 33 | L6B | 153 | LYS | 2.7 |
| 35 | L13B | 42 | TRP | 2.7 |
| 54 | L33A | 27 | LYS | 2.7 |
| 56 | L35B | 34 | TRP | 2.7 |
| 4 | S4B | 54 | TYR | 2.7 |
| 5 | S5B | 133 | TYR | 2.7 |
| 30 | L3A | 204 | ALA | 2.7 |
| 37 | L15B | 110 | TYR | 2.7 |
| 44 | L22B | 94 | ASP | 2.7 |
| 3 | S3B | 86 | VAL | 2.7 |
| 5 | S5B | 123 | LEU | 2.7 |
| 6 | S6B | 43 | LEU | 2.7 |
| 16 | S16B | 73 | LEU | 2.7 |
| 16 | S16B | 74 | LEU | 2.7 |

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| Mol | Chain | Res | Type | RSRZ |
|---|---|---|---|---|
| 20 | S20A | 13 | LEU | 2.7 |
| 31 | L4B | 201 | VAL | 2.7 |
| 34 | L9B | 127 | VAL | 2.7 |
| 35 | L13B | 122 | VAL | 2.7 |
| 43 | L21B | 47 | VAL | 2.7 |
| 48 | L27A | 3 | HIS | 2.7 |
| 54 | L33A | 10 | LEU | 2.7 |
| 42 | L20B | 103 | PRO | 2.7 |
| 57 | ASIB | 72 | C | 2.7 |
| 5 | S5B | 80 | ILE | 2.7 |
| 33 | L6A | 92 | ILE | 2.7 |
| 41 | L19A | 45 | PHE | 2.7 |
| 12 | S12B | 31 | ARG | 2.7 |
| 43 | L21B | 13 | ARG | 2.7 |
| 2 | S2B | 231 | GLU | 2.7 |
| 3 | S3A | 185 | GLY | 2.7 |
| 4 | S4A | 18 | LYS | 2.7 |
| 31 | L4B | 27 | GLU | 2.7 |
| 35 | L13B | 36 | GLY | 2.7 |
| 2 | S2B | 97 | TRP | 2.7 |
| 47 | L25B | 149 | SER | 2.7 |
| 3 | S3A | 129 | ALA | 2.7 |
| 16 | S16A | 64 | ALA | 2.7 |
| 3 | S3B | 103 | VAL | 2.7 |
| 4 | S4A | 97 | LEU | 2.7 |
| 4 | S4B | 21 | LEU | 2.7 |
| 6 | S6B | 19 | LEU | 2.7 |
| 18 | S18A | 34 | TYR | 2.7 |
| 34 | L9A | 114 | LEU | 2.7 |
| 46 | L24A | 106 | LEU | 2.7 |
| 57 | ASIB | 55 | U | 2.7 |
| 2 | S2A | 160 | ASP | 2.7 |
| 51 | L30B | 18 | ASP | 2.7 |
| 4 | S4A | 77 | ASN | 2.7 |
| 3 | S3A | 162 | GLN | 2.6 |
| 5 | S5B | 129 | ILE | 2.6 |
| 24 | ESIB | 7 | A | 2.6 |
| 33 | L6A | 154 | PRO | 2.6 |
| 46 | L24B | 44 | ILE | 2.6 |
| 4 | S4B | 79 | PHE | 2.6 |
| 4 | S4B | 122 | ARG | 2.6 |
| 47 | L25A | 82 | ARG | 2.6 |

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| Mol | Chain | Res | Type | RSRZ |
|---|---|---|---|---|
| 53 | L32B | 55 | ARG | 2.6 |
| 12 | S12B | 54 | LYS | 2.6 |
| 14 | S14B | 58 | LYS | 2.6 |
| 52 | L31A | 24 | THR | 2.6 |
| 2 | S2B | 118 | LEU | 2.6 |
| 5 | S5A | 48 | ALA | 2.6 |
| 8 | S8B | 118 | VAL | 2.6 |
| 18 | S18B | 44 | LEU | 2.6 |
| 30 | L3A | 175 | VAL | 2.6 |
| 34 | L9B | 77 | LEU | 2.6 |
| 41 | L19B | 28 | VAL | 2.6 |
| 52 | L31A | 66 | SER | 2.6 |
| 24 | ESIA | 44 | G | 2.6 |
| 28 | 5SB | 91 | G | 2.6 |
| 36 | L14B | 12 | ASP | 2.6 |
| 46 | L24B | 61 | ILE | 2.6 |
| 2 | S2B | 204 | ASN | 2.6 |
| 4 | S4A | 22 | LYS | 2.6 |
| 8 | S8B | 44 | PHE | 2.6 |
| 24 | ESIB | 47 | U | 2.6 |
| 30 | L3B | 96 | PHE | 2.6 |
| 52 | L31A | 69 | LYS | 2.6 |
| 2 | S2A | 228 | GLY | 2.6 |
| 41 | L19A | 37 | GLY | 2.6 |
| 52 | L31A | 17 | GLY | 2.6 |
| 1 | 16SB | 1071 | A | 2.6 |
| 2 | S2B | 84 | GLU | 2.6 |
| 30 | L3B | 73 | GLU | 2.6 |
| 56 | L35A | 56 | GLU | 2.6 |
| 46 | L24B | 108 | THR | 2.6 |
| 2 | S2B | 187 | LEU | 2.6 |
| 2 | S2B | 213 | LEU | 2.6 |
| 16 | S16B | 48 | TRP | 2.6 |
| 3 | S3A | 146 | ALA | 2.6 |
| 4 | S4A | 112 | VAL | 2.6 |
| 4 | S4A | 147 | ALA | 2.6 |
| 4 | S4A | 198 | VAL | 2.6 |
| 12 | S12A | 125 | ALA | 2.6 |
| 19 | S19A | 51 | VAL | 2.6 |
| 20 | S20A | 53 | LEU | 2.6 |
| 34 | L9A | 12 | LEU | 2.6 |
| 36 | L14A | 52 | VAL | 2.6 |

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| Mol | Chain | Res | Type | RSRZ |
|---|---|---|---|---|
| 42 | L20B | 105 | VAL | 2.6 |
| 47 | L25B | 150 | LEU | 2.6 |
| 49 | L28B | 98 | LEU | 2.6 |
| 4 | S4A | 83 | SER | 2.6 |
| 22 | ASIA | 42 | C | 2.6 |
| 27 | 23SB | 1201 | C | 2.6 |
| 6 | S6B | 63 | TYR | 2.6 |
| 11 | S11B | 59 | TYR | 2.6 |
| 46 | L24B | 55 | TYR | 2.6 |
| 3 | S3A | 199 | LYS | 2.6 |
| 4 | S4A | 66 | ARG | 2.6 |
| 4 | S4A | 67 | ILE | 2.6 |
| 10 | S10A | 22 | LYS | 2.6 |
| 17 | S17B | 100 | LYS | 2.6 |
| 2 | S2B | 122 | PHE | 2.6 |
| 5 | S5B | 49 | PRO | 2.6 |
| 19 | S19A | 2 | PRO | 2.6 |
| 51 | L30B | 2 | PRO | 2.6 |
| 3 | S3A | 62 | ASP | 2.6 |
| 3 | S3B | 56 | ASP | 2.6 |
| 4 | S4B | 167 | GLY | 2.6 |
| 33 | L6A | 82 | GLY | 2.6 |
| 34 | L9B | 124 | GLY | 2.6 |
| 47 | L25A | 147 | GLY | 2.6 |
| 23 | PSIA | 45 | U | 2.6 |
| 36 | L14B | 45 | GLU | 2.6 |
| 41 | L19A | 109 | GLU | 2.6 |
| 2 | S2A | 69 | LEU | 2.6 |
| 14 | S14B | 53 | LEU | 2.6 |
| 2 | S2A | 184 | VAL | 2.6 |
| 3 | S3B | 198 | VAL | 2.6 |
| 12 | S12A | 52 | VAL | 2.6 |
| 13 | S13A | 2 | ALA | 2.6 |
| 13 | S13A | 116 | THR | 2.6 |
| 16 | S16B | 44 | THR | 2.6 |
| 32 | L5A | 82 | LEU | 2.6 |
| 43 | L21B | 62 | LEU | 2.6 |
| 16 | S16B | 51 | VAL | 2.6 |
| 18 | S18B | 86 | VAL | 2.6 |
| 31 | L4B | 128 | ALA | 2.6 |
| 36 | L14A | 121 | VAL | 2.6 |
| 27 | 23SB | 1225 | A | 2.6 |

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| Mol | Chain | Res | Type | RSRZ |
|---|---|---|---|---|
| 27 | 23SB | 2644 | A | 2.6 |
| 34 | L9B | 118 | LYS | 2.6 |
| 36 | L14A | 109 | LYS | 2.6 |
| 53 | L32B | 10 | LYS | 2.6 |
| 3 | S3B | 20 | SER | 2.6 |
| 4 | S4A | 208 | SER | 2.6 |
| 10 | S10A | 62 | HIS | 2.6 |
| 21 | THXA | 21 | TYR | 2.6 |
| 35 | L13A | 130 | HIS | 2.6 |
| 2 | S2A | 163 | PHE | 2.6 |
| 15 | S15B | 2 | PRO | 2.6 |
| 19 | S19A | 74 | PHE | 2.6 |
| 27 | 23SB | 2167 | C | 2.6 |
| 35 | L13B | 50 | ASP | 2.6 |
| 41 | L19A | 18 | ASP | 2.6 |
| 3 | S3A | 158 | GLY | 2.6 |
| 6 | S6B | 7 | ASN | 2.6 |
| 7 | S7A | 133 | GLY | 2.6 |
| 30 | L3B | 192 | ASN | 2.6 |
| 7 | S7A | 22 | LEU | 2.6 |
| 20 | S20A | 104 | LEU | 2.6 |
| 30 | L3A | 195 | LEU | 2.6 |
| 47 | L25A | 70 | LEU | 2.6 |
| 5 | S5A | 115 | VAL | 2.6 |
| 3 | S3B | 67 | THR | 2.6 |
| 8 | S8B | 110 | ALA | 2.6 |
| 35 | L13B | 9 | VAL | 2.6 |
| 18 | S18B | 25 | THR | 2.6 |
| 40 | L18B | 74 | ALA | 2.6 |
| 11 | S11B | 127 | LYS | 2.6 |
| 25 | MRNA | 57 | U | 2.6 |
| 33 | L6B | 97 | ARG | 2.6 |
| 54 | L33A | 45 | LYS | 2.6 |
| 8 | S8B | 38 | ILE | 2.6 |
| 31 | L4B | 82 | ILE | 2.6 |
| 2 | S2B | 33 | TYR | 2.6 |
| 4 | S4A | 20 | TYR | 2.6 |
| 57 | ASIB | 5 | G | 2.6 |
| 6 | S6B | 12 | PRO | 2.6 |
| 8 | S8B | 57 | PRO | 2.6 |
| 33 | L6A | 117 | PRO | 2.6 |
| 33 | L6B | 173 | PRO | 2.6 |

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| Mol | Chain | Res | Type | RSRZ |
|---|---|---|---|---|
| 34 | L9B | 111 | PRO | 2.6 |
| 35 | L13B | 11 | PRO | 2.6 |
| 11 | S11A | 99 | GLN | 2.6 |
| 22 | ASIA | 64 | A | 2.6 |
| 3 | S3A | 197 | GLY | 2.6 |
| 4 | S4A | 183 | GLY | 2.6 |
| 19 | S19A | 12 | ASP | 2.6 |
| 52 | L31A | 70 | GLY | 2.6 |
| 2 | S2A | 238 | LEU | 2.6 |
| 19 | S19A | 20 | LEU | 2.6 |
| 34 | L9A | 123 | LEU | 2.6 |
| 36 | L14A | 122 | LEU | 2.6 |
| 49 | L28A | 85 | LEU | 2.6 |
| 1 | 16SB | 1948 | C | 2.6 |
| 24 | ESIB | 17 | C | 2.6 |
| 27 | 23SA | 935 | C | 2.6 |
| 33 | L6A | 127 | GLU | 2.6 |
| 54 | L33A | 12 | GLU | 2.6 |
| 2 | S2B | 136 | VAL | 2.6 |
| 4 | S4A | 8 | VAL | 2.6 |
| 7 | S7A | 40 | ALA | 2.6 |
| 12 | S12B | 36 | VAL | 2.6 |
| 20 | S20A | 66 | ALA | 2.6 |
| 47 | L25B | 56 | VAL | 2.6 |
| 49 | L28A | 77 | ALA | 2.6 |
| 54 | L33B | 33 | LYS | 2.6 |
| 3 | S3B | 167 | TRP | 2.5 |
| 2 | S2B | 108 | ILE | 2.5 |
| 31 | L4B | 10 | PRO | 2.5 |
| 33 | L6A | 173 | PRO | 2.5 |
| 16 | S16B | 11 | SER | 2.5 |
| 11 | S11A | 93 | GLN | 2.5 |
| 12 | S12B | 11 | GLY | 2.5 |
| 16 | S16B | 37 | GLY | 2.5 |
| 33 | L6A | 143 | GLN | 2.5 |
| 33 | L6B | 5 | GLY | 2.5 |
| 40 | L18A | 84 | GLN | 2.5 |
| 2 | S2A | 215 | LEU | 2.5 |
| 4 | S4A | 186 | LEU | 2.5 |
| 20 | S20A | 24 | LEU | 2.5 |
| 54 | L33B | 11 | LEU | 2.5 |
| 3 | S3B | 16 | ARG | 2.5 |

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| Mol | Chain | Res | Type | RSRZ |
|---|---|---|---|---|
| 4 | S4A | 60 | GLU | 2.5 |
| 5 | S5B | 67 | VAL | 2.5 |
| 10 | S10A | 12 | ASP | 2.5 |
| 10 | S10A | 94 | VAL | 2.5 |
| 13 | S13A | 114 | ARG | 2.5 |
| 19 | S19A | 32 | LYS | 2.5 |
| 27 | 23SB | 1137 | G | 2.5 |
| 35 | L13A | 127 | ASP | 2.5 |
| 41 | L19B | 58 | ASN | 2.5 |
| 43 | L21A | 33 | VAL | 2.5 |
| 49 | L28B | 96 | LYS | 2.5 |
| 54 | L33B | 26 | ASN | 2.5 |
| 6 | S6B | 20 | ALA | 2.5 |
| 12 | S12A | 76 | GLU | 2.5 |
| 27 | 23SB | 6 | A | 2.5 |
| 30 | L3B | 200 | GLU | 2.5 |
| 33 | L6A | 167 | GLU | 2.5 |
| 3 | S3A | 18 | TRP | 2.5 |
| 5 | S5B | 101 | ILE | 2.5 |
| 10 | S10B | 87 | THR | 2.5 |
| 12 | S12B | 64 | THR | 2.5 |
| 19 | S19A | 44 | MET | 2.5 |
| 11 | S11B | 125 | PHE | 2.5 |
| 22 | ASIA | 43 | C | 2.5 |
| 27 | 23SA | 2170 | C | 2.5 |
| 27 | 23SA | 2817 | C | 2.5 |
| 5 | S5B | 96 | PRO | 2.5 |
| 30 | L3B | 32 | PRO | 2.5 |
| 14 | S14B | 43 | CYS | 2.5 |
| 2 | S2B | 51 | LEU | 2.5 |
| 3 | S3B | 91 | LEU | 2.5 |
| 4 | S4A | 109 | GLY | 2.5 |
| 5 | S5B | 142 | LEU | 2.5 |
| 7 | S7A | 81 | GLY | 2.5 |
| 7 | S7B | 133 | GLY | 2.5 |
| 16 | S16B | 65 | GLN | 2.5 |
| 31 | L4A | 8 | GLN | 2.5 |
| 32 | L5A | 3 | LEU | 2.5 |
| 33 | L6B | 135 | GLY | 2.5 |
| 41 | L19B | 37 | GLY | 2.5 |
| 42 | L20B | 95 | LEU | 2.5 |
| 48 | L27B | 6 | GLY | 2.5 |

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| Mol | Chain | Res | Type | RSRZ |
|---|---|---|---|---|
| 12 | S12A | 50 | ARG | 2.5 |
| 17 | S17B | 68 | ARG | 2.5 |
| 36 | L14B | 49 | ARG | 2.5 |
| 41 | L19A | 39 | ARG | 2.5 |
| 54 | L33A | 17 | LYS | 2.5 |
| 3 | S3A | 50 | ALA | 2.5 |
| 3 | S3A | 163 | ALA | 2.5 |
| 5 | S5B | 122 | GLU | 2.5 |
| 6 | S6B | 100 | ASN | 2.5 |
| 7 | S7A | 152 | ALA | 2.5 |
| 8 | S8B | 77 | GLU | 2.5 |
| 32 | L5B | 57 | ALA | 2.5 |
| 54 | L33A | 20 | ASN | 2.5 |
| 54 | L33B | 35 | GLU | 2.5 |
| 10 | S10B | 98 | ILE | 2.5 |
| 13 | S13A | 9 | ILE | 2.5 |
| 13 | S13A | 39 | ILE | 2.5 |
| 15 | S15B | 82 | ILE | 2.5 |
| 36 | L14A | 96 | THR | 2.5 |
| 4 | S4A | 79 | PHE | 2.5 |
| 22 | ASIA | 65 | G | 2.5 |
| 24 | ESIA | 69 | G | 2.5 |
| 27 | 23SB | 557 | G | 2.5 |
| 4 | S4A | 54 | TYR | 2.5 |
| 4 | S4B | 29 | PRO | 2.5 |
| 3 | S3B | 33 | LEU | 2.5 |
| 5 | S5A | 43 | LEU | 2.5 |
| 1 | 16SA | 1671 | C | 2.5 |
| 9 | S9A | 128 | ARG | 2.5 |
| 18 | S18A | 78 | LEU | 2.5 |
| 32 | L5B | 152 | LEU | 2.5 |
| 28 | 5SB | 93 | C | 2.5 |
| 33 | L6A | 60 | ARG | 2.5 |
| 35 | L13B | 97 | ARG | 2.5 |
| 16 | S16B | 76 | GLN | 2.5 |
| 17 | S17B | 39 | SER | 2.5 |
| 43 | L21B | 11 | GLN | 2.5 |
| 47 | L25B | 66 | SER | 2.5 |
| 16 | S16B | 20 | VAL | 2.5 |
| 35 | L13B | 14 | VAL | 2.5 |
| 3 | S3B | 180 | ALA | 2.5 |
| 15 | S15A | 30 | ALA | 2.5 |

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| Mol | Chain | Res | Type | RSRZ |
|---|---|---|---|---|
| 35 | L13B | 124 | ALA | 2.5 |
| 42 | L20B | 96 | ALA | 2.5 |
| 2 | S2A | 117 | GLU | 2.5 |
| 13 | S13A | 8 | GLU | 2.5 |
| 27 | 23SB | 1074 | U | 2.5 |
| 33 | L6B | 116 | GLU | 2.5 |
| 5 | S5B | 11 | ILE | 2.5 |
| 8 | S8B | 121 | ASP | 2.5 |
| 41 | L19A | 88 | ILE | 2.5 |
| 42 | L20B | 80 | ILE | 2.5 |
| 2 | S2B | 28 | PHE | 2.5 |
| 4 | S4B | 173 | TRP | 2.5 |
| 8 | S8B | 138 | TRP | 2.5 |
| 10 | S10B | 81 | THR | 2.5 |
| 12 | S12A | 58 | THR | 2.5 |
| 16 | S16A | 48 | TRP | 2.5 |
| 46 | L24B | 60 | PHE | 2.5 |
| 4 | S4A | 40 | PRO | 2.5 |
| 2 | S2A | 10 | LEU | 2.5 |
| 4 | S4B | 46 | LYS | 2.5 |
| 5 | S5A | 133 | TYR | 2.5 |
| 6 | S6B | 61 | LEU | 2.5 |
| 8 | S8B | 62 | TYR | 2.5 |
| 33 | L6B | 29 | PRO | 2.5 |
| 10 | S10A | 65 | LEU | 2.5 |
| 16 | S16B | 12 | LYS | 2.5 |
| 33 | L6A | 160 | LYS | 2.5 |
| 34 | L9B | 130 | TYR | 2.5 |
| 35 | L13B | 99 | LEU | 2.5 |
| 44 | L22B | 51 | LEU | 2.5 |
| 2 | S2B | 66 | GLY | 2.5 |
| 3 | S3A | 2 | GLY | 2.5 |
| 15 | S15B | 86 | GLY | 2.5 |
| 27 | 23SB | 2823 | A | 2.5 |
| 35 | L13B | 49 | GLY | 2.5 |
| 3 | S3A | 141 | VAL | 2.5 |
| 4 | S4B | 8 | VAL | 2.5 |
| 4 | S4B | 160 | GLN | 2.5 |
| 6 | S6B | 65 | VAL | 2.5 |
| 34 | L9B | 139 | GLN | 2.5 |
| 1 | 16SA | 743 | G | 2.5 |
| 1 | 16SA | 1085 | G | 2.5 |

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| Mol | Chain | Res | Type | RSRZ |
|---|---|---|---|---|
| 3 | S3B | 200 | ALA | 2.5 |
| 7 | S7A | 2 | ALA | 2.5 |
| 9 | S9A | 81 | ILE | 2.5 |
| 31 | L4B | 28 | ILE | 2.5 |
| 38 | L16B | 68 | ILE | 2.5 |
| 43 | L21B | 98 | GLU | 2.5 |
| 7 | S7B | 73 | MET | 2.5 |
| 10 | S10A | 11 | PHE | 2.5 |
| 11 | S11B | 38 | ASN | 2.5 |
| 36 | L14A | 29 | ASN | 2.5 |
| 1 | 16SA | 727 | U | 2.5 |
| 5 | S5B | 98 | THR | 2.5 |
| 7 | S7B | 103 | TRP | 2.5 |
| 2 | S2B | 44 | LEU | 2.5 |
| 3 | S3A | 91 | LEU | 2.5 |
| 3 | S3B | 47 | LEU | 2.5 |
| 4 | S4A | 196 | LEU | 2.5 |
| 5 | S5B | 139 | LEU | 2.5 |
| 11 | S11A | 12 | ARG | 2.5 |
| 18 | S18A | 85 | LEU | 2.5 |
| 41 | L19A | 82 | LEU | 2.5 |
| 46 | L24B | 50 | ARG | 2.5 |
| 47 | L25B | 80 | ARG | 2.5 |
| 30 | L3B | 62 | PRO | 2.5 |
| 47 | L25B | 134 | PRO | 2.5 |
| 12 | S12B | 66 | TYR | 2.5 |
| 19 | S19A | 14 | HIS | 2.5 |
| 31 | L4B | 7 | TYR | 2.5 |
| 2 | S2A | 99 | GLY | 2.5 |
| 3 | S3A | 171 | GLY | 2.5 |
| 30 | L3A | 193 | GLY | 2.5 |
| 7 | S7B | 80 | VAL | 2.5 |
| 10 | S10B | 101 | VAL | 2.5 |
| 42 | L20B | 100 | VAL | 2.5 |
| 11 | S11B | 68 | ALA | 2.4 |
| 33 | L6B | 145 | ALA | 2.4 |
| 2 | S2B | 58 | ILE | 2.4 |
| 4 | S4A | 5 | ILE | 2.4 |
| 10 | S10B | 59 | SER | 2.4 |
| 14 | S14A | 27 | CYS | 2.4 |
| 33 | L6B | 92 | ILE | 2.4 |
| 34 | L9A | 91 | SER | 2.4 |

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| Mol | Chain | Res | Type | RSRZ |
|---|---|---|---|---|
| 47 | L25B | 120 | ILE | 2.4 |
| 4 | S4B | 60 | GLU | 2.4 |
| 47 | L25B | 168 | GLU | 2.4 |
| 9 | S9A | 127 | LYS | 2.4 |
| 2 | S2B | 24 | TRP | 2.4 |
| 12 | S12A | 16 | ARG | 2.4 |
| 43 | L21B | 21 | ARG | 2.4 |
| 4 | S4B | 89 | THR | 2.4 |
| 23 | PSIA | 69 | G | 2.4 |
| 24 | ESIB | 69 | G | 2.4 |
| 27 | 23SA | 1124 | C | 2.4 |
| 27 | 23SA | 2171 | C | 2.4 |
| 27 | 23SA | 2492 | C | 2.4 |
| 27 | 23SA | 2810 | C | 2.4 |
| 27 | 23SB | 1148 | C | 2.4 |
| 4 | S4A | 125 | HIS | 2.4 |
| 22 | ASIA | 50 | U | 2.4 |
| 35 | L13B | 128 | HIS | 2.4 |
| 3 | S3B | 195 | VAL | 2.4 |
| 12 | S12A | 63 | VAL | 2.4 |
| 12 | S12B | 60 | GLY | 2.4 |
| 12 | S12B | 87 | VAL | 2.4 |
| 16 | S16B | 63 | GLY | 2.4 |
| 49 | L28B | 53 | VAL | 2.4 |
| 4 | S4A | 149 | ALA | 2.4 |
| 6 | S6B | 49 | ALA | 2.4 |
| 6 | S6B | 94 | GLN | 2.4 |
| 7 | S7B | 39 | ALA | 2.4 |
| 8 | S8B | 28 | ALA | 2.4 |
| 30 | L3B | 54 | GLN | 2.4 |
| 31 | L4B | 22 | ALA | 2.4 |
| 2 | S2A | 58 | ILE | 2.4 |
| 18 | S18B | 75 | ILE | 2.4 |
| 8 | S8A | 1 | MET | 2.4 |
| 4 | S4B | 145 | GLU | 2.4 |
| 29 | L2B | 28 | GLU | 2.4 |
| 37 | L15B | 74 | GLU | 2.4 |
| 52 | L31A | 37 | SER | 2.4 |
| 2 | S2A | 153 | ARG | 2.4 |
| 5 | S5A | 14 | ARG | 2.4 |
| 11 | S11B | 51 | LYS | 2.4 |
| 15 | S15B | 88 | ARG | 2.4 |

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| Mol | Chain | Res | Type | RSRZ |
|---|---|---|---|---|
| 30 | L3B | 199 | ARG | 2.4 |
| 33 | L6A | 95 | ARG | 2.4 |
| 35 | L13B | 29 | LYS | 2.4 |
| 4 | S4B | 11 | LEU | 2.4 |
| 13 | S13B | 90 | LEU | 2.4 |
| 38 | L16B | 79 | LEU | 2.4 |
| 43 | L21B | 25 | LEU | 2.4 |
| 4 | S4B | 102 | ASP | 2.4 |
| 13 | S13B | 103 | THR | 2.4 |
| 47 | L25B | 83 | PRO | 2.4 |
| 3 | S3A | 99 | VAL | 2.4 |
| 5 | S5B | 34 | VAL | 2.4 |
| 6 | S6B | 37 | VAL | 2.4 |
| 11 | S11B | 25 | TYR | 2.4 |
| 16 | S16A | 37 | GLY | 2.4 |
| 18 | S18B | 39 | VAL | 2.4 |
| 19 | S19B | 82 | GLY | 2.4 |
| 33 | L6A | 169 | VAL | 2.4 |
| 33 | L6B | 82 | GLY | 2.4 |
| 33 | L6B | 83 | TYR | 2.4 |
| 45 | L23B | 94 | GLY | 2.4 |
| 49 | L28A | 84 | GLY | 2.4 |
| 52 | L31A | 50 | VAL | 2.4 |
| 3 | S3B | 113 | ALA | 2.4 |
| 27 | 23SB | 2165 | C | 2.4 |
| 4 | S4A | 62 | GLN | 2.4 |
| 22 | ASIA | 44 | G | 2.4 |
| 24 | ESIA | 5 | G | 2.4 |
| 30 | L3A | 1 | MET | 2.4 |
| 33 | L6A | 41 | MET | 2.4 |
| 2 | S2A | 169 | LYS | 2.4 |
| 4 | S4A | 166 | LYS | 2.4 |
| 19 | S19A | 78 | ARG | 2.4 |
| 19 | S19B | 88 | LYS | 2.4 |
| 29 | L2B | 38 | LYS | 2.4 |
| 30 | L3A | 97 | LYS | 2.4 |
| 34 | L9B | 112 | LYS | 2.4 |
| 35 | L13B | 39 | ARG | 2.4 |
| 35 | L13B | 121 | LYS | 2.4 |
| 36 | L14B | 59 | LYS | 2.4 |
| 54 | L33B | 25 | LYS | 2.4 |
| 2 | S2B | 17 | PHE | 2.4 |

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| Mol | Chain | Res | Type | RSRZ |
|---|---|---|---|---|
| 4 | S4A | 80 | GLU | 2.4 |
| 9 | S9A | 110 | GLU | 2.4 |
| 2 | S2B | 69 | LEU | 2.4 |
| 4 | S4A | 94 | LEU | 2.4 |
| 8 | S8B | 107 | LEU | 2.4 |
| 20 | S20B | 104 | LEU | 2.4 |
| 32 | L5B | 60 | LEU | 2.4 |
| 34 | L9A | 58 | LEU | 2.4 |
| 37 | L15B | 148 | LEU | 2.4 |
| 4 | S4A | 103 | ASN | 2.4 |
| 4 | S4A | 154 | ASN | 2.4 |
| 4 | S4B | 39 | PRO | 2.4 |
| 9 | S9A | 64 | THR | 2.4 |
| 36 | L14A | 65 | THR | 2.4 |
| 3 | S3B | 116 | VAL | 2.4 |
| 4 | S4B | 56 | VAL | 2.4 |
| 19 | S19B | 45 | VAL | 2.4 |
| 31 | L4A | 126 | VAL | 2.4 |
| 42 | L20B | 97 | ASP | 2.4 |
| 52 | L31B | 33 | VAL | 2.4 |
| 7 | S7A | 154 | TYR | 2.4 |
| 10 | S10B | 13 | HIS | 2.4 |
| 11 | S11B | 86 | GLY | 2.4 |
| 13 | S13A | 87 | TYR | 2.4 |
| 7 | S7B | 83 | ALA | 2.4 |
| 1 | 16SA | 696 | A | 2.4 |
| 1 | 16SA | 791 | A | 2.4 |
| 1 | 16SA | 1854 | A | 2.4 |
| 2 | S2A | 5 | ILE | 2.4 |
| 2 | S2A | 80 | ILE | 2.4 |
| 33 | L6A | 156 | ALA | 2.4 |
| 33 | L6B | 75 | ALA | 2.4 |
| 36 | L14A | 103 | ALA | 2.4 |
| 42 | L20B | 116 | ALA | 2.4 |
| 27 | 23SB | 1094 | A | 2.4 |
| 4 | S4B | 22 | LYS | 2.4 |
| 7 | S7A | 149 | ARG | 2.4 |
| 16 | S16B | 50 | LYS | 2.4 |
| 47 | L25B | 28 | MET | 2.4 |
| 2 | S2A | 84 | GLU | 2.4 |
| 3 | S3A | 12 | LEU | 2.4 |
| 4 | S4B | 176 | LEU | 2.4 |

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| Mol | Chain | Res | Type | RSRZ |
|---|---|---|---|---|
| 4 | S4B | 186 | LEU | 2.4 |
| 5 | S5B | 43 | LEU | 2.4 |
| 8 | S8B | 2 | LEU | 2.4 |
| 14 | S14B | 44 | LEU | 2.4 |
| 17 | S17B | 22 | LEU | 2.4 |
| 18 | S18B | 38 | GLU | 2.4 |
| 23 | PSIA | 20 | U | 2.4 |
| 27 | 23SB | 1199 | C | 2.4 |
| 27 | 23SB | 2813 | C | 2.4 |
| 32 | L5A | 43 | LEU | 2.4 |
| 32 | L5A | 139 | LEU | 2.4 |
| 2 | S2A | 235 | SER | 2.4 |
| 47 | L25B | 153 | SER | 2.4 |
| 1 | 16SA | 1105 | G | 2.4 |
| 1 | 16SA | 1121 | G | 2.4 |
| 1 | 16SB | 1064 | G | 2.4 |
| 27 | 23SA | 1122 | G | 2.4 |
| 54 | L33B | 13 | CYS | 2.4 |
| 3 | S3B | 130 | VAL | 2.4 |
| 4 | S4A | 7 | PRO | 2.4 |
| 4 | S4A | 148 | VAL | 2.4 |
| 5 | S5A | 41 | VAL | 2.4 |
| 5 | S5A | 67 | VAL | 2.4 |
| 5 | S5A | 96 | PRO | 2.4 |
| 7 | S7A | 93 | PRO | 2.4 |
| 35 | L13B | 13 | TRP | 2.4 |
| 11 | S11B | 14 | VAL | 2.4 |
| 34 | L9B | 142 | VAL | 2.4 |
| 35 | L13B | 53 | VAL | 2.4 |
| 43 | L21B | 16 | PRO | 2.4 |
| 43 | L21B | 29 | PRO | 2.4 |
| 2 | S2A | 195 | ASP | 2.4 |
| 3 | S3A | 69 | HIS | 2.4 |
| 4 | S4B | 143 | GLY | 2.4 |
| 11 | S11B | 52 | GLY | 2.4 |
| 18 | S18A | 77 | GLY | 2.4 |
| 40 | L18A | 109 | GLY | 2.4 |
| 46 | L24B | 104 | GLY | 2.4 |
| 4 | S4B | 207 | TYR | 2.4 |
| 16 | S16A | 39 | TYR | 2.4 |
| 18 | S18B | 73 | ALA | 2.4 |
| 42 | L20B | 62 | ILE | 2.4 |

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| Mol | Chain | Res | Type | RSRZ |
|---|---|---|---|---|
| 43 | L21B | 81 | TYR | 2.4 |
| 34 | L9B | 121 | LYS | 2.4 |
| 41 | L19A | 33 | LYS | 2.4 |
| 4 | S4A | 47 | ARG | 2.4 |
| 3 | S3A | 118 | GLN | 2.4 |
| 3 | S3A | 10 | PHE | 2.4 |
| 18 | S18B | 79 | LEU | 2.4 |
| 33 | L6A | 105 | LEU | 2.4 |
| 51 | L30B | 8 | LEU | 2.4 |
| 1 | 16SA | 701 | A | 2.4 |
| 1 | 16SA | 811 | A | 2.4 |
| 1 | 16SA | 1049 | A | 2.4 |
| 46 | L24A | 110 | GLU | 2.4 |
| 10 | S10B | 19 | SER | 2.4 |
| 11 | S11B | 101 | SER | 2.4 |
| 33 | L6B | 155 | SER | 2.4 |
| 2 | S2A | 97 | TRP | 2.4 |
| 3 | S3A | 173 | VAL | 2.4 |
| 19 | S19B | 41 | VAL | 2.4 |
| 19 | S19B | 60 | VAL | 2.4 |
| 27 | 23SA | 2169 | U | 2.4 |
| 33 | L6A | 29 | PRO | 2.4 |
| 34 | L9B | 119 | PRO | 2.4 |
| 36 | L14B | 48 | PRO | 2.4 |
| 42 | L20B | 63 | VAL | 2.4 |
| 47 | L25B | 158 | PRO | 2.4 |
| 3 | S3B | 96 | GLY | 2.3 |
| 7 | S7B | 82 | GLY | 2.3 |
| 3 | S3B | 63 | ASN | 2.3 |
| 5 | S5B | 65 | ASN | 2.3 |
| 5 | S5A | 25 | ARG | 2.3 |
| 5 | S5A | 118 | ILE | 2.3 |
| 31 | L4A | 206 | ILE | 2.3 |
| 53 | L32B | 37 | LYS | 2.3 |
| 6 | S6B | 77 | ARG | 2.3 |
| 9 | S9B | 4 | TYR | 2.3 |
| 13 | S13A | 11 | ARG | 2.3 |
| 33 | L6B | 23 | ARG | 2.3 |
| 56 | L35A | 46 | ARG | 2.3 |
| 27 | 23SB | 2816 | G | 2.3 |
| 4 | S4B | 194 | LEU | 2.3 |
| 5 | S5A | 26 | PHE | 2.3 |

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| Mol | Chain | Res | Type | RSRZ |
|---|---|---|---|---|
| 31 | L4B | 20 | LEU | 2.3 |
| 33 | L6A | 98 | LEU | 2.3 |
| 34 | L9A | 6 | LEU | 2.3 |
| 34 | L9B | 116 | LEU | 2.3 |
| 42 | L20B | 98 | LEU | 2.3 |
| 6 | S6B | 42 | GLU | 2.3 |
| 43 | L21B | 23 | GLU | 2.3 |
| 3 | S3B | 55 | VAL | 2.3 |
| 4 | S4A | 17 | VAL | 2.3 |
| 6 | S6B | 90 | VAL | 2.3 |
| 12 | S12B | 40 | VAL | 2.3 |
| 16 | S16A | 79 | VAL | 2.3 |
| 31 | L4B | 126 | VAL | 2.3 |
| 33 | L6B | 79 | VAL | 2.3 |
| 36 | L14A | 58 | VAL | 2.3 |
| 1 | 16SA | 2026 | A | 2.3 |
| 4 | S4B | 183 | GLY | 2.3 |
| 7 | S7B | 136 | LYS | 2.3 |
| 11 | S11A | 70 | LYS | 2.3 |
| 24 | ESIB | 35 | A | 2.3 |
| 27 | 23SA | 944 | A | 2.3 |
| 33 | L6A | 85 | LYS | 2.3 |
| 35 | L13B | 125 | GLY | 2.3 |
| 46 | L24B | 54 | LYS | 2.3 |
| 2 | S2B | 182 | ILE | 2.3 |
| 4 | S4A | 35 | ARG | 2.3 |
| 3 | S3A | 53 | ALA | 2.3 |
| 5 | S5A | 109 | ILE | 2.3 |
| 6 | S6B | 86 | ARG | 2.3 |
| 47 | L25A | 143 | GLY | 2.3 |
| 11 | S11B | 74 | ALA | 2.3 |
| 13 | S13A | 42 | ALA | 2.3 |
| 16 | S16B | 36 | ILE | 2.3 |
| 17 | S17B | 59 | ILE | 2.3 |
| 31 | L4B | 21 | ALA | 2.3 |
| 36 | L14B | 87 | ILE | 2.3 |
| 37 | L15A | 150 | ALA | 2.3 |
| 42 | L20B | 86 | ALA | 2.3 |
| 47 | L25A | 113 | ALA | 2.3 |
| 53 | L32B | 33 | CYS | 2.3 |
| 2 | S2B | 48 | MET | 2.3 |
| 25 | MRNA | 39 | U | 2.3 |

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| Mol | Chain | Res | Type | RSRZ |
|---|---|---|---|---|
| 33 | L6A | 164 | TYR | 2.3 |
| 36 | L14B | 13 | ASN | 2.3 |
| 4 | S4B | 177 | ASP | 2.3 |
| 3 | S3B | 175 | LEU | 2.3 |
| 14 | S14B | 39 | LEU | 2.3 |
| 27 | 23SA | 698 | C | 2.3 |
| 2 | S2A | 240 | GLN | 2.3 |
| 32 | L5B | 138 | GLN | 2.3 |
| 47 | L25A | 88 | PHE | 2.3 |
| 2 | S2A | 12 | GLU | 2.3 |
| 3 | S3B | 166 | GLU | 2.3 |
| 4 | S4B | 200 | GLU | 2.3 |
| 15 | S15B | 26 | GLU | 2.3 |
| 47 | L25A | 119 | GLU | 2.3 |
| 1 | 16SB | 652 | G | 2.3 |
| 1 | 16SB | 1660 | G | 2.3 |
| 3 | S3A | 64 | VAL | 2.3 |
| 4 | S4A | 92 | VAL | 2.3 |
| 4 | S4B | 121 | VAL | 2.3 |
| 10 | S10B | 34 | VAL | 2.3 |
| 47 | L25B | 165 | VAL | 2.3 |
| 57 | ASIB | 69 | G | 2.3 |
| 4 | S4B | 169 | LYS | 2.3 |
| 5 | S5A | 47 | LYS | 2.3 |
| 32 | L5A | 182 | LYS | 2.3 |
| 33 | L6B | 77 | LYS | 2.3 |
| 35 | L13B | 137 | LYS | 2.3 |
| 4 | S4B | 197 | PRO | 2.3 |
| 7 | S7A | 88 | PRO | 2.3 |
| 13 | S13B | 119 | GLY | 2.3 |
| 33 | L6A | 100 | GLY | 2.3 |
| 36 | L14A | 55 | GLY | 2.3 |
| 46 | L24A | 104 | GLY | 2.3 |
| 2 | S2A | 13 | ALA | 2.3 |
| 2 | S2B | 29 | ALA | 2.3 |
| 2 | S2B | 107 | THR | 2.3 |
| 5 | S5B | 94 | ALA | 2.3 |
| 36 | L14B | 14 | THR | 2.3 |
| 43 | L21B | 32 | THR | 2.3 |
| 12 | S12B | 117 | TYR | 2.3 |
| 42 | L20B | 76 | TYR | 2.3 |
| 3 | S3B | 34 | LEU | 2.3 |

