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

Nov 6, 2023 – 02:21 PM EST

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|---|---|---|
| PDB ID | : | 6UCQ |
| Title | : | Crystal structure of the Thermus thermophilus 70S ribosome recycling complex |
| Authors | : | Zhou, D.; Tanzawa, T.; Gagnon, M.G.; Lin, J. |
| Deposited on | : | 2019-09-17 |
| Resolution | : | 3.50 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:

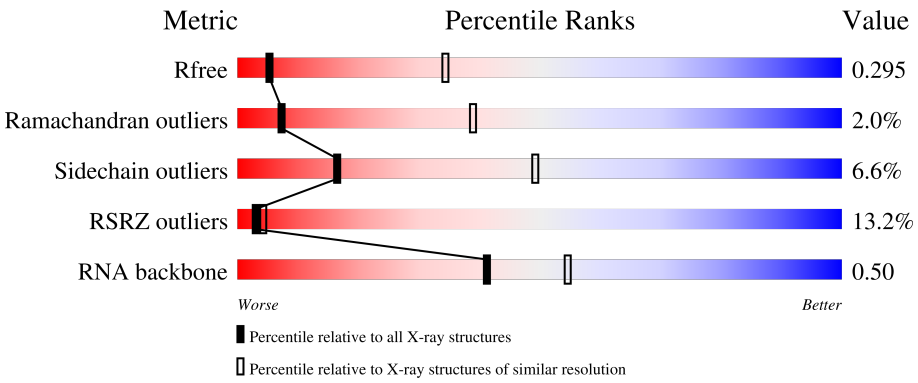
| | | |
|---|---|---|
| MolProbity | : | 4.02b-467 |
| Mogul | : | 1.8.5 (274361), CSD as541be (2020) |
| Xtriage (Phenix) | : | 1.13 |
| EDS | : | 2.36 |
| buster-report | : | 1.1.7 (2018) |
| Percentile statistics | : | 20191225.v01 (using entries in the PDB archive December 25th 2019) |
| Refmac | : | 5.8.0158 |
| CCP4 | : | 7.0.044 (Gargrove) |
| Ideal geometry (proteins) | : | Engh & Huber (2001) |
| Ideal geometry (DNA, RNA) | : | Parkinson et al. (1996) |
| Validation Pipeline (wwPDB-VP) | : | 2.36 |

# 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 3.50 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)) |
|---|---|---|
| $R_{free}$ | 130704 | 1659 (3.60-3.40) |
| Ramachandran outliers | 138981 | 1005 (3.58-3.42) |
| Sidechain outliers | 138945 | 1006 (3.58-3.42) |
| RSRZ outliers | 127900 | 1559 (3.60-3.40) |
| RNA backbone | 3102 | 1002 (4.00-3.00) |

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 | 1A | 2915 | 2% 79% 19% • • |
| 1 | 2A | 2915 | 4% 78% 17% • |
| 2 | 1B | 121 | 86% 13% • |
| 2 | 2B | 121 | % 78% 21% • |
| 3 | 1D | 276 | 6% 92% 8% |

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| Mol | Chain | Length | Quality of chain |
|---|---|---|---|
| 3 | 2D | 276 | 11% 93% 7% |
| 4 | 1E | 206 | 29% 89% 10% |
| 4 | 2E | 206 | 3% 93% 6% |
| 5 | 1F | 210 | 4% 90% 7% |
| 5 | 2F | 210 | 8% 94% |
| 6 | 1G | 182 | % 93% 6% |
| 6 | 2G | 182 | 34% 93% 6% |
| 7 | 1H | 180 | 92% |
| 7 | 2H | 180 | 21% 93% |
| 8 | 1N | 140 | 3% 91% 9% |
| 8 | 2N | 140 | 19% 94% 6% |
| 9 | 1O | 122 | 53% 93% 7% |
| 9 | 2O | 122 | 49% 98% |
| 10 | 1P | 150 | 3% 93% 7% |
| 10 | 2P | 150 | 26% 95% 5% |
| 11 | 1Q | 141 | 95% 5% |
| 11 | 2Q | 141 | 32% 95% 5% |
| 12 | 1R | 118 | 3% 84% 15% |
| 12 | 2R | 118 | 2% 95% 5% |
| 13 | 1S | 112 | 90% 8% |
| 13 | 2S | 112 | 2% 91% 7% |
| 14 | 1T | 146 | 32% 84% 6% 10% |
| 14 | 2T | 146 | 15% 86% 10% |
| 15 | 1U | 118 | 2% 94% |
| 15 | 2U | 118 | 6% 96% |

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| Mol | Chain | Length | Quality of chain |
|---|---|---|---|
| 16 | 1V | 101 | %, 90%, 10% |
| 16 | 2V | 101 | 12%, 97% |
| 17 | 1W | 113 | 7%, 93%, 6% |
| 17 | 2W | 113 | 89%, 10% |
| 18 | 1X | 96 | 2%, 93%, 6% |
| 18 | 2X | 96 | 94%, 5% |
| 19 | 1Y | 110 | %, 88%, 9% |
| 19 | 2Y | 110 | 11%, 92%, 5% |
| 20 | 1Z | 206 | 86%, 13% |
| 20 | 2Z | 206 | 20%, 86%, 12% |
| 21 | 10 | 85 | %, 87%, 12% |
| 21 | 20 | 85 | 29%, 85%, 12% |
| 22 | 11 | 98 | 15%, 94%, 5% |
| 22 | 21 | 98 | 42%, 93%, 6% |
| 23 | 12 | 72 | 89%, 6% |
| 23 | 22 | 72 | %, 96% |
| 24 | 13 | 60 | 3%, 87%, 12% |
| 24 | 23 | 60 | 17%, 93%, 5% |
| 25 | 14 | 71 | 79%, 17% |
| 25 | 24 | 71 | 20%, 83%, 14% |
| 26 | 15 | 60 | 13%, 93%, 5% |
| 26 | 25 | 60 | 93%, 5% |
| 27 | 16 | 54 | 2%, 93%, 6% |
| 27 | 26 | 54 | 74%, 94% |
| 28 | 17 | 49 | 4%, 90%, 8% |

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| Mol | Chain | Length | Quality of chain |
|---|---|---|---|
| 28 | 27 | 49 | 4% 86% 12% |
| 29 | 18 | 65 | 6% 91% 8% |
| 29 | 28 | 65 | 60% 98% |
| 30 | 19 | 37 | 97% |
| 30 | 29 | 37 | 22% 92% 8% |
| 31 | 1a | 1521 | 6% 82% 16% |
| 31 | 2a | 1521 | 7% 82% 17% |
| 32 | 1b | 256 | 4% 84% 6% 10% |
| 32 | 2b | 256 | 4% 84% 6% 10% |
| 33 | 1c | 239 | 54% 83% 14% |
| 33 | 2c | 239 | 47% 83% 14% |
| 34 | 1d | 209 | 9% 93% 6% |
| 34 | 2d | 209 | 11% 96% |
| 35 | 1e | 162 | 14% 88% 9% |
| 35 | 2e | 162 | 31% 87% 9% |
| 36 | 1f | 101 | 98% |
| 36 | 2f | 101 | 95% |
| 37 | 1g | 156 | 44% 94% 6% |
| 37 | 2g | 156 | 73% 96% |
| 38 | 1h | 138 | 4% 96% |
| 38 | 2h | 138 | 7% 94% 5% |
| 39 | 1i | 128 | 24% 95% |
| 39 | 2i | 128 | 26% 95% 5% |
| 40 | 1j | 105 | 41% 87% 6% 8% |
| 40 | 2j | 105 | 23% 88% 9% |

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| Mol | Chain | Length | Quality of chain |
|---|---|---|---|
| 41 | 1k | 129 | 35% 85% 12% |
| 41 | 2k | 129 | 47% 87% 12% |
| 42 | 1l | 132 | 13% 87% 5% 8% |
| 42 | 2l | 132 | 40% 88% 5% 8% |
| 43 | 1m | 126 | 10% 91% 6% |
| 43 | 2m | 126 | 23% 92% 5% |
| 44 | 1n | 61 | 52% 93% 5% |
| 44 | 2n | 61 | 51% 93% 5% |
| 45 | 1o | 89 | 96% |
| 45 | 2o | 89 | 6% 88% 11% |
| 46 | 1p | 88 | 6% 85% 8% 7% |
| 46 | 2p | 88 | 2% 86% 7% 7% |
| 47 | 1q | 105 | % 91% 6% |
| 47 | 2q | 105 | 46% 90% 6% |
| 48 | 1r | 88 | % 74% 23% |
| 48 | 2r | 88 | 9% 74% 23% |
| 49 | 1s | 93 | 12% 81% 9% 11% |
| 49 | 2s | 93 | 24% 84% 5% 11% |
| 50 | 1t | 106 | 3% 83% 8% 9% |
| 50 | 2t | 106 | 3% 87% 9% |
| 51 | 1u | 27 | 85% 15% |
| 51 | 2u | 27 | 19% 85% 15% |
| 52 | 1v | 758 | 11% 81% 14% |
| 52 | 2v | 758 | 31% 82% 13% |
| 53 | 1w | 185 | 8% 83% 17% |

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| Mol | Chain | Length | Quality of chain |
|---|---|---|---|
| 53 | 2w | 185 | 56% 89% 11% |
| 54 | 1x | 76 | 47% 49% 43% 5% |
| 54 | 1y | 76 | 30% 66% 30% |
| 54 | 2x | 76 | 87% 53% 41% |
| 54 | 2y | 76 | 70% 64% 32% |
| 55 | 1z | 21 | 43% 24% 24% 52% |
| 55 | 2z | 21 | 14% 19% 29% 52% |

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 |
|---|---|---|---|---|---|---|---|
| 54 | PSU | 1y | 32 | - | - | - | X |
| 54 | PSU | 2x | 32 | - | - | - | X |
| 54 | MIA | 2x | 37 | - | - | - | X |
| 54 | 7MG | 2x | 46 | - | - | - | X |
| 54 | 5MU | 2x | 54 | - | - | - | X |
| 54 | PSU | 2x | 55 | - | - | - | X |
| 54 | 4SU | 2x | 8 | - | - | - | X |
| 54 | PSU | 2y | 39 | - | - | - | X |
| 54 | 5MU | 2y | 54 | - | - | - | X |
| 54 | PSU | 2y | 55 | - | - | - | X |
| 56 | MG | 10 | 101 | - | - | - | X |
| 56 | MG | 10 | 104 | - | - | - | X |
| 56 | MG | 12 | 101 | - | - | - | X |
| 56 | MG | 13 | 301 | - | - | - | X |
| 56 | MG | 1A | 4009 | - | - | - | X |
| 56 | MG | 1A | 4012 | - | - | - | X |
| 56 | MG | 1A | 4027 | - | - | - | X |
| 56 | MG | 1A | 4036 | - | - | - | X |
| 56 | MG | 1A | 4038 | - | - | - | X |
| 56 | MG | 1A | 4047 | - | - | - | X |
| 56 | MG | 1A | 4048 | - | - | - | X |
| 56 | MG | 1A | 4052 | - | - | - | X |
| 56 | MG | 1A | 4054 | - | - | - | X |
| 56 | MG | 1A | 4060 | - | - | - | X |
| 56 | MG | 1A | 4068 | - | - | - | X |

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| Mol | Type | Chain | Res | Chirality | Geometry | Clashes | Electron density |
|---|---|---|---|---|---|---|---|
| 56 | MG | 1A | 4075 | - | - | - | X |
| 56 | MG | 1A | 4121 | - | - | - | X |
| 56 | MG | 1A | 4134 | - | - | - | X |
| 56 | MG | 1A | 4197 | - | - | - | X |
| 56 | MG | 1A | 4202 | - | - | - | X |
| 56 | MG | 1A | 4259 | - | - | - | X |
| 56 | MG | 1A | 4282 | - | - | - | X |
| 56 | MG | 1A | 4285 | - | - | - | X |
| 56 | MG | 1A | 4288 | - | - | - | X |
| 56 | MG | 1A | 4291 | - | - | - | X |
| 56 | MG | 1A | 4301 | - | - | - | X |
| 56 | MG | 1A | 4304 | - | - | - | X |
| 56 | MG | 1A | 4307 | - | - | - | X |
| 56 | MG | 1A | 4323 | - | - | - | X |
| 56 | MG | 1A | 4354 | - | - | - | X |
| 56 | MG | 1A | 4373 | - | - | - | X |
| 56 | MG | 1A | 4404 | - | - | - | X |
| 56 | MG | 1A | 4428 | - | - | - | X |
| 56 | MG | 1A | 4464 | - | - | - | X |
| 56 | MG | 1A | 4503 | - | - | - | X |
| 56 | MG | 1A | 4516 | - | - | - | X |
| 56 | MG | 1A | 4518 | - | - | - | X |
| 56 | MG | 1A | 4519 | - | - | - | X |
| 56 | MG | 1A | 4521 | - | - | - | X |
| 56 | MG | 1A | 4535 | - | - | - | X |
| 56 | MG | 1A | 4538 | - | - | - | X |
| 56 | MG | 1A | 4546 | - | - | - | X |
| 56 | MG | 1A | 4549 | - | - | - | X |
| 56 | MG | 1A | 4550 | - | - | - | X |
| 56 | MG | 1A | 4600 | - | - | - | X |
| 56 | MG | 1A | 4633 | - | - | - | X |
| 56 | MG | 1A | 4639 | - | - | - | X |
| 56 | MG | 1A | 4662 | - | - | - | X |
| 56 | MG | 1A | 4677 | - | - | - | X |
| 56 | MG | 1A | 4678 | - | - | - | X |
| 56 | MG | 1A | 4699 | - | - | - | X |
| 56 | MG | 1A | 4706 | - | - | - | X |
| 56 | MG | 1A | 4714 | - | - | - | X |
| 56 | MG | 1A | 4747 | - | - | - | X |
| 56 | MG | 1A | 4756 | - | - | - | X |
| 56 | MG | 1A | 4762 | - | - | - | X |
| 56 | MG | 1A | 4764 | - | - | - | X |

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| Mol | Type | Chain | Res | Chirality | Geometry | Clashes | Electron density |
|---|---|---|---|---|---|---|---|
| 56 | MG | 1A | 4765 | - | - | - | X |
| 56 | MG | 1A | 4772 | - | - | - | X |
| 56 | MG | 1A | 4788 | - | - | - | X |
| 56 | MG | 1A | 4790 | - | - | - | X |
| 56 | MG | 1A | 4809 | - | - | - | X |
| 56 | MG | 1A | 4861 | - | - | - | X |
| 56 | MG | 1A | 4884 | - | - | - | X |
| 56 | MG | 1A | 4888 | - | - | - | X |
| 56 | MG | 1A | 4889 | - | - | - | X |
| 56 | MG | 1A | 4895 | - | - | - | X |
| 56 | MG | 1A | 4927 | - | - | - | X |
| 56 | MG | 1A | 4933 | - | - | - | X |
| 56 | MG | 1A | 4948 | - | - | - | X |
| 56 | MG | 1A | 4960 | - | - | - | X |
| 56 | MG | 1A | 4966 | - | - | - | X |
| 56 | MG | 1A | 4973 | - | - | - | X |
| 56 | MG | 1A | 4985 | - | - | - | X |
| 56 | MG | 1A | 5006 | - | - | - | X |
| 56 | MG | 1A | 5014 | - | - | - | X |
| 56 | MG | 1A | 5033 | - | - | - | X |
| 56 | MG | 1A | 5035 | - | - | - | X |
| 56 | MG | 1B | 205 | - | - | - | X |
| 56 | MG | 1B | 212 | - | - | - | X |
| 56 | MG | 1B | 214 | - | - | - | X |
| 56 | MG | 1B | 223 | - | - | - | X |
| 56 | MG | 1D | 306 | - | - | - | X |
| 56 | MG | 1D | 308 | - | - | - | X |
| 56 | MG | 1O | 204 | - | - | - | X |
| 56 | MG | 1P | 202 | - | - | - | X |
| 56 | MG | 1Q | 201 | - | - | - | X |
| 56 | MG | 1a | 1615 | - | - | - | X |
| 56 | MG | 1a | 1621 | - | - | - | X |
| 56 | MG | 1a | 1622 | - | - | - | X |
| 56 | MG | 1a | 1629 | - | - | - | X |
| 56 | MG | 1a | 1634 | - | - | - | X |
| 56 | MG | 1a | 1642 | - | - | - | X |
| 56 | MG | 1a | 1649 | - | - | - | X |
| 56 | MG | 1a | 1669 | - | - | - | X |
| 56 | MG | 1a | 1670 | - | - | - | X |
| 56 | MG | 1a | 1682 | - | - | - | X |
| 56 | MG | 1a | 1684 | - | - | - | X |
| 56 | MG | 1a | 1685 | - | - | - | X |

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| Mol | Type | Chain | Res | Chirality | Geometry | Clashes | Electron density |
|---|---|---|---|---|---|---|---|
| 56 | MG | 1a | 1688 | - | - | - | X |
| 56 | MG | 1a | 1704 | - | - | - | X |
| 56 | MG | 1a | 1706 | - | - | - | X |
| 56 | MG | 1a | 1730 | - | - | - | X |
| 56 | MG | 1a | 1738 | - | - | - | X |
| 56 | MG | 1a | 1742 | - | - | - | X |
| 56 | MG | 1a | 1745 | - | - | - | X |
| 56 | MG | 1a | 1752 | - | - | - | X |
| 56 | MG | 1a | 1763 | - | - | - | X |
| 56 | MG | 1a | 1765 | - | - | - | X |
| 56 | MG | 1a | 1768 | - | - | - | X |
| 56 | MG | 1a | 1776 | - | - | - | X |
| 56 | MG | 1a | 1777 | - | - | - | X |
| 56 | MG | 1a | 1780 | - | - | - | X |
| 56 | MG | 1a | 1792 | - | - | - | X |
| 56 | MG | 1a | 1794 | - | - | - | X |
| 56 | MG | 1a | 1803 | - | - | - | X |
| 56 | MG | 1a | 1805 | - | - | - | X |
| 56 | MG | 1a | 1810 | - | - | - | X |
| 56 | MG | 1a | 1843 | - | - | - | X |
| 56 | MG | 1a | 1845 | - | - | - | X |
| 56 | MG | 1a | 1850 | - | - | - | X |
| 56 | MG | 1a | 1852 | - | - | - | X |
| 56 | MG | 1a | 1854 | - | - | - | X |
| 56 | MG | 1a | 1856 | - | - | - | X |
| 56 | MG | 1a | 1863 | - | - | - | X |
| 56 | MG | 1a | 1875 | - | - | - | X |
| 56 | MG | 1a | 1898 | - | - | - | X |
| 56 | MG | 1a | 1906 | - | - | - | X |
| 56 | MG | 1a | 1908 | - | - | - | X |
| 56 | MG | 1a | 1909 | - | - | - | X |
| 56 | MG | 1a | 1910 | - | - | - | X |
| 56 | MG | 1a | 1911 | - | - | - | X |
| 56 | MG | 1a | 1912 | - | - | - | X |
| 56 | MG | 1b | 304 | - | - | - | X |
| 56 | MG | 1b | 305 | - | - | - | X |
| 56 | MG | 1d | 301 | - | - | - | X |
| 56 | MG | 1m | 201 | - | - | - | X |
| 56 | MG | 1q | 201 | - | - | - | X |
| 56 | MG | 23 | 101 | - | - | - | X |
| 56 | MG | 23 | 103 | - | - | - | X |
| 56 | MG | 27 | 101 | - | - | - | X |

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| Mol | Type | Chain | Res | Chirality | Geometry | Clashes | Electron density |
|---|---|---|---|---|---|---|---|
| 56 | MG | 28 | 101 | - | - | - | X |
| 56 | MG | 2A | 3016 | - | - | - | X |
| 56 | MG | 2A | 3018 | - | - | - | X |
| 56 | MG | 2A | 3019 | - | - | - | X |
| 56 | MG | 2A | 3020 | - | - | - | X |
| 56 | MG | 2A | 3021 | - | - | - | X |
| 56 | MG | 2A | 3022 | - | - | - | X |
| 56 | MG | 2A | 3025 | - | - | - | X |
| 56 | MG | 2A | 3027 | - | - | - | X |
| 56 | MG | 2A | 3028 | - | - | - | X |
| 56 | MG | 2A | 3030 | - | - | - | X |
| 56 | MG | 2A | 3034 | - | - | - | X |
| 56 | MG | 2A | 3057 | - | - | - | X |
| 56 | MG | 2A | 3071 | - | - | - | X |
| 56 | MG | 2A | 3076 | - | - | - | X |
| 56 | MG | 2A | 3077 | - | - | - | X |
| 56 | MG | 2A | 3083 | - | - | - | X |
| 56 | MG | 2A | 3084 | - | - | - | X |
| 56 | MG | 2A | 3091 | - | - | - | X |
| 56 | MG | 2A | 3094 | - | - | - | X |
| 56 | MG | 2A | 3097 | - | - | - | X |
| 56 | MG | 2A | 3105 | - | - | - | X |
| 56 | MG | 2A | 3107 | - | - | - | X |
| 56 | MG | 2A | 3111 | - | - | - | X |
| 56 | MG | 2A | 3112 | - | - | - | X |
| 56 | MG | 2A | 3116 | - | - | - | X |
| 56 | MG | 2A | 3122 | - | - | - | X |
| 56 | MG | 2A | 3131 | - | - | - | X |
| 56 | MG | 2A | 3133 | - | - | - | X |
| 56 | MG | 2A | 3136 | - | - | - | X |
| 56 | MG | 2A | 3137 | - | - | - | X |
| 56 | MG | 2A | 3142 | - | - | - | X |
| 56 | MG | 2A | 3146 | - | - | - | X |
| 56 | MG | 2A | 3151 | - | - | - | X |
| 56 | MG | 2A | 3155 | - | - | - | X |
| 56 | MG | 2A | 3160 | - | - | - | X |
| 56 | MG | 2A | 3161 | - | - | - | X |
| 56 | MG | 2A | 3176 | - | - | - | X |
| 56 | MG | 2A | 3184 | - | - | - | X |
| 56 | MG | 2A | 3191 | - | - | - | X |
| 56 | MG | 2A | 3193 | - | - | - | X |
| 56 | MG | 2A | 3204 | - | - | - | X |

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| Mol | Type | Chain | Res | Chirality | Geometry | Clashes | Electron density |
|---|---|---|---|---|---|---|---|
| 56 | MG | 2A | 3206 | - | - | - | X |
| 56 | MG | 2A | 3245 | - | - | - | X |
| 56 | MG | 2A | 3246 | - | - | - | X |
| 56 | MG | 2A | 3248 | - | - | - | X |
| 56 | MG | 2A | 3252 | - | - | - | X |
| 56 | MG | 2A | 3257 | - | - | - | X |
| 56 | MG | 2A | 3263 | - | - | - | X |
| 56 | MG | 2A | 3272 | - | - | - | X |
| 56 | MG | 2A | 3283 | - | - | - | X |
| 56 | MG | 2A | 3284 | - | - | - | X |
| 56 | MG | 2A | 3299 | - | - | - | X |
| 56 | MG | 2A | 3302 | - | - | - | X |
| 56 | MG | 2A | 3305 | - | - | - | X |
| 56 | MG | 2A | 3307 | - | - | - | X |
| 56 | MG | 2A | 3319 | - | - | - | X |
| 56 | MG | 2A | 3327 | - | - | - | X |
| 56 | MG | 2A | 3329 | - | - | - | X |
| 56 | MG | 2A | 3337 | - | - | - | X |
| 56 | MG | 2A | 3350 | - | - | - | X |
| 56 | MG | 2A | 3351 | - | - | - | X |
| 56 | MG | 2A | 3383 | - | - | - | X |
| 56 | MG | 2A | 3389 | - | - | - | X |
| 56 | MG | 2A | 3397 | - | - | - | X |
| 56 | MG | 2A | 3398 | - | - | - | X |
| 56 | MG | 2A | 3402 | - | - | - | X |
| 56 | MG | 2A | 3403 | - | - | - | X |
| 56 | MG | 2A | 3431 | - | - | - | X |
| 56 | MG | 2A | 3440 | - | - | - | X |
| 56 | MG | 2A | 3449 | - | - | - | X |
| 56 | MG | 2A | 3451 | - | - | - | X |
| 56 | MG | 2A | 3461 | - | - | - | X |
| 56 | MG | 2A | 3464 | - | - | - | X |
| 56 | MG | 2A | 3465 | - | - | - | X |
| 56 | MG | 2A | 3470 | - | - | - | X |
| 56 | MG | 2A | 3472 | - | - | - | X |
| 56 | MG | 2A | 3476 | - | - | - | X |
| 56 | MG | 2A | 3477 | - | - | - | X |
| 56 | MG | 2A | 3482 | - | - | - | X |
| 56 | MG | 2A | 3486 | - | - | - | X |
| 56 | MG | 2A | 3502 | - | - | - | X |
| 56 | MG | 2A | 3512 | - | - | - | X |
| 56 | MG | 2A | 3517 | - | - | - | X |