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| Mol | Chain | Res | Type | RSRZ |
|---|---|---|---|---|
| 4 | S4A | 120 | LEU | 2.3 |
| 18 | S18B | 78 | LEU | 2.3 |
| 30 | L3B | 182 | LEU | 2.3 |
| 41 | L19B | 78 | LEU | 2.3 |
| 47 | L25B | 41 | LEU | 2.3 |
| 1 | 16SA | 1072 | A | 2.3 |
| 28 | 5SB | 92 | A | 2.3 |
| 41 | L19B | 45 | PHE | 2.3 |
| 2 | S2A | 60 | ASP | 2.3 |
| 30 | L3B | 89 | ASP | 2.3 |
| 1 | 16SA | 984 | U | 2.3 |
| 6 | S6B | 64 | GLN | 2.3 |
| 30 | L3A | 48 | GLN | 2.3 |
| 4 | S4B | 98 | GLU | 2.3 |
| 6 | S6B | 66 | GLU | 2.3 |
| 49 | L28B | 93 | GLU | 2.3 |
| 1 | 16SB | 1082 | C | 2.3 |
| 2 | S2A | 179 | LYS | 2.3 |
| 3 | S3A | 55 | VAL | 2.3 |
| 3 | S3A | 130 | VAL | 2.3 |
| 6 | S6B | 6 | VAL | 2.3 |
| 16 | S16B | 3 | LYS | 2.3 |
| 18 | S18B | 22 | VAL | 2.3 |
| 22 | ASIA | 67 | C | 2.3 |
| 30 | L3B | 198 | VAL | 2.3 |
| 47 | L25B | 78 | LYS | 2.3 |
| 2 | S2A | 144 | ARG | 2.3 |
| 29 | L2A | 262 | ARG | 2.3 |
| 3 | S3A | 7 | PRO | 2.3 |
| 11 | S11B | 113 | PRO | 2.3 |
| 16 | S16B | 15 | PRO | 2.3 |
| 33 | L6A | 118 | PRO | 2.3 |
| 33 | L6B | 136 | ILE | 2.3 |
| 34 | L9A | 88 | ILE | 2.3 |
| 41 | L19B | 83 | ILE | 2.3 |
| 46 | L24B | 56 | PRO | 2.3 |
| 2 | S2B | 203 | GLY | 2.3 |
| 16 | S16A | 10 | GLY | 2.3 |
| 6 | S6A | 101 | ALA | 2.3 |
| 20 | S20A | 52 | ALA | 2.3 |
| 35 | L13B | 132 | ALA | 2.3 |
| 30 | L3B | 92 | THR | 2.3 |

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| Mol | Chain | Res | Type | RSRZ |
|---|---|---|---|---|
| 3 | S3B | 69 | HIS | 2.3 |
| 34 | L9B | 143 | SER | 2.3 |
| 5 | S5B | 53 | LEU | 2.3 |
| 10 | S10A | 8 | LEU | 2.3 |
| 10 | S10A | 88 | LEU | 2.3 |
| 12 | S12B | 24 | LEU | 2.3 |
| 13 | S13B | 19 | LEU | 2.3 |
| 16 | S16A | 73 | LEU | 2.3 |
| 30 | L3A | 27 | LEU | 2.3 |
| 3 | S3B | 10 | PHE | 2.3 |
| 5 | S5B | 84 | PHE | 2.3 |
| 27 | 23SB | 1221 | G | 2.3 |
| 35 | L13B | 117 | PHE | 2.3 |
| 57 | ASIB | 65 | G | 2.3 |
| 2 | S2B | 25 | ASN | 2.3 |
| 11 | S11A | 117 | ASN | 2.3 |
| 50 | L29B | 47 | ASN | 2.3 |
| 6 | S6B | 83 | ASP | 2.3 |
| 7 | S7A | 110 | GLN | 2.3 |
| 11 | S11A | 110 | ASP | 2.3 |
| 30 | L3B | 83 | ASP | 2.3 |
| 5 | S5A | 9 | LYS | 2.3 |
| 12 | S12A | 14 | LYS | 2.3 |
| 18 | S18B | 88 | LYS | 2.3 |
| 42 | L20B | 114 | LYS | 2.3 |
| 2 | S2A | 112 | VAL | 2.3 |
| 3 | S3A | 166 | GLU | 2.3 |
| 5 | S5A | 8 | GLU | 2.3 |
| 10 | S10A | 45 | ARG | 2.3 |
| 11 | S11B | 54 | ARG | 2.3 |
| 24 | ESIA | 35 | A | 2.3 |
| 36 | L14B | 54 | GLU | 2.3 |
| 42 | L20B | 112 | ARG | 2.3 |
| 47 | L25A | 165 | VAL | 2.3 |
| 57 | ASIB | 7 | A | 2.3 |
| 27 | 23SB | 12 | U | 2.3 |
| 5 | S5B | 93 | PRO | 2.3 |
| 10 | S10B | 74 | ILE | 2.3 |
| 11 | S11B | 39 | PRO | 2.3 |
| 13 | S13B | 78 | ILE | 2.3 |
| 41 | L19B | 50 | ILE | 2.3 |
| 43 | L21B | 4 | ILE | 2.3 |

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| Mol | Chain | Res | Type | RSRZ |
|---|---|---|---|---|
| 2 | S2B | 177 | ALA | 2.3 |
| 3 | S3B | 50 | ALA | 2.3 |
| 11 | S11B | 100 | ALA | 2.3 |
| 12 | S12A | 23 | ALA | 2.3 |
| 14 | S14B | 59 | ALA | 2.3 |
| 31 | L4A | 128 | ALA | 2.3 |
| 31 | L4B | 55 | GLY | 2.3 |
| 36 | L14A | 112 | MET | 2.3 |
| 41 | L19A | 135 | ALA | 2.3 |
| 43 | L21B | 101 | GLY | 2.3 |
| 1 | 16SA | 1058 | C | 2.3 |
| 7 | S7A | 103 | TRP | 2.3 |
| 7 | S7B | 22 | LEU | 2.3 |
| 8 | S8A | 112 | LEU | 2.3 |
| 31 | L4B | 140 | LEU | 2.3 |
| 33 | L6B | 71 | LEU | 2.3 |
| 33 | L6B | 106 | THR | 2.3 |
| 34 | L9B | 108 | THR | 2.3 |
| 43 | L21B | 7 | THR | 2.3 |
| 47 | L25B | 144 | LEU | 2.3 |
| 49 | L28A | 94 | LEU | 2.3 |
| 46 | L24B | 68 | HIS | 2.3 |
| 4 | S4A | 28 | SER | 2.3 |
| 4 | S4B | 175 | SER | 2.3 |
| 47 | L25B | 48 | PHE | 2.3 |
| 48 | L27A | 9 | SER | 2.3 |
| 3 | S3B | 48 | TYR | 2.3 |
| 4 | S4B | 129 | ASN | 2.3 |
| 6 | S6B | 13 | ASN | 2.3 |
| 4 | S4A | 42 | GLN | 2.3 |
| 5 | S5A | 56 | GLN | 2.3 |
| 5 | S5A | 57 | LYS | 2.3 |
| 13 | S13B | 120 | LYS | 2.3 |
| 46 | L24B | 46 | LYS | 2.3 |
| 47 | L25B | 156 | LYS | 2.3 |
| 33 | L6A | 97 | ARG | 2.3 |
| 35 | L13B | 134 | ARG | 2.3 |
| 4 | S4A | 140 | VAL | 2.3 |
| 5 | S5A | 32 | VAL | 2.3 |
| 12 | S12A | 33 | VAL | 2.3 |
| 53 | L32A | 57 | VAL | 2.3 |
| 34 | L9A | 85 | GLU | 2.2 |

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| Mol | Chain | Res | Type | RSRZ |
|---|---|---|---|---|
| 36 | L14A | 45 | GLU | 2.2 |
| 40 | L18A | 111 | GLU | 2.2 |
| 1 | 16SA | 1782 | G | 2.2 |
| 27 | 23SA | 641 | G | 2.2 |
| 27 | 23SB | 571 | G | 2.2 |
| 30 | L3B | 26 | ILE | 2.2 |
| 41 | L19A | 7 | ILE | 2.2 |
| 43 | L21B | 70 | ILE | 2.2 |
| 50 | L29A | 50 | ILE | 2.2 |
| 2 | S2A | 202 | PRO | 2.2 |
| 2 | S2B | 99 | GLY | 2.2 |
| 3 | S3B | 185 | GLY | 2.2 |
| 4 | S4B | 37 | PRO | 2.2 |
| 8 | S8A | 72 | PRO | 2.2 |
| 12 | S12B | 22 | PRO | 2.2 |
| 13 | S13B | 10 | PRO | 2.2 |
| 35 | L13B | 86 | PRO | 2.2 |
| 20 | S20B | 52 | ALA | 2.2 |
| 41 | L19B | 5 | ALA | 2.2 |
| 1 | 16SA | 1071 | A | 2.2 |
| 5 | S5A | 12 | LEU | 2.2 |
| 11 | S11A | 98 | LEU | 2.2 |
| 24 | ESIA | 33 | U | 2.2 |
| 25 | MRNA | 44 | U | 2.2 |
| 27 | 23SA | 2909 | U | 2.2 |
| 7 | S7A | 26 | PHE | 2.2 |
| 33 | L6A | 111 | HIS | 2.2 |
| 41 | L19A | 40 | THR | 2.2 |
| 41 | L19B | 62 | THR | 2.2 |
| 4 | S4A | 184 | LYS | 2.2 |
| 7 | S7B | 151 | TYR | 2.2 |
| 8 | S8B | 94 | TYR | 2.2 |
| 9 | S9A | 116 | LYS | 2.2 |
| 16 | S16A | 38 | TYR | 2.2 |
| 18 | S18B | 68 | LYS | 2.2 |
| 19 | S19A | 35 | SER | 2.2 |
| 20 | S20A | 21 | LYS | 2.2 |
| 30 | L3B | 69 | LYS | 2.2 |
| 36 | L14B | 109 | LYS | 2.2 |
| 43 | L21B | 73 | SER | 2.2 |
| 44 | L22B | 110 | LYS | 2.2 |
| 48 | L27A | 5 | LYS | 2.2 |

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| Mol | Chain | Res | Type | RSRZ |
|---|---|---|---|---|
| 54 | L33A | 33 | LYS | 2.2 |
| 1 | 16SA | 1076 | C | 2.2 |
| 16 | S16B | 8 | ARG | 2.2 |
| 23 | PSIB | 17 | C | 2.2 |
| 27 | 23SA | 933 | C | 2.2 |
| 27 | 23SB | 2759 | C | 2.2 |
| 2 | S2B | 110 | GLN | 2.2 |
| 3 | S3A | 110 | ASN | 2.2 |
| 3 | S3B | 76 | VAL | 2.2 |
| 5 | S5A | 34 | VAL | 2.2 |
| 12 | S12A | 37 | VAL | 2.2 |
| 12 | S12B | 63 | VAL | 2.2 |
| 14 | S14A | 24 | CYS | 2.2 |
| 43 | L21B | 61 | VAL | 2.2 |
| 55 | L34B | 46 | VAL | 2.2 |
| 2 | S2B | 12 | GLU | 2.2 |
| 3 | S3B | 44 | GLU | 2.2 |
| 4 | S4A | 179 | GLU | 2.2 |
| 5 | S5A | 155 | GLU | 2.2 |
| 30 | L3A | 89 | ASP | 2.2 |
| 31 | L4B | 197 | ASP | 2.2 |
| 39 | L17B | 82 | GLU | 2.2 |
| 46 | L24B | 91 | GLU | 2.2 |
| 52 | L31A | 3 | GLU | 2.2 |
| 8 | S8B | 13 | ILE | 2.2 |
| 12 | S12A | 82 | ILE | 2.2 |
| 2 | S2A | 138 | LEU | 2.2 |
| 3 | S3B | 9 | GLY | 2.2 |
| 5 | S5A | 114 | GLY | 2.2 |
| 5 | S5B | 39 | GLY | 2.2 |
| 5 | S5B | 103 | GLY | 2.2 |
| 8 | S8B | 63 | LEU | 2.2 |
| 8 | S8B | 106 | GLY | 2.2 |
| 10 | S10A | 32 | ALA | 2.2 |
| 13 | S13A | 113 | PRO | 2.2 |
| 10 | S10A | 85 | LEU | 2.2 |
| 14 | S14A | 6 | LEU | 2.2 |
| 30 | L3B | 181 | LEU | 2.2 |
| 31 | L4A | 131 | GLY | 2.2 |
| 42 | L20B | 99 | ALA | 2.2 |
| 46 | L24B | 59 | GLY | 2.2 |
| 51 | L30B | 27 | GLY | 2.2 |

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| Mol | Chain | Res | Type | RSRZ |
|---|---|---|---|---|
| 1 | 16SA | 1050 | G | 2.2 |
| 1 | 16SA | 1106 | G | 2.2 |
| 1 | 16SB | 687 | G | 2.2 |
| 7 | S7A | 137 | LYS | 2.2 |
| 20 | S20B | 38 | LYS | 2.2 |
| 21 | THXA | 25 | LYS | 2.2 |
| 27 | 23SA | 932 | G | 2.2 |
| 29 | L2B | 5 | LYS | 2.2 |
| 33 | L6A | 77 | LYS | 2.2 |
| 37 | L15B | 46 | LYS | 2.2 |
| 42 | L20B | 79 | PHE | 2.2 |
| 1 | 16SA | 810 | U | 2.2 |
| 4 | S4A | 57 | ARG | 2.2 |
| 12 | S12B | 56 | ARG | 2.2 |
| 24 | ESIB | 16 | U | 2.2 |
| 53 | L32B | 52 | TYR | 2.2 |
| 1 | 16SA | 1001 | A | 2.2 |
| 4 | S4B | 83 | SER | 2.2 |
| 27 | 23SA | 939 | A | 2.2 |
| 27 | 23SA | 2491 | A | 2.2 |
| 27 | 23SB | 574 | A | 2.2 |
| 30 | L3B | 34 | VAL | 2.2 |
| 34 | L9A | 142 | VAL | 2.2 |
| 36 | L14B | 52 | VAL | 2.2 |
| 12 | S12B | 75 | GLN | 2.2 |
| 33 | L6B | 74 | ASN | 2.2 |
| 41 | L19B | 38 | ASN | 2.2 |
| 3 | S3A | 84 | ILE | 2.2 |
| 8 | S8B | 135 | CYS | 2.2 |
| 10 | S10A | 6 | ILE | 2.2 |
| 14 | S14A | 40 | CYS | 2.2 |
| 32 | L5B | 35 | GLU | 2.2 |
| 33 | L6A | 4 | ILE | 2.2 |
| 33 | L6A | 72 | ILE | 2.2 |
| 35 | L13B | 96 | GLU | 2.2 |
| 41 | L19A | 11 | GLU | 2.2 |
| 41 | L19A | 50 | ILE | 2.2 |
| 41 | L19A | 83 | ILE | 2.2 |
| 47 | L25B | 119 | GLU | 2.2 |
| 5 | S5B | 5 | ASP | 2.2 |
| 2 | S2A | 34 | ALA | 2.2 |
| 3 | S3A | 113 | ALA | 2.2 |

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| Mol | Chain | Res | Type | RSRZ |
|---|---|---|---|---|
| 4 | S4A | 95 | GLY | 2.2 |
| 4 | S4B | 109 | GLY | 2.2 |
| 18 | S18B | 48 | GLY | 2.2 |
| 19 | S19A | 76 | PRO | 2.2 |
| 19 | S19B | 84 | GLY | 2.2 |
| 30 | L3B | 98 | PRO | 2.2 |
| 33 | L6A | 171 | LEU | 2.2 |
| 15 | S15A | 48 | LYS | 2.2 |
| 18 | S18B | 41 | LYS | 2.2 |
| 16 | S16A | 9 | PHE | 2.2 |
| 11 | S11B | 22 | HIS | 2.2 |
| 12 | S12A | 96 | HIS | 2.2 |
| 3 | S3A | 201 | TYR | 2.2 |
| 3 | S3B | 201 | TYR | 2.2 |
| 8 | S8B | 48 | TYR | 2.2 |
| 2 | S2A | 230 | VAL | 2.2 |
| 2 | S2B | 219 | VAL | 2.2 |
| 9 | S9A | 44 | VAL | 2.2 |
| 10 | S10B | 94 | VAL | 2.2 |
| 12 | S12B | 15 | VAL | 2.2 |
| 33 | L6A | 35 | VAL | 2.2 |
| 51 | L30B | 56 | VAL | 2.2 |
| 2 | S2A | 192 | SER | 2.2 |
| 12 | S12A | 19 | SER | 2.2 |
| 41 | L19A | 31 | SER | 2.2 |
| 49 | L28B | 17 | SER | 2.2 |
| 2 | S2A | 95 | GLN | 2.2 |
| 16 | S16A | 76 | GLN | 2.2 |
| 25 | MRNA | 42 | U | 2.2 |
| 25 | MRNB | 57 | U | 2.2 |
| 8 | S8A | 134 | ILE | 2.2 |
| 12 | S12B | 97 | ILE | 2.2 |
| 34 | L9A | 97 | ILE | 2.2 |
| 46 | L24B | 75 | ILE | 2.2 |
| 47 | L25A | 120 | ILE | 2.2 |
| 2 | S2A | 204 | ASN | 2.2 |
| 12 | S12B | 5 | ASN | 2.2 |
| 18 | S18B | 36 | ASN | 2.2 |
| 1 | 16SA | 1052 | A | 2.2 |
| 22 | ASIA | 9 | A | 2.2 |
| 27 | 23SB | 2648 | G | 2.2 |
| 27 | 23SB | 2814 | A | 2.2 |

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| Mol | Chain | Res | Type | RSRZ |
|---|---|---|---|---|
| 27 | 23SB | 2903 | G | 2.2 |
| 10 | S10B | 8 | LEU | 2.2 |
| 30 | L3A | 40 | GLU | 2.2 |
| 32 | L5A | 111 | LEU | 2.2 |
| 34 | L9A | 135 | GLU | 2.2 |
| 40 | L18A | 80 | LEU | 2.2 |
| 47 | L25A | 1 | MET | 2.2 |
| 49 | L28B | 80 | LEU | 2.2 |
| 11 | S11B | 97 | ALA | 2.2 |
| 13 | S13A | 75 | ALA | 2.2 |
| 14 | S14B | 40 | CYS | 2.2 |
| 20 | S20A | 98 | PRO | 2.2 |
| 32 | L5B | 134 | GLY | 2.2 |
| 38 | L16B | 39 | PRO | 2.2 |
| 4 | S4A | 53 | ASP | 2.2 |
| 4 | S4B | 166 | LYS | 2.2 |
| 7 | S7B | 53 | LYS | 2.2 |
| 7 | S7B | 137 | LYS | 2.2 |
| 18 | S18B | 19 | LYS | 2.2 |
| 19 | S19A | 7 | LYS | 2.2 |
| 4 | S4A | 65 | ARG | 2.2 |
| 20 | S20B | 80 | ARG | 2.2 |
| 30 | L3B | 58 | ARG | 2.2 |
| 32 | L5A | 83 | ARG | 2.2 |
| 26 | TRNA | 11 | C | 2.2 |
| 26 | TRNA | 43 | C | 2.2 |
| 34 | L9A | 78 | THR | 2.2 |
| 3 | S3A | 106 | VAL | 2.2 |
| 3 | S3A | 120 | VAL | 2.2 |
| 3 | S3B | 153 | VAL | 2.2 |
| 5 | S5A | 69 | VAL | 2.2 |
| 5 | S5B | 60 | TYR | 2.2 |
| 5 | S5B | 61 | TYR | 2.2 |
| 8 | S8A | 53 | VAL | 2.2 |
| 8 | S8B | 129 | VAL | 2.2 |
| 9 | S9B | 26 | VAL | 2.2 |
| 11 | S11A | 47 | VAL | 2.2 |
| 12 | S12B | 79 | VAL | 2.2 |
| 16 | S16A | 53 | VAL | 2.2 |
| 33 | L6A | 163 | TYR | 2.2 |
| 36 | L14A | 115 | VAL | 2.2 |
| 47 | L25B | 58 | VAL | 2.2 |

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| Mol | Chain | Res | Type | RSRZ |
|---|---|---|---|---|
| 47 | L25B | 128 | VAL | 2.2 |
| 51 | L30B | 36 | VAL | 2.2 |
| 54 | L33A | 21 | TYR | 2.2 |
| 2 | S2A | 76 | GLN | 2.2 |
| 4 | S4B | 45 | GLN | 2.2 |
| 10 | S10A | 98 | ILE | 2.2 |
| 12 | S12A | 47 | SER | 2.2 |
| 33 | L6A | 121 | ILE | 2.2 |
| 41 | L19B | 12 | SER | 2.2 |
| 34 | L9A | 5 | LEU | 2.2 |
| 34 | L9B | 128 | LEU | 2.2 |
| 49 | L28A | 82 | LEU | 2.2 |
| 31 | L4B | 127 | GLU | 2.2 |
| 35 | L13A | 90 | MET | 2.2 |
| 3 | S3A | 100 | ALA | 2.2 |
| 3 | S3B | 146 | ALA | 2.2 |
| 11 | S11A | 61 | ALA | 2.2 |
| 11 | S11B | 19 | ALA | 2.2 |
| 2 | S2B | 194 | PRO | 2.2 |
| 4 | S4B | 63 | LYS | 2.2 |
| 4 | S4B | 164 | ALA | 2.2 |
| 4 | S4A | 171 | GLY | 2.2 |
| 7 | S7A | 58 | PRO | 2.2 |
| 8 | S8B | 130 | GLY | 2.2 |
| 12 | S12A | 28 | PRO | 2.2 |
| 12 | S12B | 17 | LYS | 2.2 |
| 12 | S12B | 43 | LYS | 2.2 |
| 32 | L5A | 40 | ASN | 2.2 |
| 33 | L6B | 25 | LYS | 2.2 |
| 34 | L9A | 74 | ASN | 2.2 |
| 48 | L27A | 2 | ALA | 2.2 |
| 16 | S16A | 30 | GLY | 2.2 |
| 44 | L22A | 112 | GLY | 2.2 |
| 47 | L25B | 160 | GLY | 2.2 |
| 49 | L28A | 92 | LYS | 2.2 |
| 54 | L33B | 31 | PRO | 2.2 |
| 54 | L33B | 41 | PRO | 2.2 |
| 4 | S4A | 59 | ARG | 2.2 |
| 4 | S4B | 3 | ARG | 2.2 |
| 4 | S4B | 168 | ARG | 2.2 |
| 34 | L9A | 82 | ARG | 2.2 |
| 30 | L3A | 15 | PHE | 2.2 |

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| Mol | Chain | Res | Type | RSRZ |
|---|---|---|---|---|
| 30 | L3B | 67 | PHE | 2.2 |
| 22 | ASIA | 31 | A | 2.2 |
| 1 | 16SA | 798 | G | 2.2 |
| 1 | 16SA | 1051 | G | 2.2 |
| 1 | 16SB | 1105 | G | 2.2 |
| 1 | 16SB | 1509 | G | 2.2 |
| 24 | ESIA | 65 | G | 2.2 |
| 27 | 23SA | 928 | G | 2.2 |
| 27 | 23SB | 576 | G | 2.2 |
| 2 | S2A | 174 | VAL | 2.1 |
| 3 | S3A | 68 | VAL | 2.1 |
| 4 | S4A | 127 | THR | 2.1 |
| 12 | S12B | 107 | VAL | 2.1 |
| 31 | L4A | 6 | VAL | 2.1 |
| 33 | L6B | 52 | VAL | 2.1 |
| 34 | L9B | 145 | VAL | 2.1 |
| 44 | L22B | 50 | VAL | 2.1 |
| 47 | L25A | 96 | VAL | 2.1 |
| 51 | L30B | 59 | VAL | 2.1 |
| 2 | S2B | 31 | TYR | 2.1 |
| 7 | S7B | 18 | TYR | 2.1 |
| 33 | L6B | 163 | TYR | 2.1 |
| 1 | 16SA | 2025 | C | 2.1 |
| 1 | 16SB | 1731 | C | 2.1 |
| 11 | S11B | 21 | ILE | 2.1 |
| 13 | S13A | 4 | ILE | 2.1 |
| 27 | 23SA | 2165 | C | 2.1 |
| 34 | L9B | 97 | ILE | 2.1 |
| 35 | L13A | 16 | ILE | 2.1 |
| 41 | L19B | 86 | ILE | 2.1 |
| 3 | S3A | 111 | LEU | 2.1 |
| 6 | S6B | 30 | LEU | 2.1 |
| 12 | S12B | 49 | LEU | 2.1 |
| 34 | L9A | 75 | LEU | 2.1 |
| 35 | L13B | 69 | GLN | 2.1 |
| 41 | L19A | 136 | GLN | 2.1 |
| 2 | S2B | 179 | LYS | 2.1 |
| 3 | S3A | 20 | SER | 2.1 |
| 5 | S5B | 10 | MET | 2.1 |
| 12 | S12A | 20 | LYS | 2.1 |
| 12 | S12A | 43 | LYS | 2.1 |
| 33 | L6A | 84 | SER | 2.1 |

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| Mol | Chain | Res | Type | RSRZ |
|---|---|---|---|---|
| 33 | L6B | 13 | LYS | 2.1 |
| 35 | L13B | 48 | MET | 2.1 |
| 46 | L24B | 4 | LYS | 2.1 |
| 2 | S2B | 170 | GLU | 2.1 |
| 3 | S3A | 35 | GLU | 2.1 |
| 11 | S11B | 15 | ALA | 2.1 |
| 14 | S14B | 10 | ALA | 2.1 |
| 2 | S2A | 125 | PRO | 2.1 |
| 3 | S3B | 38 | ARG | 2.1 |
| 4 | S4A | 145 | GLU | 2.1 |
| 4 | S4A | 163 | GLU | 2.1 |
| 6 | S6B | 58 | GLY | 2.1 |
| 7 | S7A | 32 | ARG | 2.1 |
| 7 | S7B | 74 | GLU | 2.1 |
| 7 | S7B | 139 | GLU | 2.1 |
| 17 | S17B | 58 | GLU | 2.1 |
| 20 | S20B | 59 | ALA | 2.1 |
| 36 | L14A | 118 | ALA | 2.1 |
| 36 | L14B | 46 | ALA | 2.1 |
| 38 | L16A | 105 | GLU | 2.1 |
| 48 | L27B | 2 | ALA | 2.1 |
| 12 | S12A | 110 | ARG | 2.1 |
| 12 | S12B | 38 | ARG | 2.1 |
| 12 | S12B | 69 | GLY | 2.1 |
| 18 | S18B | 55 | ARG | 2.1 |
| 33 | L6B | 101 | ARG | 2.1 |
| 46 | L24B | 41 | GLY | 2.1 |
| 3 | S3A | 98 | ASN | 2.1 |
| 46 | L24B | 92 | ASN | 2.1 |
| 47 | L25A | 158 | PRO | 2.1 |
| 5 | S5B | 6 | PHE | 2.1 |
| 1 | 16SA | 726 | U | 2.1 |
| 1 | 16SB | 1070 | U | 2.1 |
| 30 | L3A | 18 | ASP | 2.1 |
| 30 | L3B | 31 | CYS | 2.1 |
| 5 | S5B | 32 | VAL | 2.1 |
| 10 | S10B | 24 | VAL | 2.1 |
| 16 | S16A | 16 | HIS | 2.1 |
| 35 | L13B | 52 | VAL | 2.1 |
| 46 | L24B | 7 | VAL | 2.1 |
| 1 | 16SA | 985 | A | 2.1 |
| 1 | 16SB | 1100 | A | 2.1 |

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| Mol | Chain | Res | Type | RSRZ |
|---|---|---|---|---|
| 1 | 16SB | 1416 | A | 2.1 |
| 2 | S2B | 41 | ILE | 2.1 |
| 6 | S6B | 59 | TYR | 2.1 |
| 8 | S8A | 80 | ILE | 2.1 |
| 11 | S11B | 108 | ILE | 2.1 |
| 2 | S2A | 98 | LEU | 2.1 |
| 4 | S4B | 78 | LEU | 2.1 |
| 5 | S5A | 142 | LEU | 2.1 |
| 11 | S11B | 98 | LEU | 2.1 |
| 17 | S17B | 6 | LEU | 2.1 |
| 29 | L2B | 111 | LEU | 2.1 |
| 32 | L5A | 34 | LEU | 2.1 |
| 33 | L6B | 87 | LEU | 2.1 |
| 35 | L13B | 21 | LYS | 2.1 |
| 40 | L18B | 73 | LEU | 2.1 |
| 43 | L21B | 94 | LEU | 2.1 |
| 51 | L30A | 8 | LEU | 2.1 |
| 1 | 16SA | 1120 | G | 2.1 |
| 1 | 16SB | 857 | G | 2.1 |
| 23 | PSIA | 6 | G | 2.1 |
| 24 | ESIB | 63 | G | 2.1 |
| 27 | 23SA | 2811 | G | 2.1 |
| 43 | L21B | 1 | MET | 2.1 |
| 4 | S4B | 25 | ARG | 2.1 |
| 12 | S12A | 53 | ALA | 2.1 |
| 15 | S15B | 68 | ARG | 2.1 |
| 33 | L6B | 51 | ARG | 2.1 |
| 35 | L13B | 18 | ALA | 2.1 |
| 4 | S4A | 6 | GLY | 2.1 |
| 4 | S4A | 192 | GLU | 2.1 |
| 1 | 16SB | 1728 | C | 2.1 |
| 3 | S3A | 114 | PRO | 2.1 |
| 5 | S5A | 128 | PRO | 2.1 |
| 5 | S5B | 87 | SER | 2.1 |
| 11 | S11A | 39 | PRO | 2.1 |
| 15 | S15A | 41 | GLU | 2.1 |
| 20 | S20B | 102 | GLY | 2.1 |
| 33 | L6B | 8 | PRO | 2.1 |
| 33 | L6B | 134 | SER | 2.1 |
| 34 | L9B | 117 | GLU | 2.1 |
| 34 | L9B | 134 | PRO | 2.1 |
| 35 | L13B | 136 | GLU | 2.1 |

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| Mol | Chain | Res | Type | RSRZ |
|---|---|---|---|---|
| 41 | L19B | 36 | GLU | 2.1 |
| 43 | L21B | 50 | PRO | 2.1 |
| 5 | S5A | 28 | PHE | 2.1 |
| 20 | S20A | 26 | ASN | 2.1 |
| 30 | L3B | 85 | ASN | 2.1 |
| 2 | S2B | 191 | ASP | 2.1 |
| 5 | S5B | 51 | VAL | 2.1 |
| 6 | S6A | 83 | ASP | 2.1 |
| 8 | S8A | 138 | TRP | 2.1 |
| 14 | S14A | 33 | VAL | 2.1 |
| 16 | S16B | 52 | ASP | 2.1 |
| 30 | L3B | 159 | HIS | 2.1 |
| 1 | 16SB | 1062 | U | 2.1 |
| 2 | S2A | 208 | ILE | 2.1 |
| 3 | S3A | 150 | LYS | 2.1 |
| 4 | S4A | 151 | LYS | 2.1 |
| 5 | S5B | 116 | THR | 2.1 |
| 11 | S11B | 33 | THR | 2.1 |
| 11 | S11B | 95 | ILE | 2.1 |
| 12 | S12B | 58 | THR | 2.1 |
| 8 | S8B | 20 | TYR | 2.1 |
| 27 | 23SA | 2488 | U | 2.1 |
| 30 | L3B | 5 | LEU | 2.1 |
| 44 | L22A | 113 | LYS | 2.1 |
| 47 | L25A | 150 | LEU | 2.1 |
| 57 | ASIB | 50 | U | 2.1 |
| 3 | S3A | 127 | ARG | 2.1 |
| 4 | S4B | 107 | ARG | 2.1 |
| 4 | S4B | 209 | ARG | 2.1 |
| 47 | L25B | 1 | MET | 2.1 |
| 5 | S5A | 95 | ALA | 2.1 |
| 18 | S18B | 20 | ALA | 2.1 |
| 32 | L5A | 57 | ALA | 2.1 |
| 41 | L19A | 43 | GLN | 2.1 |
| 1 | 16SB | 1088 | A | 2.1 |
| 2 | S2A | 234 | PRO | 2.1 |
| 4 | S4A | 90 | GLY | 2.1 |
| 10 | S10A | 31 | GLY | 2.1 |
| 17 | S17B | 96 | GLU | 2.1 |
| 30 | L3A | 29 | GLY | 2.1 |
| 32 | L5A | 42 | GLY | 2.1 |
| 35 | L13A | 129 | PRO | 2.1 |

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| Mol | Chain | Res | Type | RSRZ |
|---|---|---|---|---|
| 47 | L25A | 167 | PRO | 2.1 |
| 52 | L31A | 54 | GLY | 2.1 |
| 5 | S5A | 45 | PHE | 2.1 |
| 7 | S7A | 62 | PHE | 2.1 |
| 9 | S9A | 59 | PHE | 2.1 |
| 14 | S14A | 37 | PHE | 2.1 |
| 31 | L4B | 139 | PHE | 2.1 |
| 34 | L9A | 143 | SER | 2.1 |
| 38 | L16B | 65 | PHE | 2.1 |
| 52 | L31A | 49 | PHE | 2.1 |
| 6 | S6A | 11 | ASN | 2.1 |
| 1 | 16SA | 1064 | G | 2.1 |
| 1 | 16SA | 1259 | G | 2.1 |
| 1 | 16SA | 1717 | G | 2.1 |
| 1 | 16SB | 1510 | G | 2.1 |
| 1 | 16SB | 1685 | G | 2.1 |
| 6 | S6B | 88 | VAL | 2.1 |
| 7 | S7B | 141 | VAL | 2.1 |
| 23 | PSIB | 70 | G | 2.1 |
| 26 | TRNA | 44 | G | 2.1 |
| 27 | 23SB | 2777 | G | 2.1 |
| 46 | L24B | 24 | VAL | 2.1 |
| 1 | 16SB | 680 | C | 2.1 |
| 22 | ASIA | 56 | C | 2.1 |
| 24 | ESIA | 56 | C | 2.1 |
| 2 | S2A | 113 | HIS | 2.1 |
| 4 | S4B | 184 | LYS | 2.1 |
| 2 | S2B | 138 | LEU | 2.1 |
| 2 | S2B | 158 | LEU | 2.1 |
| 5 | S5B | 71 | LEU | 2.1 |
| 8 | S8A | 121 | ASP | 2.1 |
| 11 | S11B | 34 | ASP | 2.1 |
| 30 | L3B | 64 | LYS | 2.1 |
| 41 | L19A | 85 | LYS | 2.1 |
| 42 | L20B | 93 | LYS | 2.1 |
| 16 | S16A | 4 | ILE | 2.1 |
| 20 | S20A | 20 | LEU | 2.1 |
| 20 | S20A | 41 | ILE | 2.1 |
| 30 | L3A | 5 | LEU | 2.1 |
| 33 | L6A | 33 | LEU | 2.1 |
| 36 | L14B | 117 | LEU | 2.1 |
| 38 | L16B | 37 | LEU | 2.1 |

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| Mol | Chain | Res | Type | RSRZ |
|---|---|---|---|---|
| 40 | L18A | 58 | LEU | 2.1 |
| 47 | L25A | 171 | ILE | 2.1 |
| 47 | L25B | 59 | LEU | 2.1 |
| 3 | S3A | 79 | ARG | 2.1 |
| 4 | S4A | 153 | ARG | 2.1 |
| 5 | S5A | 18 | ARG | 2.1 |
| 8 | S8B | 85 | ARG | 2.1 |
| 16 | S16B | 45 | THR | 2.1 |
| 37 | L15A | 90 | ARG | 2.1 |
| 37 | L15B | 16 | ARG | 2.1 |
| 38 | L16A | 60 | ARG | 2.1 |
| 46 | L24A | 108 | THR | 2.1 |
| 52 | L31A | 27 | THR | 2.1 |
| 52 | L31A | 44 | THR | 2.1 |
| 3 | S3B | 142 | MET | 2.1 |
| 2 | S2B | 161 | ALA | 2.1 |
| 6 | S6A | 29 | ALA | 2.1 |
| 36 | L14B | 33 | ALA | 2.1 |
| 41 | L19A | 131 | ALA | 2.1 |
| 47 | L25B | 172 | ALA | 2.1 |
| 2 | S2B | 95 | GLN | 2.1 |
| 3 | S3A | 123 | GLN | 2.1 |
| 25 | MRNA | 52 | U | 2.1 |
| 27 | 23SA | 158 | U | 2.1 |
| 5 | S5A | 39 | GLY | 2.1 |
| 48 | L27B | 8 | GLY | 2.1 |
| 3 | S3B | 114 | PRO | 2.1 |
| 3 | S3B | 161 | GLU | 2.1 |
| 7 | S7B | 71 | PRO | 2.1 |
| 10 | S10A | 47 | PHE | 2.1 |
| 30 | L3A | 171 | GLU | 2.1 |
| 33 | L6A | 21 | PRO | 2.1 |
| 33 | L6B | 40 | GLU | 2.1 |
| 33 | L6B | 126 | PRO | 2.1 |
| 35 | L13B | 40 | PRO | 2.1 |
| 54 | L33A | 24 | GLU | 2.1 |
| 54 | L33B | 24 | GLU | 2.1 |
| 2 | S2B | 210 | SER | 2.1 |
| 31 | L4B | 15 | SER | 2.1 |
| 4 | S4A | 203 | VAL | 2.1 |
| 9 | S9A | 26 | VAL | 2.1 |
| 12 | S12B | 93 | VAL | 2.1 |

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| Mol | Chain | Res | Type | RSRZ |
|---|---|---|---|---|
| 17 | S17B | 9 | VAL | 2.1 |
| 37 | L15B | 101 | VAL | 2.1 |
| 47 | L25B | 126 | VAL | 2.1 |
| 1 | 16SB | 1907 | A | 2.1 |
| 3 | S3B | 3 | ASN | 2.1 |
| 27 | 23SA | 703 | A | 2.1 |
| 30 | L3B | 2 | LYS | 2.1 |
| 33 | L6A | 25 | LYS | 2.1 |
| 35 | L13A | 137 | LYS | 2.1 |
| 43 | L21B | 44 | LYS | 2.1 |
| 46 | L24A | 95 | LYS | 2.1 |
| 2 | S2A | 102 | LEU | 2.1 |
| 3 | S3B | 39 | ILE | 2.1 |
| 3 | S3B | 52 | LEU | 2.1 |
| 3 | S3B | 111 | LEU | 2.1 |
| 2 | S2B | 19 | HIS | 2.1 |
| 5 | S5B | 15 | ARG | 2.1 |
| 5 | S5B | 89 | ILE | 2.1 |
| 8 | S8A | 35 | ILE | 2.1 |
| 9 | S9A | 47 | LEU | 2.1 |
| 11 | S11B | 103 | LEU | 2.1 |
| 13 | S13A | 64 | TRP | 2.1 |
| 20 | S20A | 10 | LEU | 2.1 |
| 35 | L13B | 116 | LEU | 2.1 |
| 38 | L16A | 66 | ILE | 2.1 |
| 44 | L22B | 92 | ARG | 2.1 |
| 47 | L25A | 125 | LEU | 2.1 |
| 47 | L25B | 133 | ILE | 2.1 |
| 51 | L30A | 37 | LEU | 2.1 |
| 52 | L31A | 22 | ILE | 2.1 |
| 3 | S3B | 15 | THR | 2.1 |
| 15 | S15A | 25 | THR | 2.1 |
| 16 | S16A | 44 | THR | 2.1 |
| 16 | S16B | 22 | THR | 2.1 |
| 16 | S16B | 38 | TYR | 2.1 |
| 33 | L6B | 122 | THR | 2.1 |
| 46 | L24B | 79 | CYS | 2.1 |
| 1 | 16SA | 795 | C | 2.1 |
| 1 | 16SA | 1830 | C | 2.1 |
| 19 | S19A | 50 | ALA | 2.1 |
| 23 | PSIB | 68 | C | 2.1 |
| 27 | 23SA | 2914 | C | 2.1 |