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| Mol | Type | Chain | Res | Chirality | Geometry | Clashes | Electron density |
|---|---|---|---|---|---|---|---|
| 56 | MG | 2A | 3521 | - | - | - | X |
| 56 | MG | 2A | 3529 | - | - | - | X |
| 56 | MG | 2A | 3536 | - | - | - | X |
| 56 | MG | 2A | 3546 | - | - | - | X |
| 56 | MG | 2A | 3552 | - | - | - | X |
| 56 | MG | 2A | 3555 | - | - | - | X |
| 56 | MG | 2A | 3556 | - | - | - | X |
| 56 | MG | 2A | 3572 | - | - | - | X |
| 56 | MG | 2A | 3574 | - | - | - | X |
| 56 | MG | 2A | 3579 | - | - | - | X |
| 56 | MG | 2A | 3582 | - | - | - | X |
| 56 | MG | 2A | 3583 | - | - | - | X |
| 56 | MG | 2A | 3591 | - | - | - | X |
| 56 | MG | 2A | 3612 | - | - | - | X |
| 56 | MG | 2A | 3615 | - | - | - | X |
| 56 | MG | 2A | 3624 | - | - | - | X |
| 56 | MG | 2A | 3629 | - | - | - | X |
| 56 | MG | 2A | 3637 | - | - | - | X |
| 56 | MG | 2A | 3639 | - | - | - | X |
| 56 | MG | 2A | 3647 | - | - | - | X |
| 56 | MG | 2A | 3675 | - | - | - | X |
| 56 | MG | 2A | 3681 | - | - | - | X |
| 56 | MG | 2A | 3692 | - | - | - | X |
| 56 | MG | 2A | 3695 | - | - | - | X |
| 56 | MG | 2A | 3719 | - | - | - | X |
| 56 | MG | 2A | 3724 | - | - | - | X |
| 56 | MG | 2A | 3735 | - | - | - | X |
| 56 | MG | 2A | 3739 | - | - | - | X |
| 56 | MG | 2A | 3770 | - | - | - | X |
| 56 | MG | 2A | 3783 | - | - | - | X |
| 56 | MG | 2A | 3789 | - | - | - | X |
| 56 | MG | 2A | 3798 | - | - | - | X |
| 56 | MG | 2A | 3800 | - | - | - | X |
| 56 | MG | 2A | 3808 | - | - | - | X |
| 56 | MG | 2A | 3826 | - | - | - | X |
| 56 | MG | 2A | 3828 | - | - | - | X |
| 56 | MG | 2A | 3830 | - | - | - | X |
| 56 | MG | 2B | 203 | - | - | - | X |
| 56 | MG | 2B | 208 | - | - | - | X |
| 56 | MG | 2B | 216 | - | - | - | X |
| 56 | MG | 2B | 218 | - | - | - | X |
| 56 | MG | 2B | 221 | - | - | - | X |

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| Mol | Type | Chain | Res | Chirality | Geometry | Clashes | Electron density |
|---|---|---|---|---|---|---|---|
| 56 | MG | 2B | 230 | - | - | - | X |
| 56 | MG | 2B | 232 | - | - | - | X |
| 56 | MG | 2F | 303 | - | - | - | X |
| 56 | MG | 2P | 203 | - | - | - | X |
| 56 | MG | 2Q | 202 | - | - | - | X |
| 56 | MG | 2Q | 206 | - | - | - | X |
| 56 | MG | 2Z | 401 | - | - | - | X |
| 56 | MG | 2Z | 403 | - | - | - | X |
| 56 | MG | 2a | 1602 | - | - | - | X |
| 56 | MG | 2a | 1606 | - | - | - | X |
| 56 | MG | 2a | 1607 | - | - | - | X |
| 56 | MG | 2a | 1608 | - | - | - | X |
| 56 | MG | 2a | 1609 | - | - | - | X |
| 56 | MG | 2a | 1617 | - | - | - | X |
| 56 | MG | 2a | 1620 | - | - | - | X |
| 56 | MG | 2a | 1622 | - | - | - | X |
| 56 | MG | 2a | 1625 | - | - | - | X |
| 56 | MG | 2a | 1627 | - | - | - | X |
| 56 | MG | 2a | 1628 | - | - | - | X |
| 56 | MG | 2a | 1634 | - | - | - | X |
| 56 | MG | 2a | 1648 | - | - | - | X |
| 56 | MG | 2a | 1663 | - | - | - | X |
| 56 | MG | 2a | 1664 | - | - | - | X |
| 56 | MG | 2a | 1666 | - | - | - | X |
| 56 | MG | 2a | 1668 | - | - | - | X |
| 56 | MG | 2a | 1669 | - | - | - | X |
| 56 | MG | 2a | 1671 | - | - | - | X |
| 56 | MG | 2a | 1673 | - | - | - | X |
| 56 | MG | 2a | 1674 | - | - | - | X |
| 56 | MG | 2a | 1676 | - | - | - | X |
| 56 | MG | 2a | 1678 | - | - | - | X |
| 56 | MG | 2a | 1682 | - | - | - | X |
| 56 | MG | 2a | 1683 | - | - | - | X |
| 56 | MG | 2a | 1684 | - | - | - | X |
| 56 | MG | 2a | 1688 | - | - | - | X |
| 56 | MG | 2a | 1700 | - | - | - | X |
| 56 | MG | 2a | 1706 | - | - | - | X |
| 56 | MG | 2a | 1709 | - | - | - | X |
| 56 | MG | 2a | 1710 | - | - | - | X |
| 56 | MG | 2a | 1713 | - | - | - | X |
| 56 | MG | 2a | 1714 | - | - | - | X |
| 56 | MG | 2a | 1716 | - | - | - | X |

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| Mol | Type | Chain | Res | Chirality | Geometry | Clashes | Electron density |
|---|---|---|---|---|---|---|---|
| 56 | MG | 2a | 1718 | - | - | - | X |
| 56 | MG | 2a | 1722 | - | - | - | X |
| 56 | MG | 2a | 1732 | - | - | - | X |
| 56 | MG | 2a | 1735 | - | - | - | X |
| 56 | MG | 2a | 1748 | - | - | - | X |
| 56 | MG | 2a | 1753 | - | - | - | X |
| 56 | MG | 2a | 1754 | - | - | - | X |
| 56 | MG | 2a | 1758 | - | - | - | X |
| 56 | MG | 2a | 1766 | - | - | - | X |
| 56 | MG | 2a | 1768 | - | - | - | X |
| 56 | MG | 2a | 1776 | - | - | - | X |
| 56 | MG | 2a | 1780 | - | - | - | X |
| 56 | MG | 2a | 1785 | - | - | - | X |
| 56 | MG | 2a | 1786 | - | - | - | X |
| 56 | MG | 2a | 1791 | - | - | - | X |
| 56 | MG | 2a | 1794 | - | - | - | X |
| 56 | MG | 2a | 1805 | - | - | - | X |
| 56 | MG | 2a | 1826 | - | - | - | X |
| 56 | MG | 2a | 1828 | - | - | - | X |
| 56 | MG | 2a | 1860 | - | - | - | X |
| 56 | MG | 2a | 1887 | - | - | - | X |
| 56 | MG | 2a | 1893 | - | - | - | X |
| 56 | MG | 2a | 1899 | - | - | - | X |
| 56 | MG | 2a | 1901 | - | - | - | X |
| 56 | MG | 2a | 1905 | - | - | - | X |
| 56 | MG | 2a | 1912 | - | - | - | X |
| 56 | MG | 2a | 1918 | - | - | - | X |
| 56 | MG | 2a | 1921 | - | - | - | X |
| 56 | MG | 2d | 301 | - | - | - | X |
| 56 | MG | 2e | 201 | - | - | - | X |
| 56 | MG | 2g | 202 | - | - | - | X |
| 56 | MG | 2g | 206 | - | - | - | X |
| 56 | MG | 2h | 203 | - | - | - | X |
| 56 | MG | 2i | 204 | - | - | - | X |
| 56 | MG | 2l | 204 | - | - | - | X |
| 56 | MG | 2l | 206 | - | - | - | X |
| 56 | MG | 2m | 201 | - | - | - | X |
| 56 | MG | 2m | 202 | - | - | - | X |
| 56 | MG | 2o | 301 | - | - | - | X |
| 56 | MG | 2p | 102 | - | - | - | X |
| 56 | MG | 2q | 201 | - | - | - | X |
| 56 | MG | 2r | 301 | - | - | - | X |

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| Mol | Type | Chain | Res | Chirality | Geometry | Clashes | Electron density |
|---|---|---|---|---|---|---|---|
| 56 | MG | 2s | 102 | - | - | - | X |
| 56 | MG | 2u | 101 | - | - | - | X |
| 56 | MG | 2v | 701 | - | - | - | X |
| 56 | MG | 2w | 202 | - | - | - | X |
| 56 | MG | 2x | 102 | - | - | - | X |
| 56 | MG | 2x | 103 | - | - | - | X |
| 56 | MG | 2x | 104 | - | - | - | X |
| 56 | MG | 2x | 105 | - | - | - | X |
| 56 | MG | 2x | 107 | - | - | - | X |
| 56 | MG | 2x | 108 | - | - | - | X |
| 56 | MG | 2y | 101 | - | - | - | X |
| 56 | MG | 2y | 103 | - | - | - | X |
| 56 | MG | 2y | 106 | - | - | - | X |
| 56 | MG | 2z | 103 | - | - | - | X |

# 2 Entry composition (i)

There are 60 unique types of molecules in this entry. The entry contains 305259 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 23S Ribosomal RNA.

| Mol | Chain | Residues | Atoms | | | | | ZeroOcc | AltConf | Trace |
|---|---|---|---|---|---|---|---|---|---|---|
| | | | Total | C | N | O | P | | | |
| 1 | 1A | 2871 | 61852 | 27531 | 11572 | 19878 | 2871 | 0 | 0 | 0 |
| 1 | 2A | 2800 | 60322 | 26848 | 11284 | 19390 | 2800 | 0 | 0 | 0 |

- Molecule 2 is a RNA chain called 5S Ribosomal RNA.

| Mol | Chain | Residues | Atoms | | | | | ZeroOcc | AltConf | Trace |
|---|---|---|---|---|---|---|---|---|---|---|
| | | | Total | C | N | O | P | | | |
| 2 | 1B | 120 | 2577 | 1146 | 476 | 835 | 120 | 0 | 0 | 0 |
| 2 | 2B | 120 | 2575 | 1146 | 476 | 833 | 120 | 0 | 0 | 0 |

- Molecule 3 is a protein called 50S ribosomal protein L2.

| Mol | Chain | Residues | Atoms | | | | | ZeroOcc | AltConf | Trace |
|---|---|---|---|---|---|---|---|---|---|---|
| | | | Total | C | N | O | S | | | |
| 3 | 1D | 275 | 2136 | 1349 | 423 | 361 | 3 | 0 | 0 | 0 |
| 3 | 2D | 275 | 2136 | 1349 | 423 | 361 | 3 | 0 | 0 | 0 |

- Molecule 4 is a protein called 50S ribosomal protein L3.

| Mol | Chain | Residues | Atoms | | | | | ZeroOcc | AltConf | Trace |
|---|---|---|---|---|---|---|---|---|---|---|
| | | | Total | C | N | O | S | | | |
| 4 | 1E | 204 | 1559 | 985 | 298 | 270 | 6 | 0 | 0 | 0 |
| 4 | 2E | 204 | 1559 | 985 | 298 | 270 | 6 | 0 | 0 | 0 |

- Molecule 5 is a protein called 50S ribosomal protein L4.

| Mol | Chain | Residues | Atoms | | | | | ZeroOcc | AltConf | Trace |
|---|---|---|---|---|---|---|---|---|---|---|
| | | | Total | C | N | O | S | | | |
| 5 | 1F | 203 | 1584 | 1009 | 298 | 275 | 2 | 0 | 0 | 1 |
| 5 | 2F | 203 | 1580 | 1007 | 297 | 274 | 2 | 0 | 0 | 1 |

- Molecule 6 is a protein called 50S ribosomal protein L5.

| Mol | Chain | Residues | Atoms | | | | | ZeroOcc | AltConf | Trace |
|---|---|---|---|---|---|---|---|---|---|---|
| | | | Total | C | N | O | S | | | |
| 6 | 1G | 181 | 1451 | 930 | 261 | 256 | 4 | 0 | 0 | 0 |
| 6 | 2G | 181 | 1453 | 930 | 263 | 256 | 4 | 0 | 0 | 0 |

- Molecule 7 is a protein called 50S ribosomal protein L6.

| Mol | Chain | Residues | Atoms | | | | | ZeroOcc | AltConf | Trace |
|---|---|---|---|---|---|---|---|---|---|---|
| | | | Total | C | N | O | S | | | |
| 7 | 1H | 174 | 1330 | 845 | 248 | 236 | 1 | 0 | 0 | 0 |
| 7 | 2H | 174 | 1330 | 845 | 248 | 236 | 1 | 0 | 0 | 0 |

- Molecule 8 is a protein called 50S ribosomal protein L13.

| Mol | Chain | Residues | Atoms | | | | | ZeroOcc | AltConf | Trace |
|---|---|---|---|---|---|---|---|---|---|---|
| | | | Total | C | N | O | S | | | |
| 8 | 1N | 140 | 1117 | 719 | 207 | 187 | 4 | 0 | 0 | 0 |
| 8 | 2N | 140 | 1117 | 719 | 207 | 187 | 4 | 0 | 0 | 0 |

- Molecule 9 is a protein called 50S ribosomal protein L14.

| Mol | Chain | Residues | Atoms | | | | | ZeroOcc | AltConf | Trace |
|---|---|---|---|---|---|---|---|---|---|---|
| | | | Total | C | N | O | S | | | |
| 9 | 1O | 122 | 933 | 588 | 171 | 170 | 4 | 0 | 0 | 0 |
| 9 | 2O | 122 | 933 | 588 | 171 | 170 | 4 | 0 | 0 | 0 |

- Molecule 10 is a protein called 50S ribosomal protein L15.

| Mol | Chain | Residues | Atoms | | | | | ZeroOcc | AltConf | Trace |
|---|---|---|---|---|---|---|---|---|---|---|
| | | | Total | C | N | O | S | | | |
| 10 | 1P | 149 | 1135 | 706 | 230 | 196 | 3 | 0 | 0 | 0 |

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| Mol | Chain | Residues | Atoms | | | | | ZeroOcc | AltConf | Trace |
|---|---|---|---|---|---|---|---|---|---|---|
| | | | Total | C | N | O | S | | | |
| 10 | 2P | 149 | 1135 | 706 | 230 | 196 | 3 | 0 | 0 | 0 |

- Molecule 11 is a protein called 50S ribosomal protein L16.

| Mol | Chain | Residues | Atoms | | | | | ZeroOcc | AltConf | Trace |
|---|---|---|---|---|---|---|---|---|---|---|
| | | | Total | C | N | O | S | | | |
| 11 | 1Q | 141 | 1122 | 715 | 212 | 188 | 7 | 0 | 0 | 0 |
| | | | Total | C | N | O | S | | | |
| 11 | 2Q | 141 | 1122 | 715 | 212 | 188 | 7 | 0 | 0 | 0 |

- Molecule 12 is a protein called 50S ribosomal protein L17.

| Mol | Chain | Residues | Atoms | | | | | ZeroOcc | AltConf | Trace |
|---|---|---|---|---|---|---|---|---|---|---|
| | | | Total | C | N | O | S | | | |
| 12 | 1R | 118 | 968 | 604 | 203 | 160 | 1 | 0 | 0 | 0 |
| | | | Total | C | N | O | S | | | |
| 12 | 2R | 118 | 968 | 604 | 203 | 160 | 1 | 0 | 0 | 0 |

- Molecule 13 is a protein called 50S ribosomal protein L18.

| Mol | Chain | Residues | Atoms | | | | ZeroOcc | AltConf | Trace |
|---|---|---|---|---|---|---|---|---|---|
| | | | Total | C | N | O | | | |
| 13 | 1S | 110 | 873 | 550 | 174 | 149 | 0 | 0 | 0 |
| | | | Total | C | N | O | | | |
| 13 | 2S | 110 | 870 | 549 | 173 | 148 | 0 | 0 | 0 |

- Molecule 14 is a protein called 50S ribosomal protein L19.

| Mol | Chain | Residues | Atoms | | | | | ZeroOcc | AltConf | Trace |
|---|---|---|---|---|---|---|---|---|---|---|
| | | | Total | C | N | O | S | | | |
| 14 | 1T | 131 | 1091 | 680 | 225 | 185 | 1 | 0 | 0 | 0 |
| | | | Total | C | N | O | S | | | |
| 14 | 2T | 131 | 1083 | 675 | 224 | 183 | 1 | 0 | 0 | 0 |

- Molecule 15 is a protein called 50S ribosomal protein L20.

| Mol | Chain | Residues | Atoms | | | | | ZeroOcc | AltConf | Trace |
|---|---|---|---|---|---|---|---|---|---|---|
| | | | Total | C | N | O | S | | | |
| 15 | 1U | 116 | 959 | 608 | 201 | 149 | 1 | 0 | 0 | 0 |
| | | | Total | C | N | O | S | | | |
| 15 | 2U | 116 | 959 | 608 | 201 | 149 | 1 | 0 | 0 | 0 |

- Molecule 16 is a protein called 50S ribosomal protein L21.

| Mol | Chain | Residues | Atoms | | | | | ZeroOcc | AltConf | Trace |
|---|---|---|---|---|---|---|---|---|---|---|
| | | | Total | C | N | O | S | | | |
| 16 | 1V | 101 | 771 | 495 | 140 | 135 | 1 | 0 | 0 | 0 |
| 16 | 2V | 101 | 771 | 495 | 140 | 135 | 1 | 0 | 0 | 0 |

- Molecule 17 is a protein called 50S ribosomal protein L22.

| Mol | Chain | Residues | Atoms | | | | | ZeroOcc | AltConf | Trace |
|---|---|---|---|---|---|---|---|---|---|---|
| | | | Total | C | N | O | S | | | |
| 17 | 1W | 112 | 886 | 557 | 174 | 153 | 2 | 0 | 0 | 0 |
| 17 | 2W | 112 | 886 | 557 | 174 | 153 | 2 | 0 | 0 | 0 |

- Molecule 18 is a protein called 50S ribosomal protein L23.

| Mol | Chain | Residues | Atoms | | | | | ZeroOcc | AltConf | Trace |
|---|---|---|---|---|---|---|---|---|---|---|
| | | | Total | C | N | O | S | | | |
| 18 | 1X | 95 | 750 | 488 | 135 | 126 | 1 | 0 | 0 | 0 |
| 18 | 2X | 95 | 750 | 488 | 135 | 126 | 1 | 0 | 0 | 0 |

- Molecule 19 is a protein called 50S ribosomal protein L24.

| Mol | Chain | Residues | Atoms | | | | | ZeroOcc | AltConf | Trace |
|---|---|---|---|---|---|---|---|---|---|---|
| | | | Total | C | N | O | S | | | |
| 19 | 1Y | 107 | 806 | 517 | 152 | 131 | 6 | 0 | 0 | 0 |
| 19 | 2Y | 107 | 806 | 517 | 152 | 131 | 6 | 0 | 0 | 0 |

- Molecule 20 is a protein called 50S ribosomal protein L25.

| Mol | Chain | Residues | Atoms | | | | | ZeroOcc | AltConf | Trace |
|---|---|---|---|---|---|---|---|---|---|---|
| | | | Total | C | N | O | S | | | |
| 20 | 1Z | 204 | 1582 | 1007 | 278 | 295 | 2 | 0 | 0 | 0 |
| 20 | 2Z | 204 | 1582 | 1007 | 278 | 295 | 2 | 0 | 0 | 0 |

- Molecule 21 is a protein called 50S ribosomal protein L27.

| Mol | Chain | Residues | Atoms | | | | | ZeroOcc | AltConf | Trace |
|---|---|---|---|---|---|---|---|---|---|---|
| | | | Total | C | N | O | S | | | |
| 21 | 10 | 75 | 598 | 370 | 127 | 100 | 1 | 0 | 0 | 0 |
| 21 | 20 | 75 | 598 | 370 | 127 | 100 | 1 | 0 | 0 | 0 |

- Molecule 22 is a protein called 50S ribosomal protein L28.

| Mol | Chain | Residues | Atoms | | | | | ZeroOcc | AltConf | Trace |
|---|---|---|---|---|---|---|---|---|---|---|
| | | | Total | C | N | O | S | | | |
| 22 | 11 | 97 | 755 | 475 | 148 | 131 | 1 | 0 | 0 | 0 |
| 22 | 21 | 97 | 755 | 475 | 148 | 131 | 1 | 0 | 0 | 0 |

- Molecule 23 is a protein called 50S ribosomal protein L29.

| Mol | Chain | Residues | Atoms | | | | | ZeroOcc | AltConf | Trace |
|---|---|---|---|---|---|---|---|---|---|---|
| | | | Total | C | N | O | S | | | |
| 23 | 12 | 70 | 588 | 365 | 118 | 103 | 2 | 0 | 0 | 0 |
| 23 | 22 | 70 | 588 | 365 | 118 | 103 | 2 | 0 | 0 | 0 |

- Molecule 24 is a protein called 50S ribosomal protein L30.

| Mol | Chain | Residues | Atoms | | | | ZeroOcc | AltConf | Trace |
|---|---|---|---|---|---|---|---|---|---|
| | | | Total | C | N | O | | | |
| 24 | 13 | 59 | 469 | 298 | 90 | 81 | 0 | 0 | 0 |
| 24 | 23 | 59 | 464 | 296 | 90 | 78 | 0 | 0 | 0 |

- Molecule 25 is a protein called 50S ribosomal protein L31.

| Mol | Chain | Residues | Atoms | | | | | ZeroOcc | AltConf | Trace |
|---|---|---|---|---|---|---|---|---|---|---|
| | | | Total | C | N | O | S | | | |
| 25 | 14 | 69 | 552 | 349 | 99 | 99 | 5 | 0 | 0 | 0 |
| 25 | 24 | 69 | 532 | 339 | 97 | 91 | 5 | 0 | 0 | 0 |

- Molecule 26 is a protein called 50S ribosomal protein L32.

| Mol | Chain | Residues | Atoms | | | | | ZeroOcc | AltConf | Trace |
|---|---|---|---|---|---|---|---|---|---|---|
| | | | Total | C | N | O | S | | | |
| 26 | 15 | 59 | 455 | 285 | 89 | 76 | 5 | 0 | 0 | 0 |

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| Mol | Chain | Residues | Atoms | | | | | ZeroOcc | AltConf | Trace |
|---|---|---|---|---|---|---|---|---|---|---|
| | | | Total | C | N | O | S | | | |
| 26 | 25 | 59 | 455 | 285 | 89 | 76 | 5 | 0 | 0 | 0 |

- Molecule 27 is a protein called 50S ribosomal protein L33.

| Mol | Chain | Residues | Atoms | | | | | ZeroOcc | AltConf | Trace |
|---|---|---|---|---|---|---|---|---|---|---|
| | | | Total | C | N | O | S | | | |
| 27 | 16 | 53 | 453 | 281 | 91 | 77 | 4 | 0 | 0 | 0 |
| | | | Total | C | N | O | S | | | |
| 27 | 26 | 53 | 449 | 279 | 91 | 75 | 4 | 0 | 0 | 0 |

- Molecule 28 is a protein called 50S ribosomal protein L34.

| Mol | Chain | Residues | Atoms | | | | | ZeroOcc | AltConf | Trace |
|---|---|---|---|---|---|---|---|---|---|---|
| | | | Total | C | N | O | S | | | |
| 28 | 17 | 48 | 418 | 257 | 104 | 55 | 2 | 0 | 0 | 0 |
| | | | Total | C | N | O | S | | | |
| 28 | 27 | 48 | 418 | 257 | 104 | 55 | 2 | 0 | 0 | 0 |

- Molecule 29 is a protein called 50S ribosomal protein L35.

| Mol | Chain | Residues | Atoms | | | | | ZeroOcc | AltConf | Trace |
|---|---|---|---|---|---|---|---|---|---|---|
| | | | Total | C | N | O | S | | | |
| 29 | 18 | 64 | 517 | 331 | 102 | 82 | 2 | 0 | 0 | 0 |
| | | | Total | C | N | O | S | | | |
| 29 | 28 | 64 | 517 | 331 | 102 | 82 | 2 | 0 | 0 | 0 |

- Molecule 30 is a protein called 50S ribosomal protein L36.

| Mol | Chain | Residues | Atoms | | | | | ZeroOcc | AltConf | Trace |
|---|---|---|---|---|---|---|---|---|---|---|
| | | | Total | C | N | O | S | | | |
| 30 | 19 | 37 | 307 | 188 | 68 | 47 | 4 | 0 | 0 | 0 |
| | | | Total | C | N | O | S | | | |
| 30 | 29 | 37 | 307 | 188 | 68 | 47 | 4 | 0 | 0 | 0 |

- Molecule 31 is a RNA chain called 16S Ribosomal RNA.

| Mol | Chain | Residues | Atoms | | | | | ZeroOcc | AltConf | Trace |
|---|---|---|---|---|---|---|---|---|---|---|
| | | | Total | C | N | O | P | | | |
| 31 | 1a | 1499 | 32224 | 14348 | 5970 | 10407 | 1499 | 0 | 0 | 0 |
| | | | Total | C | N | O | P | | | |
| 31 | 2a | 1503 | 32327 | 14396 | 5990 | 10438 | 1503 | 0 | 0 | 0 |

- Molecule 32 is a protein called 30S ribosomal protein S2.

| Mol | Chain | Residues | Atoms | | | | | ZeroOcc | AltConf | Trace |
|---|---|---|---|---|---|---|---|---|---|---|
| | | | Total | C | N | O | S | | | |
| 32 | 1b | 231 | 1846 | 1179 | 331 | 331 | 5 | 0 | 0 | 0 |
| 32 | 2b | 231 | 1825 | 1167 | 326 | 327 | 5 | 0 | 0 | 0 |

- Molecule 33 is a protein called 30S ribosomal protein S3.