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| Mol | Chain | Res | Type | RSRZ |
|---|---|---|---|---|
| 1 | 16SA | 1115 | G | 2.1 |
| 1 | 16SB | 1106 | G | 2.1 |
| 25 | MRNA | 37 | G | 2.1 |
| 54 | L33B | 22 | ALA | 2.1 |
| 3 | S3A | 74 | GLY | 2.1 |
| 4 | S4B | 201 | GLN | 2.1 |
| 7 | S7B | 106 | GLN | 2.1 |
| 12 | S12A | 118 | GLY | 2.1 |
| 33 | L6A | 91 | GLY | 2.1 |
| 33 | L6B | 28 | GLY | 2.1 |
| 43 | L21B | 17 | GLY | 2.1 |
| 2 | S2A | 232 | PRO | 2.1 |
| 4 | S4A | 24 | GLU | 2.1 |
| 4 | S4A | 81 | GLU | 2.1 |
| 8 | S8A | 44 | PHE | 2.1 |
| 9 | S9A | 18 | PHE | 2.1 |
| 9 | S9B | 90 | PRO | 2.1 |
| 12 | S12A | 124 | GLU | 2.1 |
| 14 | S14A | 36 | PHE | 2.1 |
| 15 | S15A | 26 | GLU | 2.1 |
| 15 | S15B | 19 | PRO | 2.1 |
| 36 | L14B | 108 | GLU | 2.1 |
| 37 | L15B | 98 | GLU | 2.1 |
| 41 | L19A | 22 | PHE | 2.1 |
| 52 | L31A | 30 | GLU | 2.1 |
| 53 | L32A | 48 | GLU | 2.1 |
| 4 | S4A | 169 | LYS | 2.0 |
| 8 | S8B | 103 | VAL | 2.0 |
| 10 | S10B | 99 | LYS | 2.0 |
| 25 | MRNB | 42 | U | 2.0 |
| 27 | 23SB | 2812 | U | 2.0 |
| 49 | L28A | 70 | VAL | 2.0 |
| 3 | S3A | 49 | SER | 2.0 |
| 4 | S4B | 28 | SER | 2.0 |
| 8 | S8A | 115 | SER | 2.0 |
| 20 | S20A | 11 | SER | 2.0 |
| 2 | S2A | 200 | ILE | 2.0 |
| 3 | S3A | 156 | ARG | 2.0 |
| 3 | S3A | 202 | ILE | 2.0 |
| 3 | S3A | 204 | LEU | 2.0 |
| 4 | S4B | 118 | ARG | 2.0 |
| 5 | S5A | 139 | LEU | 2.0 |

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| Mol | Chain | Res | Type | RSRZ |
|---|---|---|---|---|
| 6 | S6A | 13 | ASN | 2.0 |
| 8 | S8B | 134 | ILE | 2.0 |
| 10 | S10A | 70 | ARG | 2.0 |
| 12 | S12A | 86 | ARG | 2.0 |
| 16 | S16B | 33 | ILE | 2.0 |
| 17 | S17B | 43 | LEU | 2.0 |
| 33 | L6B | 130 | ARG | 2.0 |
| 33 | L6B | 170 | ARG | 2.0 |
| 43 | L21B | 83 | ARG | 2.0 |
| 47 | L25A | 157 | LEU | 2.0 |
| 2 | S2A | 16 | HIS | 2.0 |
| 19 | S19A | 47 | HIS | 2.0 |
| 47 | L25B | 55 | HIS | 2.0 |
| 47 | L25B | 121 | HIS | 2.0 |
| 1 | 16SB | 2115 | A | 2.0 |
| 3 | S3A | 187 | ALA | 2.0 |
| 4 | S4A | 68 | TYR | 2.0 |
| 5 | S5A | 36 | ASP | 2.0 |
| 8 | S8B | 124 | ALA | 2.0 |
| 27 | 23SA | 628 | A | 2.0 |
| 33 | L6A | 83 | TYR | 2.0 |
| 35 | L13B | 58 | ASP | 2.0 |
| 43 | L21A | 49 | THR | 2.0 |
| 47 | L25A | 170 | THR | 2.0 |
| 49 | L28B | 77 | ALA | 2.0 |
| 3 | S3B | 74 | GLY | 2.0 |
| 3 | S3B | 123 | GLN | 2.0 |
| 5 | S5B | 23 | GLY | 2.0 |
| 6 | S6B | 16 | GLN | 2.0 |
| 7 | S7A | 106 | GLN | 2.0 |
| 11 | S11B | 13 | GLN | 2.0 |
| 29 | L2A | 236 | GLY | 2.0 |
| 30 | L3B | 88 | GLY | 2.0 |
| 56 | L35A | 35 | GLN | 2.0 |
| 2 | S2B | 125 | PRO | 2.0 |
| 3 | S3A | 109 | PRO | 2.0 |
| 3 | S3B | 109 | PRO | 2.0 |
| 16 | S16B | 41 | PRO | 2.0 |
| 5 | S5A | 83 | GLU | 2.0 |
| 1 | 16SA | 1059 | C | 2.0 |
| 1 | 16SA | 1084 | C | 2.0 |
| 1 | 16SA | 1630 | C | 2.0 |

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| Mol | Chain | Res | Type | RSRZ |
|---|---|---|---|---|
| 3 | S3B | 150 | LYS | 2.0 |
| 5 | S5B | 92 | LYS | 2.0 |
| 12 | S12B | 18 | LYS | 2.0 |
| 13 | S13A | 52 | GLU | 2.0 |
| 16 | S16B | 35 | LYS | 2.0 |
| 19 | S19A | 64 | GLU | 2.0 |
| 5 | S5A | 82 | VAL | 2.0 |
| 9 | S9B | 28 | VAL | 2.0 |
| 27 | 23SA | 938 | C | 2.0 |
| 27 | 23SA | 2490 | C | 2.0 |
| 30 | L3B | 33 | VAL | 2.0 |
| 43 | L21B | 57 | VAL | 2.0 |
| 1 | 16SA | 1057 | G | 2.0 |
| 2 | S2B | 61 | LEU | 2.0 |
| 4 | S4A | 73 | ARG | 2.0 |
| 10 | S10B | 88 | LEU | 2.0 |
| 11 | S11B | 63 | LEU | 2.0 |
| 20 | S20A | 8 | ARG | 2.0 |
| 20 | S20A | 86 | ARG | 2.0 |
| 24 | ESIA | 30 | G | 2.0 |
| 24 | ESIA | 70 | G | 2.0 |
| 24 | ESIA | 71 | G | 2.0 |
| 24 | ESIB | 27 | G | 2.0 |
| 27 | 23SB | 2846 | G | 2.0 |
| 32 | L5A | 51 | ARG | 2.0 |
| 34 | L9B | 38 | LEU | 2.0 |
| 35 | L13B | 23 | LEU | 2.0 |
| 47 | L25B | 91 | LEU | 2.0 |
| 47 | L25B | 163 | LEU | 2.0 |
| 33 | L6A | 162 | ILE | 2.0 |
| 35 | L13A | 60 | ILE | 2.0 |
| 48 | L27B | 9 | SER | 2.0 |
| 1 | 16SA | 1061 | U | 2.0 |
| 1 | 16SA | 1075 | U | 2.0 |
| 23 | PSIA | 66 | U | 2.0 |
| 3 | S3B | 61 | ALA | 2.0 |
| 7 | S7B | 127 | ALA | 2.0 |
| 4 | S4B | 106 | TYR | 2.0 |
| 8 | S8A | 94 | TYR | 2.0 |
| 12 | S12A | 95 | TYR | 2.0 |
| 14 | S14B | 34 | TYR | 2.0 |
| 37 | L15B | 58 | THR | 2.0 |

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| Mol | Chain | Res | Type | RSRZ |
|---|---|---|---|---|
| 54 | L33A | 14 | THR | 2.0 |
| 32 | L5A | 49 | ASP | 2.0 |
| 36 | L14A | 12 | ASP | 2.0 |
| 36 | L14B | 56 | ASP | 2.0 |
| 47 | L25B | 77 | ASP | 2.0 |
| 2 | S2B | 65 | GLY | 2.0 |
| 2 | S2B | 152 | PHE | 2.0 |
| 11 | S11B | 102 | GLY | 2.0 |
| 15 | S15B | 15 | PHE | 2.0 |
| 16 | S16A | 63 | GLY | 2.0 |
| 33 | L6A | 166 | GLY | 2.0 |
| 2 | S2B | 46 | LYS | 2.0 |
| 5 | S5A | 70 | PRO | 2.0 |
| 13 | S13A | 10 | PRO | 2.0 |
| 17 | S17A | 4 | LYS | 2.0 |
| 29 | L2B | 4 | LYS | 2.0 |
| 35 | L13A | 133 | GLN | 2.0 |
| 47 | L25B | 167 | PRO | 2.0 |
| 50 | L29A | 38 | GLN | 2.0 |
| 3 | S3A | 138 | VAL | 2.0 |
| 4 | S4A | 25 | ARG | 2.0 |
| 8 | S8A | 93 | VAL | 2.0 |
| 9 | S9A | 65 | VAL | 2.0 |
| 14 | S14A | 8 | GLU | 2.0 |
| 19 | S19A | 43 | GLU | 2.0 |
| 24 | ESIA | 26 | A | 2.0 |
| 27 | 23SA | 5 | A | 2.0 |
| 34 | L9B | 7 | GLU | 2.0 |
| 11 | S11A | 126 | ARG | 2.0 |
| 47 | L25B | 174 | VAL | 2.0 |
| 47 | L25B | 175 | VAL | 2.0 |
| 51 | L30B | 6 | VAL | 2.0 |
| 2 | S2B | 115 | LEU | 2.0 |
| 5 | S5A | 110 | LEU | 2.0 |
| 11 | S11A | 63 | LEU | 2.0 |
| 18 | S18B | 58 | LEU | 2.0 |
| 35 | L13A | 67 | LEU | 2.0 |
| 35 | L13B | 91 | LEU | 2.0 |
| 35 | L13B | 120 | LEU | 2.0 |
| 37 | L15A | 148 | LEU | 2.0 |
| 39 | L17B | 79 | LEU | 2.0 |
| 5 | S5A | 76 | ILE | 2.0 |

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| Mol | Chain | Res | Type | RSRZ |
|---|---|---|---|---|
| 5 | S5A | 101 | ILE | 2.0 |
| 31 | L4B | 206 | ILE | 2.0 |
| 1 | 16SA | 1682 | C | 2.0 |
| 24 | ESIA | 2 | C | 2.0 |
| 27 | 23SA | 2489 | C | 2.0 |
| 27 | 23SB | 2202 | 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 | 4SU | ASIA | 8 | 20/21 | 0.49 | 0.18 | 200,201,209,209 | 0 |
| 26 | PSU | TRNA | 39 | 20/21 | 0.53 | 0.15 | 141,167,176,177 | 0 |
| 26 | PSU | TRNA | 55 | 20/21 | 0.53 | 0.12 | 140,149,172,173 | 0 |
| 22 | PSU | ASIA | 55 | 20/21 | 0.55 | 0.21 | 148,161,170,173 | 0 |
| 24 | MIA | ESIB | 37 | 29/30 | 0.55 | 0.24 | 133,151,155,159 | 0 |
| 26 | PSU | TRNA | 32 | 20/21 | 0.57 | 0.12 | 180,186,193,193 | 0 |
| 57 | 5MU | ASIB | 54 | 21/22 | 0.60 | 0.16 | 149,182,188,190 | 0 |
| 23 | 3AU | PSIB | 47 | 27/28 | 0.61 | 0.16 | 125,144,154,157 | 0 |
| 26 | MIA | TRNA | 37 | 29/30 | 0.63 | 0.21 | 115,137,156,159 | 0 |
| 26 | 5MU | TRNA | 54 | 21/22 | 0.64 | 0.13 | 150,157,163,165 | 0 |
| 23 | PSU | PSIB | 55 | 20/21 | 0.68 | 0.14 | 93,105,114,116 | 0 |
| 26 | 4SU | TRNA | 8 | 20/21 | 0.70 | 0.14 | 169,173,178,179 | 0 |
| 23 | 5MU | PSIB | 54 | 21/22 | 0.73 | 0.16 | 99,107,116,124 | 0 |
| 22 | 5MU | ASIA | 54 | 21/22 | 0.75 | 0.23 | 116,137,145,147 | 0 |
| 1 | 2MG | 16SB | 1834 | 24/25 | 0.77 | 0.12 | 112,121,124,134 | 0 |
| 12 | 0TD | S12B | 89 | 10/11 | 0.78 | 0.17 | 80,85,98,103 | 0 |
| 24 | MIA | ESIA | 37 | 29/30 | 0.78 | 0.19 | 119,144,147,154 | 0 |
| 22 | 7MG | ASIA | 46 | 24/25 | 0.79 | 0.18 | 199,203,213,220 | 0 |
| 57 | PSU | ASIB | 39 | 20/21 | 0.80 | 0.14 | 100,119,125,126 | 0 |
| 23 | 7MG | PSIB | 46 | 24/25 | 0.80 | 0.11 | 110,121,137,139 | 0 |
| 1 | 5MC | 16SB | 1590 | 21/22 | 0.82 | 0.13 | 78,90,100,102 | 0 |
| 23 | PSU | PSIA | 55 | 20/21 | 0.83 | 0.11 | 82,88,107,108 | 0 |
| 23 | 3AU | PSIA | 47 | 27/28 | 0.83 | 0.19 | 93,118,131,133 | 0 |
| 1 | 7MG | 16SB | 1156 | 24/25 | 0.84 | 0.15 | 72,84,99,102 | 0 |
| 1 | M2G | 16SB | 1589 | 25/26 | 0.84 | 0.13 | 80,89,97,102 | 0 |
| 27 | 5MU | 23SB | 1940 | 21/22 | 0.84 | 0.13 | 76,89,106,108 | 0 |
| 23 | PSU | PSIB | 32 | 20/21 | 0.84 | 0.12 | 81,89,102,107 | 0 |

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| Mol | Type | Chain | Res | Atoms | RSCC | RSR | B-factors(Å$^2$) | Q<0.9 |
|---|---|---|---|---|---|---|---|---|
| 23 | 7MG | PSIA | 46 | 24/25 | 0.84 | 0.14 | 79,89,111,120 | 0 |
| 23 | 4SU | PSIB | 8 | 20/21 | 0.85 | 0.09 | 97,105,114,118 | 0 |
| 1 | PSU | 16SB | 1145 | 20/21 | 0.85 | 0.11 | 81,88,98,101 | 0 |
| 57 | PSU | ASIB | 32 | 20/21 | 0.86 | 0.09 | 111,122,129,131 | 0 |
| 1 | PSU | 16SA | 1145 | 20/21 | 0.86 | 0.16 | 63,74,87,89 | 0 |
| 23 | 5MU | PSIA | 54 | 21/22 | 0.86 | 0.13 | 84,91,100,102 | 0 |
| 1 | 2MG | 16SA | 1834 | 24/25 | 0.87 | 0.12 | 77,82,89,99 | 0 |
| 27 | PSU | 23SB | 1942 | 20/21 | 0.87 | 0.13 | 75,81,94,96 | 0 |
| 12 | 0TD | S12A | 89 | 10/11 | 0.87 | 0.17 | 62,66,74,84 | 0 |
| 1 | 5MC | 16SB | 2028 | 21/22 | 0.87 | 0.12 | 77,87,91,96 | 0 |
| 23 | PSU | PSIB | 39 | 20/21 | 0.87 | 0.12 | 77,85,90,93 | 0 |
| 22 | PSU | ASIA | 32 | 20/21 | 0.88 | 0.17 | 84,89,99,100 | 0 |
| 23 | MIA | PSIB | 37 | 29/30 | 0.88 | 0.14 | 78,86,101,106 | 0 |
| 23 | PSU | PSIA | 32 | 20/21 | 0.89 | 0.12 | 61,71,78,79 | 0 |
| 22 | PSU | ASIA | 39 | 20/21 | 0.90 | 0.15 | 75,89,94,96 | 0 |
| 1 | 5MC | 16SB | 2032 | 21/22 | 0.90 | 0.11 | 56,69,76,84 | 0 |
| 57 | MIA | ASIB | 37 | 29/30 | 0.91 | 0.12 | 90,101,110,111 | 0 |
| 1 | 4OC | 16SB | 2030 | 22/23 | 0.91 | 0.11 | 62,74,89,92 | 0 |
| 1 | 7MG | 16SA | 1156 | 24/25 | 0.91 | 0.16 | 49,65,74,86 | 0 |
| 27 | PSU | 23SB | 1936 | 20/21 | 0.92 | 0.10 | 61,78,82,83 | 0 |
| 23 | PSU | PSIA | 39 | 20/21 | 0.92 | 0.12 | 59,63,73,76 | 0 |
| 1 | UR3 | 16SB | 2121 | 21/22 | 0.92 | 0.12 | 53,64,72,79 | 0 |
| 22 | MIA | ASIA | 37 | 29/30 | 0.92 | 0.15 | 55,69,76,81 | 0 |
| 1 | 5MC | 16SB | 2035 | 21/22 | 0.92 | 0.10 | 62,70,74,76 | 0 |
| 23 | MIA | PSIA | 37 | 29/30 | 0.92 | 0.15 | 58,65,82,85 | 0 |
| 23 | 4SU | PSIA | 8 | 20/21 | 0.92 | 0.10 | 70,77,82,84 | 0 |
| 27 | PSU | 23SA | 1936 | 20/21 | 0.93 | 0.13 | 52,56,64,70 | 0 |
| 27 | OMC | 23SB | 1945 | 21/22 | 0.93 | 0.09 | 64,75,83,85 | 0 |
| 27 | 5MC | 23SB | 1987 | 21/22 | 0.93 | 0.10 | 54,62,74,81 | 0 |
| 1 | 5MC | 16SA | 1590 | 21/22 | 0.93 | 0.12 | 59,67,77,79 | 0 |
| 27 | 5MU | 23SA | 1940 | 21/22 | 0.93 | 0.13 | 54,67,75,85 | 0 |
| 1 | 5MC | 16SA | 2028 | 21/22 | 0.93 | 0.12 | 47,64,70,72 | 0 |
| 27 | PSU | 23SA | 1942 | 20/21 | 0.93 | 0.14 | 55,63,77,83 | 0 |
| 27 | OMG | 23SB | 2266 | 24/25 | 0.94 | 0.09 | 51,57,61,63 | 0 |
| 27 | OMU | 23SB | 2567 | 21/22 | 0.94 | 0.12 | 51,62,71,79 | 0 |
| 1 | M2G | 16SA | 1589 | 25/26 | 0.94 | 0.12 | 56,63,73,79 | 0 |
| 1 | MA6 | 16SB | 2141 | 24/25 | 0.94 | 0.10 | 61,71,81,82 | 0 |
| 27 | 5MC | 23SA | 1967 | 21/22 | 0.94 | 0.11 | 41,53,60,70 | 0 |
| 1 | MA6 | 16SB | 2142 | 24/25 | 0.94 | 0.10 | 57,70,78,87 | 0 |
| 27 | OMC | 23SA | 1945 | 21/22 | 0.95 | 0.10 | 44,54,60,64 | 0 |
| 1 | 5MC | 16SA | 2032 | 21/22 | 0.95 | 0.12 | 46,52,59,63 | 0 |
| 27 | PSU | 23SB | 2620 | 20/21 | 0.95 | 0.10 | 42,49,60,66 | 0 |

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| Mol | Type | Chain | Res | Atoms | RSCC | RSR | B-factors(Å$^2$) | Q<0.9 |
|---|---|---|---|---|---|---|---|---|
| 27 | 5MU | 23SA | 1964 | 21/22 | 0.95 | 0.09 | 33,41,49,56 | 0 |
| 1 | UR3 | 16SA | 2121 | 21/22 | 0.95 | 0.13 | 39,52,60,61 | 0 |
| 27 | 5MC | 23SB | 1967 | 21/22 | 0.95 | 0.10 | 56,70,78,86 | 0 |
| 1 | 5MC | 16SA | 2035 | 21/22 | 0.95 | 0.11 | 44,49,56,62 | 0 |
| 27 | 2MA | 23SA | 2518 | 23/24 | 0.96 | 0.09 | 32,39,49,56 | 0 |
| 27 | 2MA | 23SB | 2518 | 23/24 | 0.96 | 0.10 | 40,46,52,55 | 0 |
| 27 | OMU | 23SA | 2567 | 21/22 | 0.96 | 0.10 | 41,47,53,68 | 0 |
| 1 | MA6 | 16SA | 2142 | 24/25 | 0.96 | 0.10 | 36,48,58,66 | 0 |
| 1 | MA6 | 16SA | 2141 | 24/25 | 0.96 | 0.10 | 41,48,53,58 | 0 |
| 27 | 5MC | 23SA | 1987 | 21/22 | 0.96 | 0.10 | 42,47,54,66 | 0 |
| 1 | 4OC | 16SA | 2030 | 22/23 | 0.96 | 0.11 | 49,57,64,71 | 0 |
| 27 | OMG | 23SA | 2266 | 24/25 | 0.96 | 0.09 | 35,42,51,53 | 0 |
| 27 | 5MU | 23SB | 1964 | 21/22 | 0.96 | 0.08 | 48,56,63,67 | 0 |
| 27 | PSU | 23SA | 2620 | 20/21 | 0.97 | 0.07 | 34,41,48,53 | 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 |
|---|---|---|---|---|---|---|---|---|
| 58 | MG | 23SB | 3121 | 1/1 | 0.08 | 0.21 | 105,105,105,105 | 0 |
| 59 | K | 23SA | 3390 | 1/1 | 0.28 | 0.48 | 129,129,129,129 | 0 |
| 59 | K | 16SA | 2319 | 1/1 | 0.29 | 0.24 | 109,109,109,109 | 0 |
| 58 | MG | 23SB | 3111 | 1/1 | 0.32 | 0.21 | 97,97,97,97 | 0 |
| 58 | MG | 16SB | 2247 | 1/1 | 0.33 | 0.32 | 96,96,96,96 | 0 |
| 58 | MG | 16SB | 2235 | 1/1 | 0.35 | 0.18 | 142,142,142,142 | 0 |
| 58 | MG | 23SB | 3114 | 1/1 | 0.36 | 0.27 | 95,95,95,95 | 0 |
| 59 | K | 16SA | 2299 | 1/1 | 0.36 | 0.12 | 136,136,136,136 | 0 |
| 59 | K | 16SB | 2297 | 1/1 | 0.41 | 0.17 | 125,125,125,125 | 0 |
| 58 | MG | 16SB | 2225[B] | 1/1 | 0.42 | 0.38 | 67,67,67,67 | 1 |
| 58 | MG | 16SB | 2225[A] | 1/1 | 0.42 | 0.38 | 73,73,73,73 | 1 |
| 59 | K | 16SA | 2311 | 1/1 | 0.43 | 0.21 | 107,107,107,107 | 0 |
| 58 | MG | 16SB | 2246 | 1/1 | 0.43 | 0.18 | 87,87,87,87 | 0 |
| 59 | K | 23SB | 3321 | 1/1 | 0.44 | 0.17 | 116,116,116,116 | 0 |

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| Mol | Type | Chain | Res | Atoms | RSCC | RSR | B-factors(Å$^2$) | Q<0.9 |
|---|---|---|---|---|---|---|---|---|
| 58 | MG | 23SA | 3034 | 1/1 | 0.47 | 0.20 | 79,79,79,79 | 0 |
| 58 | MG | 16SA | 2237 | 1/1 | 0.48 | 0.14 | 121,121,121,121 | 0 |
| 59 | K | 16SB | 2286 | 1/1 | 0.48 | 0.18 | 135,135,135,135 | 0 |
| 58 | MG | 23SA | 3104 | 1/1 | 0.49 | 0.18 | 86,86,86,86 | 0 |
| 59 | K | 23SB | 3315 | 1/1 | 0.50 | 0.16 | 130,130,130,130 | 0 |
| 58 | MG | 16SB | 2265 | 1/1 | 0.50 | 0.18 | 153,153,153,153 | 0 |
| 59 | K | 23SB | 3300 | 1/1 | 0.51 | 0.14 | 122,122,122,122 | 0 |
| 58 | MG | 23SB | 3063[A] | 1/1 | 0.52 | 0.38 | 57,57,57,57 | 1 |
| 59 | K | 16SB | 2316 | 1/1 | 0.52 | 0.18 | 105,105,105,105 | 0 |
| 58 | MG | 23SB | 3063[B] | 1/1 | 0.52 | 0.38 | 61,61,61,61 | 1 |
| 58 | MG | 23SB | 3219 | 1/1 | 0.52 | 0.26 | 110,110,110,110 | 0 |
| 58 | MG | 16SA | 2253 | 1/1 | 0.52 | 0.22 | 91,91,91,91 | 0 |
| 59 | K | 23SB | 3319 | 1/1 | 0.53 | 0.30 | 116,116,116,116 | 0 |
| 58 | MG | 16SA | 2250 | 1/1 | 0.54 | 0.25 | 97,97,97,97 | 0 |
| 58 | MG | 16SB | 2240 | 1/1 | 0.54 | 0.35 | 90,90,90,90 | 0 |
| 59 | K | 23SA | 3434 | 1/1 | 0.55 | 0.13 | 120,120,120,120 | 0 |
| 58 | MG | 23SA | 3093 | 1/1 | 0.56 | 0.15 | 59,59,59,59 | 0 |
| 58 | MG | 16SA | 2222 | 1/1 | 0.57 | 0.19 | 94,94,94,94 | 0 |
| 58 | MG | 16SA | 2217 | 1/1 | 0.57 | 0.41 | 80,80,80,80 | 0 |
| 58 | MG | 23SB | 3013 | 1/1 | 0.57 | 0.20 | 90,90,90,90 | 0 |
| 59 | K | 16SA | 2300 | 1/1 | 0.59 | 0.18 | 100,100,100,100 | 0 |
| 58 | MG | 23SA | 3097 | 1/1 | 0.59 | 0.18 | 71,71,71,71 | 0 |
| 58 | MG | 23SA | 3102 | 1/1 | 0.59 | 0.30 | 84,84,84,84 | 0 |
| 58 | MG | 16SA | 2243 | 1/1 | 0.59 | 0.33 | 84,84,84,84 | 0 |
| 58 | MG | 16SB | 2220 | 1/1 | 0.60 | 0.26 | 82,82,82,82 | 0 |
| 59 | K | 16SB | 2292 | 1/1 | 0.60 | 0.16 | 126,126,126,126 | 0 |
| 59 | K | 16SB | 2318 | 1/1 | 0.60 | 0.19 | 110,110,110,110 | 0 |
| 59 | K | 23SB | 3280 | 1/1 | 0.60 | 0.17 | 108,108,108,108 | 0 |
| 58 | MG | 23SA | 3116 | 1/1 | 0.61 | 0.18 | 87,87,87,87 | 0 |
| 58 | MG | 16SA | 2248 | 1/1 | 0.61 | 0.13 | 115,115,115,115 | 0 |
| 59 | K | 16SA | 2336 | 1/1 | 0.61 | 0.14 | 120,120,120,120 | 0 |
| 59 | K | 23SA | 3341 | 1/1 | 0.61 | 0.13 | 111,111,111,111 | 0 |
| 58 | MG | 16SB | 2237 | 1/1 | 0.62 | 0.22 | 94,94,94,94 | 0 |
| 58 | MG | 16SB | 2270 | 1/1 | 0.62 | 0.19 | 68,68,68,68 | 0 |
| 58 | MG | 23SB | 3110 | 1/1 | 0.62 | 0.28 | 81,81,81,81 | 0 |
| 58 | MG | 16SA | 2244 | 1/1 | 0.62 | 0.14 | 99,99,99,99 | 0 |
| 59 | K | 23SB | 3268 | 1/1 | 0.62 | 0.24 | 118,118,118,118 | 0 |
| 58 | MG | 23SA | 3117 | 1/1 | 0.63 | 0.34 | 72,72,72,72 | 0 |
| 58 | MG | 16SA | 2239 | 1/1 | 0.63 | 0.21 | 75,75,75,75 | 0 |
| 58 | MG | 16SB | 2209 | 1/1 | 0.64 | 0.32 | 91,91,91,91 | 0 |
| 59 | K | 23SA | 3421 | 1/1 | 0.64 | 0.14 | 96,96,96,96 | 0 |
| 59 | K | 23SB | 3242 | 1/1 | 0.65 | 0.15 | 124,124,124,124 | 0 |

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| Mol | Type | Chain | Res | Atoms | RSCC | RSR | B-factors(Å$^2$) | Q<0.9 |
|---|---|---|---|---|---|---|---|---|
| 58 | MG | 16SB | 2254 | 1/1 | 0.65 | 0.17 | 90,90,90,90 | 0 |
| 58 | MG | 16SA | 2231 | 1/1 | 0.65 | 0.30 | 65,65,65,65 | 0 |
| 59 | K | S20A | 201 | 1/1 | 0.65 | 0.11 | 125,125,125,125 | 0 |
| 58 | MG | 23SA | 3121 | 1/1 | 0.65 | 0.25 | 85,85,85,85 | 0 |
| 58 | MG | PSIB | 102 | 1/1 | 0.65 | 0.36 | 93,93,93,93 | 0 |
| 58 | MG | 16SB | 2204 | 1/1 | 0.65 | 0.33 | 101,101,101,101 | 0 |
| 59 | K | 16SB | 2302 | 1/1 | 0.66 | 0.16 | 129,129,129,129 | 0 |
| 58 | MG | 16SA | 2269 | 1/1 | 0.66 | 0.12 | 144,144,144,144 | 0 |
| 58 | MG | 16SB | 2233 | 1/1 | 0.66 | 0.29 | 90,90,90,90 | 0 |
| 58 | MG | 23SA | 3178 | 1/1 | 0.66 | 0.20 | 88,88,88,88 | 0 |
| 58 | MG | 16SA | 2240 | 1/1 | 0.66 | 0.18 | 88,88,88,88 | 0 |
| 59 | K | 23SB | 3322 | 1/1 | 0.66 | 0.15 | 122,122,122,122 | 0 |
| 58 | MG | 5SA | 201 | 1/1 | 0.67 | 0.14 | 66,66,66,66 | 0 |
| 58 | MG | 23SA | 3162 | 1/1 | 0.67 | 0.10 | 93,93,93,93 | 0 |
| 59 | K | 16SB | 2288 | 1/1 | 0.67 | 0.15 | 92,92,92,92 | 0 |
| 58 | MG | 16SA | 2233 | 1/1 | 0.67 | 0.25 | 92,92,92,92 | 0 |
| 58 | MG | 23SA | 3163 | 1/1 | 0.68 | 0.23 | 80,80,80,80 | 0 |
| 58 | MG | 23SA | 3172 | 1/1 | 0.68 | 0.14 | 60,60,60,60 | 0 |
| 58 | MG | 23SA | 3138 | 1/1 | 0.68 | 0.11 | 76,76,76,76 | 0 |
| 58 | MG | 23SA | 3144 | 1/1 | 0.68 | 0.14 | 86,86,86,86 | 0 |
| 58 | MG | 23SB | 3109 | 1/1 | 0.68 | 0.27 | 79,79,79,79 | 0 |
| 58 | MG | 23SA | 3149 | 1/1 | 0.68 | 0.09 | 87,87,87,87 | 0 |
| 58 | MG | 16SA | 2241 | 1/1 | 0.68 | 0.12 | 102,102,102,102 | 0 |
| 58 | MG | 16SB | 2283 | 1/1 | 0.68 | 0.16 | 127,127,127,127 | 0 |
| 58 | MG | 23SB | 3116 | 1/1 | 0.68 | 0.26 | 103,103,103,103 | 0 |
| 59 | K | L4B | 301 | 1/1 | 0.68 | 0.13 | 118,118,118,118 | 0 |
| 59 | K | 16SA | 2302 | 1/1 | 0.69 | 0.15 | 111,111,111,111 | 0 |
| 58 | MG | 23SB | 3132 | 1/1 | 0.69 | 0.24 | 80,80,80,80 | 0 |
| 58 | MG | 23SA | 3112 | 1/1 | 0.69 | 0.25 | 74,74,74,74 | 0 |
| 58 | MG | 23SB | 3068 | 1/1 | 0.69 | 0.25 | 84,84,84,84 | 0 |
| 58 | MG | 23SB | 3128 | 1/1 | 0.69 | 0.37 | 95,95,95,95 | 0 |
| 59 | K | 23SA | 3350 | 1/1 | 0.70 | 0.10 | 100,100,100,100 | 0 |
| 58 | MG | 23SA | 3241 | 1/1 | 0.70 | 0.16 | 49,49,49,49 | 0 |
| 58 | MG | 16SA | 2220 | 1/1 | 0.70 | 0.28 | 66,66,66,66 | 0 |
| 58 | MG | 23SB | 3077 | 1/1 | 0.70 | 0.32 | 77,77,77,77 | 0 |
| 58 | MG | 5SA | 202 | 1/1 | 0.70 | 0.11 | 66,66,66,66 | 0 |
| 58 | MG | 16SB | 2226 | 1/1 | 0.71 | 0.33 | 77,77,77,77 | 0 |
| 59 | K | 16SA | 2331 | 1/1 | 0.71 | 0.14 | 98,98,98,98 | 0 |
| 59 | K | 23SB | 3275 | 1/1 | 0.71 | 0.16 | 104,104,104,104 | 0 |
| 59 | K | 16SA | 2292 | 1/1 | 0.71 | 0.16 | 103,103,103,103 | 0 |
| 58 | MG | 23SB | 3084 | 1/1 | 0.71 | 0.39 | 77,77,77,77 | 0 |
| 58 | MG | 16SB | 2282 | 1/1 | 0.71 | 0.13 | 114,114,114,114 | 0 |

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| Mol | Type | Chain | Res | Atoms | RSCC | RSR | B-factors(Å$^2$) | Q<0.9 |
|---|---|---|---|---|---|---|---|---|
| 59 | K | 23SA | 3342 | 1/1 | 0.71 | 0.14 | 95,95,95,95 | 0 |
| 58 | MG | 16SB | 2202 | 1/1 | 0.71 | 0.11 | 74,74,74,74 | 0 |
| 58 | MG | MRNA | 101 | 1/1 | 0.71 | 0.13 | 81,81,81,81 | 0 |
| 59 | K | 23SA | 3409 | 1/1 | 0.71 | 0.14 | 100,100,100,100 | 0 |
| 59 | K | 16SA | 2312 | 1/1 | 0.72 | 0.10 | 114,114,114,114 | 0 |
| 58 | MG | 23SA | 3157 | 1/1 | 0.72 | 0.14 | 83,83,83,83 | 0 |
| 58 | MG | 23SB | 3087 | 1/1 | 0.72 | 0.40 | 77,77,77,77 | 0 |
| 58 | MG | 16SA | 2256 | 1/1 | 0.72 | 0.22 | 93,93,93,93 | 0 |
| 58 | MG | 23SB | 3053 | 1/1 | 0.72 | 0.20 | 80,80,80,80 | 0 |
| 58 | MG | 16SB | 2216 | 1/1 | 0.72 | 0.15 | 86,86,86,86 | 0 |
| 58 | MG | 16SB | 2243 | 1/1 | 0.72 | 0.29 | 73,73,73,73 | 0 |
| 58 | MG | 16SB | 2244 | 1/1 | 0.72 | 0.12 | 99,99,99,99 | 0 |
| 59 | K | 23SA | 3351 | 1/1 | 0.72 | 0.17 | 86,86,86,86 | 0 |
| 58 | MG | 23SA | 3015 | 1/1 | 0.72 | 0.42 | 85,85,85,85 | 0 |
| 59 | K | 23SA | 3393 | 1/1 | 0.73 | 0.21 | 101,101,101,101 | 0 |
| 58 | MG | 23SA | 3072 | 1/1 | 0.73 | 0.25 | 91,91,91,91 | 0 |
| 58 | MG | 23SA | 3148 | 1/1 | 0.73 | 0.16 | 79,79,79,79 | 0 |
| 58 | MG | 23SA | 3063 | 1/1 | 0.73 | 0.23 | 70,70,70,70 | 0 |
| 58 | MG | 23SB | 3041 | 1/1 | 0.73 | 0.24 | 64,64,64,64 | 0 |
| 58 | MG | 16SB | 2252 | 1/1 | 0.73 | 0.14 | 98,98,98,98 | 0 |
| 58 | MG | 23SB | 3059 | 1/1 | 0.73 | 0.17 | 74,74,74,74 | 0 |
| 60 | OHX | 23SB | 3497 | 7/7 | 0.73 | 0.14 | 159,164,168,271 | 0 |
| 59 | K | S13B | 201 | 1/1 | 0.74 | 0.11 | 137,137,137,137 | 0 |
| 59 | K | 23SB | 3317 | 1/1 | 0.74 | 0.10 | 102,102,102,102 | 0 |
| 59 | K | 23SA | 3427 | 1/1 | 0.74 | 0.15 | 81,81,81,81 | 0 |
| 59 | K | 16SA | 2320 | 1/1 | 0.74 | 0.19 | 123,123,123,123 | 0 |
| 58 | MG | 23SA | 3175 | 1/1 | 0.74 | 0.17 | 74,74,74,74 | 0 |
| 58 | MG | 16SB | 2210 | 1/1 | 0.74 | 0.28 | 80,80,80,80 | 0 |
| 59 | K | L16B | 201 | 1/1 | 0.74 | 0.11 | 108,108,108,108 | 0 |
| 60 | OHX | 23SB | 3388 | 7/7 | 0.74 | 0.19 | 91,102,118,203 | 0 |
| 59 | K | 16SB | 2289 | 1/1 | 0.74 | 0.25 | 109,109,109,109 | 0 |
| 59 | K | S20B | 201 | 1/1 | 0.75 | 0.13 | 119,119,119,119 | 0 |
| 58 | MG | 23SA | 3311 | 1/1 | 0.75 | 0.14 | 104,104,104,104 | 0 |
| 59 | K | 23SA | 3428 | 1/1 | 0.75 | 0.12 | 114,114,114,114 | 0 |
| 58 | MG | 16SA | 2228 | 1/1 | 0.75 | 0.29 | 71,71,71,71 | 0 |
| 58 | MG | 16SA | 2261 | 1/1 | 0.75 | 0.15 | 97,97,97,97 | 0 |
| 58 | MG | L4A | 301 | 1/1 | 0.75 | 0.09 | 60,60,60,60 | 0 |
| 58 | MG | 16SA | 2234 | 1/1 | 0.75 | 0.26 | 75,75,75,75 | 0 |
| 58 | MG | 23SA | 3080 | 1/1 | 0.75 | 0.16 | 87,87,87,87 | 0 |
| 58 | MG | S4A | 301 | 1/1 | 0.75 | 0.12 | 109,109,109,109 | 0 |
| 58 | MG | 23SA | 3124 | 1/1 | 0.75 | 0.21 | 78,78,78,78 | 0 |
| 59 | K | 16SB | 2305 | 1/1 | 0.75 | 0.11 | 93,93,93,93 | 0 |

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| Mol | Type | Chain | Res | Atoms | RSCC | RSR | B-factors(Å$^2$) | Q<0.9 |
|---|---|---|---|---|---|---|---|---|
| 58 | MG | 23SA | 3130 | 1/1 | 0.75 | 0.13 | 62,62,62,62 | 0 |
| 59 | K | L5B | 202 | 1/1 | 0.75 | 0.11 | 127,127,127,127 | 0 |
| 58 | MG | 16SA | 2235 | 1/1 | 0.75 | 0.12 | 98,98,98,98 | 0 |
| 60 | OHX | 16SA | 2407 | 7/7 | 0.75 | 0.12 | 136,147,163,250 | 0 |
| 60 | OHX | 16SB | 2383 | 7/7 | 0.75 | 0.12 | 141,154,160,266 | 0 |
| 59 | K | 16SB | 2321 | 1/1 | 0.75 | 0.11 | 101,101,101,101 | 0 |
| 58 | MG | 16SA | 2208 | 1/1 | 0.75 | 0.13 | 67,67,67,67 | 0 |
| 58 | MG | 23SB | 3099 | 1/1 | 0.76 | 0.15 | 81,81,81,81 | 0 |
| 58 | MG | 16SB | 2203 | 1/1 | 0.76 | 0.26 | 70,70,70,70 | 0 |
| 58 | MG | 16SB | 2214 | 1/1 | 0.76 | 0.36 | 67,67,67,67 | 0 |
| 59 | K | 23SB | 3303 | 1/1 | 0.76 | 0.14 | 95,95,95,95 | 0 |
| 58 | MG | 23SA | 3128 | 1/1 | 0.76 | 0.25 | 98,98,98,98 | 0 |
| 59 | K | 23SA | 3360 | 1/1 | 0.76 | 0.12 | 90,90,90,90 | 0 |
| 58 | MG | 16SB | 2234 | 1/1 | 0.76 | 0.19 | 76,76,76,76 | 0 |
| 58 | MG | 16SB | 2206 | 1/1 | 0.76 | 0.16 | 81,81,81,81 | 0 |
| 58 | MG | 23SB | 3117 | 1/1 | 0.76 | 0.17 | 75,75,75,75 | 0 |
| 58 | MG | S5B | 202 | 1/1 | 0.76 | 0.17 | 93,93,93,93 | 0 |
| 59 | K | 16SA | 2321 | 1/1 | 0.76 | 0.18 | 105,105,105,105 | 0 |
| 58 | MG | 16SB | 2249 | 1/1 | 0.76 | 0.21 | 91,91,91,91 | 0 |
| 59 | K | 23SB | 3241 | 1/1 | 0.76 | 0.12 | 96,96,96,96 | 0 |
| 58 | MG | 23SB | 3003 | 1/1 | 0.76 | 0.30 | 71,71,71,71 | 0 |
| 59 | K | 23SB | 3247 | 1/1 | 0.76 | 0.10 | 108,108,108,108 | 0 |
| 58 | MG | 5SA | 203 | 1/1 | 0.76 | 0.29 | 82,82,82,82 | 0 |
| 58 | MG | 23SB | 3169 | 1/1 | 0.77 | 0.11 | 57,57,57,57 | 0 |
| 58 | MG | 23SB | 3038 | 1/1 | 0.77 | 0.29 | 81,81,81,81 | 0 |
| 58 | MG | 23SB | 3220 | 1/1 | 0.77 | 0.18 | 45,45,45,45 | 0 |
| 59 | K | 23SB | 3311 | 1/1 | 0.77 | 0.33 | 108,108,108,108 | 0 |
| 58 | MG | 5SB | 201 | 1/1 | 0.77 | 0.14 | 89,89,89,89 | 0 |
| 58 | MG | 23SA | 3110 | 1/1 | 0.77 | 0.23 | 64,64,64,64 | 0 |
| 58 | MG | 23SA | 3100 | 1/1 | 0.77 | 0.17 | 93,93,93,93 | 0 |
| 58 | MG | 23SB | 3058 | 1/1 | 0.77 | 0.21 | 64,64,64,64 | 0 |
| 58 | MG | 16SA | 2252 | 1/1 | 0.77 | 0.34 | 72,72,72,72 | 0 |
| 58 | MG | 23SA | 3168 | 1/1 | 0.77 | 0.21 | 85,85,85,85 | 0 |
| 58 | MG | 23SA | 3324 | 1/1 | 0.77 | 0.27 | 111,111,111,111 | 0 |
| 58 | MG | 23SB | 3064 | 1/1 | 0.77 | 0.33 | 57,57,57,57 | 0 |
| 58 | MG | 23SB | 3119 | 1/1 | 0.77 | 0.27 | 91,91,91,91 | 0 |
| 58 | MG | 16SB | 2217 | 1/1 | 0.77 | 0.36 | 71,71,71,71 | 0 |
| 58 | MG | 23SA | 3065 | 1/1 | 0.77 | 0.19 | 72,72,72,72 | 0 |
| 60 | OHX | 23SB | 3448 | 7/7 | 0.77 | 0.14 | 108,113,129,237 | 0 |
| 58 | MG | 16SB | 2238 | 1/1 | 0.77 | 0.26 | 85,85,85,85 | 0 |
| 59 | K | 23SA | 3413 | 1/1 | 0.78 | 0.21 | 97,97,97,97 | 0 |
| 58 | MG | 23SB | 3124 | 1/1 | 0.78 | 0.21 | 68,68,68,68 | 0 |

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| Mol | Type | Chain | Res | Atoms | RSCC | RSR | B-factors(Å$^2$) | Q<0.9 |
|---|---|---|---|---|---|---|---|---|
| 59 | K | 23SB | 3274 | 1/1 | 0.78 | 0.12 | 114,114,114,114 | 0 |
| 58 | MG | 23SA | 3166 | 1/1 | 0.78 | 0.33 | 67,67,67,67 | 0 |
| 58 | MG | 23SA | 3107 | 1/1 | 0.78 | 0.34 | 85,85,85,85 | 0 |
| 58 | MG | 16SB | 2212 | 1/1 | 0.78 | 0.21 | 95,95,95,95 | 0 |
| 58 | MG | 23SB | 3108 | 1/1 | 0.78 | 0.14 | 76,76,76,76 | 0 |
| 58 | MG | 16SA | 2212 | 1/1 | 0.78 | 0.33 | 85,85,85,85 | 0 |
| 58 | MG | 16SA | 2247 | 1/1 | 0.78 | 0.27 | 74,74,74,74 | 0 |
| 58 | MG | 16SB | 2273 | 1/1 | 0.78 | 0.12 | 70,70,70,70 | 0 |
| 59 | K | 23SA | 3345 | 1/1 | 0.78 | 0.15 | 104,104,104,104 | 0 |
| 59 | K | 23SA | 3346 | 1/1 | 0.78 | 0.17 | 108,108,108,108 | 0 |
| 59 | K | 16SA | 2295 | 1/1 | 0.78 | 0.13 | 108,108,108,108 | 0 |
| 58 | MG | 16SB | 2201 | 1/1 | 0.78 | 0.24 | 69,69,69,69 | 0 |
| 59 | K | 23SA | 3352 | 1/1 | 0.78 | 0.19 | 80,80,80,80 | 0 |
| 58 | MG | 23SA | 3153 | 1/1 | 0.78 | 0.32 | 79,79,79,79 | 0 |
| 59 | K | S4B | 301 | 1/1 | 0.78 | 0.24 | 101,101,101,101 | 0 |
| 60 | OHX | 23SA | 3560 | 7/7 | 0.78 | 0.14 | 60,91,113,235 | 0 |
| 60 | OHX | 23SA | 3600 | 7/7 | 0.78 | 0.12 | 122,125,155,245 | 0 |
| 60 | OHX | 23SA | 3603 | 7/7 | 0.78 | 0.13 | 141,147,166,236 | 0 |
| 59 | K | 23SA | 3381 | 1/1 | 0.78 | 0.10 | 94,94,94,94 | 0 |
| 58 | MG | 23SA | 3085 | 1/1 | 0.78 | 0.07 | 77,77,77,77 | 0 |
| 58 | MG | 16SA | 2255 | 1/1 | 0.78 | 0.27 | 65,65,65,65 | 0 |
| 58 | MG | 23SA | 3139 | 1/1 | 0.78 | 0.12 | 59,59,59,59 | 0 |
| 59 | K | L5A | 302 | 1/1 | 0.79 | 0.14 | 102,102,102,102 | 0 |
| 58 | MG | 23SB | 3080 | 1/1 | 0.79 | 0.24 | 85,85,85,85 | 0 |
| 58 | MG | 16SB | 2211 | 1/1 | 0.79 | 0.17 | 87,87,87,87 | 0 |
| 58 | MG | 23SA | 3328 | 1/1 | 0.79 | 0.09 | 110,110,110,110 | 0 |
| 58 | MG | 23SA | 3089 | 1/1 | 0.79 | 0.10 | 60,60,60,60 | 0 |
| 59 | K | 23SA | 3404 | 1/1 | 0.79 | 0.10 | 73,73,73,73 | 0 |
| 58 | MG | 23SB | 3105 | 1/1 | 0.79 | 0.13 | 76,76,76,76 | 0 |
| 58 | MG | 23SA | 3031 | 1/1 | 0.79 | 0.24 | 65,65,65,65 | 0 |
| 59 | K | 16SB | 2311 | 1/1 | 0.79 | 0.14 | 107,107,107,107 | 0 |
| 58 | MG | 23SA | 3111 | 1/1 | 0.79 | 0.23 | 111,111,111,111 | 0 |
| 59 | K | 23SB | 3301 | 1/1 | 0.79 | 0.11 | 88,88,88,88 | 0 |
| 60 | OHX | 16SB | 2359 | 7/7 | 0.79 | 0.13 | 119,129,145,253 | 0 |
| 58 | MG | 16SB | 2219 | 1/1 | 0.79 | 0.23 | 81,81,81,81 | 0 |
| 59 | K | 16SA | 2334 | 1/1 | 0.79 | 0.23 | 97,97,97,97 | 0 |
| 59 | K | 23SB | 3313 | 1/1 | 0.79 | 0.13 | 126,126,126,126 | 0 |
| 59 | K | 23SA | 3357 | 1/1 | 0.79 | 0.11 | 94,94,94,94 | 0 |
| 59 | K | 23SB | 3295 | 1/1 | 0.80 | 0.18 | 98,98,98,98 | 0 |
| 58 | MG | 23SA | 3087 | 1/1 | 0.80 | 0.09 | 73,73,73,73 | 0 |
| 59 | K | 16SA | 2301 | 1/1 | 0.80 | 0.19 | 115,115,115,115 | 0 |
| 59 | K | 23SA | 3349 | 1/1 | 0.80 | 0.30 | 103,103,103,103 | 0 |

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| Mol | Type | Chain | Res | Atoms | RSCC | RSR | B-factors(Å$^2$) | Q<0.9 |
|---|---|---|---|---|---|---|---|---|
| 58 | MG | 16SB | 2248 | 1/1 | 0.80 | 0.43 | 79,79,79,79 | 0 |
| 59 | K | 16SA | 2307 | 1/1 | 0.80 | 0.15 | 75,75,75,75 | 0 |
| 59 | K | 23SB | 3314 | 1/1 | 0.80 | 0.12 | 75,75,75,75 | 0 |
| 58 | MG | 23SA | 3217 | 1/1 | 0.80 | 0.14 | 66,66,66,66 | 0 |
| 58 | MG | 23SA | 3020 | 1/1 | 0.80 | 0.23 | 38,38,38,38 | 0 |
| 59 | K | 23SA | 3359 | 1/1 | 0.80 | 0.07 | 101,101,101,101 | 0 |
| 58 | MG | 16SA | 2257 | 1/1 | 0.80 | 0.28 | 55,55,55,55 | 0 |
| 58 | MG | 23SA | 3096 | 1/1 | 0.80 | 0.19 | 66,66,66,66 | 0 |
| 59 | K | 23SA | 3387 | 1/1 | 0.80 | 0.13 | 64,64,64,64 | 0 |
| 58 | MG | 16SA | 2232 | 1/1 | 0.80 | 0.25 | 74,74,74,74 | 0 |
| 58 | MG | 16SB | 2242 | 1/1 | 0.80 | 0.28 | 61,61,61,61 | 0 |
| 59 | K | 16SA | 2332 | 1/1 | 0.80 | 0.17 | 94,94,94,94 | 0 |
| 60 | OHX | 23SA | 3512 | 7/7 | 0.80 | 0.14 | 128,135,145,228 | 0 |
| 59 | K | 16SA | 2333 | 1/1 | 0.80 | 0.24 | 99,99,99,99 | 0 |
| 58 | MG | 23SA | 3098 | 1/1 | 0.80 | 0.31 | 65,65,65,65 | 0 |
| 58 | MG | 23SA | 3050 | 1/1 | 0.80 | 0.23 | 64,64,64,64 | 0 |
| 59 | K | 16SA | 2293 | 1/1 | 0.80 | 0.10 | 102,102,102,102 | 0 |
| 59 | K | PSIA | 104 | 1/1 | 0.80 | 0.17 | 98,98,98,98 | 0 |
| 58 | MG | 16SB | 2245 | 1/1 | 0.80 | 0.15 | 93,93,93,93 | 0 |
| 58 | MG | 23SA | 3052 | 1/1 | 0.80 | 0.29 | 62,62,62,62 | 0 |
| 59 | K | 23SB | 3282 | 1/1 | 0.80 | 0.20 | 81,81,81,81 | 0 |
| 59 | K | 23SA | 3336 | 1/1 | 0.81 | 0.11 | 120,120,120,120 | 0 |
| 58 | MG | 23SA | 3037 | 1/1 | 0.81 | 0.23 | 89,89,89,89 | 0 |
| 59 | K | 16SA | 2294 | 1/1 | 0.81 | 0.14 | 89,89,89,89 | 0 |
| 59 | K | 16SB | 2287 | 1/1 | 0.81 | 0.13 | 127,127,127,127 | 0 |
| 59 | K | 23SB | 3304 | 1/1 | 0.81 | 0.12 | 98,98,98,98 | 0 |
| 59 | K | 23SB | 3306 | 1/1 | 0.81 | 0.13 | 88,88,88,88 | 0 |
| 58 | MG | 23SB | 3046 | 1/1 | 0.81 | 0.27 | 50,50,50,50 | 0 |
| 58 | MG | 23SA | 3280 | 1/1 | 0.81 | 0.13 | 84,84,84,84 | 0 |
| 58 | MG | 16SB | 2266 | 1/1 | 0.81 | 0.12 | 113,113,113,113 | 0 |
| 58 | MG | 16SB | 2269 | 1/1 | 0.81 | 0.11 | 105,105,105,105 | 0 |
| 58 | MG | 16SA | 2276 | 1/1 | 0.81 | 0.12 | 87,87,87,87 | 0 |
| 58 | MG | 23SA | 3143 | 1/1 | 0.81 | 0.21 | 44,44,44,44 | 0 |
| 59 | K | 23SA | 3356 | 1/1 | 0.81 | 0.21 | 89,89,89,89 | 0 |
| 58 | MG | 23SA | 3090 | 1/1 | 0.81 | 0.20 | 77,77,77,77 | 0 |
| 58 | MG | 23SB | 3120 | 1/1 | 0.81 | 0.15 | 100,100,100,100 | 0 |
| 58 | MG | 23SA | 3170 | 1/1 | 0.81 | 0.26 | 77,77,77,77 | 0 |
| 58 | MG | 16SB | 2231 | 1/1 | 0.81 | 0.22 | 87,87,87,87 | 0 |
| 58 | MG | 23SA | 3126 | 1/1 | 0.81 | 0.13 | 61,61,61,61 | 0 |
| 59 | K | 16SA | 2330 | 1/1 | 0.81 | 0.11 | 100,100,100,100 | 0 |
| 58 | MG | 23SA | 3127 | 1/1 | 0.81 | 0.15 | 67,67,67,67 | 0 |
| 58 | MG | 23SB | 3006 | 1/1 | 0.81 | 0.33 | 54,54,54,54 | 0 |

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| Mol | Type | Chain | Res | Atoms | RSCC | RSR | B-factors(Å$^2$) | Q<0.9 |
|---|---|---|---|---|---|---|---|---|
| 59 | K | 23SA | 3407 | 1/1 | 0.81 | 0.09 | 112,112,112,112 | 0 |
| 60 | OHX | 23SA | 3633 | 7/7 | 0.81 | 0.10 | 87,94,101,243 | 0 |
| 58 | MG | 23SB | 3094 | 1/1 | 0.81 | 0.31 | 62,62,62,62 | 0 |
| 58 | MG | 23SA | 3013 | 1/1 | 0.81 | 0.38 | 69,69,69,69 | 0 |
| 60 | OHX | 16SB | 2392 | 7/7 | 0.81 | 0.12 | 157,166,172,266 | 0 |
| 58 | MG | 23SB | 3104 | 1/1 | 0.81 | 0.32 | 89,89,89,89 | 0 |
| 58 | MG | L5B | 201 | 1/1 | 0.81 | 0.11 | 123,123,123,123 | 0 |
| 60 | OHX | 23SB | 3485 | 7/7 | 0.81 | 0.12 | 145,151,159,232 | 0 |
| 58 | MG | 16SA | 2245 | 1/1 | 0.81 | 0.21 | 70,70,70,70 | 0 |
| 58 | MG | 16SA | 2254 | 1/1 | 0.82 | 0.15 | 70,70,70,70 | 0 |
| 58 | MG | 23SA | 3155 | 1/1 | 0.82 | 0.28 | 67,67,67,67 | 0 |
| 58 | MG | 23SB | 3086 | 1/1 | 0.82 | 0.28 | 77,77,77,77 | 0 |
| 58 | MG | 16SB | 2255 | 1/1 | 0.82 | 0.17 | 73,73,73,73 | 0 |
| 59 | K | 23SA | 3430 | 1/1 | 0.82 | 0.17 | 112,112,112,112 | 0 |
| 58 | MG | 16SB | 2261 | 1/1 | 0.82 | 0.07 | 133,133,133,133 | 0 |
| 59 | K | L3A | 303 | 1/1 | 0.82 | 0.10 | 87,87,87,87 | 0 |
| 58 | MG | 23SA | 3131 | 1/1 | 0.82 | 0.18 | 81,81,81,81 | 0 |
| 60 | OHX | 16SA | 2391 | 7/7 | 0.82 | 0.15 | 88,112,122,226 | 0 |
| 58 | MG | 23SB | 3103 | 1/1 | 0.82 | 0.21 | 75,75,75,75 | 0 |
| 59 | K | 16SA | 2322 | 1/1 | 0.82 | 0.14 | 92,92,92,92 | 0 |
| 58 | MG | 23SA | 3257 | 1/1 | 0.82 | 0.17 | 37,37,37,37 | 0 |
| 59 | K | 23SB | 3283 | 1/1 | 0.82 | 0.12 | 101,101,101,101 | 0 |
| 58 | MG | 23SA | 3074 | 1/1 | 0.82 | 0.25 | 52,52,52,52 | 0 |
| 60 | OHX | 23SA | 3604 | 7/7 | 0.82 | 0.12 | 122,137,150,246 | 0 |
| 58 | MG | 23SB | 3054 | 1/1 | 0.82 | 0.08 | 71,71,71,71 | 0 |
| 58 | MG | 16SA | 2279 | 1/1 | 0.82 | 0.13 | 84,84,84,84 | 0 |
| 60 | OHX | 16SB | 2368 | 7/7 | 0.82 | 0.13 | 101,107,114,229 | 0 |
| 58 | MG | 23SA | 3109 | 1/1 | 0.82 | 0.24 | 60,60,60,60 | 0 |
| 58 | MG | 16SA | 2287 | 1/1 | 0.82 | 0.11 | 100,100,100,100 | 0 |
| 60 | OHX | S8B | 201 | 7/7 | 0.82 | 0.10 | 133,155,169,246 | 0 |
| 58 | MG | 16SA | 2238 | 1/1 | 0.82 | 0.33 | 75,75,75,75 | 0 |
| 58 | MG | 16SB | 2284 | 1/1 | 0.82 | 0.10 | 112,112,112,112 | 0 |
| 58 | MG | 16SA | 2225 | 1/1 | 0.82 | 0.13 | 83,83,83,83 | 0 |
| 58 | MG | 23SA | 3150 | 1/1 | 0.82 | 0.29 | 74,74,74,74 | 0 |
| 60 | OHX | 23SB | 3508 | 7/7 | 0.82 | 0.11 | 163,169,177,258 | 0 |
| 60 | OHX | 23SB | 3509 | 7/7 | 0.82 | 0.11 | 135,148,161,244 | 0 |
| 60 | OHX | 23SB | 3510 | 7/7 | 0.82 | 0.10 | 144,156,172,247 | 0 |
| 58 | MG | 23SB | 3040 | 1/1 | 0.83 | 0.27 | 53,53,53,53 | 0 |
| 58 | MG | L23A | 101 | 1/1 | 0.83 | 0.13 | 57,57,57,57 | 0 |
| 58 | MG | 16SB | 2236 | 1/1 | 0.83 | 0.30 | 82,82,82,82 | 0 |
| 58 | MG | 16SB | 2279 | 1/1 | 0.83 | 0.11 | 103,103,103,103 | 0 |
| 58 | MG | 16SB | 2222 | 1/1 | 0.83 | 0.21 | 68,68,68,68 | 0 |

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| Mol | Type | Chain | Res | Atoms | RSCC | RSR | B-factors(Å$^2$) | Q<0.9 |
|---|---|---|---|---|---|---|---|---|
| 58 | MG | 23SB | 3056 | 1/1 | 0.83 | 0.22 | 59,59,59,59 | 0 |
| 58 | MG | 23SA | 3270 | 1/1 | 0.83 | 0.11 | 63,63,63,63 | 0 |
| 59 | K | 23SA | 3343 | 1/1 | 0.83 | 0.40 | 110,110,110,110 | 0 |
| 59 | K | 23SA | 3344 | 1/1 | 0.83 | 0.09 | 86,86,86,86 | 0 |
| 58 | MG | 23SB | 3147 | 1/1 | 0.83 | 0.15 | 56,56,56,56 | 0 |
| 58 | MG | 23SB | 3160 | 1/1 | 0.83 | 0.11 | 111,111,111,111 | 0 |
| 59 | K | 23SB | 3252 | 1/1 | 0.83 | 0.19 | 84,84,84,84 | 0 |
| 59 | K | 23SA | 3432 | 1/1 | 0.83 | 0.12 | 93,93,93,93 | 0 |
| 59 | K | 23SB | 3272 | 1/1 | 0.83 | 0.16 | 111,111,111,111 | 0 |
| 59 | K | 23SB | 3273 | 1/1 | 0.83 | 0.17 | 83,83,83,83 | 0 |
| 59 | K | 23SA | 3348 | 1/1 | 0.83 | 0.08 | 85,85,85,85 | 0 |
| 58 | MG | 16SB | 2253 | 1/1 | 0.83 | 0.35 | 71,71,71,71 | 0 |
| 59 | K | 23SB | 3278 | 1/1 | 0.83 | 0.24 | 82,82,82,82 | 0 |
| 58 | MG | 23SA | 3167 | 1/1 | 0.83 | 0.21 | 42,42,42,42 | 0 |
| 58 | MG | 16SA | 2249 | 1/1 | 0.83 | 0.35 | 72,72,72,72 | 0 |
| 60 | OHX | 16SB | 2379 | 7/7 | 0.83 | 0.11 | 150,159,165,251 | 0 |
| 58 | MG | 23SB | 3224 | 1/1 | 0.83 | 0.12 | 79,79,79,79 | 0 |
| 60 | OHX | 16SB | 2385 | 7/7 | 0.83 | 0.12 | 160,164,166,249 | 0 |
| 59 | K | 23SB | 3291 | 1/1 | 0.83 | 0.10 | 76,76,76,76 | 0 |
| 59 | K | 23SB | 3294 | 1/1 | 0.83 | 0.10 | 131,131,131,131 | 0 |
| 59 | K | 16SA | 2328 | 1/1 | 0.83 | 0.17 | 103,103,103,103 | 0 |
| 58 | MG | 16SB | 2227 | 1/1 | 0.83 | 0.22 | 61,61,61,61 | 0 |
| 58 | MG | 23SA | 3312 | 1/1 | 0.83 | 0.11 | 86,86,86,86 | 0 |
| 58 | MG | 16SA | 2236 | 1/1 | 0.83 | 0.36 | 61,61,61,61 | 0 |
| 59 | K | 16SB | 2298 | 1/1 | 0.83 | 0.08 | 104,104,104,104 | 0 |
| 58 | MG | L17A | 201 | 1/1 | 0.83 | 0.23 | 89,89,89,89 | 0 |
| 59 | K | 16SB | 2304 | 1/1 | 0.83 | 0.10 | 96,96,96,96 | 0 |
| 60 | OHX | 5SB | 214 | 7/7 | 0.83 | 0.12 | 126,136,154,239 | 0 |
| 60 | OHX | 16SA | 2376 | 7/7 | 0.84 | 0.13 | 99,103,107,223 | 0 |
| 58 | MG | L5A | 301 | 1/1 | 0.84 | 0.25 | 71,71,71,71 | 0 |
| 58 | MG | 23SA | 3007 | 1/1 | 0.84 | 0.26 | 67,67,67,67 | 0 |
| 58 | MG | 23SA | 3161 | 1/1 | 0.84 | 0.13 | 48,48,48,48 | 0 |
| 58 | MG | L32A | 101 | 1/1 | 0.84 | 0.14 | 68,68,68,68 | 0 |
| 60 | OHX | 23SA | 3598 | 7/7 | 0.84 | 0.11 | 123,128,144,226 | 0 |
| 58 | MG | 16SB | 2263 | 1/1 | 0.84 | 0.11 | 122,122,122,122 | 0 |
| 59 | K | 23SA | 3338 | 1/1 | 0.84 | 0.18 | 105,105,105,105 | 0 |
| 58 | MG | PSIB | 103 | 1/1 | 0.84 | 0.22 | 66,66,66,66 | 0 |
| 59 | K | 16SB | 2315 | 1/1 | 0.84 | 0.16 | 122,122,122,122 | 0 |
| 60 | OHX | L28A | 101 | 7/7 | 0.84 | 0.10 | 82,89,94,243 | 0 |
| 58 | MG | 23SB | 3062 | 1/1 | 0.84 | 0.17 | 67,67,67,67 | 0 |
| 58 | MG | 16SA | 2201 | 1/1 | 0.84 | 0.26 | 72,72,72,72 | 0 |
| 58 | MG | 16SA | 2226 | 1/1 | 0.84 | 0.21 | 66,66,66,66 | 0 |

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| Mol | Type | Chain | Res | Atoms | RSCC | RSR | B-factors(Å$^2$) | Q<0.9 |
|---|---|---|---|---|---|---|---|---|
| 59 | K | 23SA | 3422 | 1/1 | 0.84 | 0.10 | 75,75,75,75 | 0 |
| 58 | MG | 23SB | 3177 | 1/1 | 0.84 | 0.12 | 57,57,57,57 | 0 |
| 58 | MG | 23SB | 3188 | 1/1 | 0.84 | 0.13 | 37,37,37,37 | 0 |
| 58 | MG | 23SB | 3199 | 1/1 | 0.84 | 0.19 | 79,79,79,79 | 0 |
| 58 | MG | 23SA | 3017 | 1/1 | 0.84 | 0.14 | 90,90,90,90 | 0 |
| 58 | MG | 23SA | 3137 | 1/1 | 0.84 | 0.14 | 75,75,75,75 | 0 |
| 60 | OHX | 23SB | 3470 | 7/7 | 0.84 | 0.13 | 106,129,148,206 | 0 |
| 58 | MG | 23SB | 3076 | 1/1 | 0.84 | 0.23 | 62,62,62,62 | 0 |
| 58 | MG | 23SB | 3237 | 1/1 | 0.84 | 0.30 | 91,91,91,91 | 0 |
| 58 | MG | 23SA | 3066 | 1/1 | 0.84 | 0.14 | 60,60,60,60 | 0 |
| 58 | MG | 23SA | 3070 | 1/1 | 0.84 | 0.22 | 72,72,72,72 | 0 |
| 59 | K | 23SA | 3358 | 1/1 | 0.84 | 0.12 | 83,83,83,83 | 0 |
| 58 | MG | 23SB | 3082 | 1/1 | 0.84 | 0.22 | 77,77,77,77 | 0 |
| 58 | MG | 23SB | 3112 | 1/1 | 0.85 | 0.22 | 57,57,57,57 | 0 |
| 58 | MG | 23SA | 3140 | 1/1 | 0.85 | 0.17 | 77,77,77,77 | 0 |
| 59 | K | 23SB | 3245 | 1/1 | 0.85 | 0.13 | 81,81,81,81 | 0 |
| 58 | MG | 23SB | 3083 | 1/1 | 0.85 | 0.20 | 75,75,75,75 | 0 |
| 58 | MG | 23SB | 3223 | 1/1 | 0.85 | 0.11 | 80,80,80,80 | 0 |
| 59 | K | 23SB | 3254 | 1/1 | 0.85 | 0.12 | 65,65,65,65 | 0 |
| 58 | MG | 23SA | 3141 | 1/1 | 0.85 | 0.21 | 69,69,69,69 | 0 |
| 59 | K | 23SA | 3435 | 1/1 | 0.85 | 0.11 | 78,78,78,78 | 0 |
| 60 | OHX | 23SA | 3539 | 7/7 | 0.85 | 0.10 | 81,91,100,236 | 0 |
| 58 | MG | 23SB | 3057 | 1/1 | 0.85 | 0.21 | 59,59,59,59 | 0 |
| 58 | MG | 16SA | 2211 | 1/1 | 0.85 | 0.17 | 52,52,52,52 | 0 |
| 58 | MG | 5SB | 203 | 1/1 | 0.85 | 0.28 | 55,55,55,55 | 0 |
| 58 | MG | L2B | 301 | 1/1 | 0.85 | 0.30 | 78,78,78,78 | 0 |
| 58 | MG | 16SA | 2219 | 1/1 | 0.85 | 0.24 | 65,65,65,65 | 0 |
| 58 | MG | 16SA | 2227 | 1/1 | 0.85 | 0.32 | 67,67,67,67 | 0 |
| 58 | MG | 23SA | 3136 | 1/1 | 0.85 | 0.15 | 61,61,61,61 | 0 |
| 59 | K | 23SB | 3286 | 1/1 | 0.85 | 0.14 | 92,92,92,92 | 0 |
| 59 | K | 16SB | 2293 | 1/1 | 0.85 | 0.08 | 102,102,102,102 | 0 |
| 58 | MG | 23SA | 3278 | 1/1 | 0.85 | 0.14 | 67,67,67,67 | 0 |
| 60 | OHX | 16SB | 2382 | 7/7 | 0.85 | 0.12 | 143,150,162,242 | 0 |
| 59 | K | 23SA | 3384 | 1/1 | 0.85 | 0.07 | 89,89,89,89 | 0 |
| 58 | MG | 23SB | 3133 | 1/1 | 0.85 | 0.20 | 83,83,83,83 | 0 |
| 60 | OHX | 16SB | 2388 | 7/7 | 0.85 | 0.12 | 111,113,150,236 | 0 |
| 59 | K | PSIA | 103 | 1/1 | 0.85 | 0.10 | 84,84,84,84 | 0 |
| 59 | K | 16SA | 2296 | 1/1 | 0.85 | 0.12 | 93,93,93,93 | 0 |
| 59 | K | 16SA | 2298 | 1/1 | 0.85 | 0.13 | 90,90,90,90 | 0 |
| 58 | MG | 23SA | 3088 | 1/1 | 0.85 | 0.22 | 68,68,68,68 | 0 |
| 60 | OHX | 23SB | 3461 | 7/7 | 0.85 | 0.09 | 112,118,121,252 | 0 |
| 58 | MG | 23SA | 3002 | 1/1 | 0.85 | 0.30 | 54,54,54,54 | 0 |

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| Mol | Type | Chain | Res | Atoms | RSCC | RSR | B-factors(Å$^2$) | Q<0.9 |
|---|---|---|---|---|---|---|---|---|
| 58 | MG | 23SB | 3045 | 1/1 | 0.85 | 0.28 | 45,45,45,45 | 0 |
| 59 | K | 16SB | 2319 | 1/1 | 0.85 | 0.23 | 84,84,84,84 | 0 |
| 59 | K | 23SA | 3418 | 1/1 | 0.85 | 0.09 | 62,62,62,62 | 0 |
| 59 | K | 23SA | 3419 | 1/1 | 0.85 | 0.09 | 78,78,78,78 | 0 |
| 58 | MG | 16SA | 2223 | 1/1 | 0.85 | 0.18 | 69,69,69,69 | 0 |
| 60 | OHX | 23SB | 3512 | 7/7 | 0.85 | 0.10 | 154,161,175,244 | 0 |
| 58 | MG | S5B | 201 | 1/1 | 0.85 | 0.28 | 69,69,69,69 | 0 |
| 61 | SJH | 23SB | 3323 | 83/83 | 0.85 | 0.19 | 50,50,50,50 | 0 |
| 58 | MG | 23SB | 3070 | 1/1 | 0.86 | 0.27 | 56,56,56,56 | 0 |
| 58 | MG | 23SB | 3073 | 1/1 | 0.86 | 0.34 | 75,75,75,75 | 0 |
| 58 | MG | 23SA | 3003 | 1/1 | 0.86 | 0.16 | 62,62,62,62 | 0 |
| 60 | OHX | 16SA | 2399 | 7/7 | 0.86 | 0.11 | 162,172,178,247 | 0 |
| 59 | K | 23SA | 3431 | 1/1 | 0.86 | 0.06 | 70,70,70,70 | 0 |
| 60 | OHX | 23SA | 3511 | 7/7 | 0.86 | 0.12 | 129,155,160,239 | 0 |
| 58 | MG | 23SB | 3123 | 1/1 | 0.86 | 0.30 | 61,61,61,61 | 0 |
| 58 | MG | 23SA | 3263 | 1/1 | 0.86 | 0.10 | 45,45,45,45 | 0 |
| 60 | OHX | 23SA | 3559 | 7/7 | 0.86 | 0.09 | 106,114,120,233 | 0 |
| 58 | MG | 23SA | 3060 | 1/1 | 0.86 | 0.23 | 80,80,80,80 | 0 |
| 58 | MG | 23SB | 3031 | 1/1 | 0.86 | 0.27 | 69,69,69,69 | 0 |
| 59 | K | 16SA | 2303 | 1/1 | 0.86 | 0.13 | 111,111,111,111 | 0 |
| 58 | MG | 23SB | 3035 | 1/1 | 0.86 | 0.24 | 60,60,60,60 | 0 |
| 58 | MG | 16SA | 2213 | 1/1 | 0.86 | 0.17 | 60,60,60,60 | 0 |
| 60 | OHX | 23SA | 3613 | 7/7 | 0.86 | 0.12 | 100,119,125,217 | 0 |
| 60 | OHX | 23SA | 3614 | 7/7 | 0.86 | 0.09 | 109,128,161,248 | 0 |
| 60 | OHX | 23SA | 3628 | 7/7 | 0.86 | 0.10 | 149,156,162,258 | 0 |
| 58 | MG | 23SA | 3008 | 1/1 | 0.86 | 0.08 | 84,84,84,84 | 0 |
| 58 | MG | 16SB | 2205 | 1/1 | 0.86 | 0.23 | 55,55,55,55 | 0 |
| 59 | K | 16SB | 2291 | 1/1 | 0.86 | 0.23 | 85,85,85,85 | 0 |
| 58 | MG | 23SA | 3300 | 1/1 | 0.86 | 0.09 | 65,65,65,65 | 0 |
| 60 | OHX | 16SB | 2372 | 7/7 | 0.86 | 0.11 | 94,114,129,214 | 0 |
| 60 | OHX | 16SB | 2378 | 7/7 | 0.86 | 0.12 | 125,127,138,207 | 0 |
| 58 | MG | 23SB | 3097 | 1/1 | 0.86 | 0.18 | 75,75,75,75 | 0 |
| 58 | MG | 23SA | 3129 | 1/1 | 0.86 | 0.17 | 54,54,54,54 | 0 |
| 59 | K | 16SA | 2327 | 1/1 | 0.86 | 0.29 | 82,82,82,82 | 0 |
| 58 | MG | 23SB | 3101 | 1/1 | 0.86 | 0.20 | 74,74,74,74 | 0 |
| 58 | MG | 23SA | 3009 | 1/1 | 0.86 | 0.20 | 51,51,51,51 | 0 |
| 58 | MG | 23SA | 3114 | 1/1 | 0.86 | 0.21 | 65,65,65,65 | 0 |
| 60 | OHX | 16SB | 2396 | 7/7 | 0.86 | 0.11 | 118,139,162,230 | 0 |
| 58 | MG | 23SA | 3132 | 1/1 | 0.86 | 0.13 | 62,62,62,62 | 0 |
| 60 | OHX | MRNB | 101 | 7/7 | 0.86 | 0.11 | 140,145,154,244 | 0 |
| 59 | K | 23SB | 3310 | 1/1 | 0.86 | 0.14 | 74,74,74,74 | 0 |
| 59 | K | 23SA | 3391 | 1/1 | 0.86 | 0.12 | 72,72,72,72 | 0 |

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| Mol | Type | Chain | Res | Atoms | RSCC | RSR | B-factors(Å$^2$) | Q<0.9 |
|---|---|---|---|---|---|---|---|---|
| 58 | MG | 23SA | 3174 | 1/1 | 0.86 | 0.10 | 60,60,60,60 | 0 |
| 58 | MG | 16SA | 2218 | 1/1 | 0.86 | 0.14 | 71,71,71,71 | 0 |
| 59 | K | 16SA | 2335 | 1/1 | 0.86 | 0.08 | 108,108,108,108 | 0 |
| 58 | MG | 23SA | 3177 | 1/1 | 0.86 | 0.33 | 65,65,65,65 | 0 |
| 59 | K | 23SB | 3318 | 1/1 | 0.86 | 0.15 | 73,73,73,73 | 0 |
| 58 | MG | 23SA | 3103 | 1/1 | 0.86 | 0.32 | 60,60,60,60 | 0 |
| 58 | MG | 16SA | 2246 | 1/1 | 0.86 | 0.27 | 73,73,73,73 | 0 |
| 58 | MG | 23SA | 3239 | 1/1 | 0.86 | 0.16 | 35,35,35,35 | 0 |
| 60 | OHX | 23SB | 3515 | 7/7 | 0.86 | 0.10 | 98,102,106,258 | 0 |
| 58 | MG | 16SB | 2223 | 1/1 | 0.86 | 0.29 | 68,68,68,68 | 0 |
| 58 | MG | 23SA | 3159 | 1/1 | 0.86 | 0.30 | 63,63,63,63 | 0 |
| 60 | OHX | ASIA | 102 | 7/7 | 0.87 | 0.12 | 99,122,129,226 | 0 |
| 58 | MG | 23SA | 3055 | 1/1 | 0.87 | 0.29 | 62,62,62,62 | 0 |
| 58 | MG | 16SA | 2272 | 1/1 | 0.87 | 0.12 | 56,56,56,56 | 0 |
| 58 | MG | 23SB | 3115 | 1/1 | 0.87 | 0.10 | 53,53,53,53 | 0 |
| 58 | MG | 16SA | 2202 | 1/1 | 0.87 | 0.23 | 64,64,64,64 | 0 |
| 58 | MG | 23SB | 3065 | 1/1 | 0.87 | 0.14 | 59,59,59,59 | 0 |
| 58 | MG | 23SA | 3325 | 1/1 | 0.87 | 0.12 | 42,42,42,42 | 0 |
| 58 | MG | 23SB | 3069 | 1/1 | 0.87 | 0.21 | 67,67,67,67 | 0 |
| 58 | MG | 23SA | 3006 | 1/1 | 0.87 | 0.27 | 54,54,54,54 | 0 |
| 58 | MG | 23SA | 3024 | 1/1 | 0.87 | 0.15 | 53,53,53,53 | 0 |
| 58 | MG | 23SA | 3214 | 1/1 | 0.87 | 0.09 | 43,43,43,43 | 0 |
| 58 | MG | 23SB | 3127 | 1/1 | 0.87 | 0.08 | 63,63,63,63 | 0 |
| 58 | MG | 16SA | 2258 | 1/1 | 0.87 | 0.10 | 88,88,88,88 | 0 |
| 59 | K | 23SB | 3288 | 1/1 | 0.87 | 0.09 | 88,88,88,88 | 0 |
| 58 | MG | 23SA | 3230 | 1/1 | 0.87 | 0.14 | 114,114,114,114 | 0 |
| 58 | MG | 23SA | 3160 | 1/1 | 0.87 | 0.11 | 75,75,75,75 | 0 |
| 58 | MG | 16SB | 2224 | 1/1 | 0.87 | 0.23 | 70,70,70,70 | 0 |
| 58 | MG | 23SB | 3150 | 1/1 | 0.87 | 0.11 | 65,65,65,65 | 0 |
| 60 | OHX | 16SB | 2375 | 7/7 | 0.87 | 0.12 | 112,129,142,222 | 0 |
| 58 | MG | 16SA | 2229 | 1/1 | 0.87 | 0.17 | 48,48,48,48 | 0 |
| 59 | K | 16SB | 2299 | 1/1 | 0.87 | 0.10 | 84,84,84,84 | 0 |
| 60 | OHX | 16SB | 2381 | 7/7 | 0.87 | 0.10 | 141,152,160,225 | 0 |
| 58 | MG | 16SA | 2267 | 1/1 | 0.87 | 0.11 | 102,102,102,102 | 0 |
| 59 | K | 16SA | 2324 | 1/1 | 0.87 | 0.21 | 79,79,79,79 | 0 |
| 58 | MG | 23SA | 3077 | 1/1 | 0.87 | 0.23 | 57,57,57,57 | 0 |
| 59 | K | 16SB | 2308 | 1/1 | 0.87 | 0.10 | 105,105,105,105 | 0 |
| 58 | MG | 23SB | 3044 | 1/1 | 0.87 | 0.35 | 45,45,45,45 | 0 |
| 60 | OHX | 16SB | 2393 | 7/7 | 0.87 | 0.10 | 134,138,165,251 | 0 |
| 58 | MG | 23SA | 3101 | 1/1 | 0.87 | 0.15 | 62,62,62,62 | 0 |
| 60 | OHX | 16SB | 2398 | 7/7 | 0.87 | 0.09 | 93,103,110,241 | 0 |
| 58 | MG | 16SB | 2228 | 1/1 | 0.87 | 0.32 | 66,66,66,66 | 0 |