| Mol | Chain | Residues | Atoms | | | | | ZeroOcc | AltConf | Trace |
|---|---|---|---|---|---|---|---|---|---|---|
| | | | Total | C | N | O | S | | | |
| 33 | 1c | 206 | 1548 | 973 | 301 | 273 | 1 | 0 | 0 | 0 |
| 33 | 2c | 206 | 1542 | 968 | 300 | 273 | 1 | 0 | 0 | 0 |

- Molecule 34 is a protein called 30S ribosomal protein S4.

| Mol | Chain | Residues | Atoms | | | | | ZeroOcc | AltConf | Trace |
|---|---|---|---|---|---|---|---|---|---|---|
| | | | Total | C | N | O | S | | | |
| 34 | 1d | 208 | 1655 | 1038 | 326 | 284 | 7 | 0 | 0 | 0 |
| 34 | 2d | 208 | 1674 | 1050 | 333 | 284 | 7 | 0 | 0 | 0 |

- Molecule 35 is a protein called 30S ribosomal protein S5.

| Mol | Chain | Residues | Atoms | | | | | ZeroOcc | AltConf | Trace |
|---|---|---|---|---|---|---|---|---|---|---|
| | | | Total | C | N | O | S | | | |
| 35 | 1e | 148 | 1129 | 714 | 213 | 198 | 4 | 0 | 0 | 0 |
| 35 | 2e | 148 | 1133 | 716 | 214 | 199 | 4 | 0 | 0 | 0 |

- Molecule 36 is a protein called 30S ribosomal protein S6.

| Mol | Chain | Residues | Atoms | | | | | ZeroOcc | AltConf | Trace |
|---|---|---|---|---|---|---|---|---|---|---|
| | | | Total | C | N | O | S | | | |
| 36 | 1f | 100 | 810 | 514 | 144 | 149 | 3 | 0 | 0 | 0 |
| 36 | 2f | 100 | 816 | 516 | 146 | 151 | 3 | 0 | 0 | 0 |

- Molecule 37 is a protein called 30S ribosomal protein S7.

| Mol | Chain | Residues | Atoms | | | | | ZeroOcc | AltConf | Trace |
|---|---|---|---|---|---|---|---|---|---|---|
| | | | Total | C | N | O | S | | | |
| 37 | 1g | 155 | 1231 | 766 | 243 | 216 | 6 | 0 | 0 | 0 |
| 37 | 2g | 155 | 1235 | 769 | 244 | 216 | 6 | 0 | 0 | 0 |

- Molecule 38 is a protein called 30S ribosomal protein S8.

| Mol | Chain | Residues | Atoms | | | | | ZeroOcc | AltConf | Trace |
|---|---|---|---|---|---|---|---|---|---|---|
| | | | Total | C | N | O | S | | | |
| 38 | 1h | 137 | 1088 | 689 | 206 | 191 | 2 | 0 | 0 | 0 |
| 38 | 2h | 137 | 1088 | 689 | 206 | 191 | 2 | 0 | 0 | 0 |

- Molecule 39 is a protein called 30S ribosomal protein S9.

| Mol | Chain | Residues | Atoms | | | | ZeroOcc | AltConf | Trace |
|---|---|---|---|---|---|---|---|---|---|
| | | | Total | C | N | O | | | |
| 39 | 1i | 127 | 983 | 623 | 193 | 167 | 0 | 0 | 0 |
| 39 | 2i | 127 | 978 | 619 | 190 | 169 | 0 | 0 | 0 |

- Molecule 40 is a protein called 30S ribosomal protein S10.

| Mol | Chain | Residues | Atoms | | | | ZeroOcc | AltConf | Trace |
|---|---|---|---|---|---|---|---|---|---|
| | | | Total | C | N | O | | | |
| 40 | 1j | 97 | 709 | 440 | 138 | 131 | 0 | 0 | 0 |
| 40 | 2j | 96 | 714 | 445 | 138 | 131 | 0 | 0 | 0 |

- Molecule 41 is a protein called 30S ribosomal protein S11.

| Mol | Chain | Residues | Atoms | | | | | ZeroOcc | AltConf | Trace |
|---|---|---|---|---|---|---|---|---|---|---|
| | | | Total | C | N | O | S | | | |
| 41 | 1k | 114 | 829 | 516 | 155 | 155 | 3 | 0 | 0 | 0 |
| 41 | 2k | 114 | 833 | 519 | 156 | 155 | 3 | 0 | 0 | 0 |

- Molecule 42 is a protein called 30S ribosomal protein S12.

| Mol | Chain | Residues | Atoms | | | | | ZeroOcc | AltConf | Trace |
|---|---|---|---|---|---|---|---|---|---|---|
| | | | Total | C | N | O | S | | | |
| 42 | 1l | 122 | 932 | 586 | 185 | 159 | 2 | 0 | 0 | 0 |

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| Mol | Chain | Residues | Atoms | | | | | ZeroOcc | AltConf | Trace |
|---|---|---|---|---|---|---|---|---|---|---|
| | | | Total | C | N | O | S | | | |
| 42 | 2l | 122 | 932 | 586 | 185 | 159 | 2 | 0 | 0 | 0 |

- Molecule 43 is a protein called 30S ribosomal protein S13.

| Mol | Chain | Residues | Atoms | | | | | ZeroOcc | AltConf | Trace |
|---|---|---|---|---|---|---|---|---|---|---|
| | | | Total | C | N | O | S | | | |
| 43 | 1m | 118 | 919 | 566 | 190 | 161 | 2 | 0 | 0 | 0 |
| 43 | 2m | 122 | 950 | 586 | 197 | 165 | 2 | 0 | 0 | 0 |

- Molecule 44 is a protein called 30S ribosomal protein S14 type Z.

| Mol | Chain | Residues | Atoms | | | | | ZeroOcc | AltConf | Trace |
|---|---|---|---|---|---|---|---|---|---|---|
| | | | Total | C | N | O | S | | | |
| 44 | 1n | 60 | 492 | 312 | 104 | 72 | 4 | 0 | 0 | 0 |
| 44 | 2n | 60 | 492 | 312 | 104 | 72 | 4 | 0 | 0 | 0 |

- Molecule 45 is a protein called 30S ribosomal protein S15.

| Mol | Chain | Residues | Atoms | | | | | ZeroOcc | AltConf | Trace |
|---|---|---|---|---|---|---|---|---|---|---|
| | | | Total | C | N | O | S | | | |
| 45 | 1o | 88 | 728 | 456 | 144 | 126 | 2 | 0 | 0 | 0 |
| 45 | 2o | 88 | 728 | 456 | 144 | 126 | 2 | 0 | 0 | 0 |

- Molecule 46 is a protein called 30S ribosomal protein S16.

| Mol | Chain | Residues | Atoms | | | | | ZeroOcc | AltConf | Trace |
|---|---|---|---|---|---|---|---|---|---|---|
| | | | Total | C | N | O | S | | | |
| 46 | 1p | 82 | 681 | 433 | 134 | 113 | 1 | 0 | 0 | 0 |
| 46 | 2p | 82 | 677 | 430 | 133 | 113 | 1 | 0 | 0 | 0 |

- Molecule 47 is a protein called 30S ribosomal protein S17.

| Mol | Chain | Residues | Atoms | | | | | ZeroOcc | AltConf | Trace |
|---|---|---|---|---|---|---|---|---|---|---|
| | | | Total | C | N | O | S | | | |
| 47 | 1q | 99 | 823 | 528 | 151 | 142 | 2 | 0 | 0 | 0 |
| 47 | 2q | 99 | 823 | 528 | 151 | 142 | 2 | 0 | 0 | 0 |

- Molecule 48 is a protein called 30S ribosomal protein S18.

| Mol | Chain | Residues | Atoms | | | | ZeroOcc | AltConf | Trace |
|---|---|---|---|---|---|---|---|---|---|
| | | | Total | C | N | O | | | |
| 48 | 1r | 68 | 555 | 355 | 108 | 92 | 0 | 0 | 0 |
| 48 | 2r | 68 | 555 | 355 | 108 | 92 | 0 | 0 | 0 |

- Molecule 49 is a protein called 30S ribosomal protein S19.

| Mol | Chain | Residues | Atoms | | | | | ZeroOcc | AltConf | Trace |
|---|---|---|---|---|---|---|---|---|---|---|
| | | | Total | C | N | O | S | | | |
| 49 | 1s | 83 | 652 | 417 | 120 | 113 | 2 | 0 | 0 | 0 |
| 49 | 2s | 83 | 646 | 412 | 119 | 113 | 2 | 0 | 0 | 0 |

- Molecule 50 is a protein called 30S ribosomal protein S20.

| Mol | Chain | Residues | Atoms | | | | | ZeroOcc | AltConf | Trace |
|---|---|---|---|---|---|---|---|---|---|---|
| | | | Total | C | N | O | S | | | |
| 50 | 1t | 96 | 728 | 446 | 156 | 124 | 2 | 0 | 0 | 0 |
| 50 | 2t | 96 | 727 | 446 | 155 | 124 | 2 | 0 | 0 | 0 |

- Molecule 51 is a protein called 30S ribosomal protein Thx.

| Mol | Chain | Residues | Atoms | | | | ZeroOcc | AltConf | Trace |
|---|---|---|---|---|---|---|---|---|---|
| | | | Total | C | N | O | | | |
| 51 | 1u | 23 | 199 | 122 | 48 | 29 | 0 | 0 | 0 |
| 51 | 2u | 23 | 199 | 122 | 48 | 29 | 0 | 0 | 0 |

- Molecule 52 is a protein called 50S ribosomal protein L9,Elongation factor G.

| Mol | Chain | Residues | Atoms | | | | | ZeroOcc | AltConf | Trace |
|---|---|---|---|---|---|---|---|---|---|---|
| | | | Total | C | N | O | S | | | |
| 52 | 1v | 728 | 5664 | 3599 | 974 | 1072 | 19 | 0 | 0 | 0 |
| 52 | 2v | 728 | 5664 | 3599 | 974 | 1072 | 19 | 0 | 0 | 0 |

- Molecule 53 is a protein called Ribosome-recycling factor.

| Mol | Chain | Residues | Atoms | | | | | ZeroOcc | AltConf | Trace |
|---|---|---|---|---|---|---|---|---|---|---|
| | | | Total | C | N | O | S | | | |
| 53 | 1w | 185 | 1478 | 924 | 270 | 282 | 2 | 0 | 0 | 0 |
| 53 | 2w | 185 | 1478 | 924 | 270 | 282 | 2 | 0 | 0 | 0 |

- Molecule 54 is a RNA chain called P-site and E-site tRNAs.

| Mol | Chain | Residues | Atoms | | | | | | ZeroOcc | AltConf | Trace |
|---|---|---|---|---|---|---|---|---|---|---|---|
| | | | Total | C | N | O | P | S | | | |
| 54 | 1x | 74 | 1581 | 707 | 285 | 515 | 73 | 1 | 0 | 0 | 0 |
| 54 | 1y | 74 | 1581 | 707 | 285 | 515 | 73 | 1 | 0 | 0 | 0 |
| 54 | 2x | 74 | 1581 | 707 | 285 | 515 | 73 | 1 | 0 | 0 | 0 |
| 54 | 2y | 74 | 1581 | 707 | 285 | 515 | 73 | 1 | 0 | 0 | 0 |

- Molecule 55 is a RNA chain called mRNA.

| Mol | Chain | Residues | Atoms | | | | | ZeroOcc | AltConf | Trace |
|---|---|---|---|---|---|---|---|---|---|---|
| | | | Total | C | N | O | P | | | |
| 55 | 1z | 10 | 212 | 96 | 39 | 67 | 10 | 0 | 0 | 0 |
| 55 | 2z | 10 | 212 | 96 | 39 | 67 | 10 | 0 | 0 | 0 |

- Molecule 56 is MAGNESIUM ION (three-letter code: MG) (formula: Mg).

| Mol | Chain | Residues | Atoms | | ZeroOcc | AltConf |
|---|---|---|---|---|---|---|
| | | | Total | Mg | | |
| 56 | 1A | 1063 | 1063 | 1063 | 0 | 0 |
| 56 | 1B | 26 | 26 | 26 | 0 | 0 |
| 56 | 1D | 8 | 8 | 8 | 0 | 0 |
| 56 | 1E | 8 | 8 | 8 | 0 | 0 |
| 56 | 1F | 1 | 1 | 1 | 0 | 0 |
| 56 | 1H | 2 | 2 | 2 | 0 | 0 |
| 56 | 1N | 1 | 1 | 1 | 0 | 0 |
| 56 | 1O | 5 | 5 | 5 | 0 | 0 |

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| Mol | Chain | Residues | Atoms | | ZeroOcc | AltConf |
|---|---|---|---|---|---|---|
| | | | Total | Mg | | |
| 56 | 1P | 5 | 5 | 5 | 0 | 0 |
| 56 | 1Q | 3 | 3 | 3 | 0 | 0 |
| 56 | 1R | 3 | 3 | 3 | 0 | 0 |
| 56 | 1S | 2 | 2 | 2 | 0 | 0 |
| 56 | 1T | 5 | 5 | 5 | 0 | 0 |
| 56 | 1U | 3 | 3 | 3 | 0 | 0 |
| 56 | 1V | 1 | 1 | 1 | 0 | 0 |
| 56 | 1W | 2 | 2 | 2 | 0 | 0 |
| 56 | 1Y | 1 | 1 | 1 | 0 | 0 |
| 56 | 1Z | 5 | 5 | 5 | 0 | 0 |
| 56 | 10 | 4 | 4 | 4 | 0 | 0 |
| 56 | 11 | 1 | 1 | 1 | 0 | 0 |
| 56 | 12 | 1 | 1 | 1 | 0 | 0 |
| 56 | 13 | 1 | 1 | 1 | 0 | 0 |
| 56 | 15 | 2 | 2 | 2 | 0 | 0 |
| 56 | 16 | 1 | 1 | 1 | 0 | 0 |
| 56 | 17 | 3 | 3 | 3 | 0 | 0 |
| 56 | 18 | 3 | 3 | 3 | 0 | 0 |
| 56 | 19 | 1 | 1 | 1 | 0 | 0 |
| 56 | 1a | 319 | 319 | 319 | 0 | 0 |
| 56 | 1b | 9 | 9 | 9 | 0 | 0 |

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| Mol | Chain | Residues | Atoms | | ZeroOcc | AltConf |
|---|---|---|---|---|---|---|
| | | | Total | Mg | | |
| 56 | 1d | 4 | 4 | 4 | 0 | 0 |
| 56 | 1e | 2 | 2 | 2 | 0 | 0 |
| 56 | 1g | 2 | 2 | 2 | 0 | 0 |
| 56 | 1i | 1 | 1 | 1 | 0 | 0 |
| 56 | 1l | 1 | 1 | 1 | 0 | 0 |
| 56 | 1m | 2 | 2 | 2 | 0 | 0 |
| 56 | 1n | 2 | 2 | 2 | 0 | 0 |
| 56 | 1o | 1 | 1 | 1 | 0 | 0 |
| 56 | 1p | 1 | 1 | 1 | 0 | 0 |
| 56 | 1q | 1 | 1 | 1 | 0 | 0 |
| 56 | 1s | 3 | 3 | 3 | 0 | 0 |
| 56 | 1t | 1 | 1 | 1 | 0 | 0 |
| 56 | 1u | 1 | 1 | 1 | 0 | 0 |
| 56 | 1v | 3 | 3 | 3 | 0 | 0 |
| 56 | 1x | 2 | 2 | 2 | 0 | 0 |
| 56 | 1y | 6 | 6 | 6 | 0 | 0 |
| 56 | 1z | 1 | 1 | 1 | 0 | 0 |
| 56 | 2A | 852 | 852 | 852 | 0 | 0 |
| 56 | 2B | 32 | 32 | 32 | 0 | 0 |
| 56 | 2D | 6 | 6 | 6 | 0 | 0 |
| 56 | 2E | 5 | 5 | 5 | 0 | 0 |

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| Mol | Chain | Residues | Atoms | | ZeroOcc | AltConf |
|---|---|---|---|---|---|---|
| | | | Total | Mg | | |
| 56 | 2F | 4 | 4 | 4 | 0 | 0 |
| 56 | 2N | 2 | 2 | 2 | 0 | 0 |
| 56 | 2O | 1 | 1 | 1 | 0 | 0 |
| 56 | 2P | 3 | 3 | 3 | 0 | 0 |
| 56 | 2Q | 6 | 6 | 6 | 0 | 0 |
| 56 | 2S | 1 | 1 | 1 | 0 | 0 |
| 56 | 2T | 2 | 2 | 2 | 0 | 0 |
| 56 | 2V | 1 | 1 | 1 | 0 | 0 |
| 56 | 2X | 1 | 1 | 1 | 0 | 0 |
| 56 | 2Y | 2 | 2 | 2 | 0 | 0 |
| 56 | 2Z | 4 | 4 | 4 | 0 | 0 |
| 56 | 20 | 6 | 6 | 6 | 0 | 0 |
| 56 | 21 | 1 | 1 | 1 | 0 | 0 |
| 56 | 23 | 3 | 3 | 3 | 0 | 0 |
| 56 | 24 | 1 | 1 | 1 | 0 | 0 |
| 56 | 25 | 1 | 1 | 1 | 0 | 0 |
| 56 | 26 | 2 | 2 | 2 | 0 | 0 |
| 56 | 27 | 3 | 3 | 3 | 0 | 0 |
| 56 | 28 | 6 | 6 | 6 | 0 | 0 |
| 56 | 29 | 2 | 2 | 2 | 0 | 0 |
| 56 | 2a | 321 | 321 | 321 | 0 | 0 |

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| Mol | Chain | Residues | Atoms | | ZeroOcc | AltConf |
|---|---|---|---|---|---|---|
| | | | Total | Mg | | |
| 56 | 2b | 3 | 3 | 3 | 0 | 0 |
| 56 | 2c | 1 | 1 | 1 | 0 | 0 |
| 56 | 2d | 3 | 3 | 3 | 0 | 0 |
| 56 | 2e | 2 | 2 | 2 | 0 | 0 |
| 56 | 2f | 4 | 4 | 4 | 0 | 0 |
| 56 | 2g | 6 | 6 | 6 | 0 | 0 |
| 56 | 2h | 5 | 5 | 5 | 0 | 0 |
| 56 | 2i | 4 | 4 | 4 | 0 | 0 |
| 56 | 2k | 2 | 2 | 2 | 0 | 0 |
| 56 | 2l | 6 | 6 | 6 | 0 | 0 |
| 56 | 2m | 3 | 3 | 3 | 0 | 0 |
| 56 | 2o | 1 | 1 | 1 | 0 | 0 |
| 56 | 2p | 3 | 3 | 3 | 0 | 0 |
| 56 | 2q | 4 | 4 | 4 | 0 | 0 |
| 56 | 2r | 2 | 2 | 2 | 0 | 0 |
| 56 | 2s | 3 | 3 | 3 | 0 | 0 |
| 56 | 2t | 1 | 1 | 1 | 0 | 0 |
| 56 | 2u | 3 | 3 | 3 | 0 | 0 |
| 56 | 2v | 3 | 3 | 3 | 0 | 0 |
| 56 | 2w | 2 | 2 | 2 | 0 | 0 |
| 56 | 2x | 8 | 8 | 8 | 0 | 0 |

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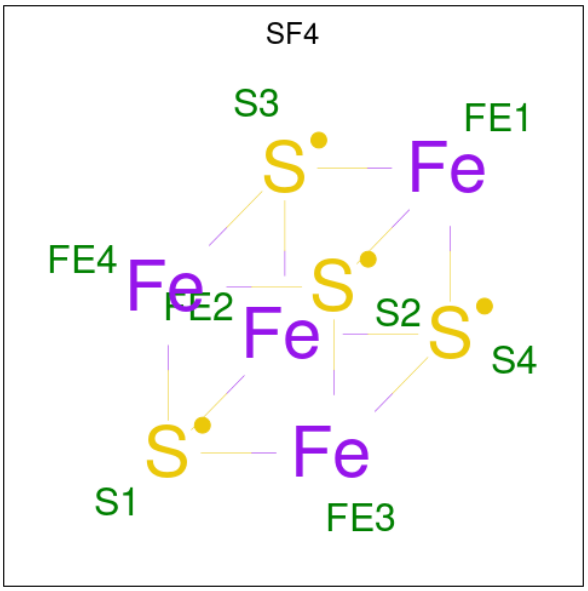
| Mol | Chain | Residues | Atoms | ZeroOcc | AltConf |
|---|---|---|---|---|---|
| 56 | 2y | 10 | Total Mg<br>10 10 | 0 | 0 |
| 56 | 2z | 3 | Total Mg<br>3 3 | 0 | 0 |

- Molecule 57 is ZINC ION (three-letter code: ZN) (formula: Zn).

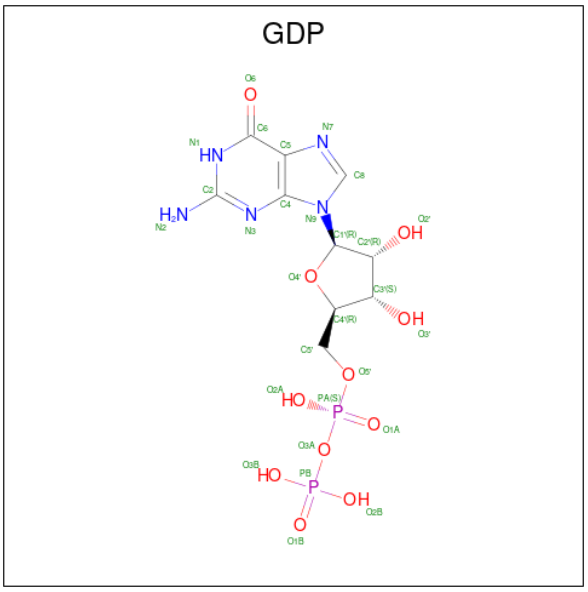
| Mol | Chain | Residues | Atoms | ZeroOcc | AltConf |
|---|---|---|---|---|---|
| 57 | 1Y | 1 | Total Zn<br>1 1 | 0 | 0 |
| 57 | 14 | 1 | Total Zn<br>1 1 | 0 | 0 |
| 57 | 15 | 1 | Total Zn<br>1 1 | 0 | 0 |
| 57 | 16 | 1 | Total Zn<br>1 1 | 0 | 0 |
| 57 | 19 | 1 | Total Zn<br>1 1 | 0 | 0 |
| 57 | 1n | 1 | Total Zn<br>1 1 | 0 | 0 |
| 57 | 2Y | 1 | Total Zn<br>1 1 | 0 | 0 |
| 57 | 24 | 1 | Total Zn<br>1 1 | 0 | 0 |
| 57 | 25 | 1 | Total Zn<br>1 1 | 0 | 0 |
| 57 | 26 | 1 | Total Zn<br>1 1 | 0 | 0 |
| 57 | 29 | 1 | Total Zn<br>1 1 | 0 | 0 |
| 57 | 2n | 1 | Total Zn<br>1 1 | 0 | 0 |

- Molecule 58 is IRON/SULFUR CLUSTER (three-letter code: SF4) (formula: $Fe_4S_4$).




| Mol | Chain | Residues | Atoms | | | ZeroOcc | AltConf |
|---|---|---|---|---|---|---|---|
| | | | Total | Fe | S | | |
| 58 | 1d | 1 | 8 | 4 | 4 | 0 | 0 |
| | | | Total | Fe | S | | |
| 58 | 2d | 1 | 8 | 4 | 4 | 0 | 0 |

- Molecule 59 is GUANOSINE-5'-DIPHOSPHATE (three-letter code: GDP) (formula: $C_{10}H_{15}N_5O_{11}P_2$).




| Mol | Chain | Residues | Atoms | | | | | ZeroOcc | AltConf |
|---|---|---|---|---|---|---|---|---|---|
| | | | Total | C | N | O | P | | |
| 59 | 1v | 1 | 28 | 10 | 5 | 11 | 2 | 0 | 0 |

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| Mol | Chain | Residues | Atoms | | | | | ZeroOcc | AltConf |
|---|---|---|---|---|---|---|---|---|---|
| | | | Total | C | N | O | P | | |
| 59 | 2v | 1 | 28 | 10 | 5 | 11 | 2 | 0 | 0 |

- Molecule 60 is POTASSIUM ION (three-letter code: K) (formula: K).