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| Mol | Type | Chain | Res | Atoms | RSCC | RSR | B-factors(Å$^2$) | Q<0.9 |
|---|---|---|---|---|---|---|---|---|
| 59 | K | 23SA | 3399 | 1/1 | 0.87 | 0.14 | 79,79,79,79 | 0 |
| 60 | OHX | 23SB | 3358 | 7/7 | 0.87 | 0.15 | 54,81,112,155 | 0 |
| 58 | MG | 23SB | 3051 | 1/1 | 0.87 | 0.23 | 46,46,46,46 | 0 |
| 58 | MG | 23SA | 3012 | 1/1 | 0.87 | 0.10 | 98,98,98,98 | 0 |
| 60 | OHX | 23SB | 3456 | 7/7 | 0.87 | 0.11 | 83,92,104,232 | 0 |
| 58 | MG | 16SB | 2232 | 1/1 | 0.87 | 0.31 | 69,69,69,69 | 0 |
| 59 | K | S6B | 201 | 1/1 | 0.87 | 0.16 | 97,97,97,97 | 0 |
| 58 | MG | 23SA | 3083 | 1/1 | 0.87 | 0.15 | 58,58,58,58 | 0 |
| 58 | MG | 23SA | 3283 | 1/1 | 0.87 | 0.12 | 39,39,39,39 | 0 |
| 60 | OHX | 23SB | 3506 | 7/7 | 0.87 | 0.10 | 150,165,174,249 | 0 |
| 58 | MG | 5SB | 202 | 1/1 | 0.87 | 0.09 | 77,77,77,77 | 0 |
| 58 | MG | 23SA | 3291 | 1/1 | 0.87 | 0.10 | 60,60,60,60 | 0 |
| 59 | K | 23SB | 3243 | 1/1 | 0.87 | 0.15 | 110,110,110,110 | 0 |
| 60 | OHX | 23SB | 3511 | 7/7 | 0.87 | 0.10 | 185,187,188,263 | 0 |
| 58 | MG | 23SA | 3295 | 1/1 | 0.87 | 0.17 | 62,62,62,62 | 0 |
| 60 | OHX | 16SA | 2400 | 7/7 | 0.87 | 0.10 | 131,143,159,239 | 0 |
| 60 | OHX | 16SA | 2406 | 7/7 | 0.87 | 0.11 | 130,144,148,254 | 0 |
| 58 | MG | 16SA | 2230 | 1/1 | 0.87 | 0.19 | 68,68,68,68 | 0 |
| 58 | MG | 23SB | 3164 | 1/1 | 0.88 | 0.13 | 63,63,63,63 | 0 |
| 58 | MG | 23SB | 3093 | 1/1 | 0.88 | 0.13 | 67,67,67,67 | 0 |
| 58 | MG | 16SB | 2276 | 1/1 | 0.88 | 0.08 | 104,104,104,104 | 0 |
| 59 | K | 23SA | 3415 | 1/1 | 0.88 | 0.09 | 91,91,91,91 | 0 |
| 58 | MG | 23SB | 3095 | 1/1 | 0.88 | 0.15 | 66,66,66,66 | 0 |
| 60 | OHX | 23SA | 3552 | 7/7 | 0.88 | 0.10 | 94,98,103,214 | 0 |
| 60 | OHX | 23SA | 3555 | 7/7 | 0.88 | 0.10 | 109,119,127,236 | 0 |
| 58 | MG | 23SB | 3192 | 1/1 | 0.88 | 0.13 | 59,59,59,59 | 0 |
| 59 | K | 23SB | 3264 | 1/1 | 0.88 | 0.11 | 84,84,84,84 | 0 |
| 60 | OHX | 23SA | 3564 | 7/7 | 0.88 | 0.10 | 75,83,93,207 | 0 |
| 60 | OHX | 23SA | 3597 | 7/7 | 0.88 | 0.10 | 136,148,161,225 | 0 |
| 58 | MG | 23SA | 3029 | 1/1 | 0.88 | 0.17 | 45,45,45,45 | 0 |
| 59 | K | 23SB | 3271 | 1/1 | 0.88 | 0.22 | 85,85,85,85 | 0 |
| 58 | MG | 23SB | 3052 | 1/1 | 0.88 | 0.34 | 56,56,56,56 | 0 |
| 58 | MG | 23SB | 3100 | 1/1 | 0.88 | 0.21 | 81,81,81,81 | 0 |
| 60 | OHX | 23SA | 3608 | 7/7 | 0.88 | 0.10 | 152,160,170,242 | 0 |
| 58 | MG | 23SA | 3223 | 1/1 | 0.88 | 0.12 | 47,47,47,47 | 0 |
| 59 | K | S13A | 201 | 1/1 | 0.88 | 0.09 | 90,90,90,90 | 0 |
| 60 | OHX | 23SA | 3625 | 7/7 | 0.88 | 0.11 | 125,130,156,230 | 0 |
| 58 | MG | 23SB | 3102 | 1/1 | 0.88 | 0.38 | 65,65,65,65 | 0 |
| 60 | OHX | 23SA | 3631 | 7/7 | 0.88 | 0.10 | 97,104,111,227 | 0 |
| 58 | MG | 23SB | 3229 | 1/1 | 0.88 | 0.15 | 94,94,94,94 | 0 |
| 60 | OHX | 5SA | 213 | 7/7 | 0.88 | 0.11 | 75,92,112,197 | 0 |
| 58 | MG | 23SA | 3115 | 1/1 | 0.88 | 0.09 | 62,62,62,62 | 0 |

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| Mol | Type | Chain | Res | Atoms | RSCC | RSR | B-factors(Å$^2$) | Q<0.9 |
|---|---|---|---|---|---|---|---|---|
| 58 | MG | 23SA | 3054 | 1/1 | 0.88 | 0.23 | 42,42,42,42 | 0 |
| 60 | OHX | 16SB | 2365 | 7/7 | 0.88 | 0.10 | 94,104,122,243 | 0 |
| 58 | MG | 23SA | 3135 | 1/1 | 0.88 | 0.12 | 84,84,84,84 | 0 |
| 58 | MG | 16SB | 2230 | 1/1 | 0.88 | 0.22 | 68,68,68,68 | 0 |
| 58 | MG | 23SA | 3169 | 1/1 | 0.88 | 0.21 | 87,87,87,87 | 0 |
| 58 | MG | 23SA | 3073 | 1/1 | 0.88 | 0.11 | 71,71,71,71 | 0 |
| 58 | MG | 23SB | 3001 | 1/1 | 0.88 | 0.21 | 42,42,42,42 | 0 |
| 59 | K | 23SB | 3298 | 1/1 | 0.88 | 0.06 | 89,89,89,89 | 0 |
| 58 | MG | 16SA | 2286 | 1/1 | 0.88 | 0.10 | 98,98,98,98 | 0 |
| 58 | MG | 23SA | 3033 | 1/1 | 0.88 | 0.15 | 78,78,78,78 | 0 |
| 58 | MG | 16SA | 2275 | 1/1 | 0.88 | 0.13 | 58,58,58,58 | 0 |
| 58 | MG | 23SB | 3016 | 1/1 | 0.88 | 0.25 | 42,42,42,42 | 0 |
| 58 | MG | 23SB | 3020 | 1/1 | 0.88 | 0.19 | 51,51,51,51 | 0 |
| 58 | MG | 23SB | 3118 | 1/1 | 0.88 | 0.18 | 80,80,80,80 | 0 |
| 58 | MG | 23SB | 3023 | 1/1 | 0.88 | 0.26 | 66,66,66,66 | 0 |
| 59 | K | 23SB | 3312 | 1/1 | 0.88 | 0.07 | 89,89,89,89 | 0 |
| 58 | MG | 23SB | 3028 | 1/1 | 0.88 | 0.07 | 70,70,70,70 | 0 |
| 58 | MG | 16SB | 2262 | 1/1 | 0.88 | 0.12 | 77,77,77,77 | 0 |
| 58 | MG | 23SB | 3033 | 1/1 | 0.88 | 0.23 | 68,68,68,68 | 0 |
| 59 | K | 16SB | 2306 | 1/1 | 0.88 | 0.12 | 81,81,81,81 | 0 |
| 60 | OHX | 23SB | 3417 | 7/7 | 0.88 | 0.10 | 84,93,104,216 | 0 |
| 60 | OHX | 23SB | 3441 | 7/7 | 0.88 | 0.11 | 80,90,114,205 | 0 |
| 58 | MG | 23SA | 3081 | 1/1 | 0.88 | 0.13 | 59,59,59,59 | 0 |
| 60 | OHX | 23SB | 3453 | 7/7 | 0.88 | 0.09 | 108,109,124,237 | 0 |
| 59 | K | 16SA | 2310 | 1/1 | 0.88 | 0.07 | 79,79,79,79 | 0 |
| 60 | OHX | 23SB | 3459 | 7/7 | 0.88 | 0.11 | 142,161,168,231 | 0 |
| 59 | K | 23SB | 3320 | 1/1 | 0.88 | 0.13 | 82,82,82,82 | 0 |
| 60 | OHX | 23SB | 3465 | 7/7 | 0.88 | 0.08 | 106,109,117,246 | 0 |
| 59 | K | 23SA | 3372 | 1/1 | 0.88 | 0.14 | 69,69,69,69 | 0 |
| 58 | MG | 23SB | 3081 | 1/1 | 0.88 | 0.12 | 54,54,54,54 | 0 |
| 59 | K | L3B | 303 | 1/1 | 0.88 | 0.12 | 98,98,98,98 | 0 |
| 60 | OHX | 23SB | 3498 | 7/7 | 0.88 | 0.11 | 110,121,148,223 | 0 |
| 60 | OHX | 23SB | 3499 | 7/7 | 0.88 | 0.10 | 117,142,151,221 | 0 |
| 58 | MG | 23SA | 3285 | 1/1 | 0.88 | 0.14 | 42,42,42,42 | 0 |
| 59 | K | 16SA | 2316 | 1/1 | 0.88 | 0.09 | 92,92,92,92 | 0 |
| 58 | MG | 16SA | 2210 | 1/1 | 0.88 | 0.36 | 53,53,53,53 | 0 |
| 58 | MG | L33A | 101 | 1/1 | 0.88 | 0.25 | 87,87,87,87 | 0 |
| 58 | MG | 23SB | 3085 | 1/1 | 0.88 | 0.33 | 61,61,61,61 | 0 |
| 58 | MG | 23SA | 3189 | 1/1 | 0.88 | 0.12 | 51,51,51,51 | 0 |
| 59 | K | 23SA | 3402 | 1/1 | 0.88 | 0.09 | 61,61,61,61 | 0 |
| 60 | OHX | 16SA | 2404 | 7/7 | 0.88 | 0.11 | 156,159,166,251 | 0 |
| 58 | MG | 16SA | 2204 | 1/1 | 0.88 | 0.19 | 56,56,56,56 | 0 |

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| Mol | Type | Chain | Res | Atoms | RSCC | RSR | B-factors(Å$^2$) | Q<0.9 |
|---|---|---|---|---|---|---|---|---|
| 58 | MG | 23SB | 3022 | 1/1 | 0.89 | 0.14 | 46,46,46,46 | 0 |
| 58 | MG | 16SA | 2214 | 1/1 | 0.89 | 0.39 | 54,54,54,54 | 0 |
| 59 | K | 23SA | 3367 | 1/1 | 0.89 | 0.09 | 57,57,57,57 | 0 |
| 60 | OHX | 23SA | 3622 | 7/7 | 0.89 | 0.10 | 128,144,153,225 | 0 |
| 59 | K | 16SA | 2323 | 1/1 | 0.89 | 0.08 | 75,75,75,75 | 0 |
| 59 | K | 23SB | 3302 | 1/1 | 0.89 | 0.10 | 91,91,91,91 | 0 |
| 58 | MG | 23SB | 3027 | 1/1 | 0.89 | 0.18 | 63,63,63,63 | 0 |
| 58 | MG | 16SA | 2221 | 1/1 | 0.89 | 0.25 | 59,59,59,59 | 0 |
| 58 | MG | 23SB | 3072 | 1/1 | 0.89 | 0.21 | 56,56,56,56 | 0 |
| 58 | MG | 23SA | 3084 | 1/1 | 0.89 | 0.14 | 46,46,46,46 | 0 |
| 60 | OHX | 16SB | 2348 | 7/7 | 0.89 | 0.10 | 112,114,120,229 | 0 |
| 60 | OHX | 16SB | 2349 | 7/7 | 0.89 | 0.11 | 89,98,117,198 | 0 |
| 59 | K | 16SB | 2313 | 1/1 | 0.89 | 0.12 | 91,91,91,91 | 0 |
| 58 | MG | 23SB | 3236 | 1/1 | 0.89 | 0.10 | 106,106,106,106 | 0 |
| 58 | MG | 23SA | 3171 | 1/1 | 0.89 | 0.07 | 63,63,63,63 | 0 |
| 58 | MG | 23SB | 3034 | 1/1 | 0.89 | 0.21 | 59,59,59,59 | 0 |
| 58 | MG | 23SA | 3273 | 1/1 | 0.89 | 0.12 | 100,100,100,100 | 0 |
| 58 | MG | 23SA | 3151 | 1/1 | 0.89 | 0.18 | 72,72,72,72 | 0 |
| 58 | MG | 23SA | 3044 | 1/1 | 0.89 | 0.15 | 69,69,69,69 | 0 |
| 59 | K | S6A | 201 | 1/1 | 0.89 | 0.26 | 98,98,98,98 | 0 |
| 58 | MG | 23SA | 3023 | 1/1 | 0.89 | 0.19 | 70,70,70,70 | 0 |
| 58 | MG | 16SA | 2207 | 1/1 | 0.89 | 0.13 | 79,79,79,79 | 0 |
| 58 | MG | 23SA | 3123 | 1/1 | 0.89 | 0.23 | 78,78,78,78 | 0 |
| 58 | MG | 16SB | 2285 | 1/1 | 0.89 | 0.10 | 91,91,91,91 | 0 |
| 58 | MG | 23SA | 3293 | 1/1 | 0.89 | 0.08 | 67,67,67,67 | 0 |
| 59 | K | 23SA | 3337 | 1/1 | 0.89 | 0.18 | 88,88,88,88 | 0 |
| 60 | OHX | 16SB | 2395 | 7/7 | 0.89 | 0.10 | 132,140,148,232 | 0 |
| 59 | K | 23SB | 3246 | 1/1 | 0.89 | 0.26 | 91,91,91,91 | 0 |
| 58 | MG | 16SA | 2282 | 1/1 | 0.89 | 0.07 | 105,105,105,105 | 0 |
| 60 | OHX | 16SA | 2390 | 7/7 | 0.89 | 0.09 | 109,122,132,247 | 0 |
| 59 | K | 23SA | 3339 | 1/1 | 0.89 | 0.12 | 113,113,113,113 | 0 |
| 59 | K | 16SA | 2297 | 1/1 | 0.89 | 0.19 | 95,95,95,95 | 0 |
| 59 | K | 23SB | 3258 | 1/1 | 0.89 | 0.07 | 58,58,58,58 | 0 |
| 60 | OHX | 23SB | 3411 | 7/7 | 0.89 | 0.09 | 103,109,121,218 | 0 |
| 59 | K | 23SB | 3259 | 1/1 | 0.89 | 0.09 | 69,69,69,69 | 0 |
| 60 | OHX | 23SB | 3421 | 7/7 | 0.89 | 0.09 | 93,96,114,233 | 0 |
| 60 | OHX | 23SB | 3433 | 7/7 | 0.89 | 0.11 | 94,104,115,211 | 0 |
| 58 | MG | 23SB | 3129 | 1/1 | 0.89 | 0.22 | 56,56,56,56 | 0 |
| 58 | MG | 23SB | 3131 | 1/1 | 0.89 | 0.25 | 59,59,59,59 | 0 |
| 60 | OHX | 16SA | 2409 | 7/7 | 0.89 | 0.10 | 123,137,158,221 | 0 |
| 58 | MG | PSIB | 101 | 1/1 | 0.89 | 0.18 | 66,66,66,66 | 0 |
| 58 | MG | 23SA | 3198 | 1/1 | 0.89 | 0.12 | 46,46,46,46 | 0 |

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| Mol | Type | Chain | Res | Atoms | RSCC | RSR | B-factors(Å$^2$) | Q<0.9 |
|---|---|---|---|---|---|---|---|---|
| 58 | MG | 16SA | 2285 | 1/1 | 0.89 | 0.09 | 118,118,118,118 | 0 |
| 60 | OHX | 23SB | 3462 | 7/7 | 0.89 | 0.09 | 100,106,116,237 | 0 |
| 58 | MG | 23SA | 3091 | 1/1 | 0.89 | 0.18 | 53,53,53,53 | 0 |
| 60 | OHX | 23SA | 3546 | 7/7 | 0.89 | 0.12 | 117,124,152,208 | 0 |
| 60 | OHX | 23SB | 3483 | 7/7 | 0.89 | 0.09 | 127,135,150,240 | 0 |
| 60 | OHX | 23SA | 3550 | 7/7 | 0.89 | 0.09 | 97,104,114,218 | 0 |
| 60 | OHX | 23SB | 3493 | 7/7 | 0.89 | 0.09 | 123,130,149,234 | 0 |
| 58 | MG | 23SB | 3158 | 1/1 | 0.89 | 0.10 | 72,72,72,72 | 0 |
| 58 | MG | 23SA | 3142 | 1/1 | 0.89 | 0.27 | 61,61,61,61 | 0 |
| 58 | MG | 23SB | 3004 | 1/1 | 0.89 | 0.22 | 47,47,47,47 | 0 |
| 60 | OHX | 23SB | 3501 | 7/7 | 0.89 | 0.09 | 152,156,161,252 | 0 |
| 60 | OHX | 23SB | 3503 | 7/7 | 0.89 | 0.09 | 126,131,152,227 | 0 |
| 58 | MG | 16SB | 2260 | 1/1 | 0.89 | 0.10 | 96,96,96,96 | 0 |
| 59 | K | 16SB | 2290 | 1/1 | 0.89 | 0.07 | 112,112,112,112 | 0 |
| 60 | OHX | 23SA | 3588 | 7/7 | 0.89 | 0.11 | 115,116,136,199 | 0 |
| 59 | K | 23SA | 3355 | 1/1 | 0.89 | 0.12 | 65,65,65,65 | 0 |
| 58 | MG | 16SA | 2260 | 1/1 | 0.89 | 0.09 | 93,93,93,93 | 0 |
| 59 | K | 23SB | 3289 | 1/1 | 0.89 | 0.07 | 79,79,79,79 | 0 |
| 58 | MG | 23SA | 3062 | 1/1 | 0.89 | 0.10 | 78,78,78,78 | 0 |
| 58 | MG | 23SA | 3334 | 1/1 | 0.89 | 0.11 | 65,65,65,65 | 0 |
| 61 | SJH | 23SA | 3436 | 83/83 | 0.89 | 0.14 | 50,50,50,50 | 0 |
| 60 | OHX | 23SA | 3607 | 7/7 | 0.89 | 0.10 | 108,129,141,206 | 0 |
| 58 | MG | 23SA | 3113 | 1/1 | 0.90 | 0.07 | 59,59,59,59 | 0 |
| 59 | K | 23SA | 3408 | 1/1 | 0.90 | 0.07 | 76,76,76,76 | 0 |
| 58 | MG | 23SA | 3146 | 1/1 | 0.90 | 0.07 | 69,69,69,69 | 0 |
| 58 | MG | 16SB | 2258 | 1/1 | 0.90 | 0.08 | 95,95,95,95 | 0 |
| 59 | K | 23SA | 3414 | 1/1 | 0.90 | 0.08 | 70,70,70,70 | 0 |
| 58 | MG | 16SB | 2208 | 1/1 | 0.90 | 0.14 | 74,74,74,74 | 0 |
| 59 | K | 23SB | 3240 | 1/1 | 0.90 | 0.09 | 87,87,87,87 | 0 |
| 58 | MG | 23SB | 3008 | 1/1 | 0.90 | 0.10 | 43,43,43,43 | 0 |
| 58 | MG | 23SB | 3010 | 1/1 | 0.90 | 0.34 | 52,52,52,52 | 0 |
| 58 | MG | 23SA | 3014 | 1/1 | 0.90 | 0.38 | 65,65,65,65 | 0 |
| 59 | K | 5SB | 205 | 1/1 | 0.90 | 0.06 | 102,102,102,102 | 0 |
| 59 | K | 23SA | 3340 | 1/1 | 0.90 | 0.09 | 84,84,84,84 | 0 |
| 60 | OHX | 16SB | 2376 | 7/7 | 0.90 | 0.12 | 99,115,127,194 | 0 |
| 58 | MG | 16SA | 2251 | 1/1 | 0.90 | 0.34 | 59,59,59,59 | 0 |
| 58 | MG | 23SB | 3161 | 1/1 | 0.90 | 0.12 | 51,51,51,51 | 0 |
| 58 | MG | 23SA | 3069 | 1/1 | 0.90 | 0.12 | 65,65,65,65 | 0 |
| 60 | OHX | 16SA | 2356 | 7/7 | 0.90 | 0.11 | 115,120,125,207 | 0 |
| 59 | K | 16SA | 2305 | 1/1 | 0.90 | 0.22 | 78,78,78,78 | 0 |
| 60 | OHX | 16SB | 2384 | 7/7 | 0.90 | 0.09 | 159,166,170,246 | 0 |
| 58 | MG | 23SB | 3165 | 1/1 | 0.90 | 0.09 | 57,57,57,57 | 0 |

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| Mol | Type | Chain | Res | Atoms | RSCC | RSR | B-factors(Å$^2$) | Q<0.9 |
|---|---|---|---|---|---|---|---|---|
| 58 | MG | 23SB | 3166 | 1/1 | 0.90 | 0.15 | 41,41,41,41 | 0 |
| 60 | OHX | 16SA | 2392 | 7/7 | 0.90 | 0.10 | 110,128,151,224 | 0 |
| 58 | MG | 23SA | 3005 | 1/1 | 0.90 | 0.20 | 57,57,57,57 | 0 |
| 58 | MG | 23SB | 3106 | 1/1 | 0.90 | 0.14 | 87,87,87,87 | 0 |
| 60 | OHX | 16SA | 2401 | 7/7 | 0.90 | 0.09 | 128,136,164,243 | 0 |
| 60 | OHX | 16SA | 2402 | 7/7 | 0.90 | 0.10 | 138,140,154,213 | 0 |
| 59 | K | 23SB | 3270 | 1/1 | 0.90 | 0.13 | 68,68,68,68 | 0 |
| 60 | OHX | ASIB | 103 | 7/7 | 0.90 | 0.09 | 123,125,144,231 | 0 |
| 60 | OHX | PSIB | 105 | 7/7 | 0.90 | 0.09 | 144,155,165,240 | 0 |
| 60 | OHX | PSIB | 106 | 7/7 | 0.90 | 0.09 | 133,142,147,228 | 0 |
| 60 | OHX | 16SA | 2405 | 7/7 | 0.90 | 0.09 | 153,161,170,238 | 0 |
| 58 | MG | 16SB | 2213 | 1/1 | 0.90 | 0.21 | 72,72,72,72 | 0 |
| 59 | K | L16A | 201 | 1/1 | 0.90 | 0.14 | 89,89,89,89 | 0 |
| 60 | OHX | 16SA | 2408 | 7/7 | 0.90 | 0.08 | 162,169,175,253 | 0 |
| 59 | K | 16SA | 2318 | 1/1 | 0.90 | 0.13 | 97,97,97,97 | 0 |
| 60 | OHX | 16SA | 2410 | 7/7 | 0.90 | 0.09 | 109,114,126,227 | 0 |
| 60 | OHX | 23SB | 3426 | 7/7 | 0.90 | 0.08 | 106,114,129,238 | 0 |
| 60 | OHX | 23SB | 3432 | 7/7 | 0.90 | 0.08 | 100,106,118,232 | 0 |
| 60 | OHX | 16SA | 2414 | 7/7 | 0.90 | 0.09 | 101,104,112,212 | 0 |
| 58 | MG | 23SA | 3071 | 1/1 | 0.90 | 0.26 | 74,74,74,74 | 0 |
| 60 | OHX | 23SA | 3478 | 7/7 | 0.90 | 0.11 | 68,79,105,167 | 0 |
| 58 | MG | 23SB | 3193 | 1/1 | 0.90 | 0.10 | 70,70,70,70 | 0 |
| 58 | MG | 16SB | 2215 | 1/1 | 0.90 | 0.17 | 42,42,42,42 | 0 |
| 60 | OHX | 23SA | 3527 | 7/7 | 0.90 | 0.08 | 76,87,107,193 | 0 |
| 58 | MG | 16SB | 2239 | 1/1 | 0.90 | 0.12 | 97,97,97,97 | 0 |
| 58 | MG | 23SA | 3154 | 1/1 | 0.90 | 0.24 | 76,76,76,76 | 0 |
| 58 | MG | 23SA | 3019 | 1/1 | 0.90 | 0.12 | 38,38,38,38 | 0 |
| 60 | OHX | 23SB | 3469 | 7/7 | 0.90 | 0.12 | 114,120,138,183 | 0 |
| 59 | K | 16SA | 2326 | 1/1 | 0.90 | 0.06 | 80,80,80,80 | 0 |
| 58 | MG | 23SA | 3156 | 1/1 | 0.90 | 0.22 | 59,59,59,59 | 0 |
| 60 | OHX | 23SB | 3484 | 7/7 | 0.90 | 0.10 | 122,131,158,229 | 0 |
| 58 | MG | 23SB | 3036 | 1/1 | 0.90 | 0.27 | 53,53,53,53 | 0 |
| 58 | MG | 16SA | 2280 | 1/1 | 0.90 | 0.10 | 87,87,87,87 | 0 |
| 60 | OHX | 23SB | 3496 | 7/7 | 0.90 | 0.09 | 104,118,141,241 | 0 |
| 58 | MG | 16SA | 2273 | 1/1 | 0.90 | 0.09 | 69,69,69,69 | 0 |
| 59 | K | 23SA | 3385 | 1/1 | 0.90 | 0.23 | 74,74,74,74 | 0 |
| 59 | K | 23SB | 3296 | 1/1 | 0.90 | 0.14 | 103,103,103,103 | 0 |
| 58 | MG | 23SA | 3187 | 1/1 | 0.90 | 0.11 | 39,39,39,39 | 0 |
| 58 | MG | 23SA | 3061 | 1/1 | 0.90 | 0.23 | 67,67,67,67 | 0 |
| 60 | OHX | 23SB | 3504 | 7/7 | 0.90 | 0.08 | 137,145,154,245 | 0 |
| 60 | OHX | 23SB | 3505 | 7/7 | 0.90 | 0.09 | 136,158,167,230 | 0 |
| 58 | MG | 23SA | 3191 | 1/1 | 0.90 | 0.11 | 42,42,42,42 | 0 |

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| Mol | Type | Chain | Res | Atoms | RSCC | RSR | B-factors(Å$^2$) | Q<0.9 |
|---|---|---|---|---|---|---|---|---|
| 58 | MG | 23SA | 3041 | 1/1 | 0.90 | 0.16 | 60,60,60,60 | 0 |
| 60 | OHX | 23SA | 3605 | 7/7 | 0.90 | 0.12 | 111,117,144,211 | 0 |
| 59 | K | 23SA | 3398 | 1/1 | 0.90 | 0.08 | 65,65,65,65 | 0 |
| 58 | MG | 23SB | 3049 | 1/1 | 0.90 | 0.34 | 56,56,56,56 | 0 |
| 58 | MG | 23SA | 3043 | 1/1 | 0.90 | 0.27 | 73,73,73,73 | 0 |
| 60 | OHX | 23SB | 3513 | 7/7 | 0.90 | 0.08 | 98,102,105,234 | 0 |
| 59 | K | 23SB | 3309 | 1/1 | 0.90 | 0.08 | 71,71,71,71 | 0 |
| 60 | OHX | 23SA | 3616 | 7/7 | 0.90 | 0.10 | 180,184,189,253 | 0 |
| 59 | K | 16SB | 2317 | 1/1 | 0.90 | 0.15 | 82,82,82,82 | 0 |
| 58 | MG | 23SA | 3216 | 1/1 | 0.90 | 0.09 | 63,63,63,63 | 0 |
| 58 | MG | 23SA | 3248 | 1/1 | 0.91 | 0.15 | 51,51,51,51 | 0 |
| 58 | MG | 23SA | 3152 | 1/1 | 0.91 | 0.10 | 65,65,65,65 | 0 |
| 60 | OHX | 5SA | 218 | 7/7 | 0.91 | 0.08 | 138,150,160,226 | 0 |
| 59 | K | 23SA | 3423 | 1/1 | 0.91 | 0.12 | 72,72,72,72 | 0 |
| 59 | K | 23SB | 3244 | 1/1 | 0.91 | 0.12 | 95,95,95,95 | 0 |
| 59 | K | 23SA | 3426 | 1/1 | 0.91 | 0.12 | 102,102,102,102 | 0 |
| 58 | MG | 23SA | 3261 | 1/1 | 0.91 | 0.10 | 37,37,37,37 | 0 |
| 58 | MG | 23SB | 3173 | 1/1 | 0.91 | 0.10 | 34,34,34,34 | 0 |
| 59 | K | 23SB | 3250 | 1/1 | 0.91 | 0.08 | 65,65,65,65 | 0 |
| 58 | MG | 23SB | 3075 | 1/1 | 0.91 | 0.33 | 63,63,63,63 | 0 |
| 60 | OHX | 16SB | 2373 | 7/7 | 0.91 | 0.10 | 122,126,140,219 | 0 |
| 60 | OHX | 16SA | 2361 | 7/7 | 0.91 | 0.10 | 116,140,162,226 | 0 |
| 60 | OHX | 16SA | 2366 | 7/7 | 0.91 | 0.11 | 79,89,113,211 | 0 |
| 60 | OHX | 16SA | 2368 | 7/7 | 0.91 | 0.10 | 76,97,115,198 | 0 |
| 60 | OHX | 16SA | 2369 | 7/7 | 0.91 | 0.11 | 92,97,108,196 | 0 |
| 58 | MG | 23SB | 3183 | 1/1 | 0.91 | 0.08 | 65,65,65,65 | 0 |
| 60 | OHX | 16SA | 2383 | 7/7 | 0.91 | 0.09 | 102,107,121,224 | 0 |
| 60 | OHX | 16SA | 2385 | 7/7 | 0.91 | 0.10 | 122,136,150,215 | 0 |
| 59 | K | 23SB | 3256 | 1/1 | 0.91 | 0.12 | 69,69,69,69 | 0 |
| 58 | MG | 23SB | 3184 | 1/1 | 0.91 | 0.08 | 71,71,71,71 | 0 |
| 59 | K | 16SA | 2315 | 1/1 | 0.91 | 0.10 | 76,76,76,76 | 0 |
| 60 | OHX | 16SB | 2391 | 7/7 | 0.91 | 0.09 | 122,127,148,225 | 0 |
| 60 | OHX | 16SA | 2397 | 7/7 | 0.91 | 0.09 | 154,160,167,245 | 0 |
| 59 | K | 23SB | 3261 | 1/1 | 0.91 | 0.10 | 59,59,59,59 | 0 |
| 58 | MG | 23SB | 3002 | 1/1 | 0.91 | 0.23 | 65,65,65,65 | 0 |
| 59 | K | 5SA | 208 | 1/1 | 0.91 | 0.08 | 81,81,81,81 | 0 |
| 59 | K | 23SB | 3269 | 1/1 | 0.91 | 0.09 | 100,100,100,100 | 0 |
| 58 | MG | 16SA | 2288 | 1/1 | 0.91 | 0.09 | 88,88,88,88 | 0 |
| 58 | MG | 23SB | 3078 | 1/1 | 0.91 | 0.11 | 48,48,48,48 | 0 |
| 58 | MG | 23SB | 3079 | 1/1 | 0.91 | 0.17 | 51,51,51,51 | 0 |
| 58 | MG | 23SA | 3027 | 1/1 | 0.91 | 0.14 | 38,38,38,38 | 0 |
| 58 | MG | L35A | 101 | 1/1 | 0.91 | 0.22 | 68,68,68,68 | 0 |

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| Mol | Type | Chain | Res | Atoms | RSCC | RSR | B-factors(Å$^2$) | Q<0.9 |
|---|---|---|---|---|---|---|---|---|
| 58 | MG | 23SB | 3222 | 1/1 | 0.91 | 0.10 | 77,77,77,77 | 0 |
| 59 | K | 23SB | 3276 | 1/1 | 0.91 | 0.07 | 65,65,65,65 | 0 |
| 59 | K | 23SB | 3277 | 1/1 | 0.91 | 0.10 | 78,78,78,78 | 0 |
| 60 | OHX | 16SA | 2415 | 7/7 | 0.91 | 0.09 | 125,133,149,248 | 0 |
| 58 | MG | 16SB | 2229 | 1/1 | 0.91 | 0.30 | 55,55,55,55 | 0 |
| 60 | OHX | MRNA | 102 | 7/7 | 0.91 | 0.11 | 105,114,119,213 | 0 |
| 59 | K | 23SA | 3361 | 1/1 | 0.91 | 0.18 | 79,79,79,79 | 0 |
| 60 | OHX | 23SA | 3495 | 7/7 | 0.91 | 0.10 | 85,95,107,177 | 0 |
| 60 | OHX | 23SB | 3440 | 7/7 | 0.91 | 0.09 | 109,113,121,229 | 0 |
| 58 | MG | 16SB | 2271 | 1/1 | 0.91 | 0.11 | 97,97,97,97 | 0 |
| 58 | MG | 16SA | 2205 | 1/1 | 0.91 | 0.28 | 54,54,54,54 | 0 |
| 60 | OHX | 23SA | 3513 | 7/7 | 0.91 | 0.08 | 75,97,110,190 | 0 |
| 58 | MG | 23SB | 3230 | 1/1 | 0.91 | 0.12 | 67,67,67,67 | 0 |
| 60 | OHX | 23SA | 3529 | 7/7 | 0.91 | 0.09 | 81,94,113,196 | 0 |
| 60 | OHX | 23SA | 3530 | 7/7 | 0.91 | 0.10 | 87,108,124,202 | 0 |
| 59 | K | 16SB | 2294 | 1/1 | 0.91 | 0.06 | 109,109,109,109 | 0 |
| 60 | OHX | 23SB | 3464 | 7/7 | 0.91 | 0.09 | 97,102,112,211 | 0 |
| 58 | MG | 23SB | 3014 | 1/1 | 0.91 | 0.21 | 49,49,49,49 | 0 |
| 58 | MG | 23SB | 3055 | 1/1 | 0.91 | 0.26 | 56,56,56,56 | 0 |
| 58 | MG | 23SA | 3176 | 1/1 | 0.91 | 0.10 | 61,61,61,61 | 0 |
| 60 | OHX | 23SB | 3472 | 7/7 | 0.91 | 0.09 | 132,136,154,230 | 0 |
| 60 | OHX | 23SB | 3477 | 7/7 | 0.91 | 0.11 | 113,132,148,190 | 0 |
| 58 | MG | 23SB | 3088 | 1/1 | 0.91 | 0.15 | 64,64,64,64 | 0 |
| 58 | MG | 23SB | 3091 | 1/1 | 0.91 | 0.34 | 58,58,58,58 | 0 |
| 58 | MG | 23SB | 3092 | 1/1 | 0.91 | 0.14 | 83,83,83,83 | 0 |
| 59 | K | 23SB | 3299 | 1/1 | 0.91 | 0.10 | 56,56,56,56 | 0 |
| 60 | OHX | 23SA | 3576 | 7/7 | 0.91 | 0.09 | 75,83,109,209 | 0 |
| 58 | MG | L3B | 302 | 1/1 | 0.91 | 0.10 | 45,45,45,45 | 0 |
| 59 | K | 16SB | 2307 | 1/1 | 0.91 | 0.09 | 88,88,88,88 | 0 |
| 58 | MG | 23SA | 3218 | 1/1 | 0.91 | 0.14 | 59,59,59,59 | 0 |
| 59 | K | 23SA | 3401 | 1/1 | 0.91 | 0.07 | 77,77,77,77 | 0 |
| 58 | MG | 23SB | 3130 | 1/1 | 0.91 | 0.25 | 56,56,56,56 | 0 |
| 59 | K | 23SA | 3403 | 1/1 | 0.91 | 0.07 | 61,61,61,61 | 0 |
| 58 | MG | 16SB | 2280 | 1/1 | 0.91 | 0.07 | 104,104,104,104 | 0 |
| 60 | OHX | 23SA | 3606 | 7/7 | 0.91 | 0.08 | 118,126,147,227 | 0 |
| 58 | MG | 16SB | 2281 | 1/1 | 0.91 | 0.10 | 85,85,85,85 | 0 |
| 58 | MG | 16SB | 2251 | 1/1 | 0.91 | 0.07 | 54,54,54,54 | 0 |
| 58 | MG | 16SB | 2218 | 1/1 | 0.91 | 0.21 | 64,64,64,64 | 0 |
| 58 | MG | 23SA | 3035 | 1/1 | 0.91 | 0.19 | 63,63,63,63 | 0 |
| 58 | MG | 23SA | 3092 | 1/1 | 0.91 | 0.18 | 61,61,61,61 | 0 |
| 58 | MG | 16SB | 2221 | 1/1 | 0.91 | 0.23 | 42,42,42,42 | 0 |
| 59 | K | 23SA | 3416 | 1/1 | 0.91 | 0.07 | 79,79,79,79 | 0 |

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| Mol | Type | Chain | Res | Atoms | RSCC | RSR | B-factors(Å$^2$) | Q<0.9 |
|---|---|---|---|---|---|---|---|---|
| 60 | OHX | 5SB | 212 | 7/7 | 0.91 | 0.09 | 89,113,122,208 | 0 |
| 60 | OHX | 5SB | 213 | 7/7 | 0.91 | 0.09 | 110,122,136,226 | 0 |
| 58 | MG | 23SA | 3067 | 1/1 | 0.91 | 0.28 | 71,71,71,71 | 0 |
| 58 | MG | 23SA | 3036 | 1/1 | 0.91 | 0.18 | 64,64,64,64 | 0 |
| 60 | OHX | 23SA | 3632 | 7/7 | 0.91 | 0.08 | 79,85,98,239 | 0 |
| 60 | OHX | 16SB | 2360 | 7/7 | 0.92 | 0.09 | 106,120,137,211 | 0 |
| 58 | MG | 23SA | 3048 | 1/1 | 0.92 | 0.23 | 62,62,62,62 | 0 |
| 59 | K | 23SA | 3382 | 1/1 | 0.92 | 0.11 | 69,69,69,69 | 0 |
| 60 | OHX | 16SB | 2371 | 7/7 | 0.92 | 0.08 | 95,106,111,208 | 0 |
| 58 | MG | 16SA | 2290 | 1/1 | 0.92 | 0.20 | 71,71,71,71 | 0 |
| 60 | OHX | 16SA | 2403 | 7/7 | 0.92 | 0.08 | 145,149,153,234 | 0 |
| 58 | MG | 23SB | 3125 | 1/1 | 0.92 | 0.15 | 52,52,52,52 | 0 |
| 58 | MG | 23SB | 3235 | 1/1 | 0.92 | 0.10 | 109,109,109,109 | 0 |
| 58 | MG | 16SB | 2277 | 1/1 | 0.92 | 0.07 | 98,98,98,98 | 0 |
| 58 | MG | 23SA | 3286 | 1/1 | 0.92 | 0.08 | 42,42,42,42 | 0 |
| 58 | MG | L15A | 202 | 1/1 | 0.92 | 0.08 | 62,62,62,62 | 0 |
| 58 | MG | 16SB | 2250 | 1/1 | 0.92 | 0.10 | 58,58,58,58 | 0 |
| 59 | K | 23SB | 3290 | 1/1 | 0.92 | 0.07 | 81,81,81,81 | 0 |
| 60 | OHX | 16SA | 2411 | 7/7 | 0.92 | 0.08 | 196,200,203,282 | 0 |
| 58 | MG | 23SB | 3025 | 1/1 | 0.92 | 0.16 | 61,61,61,61 | 0 |
| 58 | MG | 23SA | 3082 | 1/1 | 0.92 | 0.16 | 40,40,40,40 | 0 |
| 60 | OHX | 16SB | 2389 | 7/7 | 0.92 | 0.09 | 118,137,157,208 | 0 |
| 60 | OHX | 16SB | 2390 | 7/7 | 0.92 | 0.09 | 147,151,155,217 | 0 |
| 58 | MG | 23SB | 3098 | 1/1 | 0.92 | 0.17 | 67,67,67,67 | 0 |
| 59 | K | 16SB | 2309 | 1/1 | 0.92 | 0.11 | 89,89,89,89 | 0 |
| 60 | OHX | 23SA | 3470 | 7/7 | 0.92 | 0.13 | 46,51,99,161 | 0 |
| 60 | OHX | 16SB | 2394 | 7/7 | 0.92 | 0.08 | 131,145,156,224 | 0 |
| 59 | K | 23SB | 3297 | 1/1 | 0.92 | 0.08 | 79,79,79,79 | 0 |
| 59 | K | 16SB | 2310 | 1/1 | 0.92 | 0.26 | 96,96,96,96 | 0 |
| 60 | OHX | 16SB | 2397 | 7/7 | 0.92 | 0.08 | 132,141,150,237 | 0 |
| 58 | MG | 23SA | 3038 | 1/1 | 0.92 | 0.24 | 58,58,58,58 | 0 |
| 60 | OHX | 16SB | 2399 | 7/7 | 0.92 | 0.08 | 107,114,120,238 | 0 |
| 59 | K | 16SB | 2312 | 1/1 | 0.92 | 0.07 | 82,82,82,82 | 0 |
| 59 | K | 16SA | 2291 | 1/1 | 0.92 | 0.07 | 95,95,95,95 | 0 |
| 58 | MG | 23SA | 3147 | 1/1 | 0.92 | 0.25 | 41,41,41,41 | 0 |
| 58 | MG | 16SA | 2271 | 1/1 | 0.92 | 0.10 | 49,49,49,49 | 0 |
| 58 | MG | 23SB | 3066 | 1/1 | 0.92 | 0.27 | 57,57,57,57 | 0 |
| 59 | K | 23SA | 3410 | 1/1 | 0.92 | 0.07 | 73,73,73,73 | 0 |
| 60 | OHX | 23SB | 3385 | 7/7 | 0.92 | 0.10 | 87,99,111,177 | 0 |
| 58 | MG | L34A | 101 | 1/1 | 0.92 | 0.29 | 63,63,63,63 | 0 |
| 58 | MG | 23SA | 3042 | 1/1 | 0.92 | 0.11 | 40,40,40,40 | 0 |
| 58 | MG | 23SA | 3056 | 1/1 | 0.92 | 0.24 | 57,57,57,57 | 0 |

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| Mol | Type | Chain | Res | Atoms | RSCC | RSR | B-factors(Å$^2$) | Q<0.9 |
|---|---|---|---|---|---|---|---|---|
| 58 | MG | 23SA | 3010 | 1/1 | 0.92 | 0.19 | 41,41,41,41 | 0 |
| 58 | MG | 23SB | 3039 | 1/1 | 0.92 | 0.24 | 44,44,44,44 | 0 |
| 58 | MG | 23SA | 3032 | 1/1 | 0.92 | 0.13 | 61,61,61,61 | 0 |
| 58 | MG | 23SA | 3327 | 1/1 | 0.92 | 0.10 | 75,75,75,75 | 0 |
| 60 | OHX | 23SB | 3438 | 7/7 | 0.92 | 0.10 | 118,134,139,208 | 0 |
| 60 | OHX | 23SA | 3570 | 7/7 | 0.92 | 0.09 | 133,152,161,233 | 0 |
| 58 | MG | 23SB | 3181 | 1/1 | 0.92 | 0.09 | 53,53,53,53 | 0 |
| 60 | OHX | 23SB | 3442 | 7/7 | 0.92 | 0.09 | 89,106,113,212 | 0 |
| 58 | MG | 23SB | 3042 | 1/1 | 0.92 | 0.14 | 53,53,53,53 | 0 |
| 60 | OHX | 23SA | 3590 | 7/7 | 0.92 | 0.08 | 141,152,157,234 | 0 |
| 60 | OHX | 23SA | 3591 | 7/7 | 0.92 | 0.08 | 99,119,144,202 | 0 |
| 60 | OHX | 23SA | 3595 | 7/7 | 0.92 | 0.10 | 91,115,138,225 | 0 |
| 59 | K | 23SA | 3424 | 1/1 | 0.92 | 0.22 | 100,100,100,100 | 0 |
| 59 | K | 23SA | 3425 | 1/1 | 0.92 | 0.06 | 65,65,65,65 | 0 |
| 60 | OHX | 23SB | 3463 | 7/7 | 0.92 | 0.07 | 134,143,146,248 | 0 |
| 58 | MG | 16SB | 2264 | 1/1 | 0.92 | 0.08 | 98,98,98,98 | 0 |
| 60 | OHX | 23SA | 3602 | 7/7 | 0.92 | 0.08 | 113,120,138,213 | 0 |
| 60 | OHX | 23SB | 3466 | 7/7 | 0.92 | 0.09 | 104,123,142,206 | 0 |
| 58 | MG | 23SB | 3186 | 1/1 | 0.92 | 0.06 | 87,87,87,87 | 0 |
| 58 | MG | 16SB | 2241 | 1/1 | 0.92 | 0.23 | 49,49,49,49 | 0 |
| 58 | MG | 23SB | 3191 | 1/1 | 0.92 | 0.09 | 80,80,80,80 | 0 |
| 60 | OHX | 23SB | 3474 | 7/7 | 0.92 | 0.09 | 126,129,149,216 | 0 |
| 58 | MG | 23SA | 3046 | 1/1 | 0.92 | 0.22 | 56,56,56,56 | 0 |
| 60 | OHX | 23SB | 3479 | 7/7 | 0.92 | 0.10 | 118,134,146,193 | 0 |
| 60 | OHX | 23SB | 3481 | 7/7 | 0.92 | 0.07 | 143,153,167,246 | 0 |
| 59 | K | 16SA | 2314 | 1/1 | 0.92 | 0.09 | 65,65,65,65 | 0 |
| 59 | K | 23SA | 3353 | 1/1 | 0.92 | 0.09 | 64,64,64,64 | 0 |
| 60 | OHX | 23SA | 3612 | 7/7 | 0.92 | 0.08 | 91,119,133,210 | 0 |
| 60 | OHX | 23SB | 3488 | 7/7 | 0.92 | 0.09 | 129,138,150,229 | 0 |
| 60 | OHX | 23SB | 3490 | 7/7 | 0.92 | 0.09 | 135,138,156,200 | 0 |
| 58 | MG | 23SB | 3047 | 1/1 | 0.92 | 0.32 | 59,59,59,59 | 0 |
| 60 | OHX | 23SB | 3494 | 7/7 | 0.92 | 0.09 | 135,141,158,212 | 0 |
| 60 | OHX | 16SA | 2358 | 7/7 | 0.92 | 0.09 | 105,106,129,192 | 0 |
| 59 | K | 5SA | 207 | 1/1 | 0.92 | 0.09 | 70,70,70,70 | 0 |
| 60 | OHX | 23SA | 3618 | 7/7 | 0.92 | 0.09 | 127,141,163,218 | 0 |
| 60 | OHX | 23SA | 3619 | 7/7 | 0.92 | 0.09 | 114,133,137,209 | 0 |
| 58 | MG | 23SB | 3197 | 1/1 | 0.92 | 0.08 | 66,66,66,66 | 0 |
| 59 | K | 23SB | 3263 | 1/1 | 0.92 | 0.25 | 93,93,93,93 | 0 |
| 60 | OHX | 23SA | 3627 | 7/7 | 0.92 | 0.09 | 123,131,152,228 | 0 |
| 58 | MG | 23SB | 3048 | 1/1 | 0.92 | 0.10 | 43,43,43,43 | 0 |
| 58 | MG | 23SB | 3208 | 1/1 | 0.92 | 0.18 | 53,53,53,53 | 0 |
| 60 | OHX | 16SA | 2380 | 7/7 | 0.92 | 0.10 | 75,91,104,201 | 0 |

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| Mol | Type | Chain | Res | Atoms | RSCC | RSR | B-factors(Å$^2$) | Q<0.9 |
|---|---|---|---|---|---|---|---|---|
| 58 | MG | 23SB | 3216 | 1/1 | 0.92 | 0.08 | 88,88,88,88 | 0 |
| 58 | MG | 23SB | 3005 | 1/1 | 0.92 | 0.24 | 53,53,53,53 | 0 |
| 58 | MG | 23SA | 3076 | 1/1 | 0.92 | 0.31 | 62,62,62,62 | 0 |
| 60 | OHX | L27A | 103 | 7/7 | 0.92 | 0.10 | 88,92,103,211 | 0 |
| 59 | K | 23SA | 3365 | 1/1 | 0.92 | 0.06 | 67,67,67,67 | 0 |
| 60 | OHX | 16SB | 2338 | 7/7 | 0.92 | 0.12 | 82,95,114,179 | 0 |
| 60 | OHX | 5SB | 209 | 7/7 | 0.92 | 0.09 | 112,121,129,202 | 0 |
| 60 | OHX | 5SB | 210 | 7/7 | 0.92 | 0.07 | 111,121,129,222 | 0 |
| 59 | K | 23SA | 3366 | 1/1 | 0.92 | 0.07 | 48,48,48,48 | 0 |
| 58 | MG | 23SA | 3279 | 1/1 | 0.92 | 0.06 | 99,99,99,99 | 0 |
| 60 | OHX | 16SB | 2353 | 7/7 | 0.92 | 0.09 | 112,131,139,226 | 0 |
| 60 | OHX | 5SB | 215 | 7/7 | 0.92 | 0.09 | 137,146,158,239 | 0 |
| 60 | OHX | 16SB | 2355 | 7/7 | 0.92 | 0.09 | 110,116,123,197 | 0 |
| 58 | MG | 23SA | 3047 | 1/1 | 0.92 | 0.15 | 59,59,59,59 | 0 |
| 58 | MG | 23SA | 3268 | 1/1 | 0.93 | 0.12 | 31,31,31,31 | 0 |
| 59 | K | 23SA | 3383 | 1/1 | 0.93 | 0.11 | 75,75,75,75 | 0 |
| 60 | OHX | 23SA | 3543 | 7/7 | 0.93 | 0.08 | 76,92,101,198 | 0 |
| 60 | OHX | 16SB | 2386 | 7/7 | 0.93 | 0.10 | 116,126,138,198 | 0 |
| 60 | OHX | 16SB | 2387 | 7/7 | 0.93 | 0.08 | 139,144,150,218 | 0 |
| 58 | MG | 23SB | 3178 | 1/1 | 0.93 | 0.09 | 57,57,57,57 | 0 |
| 58 | MG | 23SB | 3030 | 1/1 | 0.93 | 0.29 | 54,54,54,54 | 0 |
| 59 | K | 23SA | 3386 | 1/1 | 0.93 | 0.06 | 64,64,64,64 | 0 |
| 60 | OHX | 23SA | 3554 | 7/7 | 0.93 | 0.07 | 98,107,109,231 | 0 |
| 58 | MG | 23SA | 3203 | 1/1 | 0.93 | 0.10 | 45,45,45,45 | 0 |
| 60 | OHX | 23SA | 3558 | 7/7 | 0.93 | 0.08 | 94,112,120,185 | 0 |
| 59 | K | 23SB | 3262 | 1/1 | 0.93 | 0.08 | 61,61,61,61 | 0 |
| 58 | MG | 23SA | 3039 | 1/1 | 0.93 | 0.17 | 29,29,29,29 | 0 |
| 60 | OHX | 23SA | 3561 | 7/7 | 0.93 | 0.10 | 79,83,104,176 | 0 |
| 60 | OHX | 23SA | 3562 | 7/7 | 0.93 | 0.07 | 94,100,111,223 | 0 |
| 58 | MG | 23SB | 3060 | 1/1 | 0.93 | 0.29 | 44,44,44,44 | 0 |
| 60 | OHX | 23SA | 3567 | 7/7 | 0.93 | 0.07 | 97,99,113,230 | 0 |
| 59 | K | 23SB | 3266 | 1/1 | 0.93 | 0.16 | 82,82,82,82 | 0 |
| 60 | OHX | 23SA | 3575 | 7/7 | 0.93 | 0.09 | 76,80,105,188 | 0 |
| 58 | MG | 16SA | 2206 | 1/1 | 0.93 | 0.31 | 31,31,31,31 | 0 |
| 59 | K | 23SA | 3397 | 1/1 | 0.93 | 0.07 | 52,52,52,52 | 0 |
| 60 | OHX | 16SA | 2348 | 7/7 | 0.93 | 0.11 | 77,89,99,143 | 0 |
| 58 | MG | 23SB | 3190 | 1/1 | 0.93 | 0.12 | 51,51,51,51 | 0 |
| 60 | OHX | 23SA | 3592 | 7/7 | 0.93 | 0.09 | 142,146,163,235 | 0 |
| 60 | OHX | 23SA | 3593 | 7/7 | 0.93 | 0.08 | 117,129,149,224 | 0 |
| 60 | OHX | 23SB | 3407 | 7/7 | 0.93 | 0.08 | 92,104,113,194 | 0 |
| 58 | MG | 23SA | 3145 | 1/1 | 0.93 | 0.20 | 53,53,53,53 | 0 |
| 60 | OHX | 23SB | 3415 | 7/7 | 0.93 | 0.09 | 89,94,111,191 | 0 |

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| Mol | Type | Chain | Res | Atoms | RSCC | RSR | B-factors(Å$^2$) | Q<0.9 |
|---|---|---|---|---|---|---|---|---|
| 58 | MG | 23SA | 3119 | 1/1 | 0.93 | 0.15 | 59,59,59,59 | 0 |
| 58 | MG | 23SA | 3220 | 1/1 | 0.93 | 0.11 | 32,32,32,32 | 0 |
| 58 | MG | 23SB | 3195 | 1/1 | 0.93 | 0.10 | 46,46,46,46 | 0 |
| 58 | MG | 23SA | 3026 | 1/1 | 0.93 | 0.21 | 57,57,57,57 | 0 |
| 60 | OHX | 16SA | 2371 | 7/7 | 0.93 | 0.10 | 89,93,120,170 | 0 |
| 60 | OHX | 23SB | 3436 | 7/7 | 0.93 | 0.08 | 92,97,106,198 | 0 |
| 60 | OHX | 16SA | 2375 | 7/7 | 0.93 | 0.10 | 98,106,121,189 | 0 |
| 60 | OHX | 23SB | 3439 | 7/7 | 0.93 | 0.08 | 79,91,98,201 | 0 |
| 58 | MG | 23SB | 3096 | 1/1 | 0.93 | 0.52 | 80,80,80,80 | 0 |
| 60 | OHX | 16SA | 2379 | 7/7 | 0.93 | 0.08 | 107,116,125,210 | 0 |
| 58 | MG | 23SB | 3202 | 1/1 | 0.93 | 0.09 | 45,45,45,45 | 0 |
| 60 | OHX | 23SB | 3444 | 7/7 | 0.93 | 0.08 | 89,96,108,221 | 0 |
| 58 | MG | 16SA | 2224 | 1/1 | 0.93 | 0.19 | 36,36,36,36 | 0 |
| 60 | OHX | 23SA | 3609 | 7/7 | 0.93 | 0.07 | 128,133,141,224 | 0 |
| 60 | OHX | 23SA | 3611 | 7/7 | 0.93 | 0.09 | 97,100,101,213 | 0 |
| 58 | MG | 16SA | 2274 | 1/1 | 0.93 | 0.10 | 57,57,57,57 | 0 |
| 60 | OHX | 16SA | 2388 | 7/7 | 0.93 | 0.09 | 88,100,107,202 | 0 |
| 58 | MG | 23SA | 3125 | 1/1 | 0.93 | 0.10 | 59,59,59,59 | 0 |
| 60 | OHX | 23SA | 3615 | 7/7 | 0.93 | 0.08 | 94,104,121,185 | 0 |
| 58 | MG | 23SB | 3043 | 1/1 | 0.93 | 0.23 | 34,34,34,34 | 0 |
| 58 | MG | 23SB | 3071 | 1/1 | 0.93 | 0.27 | 53,53,53,53 | 0 |
| 60 | OHX | 16SA | 2395 | 7/7 | 0.93 | 0.08 | 130,134,147,229 | 0 |
| 60 | OHX | 23SA | 3620 | 7/7 | 0.93 | 0.08 | 122,127,151,215 | 0 |
| 59 | K | 23SB | 3287 | 1/1 | 0.93 | 0.10 | 80,80,80,80 | 0 |
| 60 | OHX | 23SA | 3624 | 7/7 | 0.93 | 0.08 | 94,112,133,228 | 0 |
| 58 | MG | 23SA | 3294 | 1/1 | 0.93 | 0.08 | 44,44,44,44 | 0 |
| 60 | OHX | 23SB | 3476 | 7/7 | 0.93 | 0.08 | 123,129,146,201 | 0 |
| 59 | K | 16SB | 2314 | 1/1 | 0.93 | 0.10 | 102,102,102,102 | 0 |
| 60 | OHX | 23SB | 3478 | 7/7 | 0.93 | 0.10 | 99,109,121,194 | 0 |
| 58 | MG | 23SB | 3138 | 1/1 | 0.93 | 0.10 | 41,41,41,41 | 0 |
| 60 | OHX | 23SA | 3630 | 7/7 | 0.93 | 0.08 | 102,118,137,188 | 0 |
| 58 | MG | 23SB | 3227 | 1/1 | 0.93 | 0.17 | 63,63,63,63 | 0 |
| 58 | MG | L30A | 101 | 1/1 | 0.93 | 0.09 | 54,54,54,54 | 0 |
| 59 | K | 23SA | 3354 | 1/1 | 0.93 | 0.13 | 92,92,92,92 | 0 |
| 60 | OHX | 23SB | 3487 | 7/7 | 0.93 | 0.08 | 124,135,141,225 | 0 |
| 58 | MG | 23SA | 3001 | 1/1 | 0.93 | 0.21 | 41,41,41,41 | 0 |
| 60 | OHX | 5SA | 217 | 7/7 | 0.93 | 0.09 | 114,124,140,203 | 0 |
| 58 | MG | 23SB | 3017 | 1/1 | 0.93 | 0.10 | 38,38,38,38 | 0 |
| 58 | MG | 23SB | 3018 | 1/1 | 0.93 | 0.07 | 47,47,47,47 | 0 |
| 58 | MG | 23SA | 3249 | 1/1 | 0.93 | 0.08 | 35,35,35,35 | 0 |
| 58 | MG | 23SA | 3307 | 1/1 | 0.93 | 0.06 | 37,37,37,37 | 0 |
| 60 | OHX | 16SB | 2343 | 7/7 | 0.93 | 0.10 | 98,100,125,168 | 0 |

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| Mol | Type | Chain | Res | Atoms | RSCC | RSR | B-factors(Å$^2$) | Q<0.9 |
|---|---|---|---|---|---|---|---|---|
| 60 | OHX | 16SB | 2345 | 7/7 | 0.93 | 0.09 | 92,101,115,193 | 0 |
| 60 | OHX | 23SB | 3500 | 7/7 | 0.93 | 0.08 | 188,188,201,242 | 0 |
| 58 | MG | 23SA | 3079 | 1/1 | 0.93 | 0.33 | 66,66,66,66 | 0 |
| 60 | OHX | 23SB | 3502 | 7/7 | 0.93 | 0.08 | 111,132,143,216 | 0 |
| 58 | MG | 23SB | 3024 | 1/1 | 0.93 | 0.15 | 76,76,76,76 | 0 |
| 58 | MG | 23SA | 3058 | 1/1 | 0.93 | 0.16 | 49,49,49,49 | 0 |
| 58 | MG | L3B | 301 | 1/1 | 0.93 | 0.23 | 47,47,47,47 | 0 |
| 59 | K | 23SB | 3305 | 1/1 | 0.93 | 0.11 | 69,69,69,69 | 0 |
| 60 | OHX | 23SB | 3507 | 7/7 | 0.93 | 0.09 | 110,119,128,207 | 0 |
| 58 | MG | 23SB | 3172 | 1/1 | 0.93 | 0.08 | 46,46,46,46 | 0 |
| 60 | OHX | 16SB | 2363 | 7/7 | 0.93 | 0.09 | 139,140,164,204 | 0 |
| 59 | K | 23SB | 3307 | 1/1 | 0.93 | 0.11 | 88,88,88,88 | 0 |
| 59 | K | 23SB | 3308 | 1/1 | 0.93 | 0.07 | 85,85,85,85 | 0 |
| 60 | OHX | 16SB | 2369 | 7/7 | 0.93 | 0.09 | 88,99,116,191 | 0 |
| 58 | MG | 16SA | 2289 | 1/1 | 0.93 | 0.10 | 102,102,102,102 | 0 |
| 59 | K | 23SA | 3375 | 1/1 | 0.93 | 0.07 | 52,52,52,52 | 0 |
| 59 | K | 23SA | 3378 | 1/1 | 0.93 | 0.08 | 70,70,70,70 | 0 |
| 59 | K | 23SA | 3380 | 1/1 | 0.93 | 0.08 | 78,78,78,78 | 0 |
| 60 | OHX | 23SA | 3514 | 7/7 | 0.93 | 0.09 | 79,100,109,186 | 0 |
| 60 | OHX | 16SB | 2377 | 7/7 | 0.93 | 0.08 | 138,140,149,221 | 0 |
| 60 | OHX | 23SA | 3515 | 7/7 | 0.93 | 0.15 | 73,81,96,166 | 0 |
| 60 | OHX | 23SA | 3521 | 7/7 | 0.93 | 0.20 | 82,84,100,161 | 0 |
| 60 | OHX | L35B | 103 | 7/7 | 0.93 | 0.10 | 121,122,130,188 | 0 |
| 59 | K | 23SB | 3248 | 1/1 | 0.93 | 0.24 | 100,100,100,100 | 0 |
| 58 | MG | L35B | 102 | 1/1 | 0.93 | 0.20 | 89,89,89,89 | 0 |
| 58 | MG | 23SB | 3157 | 1/1 | 0.94 | 0.08 | 42,42,42,42 | 0 |
| 58 | MG | 16SB | 2256 | 1/1 | 0.94 | 0.09 | 72,72,72,72 | 0 |
| 58 | MG | 23SB | 3007 | 1/1 | 0.94 | 0.27 | 34,34,34,34 | 0 |
| 58 | MG | 23SA | 3190 | 1/1 | 0.94 | 0.12 | 89,89,89,89 | 0 |
| 58 | MG | 23SB | 3162 | 1/1 | 0.94 | 0.07 | 53,53,53,53 | 0 |
| 58 | MG | 23SB | 3009 | 1/1 | 0.94 | 0.20 | 40,40,40,40 | 0 |
| 60 | OHX | 23SA | 3563 | 7/7 | 0.94 | 0.06 | 93,103,112,234 | 0 |
| 59 | K | 23SB | 3249 | 1/1 | 0.94 | 0.07 | 66,66,66,66 | 0 |
| 59 | K | 23SA | 3347 | 1/1 | 0.94 | 0.07 | 72,72,72,72 | 0 |
| 60 | OHX | 23SA | 3569 | 7/7 | 0.94 | 0.07 | 99,109,119,234 | 0 |
| 59 | K | 23SB | 3251 | 1/1 | 0.94 | 0.06 | 56,56,56,56 | 0 |
| 58 | MG | L27A | 101 | 1/1 | 0.94 | 0.18 | 40,40,40,40 | 0 |
| 60 | OHX | 16SA | 2355 | 7/7 | 0.94 | 0.08 | 90,108,124,164 | 0 |
| 60 | OHX | 23SA | 3578 | 7/7 | 0.94 | 0.07 | 138,140,158,239 | 0 |
| 60 | OHX | S4B | 302 | 7/7 | 0.94 | 0.08 | 112,116,130,195 | 0 |
| 58 | MG | 23SA | 3018 | 1/1 | 0.94 | 0.20 | 34,34,34,34 | 0 |
| 58 | MG | 23SA | 3122 | 1/1 | 0.94 | 0.24 | 49,49,49,49 | 0 |

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| Mol | Type | Chain | Res | Atoms | RSCC | RSR | B-factors(Å$^2$) | Q<0.9 |
|---|---|---|---|---|---|---|---|---|
| 58 | MG | 23SB | 3170 | 1/1 | 0.94 | 0.09 | 57,57,57,57 | 0 |
| 58 | MG | 23SA | 3086 | 1/1 | 0.94 | 0.19 | 62,62,62,62 | 0 |
| 60 | OHX | ESIB | 101 | 7/7 | 0.94 | 0.08 | 152,164,172,232 | 0 |
| 58 | MG | 23SA | 3211 | 1/1 | 0.94 | 0.07 | 61,61,61,61 | 0 |
| 59 | K | 23SA | 3433 | 1/1 | 0.94 | 0.09 | 57,57,57,57 | 0 |
| 60 | OHX | 23SB | 3359 | 7/7 | 0.94 | 0.09 | 110,120,133,166 | 0 |
| 60 | OHX | 23SB | 3366 | 7/7 | 0.94 | 0.10 | 68,87,109,158 | 0 |
| 60 | OHX | 23SB | 3372 | 7/7 | 0.94 | 0.08 | 91,97,114,160 | 0 |
| 58 | MG | 23SA | 3059 | 1/1 | 0.94 | 0.08 | 61,61,61,61 | 0 |
| 58 | MG | 23SA | 3105 | 1/1 | 0.94 | 0.10 | 73,73,73,73 | 0 |
| 60 | OHX | 23SB | 3389 | 7/7 | 0.94 | 0.08 | 61,98,105,173 | 0 |
| 60 | OHX | 23SA | 3599 | 7/7 | 0.94 | 0.08 | 140,146,155,214 | 0 |
| 60 | OHX | 23SB | 3410 | 7/7 | 0.94 | 0.09 | 113,115,120,199 | 0 |
| 59 | K | 23SB | 3265 | 1/1 | 0.94 | 0.07 | 51,51,51,51 | 0 |
| 60 | OHX | 23SA | 3601 | 7/7 | 0.94 | 0.07 | 119,135,151,211 | 0 |
| 58 | MG | 16SB | 2267 | 1/1 | 0.94 | 0.07 | 72,72,72,72 | 0 |
| 58 | MG | 23SA | 3106 | 1/1 | 0.94 | 0.22 | 63,63,63,63 | 0 |
| 60 | OHX | 23SB | 3424 | 7/7 | 0.94 | 0.07 | 102,113,118,190 | 0 |
| 60 | OHX | 16SA | 2381 | 7/7 | 0.94 | 0.08 | 134,138,146,225 | 0 |
| 60 | OHX | 23SB | 3428 | 7/7 | 0.94 | 0.11 | 92,112,132,177 | 0 |
| 58 | MG | 23SA | 3028 | 1/1 | 0.94 | 0.25 | 41,41,41,41 | 0 |
| 60 | OHX | 16SA | 2384 | 7/7 | 0.94 | 0.07 | 104,120,127,210 | 0 |
| 60 | OHX | 23SB | 3434 | 7/7 | 0.94 | 0.08 | 98,99,117,181 | 0 |
| 60 | OHX | 23SB | 3435 | 7/7 | 0.94 | 0.07 | 111,113,124,228 | 0 |
| 59 | K | 16SA | 2308 | 1/1 | 0.94 | 0.06 | 78,78,78,78 | 0 |
| 60 | OHX | 16SA | 2387 | 7/7 | 0.94 | 0.09 | 100,103,114,193 | 0 |
| 58 | MG | 16SA | 2284 | 1/1 | 0.94 | 0.07 | 95,95,95,95 | 0 |
| 60 | OHX | 23SA | 3610 | 7/7 | 0.94 | 0.07 | 132,141,164,238 | 0 |
| 58 | MG | 23SA | 3296 | 1/1 | 0.94 | 0.10 | 48,48,48,48 | 0 |
| 59 | K | 23SA | 3362 | 1/1 | 0.94 | 0.05 | 39,39,39,39 | 0 |
| 58 | MG | 23SA | 3030 | 1/1 | 0.94 | 0.22 | 54,54,54,54 | 0 |
| 60 | OHX | 16SA | 2394 | 7/7 | 0.94 | 0.07 | 114,116,133,196 | 0 |
| 60 | OHX | 23SB | 3450 | 7/7 | 0.94 | 0.07 | 105,107,114,220 | 0 |
| 58 | MG | 23SB | 3029 | 1/1 | 0.94 | 0.27 | 44,44,44,44 | 0 |
| 58 | MG | 23SA | 3303 | 1/1 | 0.94 | 0.09 | 54,54,54,54 | 0 |
| 58 | MG | 16SA | 2203 | 1/1 | 0.94 | 0.31 | 62,62,62,62 | 0 |
| 60 | OHX | 23SB | 3460 | 7/7 | 0.94 | 0.07 | 88,91,110,224 | 0 |
| 59 | K | 23SA | 3374 | 1/1 | 0.94 | 0.08 | 69,69,69,69 | 0 |
| 58 | MG | 23SA | 3078 | 1/1 | 0.94 | 0.19 | 54,54,54,54 | 0 |
| 58 | MG | 23SA | 3240 | 1/1 | 0.94 | 0.12 | 28,28,28,28 | 0 |
| 60 | OHX | 23SA | 3623 | 7/7 | 0.94 | 0.08 | 106,117,141,204 | 0 |
| 59 | K | 16SB | 2296 | 1/1 | 0.94 | 0.08 | 87,87,87,87 | 0 |

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| Mol | Type | Chain | Res | Atoms | RSCC | RSR | B-factors(Å$^2$) | Q<0.9 |
|---|---|---|---|---|---|---|---|---|
| 59 | K | 23SA | 3379 | 1/1 | 0.94 | 0.11 | 60,60,60,60 | 0 |
| 58 | MG | 23SB | 3198 | 1/1 | 0.94 | 0.08 | 54,54,54,54 | 0 |
| 58 | MG | 23SB | 3074 | 1/1 | 0.94 | 0.36 | 58,58,58,58 | 0 |
| 60 | OHX | 23SB | 3471 | 7/7 | 0.94 | 0.07 | 134,141,156,215 | 0 |
| 59 | K | 16SB | 2300 | 1/1 | 0.94 | 0.06 | 72,72,72,72 | 0 |
| 60 | OHX | 23SB | 3473 | 7/7 | 0.94 | 0.08 | 106,109,130,178 | 0 |
| 58 | MG | 23SA | 3314 | 1/1 | 0.94 | 0.17 | 57,57,57,57 | 0 |
| 58 | MG | 23SA | 3321 | 1/1 | 0.94 | 0.08 | 43,43,43,43 | 0 |
| 58 | MG | 23SB | 3037 | 1/1 | 0.94 | 0.34 | 56,56,56,56 | 0 |
| 58 | MG | 23SB | 3217 | 1/1 | 0.94 | 0.05 | 88,88,88,88 | 0 |
| 60 | OHX | 5SA | 216 | 7/7 | 0.94 | 0.08 | 84,97,113,216 | 0 |
| 60 | OHX | 16SA | 2412 | 7/7 | 0.94 | 0.09 | 99,106,111,207 | 0 |
| 60 | OHX | 23SB | 3482 | 7/7 | 0.94 | 0.07 | 129,137,145,231 | 0 |
| 58 | MG | 23SA | 3064 | 1/1 | 0.94 | 0.22 | 57,57,57,57 | 0 |
| 58 | MG | 23SA | 3173 | 1/1 | 0.94 | 0.25 | 46,46,46,46 | 0 |
| 59 | K | 16SA | 2329 | 1/1 | 0.94 | 0.09 | 94,94,94,94 | 0 |
| 60 | OHX | 16SB | 2328 | 7/7 | 0.94 | 0.10 | 83,93,105,146 | 0 |
| 58 | MG | 23SA | 3134 | 1/1 | 0.94 | 0.09 | 60,60,60,60 | 0 |
| 60 | OHX | TRNA | 102 | 7/7 | 0.94 | 0.07 | 118,122,143,229 | 0 |
| 58 | MG | 23SA | 3051 | 1/1 | 0.94 | 0.18 | 69,69,69,69 | 0 |
| 58 | MG | 23SA | 3040 | 1/1 | 0.94 | 0.12 | 53,53,53,53 | 0 |
| 60 | OHX | 23SA | 3479 | 7/7 | 0.94 | 0.09 | 92,105,110,166 | 0 |
| 60 | OHX | 16SB | 2350 | 7/7 | 0.94 | 0.07 | 101,111,113,186 | 0 |
| 58 | MG | 23SB | 3225 | 1/1 | 0.94 | 0.11 | 85,85,85,85 | 0 |
| 60 | OHX | 16SB | 2354 | 7/7 | 0.94 | 0.08 | 87,94,105,178 | 0 |
| 58 | MG | 16SA | 2259 | 1/1 | 0.94 | 0.08 | 77,77,77,77 | 0 |
| 60 | OHX | 16SB | 2356 | 7/7 | 0.94 | 0.09 | 96,103,117,193 | 0 |
| 58 | MG | 23SA | 3264 | 1/1 | 0.94 | 0.12 | 45,45,45,45 | 0 |
| 58 | MG | 16SA | 2216 | 1/1 | 0.94 | 0.12 | 36,36,36,36 | 0 |
| 58 | MG | PSIA | 102 | 1/1 | 0.94 | 0.09 | 84,84,84,84 | 0 |
| 60 | OHX | 16SB | 2364 | 7/7 | 0.94 | 0.09 | 109,111,126,185 | 0 |
| 58 | MG | 23SA | 3158 | 1/1 | 0.94 | 0.19 | 39,39,39,39 | 0 |
| 60 | OHX | 23SA | 3519 | 7/7 | 0.94 | 0.07 | 93,100,111,208 | 0 |
| 58 | MG | 23SA | 3274 | 1/1 | 0.94 | 0.08 | 47,47,47,47 | 0 |
| 60 | OHX | 16SB | 2370 | 7/7 | 0.94 | 0.07 | 123,128,137,241 | 0 |
| 60 | OHX | 23SA | 3523 | 7/7 | 0.94 | 0.20 | 71,90,93,140 | 0 |
| 60 | OHX | 23SA | 3524 | 7/7 | 0.94 | 0.18 | 82,85,101,153 | 0 |
| 60 | OHX | 23SA | 3525 | 7/7 | 0.94 | 0.08 | 107,110,130,195 | 0 |
| 60 | OHX | 16SB | 2374 | 7/7 | 0.94 | 0.09 | 105,117,136,182 | 0 |
| 60 | OHX | 23SB | 3514 | 7/7 | 0.94 | 0.06 | 102,108,117,230 | 0 |
| 59 | K | 16SB | 2320 | 1/1 | 0.94 | 0.10 | 97,97,97,97 | 0 |
| 60 | OHX | 5SB | 206 | 7/7 | 0.94 | 0.09 | 90,101,122,161 | 0 |