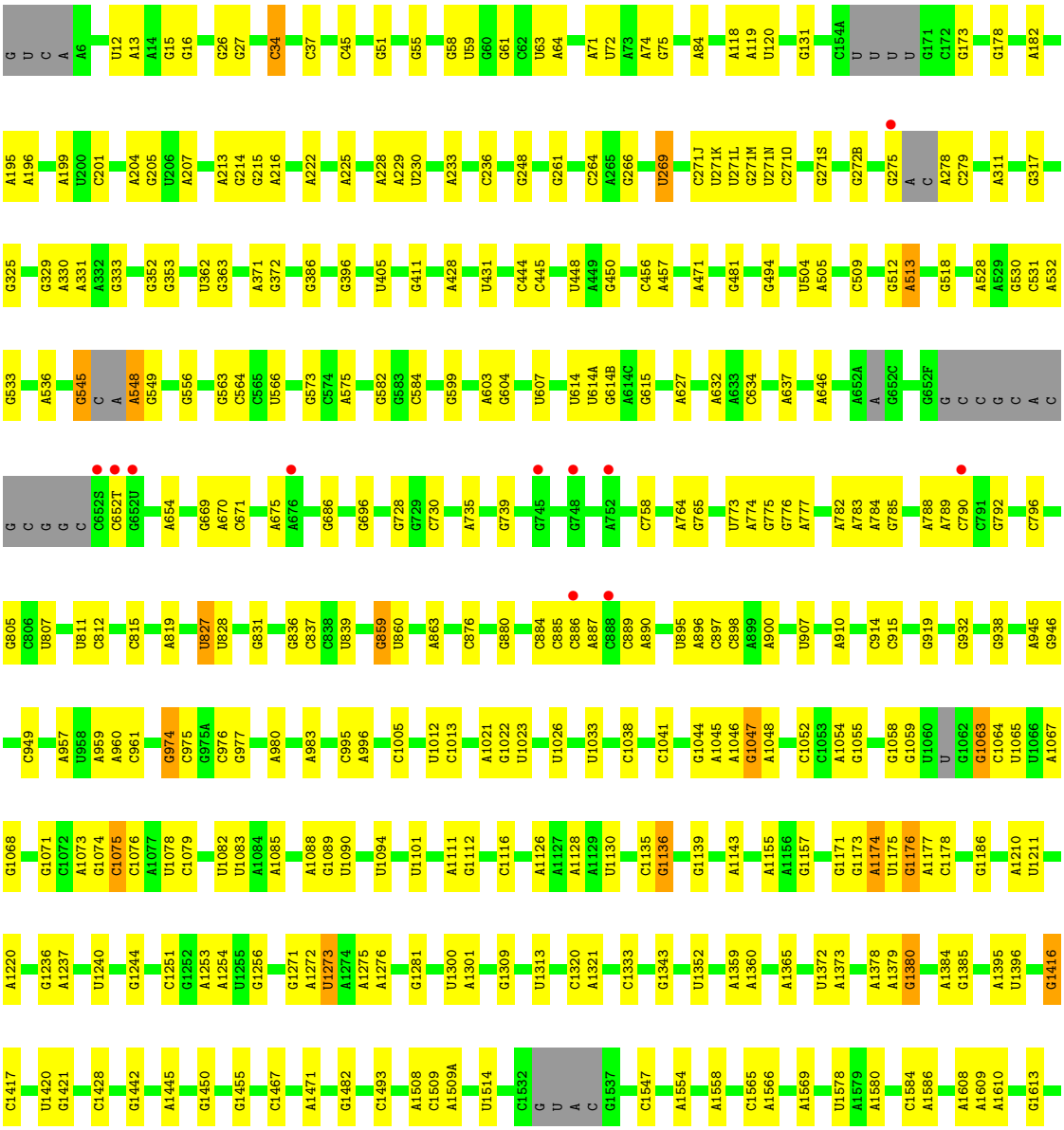
| Mol | Chain | Residues | Atoms | | ZeroOcc | AltConf |
|---|---|---|---|---|---|---|
| | | | Total | K | | |
| 60 | 2A | 1 | 1 | 1 | 0 | 0 |

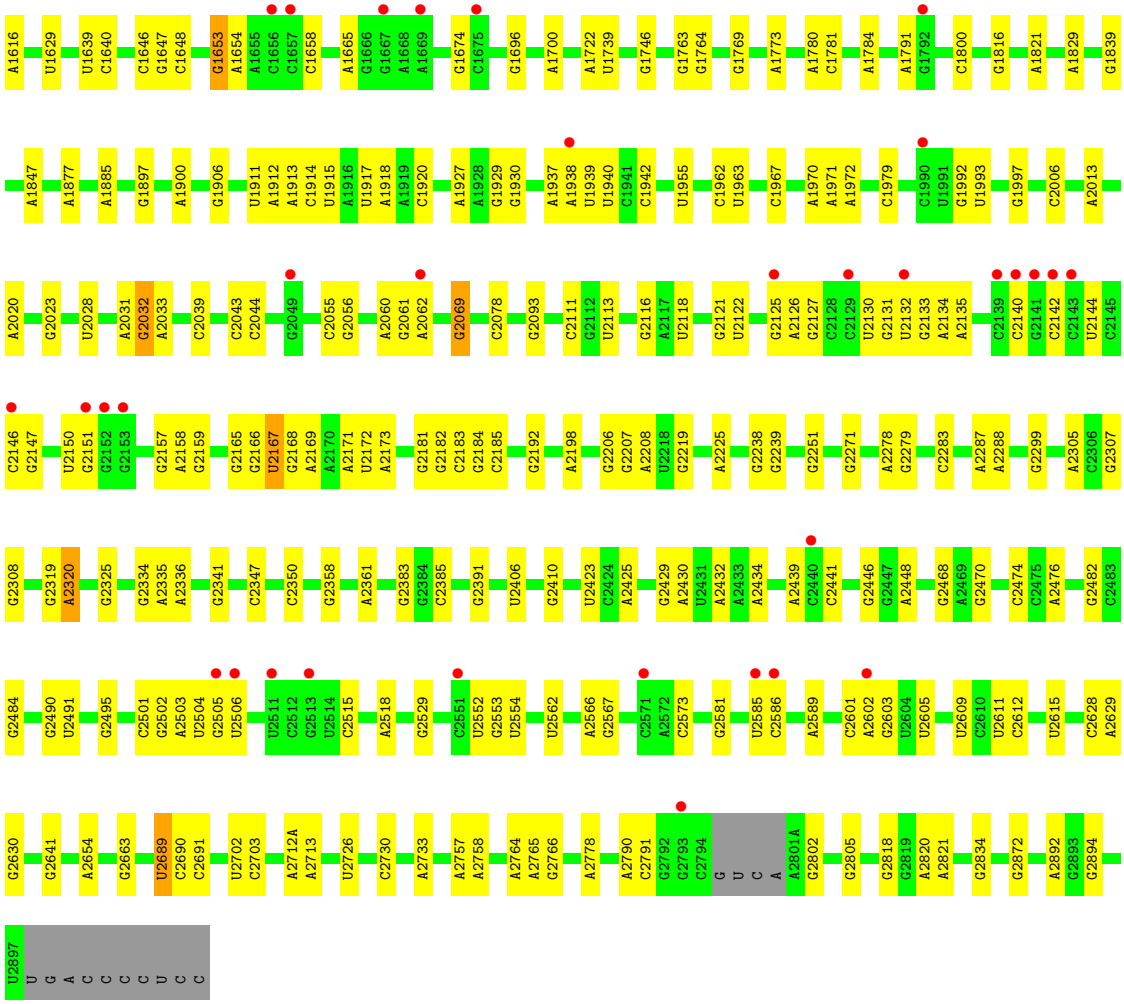
# 3 Residue-property plots (i)

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: 23S Ribosomal RNA

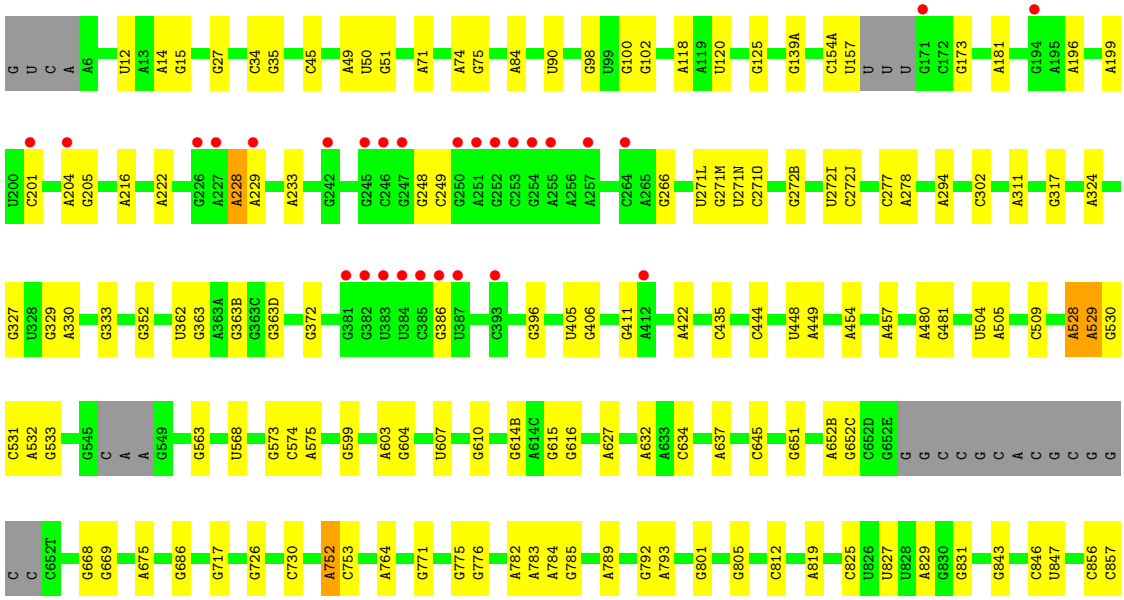
Chain 1A: 2% 79% 19%

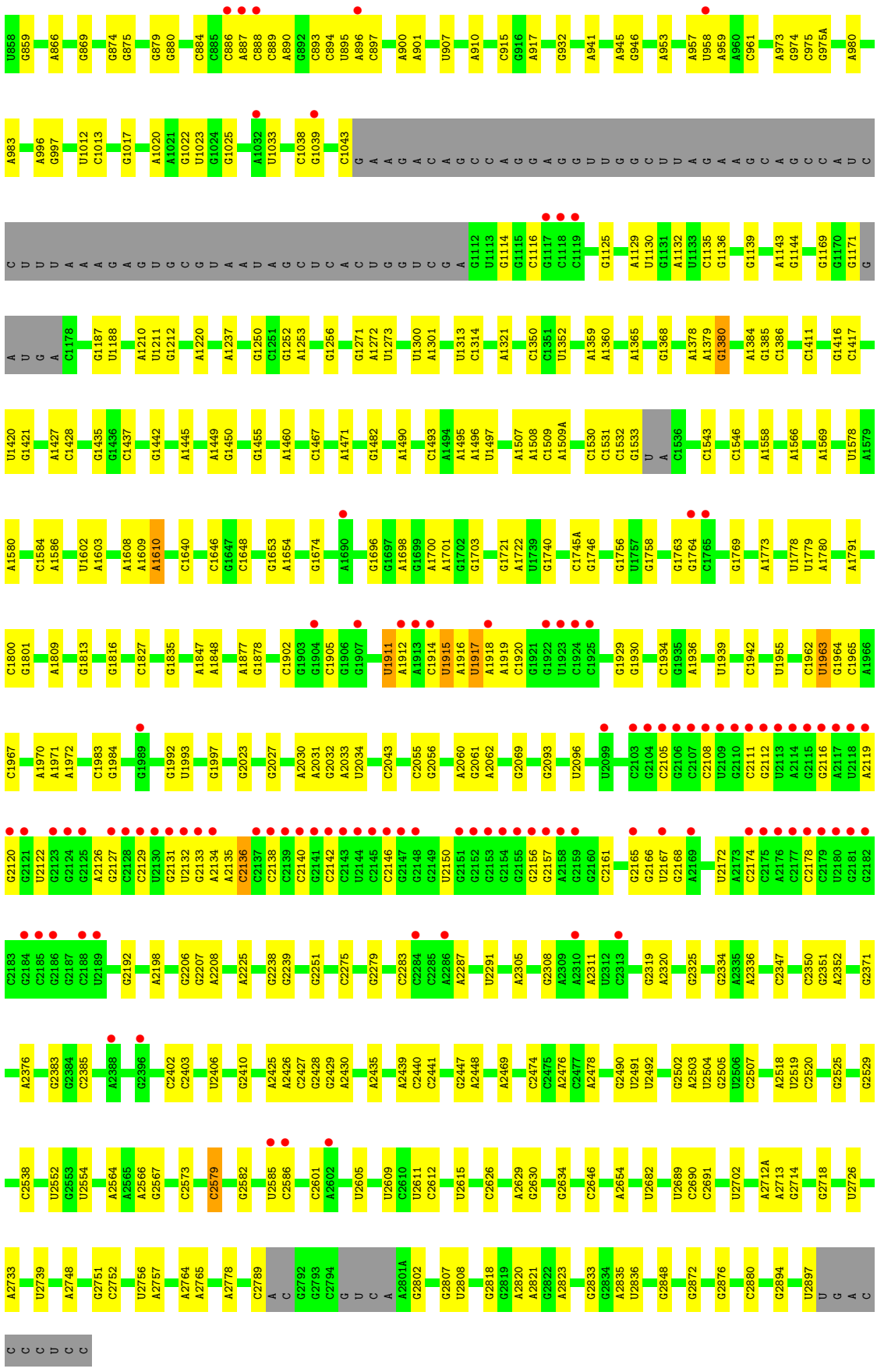





- Molecule 1: 23S Ribosomal RNA

Chain 2A:




U858 G859 A866 G869 G874 G875 G879 G880 C884 C885 C886 A887 C888 C889 A890 G892 C893 C894 U895 A896 C897 A900 A901 U907 A910 C915 G916 A917 G932 A941 A945 G946 A953 A957 U958 A959 A960 C961 A973 G974 C975 G975A A980
A983 A996 G997 U1012 C1013 G1017 A1020 A1021 G1022 U1023 G1024 G1025 A1032 U1033 C1038 G1039 C1043 G A A G A C A G C C G A A G G U U G C C C A U C
C U U U A A A G A G U G C G U A A U A G C U C A C U G G A G1112 U1113 G1114 G1115 C1116 G1117 C1118 C1119 G1125 A1129 U1130 G1131 A1132 U1133 C1135 G1136 G1139 A1143 G1144 G1169 G1170 G1171 G
A U G A C1178 G1187 U1188 A1210 U1211 G1212 A1220 A1237 G1250 C1251 G1252 A1253 G1256 G1271 A1272 U1273 U1300 A1301 U1313 C1314 A1321 C1350 C1351 U1352 A1359 A1360 A1365 G1368 A1378 A1379 G1380 A1384 G1385 C1386 C1411 G1416 C1417
U1420 G1421 A1427 C1428 G1435 G1436 C1437 G1442 A1445 A1449 G1450 G1455 A1460 C1467 A1471 G1482 A1490 C1493 A1494 A1495 A1496 U1497 A1507 A1508 C1509 A1509A C1530 C1531 C1532 G1533 U A C1536 C1543 C1546 A1558 A1566 A1569 U1578 A1579
A1580 C1584 A1586 U1602 A1603 A1608 A1609 A1610 C1640 C1646 G1647 C1648 G1653 A1654 G1674 A1690 G1696 G1697 A1698 G1699 A1700 A1701 G1702 G1703 G1721 A1722 U1739 G1740 C1745A G1746 G1756 U1757 G1758 G1763 G1764 C1765 G1769 A1773 U1778 U1779 A1780 A1791
C1800 G1801 A1809 G1813 G1816 C1827 G1835 A1847 A1848 A1877 G1878 C1902 G1903 G1904 C1905 G1906 G1907 U1911 A1912 A1913 C1914 U1915 A1916 U1917 A1918 A1919 C1920 G1921 G1922 U1923 C1924 C1925 G1929 G1930 C1934 G1935 A1936 U1939 C1942 U1955 C1962 U1963 G1964 C1965 A1966
C1967 A1970 A1971 A1972 C1983 G1984 G1989 G1992 U1993 G1997 G2023 G2027 A2030 A2031 G2032 A2033 U2034 C2043 C2055 G2056 A2060 G2061 A2062 G2069 G2093 U2096 U2099 C2103 G2104 C2105 G2106 C2107 C2108 U2109 G2110 C2111 G2112 U2113 A2114 G2115 G2116 A2117 U2118 A2119
G2120 G2121 U2122 G2123 G2124 G2125 A2126 G2127 C2128 C2129 U2130 G2131 U2132 G2133 A2134 A2135 C2136 C2137 C2138 C2139 C2140 G2141 C2142 C2143 U2144 C2145 C2146 G2147 G2148 G2149 U2150 G2151 G2152 G2153 G2154 G2155 G2156 G2157 A2158 G2159 G2160 C2161 G2165 G2166 U2167 G2168 A2169 U2172 A2173 C2174 C2175 A2176 C2177 C2178 C2179 U2180 G2181 G2182
C2183 G2184 C2185 G2186 G2187 C2188 U2189 G2192 A2198 G2206 G2207 A2208 A2225 G2238 G2239 G2251 C2275 G2279 C2283 C2284 C2285 A2286 A2287 U2291 A2305 G2308 A2309 A2310 A2311 U2312 C2313 G2319 A2320 G2325 G2334 A2335 A2336 C2347 C2350 G2351 A2352 G2371
A2376 G2383 G2384 C2385 A2388 G2396 C2402 C2403 U2406 G2410 A2425 A2426 C2427 G2428 G2429 A2430 A2435 A2439 C2440 C2441 G2447 A2448 A2469 C2474 C2475 A2476 C2477 A2478 G2490 U2491 U2492 G2502 A2503 U2504 G2505 U2506 C2507 A2518 U2519 C2520 G2525 G2529
C2538 U2552 G2553 U2554 A2564 A2565 A2566 G2567 C2573 C2579 G2582 U2585 C2586 C2601 A2602 U2605 U2609 C2610 U2611 C2612 U2615 C2626 A2629 G2630 G2634 C2646 A2654 U2682 U2689 C2690 C2691 U2702 A2712A A2713 G2714 G2718 U2726
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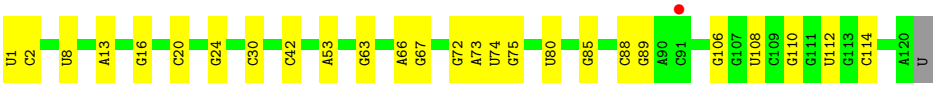
C C C U C C

- Molecule 2: 5S Ribosomal RNA

Chain 1B:

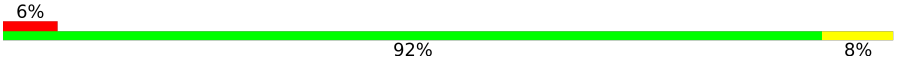
- Molecule 2: 5S Ribosomal RNA

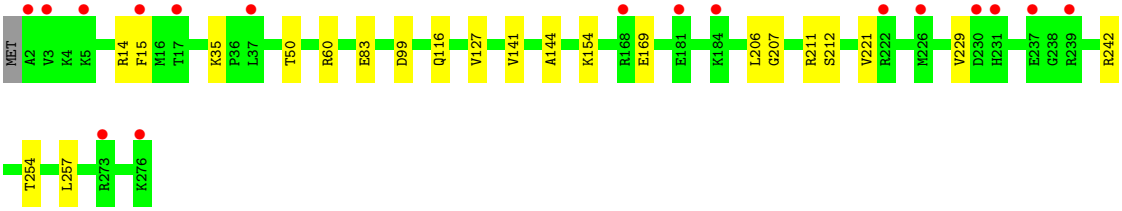
Chain 2B:




- Molecule 3: 50S ribosomal protein L2

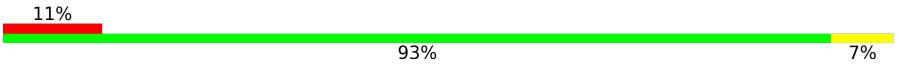
Chain 1D:

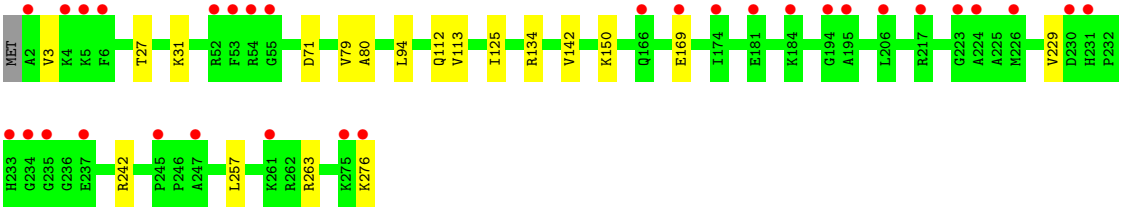



- Molecule 3: 50S ribosomal protein L2

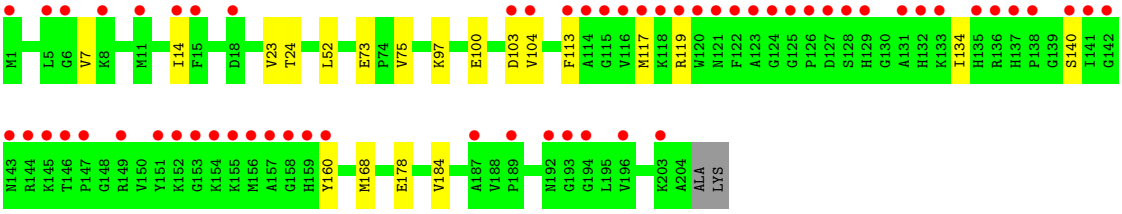
Chain 2D:



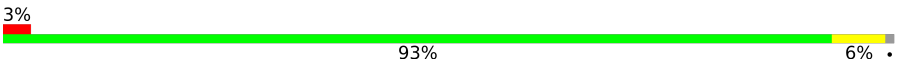

- Molecule 4: 50S ribosomal protein L3

Chain 1E:



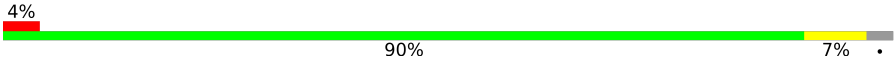

- Molecule 4: 50S ribosomal protein L3

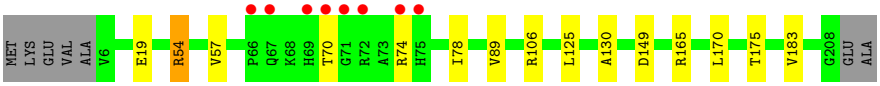
Chain 2E:



• Molecule 5: 50S ribosomal protein L4

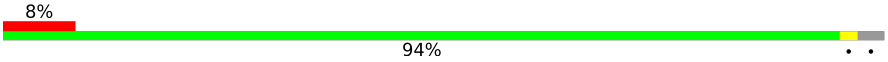
Chain 1F:

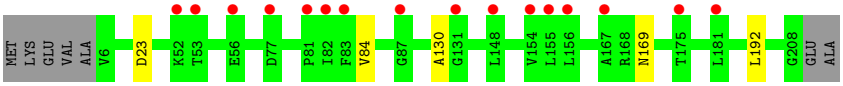



• Molecule 5: 50S ribosomal protein L4

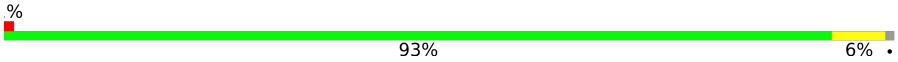
Chain 2F:



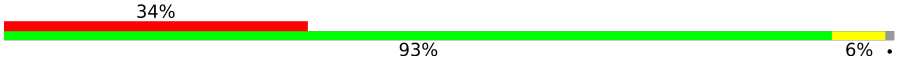

• Molecule 6: 50S ribosomal protein L5

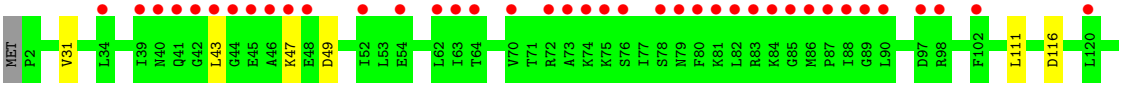
Chain 1G:

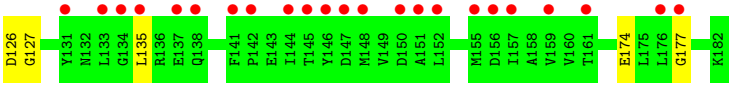


• Molecule 6: 50S ribosomal protein L5

Chain 2G:

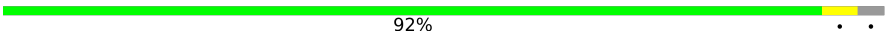


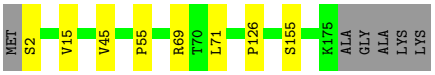




• Molecule 7: 50S ribosomal protein L6

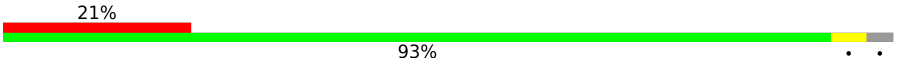
Chain 1H:

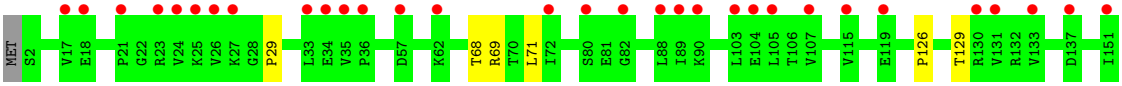


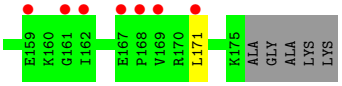




• Molecule 7: 50S ribosomal protein L6

Chain 2H:

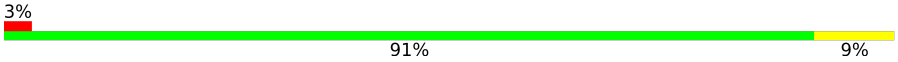


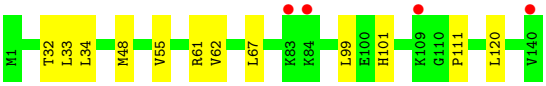






• Molecule 8: 50S ribosomal protein L13

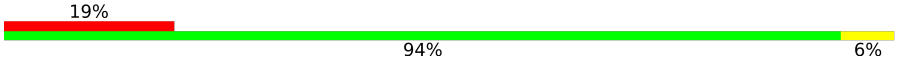
Chain 1N:

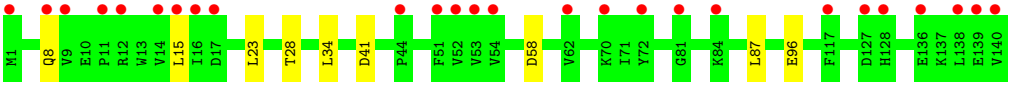



• Molecule 8: 50S ribosomal protein L13

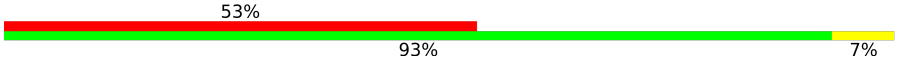
Chain 2N:

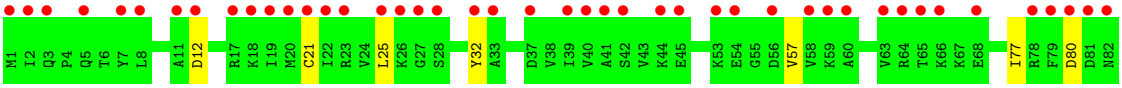


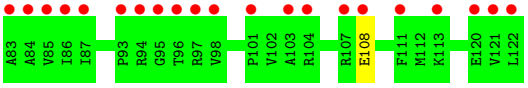




• Molecule 9: 50S ribosomal protein L14

Chain 1O:

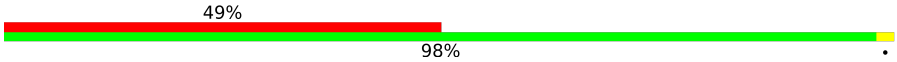


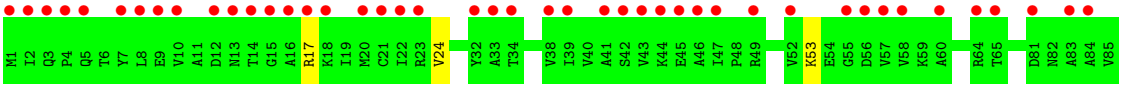



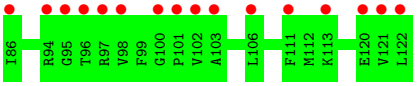




• Molecule 9: 50S ribosomal protein L14

Chain 2O:

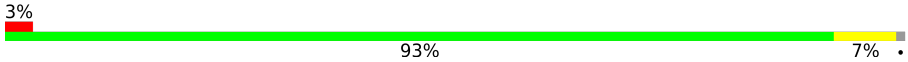


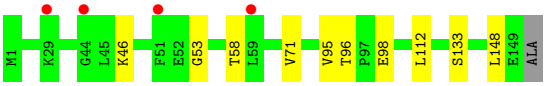




• Molecule 10: 50S ribosomal protein L15

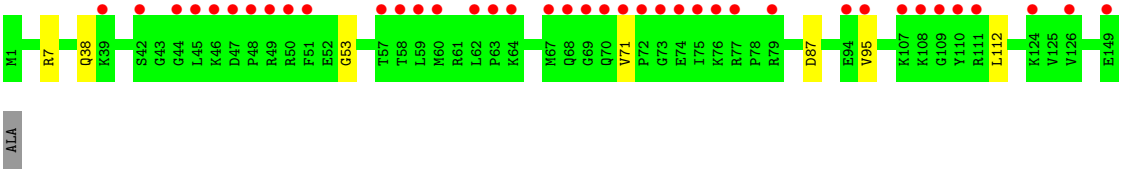
Chain 1P:



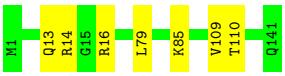

• Molecule 10: 50S ribosomal protein L15

Chain 2P: 26% 95% 5%



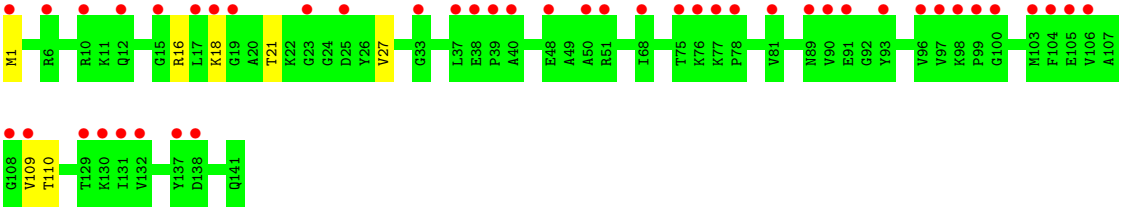

• Molecule 11: 50S ribosomal protein L16

Chain 1Q: 95% 5%



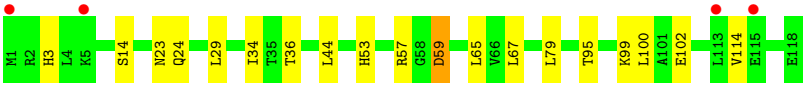

• Molecule 11: 50S ribosomal protein L16

Chain 2Q: 32% 95% 5%



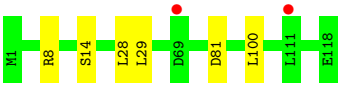

• Molecule 12: 50S ribosomal protein L17

Chain 1R: 3% 84% 15%




• Molecule 12: 50S ribosomal protein L17

Chain 2R: 2% 95% 5%

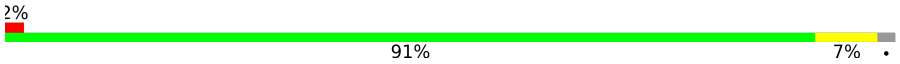


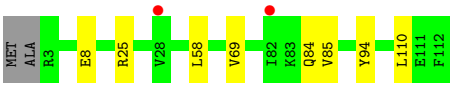

• Molecule 13: 50S ribosomal protein L18

Chain 1S: 90% 8%

• Molecule 13: 50S ribosomal protein L18

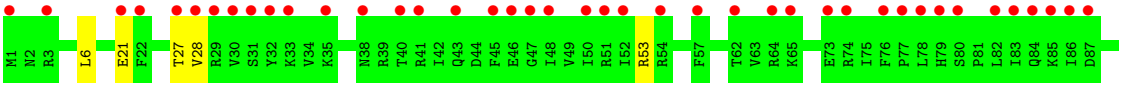
Chain 2S:



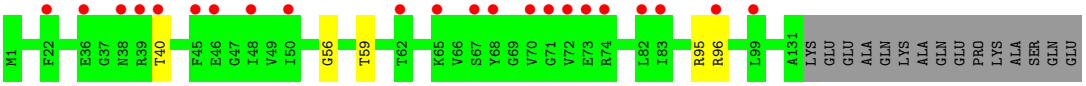

• Molecule 14: 50S ribosomal protein L19

Chain 1T:



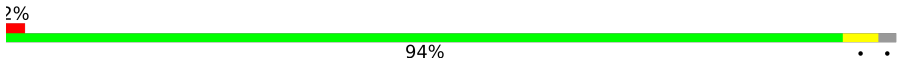
• Molecule 14: 50S ribosomal protein L19

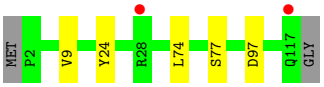
Chain 2T:




• Molecule 15: 50S ribosomal protein L20

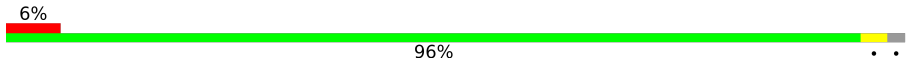
Chain 1U:

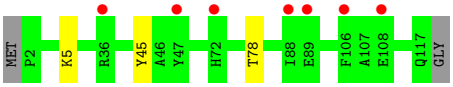



• Molecule 15: 50S ribosomal protein L20

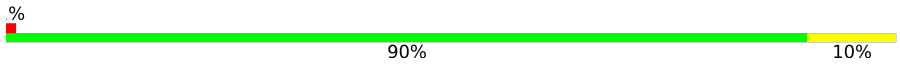
Chain 2U:



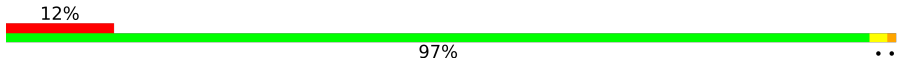

• Molecule 16: 50S ribosomal protein L21

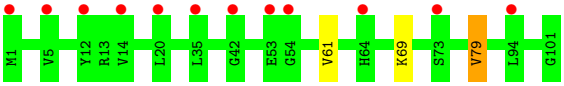
Chain 1V:



• Molecule 16: 50S ribosomal protein L21

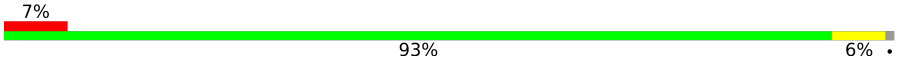
Chain 2V:

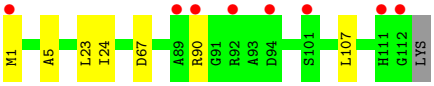





• Molecule 17: 50S ribosomal protein L22

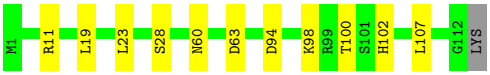
Chain 1W:



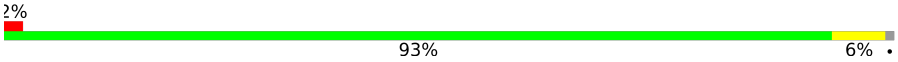

• Molecule 17: 50S ribosomal protein L22

Chain 2W:



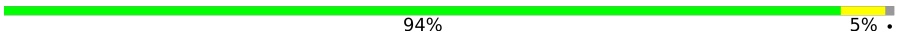

• Molecule 18: 50S ribosomal protein L23

Chain 1X:



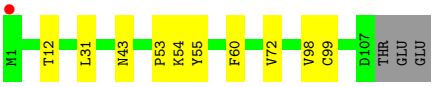
• Molecule 18: 50S ribosomal protein L23

Chain 2X:



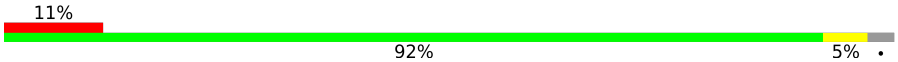
• Molecule 19: 50S ribosomal protein L24

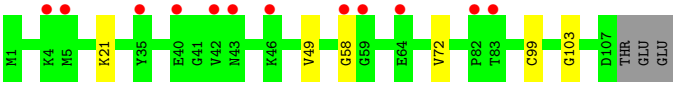
Chain 1Y:




• Molecule 19: 50S ribosomal protein L24

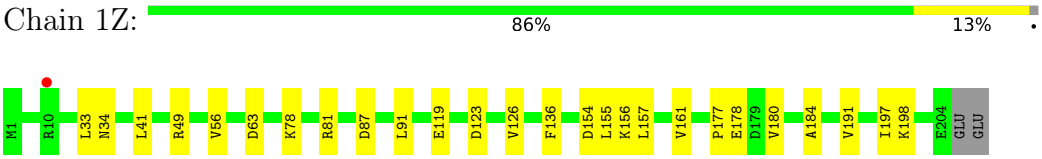
Chain 2Y:



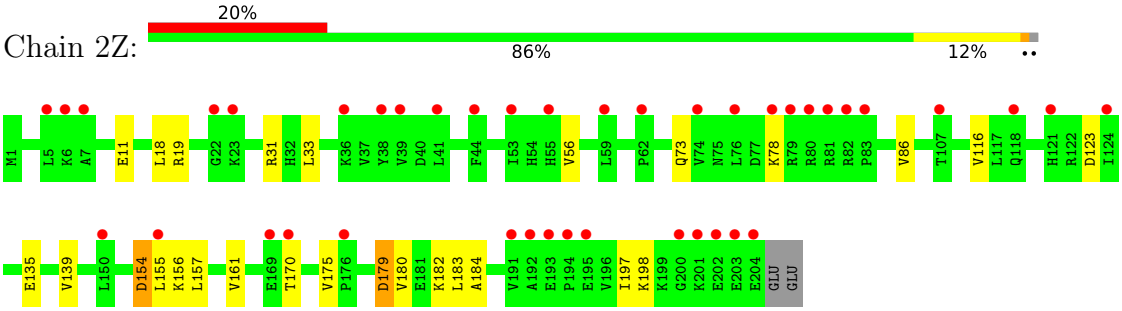

• Molecule 20: 50S ribosomal protein L25

Chain 1Z:



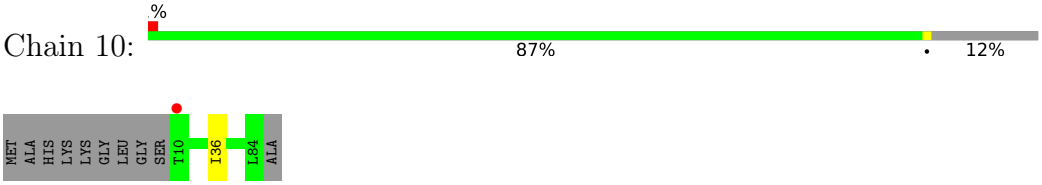

• Molecule 20: 50S ribosomal protein L25

Chain 2Z:



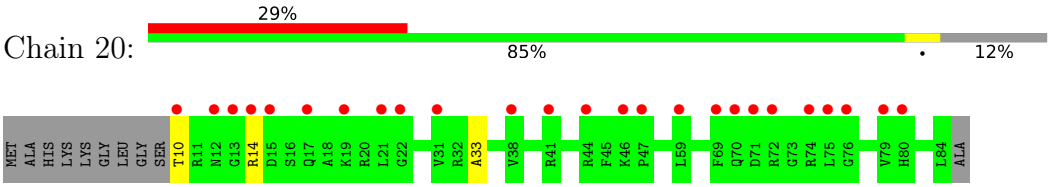

• Molecule 21: 50S ribosomal protein L27

Chain 10:



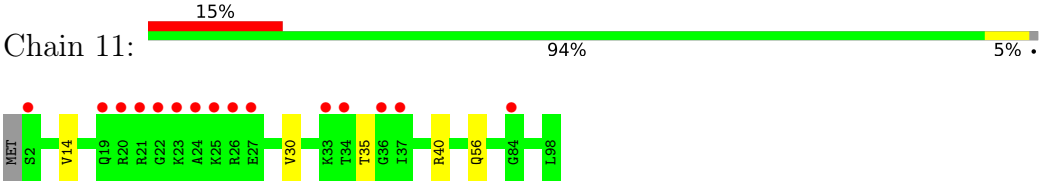

• Molecule 21: 50S ribosomal protein L27

Chain 20:



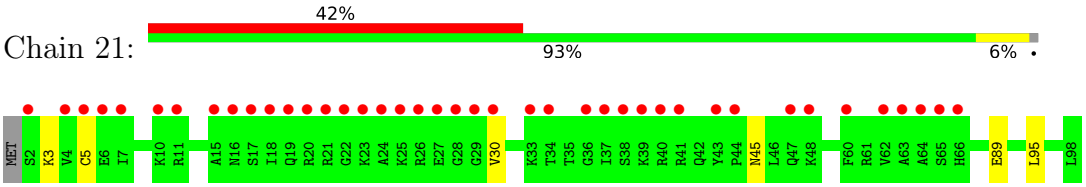

• Molecule 22: 50S ribosomal protein L28

Chain 11:



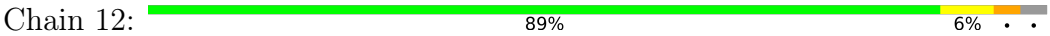

• Molecule 22: 50S ribosomal protein L28

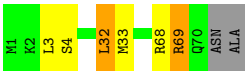
Chain 21:




• Molecule 23: 50S ribosomal protein L29

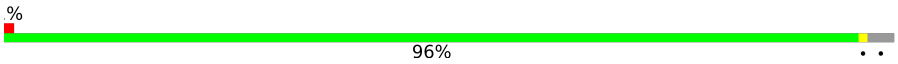
Chain 12:

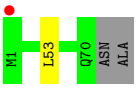





• Molecule 23: 50S ribosomal protein L29

Chain 22:



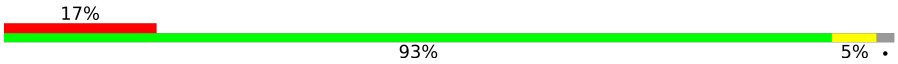



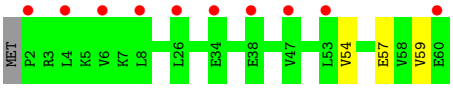

• Molecule 24: 50S ribosomal protein L30

Chain 13:

• Molecule 24: 50S ribosomal protein L30

Chain 23:



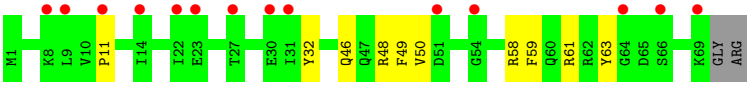




• Molecule 25: 50S ribosomal protein L31

Chain 14:

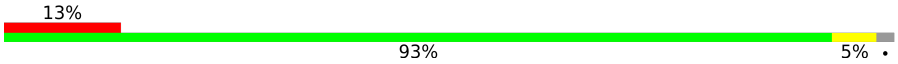
• Molecule 25: 50S ribosomal protein L31

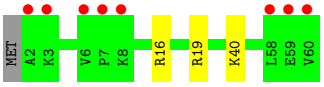
Chain 24:




• Molecule 26: 50S ribosomal protein L32

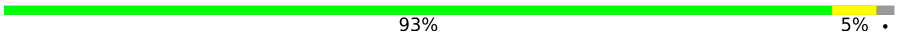
Chain 15:



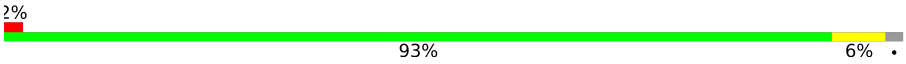

• Molecule 26: 50S ribosomal protein L32

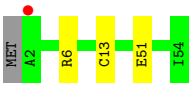
Chain 25:



• Molecule 27: 50S ribosomal protein L33

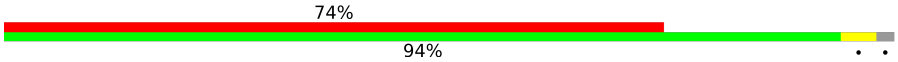
Chain 16:

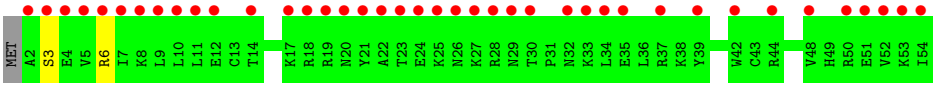



• Molecule 27: 50S ribosomal protein L33

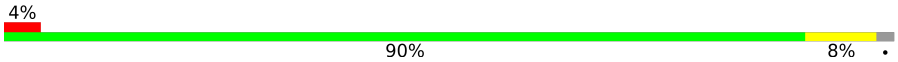
Chain 26:



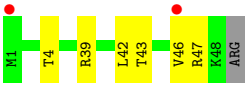

• Molecule 28: 50S ribosomal protein L34

Chain 17:



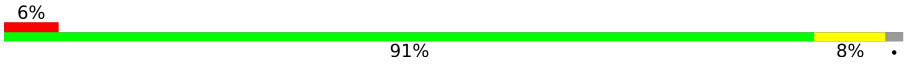
• Molecule 28: 50S ribosomal protein L34

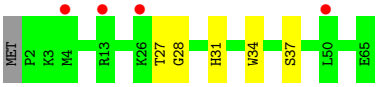
Chain 27:




• Molecule 29: 50S ribosomal protein L35

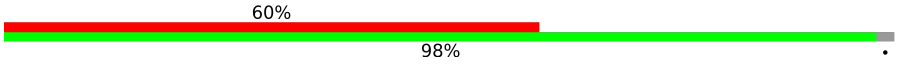
Chain 18:

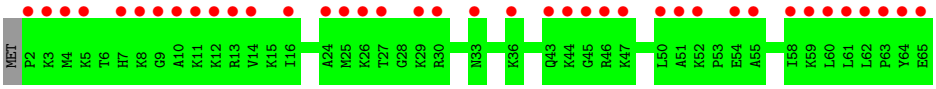



• Molecule 29: 50S ribosomal protein L35

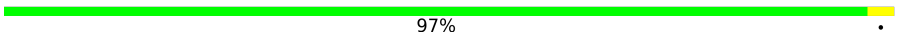
Chain 28:



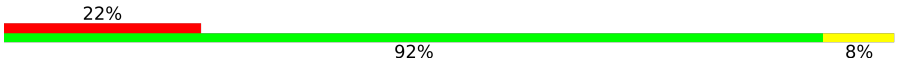
- Molecule 30: 50S ribosomal protein L36

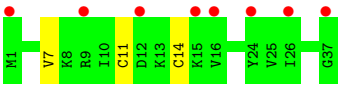
Chain 19:



- Molecule 30: 50S ribosomal protein L36

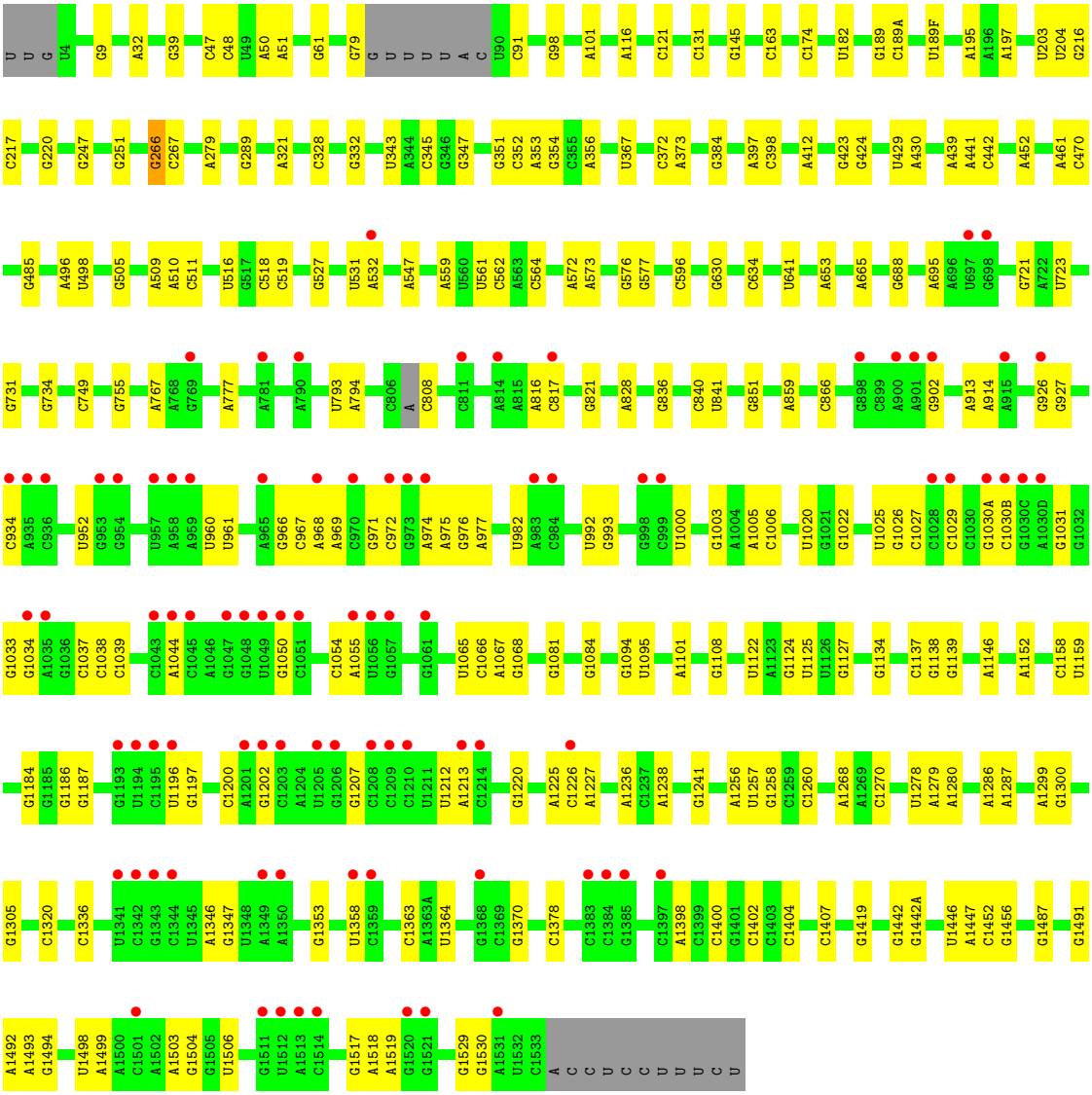
Chain 29:



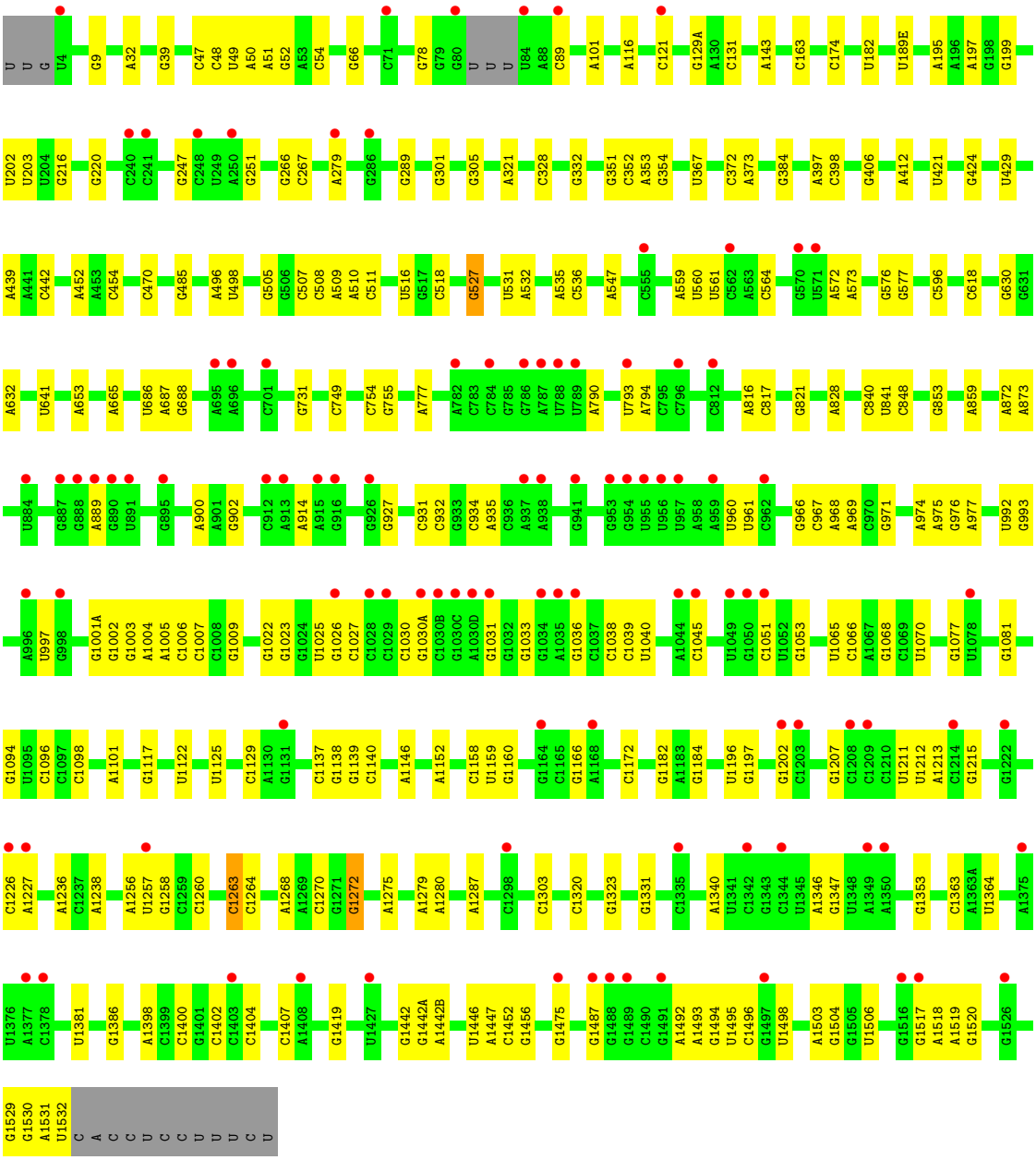

- Molecule 31: 16S Ribosomal RNA

Chain 1a:



• Molecule 31: 16S Ribosomal RNA

Chain 2a:

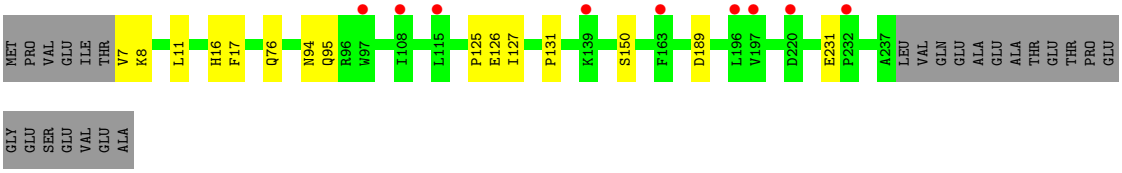



• Molecule 32: 30S ribosomal protein S2

Chain 1b:

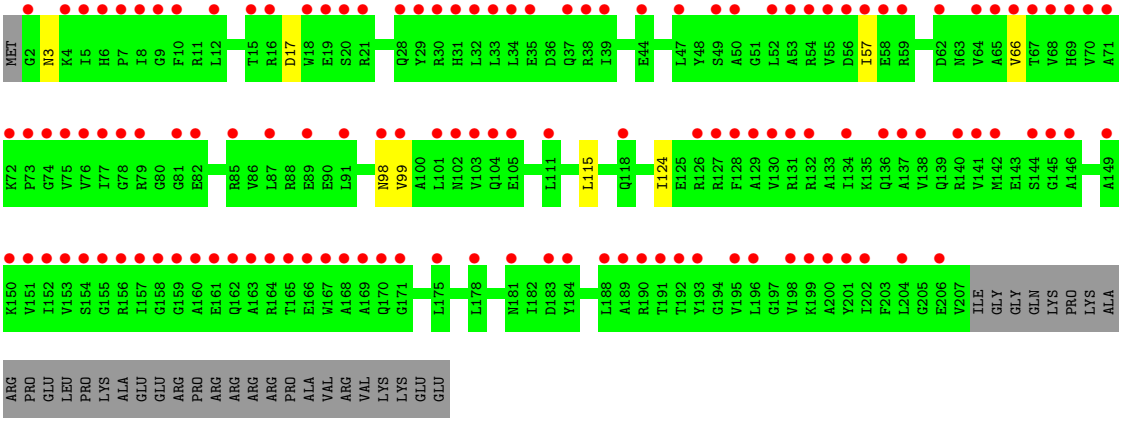
- Molecule 32: 30S ribosomal protein S2

Chain 2b:



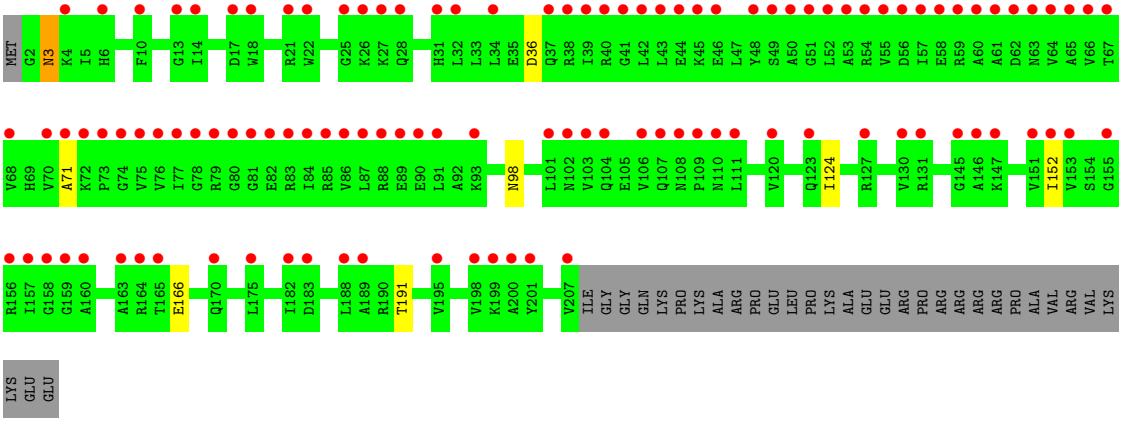

- Molecule 33: 30S ribosomal protein S3

Chain 1c:



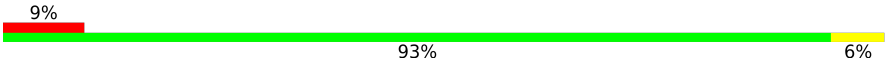

- Molecule 33: 30S ribosomal protein S3

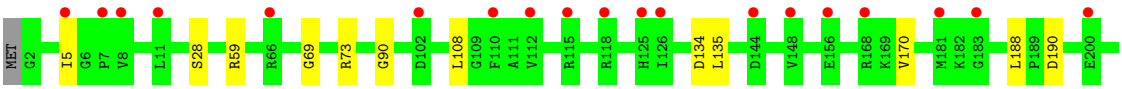
Chain 2c:




- Molecule 34: 30S ribosomal protein S4

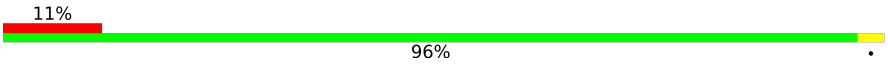
Chain 1d:

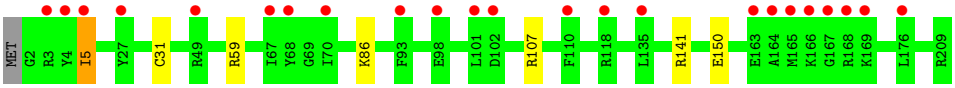


• Molecule 34: 30S ribosomal protein S4

Chain 2d:



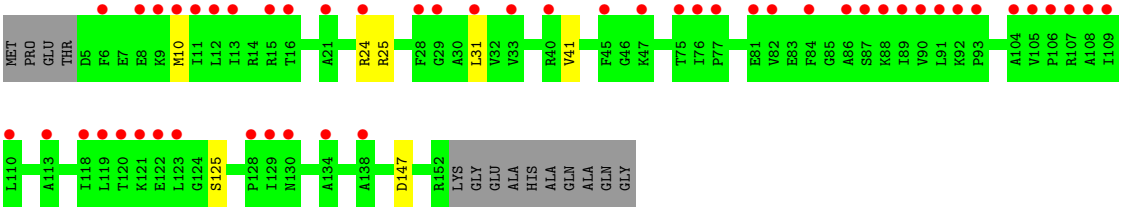




• Molecule 35: 30S ribosomal protein S5

Chain 1e:

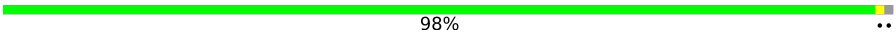
• Molecule 35: 30S ribosomal protein S5

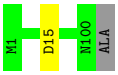
Chain 2e:




• Molecule 36: 30S ribosomal protein S6

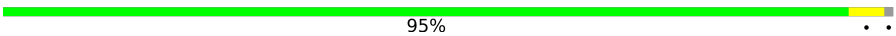
Chain 1f:



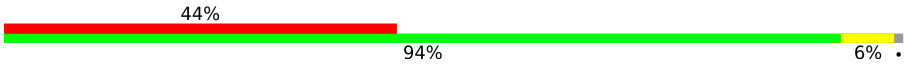

• Molecule 36: 30S ribosomal protein S6

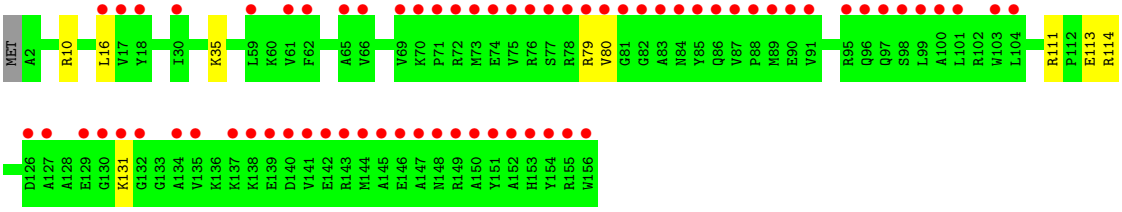
Chain 2f:



• Molecule 37: 30S ribosomal protein S7

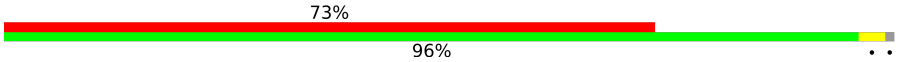
Chain 1g:

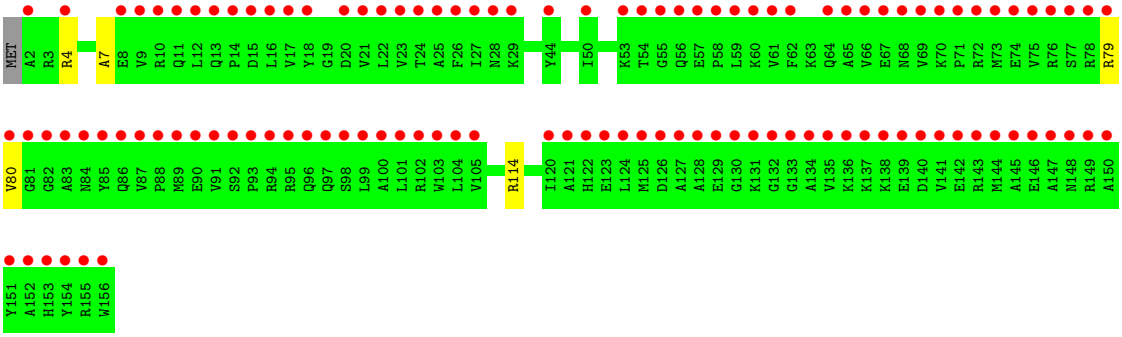





- Molecule 37: 30S ribosomal protein S7

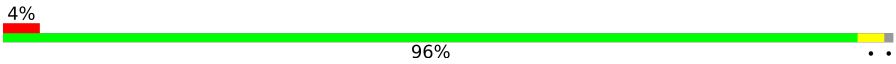
Chain 2g:



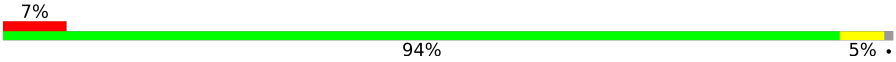

- Molecule 38: 30S ribosomal protein S8

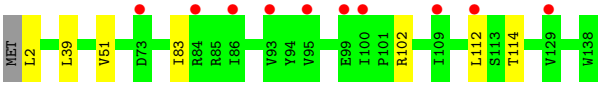
Chain 1h:



- Molecule 38: 30S ribosomal protein S8

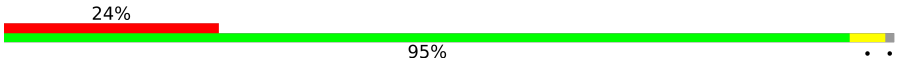
Chain 2h:

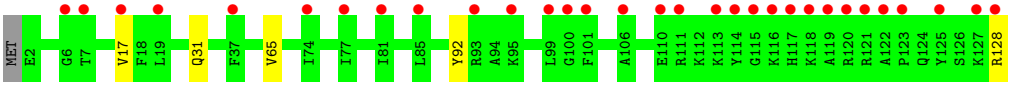



- Molecule 39: 30S ribosomal protein S9

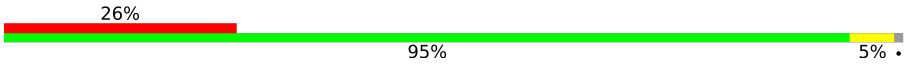
Chain 1i:

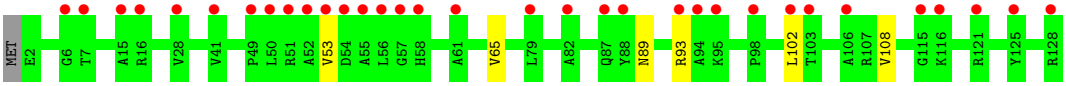



- Molecule 39: 30S ribosomal protein S9

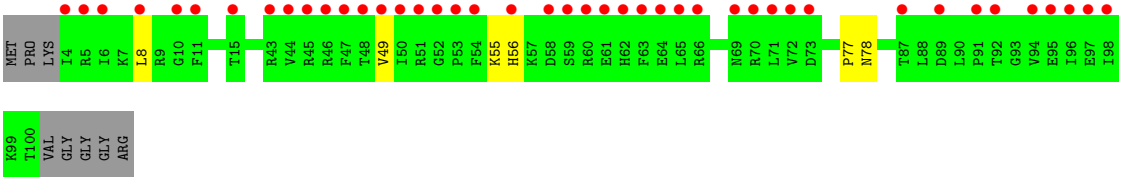
Chain 2i:





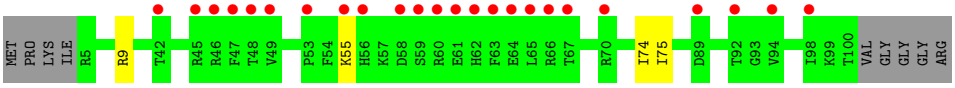

• Molecule 40: 30S ribosomal protein S10

Chain 1j:



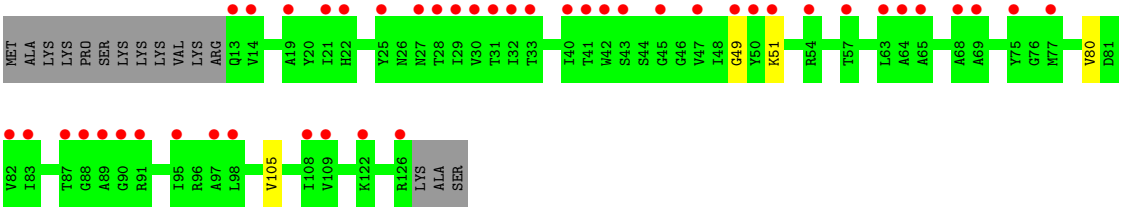

• Molecule 40: 30S ribosomal protein S10

Chain 2j:



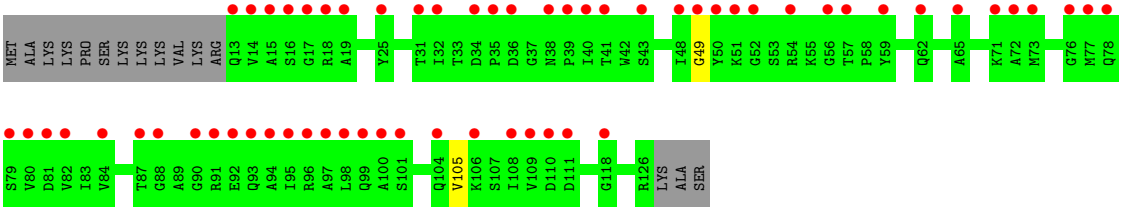

• Molecule 41: 30S ribosomal protein S11

Chain 1k:



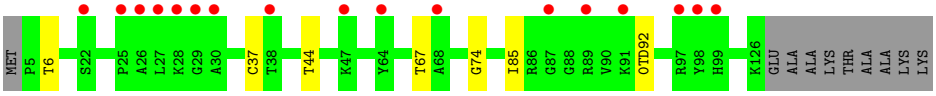

• Molecule 41: 30S ribosomal protein S11

Chain 2k:



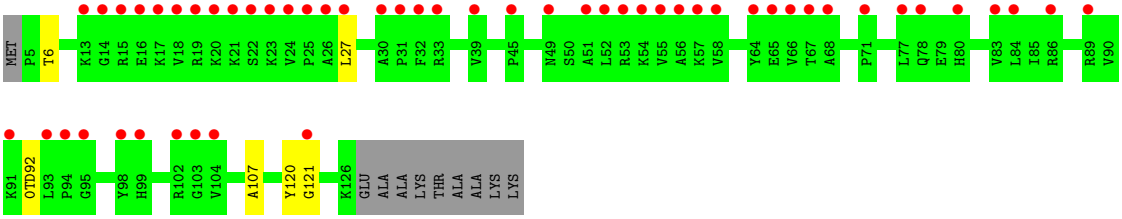

• Molecule 42: 30S ribosomal protein S12

Chain 1l:



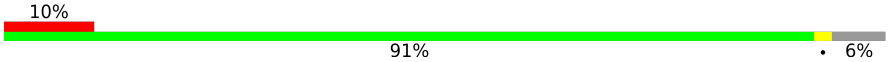
- Molecule 42: 30S ribosomal protein S12

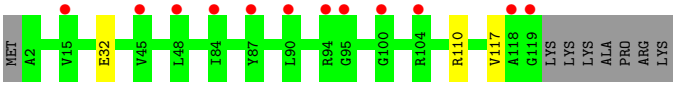
Chain 2l:




- Molecule 43: 30S ribosomal protein S13

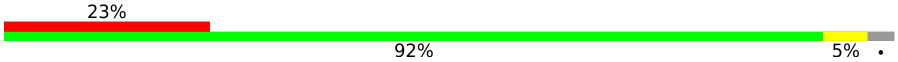
Chain 1m:

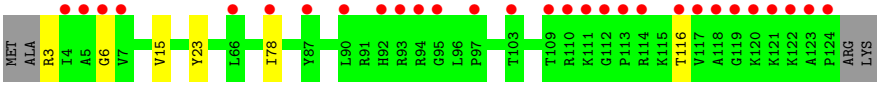



- Molecule 43: 30S ribosomal protein S13

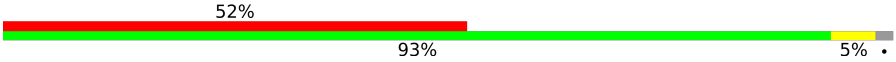
Chain 2m:

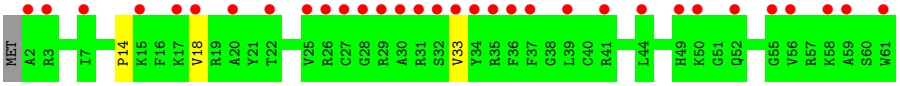



- Molecule 44: 30S ribosomal protein S14 type Z

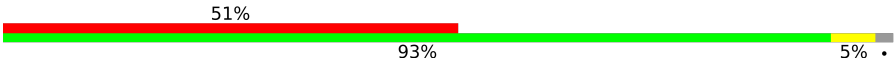
Chain 1n:

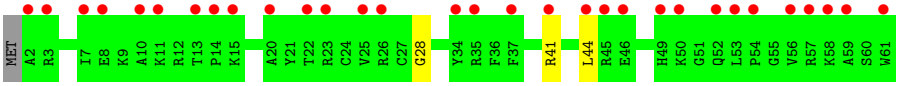



- Molecule 44: 30S ribosomal protein S14 type Z

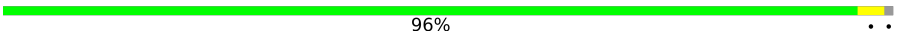
Chain 2n:

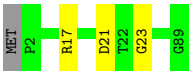



- Molecule 45: 30S ribosomal protein S15

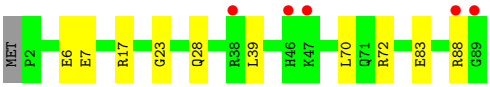
Chain 1o:



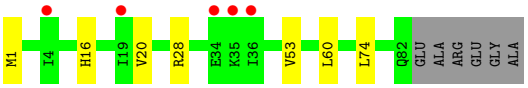

- Molecule 45: 30S ribosomal protein S15

Chain 2o:



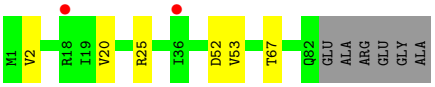

• Molecule 46: 30S ribosomal protein S16

Chain 1p:



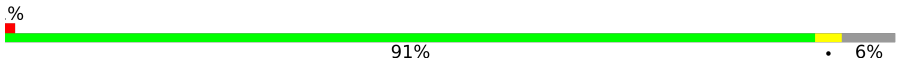

• Molecule 46: 30S ribosomal protein S16

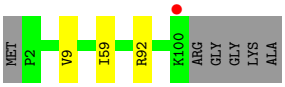
Chain 2p:




• Molecule 47: 30S ribosomal protein S17

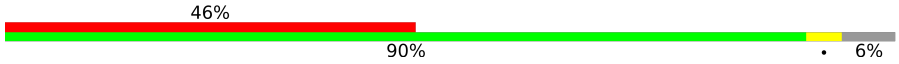
Chain 1q:

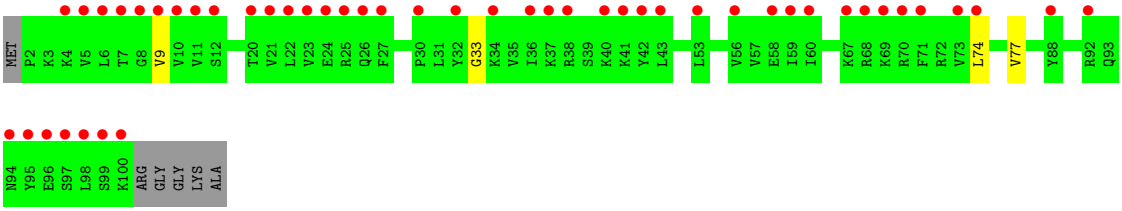



• Molecule 47: 30S ribosomal protein S17

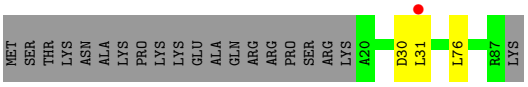
Chain 2q:



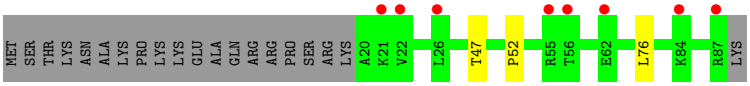

• Molecule 48: 30S ribosomal protein S18

Chain 1r:



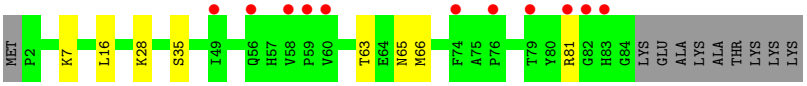

• Molecule 48: 30S ribosomal protein S18

Chain 2r:



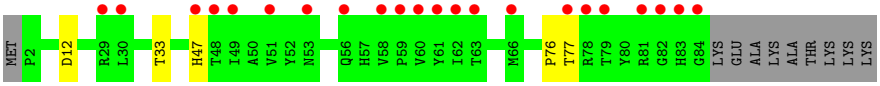

• Molecule 49: 30S ribosomal protein S19

Chain 1s:



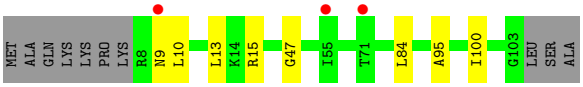

• Molecule 49: 30S ribosomal protein S19

Chain 2s:



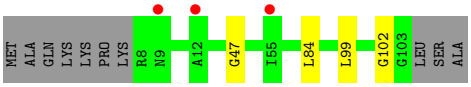

• Molecule 50: 30S ribosomal protein S20

Chain 1t:



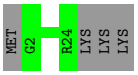

• Molecule 50: 30S ribosomal protein S20

Chain 2t:



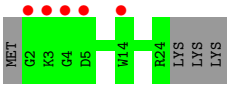

• Molecule 51: 30S ribosomal protein Thx

Chain 1u:



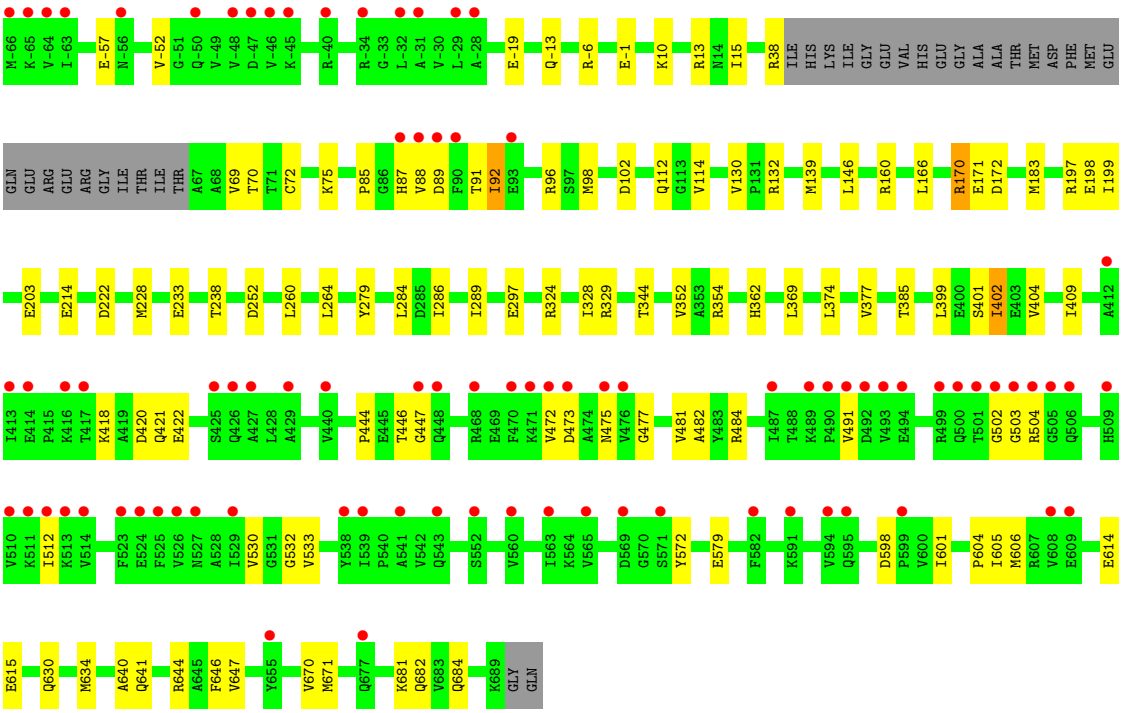

• Molecule 51: 30S ribosomal protein Thx

Chain 2u:



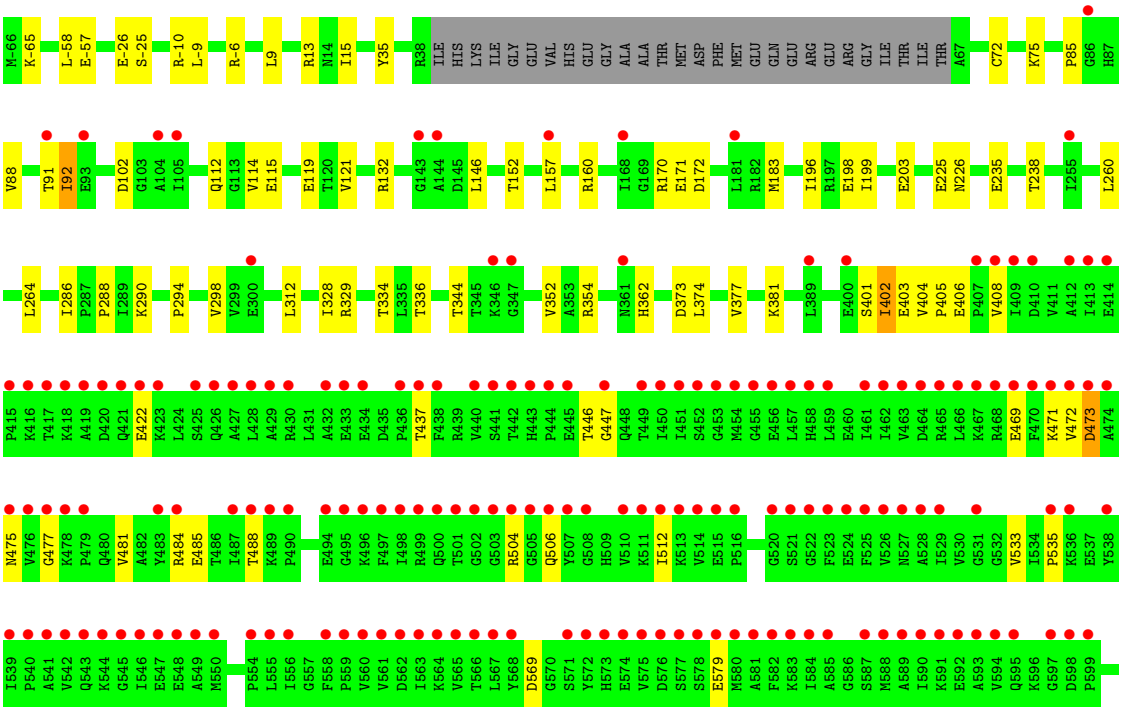

• Molecule 52: 50S ribosomal protein L9,Elongation factor G

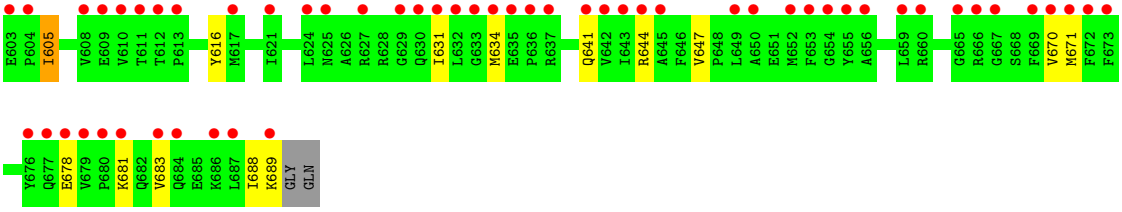
Chain 1v:




- Molecule 52: 50S ribosomal protein L9,Elongation factor G

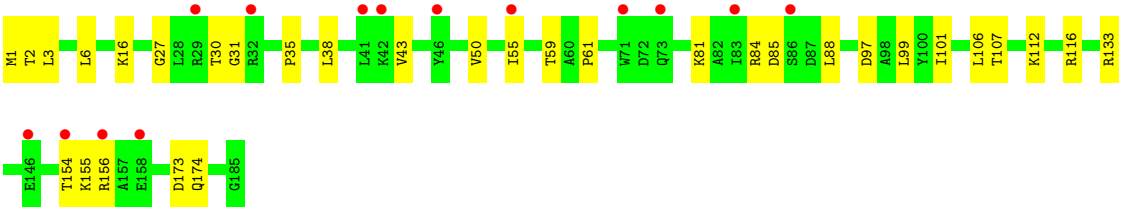
Chain 2v:





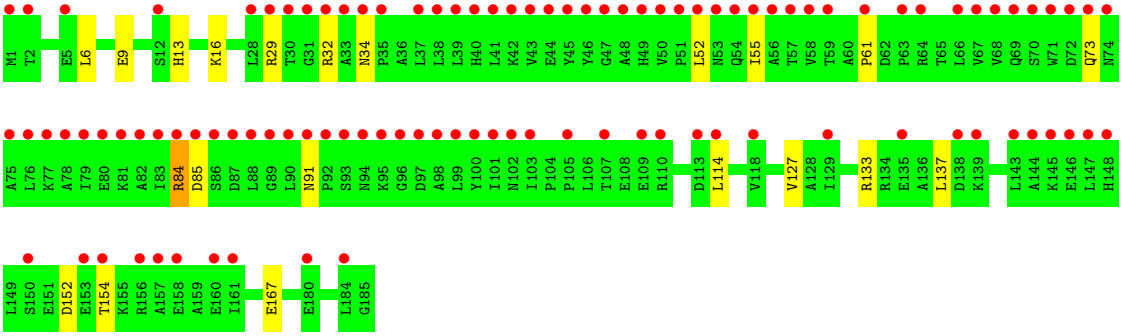

- Molecule 53: Ribosome-recycling factor

Chain 1w:



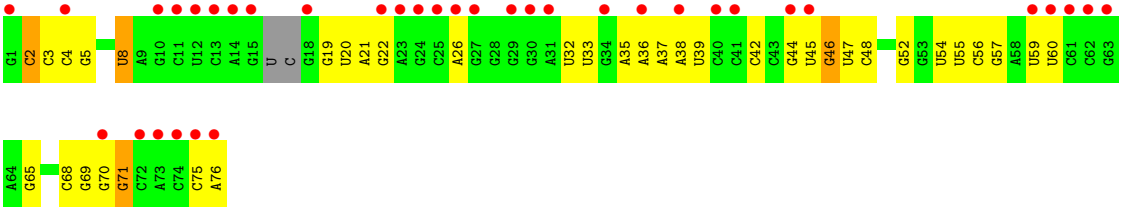

- Molecule 53: Ribosome-recycling factor

Chain 2w:



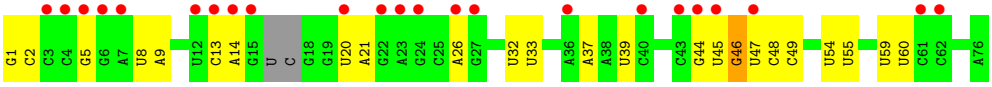

- Molecule 54: P-site and E-site tRNAs

Chain 1x:



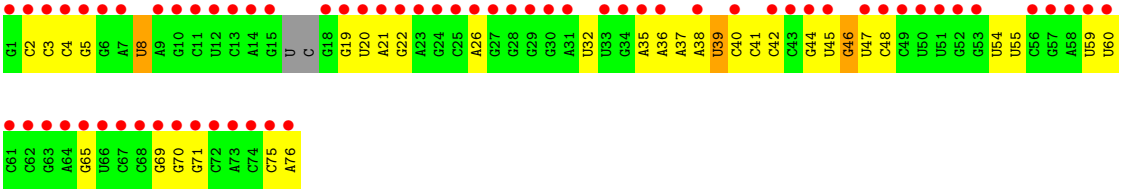

- Molecule 54: P-site and E-site tRNAs

Chain 1y:



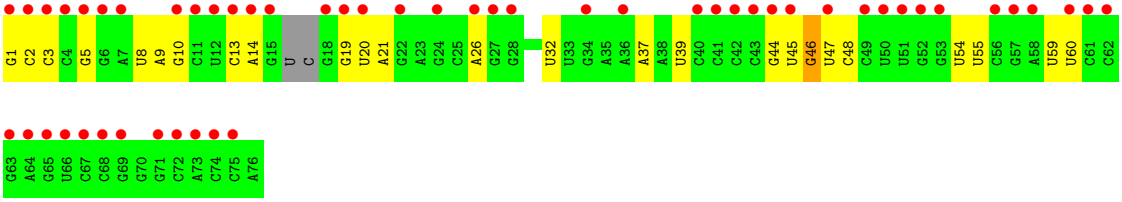
- Molecule 54: P-site and E-site tRNAs

Chain 2x:



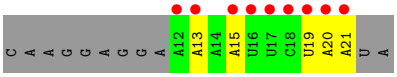

- Molecule 54: P-site and E-site tRNAs

Chain 2y:



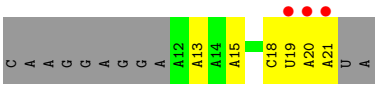

- Molecule 55: mRNA

Chain 1z:




- Molecule 55: mRNA

Chain 2z:



# 4 Data and refinement statistics (i)

| Property | Value | Source |
|---|---|---|
| Space group | P 21 21 21 | Depositor |
| Cell constants<br>a, b, c, $\alpha$, $\beta$, $\gamma$ | 209.66Å 448.74Å 623.99Å<br>90.00° 90.00° 90.00° | Depositor |
| Resolution (Å) | 49.89 – 3.50<br>188.71 – 3.50 | Depositor<br>EDS |
| % Data completeness<br>(in resolution range) | 98.4 (49.89-3.50)<br>98.3 (188.71-3.50) | Depositor<br>EDS |
| $R_{merge}$ | 0.33 | Depositor |
| $R_{sym}$ | (Not available) | Depositor |
| $< I/\sigma(I) >$ [1] | 1.09 (at 3.49Å) | Xtriage |
| Refinement program | PHENIX 1.13_2998 | Depositor |
| R, $R_{free}$ | 0.244 , 0.294<br>0.245 , 0.295 | Depositor<br>DCC |
| $R_{free}$ test set | 36340 reflections (5.04%) | wwPDB-VP |
| Wilson B-factor (Å$^2$) | 112.7 | Xtriage |
| Anisotropy | 0.257 | Xtriage |
| Bulk solvent $k_{sol}$(e/Å$^3$), $B_{sol}$(Å$^2$) | 0.25 , 93.5 | EDS |
| L-test for twinning[2] | $< \|L\| > = 0.36$, $< L^2 > = 0.19$ | Xtriage |
| Estimated twinning fraction | No twinning to report. | Xtriage |
| $F_o$,$F_c$ correlation | 0.89 | EDS |
| Total number of atoms | 305259 | wwPDB-VP |
| Average B, all atoms (Å$^2$) | 135.0 | wwPDB-VP |

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 1.56% 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 (i)

## 5.1 Standard geometry (i)

Bond lengths and bond angles in the following residue types are not validated in this section: ZN, 2MG, PSU, MIA, UR3, GDP, 0TD, M2G, 4SU, 5MU, 7MG, MG, 5MC, K, OMC, 2MA, 4OC, MA6, SF4, OMG, 2MU

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 | 1A | 0.62 | 0/69010 | 1.08 | 104/107716 (0.1%) |
| 1 | 2A | 0.41 | 2/67294 (0.0%) | 0.87 | 15/105038 (0.0%) |
| 2 | 1B | 0.56 | 1/2882 (0.0%) | 0.94 | 0/4494 |
| 2 | 2B | 0.35 | 1/2879 (0.0%) | 0.80 | 1/4487 (0.0%) |
| 3 | 1D | 0.41 | 0/2186 | 0.58 | 0/2944 |
| 3 | 2D | 0.34 | 0/2186 | 0.51 | 0/2944 |
| 4 | 1E | 0.42 | 0/1592 | 0.57 | 0/2149 |
| 4 | 2E | 0.31 | 0/1592 | 0.51 | 0/2149 |
| 5 | 1F | 0.42 | 0/1619 | 0.55 | 0/2193 |
| 5 | 2F | 0.31 | 0/1615 | 0.48 | 0/2188 |
| 6 | 1G | 0.31 | 0/1476 | 0.49 | 0/1989 |
| 6 | 2G | 0.26 | 0/1478 | 0.45 | 0/1992 |
| 7 | 1H | 0.38 | 0/1356 | 0.52 | 0/1834 |
| 7 | 2H | 0.28 | 0/1356 | 0.46 | 0/1834 |
| 8 | 1N | 0.41 | 0/1144 | 0.54 | 0/1543 |
| 8 | 2N | 0.29 | 0/1144 | 0.47 | 0/1543 |
| 9 | 1O | 0.38 | 0/943 | 0.54 | 0/1269 |
| 9 | 2O | 0.32 | 0/943 | 0.50 | 0/1269 |
| 10 | 1P | 0.38 | 0/1152 | 0.61 | 0/1533 |
| 10 | 2P | 0.31 | 0/1152 | 0.51 | 0/1533 |
| 11 | 1Q | 0.43 | 0/1143 | 0.58 | 0/1527 |
| 11 | 2Q | 0.30 | 0/1143 | 0.48 | 0/1527 |
| 12 | 1R | 0.39 | 0/982 | 0.58 | 0/1312 |
| 12 | 2R | 0.30 | 0/982 | 0.47 | 0/1312 |
| 13 | 1S | 0.36 | 0/883 | 0.52 | 0/1176 |
| 13 | 2S | 0.28 | 0/880 | 0.45 | 0/1172 |
| 14 | 1T | 0.37 | 0/1105 | 0.53 | 0/1477 |
| 14 | 2T | 0.30 | 0/1097 | 0.46 | 0/1468 |
| 15 | 1U | 0.47 | 0/977 | 0.57 | 0/1301 |
| 15 | 2U | 0.29 | 0/977 | 0.42 | 0/1301 |
| 16 | 1V | 0.43 | 0/782 | 0.59 | 0/1049 |

| Mol | Chain | Bond lengths | | Bond angles | |
|---|---|---|---|---|---|
| | | RMSZ | #\|Z\| >5 | RMSZ | #\|Z\| >5 |
| 16 | 2V | 0.31 | 0/782 | 0.49 | 0/1049 |
| 17 | 1W | 0.45 | 0/897 | 0.60 | 0/1205 |
| 17 | 2W | 0.33 | 0/897 | 0.50 | 0/1205 |
| 18 | 1X | 0.46 | 0/764 | 0.58 | 0/1025 |
| 18 | 2X | 0.35 | 0/764 | 0.49 | 0/1025 |
| 19 | 1Y | 0.46 | 0/819 | 0.58 | 0/1095 |
| 19 | 2Y | 0.32 | 0/819 | 0.48 | 0/1095 |
| 20 | 1Z | 0.40 | 0/1615 | 0.57 | 0/2197 |
| 20 | 2Z | 0.28 | 0/1615 | 0.50 | 0/2197 |
| 21 | 10 | 0.40 | 0/606 | 0.56 | 0/808 |
| 21 | 20 | 0.30 | 0/606 | 0.48 | 0/808 |
| 22 | 11 | 0.39 | 0/762 | 0.55 | 0/1014 |
| 22 | 21 | 0.31 | 0/762 | 0.49 | 0/1014 |
| 23 | 12 | 0.41 | 0/590 | 0.55 | 0/781 |
| 23 | 22 | 0.30 | 0/590 | 0.41 | 0/781 |
| 24 | 13 | 0.45 | 0/474 | 0.58 | 0/635 |
| 24 | 23 | 0.34 | 0/469 | 0.50 | 0/630 |
| 25 | 14 | 0.32 | 0/565 | 0.54 | 0/761 |
| 25 | 24 | 0.26 | 0/545 | 0.46 | 0/737 |
| 26 | 15 | 0.47 | 0/469 | 0.63 | 0/635 |
| 26 | 25 | 0.34 | 0/469 | 0.52 | 0/635 |
| 27 | 16 | 0.44 | 0/460 | 0.57 | 0/613 |
| 27 | 26 | 0.30 | 0/456 | 0.48 | 0/608 |
| 28 | 17 | 0.45 | 0/426 | 0.59 | 0/561 |
| 28 | 27 | 0.35 | 0/426 | 0.53 | 0/561 |
| 29 | 18 | 0.45 | 0/525 | 0.59 | 0/691 |
| 29 | 28 | 0.33 | 0/525 | 0.48 | 0/691 |
| 30 | 19 | 0.38 | 0/310 | 0.55 | 0/407 |
| 30 | 29 | 0.29 | 0/310 | 0.52 | 0/407 |
| 31 | 1a | 0.34 | 0/35769 | 0.83 | 14/55821 (0.0%) |
| 31 | 2a | 0.31 | 0/35886 | 0.82 | 11/56005 (0.0%) |
| 32 | 1b | 0.28 | 0/1881 | 0.46 | 0/2542 |
| 32 | 2b | 0.26 | 0/1860 | 0.44 | 0/2518 |
| 33 | 1c | 0.25 | 0/1572 | 0.43 | 0/2126 |
| 33 | 2c | 0.25 | 0/1566 | 0.44 | 0/2119 |
| 34 | 1d | 0.28 | 0/1685 | 0.44 | 0/2262 |
| 34 | 2d | 0.27 | 0/1704 | 0.43 | 0/2284 |
| 35 | 1e | 0.29 | 0/1145 | 0.46 | 0/1543 |
| 35 | 2e | 0.29 | 0/1149 | 0.47 | 0/1548 |
| 36 | 1f | 0.28 | 0/823 | 0.45 | 0/1115 |
| 36 | 2f | 0.28 | 0/829 | 0.46 | 0/1123 |
| 37 | 1g | 0.25 | 0/1250 | 0.40 | 0/1679 |
| 37 | 2g | 0.25 | 0/1254 | 0.41 | 0/1683 |

| Mol | Chain | Bond lengths | | Bond angles | |
|---|---|---|---|---|---|
| | | RMSZ | #\|Z\| >5 | RMSZ | #\|Z\| >5 |
| 38 | 1h | 0.29 | 0/1108 | 0.45 | 0/1494 |
| 38 | 2h | 0.28 | 0/1108 | 0.46 | 0/1494 |
| 39 | 1i | 0.26 | 0/1002 | 0.44 | 0/1346 |
| 39 | 2i | 0.26 | 0/997 | 0.43 | 0/1343 |
| 40 | 1j | 0.24 | 0/722 | 0.46 | 0/982 |
| 40 | 2j | 0.24 | 0/727 | 0.44 | 0/988 |
| 41 | 1k | 0.29 | 0/844 | 0.47 | 0/1145 |
| 41 | 2k | 0.28 | 0/848 | 0.46 | 0/1149 |
| 42 | 1l | 0.30 | 0/937 | 0.47 | 0/1260 |
| 42 | 2l | 0.29 | 0/937 | 0.50 | 0/1260 |
| 43 | 1m | 0.25 | 0/929 | 0.44 | 0/1250 |
| 43 | 2m | 0.25 | 0/961 | 0.45 | 0/1291 |
| 44 | 1n | 0.25 | 0/501 | 0.42 | 0/664 |
| 44 | 2n | 0.26 | 0/501 | 0.46 | 0/664 |
| 45 | 1o | 0.29 | 0/739 | 0.43 | 0/985 |
| 45 | 2o | 0.26 | 0/739 | 0.43 | 0/985 |
| 46 | 1p | 0.29 | 0/697 | 0.44 | 0/939 |
| 46 | 2p | 0.28 | 0/693 | 0.46 | 0/935 |
| 47 | 1q | 0.34 | 0/836 | 0.49 | 0/1117 |
| 47 | 2q | 0.29 | 0/836 | 0.44 | 0/1117 |
| 48 | 1r | 0.28 | 0/560 | 0.46 | 0/746 |
| 48 | 2r | 0.27 | 0/560 | 0.43 | 0/746 |
| 49 | 1s | 0.26 | 0/667 | 0.48 | 0/900 |
| 49 | 2s | 0.25 | 0/661 | 0.48 | 0/893 |
| 50 | 1t | 0.28 | 0/730 | 0.42 | 0/965 |
| 50 | 2t | 0.26 | 0/729 | 0.40 | 0/965 |
| 51 | 1u | 0.26 | 0/203 | 0.44 | 0/266 |
| 51 | 2u | 0.22 | 0/203 | 0.40 | 0/266 |
| 52 | 1v | 0.32 | 1/5765 (0.0%) | 0.51 | 0/7809 |
| 52 | 2v | 0.29 | 0/5765 | 0.49 | 0/7809 |
| 53 | 1w | 0.35 | 0/1497 | 0.51 | 0/2017 |
| 53 | 2w | 0.30 | 0/1497 | 0.45 | 0/2017 |
| 54 | 1x | 0.39 | 0/1602 | 1.06 | 6/2493 (0.2%) |
| 54 | 1y | 0.36 | 0/1602 | 0.98 | 3/2493 (0.1%) |
| 54 | 2x | 0.32 | 0/1602 | 0.96 | 2/2493 (0.1%) |
| 54 | 2y | 0.32 | 0/1602 | 0.92 | 1/2493 (0.0%) |
| 55 | 1z | 0.36 | 0/237 | 0.74 | 0/366 |
| 55 | 2z | 0.30 | 0/237 | 0.73 | 0/366 |
| All | All | 0.43 | 5/326021 (0.0%) | 0.83 | 157/486013 (0.0%) |

All (5) bond length outliers are listed below:

| Mol | Chain | Res | Type | Atoms | Z | Observed(Å) | Ideal(Å) |
|---|---|---|---|---|---|---|---|
| 1 | 2A | 2426 | A | O3'-P | -10.56 | 1.48 | 1.61 |
| 2 | 1B | 1 | U | OP3-P | -10.13 | 1.49 | 1.61 |
| 2 | 2B | 1 | U | OP3-P | -10.12 | 1.49 | 1.61 |
| 52 | 1v | 199 | ILE | C-N | 8.10 | 1.49 | 1.34 |
| 1 | 2A | 2440 | C | O3'-P | 6.55 | 1.69 | 1.61 |