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| Mol | Type | Chain | Res | Atoms | RSCC | RSR | B-factors(Å$^2$) | Q<0.9 |
|---|---|---|---|---|---|---|---|---|
| 58 | MG | 23SB | 3238 | 1/1 | 0.94 | 0.07 | 40,40,40,40 | 0 |
| 58 | MG | 23SB | 3134 | 1/1 | 0.94 | 0.13 | 53,53,53,53 | 0 |
| 58 | MG | 23SB | 3137 | 1/1 | 0.94 | 0.06 | 60,60,60,60 | 0 |
| 60 | OHX | 23SA | 3541 | 7/7 | 0.94 | 0.16 | 69,83,95,155 | 0 |
| 59 | K | 23SA | 3411 | 1/1 | 0.94 | 0.09 | 81,81,81,81 | 0 |
| 58 | MG | 23SB | 3089 | 1/1 | 0.94 | 0.16 | 72,72,72,72 | 0 |
| 60 | OHX | L20B | 201 | 7/7 | 0.94 | 0.08 | 88,98,107,189 | 0 |
| 58 | MG | 23SA | 3275 | 1/1 | 0.94 | 0.10 | 71,71,71,71 | 0 |
| 58 | MG | 23SB | 3050 | 1/1 | 0.94 | 0.16 | 55,55,55,55 | 0 |
| 58 | MG | 23SB | 3156 | 1/1 | 0.94 | 0.07 | 48,48,48,48 | 0 |
| 58 | MG | 16SA | 2283 | 1/1 | 0.95 | 0.12 | 85,85,85,85 | 0 |
| 58 | MG | L3A | 301 | 1/1 | 0.95 | 0.13 | 54,54,54,54 | 0 |
| 60 | OHX | 23SA | 3572 | 7/7 | 0.95 | 0.07 | 89,101,111,205 | 0 |
| 60 | OHX | 23SA | 3573 | 7/7 | 0.95 | 0.07 | 77,83,98,186 | 0 |
| 58 | MG | 23SA | 3068 | 1/1 | 0.95 | 0.38 | 60,60,60,60 | 0 |
| 58 | MG | 23SA | 3022 | 1/1 | 0.95 | 0.20 | 49,49,49,49 | 0 |
| 60 | OHX | 23SA | 3577 | 7/7 | 0.95 | 0.07 | 80,96,102,220 | 0 |
| 58 | MG | 23SA | 3004 | 1/1 | 0.95 | 0.27 | 40,40,40,40 | 0 |
| 60 | OHX | 23SA | 3579 | 7/7 | 0.95 | 0.06 | 92,103,109,213 | 0 |
| 60 | OHX | ASIB | 102 | 7/7 | 0.95 | 0.09 | 150,170,188,213 | 0 |
| 60 | OHX | 23SA | 3582 | 7/7 | 0.95 | 0.07 | 109,116,130,206 | 0 |
| 60 | OHX | 16SA | 2378 | 7/7 | 0.95 | 0.08 | 104,108,111,178 | 0 |
| 58 | MG | 23SA | 3016 | 1/1 | 0.95 | 0.16 | 66,66,66,66 | 0 |
| 58 | MG | 23SB | 3189 | 1/1 | 0.95 | 0.08 | 52,52,52,52 | 0 |
| 59 | K | 23SB | 3267 | 1/1 | 0.95 | 0.13 | 65,65,65,65 | 0 |
| 60 | OHX | 16SA | 2382 | 7/7 | 0.95 | 0.07 | 101,104,120,187 | 0 |
| 60 | OHX | 23SA | 3594 | 7/7 | 0.95 | 0.07 | 86,92,102,199 | 0 |
| 58 | MG | 23SA | 3281 | 1/1 | 0.95 | 0.06 | 39,39,39,39 | 0 |
| 58 | MG | 23SA | 3133 | 1/1 | 0.95 | 0.13 | 58,58,58,58 | 0 |
| 60 | OHX | 23SB | 3383 | 7/7 | 0.95 | 0.08 | 95,102,112,175 | 0 |
| 59 | K | L4A | 303 | 1/1 | 0.95 | 0.06 | 80,80,80,80 | 0 |
| 60 | OHX | 16SA | 2386 | 7/7 | 0.95 | 0.08 | 101,109,118,167 | 0 |
| 59 | K | 16SA | 2309 | 1/1 | 0.95 | 0.08 | 85,85,85,85 | 0 |
| 60 | OHX | 23SB | 3395 | 7/7 | 0.95 | 0.09 | 86,95,112,173 | 0 |
| 60 | OHX | 23SB | 3399 | 7/7 | 0.95 | 0.10 | 89,90,102,150 | 0 |
| 60 | OHX | 23SB | 3406 | 7/7 | 0.95 | 0.07 | 90,98,104,195 | 0 |
| 58 | MG | 23SA | 3226 | 1/1 | 0.95 | 0.06 | 76,76,76,76 | 0 |
| 60 | OHX | 23SB | 3409 | 7/7 | 0.95 | 0.08 | 84,92,100,160 | 0 |
| 60 | OHX | 16SA | 2389 | 7/7 | 0.95 | 0.08 | 108,111,117,198 | 0 |
| 59 | K | 23SA | 3364 | 1/1 | 0.95 | 0.07 | 46,46,46,46 | 0 |
| 58 | MG | 23SB | 3122 | 1/1 | 0.95 | 0.15 | 38,38,38,38 | 0 |
| 58 | MG | 23SA | 3120 | 1/1 | 0.95 | 0.08 | 70,70,70,70 | 0 |

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| Mol | Type | Chain | Res | Atoms | RSCC | RSR | B-factors(Å$^2$) | Q<0.9 |
|---|---|---|---|---|---|---|---|---|
| 60 | OHX | 16SA | 2393 | 7/7 | 0.95 | 0.08 | 108,114,137,185 | 0 |
| 60 | OHX | 23SB | 3423 | 7/7 | 0.95 | 0.08 | 96,107,117,182 | 0 |
| 59 | K | 16SA | 2313 | 1/1 | 0.95 | 0.07 | 62,62,62,62 | 0 |
| 59 | K | 23SA | 3369 | 1/1 | 0.95 | 0.05 | 50,50,50,50 | 0 |
| 60 | OHX | 16SA | 2396 | 7/7 | 0.95 | 0.10 | 99,106,128,172 | 0 |
| 60 | OHX | 23SB | 3431 | 7/7 | 0.95 | 0.06 | 113,115,123,203 | 0 |
| 58 | MG | 23SB | 3196 | 1/1 | 0.95 | 0.11 | 53,53,53,53 | 0 |
| 58 | MG | 23SA | 3233 | 1/1 | 0.95 | 0.16 | 70,70,70,70 | 0 |
| 58 | MG | 23SA | 3236 | 1/1 | 0.95 | 0.17 | 102,102,102,102 | 0 |
| 58 | MG | 23SA | 3237 | 1/1 | 0.95 | 0.07 | 46,46,46,46 | 0 |
| 59 | K | 16SB | 2295 | 1/1 | 0.95 | 0.09 | 90,90,90,90 | 0 |
| 58 | MG | 23SA | 3180 | 1/1 | 0.95 | 0.14 | 37,37,37,37 | 0 |
| 58 | MG | 23SB | 3204 | 1/1 | 0.95 | 0.08 | 34,34,34,34 | 0 |
| 60 | OHX | 23SA | 3617 | 7/7 | 0.95 | 0.07 | 93,106,124,185 | 0 |
| 58 | MG | 23SB | 3206 | 1/1 | 0.95 | 0.13 | 63,63,63,63 | 0 |
| 58 | MG | 23SA | 3185 | 1/1 | 0.95 | 0.07 | 35,35,35,35 | 0 |
| 58 | MG | 23SA | 3025 | 1/1 | 0.95 | 0.25 | 58,58,58,58 | 0 |
| 60 | OHX | 23SB | 3447 | 7/7 | 0.95 | 0.08 | 86,91,103,193 | 0 |
| 59 | K | 23SB | 3292 | 1/1 | 0.95 | 0.06 | 80,80,80,80 | 0 |
| 58 | MG | 23SB | 3011 | 1/1 | 0.95 | 0.30 | 43,43,43,43 | 0 |
| 60 | OHX | 23SB | 3451 | 7/7 | 0.95 | 0.07 | 96,110,128,184 | 0 |
| 60 | OHX | 23SB | 3452 | 7/7 | 0.95 | 0.07 | 105,116,122,211 | 0 |
| 58 | MG | 23SB | 3218 | 1/1 | 0.95 | 0.06 | 42,42,42,42 | 0 |
| 58 | MG | 23SA | 3301 | 1/1 | 0.95 | 0.10 | 37,37,37,37 | 0 |
| 60 | OHX | 23SB | 3457 | 7/7 | 0.95 | 0.10 | 90,92,116,167 | 0 |
| 60 | OHX | 23SB | 3458 | 7/7 | 0.95 | 0.07 | 98,102,111,227 | 0 |
| 58 | MG | 23SA | 3245 | 1/1 | 0.95 | 0.07 | 51,51,51,51 | 0 |
| 60 | OHX | 16SA | 2413 | 7/7 | 0.95 | 0.08 | 87,97,103,201 | 0 |
| 59 | K | 23SA | 3388 | 1/1 | 0.95 | 0.08 | 74,74,74,74 | 0 |
| 58 | MG | 23SB | 3015 | 1/1 | 0.95 | 0.16 | 44,44,44,44 | 0 |
| 60 | OHX | S19A | 101 | 7/7 | 0.95 | 0.09 | 105,123,131,174 | 0 |
| 58 | MG | 23SB | 3136 | 1/1 | 0.95 | 0.09 | 47,47,47,47 | 0 |
| 60 | OHX | ESIA | 101 | 7/7 | 0.95 | 0.07 | 143,154,174,216 | 0 |
| 58 | MG | 16SB | 2268 | 1/1 | 0.95 | 0.06 | 86,86,86,86 | 0 |
| 60 | OHX | 23SB | 3468 | 7/7 | 0.95 | 0.08 | 110,122,131,185 | 0 |
| 59 | K | 23SA | 3395 | 1/1 | 0.95 | 0.08 | 61,61,61,61 | 0 |
| 60 | OHX | 23SA | 3465 | 7/7 | 0.95 | 0.11 | 73,76,89,133 | 0 |
| 58 | MG | 23SA | 3094 | 1/1 | 0.95 | 0.05 | 77,77,77,77 | 0 |
| 60 | OHX | L27A | 104 | 7/7 | 0.95 | 0.08 | 111,116,145,172 | 0 |
| 58 | MG | 23SB | 3144 | 1/1 | 0.95 | 0.09 | 58,58,58,58 | 0 |
| 60 | OHX | L35A | 102 | 7/7 | 0.95 | 0.09 | 98,107,111,169 | 0 |
| 58 | MG | 23SB | 3145 | 1/1 | 0.95 | 0.08 | 60,60,60,60 | 0 |

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| Mol | Type | Chain | Res | Atoms | RSCC | RSR | B-factors(Å$^2$) | Q<0.9 |
|---|---|---|---|---|---|---|---|---|
| 60 | OHX | 16SB | 2334 | 7/7 | 0.95 | 0.09 | 118,127,134,170 | 0 |
| 60 | OHX | 16SB | 2336 | 7/7 | 0.95 | 0.10 | 68,90,111,131 | 0 |
| 60 | OHX | 23SA | 3492 | 7/7 | 0.95 | 0.15 | 69,79,89,131 | 0 |
| 60 | OHX | 16SB | 2341 | 7/7 | 0.95 | 0.07 | 96,100,117,187 | 0 |
| 59 | K | 23SA | 3400 | 1/1 | 0.95 | 0.12 | 56,56,56,56 | 0 |
| 60 | OHX | 23SA | 3497 | 7/7 | 0.95 | 0.11 | 62,85,98,140 | 0 |
| 60 | OHX | 23SA | 3508 | 7/7 | 0.95 | 0.08 | 73,82,110,156 | 0 |
| 58 | MG | 23SA | 3095 | 1/1 | 0.95 | 0.23 | 51,51,51,51 | 0 |
| 60 | OHX | 23SB | 3486 | 7/7 | 0.95 | 0.07 | 96,100,116,205 | 0 |
| 58 | MG | 23SB | 3231 | 1/1 | 0.95 | 0.07 | 111,111,111,111 | 0 |
| 58 | MG | 23SB | 3232 | 1/1 | 0.95 | 0.06 | 50,50,50,50 | 0 |
| 58 | MG | 23SB | 3233 | 1/1 | 0.95 | 0.08 | 102,102,102,102 | 0 |
| 60 | OHX | 23SB | 3491 | 7/7 | 0.95 | 0.07 | 132,134,135,208 | 0 |
| 60 | OHX | 23SB | 3492 | 7/7 | 0.95 | 0.07 | 97,109,131,185 | 0 |
| 58 | MG | 23SB | 3148 | 1/1 | 0.95 | 0.07 | 69,69,69,69 | 0 |
| 60 | OHX | 23SA | 3516 | 7/7 | 0.95 | 0.13 | 70,77,90,165 | 0 |
| 60 | OHX | 23SB | 3495 | 7/7 | 0.95 | 0.07 | 143,146,157,198 | 0 |
| 60 | OHX | 16SB | 2357 | 7/7 | 0.95 | 0.07 | 103,106,112,188 | 0 |
| 58 | MG | 16SA | 2281 | 1/1 | 0.95 | 0.06 | 40,40,40,40 | 0 |
| 58 | MG | 23SA | 3258 | 1/1 | 0.95 | 0.06 | 42,42,42,42 | 0 |
| 58 | MG | 16SB | 2274 | 1/1 | 0.95 | 0.07 | 80,80,80,80 | 0 |
| 58 | MG | 16SB | 2275 | 1/1 | 0.95 | 0.11 | 80,80,80,80 | 0 |
| 59 | K | 23SA | 3412 | 1/1 | 0.95 | 0.07 | 40,40,40,40 | 0 |
| 60 | OHX | 16SB | 2367 | 7/7 | 0.95 | 0.08 | 191,194,215,295 | 0 |
| 58 | MG | 23SB | 3159 | 1/1 | 0.95 | 0.07 | 56,56,56,56 | 0 |
| 58 | MG | 16SA | 2277 | 1/1 | 0.95 | 0.07 | 63,63,63,63 | 0 |
| 58 | MG | 23SB | 3026 | 1/1 | 0.95 | 0.16 | 47,47,47,47 | 0 |
| 60 | OHX | 23SA | 3532 | 7/7 | 0.95 | 0.11 | 60,78,105,175 | 0 |
| 58 | MG | PSIA | 101 | 1/1 | 0.95 | 0.29 | 56,56,56,56 | 0 |
| 60 | OHX | 23SA | 3540 | 7/7 | 0.95 | 0.06 | 77,94,109,196 | 0 |
| 58 | MG | 23SA | 3207 | 1/1 | 0.95 | 0.13 | 40,40,40,40 | 0 |
| 60 | OHX | 23SA | 3542 | 7/7 | 0.95 | 0.08 | 90,100,107,188 | 0 |
| 58 | MG | 23SA | 3265 | 1/1 | 0.95 | 0.07 | 41,41,41,41 | 0 |
| 59 | K | 23SA | 3420 | 1/1 | 0.95 | 0.07 | 71,71,71,71 | 0 |
| 58 | MG | 23SA | 3210 | 1/1 | 0.95 | 0.06 | 38,38,38,38 | 0 |
| 58 | MG | 23SB | 3107 | 1/1 | 0.95 | 0.29 | 75,75,75,75 | 0 |
| 60 | OHX | 23SA | 3553 | 7/7 | 0.95 | 0.08 | 71,80,96,181 | 0 |
| 58 | MG | 23SA | 3045 | 1/1 | 0.95 | 0.17 | 33,33,33,33 | 0 |
| 58 | MG | 23SB | 3032 | 1/1 | 0.95 | 0.15 | 55,55,55,55 | 0 |
| 60 | OHX | 16SA | 2351 | 7/7 | 0.95 | 0.09 | 85,94,107,150 | 0 |
| 60 | OHX | 5SB | 211 | 7/7 | 0.95 | 0.07 | 107,114,125,191 | 0 |
| 58 | MG | 23SA | 3272 | 1/1 | 0.95 | 0.07 | 63,63,63,63 | 0 |

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| Mol | Type | Chain | Res | Atoms | RSCC | RSR | B-factors(Å$^2$) | Q<0.9 |
|---|---|---|---|---|---|---|---|---|
| 58 | MG | 23SB | 3174 | 1/1 | 0.95 | 0.12 | 54,54,54,54 | 0 |
| 58 | MG | 23SB | 3175 | 1/1 | 0.95 | 0.08 | 62,62,62,62 | 0 |
| 60 | OHX | 16SA | 2360 | 7/7 | 0.95 | 0.07 | 92,94,119,193 | 0 |
| 58 | MG | 23SA | 3213 | 1/1 | 0.95 | 0.09 | 49,49,49,49 | 0 |
| 60 | OHX | 16SA | 2364 | 7/7 | 0.95 | 0.08 | 72,94,101,159 | 0 |
| 59 | K | 23SA | 3429 | 1/1 | 0.95 | 0.17 | 76,76,76,76 | 0 |
| 60 | OHX | 23SA | 3568 | 7/7 | 0.95 | 0.08 | 84,98,111,175 | 0 |
| 60 | OHX | 23SB | 3396 | 7/7 | 0.96 | 0.07 | 86,89,98,176 | 0 |
| 60 | OHX | 23SB | 3397 | 7/7 | 0.96 | 0.06 | 82,86,94,166 | 0 |
| 60 | OHX | 23SB | 3398 | 7/7 | 0.96 | 0.06 | 102,110,115,193 | 0 |
| 58 | MG | 23SA | 3323 | 1/1 | 0.96 | 0.07 | 25,25,25,25 | 0 |
| 60 | OHX | 23SB | 3400 | 7/7 | 0.96 | 0.07 | 110,122,130,188 | 0 |
| 60 | OHX | 23SB | 3403 | 7/7 | 0.96 | 0.08 | 89,99,119,158 | 0 |
| 60 | OHX | 5SA | 210 | 7/7 | 0.96 | 0.08 | 68,97,110,132 | 0 |
| 60 | OHX | 5SA | 212 | 7/7 | 0.96 | 0.08 | 83,95,112,163 | 0 |
| 60 | OHX | 23SB | 3408 | 7/7 | 0.96 | 0.08 | 78,89,99,156 | 0 |
| 59 | K | 23SA | 3373 | 1/1 | 0.96 | 0.04 | 37,37,37,37 | 0 |
| 60 | OHX | 23SA | 3548 | 7/7 | 0.96 | 0.12 | 66,73,104,175 | 0 |
| 60 | OHX | 23SA | 3549 | 7/7 | 0.96 | 0.07 | 82,94,102,158 | 0 |
| 60 | OHX | 23SB | 3413 | 7/7 | 0.96 | 0.08 | 79,83,95,170 | 0 |
| 60 | OHX | 23SB | 3414 | 7/7 | 0.96 | 0.11 | 76,79,91,152 | 0 |
| 60 | OHX | 16SA | 2398 | 7/7 | 0.96 | 0.07 | 120,122,129,185 | 0 |
| 60 | OHX | 23SB | 3416 | 7/7 | 0.96 | 0.08 | 94,107,122,167 | 0 |
| 60 | OHX | L15A | 203 | 7/7 | 0.96 | 0.14 | 76,83,97,140 | 0 |
| 59 | K | 23SB | 3316 | 1/1 | 0.96 | 0.27 | 89,89,89,89 | 0 |
| 58 | MG | 16SA | 2242 | 1/1 | 0.96 | 0.33 | 63,63,63,63 | 0 |
| 58 | MG | 23SA | 3099 | 1/1 | 0.96 | 0.07 | 54,54,54,54 | 0 |
| 60 | OHX | 23SB | 3425 | 7/7 | 0.96 | 0.08 | 74,89,96,169 | 0 |
| 59 | K | 23SA | 3376 | 1/1 | 0.96 | 0.05 | 59,59,59,59 | 0 |
| 60 | OHX | 23SA | 3556 | 7/7 | 0.96 | 0.07 | 87,91,98,175 | 0 |
| 60 | OHX | 23SB | 3429 | 7/7 | 0.96 | 0.07 | 105,111,115,204 | 0 |
| 60 | OHX | 23SB | 3430 | 7/7 | 0.96 | 0.07 | 96,102,106,185 | 0 |
| 60 | OHX | 23SA | 3557 | 7/7 | 0.96 | 0.06 | 94,104,119,199 | 0 |
| 60 | OHX | 16SB | 2335 | 7/7 | 0.96 | 0.08 | 110,123,134,166 | 0 |
| 59 | K | 16SA | 2304 | 1/1 | 0.96 | 0.23 | 77,77,77,77 | 0 |
| 58 | MG | 23SA | 3075 | 1/1 | 0.96 | 0.05 | 73,73,73,73 | 0 |
| 58 | MG | 23SA | 3118 | 1/1 | 0.96 | 0.10 | 52,52,52,52 | 0 |
| 58 | MG | 23SA | 3243 | 1/1 | 0.96 | 0.06 | 36,36,36,36 | 0 |
| 58 | MG | 16SA | 2262 | 1/1 | 0.96 | 0.08 | 70,70,70,70 | 0 |
| 60 | OHX | 16SB | 2346 | 7/7 | 0.96 | 0.07 | 84,98,106,161 | 0 |
| 60 | OHX | 16SB | 2347 | 7/7 | 0.96 | 0.07 | 113,116,121,183 | 0 |
| 58 | MG | 23SA | 3206 | 1/1 | 0.96 | 0.07 | 55,55,55,55 | 0 |

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| Mol | Type | Chain | Res | Atoms | RSCC | RSR | B-factors(Å$^2$) | Q<0.9 |
|---|---|---|---|---|---|---|---|---|
| 58 | MG | 16SB | 2207 | 1/1 | 0.96 | 0.11 | 61,61,61,61 | 0 |
| 60 | OHX | 23SB | 3443 | 7/7 | 0.96 | 0.07 | 90,95,107,189 | 0 |
| 60 | OHX | 23SA | 3566 | 7/7 | 0.96 | 0.06 | 95,99,108,197 | 0 |
| 60 | OHX | 23SB | 3445 | 7/7 | 0.96 | 0.07 | 97,105,117,180 | 0 |
| 60 | OHX | 23SB | 3446 | 7/7 | 0.96 | 0.06 | 83,97,99,203 | 0 |
| 60 | OHX | 16SB | 2352 | 7/7 | 0.96 | 0.07 | 85,96,108,177 | 0 |
| 58 | MG | 23SA | 3224 | 1/1 | 0.96 | 0.06 | 69,69,69,69 | 0 |
| 60 | OHX | 23SB | 3449 | 7/7 | 0.96 | 0.06 | 102,106,109,189 | 0 |
| 58 | MG | 23SB | 3234 | 1/1 | 0.96 | 0.05 | 102,102,102,102 | 0 |
| 59 | K | 23SB | 3281 | 1/1 | 0.96 | 0.07 | 75,75,75,75 | 0 |
| 58 | MG | 23SA | 3252 | 1/1 | 0.96 | 0.07 | 50,50,50,50 | 0 |
| 60 | OHX | 23SA | 3571 | 7/7 | 0.96 | 0.13 | 70,83,95,178 | 0 |
| 60 | OHX | 23SB | 3454 | 7/7 | 0.96 | 0.07 | 91,102,107,180 | 0 |
| 58 | MG | 23SB | 3141 | 1/1 | 0.96 | 0.06 | 44,44,44,44 | 0 |
| 60 | OHX | 16SA | 2357 | 7/7 | 0.96 | 0.07 | 93,100,111,175 | 0 |
| 60 | OHX | 16SB | 2361 | 7/7 | 0.96 | 0.07 | 120,121,125,206 | 0 |
| 60 | OHX | 23SA | 3574 | 7/7 | 0.96 | 0.06 | 84,98,110,186 | 0 |
| 60 | OHX | 16SA | 2416 | 7/7 | 0.96 | 0.08 | 96,107,111,178 | 0 |
| 59 | K | 23SB | 3285 | 1/1 | 0.96 | 0.05 | 70,70,70,70 | 0 |
| 60 | OHX | 16SB | 2366 | 7/7 | 0.96 | 0.07 | 98,106,112,182 | 0 |
| 59 | K | 23SA | 3389 | 1/1 | 0.96 | 0.05 | 68,68,68,68 | 0 |
| 60 | OHX | ASIA | 103 | 7/7 | 0.96 | 0.10 | 138,148,166,192 | 0 |
| 58 | MG | 23SA | 3306 | 1/1 | 0.96 | 0.10 | 73,73,73,73 | 0 |
| 59 | K | 16SA | 2317 | 1/1 | 0.96 | 0.04 | 50,50,50,50 | 0 |
| 60 | OHX | 23SA | 3585 | 7/7 | 0.96 | 0.07 | 95,99,129,168 | 0 |
| 60 | OHX | 23SA | 3586 | 7/7 | 0.96 | 0.07 | 101,106,128,162 | 0 |
| 58 | MG | 16SA | 2263 | 1/1 | 0.96 | 0.07 | 70,70,70,70 | 0 |
| 60 | OHX | 23SA | 3589 | 7/7 | 0.96 | 0.08 | 112,126,132,194 | 0 |
| 60 | OHX | 23SA | 3459 | 7/7 | 0.96 | 0.12 | 55,83,96,117 | 0 |
| 58 | MG | 23SB | 3061 | 1/1 | 0.96 | 0.32 | 59,59,59,59 | 0 |
| 58 | MG | 23SB | 3113 | 1/1 | 0.96 | 0.07 | 52,52,52,52 | 0 |
| 60 | OHX | 23SB | 3475 | 7/7 | 0.96 | 0.08 | 166,169,173,226 | 0 |
| 60 | OHX | 16SA | 2370 | 7/7 | 0.96 | 0.08 | 85,94,98,186 | 0 |
| 58 | MG | L15A | 201 | 1/1 | 0.96 | 0.09 | 52,52,52,52 | 0 |
| 60 | OHX | 16SB | 2380 | 7/7 | 0.96 | 0.07 | 141,148,159,212 | 0 |
| 60 | OHX | 23SA | 3480 | 7/7 | 0.96 | 0.09 | 74,80,103,129 | 0 |
| 60 | OHX | 23SB | 3480 | 7/7 | 0.96 | 0.06 | 121,142,146,213 | 0 |
| 60 | OHX | 23SA | 3486 | 7/7 | 0.96 | 0.10 | 55,72,99,142 | 0 |
| 60 | OHX | 16SA | 2372 | 7/7 | 0.96 | 0.08 | 73,90,105,162 | 0 |
| 60 | OHX | 16SA | 2373 | 7/7 | 0.96 | 0.06 | 113,116,123,191 | 0 |
| 58 | MG | 23SB | 3153 | 1/1 | 0.96 | 0.08 | 52,52,52,52 | 0 |
| 60 | OHX | 23SA | 3498 | 7/7 | 0.96 | 0.19 | 62,67,77,108 | 0 |

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| Mol | Type | Chain | Res | Atoms | RSCC | RSR | B-factors(Å$^2$) | Q<0.9 |
|---|---|---|---|---|---|---|---|---|
| 60 | OHX | 23SA | 3501 | 7/7 | 0.96 | 0.08 | 86,95,99,151 | 0 |
| 58 | MG | 23SA | 3108 | 1/1 | 0.96 | 0.12 | 51,51,51,51 | 0 |
| 60 | OHX | 23SA | 3510 | 7/7 | 0.96 | 0.13 | 73,82,88,134 | 0 |
| 60 | OHX | 16SA | 2377 | 7/7 | 0.96 | 0.07 | 104,109,116,184 | 0 |
| 58 | MG | 23SA | 3259 | 1/1 | 0.96 | 0.07 | 64,64,64,64 | 0 |
| 59 | K | 16SA | 2325 | 1/1 | 0.96 | 0.07 | 80,80,80,80 | 0 |
| 58 | MG | 23SB | 3090 | 1/1 | 0.96 | 0.13 | 65,65,65,65 | 0 |
| 58 | MG | 23SA | 3186 | 1/1 | 0.96 | 0.06 | 23,23,23,23 | 0 |
| 58 | MG | 16SB | 2257 | 1/1 | 0.96 | 0.07 | 64,64,64,64 | 0 |
| 60 | OHX | 23SA | 3517 | 7/7 | 0.96 | 0.07 | 75,89,104,170 | 0 |
| 58 | MG | 23SB | 3205 | 1/1 | 0.96 | 0.08 | 54,54,54,54 | 0 |
| 58 | MG | 23SA | 3315 | 1/1 | 0.96 | 0.07 | 101,101,101,101 | 0 |
| 58 | MG | 16SB | 2259 | 1/1 | 0.96 | 0.06 | 96,96,96,96 | 0 |
| 58 | MG | 23SB | 3212 | 1/1 | 0.96 | 0.05 | 56,56,56,56 | 0 |
| 59 | K | 23SA | 3363 | 1/1 | 0.96 | 0.05 | 53,53,53,53 | 0 |
| 60 | OHX | S14B | 101 | 7/7 | 0.96 | 0.08 | 102,124,132,165 | 0 |
| 59 | K | 23SB | 3257 | 1/1 | 0.96 | 0.04 | 77,77,77,77 | 0 |
| 60 | OHX | 23SA | 3528 | 7/7 | 0.96 | 0.07 | 87,90,100,182 | 0 |
| 58 | MG | 23SA | 3319 | 1/1 | 0.96 | 0.05 | 68,68,68,68 | 0 |
| 58 | MG | 23SB | 3021 | 1/1 | 0.96 | 0.05 | 66,66,66,66 | 0 |
| 60 | OHX | 23SA | 3621 | 7/7 | 0.96 | 0.08 | 96,102,123,180 | 0 |
| 58 | MG | 23SA | 3165 | 1/1 | 0.96 | 0.26 | 64,64,64,64 | 0 |
| 60 | OHX | 23SB | 3357 | 7/7 | 0.96 | 0.07 | 81,94,106,158 | 0 |
| 60 | OHX | 23SA | 3533 | 7/7 | 0.96 | 0.06 | 85,91,99,178 | 0 |
| 60 | OHX | 23SA | 3534 | 7/7 | 0.96 | 0.08 | 75,93,110,174 | 0 |
| 60 | OHX | 23SB | 3361 | 7/7 | 0.96 | 0.08 | 76,89,106,161 | 0 |
| 60 | OHX | 23SB | 3364 | 7/7 | 0.96 | 0.11 | 77,86,99,142 | 0 |
| 60 | OHX | 23SA | 3537 | 7/7 | 0.96 | 0.06 | 98,104,109,202 | 0 |
| 60 | OHX | 23SA | 3626 | 7/7 | 0.96 | 0.07 | 106,109,123,185 | 0 |
| 60 | OHX | 23SB | 3373 | 7/7 | 0.96 | 0.15 | 72,84,91,148 | 0 |
| 60 | OHX | 5SB | 208 | 7/7 | 0.96 | 0.07 | 99,101,116,175 | 0 |
| 60 | OHX | 23SB | 3378 | 7/7 | 0.96 | 0.10 | 71,85,90,156 | 0 |
| 60 | OHX | 23SB | 3381 | 7/7 | 0.96 | 0.08 | 82,98,103,149 | 0 |
| 60 | OHX | 23SB | 3382 | 7/7 | 0.96 | 0.07 | 92,100,102,184 | 0 |
| 60 | OHX | 23SA | 3538 | 7/7 | 0.96 | 0.07 | 95,114,124,179 | 0 |
| 60 | OHX | 23SB | 3384 | 7/7 | 0.96 | 0.07 | 90,103,109,158 | 0 |
| 59 | K | 16SB | 2301 | 1/1 | 0.96 | 0.07 | 92,92,92,92 | 0 |
| 58 | MG | 23SA | 3322 | 1/1 | 0.96 | 0.07 | 43,43,43,43 | 0 |
| 59 | K | 23SA | 3417 | 1/1 | 0.96 | 0.06 | 68,68,68,68 | 0 |
| 60 | OHX | 23SB | 3392 | 7/7 | 0.96 | 0.12 | 67,88,95,140 | 0 |
| 60 | OHX | 23SB | 3393 | 7/7 | 0.96 | 0.08 | 79,88,96,165 | 0 |
| 58 | MG | 23SB | 3126 | 1/1 | 0.96 | 0.07 | 59,59,59,59 | 0 |

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| Mol | Type | Chain | Res | Atoms | RSCC | RSR | B-factors(Å$^2$) | Q<0.9 |
|---|---|---|---|---|---|---|---|---|
| 60 | OHX | 16SB | 2351 | 7/7 | 0.97 | 0.06 | 116,129,145,187 | 0 |
| 60 | OHX | 23SA | 3477 | 7/7 | 0.97 | 0.08 | 71,87,97,132 | 0 |
| 59 | K | L2A | 301 | 1/1 | 0.97 | 0.07 | 52,52,52,52 | 0 |
| 59 | K | 23SA | 3394 | 1/1 | 0.97 | 0.07 | 59,59,59,59 | 0 |
| 60 | OHX | 23SB | 3418 | 7/7 | 0.97 | 0.07 | 122,132,139,198 | 0 |
| 60 | OHX | 23SB | 3420 | 7/7 | 0.97 | 0.07 | 99,102,107,176 | 0 |
| 58 | MG | 23SA | 3282 | 1/1 | 0.97 | 0.05 | 30,30,30,30 | 0 |
| 60 | OHX | 23SA | 3481 | 7/7 | 0.97 | 0.07 | 81,94,105,138 | 0 |
| 60 | OHX | 23SA | 3483 | 7/7 | 0.97 | 0.10 | 68,75,84,124 | 0 |
| 60 | OHX | 16SB | 2358 | 7/7 | 0.97 | 0.06 | 104,114,122,205 | 0 |
| 59 | K | 23SA | 3396 | 1/1 | 0.97 | 0.06 | 68,68,68,68 | 0 |
| 60 | OHX | 23SA | 3487 | 7/7 | 0.97 | 0.14 | 68,87,98,133 | 0 |
| 60 | OHX | 23SA | 3580 | 7/7 | 0.97 | 0.06 | 90,92,101,178 | 0 |
| 60 | OHX | 23SA | 3489 | 7/7 | 0.97 | 0.10 | 83,85,99,126 | 0 |
| 60 | OHX | 23SA | 3584 | 7/7 | 0.97 | 0.05 | 92,105,118,200 | 0 |
| 58 | MG | 23SA | 3188 | 1/1 | 0.97 | 0.05 | 50,50,50,50 | 0 |
| 58 | MG | 16SA | 2278 | 1/1 | 0.97 | 0.15 | 93,93,93,93 | 0 |
| 60 | OHX | 23SA | 3587 | 7/7 | 0.97 | 0.09 | 81,88,96,150 | 0 |
| 60 | OHX | 23SA | 3496 | 7/7 | 0.97 | 0.11 | 72,80,86,150 | 0 |
| 58 | MG | 23SA | 3179 | 1/1 | 0.97 | 0.07 | 31,31,31,31 | 0 |
| 58 | MG | 23SA | 3316 | 1/1 | 0.97 | 0.12 | 86,86,86,86 | 0 |
| 60 | OHX | 23SA | 3499 | 7/7 | 0.97 | 0.08 | 68,88,99,163 | 0 |
| 58 | MG | 23SA | 3318 | 1/1 | 0.97 | 0.06 | 64,64,64,64 | 0 |
| 60 | OHX | 23SA | 3503 | 7/7 | 0.97 | 0.14 | 80,89,99,149 | 0 |
| 60 | OHX | 23SA | 3504 | 7/7 | 0.97 | 0.13 | 87,89,95,142 | 0 |
| 60 | OHX | 23SA | 3505 | 7/7 | 0.97 | 0.12 | 79,87,103,142 | 0 |
| 60 | OHX | 23SA | 3596 | 7/7 | 0.97 | 0.07 | 95,124,136,188 | 0 |
| 60 | OHX | 23SA | 3506 | 7/7 | 0.97 | 0.10 | 58,69,82,144 | 0 |
| 58 | MG | 23SA | 3287 | 1/1 | 0.97 | 0.04 | 43,43,43,43 | 0 |
| 60 | OHX | 23SA | 3509 | 7/7 | 0.97 | 0.07 | 103,106,119,151 | 0 |
| 58 | MG | 23SA | 3320 | 1/1 | 0.97 | 0.07 | 93,93,93,93 | 0 |
| 58 | MG | 23SB | 3200 | 1/1 | 0.97 | 0.07 | 82,82,82,82 | 0 |
| 59 | K | 23SA | 3405 | 1/1 | 0.97 | 0.07 | 72,72,72,72 | 0 |
| 59 | K | 23SB | 3253 | 1/1 | 0.97 | 0.06 | 54,54,54,54 | 0 |
| 58 | MG | 23SB | 3201 | 1/1 | 0.97 | 0.06 | 73,73,73,73 | 0 |
| 58 | MG | L35B | 101 | 1/1 | 0.97 | 0.09 | 91,91,91,91 | 0 |
| 58 | MG | 23SA | 3289 | 1/1 | 0.97 | 0.05 | 33,33,33,33 | 0 |
| 60 | OHX | 23SB | 3455 | 7/7 | 0.97 | 0.06 | 80,87,94,174 | 0 |
| 58 | MG | 16SB | 2272 | 1/1 | 0.97 | 0.07 | 90,90,90,90 | 0 |
| 58 | MG | 23SA | 3247 | 1/1 | 0.97 | 0.05 | 26,26,26,26 | 0 |
| 60 | OHX | 23SA | 3520 | 7/7 | 0.97 | 0.08 | 81,88,104,156 | 0 |
| 59 | K | 23SB | 3260 | 1/1 | 0.97 | 0.06 | 53,53,53,53 | 0 |

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| Mol | Type | Chain | Res | Atoms | RSCC | RSR | B-factors(Å$^2$) | Q<0.9 |
|---|---|---|---|---|---|---|---|---|
| 58 | MG | 23SA | 3271 | 1/1 | 0.97 | 0.10 | 67,67,67,67 | 0 |
| 58 | MG | 23SB | 3207 | 1/1 | 0.97 | 0.14 | 51,51,51,51 | 0 |
| 58 | MG | 16SA | 2266 | 1/1 | 0.97 | 0.06 | 86,86,86,86 | 0 |
| 58 | MG | 23SB | 3067 | 1/1 | 0.97 | 0.13 | 36,36,36,36 | 0 |
| 59 | K | 16SB | 2303 | 1/1 | 0.97 | 0.06 | 74,74,74,74 | 0 |
| 59 | K | 23SA | 3368 | 1/1 | 0.97 | 0.04 | 39,39,39,39 | 0 |
| 58 | MG | 23SB | 3213 | 1/1 | 0.97 | 0.08 | 42,42,42,42 | 0 |
| 60 | OHX | 23SB | 3467 | 7/7 | 0.97 | 0.07 | 94,109,115,181 | 0 |
| 58 | MG | 23SB | 3215 | 1/1 | 0.97 | 0.06 | 42,42,42,42 | 0 |
| 58 | MG | 23SB | 3012 | 1/1 | 0.97 | 0.05 | 54,54,54,54 | 0 |
| 58 | MG | 23SA | 3232 | 1/1 | 0.97 | 0.07 | 82,82,82,82 | 0 |
| 60 | OHX | 23SA | 3535 | 7/7 | 0.97 | 0.05 | 90,95,110,191 | 0 |
| 58 | MG | 23SA | 3197 | 1/1 | 0.97 | 0.07 | 52,52,52,52 | 0 |
| 60 | OHX | ASIB | 101 | 7/7 | 0.97 | 0.07 | 107,120,125,167 | 0 |
| 58 | MG | 16SB | 2278 | 1/1 | 0.97 | 0.08 | 73,73,73,73 | 0 |
| 59 | K | 23SA | 3335 | 1/1 | 0.97 | 0.05 | 70,70,70,70 | 0 |
| 59 | K | L2B | 302 | 1/1 | 0.97 | 0.07 | 65,65,65,65 | 0 |
| 58 | MG | 23SA | 3298 | 1/1 | 0.97 | 0.05 | 32,32,32,32 | 0 |
| 58 | MG | 23SB | 3221 | 1/1 | 0.97 | 0.04 | 94,94,94,94 | 0 |
| 58 | MG | 23SA | 3332 | 1/1 | 0.97 | 0.10 | 32,32,32,32 | 0 |
| 60 | OHX | 23SB | 3326 | 7/7 | 0.97 | 0.16 | 56,72,101,137 | 0 |
| 60 | OHX | 23SB | 3335 | 7/7 | 0.97 | 0.16 | 60,83,91,162 | 0 |
| 60 | OHX | 23SB | 3342 | 7/7 | 0.97 | 0.09 | 47,60,90,114 | 0 |
| 60 | OHX | 23SB | 3344 | 7/7 | 0.97 | 0.08 | 80,88,104,133 | 0 |
| 60 | OHX | 23SB | 3346 | 7/7 | 0.97 | 0.09 | 85,96,101,143 | 0 |
| 60 | OHX | 23SB | 3349 | 7/7 | 0.97 | 0.11 | 84,92,100,127 | 0 |
| 60 | OHX | 23SB | 3352 | 7/7 | 0.97 | 0.08 | 69,81,101,121 | 0 |
| 60 | OHX | 23SB | 3355 | 7/7 | 0.97 | 0.08 | 89,92,104,140 | 0 |
| 60 | OHX | 23SA | 3629 | 7/7 | 0.97 | 0.06 | 87,91,106,176 | 0 |
| 60 | OHX | 23SB | 3489 | 7/7 | 0.97 | 0.06 | 111,122,129,189 | 0 |
| 60 | OHX | 23SA | 3544 | 7/7 | 0.97 | 0.12 | 64,81,89,161 | 0 |
| 60 | OHX | 23SA | 3545 | 7/7 | 0.97 | 0.06 | 77,91,112,179 | 0 |
| 58 | MG | 23SA | 3234 | 1/1 | 0.97 | 0.07 | 93,93,93,93 | 0 |
| 60 | OHX | 23SA | 3547 | 7/7 | 0.97 | 0.08 | 69,73,100,135 | 0 |
| 60 | OHX | 16SA | 2342 | 7/7 | 0.97 | 0.09 | 98,105,114,137 | 0 |
| 60 | OHX | 23SB | 3369 | 7/7 | 0.97 | 0.09 | 60,77,90,136 | 0 |
| 60 | OHX | 23SB | 3371 | 7/7 | 0.97 | 0.08 | 104,112,125,154 | 0 |
| 60 | OHX | 5SA | 211 | 7/7 | 0.97 | 0.06 | 90,102,112,165 | 0 |
| 60 | OHX | 16SA | 2347 | 7/7 | 0.97 | 0.08 | 107,109,124,145 | 0 |
| 60 | OHX | 23SB | 3374 | 7/7 | 0.97 | 0.09 | 82,95,101,131 | 0 |
| 60 | OHX | 23SB | 3375 | 7/7 | 0.97 | 0.07 | 82,94,101,135 | 0 |
| 58 | MG | 23SB | 3019 | 1/1 | 0.97 | 0.10 | 51,51,51,51 | 0 |

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| Mol | Type | Chain | Res | Atoms | RSCC | RSR | B-factors(Å$^2$) | Q<0.9 |
|---|---|---|---|---|---|---|---|---|
| 60 | OHX | 23SA | 3551 | 7/7 | 0.97 | 0.06 | 90,96,108,182 | 0 |
| 59 | K | 23SB | 3279 | 1/1 | 0.97 | 0.03 | 52,52,52,52 | 0 |
| 60 | OHX | 16SA | 2353 | 7/7 | 0.97 | 0.07 | 89,94,102,156 | 0 |
| 58 | MG | 16SA | 2265 | 1/1 | 0.97 | 0.09 | 73,73,73,73 | 0 |
| 58 | MG | 23SB | 3182 | 1/1 | 0.97 | 0.05 | 62,62,62,62 | 0 |
| 58 | MG | 23SA | 3302 | 1/1 | 0.97 | 0.06 | 39,39,39,39 | 0 |
| 58 | MG | 23SA | 3202 | 1/1 | 0.97 | 0.07 | 74,74,74,74 | 0 |
| 60 | OHX | 23SB | 3390 | 7/7 | 0.97 | 0.06 | 82,92,101,166 | 0 |
| 60 | OHX | 23SB | 3391 | 7/7 | 0.97 | 0.08 | 92,101,112,165 | 0 |
| 60 | OHX | 16SA | 2359 | 7/7 | 0.97 | 0.13 | 75,86,97,154 | 0 |
| 58 | MG | 23SB | 3185 | 1/1 | 0.97 | 0.06 | 77,77,77,77 | 0 |
| 58 | MG | 23SA | 3011 | 1/1 | 0.97 | 0.28 | 43,43,43,43 | 0 |
| 60 | OHX | 16SA | 2362 | 7/7 | 0.97 | 0.06 | 68,86,95,171 | 0 |
| 60 | OHX | 16SA | 2363 | 7/7 | 0.97 | 0.07 | 87,99,108,136 | 0 |
| 60 | OHX | TRNA | 101 | 7/7 | 0.97 | 0.07 | 126,128,151,181 | 0 |
| 60 | OHX | 16SB | 2340 | 7/7 | 0.97 | 0.07 | 95,106,110,161 | 0 |
| 58 | MG | 23SA | 3049 | 1/1 | 0.97 | 0.10 | 40,40,40,40 | 0 |
| 60 | OHX | 23SB | 3402 | 7/7 | 0.97 | 0.06 | 96,103,111,160 | 0 |
| 60 | OHX | 16SB | 2342 | 7/7 | 0.97 | 0.06 | 98,111,117,180 | 0 |
| 60 | OHX | 23SB | 3405 | 7/7 | 0.97 | 0.07 | 100,109,116,160 | 0 |
| 60 | OHX | 23SA | 3565 | 7/7 | 0.97 | 0.09 | 67,68,89,172 | 0 |
| 60 | OHX | 23SA | 3454 | 7/7 | 0.97 | 0.11 | 62,77,97,102 | 0 |
| 60 | OHX | 16SA | 2365 | 7/7 | 0.97 | 0.07 | 82,95,103,153 | 0 |
| 58 | MG | 23SA | 3308 | 1/1 | 0.97 | 0.11 | 38,38,38,38 | 0 |
| 60 | OHX | 23SA | 3466 | 7/7 | 0.97 | 0.10 | 53,79,99,128 | 0 |
| 60 | OHX | 23SA | 3468 | 7/7 | 0.97 | 0.08 | 51,67,97,150 | 0 |
| 58 | MG | 23SA | 3310 | 1/1 | 0.97 | 0.15 | 57,57,57,57 | 0 |
| 58 | MG | L27B | 101 | 1/1 | 0.98 | 0.11 | 63,63,63,63 | 0 |
| 58 | MG | 23SA | 3305 | 1/1 | 0.98 | 0.08 | 48,48,48,48 | 0 |
| 58 | MG | 23SA | 3164 | 1/1 | 0.98 | 0.09 | 33,33,33,33 | 0 |
| 60 | OHX | 23SB | 3386 | 7/7 | 0.98 | 0.09 | 58,74,95,127 | 0 |
| 60 | OHX | 23SB | 3387 | 7/7 | 0.98 | 0.06 | 80,92,108,123 | 0 |
| 58 | MG | 23SA | 3181 | 1/1 | 0.98 | 0.05 | 42,42,42,42 | 0 |
| 60 | OHX | 5SA | 214 | 7/7 | 0.98 | 0.06 | 71,90,101,152 | 0 |
| 60 | OHX | 5SA | 215 | 7/7 | 0.98 | 0.04 | 98,108,110,190 | 0 |
| 60 | OHX | 23SA | 3531 | 7/7 | 0.98 | 0.05 | 86,94,101,174 | 0 |
| 58 | MG | 23SA | 3242 | 1/1 | 0.98 | 0.04 | 38,38,38,38 | 0 |
| 58 | MG | 23SB | 3135 | 1/1 | 0.98 | 0.05 | 62,62,62,62 | 0 |
| 60 | OHX | 23SB | 3394 | 7/7 | 0.98 | 0.07 | 72,84,101,133 | 0 |
| 58 | MG | 23SA | 3309 | 1/1 | 0.98 | 0.04 | 71,71,71,71 | 0 |
| 58 | MG | 23SB | 3194 | 1/1 | 0.98 | 0.04 | 71,71,71,71 | 0 |
| 60 | OHX | 23SA | 3536 | 7/7 | 0.98 | 0.06 | 72,84,94,136 | 0 |

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| Mol | Type | Chain | Res | Atoms | RSCC | RSR | B-factors(Å$^2$) | Q<0.9 |
|---|---|---|---|---|---|---|---|---|
| 58 | MG | 23SA | 3199 | 1/1 | 0.98 | 0.07 | 36,36,36,36 | 0 |
| 58 | MG | 23SA | 3276 | 1/1 | 0.98 | 0.06 | 74,74,74,74 | 0 |
| 60 | OHX | 16SB | 2325 | 7/7 | 0.98 | 0.09 | 84,96,101,124 | 0 |
| 60 | OHX | 23SB | 3401 | 7/7 | 0.98 | 0.05 | 87,94,107,156 | 0 |
| 58 | MG | 23SB | 3140 | 1/1 | 0.98 | 0.04 | 44,44,44,44 | 0 |
| 60 | OHX | 16SB | 2330 | 7/7 | 0.98 | 0.07 | 85,93,109,126 | 0 |
| 60 | OHX | 23SB | 3404 | 7/7 | 0.98 | 0.06 | 70,80,97,130 | 0 |
| 60 | OHX | 16SB | 2331 | 7/7 | 0.98 | 0.06 | 97,100,108,156 | 0 |
| 60 | OHX | 16SB | 2332 | 7/7 | 0.98 | 0.08 | 99,104,117,138 | 0 |
| 58 | MG | 23SA | 3277 | 1/1 | 0.98 | 0.07 | 59,59,59,59 | 0 |
| 58 | MG | 23SB | 3142 | 1/1 | 0.98 | 0.06 | 50,50,50,50 | 0 |
| 58 | MG | 23SA | 3313 | 1/1 | 0.98 | 0.12 | 86,86,86,86 | 0 |
| 60 | OHX | 16SB | 2337 | 7/7 | 0.98 | 0.05 | 90,94,105,154 | 0 |
| 58 | MG | 23SA | 3244 | 1/1 | 0.98 | 0.06 | 20,20,20,20 | 0 |
| 60 | OHX | 23SB | 3412 | 7/7 | 0.98 | 0.06 | 104,109,121,169 | 0 |
| 60 | OHX | 16SB | 2339 | 7/7 | 0.98 | 0.05 | 88,95,111,154 | 0 |
| 58 | MG | 23SA | 3183 | 1/1 | 0.98 | 0.06 | 50,50,50,50 | 0 |
| 58 | MG | 23SB | 3203 | 1/1 | 0.98 | 0.05 | 53,53,53,53 | 0 |
| 58 | MG | 23SA | 3221 | 1/1 | 0.98 | 0.07 | 60,60,60,60 | 0 |
| 59 | K | 16SA | 2306 | 1/1 | 0.98 | 0.09 | 69,69,69,69 | 0 |
| 60 | OHX | 16SB | 2344 | 7/7 | 0.98 | 0.05 | 101,109,122,168 | 0 |
| 60 | OHX | 23SB | 3419 | 7/7 | 0.98 | 0.08 | 79,86,91,139 | 0 |
| 58 | MG | 23SA | 3222 | 1/1 | 0.98 | 0.05 | 32,32,32,32 | 0 |
| 58 | MG | 23SB | 3151 | 1/1 | 0.98 | 0.11 | 33,33,33,33 | 0 |
| 60 | OHX | 23SB | 3422 | 7/7 | 0.98 | 0.05 | 81,92,100,148 | 0 |
| 58 | MG | 23SB | 3152 | 1/1 | 0.98 | 0.06 | 53,53,53,53 | 0 |
| 58 | MG | 16SA | 2209 | 1/1 | 0.98 | 0.11 | 62,62,62,62 | 0 |
| 58 | MG | 23SB | 3209 | 1/1 | 0.98 | 0.04 | 59,59,59,59 | 0 |
| 58 | MG | 23SB | 3211 | 1/1 | 0.98 | 0.04 | 41,41,41,41 | 0 |
| 60 | OHX | 23SB | 3427 | 7/7 | 0.98 | 0.06 | 78,91,105,136 | 0 |
| 58 | MG | 23SB | 3154 | 1/1 | 0.98 | 0.04 | 55,55,55,55 | 0 |
| 58 | MG | 23SB | 3155 | 1/1 | 0.98 | 0.05 | 73,73,73,73 | 0 |
| 58 | MG | 23SB | 3214 | 1/1 | 0.98 | 0.06 | 69,69,69,69 | 0 |
| 59 | K | 23SA | 3370 | 1/1 | 0.98 | 0.02 | 61,61,61,61 | 0 |
| 59 | K | 23SA | 3371 | 1/1 | 0.98 | 0.03 | 41,41,41,41 | 0 |
| 60 | OHX | 16SA | 2343 | 7/7 | 0.98 | 0.08 | 81,94,106,121 | 0 |
| 60 | OHX | 16SA | 2346 | 7/7 | 0.98 | 0.07 | 78,80,100,113 | 0 |
| 58 | MG | 23SA | 3205 | 1/1 | 0.98 | 0.06 | 39,39,39,39 | 0 |
| 60 | OHX | 23SA | 3437 | 7/7 | 0.98 | 0.17 | 54,56,72,138 | 0 |
| 60 | OHX | 23SB | 3437 | 7/7 | 0.98 | 0.05 | 93,101,104,163 | 0 |
| 60 | OHX | 23SA | 3440 | 7/7 | 0.98 | 0.14 | 43,67,70,125 | 0 |
| 60 | OHX | 23SA | 3441 | 7/7 | 0.98 | 0.12 | 78,81,98,141 | 0 |

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| Mol | Type | Chain | Res | Atoms | RSCC | RSR | B-factors(Å$^2$) | Q<0.9 |
|---|---|---|---|---|---|---|---|---|
| 60 | OHX | 16SB | 2362 | 7/7 | 0.98 | 0.06 | 94,96,112,155 | 0 |
| 60 | OHX | 23SA | 3453 | 7/7 | 0.98 | 0.09 | 63,75,88,98 | 0 |
| 58 | MG | 23SA | 3284 | 1/1 | 0.98 | 0.05 | 42,42,42,42 | 0 |
| 60 | OHX | 23SA | 3457 | 7/7 | 0.98 | 0.07 | 50,69,94,96 | 0 |
| 60 | OHX | 23SA | 3458 | 7/7 | 0.98 | 0.06 | 60,71,82,107 | 0 |
| 60 | OHX | 16SA | 2349 | 7/7 | 0.98 | 0.07 | 90,104,118,118 | 0 |
| 60 | OHX | 23SA | 3460 | 7/7 | 0.98 | 0.06 | 66,80,100,111 | 0 |
| 60 | OHX | 23SA | 3461 | 7/7 | 0.98 | 0.06 | 70,73,97,117 | 0 |
| 60 | OHX | 23SA | 3463 | 7/7 | 0.98 | 0.09 | 35,55,79,103 | 0 |
| 60 | OHX | 23SA | 3464 | 7/7 | 0.98 | 0.08 | 70,74,94,129 | 0 |
| 60 | OHX | 16SA | 2350 | 7/7 | 0.98 | 0.06 | 100,101,107,154 | 0 |
| 58 | MG | 23SA | 3253 | 1/1 | 0.98 | 0.09 | 29,29,29,29 | 0 |
| 60 | OHX | 16SA | 2352 | 7/7 | 0.98 | 0.07 | 78,83,104,130 | 0 |
| 60 | OHX | 23SA | 3469 | 7/7 | 0.98 | 0.09 | 60,67,79,108 | 0 |
| 58 | MG | 23SA | 3256 | 1/1 | 0.98 | 0.06 | 34,34,34,34 | 0 |
| 60 | OHX | 23SA | 3471 | 7/7 | 0.98 | 0.07 | 72,75,95,114 | 0 |
| 60 | OHX | 23SA | 3472 | 7/7 | 0.98 | 0.07 | 57,69,75,136 | 0 |
| 60 | OHX | 23SA | 3581 | 7/7 | 0.98 | 0.06 | 83,96,108,158 | 0 |
| 60 | OHX | 23SA | 3474 | 7/7 | 0.98 | 0.05 | 85,92,102,143 | 0 |
| 60 | OHX | 23SA | 3583 | 7/7 | 0.98 | 0.05 | 86,90,110,172 | 0 |
| 60 | OHX | 23SA | 3475 | 7/7 | 0.98 | 0.08 | 69,79,97,138 | 0 |
| 60 | OHX | 23SA | 3476 | 7/7 | 0.98 | 0.06 | 76,91,98,125 | 0 |
| 60 | OHX | 16SA | 2354 | 7/7 | 0.98 | 0.06 | 84,96,105,152 | 0 |
| 58 | MG | 23SA | 3053 | 1/1 | 0.98 | 0.30 | 36,36,36,36 | 0 |
| 59 | K | 23SA | 3377 | 1/1 | 0.98 | 0.06 | 38,38,38,38 | 0 |
| 58 | MG | 23SA | 3288 | 1/1 | 0.98 | 0.04 | 44,44,44,44 | 0 |
| 58 | MG | 23SA | 3228 | 1/1 | 0.98 | 0.04 | 56,56,56,56 | 0 |
| 60 | OHX | 23SA | 3482 | 7/7 | 0.98 | 0.12 | 64,70,94,116 | 0 |
| 58 | MG | 23SA | 3290 | 1/1 | 0.98 | 0.05 | 50,50,50,50 | 0 |
| 60 | OHX | 23SA | 3485 | 7/7 | 0.98 | 0.06 | 80,92,101,147 | 0 |
| 58 | MG | 23SA | 3329 | 1/1 | 0.98 | 0.09 | 49,49,49,49 | 0 |
| 58 | MG | 23SA | 3331 | 1/1 | 0.98 | 0.14 | 42,42,42,42 | 0 |
| 60 | OHX | 23SA | 3488 | 7/7 | 0.98 | 0.07 | 76,78,90,125 | 0 |
| 58 | MG | 23SB | 3167 | 1/1 | 0.98 | 0.07 | 50,50,50,50 | 0 |
| 60 | OHX | 23SA | 3490 | 7/7 | 0.98 | 0.06 | 86,96,102,157 | 0 |
| 60 | OHX | 23SA | 3491 | 7/7 | 0.98 | 0.07 | 74,84,104,130 | 0 |
| 58 | MG | 23SB | 3226 | 1/1 | 0.98 | 0.08 | 76,76,76,76 | 0 |
| 60 | OHX | 23SA | 3493 | 7/7 | 0.98 | 0.07 | 78,81,99,132 | 0 |
| 58 | MG | 23SB | 3168 | 1/1 | 0.98 | 0.04 | 45,45,45,45 | 0 |
| 58 | MG | 23SB | 3228 | 1/1 | 0.98 | 0.05 | 91,91,91,91 | 0 |
| 58 | MG | 16SA | 2268 | 1/1 | 0.98 | 0.04 | 50,50,50,50 | 0 |
| 58 | MG | 23SA | 3333 | 1/1 | 0.98 | 0.07 | 95,95,95,95 | 0 |

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| Mol | Type | Chain | Res | Atoms | RSCC | RSR | B-factors(Å$^2$) | Q<0.9 |
|---|---|---|---|---|---|---|---|---|
| 58 | MG | 23SB | 3171 | 1/1 | 0.98 | 0.05 | 42,42,42,42 | 0 |
| 60 | OHX | 23SA | 3500 | 7/7 | 0.98 | 0.08 | 76,80,87,134 | 0 |
| 60 | OHX | PSIB | 104 | 7/7 | 0.98 | 0.07 | 100,109,114,132 | 0 |
| 58 | MG | 23SA | 3231 | 1/1 | 0.98 | 0.06 | 78,78,78,78 | 0 |
| 60 | OHX | 23SA | 3502 | 7/7 | 0.98 | 0.07 | 74,89,108,136 | 0 |
| 58 | MG | 23SA | 3262 | 1/1 | 0.98 | 0.04 | 63,63,63,63 | 0 |
| 59 | K | 23SA | 3392 | 1/1 | 0.98 | 0.03 | 47,47,47,47 | 0 |
| 58 | MG | 23SA | 3209 | 1/1 | 0.98 | 0.06 | 48,48,48,48 | 0 |
| 60 | OHX | 23SB | 3332 | 7/7 | 0.98 | 0.07 | 75,95,101,131 | 0 |
| 60 | OHX | 16SA | 2374 | 7/7 | 0.98 | 0.08 | 78,87,97,143 | 0 |
| 60 | OHX | 23SA | 3507 | 7/7 | 0.98 | 0.06 | 91,98,112,138 | 0 |
| 60 | OHX | 23SB | 3343 | 7/7 | 0.98 | 0.07 | 65,75,88,109 | 0 |
| 59 | K | 23SB | 3284 | 1/1 | 0.98 | 0.03 | 64,64,64,64 | 0 |
| 60 | OHX | 23SB | 3345 | 7/7 | 0.98 | 0.09 | 66,76,89,118 | 0 |
| 58 | MG | 16SA | 2215 | 1/1 | 0.98 | 0.21 | 40,40,40,40 | 0 |
| 60 | OHX | 23SB | 3348 | 7/7 | 0.98 | 0.12 | 64,74,82,129 | 0 |
| 58 | MG | 5SA | 206 | 1/1 | 0.98 | 0.09 | 75,75,75,75 | 0 |
| 60 | OHX | 23SB | 3350 | 7/7 | 0.98 | 0.08 | 78,81,103,108 | 0 |
| 58 | MG | 23SA | 3297 | 1/1 | 0.98 | 0.06 | 59,59,59,59 | 0 |
| 60 | OHX | 23SB | 3353 | 7/7 | 0.98 | 0.06 | 86,93,106,141 | 0 |
| 58 | MG | 23SB | 3179 | 1/1 | 0.98 | 0.06 | 47,47,47,47 | 0 |
| 60 | OHX | 23SB | 3356 | 7/7 | 0.98 | 0.07 | 75,88,102,144 | 0 |
| 58 | MG | 23SB | 3239 | 1/1 | 0.98 | 0.07 | 85,85,85,85 | 0 |
| 58 | MG | 16SA | 2270 | 1/1 | 0.98 | 0.06 | 73,73,73,73 | 0 |
| 58 | MG | 23SA | 3212 | 1/1 | 0.98 | 0.05 | 56,56,56,56 | 0 |
| 60 | OHX | 23SB | 3360 | 7/7 | 0.98 | 0.06 | 90,95,105,131 | 0 |
| 58 | MG | 23SA | 3269 | 1/1 | 0.98 | 0.04 | 52,52,52,52 | 0 |
| 60 | OHX | 23SB | 3362 | 7/7 | 0.98 | 0.05 | 91,96,101,157 | 0 |
| 60 | OHX | 23SB | 3363 | 7/7 | 0.98 | 0.07 | 67,75,85,121 | 0 |
| 59 | K | 23SB | 3293 | 1/1 | 0.98 | 0.06 | 67,67,67,67 | 0 |
| 60 | OHX | 23SA | 3518 | 7/7 | 0.98 | 0.07 | 60,64,93,123 | 0 |
| 60 | OHX | 23SB | 3367 | 7/7 | 0.98 | 0.10 | 68,73,95,125 | 0 |
| 60 | OHX | 23SB | 3368 | 7/7 | 0.98 | 0.07 | 79,91,110,135 | 0 |
| 58 | MG | 5SB | 204 | 1/1 | 0.98 | 0.04 | 81,81,81,81 | 0 |
| 60 | OHX | 23SB | 3370 | 7/7 | 0.98 | 0.10 | 69,86,96,123 | 0 |
| 60 | OHX | 5SB | 207 | 7/7 | 0.98 | 0.08 | 80,94,115,116 | 0 |
| 58 | MG | 23SA | 3057 | 1/1 | 0.98 | 0.05 | 45,45,45,45 | 0 |
| 58 | MG | 23SA | 3021 | 1/1 | 0.98 | 0.16 | 43,43,43,43 | 0 |
| 60 | OHX | 23SA | 3522 | 7/7 | 0.98 | 0.05 | 88,94,101,161 | 0 |
| 58 | MG | 23SA | 3304 | 1/1 | 0.98 | 0.04 | 39,39,39,39 | 0 |
| 59 | K | 23SA | 3406 | 1/1 | 0.98 | 0.09 | 60,60,60,60 | 0 |
| 60 | OHX | 23SB | 3376 | 7/7 | 0.98 | 0.07 | 89,92,107,148 | 0 |

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| Mol | Type | Chain | Res | Atoms | RSCC | RSR | B-factors(Å$^2$) | Q<0.9 |
|---|---|---|---|---|---|---|---|---|
| 60 | OHX | 23SB | 3377 | 7/7 | 0.98 | 0.06 | 76,93,102,145 | 0 |
| 58 | MG | 23SB | 3187 | 1/1 | 0.98 | 0.09 | 54,54,54,54 | 0 |
| 60 | OHX | 23SB | 3379 | 7/7 | 0.98 | 0.06 | 92,100,107,135 | 0 |
| 60 | OHX | 23SB | 3380 | 7/7 | 0.98 | 0.07 | 86,93,108,134 | 0 |
| 60 | OHX | 23SA | 3526 | 7/7 | 0.98 | 0.06 | 68,76,93,135 | 0 |
| 60 | OHX | 5SA | 209 | 7/7 | 0.98 | 0.08 | 73,79,90,91 | 0 |
| 58 | MG | 23SA | 3330 | 1/1 | 0.99 | 0.03 | 47,47,47,47 | 0 |
| 60 | OHX | 16SA | 2337 | 7/7 | 0.99 | 0.09 | 67,67,82,96 | 0 |
| 60 | OHX | 16SA | 2338 | 7/7 | 0.99 | 0.10 | 64,86,90,90 | 0 |
| 60 | OHX | 23SB | 3347 | 7/7 | 0.99 | 0.06 | 72,78,92,131 | 0 |
| 60 | OHX | 16SA | 2339 | 7/7 | 0.99 | 0.09 | 60,69,87,91 | 0 |
| 60 | OHX | 23SA | 3462 | 7/7 | 0.99 | 0.06 | 61,68,88,100 | 0 |
| 60 | OHX | 16SA | 2340 | 7/7 | 0.99 | 0.07 | 74,81,92,100 | 0 |
| 60 | OHX | 23SB | 3351 | 7/7 | 0.99 | 0.08 | 68,84,98,103 | 0 |
| 60 | OHX | 16SA | 2341 | 7/7 | 0.99 | 0.06 | 82,101,107,124 | 0 |
| 58 | MG | 23SA | 3225 | 1/1 | 0.99 | 0.07 | 60,60,60,60 | 0 |
| 60 | OHX | 23SB | 3354 | 7/7 | 0.99 | 0.07 | 83,92,96,126 | 0 |
| 58 | MG | 16SA | 2264 | 1/1 | 0.99 | 0.03 | 45,45,45,45 | 0 |
| 60 | OHX | 23SA | 3467 | 7/7 | 0.99 | 0.06 | 67,87,98,117 | 0 |
| 60 | OHX | 16SA | 2344 | 7/7 | 0.99 | 0.06 | 78,92,99,110 | 0 |
| 60 | OHX | 16SA | 2345 | 7/7 | 0.99 | 0.06 | 85,99,115,130 | 0 |
| 58 | MG | 23SA | 3260 | 1/1 | 0.99 | 0.05 | 44,44,44,44 | 0 |
| 58 | MG | 23SA | 3227 | 1/1 | 0.99 | 0.04 | 68,68,68,68 | 0 |
| 59 | K | 23SB | 3255 | 1/1 | 0.99 | 0.04 | 51,51,51,51 | 0 |
| 60 | OHX | 23SA | 3473 | 7/7 | 0.99 | 0.05 | 72,78,93,118 | 0 |
| 58 | MG | 23SA | 3192 | 1/1 | 0.99 | 0.09 | 40,40,40,40 | 0 |
| 58 | MG | 23SB | 3163 | 1/1 | 0.99 | 0.06 | 45,45,45,45 | 0 |
| 60 | OHX | 23SB | 3365 | 7/7 | 0.99 | 0.05 | 102,104,111,148 | 0 |
| 58 | MG | 23SA | 3229 | 1/1 | 0.99 | 0.05 | 69,69,69,69 | 0 |
| 58 | MG | 23SA | 3201 | 1/1 | 0.99 | 0.04 | 36,36,36,36 | 0 |
| 58 | MG | 5SA | 204 | 1/1 | 0.99 | 0.03 | 60,60,60,60 | 0 |
| 58 | MG | 5SA | 205 | 1/1 | 0.99 | 0.04 | 54,54,54,54 | 0 |
| 58 | MG | 23SA | 3219 | 1/1 | 0.99 | 0.05 | 46,46,46,46 | 0 |
| 58 | MG | 23SA | 3266 | 1/1 | 0.99 | 0.09 | 45,45,45,45 | 0 |
| 58 | MG | 23SA | 3267 | 1/1 | 0.99 | 0.04 | 43,43,43,43 | 0 |
| 58 | MG | L4A | 302 | 1/1 | 0.99 | 0.04 | 72,72,72,72 | 0 |
| 60 | OHX | 23SA | 3484 | 7/7 | 0.99 | 0.06 | 68,80,83,121 | 0 |
| 58 | MG | 23SA | 3246 | 1/1 | 0.99 | 0.04 | 41,41,41,41 | 0 |
| 58 | MG | 23SB | 3210 | 1/1 | 0.99 | 0.09 | 73,73,73,73 | 0 |
| 58 | MG | 23SA | 3193 | 1/1 | 0.99 | 0.05 | 46,46,46,46 | 0 |
| 58 | MG | 23SB | 3139 | 1/1 | 0.99 | 0.03 | 42,42,42,42 | 0 |
| 58 | MG | 23SA | 3292 | 1/1 | 0.99 | 0.07 | 55,55,55,55 | 0 |

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| Mol | Type | Chain | Res | Atoms | RSCC | RSR | B-factors(Å$^2$) | Q<0.9 |
|---|---|---|---|---|---|---|---|---|
| 58 | MG | 23SB | 3176 | 1/1 | 0.99 | 0.03 | 44,44,44,44 | 0 |
| 58 | MG | 23SA | 3195 | 1/1 | 0.99 | 0.05 | 33,33,33,33 | 0 |
| 58 | MG | 23SA | 3196 | 1/1 | 0.99 | 0.09 | 65,65,65,65 | 0 |
| 60 | OHX | 16SA | 2367 | 7/7 | 0.99 | 0.06 | 88,96,101,142 | 0 |
| 60 | OHX | 23SA | 3494 | 7/7 | 0.99 | 0.06 | 48,58,79,112 | 0 |
| 58 | MG | 23SB | 3143 | 1/1 | 0.99 | 0.06 | 46,46,46,46 | 0 |
| 58 | MG | 23SB | 3180 | 1/1 | 0.99 | 0.06 | 42,42,42,42 | 0 |
| 58 | MG | 23SA | 3250 | 1/1 | 0.99 | 0.06 | 49,49,49,49 | 0 |
| 60 | OHX | ASIA | 101 | 7/7 | 0.99 | 0.06 | 94,101,119,138 | 0 |
| 58 | MG | L27A | 102 | 1/1 | 0.99 | 0.04 | 63,63,63,63 | 0 |
| 58 | MG | 23SB | 3146 | 1/1 | 0.99 | 0.09 | 61,61,61,61 | 0 |
| 60 | OHX | PSIA | 105 | 7/7 | 0.99 | 0.06 | 84,94,100,118 | 0 |
| 58 | MG | 23SA | 3251 | 1/1 | 0.99 | 0.10 | 39,39,39,39 | 0 |
| 58 | MG | 23SA | 3235 | 1/1 | 0.99 | 0.06 | 38,38,38,38 | 0 |
| 58 | MG | 23SB | 3149 | 1/1 | 0.99 | 0.11 | 64,64,64,64 | 0 |
| 58 | MG | 23SA | 3184 | 1/1 | 0.99 | 0.04 | 23,23,23,23 | 0 |
| 58 | MG | 23SA | 3299 | 1/1 | 0.99 | 0.03 | 58,58,58,58 | 0 |
| 60 | OHX | 23SA | 3438 | 7/7 | 0.99 | 0.10 | 37,46,60,76 | 0 |
| 58 | MG | 23SA | 3254 | 1/1 | 0.99 | 0.03 | 46,46,46,46 | 0 |
| 58 | MG | 23SA | 3326 | 1/1 | 0.99 | 0.06 | 60,60,60,60 | 0 |
| 60 | OHX | L4A | 304 | 7/7 | 0.99 | 0.20 | 33,37,51,146 | 0 |
| 60 | OHX | 23SA | 3442 | 7/7 | 0.99 | 0.10 | 56,63,82,104 | 0 |
| 60 | OHX | L17A | 202 | 7/7 | 0.99 | 0.08 | 61,71,78,89 | 0 |
| 60 | OHX | L19A | 201 | 7/7 | 0.99 | 0.06 | 79,85,96,119 | 0 |
| 60 | OHX | 23SA | 3443 | 7/7 | 0.99 | 0.09 | 44,56,64,99 | 0 |
| 60 | OHX | 23SA | 3444 | 7/7 | 0.99 | 0.07 | 59,69,82,94 | 0 |
| 60 | OHX | 23SA | 3446 | 7/7 | 0.99 | 0.06 | 56,65,79,90 | 0 |
| 60 | OHX | 23SA | 3447 | 7/7 | 0.99 | 0.11 | 49,60,75,116 | 0 |
| 60 | OHX | 16SB | 2322 | 7/7 | 0.99 | 0.08 | 72,83,93,94 | 0 |
| 60 | OHX | 16SB | 2323 | 7/7 | 0.99 | 0.08 | 77,87,98,102 | 0 |
| 60 | OHX | 16SB | 2324 | 7/7 | 0.99 | 0.07 | 86,88,100,108 | 0 |
| 60 | OHX | 23SA | 3448 | 7/7 | 0.99 | 0.06 | 60,70,78,91 | 0 |
| 60 | OHX | 16SB | 2326 | 7/7 | 0.99 | 0.06 | 96,105,113,125 | 0 |
| 60 | OHX | 16SB | 2327 | 7/7 | 0.99 | 0.06 | 87,94,111,120 | 0 |
| 60 | OHX | 23SA | 3449 | 7/7 | 0.99 | 0.08 | 69,80,87,90 | 0 |
| 60 | OHX | 16SB | 2329 | 7/7 | 0.99 | 0.06 | 67,78,92,96 | 0 |
| 60 | OHX | 23SA | 3450 | 7/7 | 0.99 | 0.07 | 77,87,96,98 | 0 |
| 60 | OHX | 23SA | 3451 | 7/7 | 0.99 | 0.08 | 63,74,84,95 | 0 |
| 60 | OHX | 23SA | 3452 | 7/7 | 0.99 | 0.07 | 54,64,86,94 | 0 |
| 60 | OHX | 16SB | 2333 | 7/7 | 0.99 | 0.05 | 92,96,103,121 | 0 |
| 60 | OHX | 23SB | 3324 | 7/7 | 0.99 | 0.14 | 37,44,75,112 | 0 |
| 58 | MG | 23SA | 3255 | 1/1 | 0.99 | 0.03 | 72,72,72,72 | 0 |

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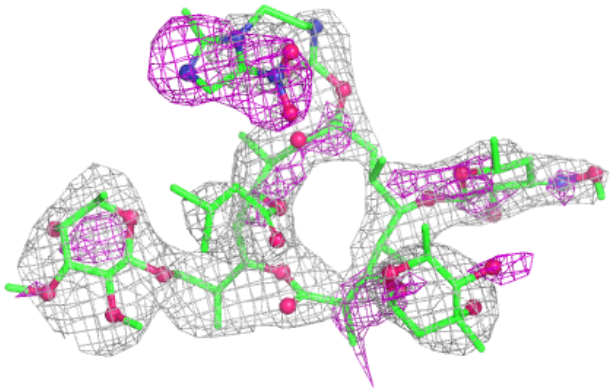
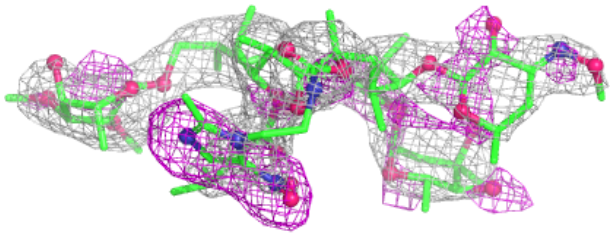
| Mol | Type | Chain | Res | Atoms | RSCC | RSR | B-factors(Å$^2$) | Q<0.9 |
|---|---|---|---|---|---|---|---|---|
| 60 | OHX | 23SB | 3328 | 7/7 | 0.99 | 0.10 | 53,62,75,105 | 0 |
| 60 | OHX | 23SB | 3329 | 7/7 | 0.99 | 0.08 | 65,75,94,96 | 0 |
| 60 | OHX | 23SB | 3330 | 7/7 | 0.99 | 0.05 | 58,71,85,87 | 0 |
| 60 | OHX | 23SB | 3331 | 7/7 | 0.99 | 0.07 | 83,87,102,104 | 0 |
| 58 | MG | 23SA | 3215 | 1/1 | 0.99 | 0.04 | 47,47,47,47 | 0 |
| 60 | OHX | 23SB | 3334 | 7/7 | 0.99 | 0.08 | 72,79,82,102 | 0 |
| 60 | OHX | 23SA | 3455 | 7/7 | 0.99 | 0.08 | 56,72,90,98 | 0 |
| 60 | OHX | 23SB | 3336 | 7/7 | 0.99 | 0.06 | 58,76,89,104 | 0 |
| 60 | OHX | 23SB | 3337 | 7/7 | 0.99 | 0.06 | 79,83,95,96 | 0 |
| 60 | OHX | 23SB | 3338 | 7/7 | 0.99 | 0.07 | 74,84,95,113 | 0 |
| 60 | OHX | 23SB | 3339 | 7/7 | 0.99 | 0.08 | 95,104,111,114 | 0 |
| 60 | OHX | L17B | 201 | 7/7 | 0.99 | 0.10 | 67,75,89,93 | 0 |
| 60 | OHX | 23SB | 3340 | 7/7 | 0.99 | 0.07 | 79,82,103,105 | 0 |
| 60 | OHX | 23SB | 3341 | 7/7 | 0.99 | 0.06 | 72,88,98,114 | 0 |
| 60 | OHX | 23SA | 3456 | 7/7 | 0.99 | 0.07 | 69,75,93,104 | 0 |
| 58 | MG | 23SA | 3238 | 1/1 | 0.99 | 0.03 | 33,33,33,33 | 0 |
| 60 | OHX | 23SB | 3327 | 7/7 | 1.00 | 0.08 | 67,73,94,97 | 0 |
| 58 | MG | 23SA | 3317 | 1/1 | 1.00 | 0.03 | 52,52,52,52 | 0 |
| 58 | MG | L3A | 302 | 1/1 | 1.00 | 0.01 | 29,29,29,29 | 0 |
| 60 | OHX | 23SA | 3439 | 7/7 | 1.00 | 0.06 | 65,75,79,85 | 0 |
| 58 | MG | 23SA | 3200 | 1/1 | 1.00 | 0.09 | 39,39,39,39 | 0 |
| 58 | MG | 23SA | 3208 | 1/1 | 1.00 | 0.07 | 33,33,33,33 | 0 |
| 60 | OHX | 23SB | 3333 | 7/7 | 1.00 | 0.05 | 67,70,73,93 | 0 |
| 58 | MG | 23SA | 3204 | 1/1 | 1.00 | 0.02 | 32,32,32,32 | 0 |
| 58 | MG | 23SA | 3194 | 1/1 | 1.00 | 0.04 | 33,33,33,33 | 0 |
| 58 | MG | 23SA | 3182 | 1/1 | 1.00 | 0.07 | 46,46,46,46 | 0 |
| 60 | OHX | 23SB | 3325 | 7/7 | 1.00 | 0.10 | 57,58,71,96 | 0 |
| 60 | OHX | 23SA | 3445 | 7/7 | 1.00 | 0.06 | 58,63,73,86 | 0 |

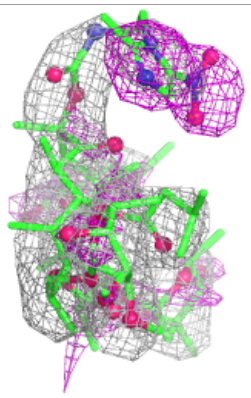
The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation to approximate a three-dimensional view.

**Electron density around SJH 23SB 3323:**

$2mF_o$-$DF_c$ (at 0.7 rmsd) in gray
$mF_o$-$DF_c$ (at 3 rmsd) in purple (negative) and green (positive)

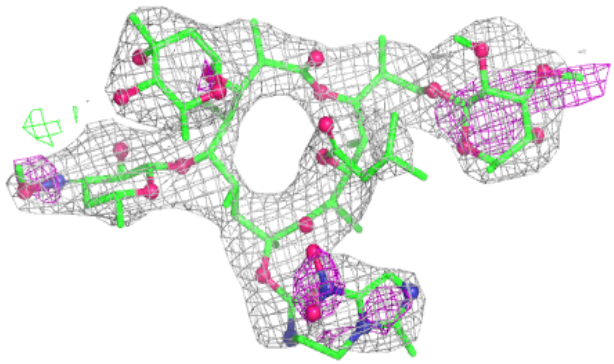


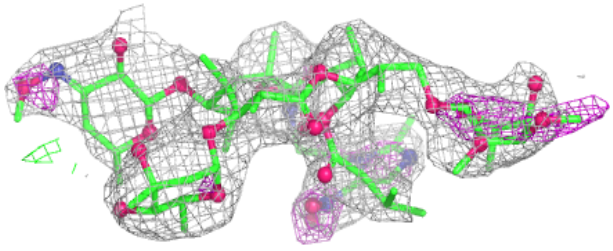


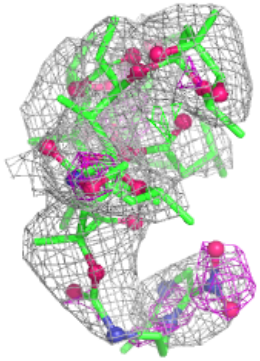


**Electron density around SJH 23SA 3436:**

$2mF_o$-$DF_c$ (at 0.7 rmsd) in gray
$mF_o$-$DF_c$ (at 3 rmsd) in purple (negative) and green (positive)







## 6.5 Other polymers (i)

There are no such residues in this entry.