All (157) bond angle outliers are listed below:

| Mol | Chain | Res | Type | Atoms | Z | Observed($^o$) | Ideal($^o$) |
|---|---|---|---|---|---|---|---|
| 31 | 2a | 1272 | G | C5-C6-O6 | 11.42 | 135.45 | 128.60 |
| 31 | 1a | 1030(B) | C | C2-N1-C1' | 8.79 | 128.47 | 118.80 |
| 1 | 1A | 1075 | C | N1-C2-O2 | 8.70 | 124.12 | 118.90 |
| 31 | 2a | 1272 | G | N3-C2-N2 | 8.58 | 125.91 | 119.90 |
| 31 | 1a | 1030(B) | C | N1-C2-O2 | 8.46 | 123.98 | 118.90 |
| 31 | 2a | 1272 | G | N1-C6-O6 | -8.31 | 114.92 | 119.90 |
| 31 | 2a | 1272 | G | N1-C2-N2 | -8.17 | 108.85 | 116.20 |
| 1 | 1A | 1979 | C | C6-N1-C2 | -8.01 | 117.10 | 120.30 |
| 1 | 1A | 974 | G | C8-N9-C4 | -7.83 | 103.27 | 106.40 |
| 31 | 1a | 1158 | C | C2-N1-C1' | 7.59 | 127.15 | 118.80 |
| 1 | 1A | 2167 | U | C2-N1-C1' | 7.56 | 126.77 | 117.70 |
| 1 | 1A | 1380 | G | O5'-P-OP2 | -7.50 | 98.95 | 105.70 |
| 1 | 1A | 1075 | C | C2-N3-C4 | 7.40 | 123.60 | 119.90 |
| 1 | 1A | 2167 | U | N1-C2-O2 | 7.25 | 127.88 | 122.80 |
| 1 | 1A | 2167 | U | N3-C2-O2 | -7.02 | 117.28 | 122.20 |
| 31 | 1a | 1030(B) | C | N3-C2-O2 | -6.96 | 117.03 | 121.90 |
| 31 | 1a | 808 | C | C6-N1-C2 | -6.91 | 117.53 | 120.30 |
| 31 | 2a | 754 | C | C2-N1-C1' | 6.83 | 126.31 | 118.80 |
| 1 | 1A | 977 | G | O5'-P-OP1 | -6.82 | 99.56 | 105.70 |
| 31 | 1a | 266 | G | P-O3'-C3' | 6.81 | 127.87 | 119.70 |
| 54 | 1x | 56 | C | C2-N3-C4 | 6.78 | 123.29 | 119.90 |
| 1 | 1A | 1653 | G | P-O3'-C3' | 6.72 | 127.76 | 119.70 |
| 1 | 1A | 1665 | A | O5'-P-OP1 | -6.70 | 99.67 | 105.70 |
| 1 | 1A | 859 | G | N3-C4-C5 | 6.66 | 131.93 | 128.60 |
| 1 | 1A | 512 | G | O4'-C1'-N9 | 6.64 | 113.52 | 108.20 |
| 2 | 2B | 80 | U | O4'-C1'-N1 | 6.64 | 113.51 | 108.20 |
| 54 | 1x | 2 | C | C2-N3-C4 | 6.63 | 123.21 | 119.90 |
| 1 | 1A | 513 | A | N1-C6-N6 | -6.62 | 114.63 | 118.60 |
| 1 | 1A | 837 | C | C6-N1-C2 | -6.56 | 117.68 | 120.30 |
| 1 | 1A | 1629 | U | C5-C6-N1 | 6.55 | 125.97 | 122.70 |
| 31 | 1a | 1030(B) | C | C6-N1-C2 | -6.51 | 117.69 | 120.30 |
| 1 | 2A | 529 | A | O5'-P-OP1 | -6.48 | 99.87 | 105.70 |
| 1 | 2A | 1380 | G | O5'-P-OP2 | -6.41 | 99.93 | 105.70 |
| 54 | 2x | 2 | C | N1-C2-O2 | 6.34 | 122.70 | 118.90 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed($^o$) | Ideal($^o$) |
|---|---|---|---|---|---|---|---|
| 1 | 1A | 1653 | G | N3-C4-C5 | -6.33 | 125.43 | 128.60 |
| 54 | 1x | 56 | C | C5-C4-N4 | 6.31 | 124.61 | 120.20 |
| 1 | 2A | 1983 | C | C6-N1-C2 | -6.25 | 117.80 | 120.30 |
| 1 | 1A | 59 | U | C5-C6-N1 | 6.23 | 125.82 | 122.70 |
| 1 | 1A | 450 | G | C8-N9-C4 | -6.23 | 103.91 | 106.40 |
| 1 | 1A | 445 | C | C6-N1-C2 | -6.22 | 117.81 | 120.30 |
| 1 | 1A | 1653 | G | C4-N9-C1' | 6.21 | 134.58 | 126.50 |
| 1 | 1A | 2423 | U | C6-N1-C2 | 6.20 | 124.72 | 121.00 |
| 1 | 1A | 2006 | C | C2-N1-C1' | 6.06 | 125.47 | 118.80 |
| 31 | 1a | 1158 | C | C6-N1-C2 | -6.05 | 117.88 | 120.30 |
| 1 | 1A | 269 | U | P-O3'-C3' | 6.04 | 126.95 | 119.70 |
| 1 | 1A | 582 | G | C8-N9-C4 | 6.04 | 108.81 | 106.40 |
| 1 | 1A | 518 | G | N3-C4-C5 | -6.04 | 125.58 | 128.60 |
| 1 | 1A | 859 | G | C8-N9-C4 | 6.03 | 108.81 | 106.40 |
| 1 | 2A | 1779 | U | C2-N1-C1' | 6.02 | 124.93 | 117.70 |
| 54 | 1y | 33 | U | C2-N1-C1' | 6.01 | 124.91 | 117.70 |
| 1 | 1A | 2501 | C | C6-N1-C2 | 5.99 | 122.70 | 120.30 |
| 1 | 1A | 548 | A | P-O3'-C3' | 5.99 | 126.88 | 119.70 |
| 1 | 2A | 228 | A | OP1-P-O3' | 5.98 | 118.35 | 105.20 |
| 1 | 1A | 26 | G | N3-C4-C5 | -5.95 | 125.62 | 128.60 |
| 1 | 1A | 614 | U | N3-C2-O2 | -5.95 | 118.04 | 122.20 |
| 31 | 1a | 1158 | C | N1-C2-O2 | 5.95 | 122.47 | 118.90 |
| 31 | 1a | 1030(B) | C | C6-N1-C1' | -5.89 | 113.73 | 120.80 |
| 1 | 2A | 1610 | A | C8-N9-C4 | -5.83 | 103.47 | 105.80 |
| 1 | 2A | 2136 | C | N1-C2-O2 | 5.81 | 122.39 | 118.90 |
| 54 | 1x | 2 | C | N1-C2-O2 | 5.80 | 122.38 | 118.90 |
| 1 | 1A | 1174 | A | P-O3'-C3' | 5.79 | 126.65 | 119.70 |
| 1 | 1A | 739 | G | N3-C4-C5 | -5.79 | 125.71 | 128.60 |
| 1 | 1A | 2044 | C | C6-N1-C2 | -5.71 | 118.01 | 120.30 |
| 31 | 2a | 754 | C | N1-C2-O2 | 5.71 | 122.33 | 118.90 |
| 54 | 1y | 1 | G | P-O3'-C3' | 5.71 | 126.56 | 119.70 |
| 1 | 1A | 1640 | C | O4'-C1'-N1 | 5.71 | 112.77 | 108.20 |
| 1 | 1A | 1176 | G | OP1-P-O3' | 5.70 | 117.74 | 105.20 |
| 1 | 1A | 1251 | C | C5-C6-N1 | -5.68 | 118.16 | 121.00 |
| 54 | 2x | 2 | C | C2-N3-C4 | 5.66 | 122.73 | 119.90 |
| 1 | 1A | 728 | G | N3-C4-N9 | 5.65 | 129.39 | 126.00 |
| 1 | 1A | 774 | A | O5'-P-OP2 | -5.65 | 100.62 | 105.70 |
| 1 | 1A | 1136 | G | N3-C4-C5 | -5.64 | 125.78 | 128.60 |
| 1 | 2A | 2848 | G | O4'-C1'-N9 | 5.63 | 112.71 | 108.20 |
| 1 | 1A | 2515 | C | N3-C2-O2 | -5.63 | 117.96 | 121.90 |
| 1 | 1A | 333 | G | C4-N9-C1' | 5.63 | 133.81 | 126.50 |
| 1 | 1A | 1658 | C | C6-N1-C2 | -5.62 | 118.05 | 120.30 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed($^o$) | Ideal($^o$) |
|---|---|---|---|---|---|---|---|
| 1 | 1A | 2589 | A | C8-N9-C4 | 5.60 | 108.04 | 105.80 |
| 1 | 1A | 1653 | G | N3-C4-N9 | 5.59 | 129.35 | 126.00 |
| 1 | 1A | 827 | U | C6-N1-C2 | 5.59 | 124.35 | 121.00 |
| 1 | 1A | 1372 | U | C5-C4-O4 | -5.59 | 122.55 | 125.90 |
| 1 | 1A | 1174 | A | OP1-P-O3' | 5.57 | 117.45 | 105.20 |
| 1 | 1A | 178 | G | C8-N9-C4 | 5.55 | 108.62 | 106.40 |
| 1 | 1A | 2432 | A | N1-C6-N6 | 5.55 | 121.93 | 118.60 |
| 31 | 2a | 1263 | C | N1-C2-O2 | 5.55 | 122.23 | 118.90 |
| 54 | 1x | 71 | G | N3-C2-N2 | 5.53 | 123.77 | 119.90 |
| 1 | 1A | 2271 | G | N3-C4-N9 | 5.52 | 129.31 | 126.00 |
| 1 | 1A | 2320 | A | C8-N9-C4 | -5.50 | 103.60 | 105.80 |
| 1 | 1A | 545 | G | C8-N9-C4 | -5.48 | 104.21 | 106.40 |
| 1 | 1A | 2271 | G | N3-C4-C5 | -5.48 | 125.86 | 128.60 |
| 1 | 1A | 1082 | U | N3-C4-O4 | -5.47 | 115.57 | 119.40 |
| 31 | 1a | 1034 | G | C6-N1-C2 | 5.47 | 128.38 | 125.10 |
| 1 | 1A | 1251 | C | C6-N1-C2 | 5.46 | 122.48 | 120.30 |
| 1 | 1A | 1416 | G | O4'-C1'-N9 | 5.46 | 112.56 | 108.20 |
| 1 | 1A | 34 | C | C6-N1-C2 | 5.45 | 122.48 | 120.30 |
| 1 | 1A | 2335 | A | O4'-C1'-N9 | 5.45 | 112.56 | 108.20 |
| 1 | 1A | 807 | U | C5-C4-O4 | -5.44 | 122.63 | 125.90 |
| 31 | 1a | 1067 | A | P-O3'-C3' | 5.43 | 126.22 | 119.70 |
| 1 | 1A | 2423 | U | C5-C6-N1 | -5.38 | 120.01 | 122.70 |
| 1 | 1A | 1186 | G | N1-C6-O6 | -5.38 | 116.67 | 119.90 |
| 1 | 1A | 1157 | G | C4-N9-C1' | 5.38 | 133.49 | 126.50 |
| 31 | 2a | 1158 | C | C2-N1-C1' | 5.38 | 124.72 | 118.80 |
| 1 | 2A | 2579 | C | C5-C6-N1 | 5.37 | 123.68 | 121.00 |
| 1 | 1A | 859 | G | N1-C6-O6 | 5.36 | 123.11 | 119.90 |
| 1 | 1A | 59 | U | C6-N1-C2 | -5.35 | 117.79 | 121.00 |
| 1 | 1A | 518 | G | N3-C4-N9 | 5.35 | 129.21 | 126.00 |
| 1 | 1A | 1784 | A | N1-C6-N6 | -5.35 | 115.39 | 118.60 |
| 1 | 1A | 2319 | G | O4'-C1'-N9 | 5.35 | 112.48 | 108.20 |
| 1 | 1A | 735 | A | C8-N9-C4 | 5.34 | 107.94 | 105.80 |
| 1 | 1A | 773 | U | C5-C6-N1 | -5.34 | 120.03 | 122.70 |
| 54 | 1x | 68 | C | N1-C2-O2 | 5.34 | 122.10 | 118.90 |
| 1 | 1A | 207 | A | C8-N9-C4 | 5.34 | 107.94 | 105.80 |
| 1 | 1A | 431 | U | C5-C6-N1 | 5.34 | 125.37 | 122.70 |
| 1 | 1A | 236 | C | C6-N1-C2 | 5.33 | 122.43 | 120.30 |
| 1 | 1A | 1047 | G | C8-N9-C4 | -5.33 | 104.27 | 106.40 |
| 1 | 2A | 1350 | C | C6-N1-C2 | 5.32 | 122.43 | 120.30 |
| 1 | 1A | 2689 | U | P-O3'-C3' | 5.32 | 126.08 | 119.70 |
| 1 | 1A | 16 | G | N1-C6-O6 | 5.32 | 123.09 | 119.90 |
| 1 | 1A | 2446 | G | O5'-P-OP2 | -5.30 | 100.93 | 105.70 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed($^o$) | Ideal($^o$) |
|---|---|---|---|---|---|---|---|
| 1 | 1A | 26 | G | N3-C4-N9 | 5.30 | 129.18 | 126.00 |
| 1 | 1A | 333 | G | C8-N9-C1' | -5.30 | 120.11 | 127.00 |
| 1 | 2A | 752 | A | P-O3'-C3' | 5.30 | 126.06 | 119.70 |
| 1 | 1A | 783 | A | C4-C5-C6 | 5.28 | 119.64 | 117.00 |
| 1 | 1A | 1273 | U | N1-C2-N3 | 5.28 | 118.07 | 114.90 |
| 31 | 1a | 1030(B) | C | C5-C6-N1 | 5.28 | 123.64 | 121.00 |
| 1 | 1A | 2006 | C | C5-C4-N4 | -5.27 | 116.51 | 120.20 |
| 1 | 1A | 974 | G | N7-C8-N9 | 5.23 | 115.72 | 113.10 |
| 1 | 1A | 976 | C | C6-N1-C2 | -5.23 | 118.21 | 120.30 |
| 1 | 1A | 863 | A | O5'-P-OP2 | -5.21 | 101.01 | 105.70 |
| 1 | 1A | 1653 | G | C8-N9-C1' | -5.20 | 120.24 | 127.00 |
| 54 | 2y | 1 | G | P-O3'-C3' | 5.20 | 125.94 | 119.70 |
| 1 | 2A | 1905 | C | N1-C2-O2 | 5.19 | 122.02 | 118.90 |
| 1 | 1A | 1333 | C | N3-C4-C5 | 5.19 | 123.98 | 121.90 |
| 1 | 1A | 1781 | C | C6-N1-C2 | 5.18 | 122.37 | 120.30 |
| 1 | 1A | 836 | G | C8-N9-C4 | -5.18 | 104.33 | 106.40 |
| 1 | 2A | 528 | A | OP1-P-O3' | 5.17 | 116.58 | 105.20 |
| 1 | 1A | 783 | A | N3-C4-C5 | -5.16 | 123.19 | 126.80 |
| 1 | 1A | 1885 | A | C8-N9-C4 | 5.15 | 107.86 | 105.80 |
| 54 | 1y | 33 | U | N1-C2-O2 | 5.15 | 126.40 | 122.80 |
| 1 | 1A | 599 | G | N3-C4-N9 | 5.14 | 129.09 | 126.00 |
| 1 | 1A | 2069 | G | N3-C4-C5 | -5.13 | 126.03 | 128.60 |
| 1 | 2A | 228 | A | P-O3'-C3' | 5.12 | 125.85 | 119.70 |
| 31 | 2a | 1263 | C | C2-N3-C4 | 5.12 | 122.46 | 119.90 |
| 31 | 2a | 1158 | C | N1-C2-O2 | 5.12 | 121.97 | 118.90 |
| 1 | 1A | 671 | C | C6-N1-C2 | -5.11 | 118.25 | 120.30 |
| 31 | 2a | 1272 | G | C4-N9-C1' | 5.10 | 133.13 | 126.50 |
| 1 | 1A | 1063 | G | C5-C6-O6 | 5.09 | 131.66 | 128.60 |
| 1 | 1A | 2553 | G | N3-C4-N9 | 5.08 | 129.05 | 126.00 |
| 1 | 1A | 790 | C | N1-C2-O2 | 5.08 | 121.95 | 118.90 |
| 31 | 1a | 913 | A | P-O3'-C3' | 5.07 | 125.79 | 119.70 |
| 1 | 1A | 815 | C | OP2-P-O3' | 5.06 | 116.34 | 105.20 |
| 1 | 1A | 2028 | U | N3-C4-C5 | -5.05 | 111.57 | 114.60 |
| 1 | 1A | 1157 | G | C8-N9-C1' | -5.05 | 120.44 | 127.00 |
| 1 | 1A | 949 | C | C6-N1-C2 | 5.04 | 122.32 | 120.30 |
| 1 | 2A | 1963 | U | N1-C2-N3 | -5.04 | 111.88 | 114.90 |
| 1 | 1A | 2032 | G | C5-N7-C8 | -5.01 | 101.80 | 104.30 |
| 1 | 1A | 2432 | A | C6-C5-N7 | -5.01 | 128.79 | 132.30 |
| 1 | 1A | 859 | G | C4-N9-C1' | -5.01 | 119.99 | 126.50 |

There are no chirality outliers.

There are no planarity outliers.

## 5.2 Too-close contacts (i)

Due to software issues we are unable to calculate clashes - this section is therefore empty.

## 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 | |
|---|---|---|---|---|---|---|---|
| 3 | 1D | 273/276 (99%) | 241 (88%) | 26 (10%) | 6 (2%) | 6 | 37 |
| 3 | 2D | 273/276 (99%) | 234 (86%) | 33 (12%) | 6 (2%) | 6 | 37 |
| 4 | 1E | 202/206 (98%) | 179 (89%) | 19 (9%) | 4 (2%) | 7 | 39 |
| 4 | 2E | 202/206 (98%) | 174 (86%) | 26 (13%) | 2 (1%) | 15 | 54 |
| 5 | 1F | 201/210 (96%) | 182 (90%) | 17 (8%) | 2 (1%) | 15 | 54 |
| 5 | 2F | 201/210 (96%) | 183 (91%) | 15 (8%) | 3 (2%) | 10 | 45 |
| 6 | 1G | 179/182 (98%) | 155 (87%) | 23 (13%) | 1 (1%) | 25 | 64 |
| 6 | 2G | 179/182 (98%) | 147 (82%) | 27 (15%) | 5 (3%) | 5 | 32 |
| 7 | 1H | 172/180 (96%) | 152 (88%) | 18 (10%) | 2 (1%) | 13 | 50 |
| 7 | 2H | 172/180 (96%) | 151 (88%) | 19 (11%) | 2 (1%) | 13 | 50 |
| 8 | 1N | 138/140 (99%) | 121 (88%) | 16 (12%) | 1 (1%) | 22 | 61 |
| 8 | 2N | 138/140 (99%) | 127 (92%) | 8 (6%) | 3 (2%) | 6 | 37 |
| 9 | 1O | 120/122 (98%) | 105 (88%) | 13 (11%) | 2 (2%) | 9 | 42 |
| 9 | 2O | 120/122 (98%) | 103 (86%) | 16 (13%) | 1 (1%) | 19 | 58 |
| 10 | 1P | 147/150 (98%) | 134 (91%) | 11 (8%) | 2 (1%) | 11 | 46 |
| 10 | 2P | 147/150 (98%) | 132 (90%) | 13 (9%) | 2 (1%) | 11 | 46 |
| 11 | 1Q | 139/141 (99%) | 123 (88%) | 14 (10%) | 2 (1%) | 11 | 46 |
| 11 | 2Q | 139/141 (99%) | 122 (88%) | 16 (12%) | 1 (1%) | 22 | 61 |
| 12 | 1R | 116/118 (98%) | 91 (78%) | 21 (18%) | 4 (3%) | 3 | 28 |
| 12 | 2R | 116/118 (98%) | 110 (95%) | 5 (4%) | 1 (1%) | 17 | 56 |
| 13 | 1S | 108/112 (96%) | 96 (89%) | 12 (11%) | 0 | 100 | 100 |

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| Mol | Chain | Analysed | Favoured | Allowed | Outliers | Percentiles | |
|---|---|---|---|---|---|---|---|
| 13 | 2S | 108/112 (96%) | 96 (89%) | 10 (9%) | 2 (2%) | 8 | 40 |
| 14 | 1T | 129/146 (88%) | 117 (91%) | 12 (9%) | 0 | 100 | 100 |
| 14 | 2T | 129/146 (88%) | 115 (89%) | 13 (10%) | 1 (1%) | 19 | 58 |
| 15 | 1U | 114/118 (97%) | 104 (91%) | 8 (7%) | 2 (2%) | 8 | 41 |
| 15 | 2U | 114/118 (97%) | 109 (96%) | 4 (4%) | 1 (1%) | 17 | 56 |
| 16 | 1V | 99/101 (98%) | 85 (86%) | 12 (12%) | 2 (2%) | 7 | 39 |
| 16 | 2V | 99/101 (98%) | 86 (87%) | 12 (12%) | 1 (1%) | 15 | 54 |
| 17 | 1W | 110/113 (97%) | 98 (89%) | 10 (9%) | 2 (2%) | 8 | 41 |
| 17 | 2W | 110/113 (97%) | 102 (93%) | 7 (6%) | 1 (1%) | 17 | 56 |
| 18 | 1X | 93/96 (97%) | 84 (90%) | 6 (6%) | 3 (3%) | 4 | 29 |
| 18 | 2X | 93/96 (97%) | 81 (87%) | 11 (12%) | 1 (1%) | 14 | 52 |
| 19 | 1Y | 105/110 (96%) | 88 (84%) | 15 (14%) | 2 (2%) | 8 | 40 |
| 19 | 2Y | 105/110 (96%) | 92 (88%) | 10 (10%) | 3 (3%) | 4 | 31 |
| 20 | 1Z | 202/206 (98%) | 159 (79%) | 34 (17%) | 9 (4%) | 2 | 21 |
| 20 | 2Z | 202/206 (98%) | 161 (80%) | 28 (14%) | 13 (6%) | 1 | 14 |
| 21 | 10 | 73/85 (86%) | 69 (94%) | 4 (6%) | 0 | 100 | 100 |
| 21 | 20 | 73/85 (86%) | 67 (92%) | 5 (7%) | 1 (1%) | 11 | 46 |
| 22 | 11 | 95/98 (97%) | 90 (95%) | 5 (5%) | 0 | 100 | 100 |
| 22 | 21 | 95/98 (97%) | 89 (94%) | 4 (4%) | 2 (2%) | 7 | 38 |
| 23 | 12 | 68/72 (94%) | 60 (88%) | 5 (7%) | 3 (4%) | 2 | 21 |
| 23 | 22 | 68/72 (94%) | 63 (93%) | 5 (7%) | 0 | 100 | 100 |
| 24 | 13 | 57/60 (95%) | 51 (90%) | 5 (9%) | 1 (2%) | 8 | 41 |
| 24 | 23 | 57/60 (95%) | 51 (90%) | 5 (9%) | 1 (2%) | 8 | 41 |
| 25 | 14 | 67/71 (94%) | 51 (76%) | 10 (15%) | 6 (9%) | 1 | 8 |
| 25 | 24 | 67/71 (94%) | 53 (79%) | 10 (15%) | 4 (6%) | 1 | 15 |
| 26 | 15 | 57/60 (95%) | 53 (93%) | 4 (7%) | 0 | 100 | 100 |
| 26 | 25 | 57/60 (95%) | 53 (93%) | 4 (7%) | 0 | 100 | 100 |
| 27 | 16 | 51/54 (94%) | 46 (90%) | 5 (10%) | 0 | 100 | 100 |
| 27 | 26 | 51/54 (94%) | 48 (94%) | 2 (4%) | 1 (2%) | 7 | 39 |
| 28 | 17 | 46/49 (94%) | 43 (94%) | 3 (6%) | 0 | 100 | 100 |
| 28 | 27 | 46/49 (94%) | 40 (87%) | 5 (11%) | 1 (2%) | 6 | 37 |

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| Mol | Chain | Analysed | Favoured | Allowed | Outliers | Percentiles | |
|---|---|---|---|---|---|---|---|
| 29 | 18 | 62/65 (95%) | 54 (87%) | 7 (11%) | 1 (2%) | 9 | 43 |
| 29 | 28 | 62/65 (95%) | 57 (92%) | 5 (8%) | 0 | 100 | 100 |
| 30 | 19 | 35/37 (95%) | 30 (86%) | 5 (14%) | 0 | 100 | 100 |
| 30 | 29 | 35/37 (95%) | 31 (89%) | 4 (11%) | 0 | 100 | 100 |
| 32 | 1b | 229/256 (90%) | 190 (83%) | 32 (14%) | 7 (3%) | 4 | 30 |
| 32 | 2b | 229/256 (90%) | 199 (87%) | 22 (10%) | 8 (4%) | 3 | 27 |
| 33 | 1c | 204/239 (85%) | 183 (90%) | 17 (8%) | 4 (2%) | 7 | 39 |
| 33 | 2c | 204/239 (85%) | 172 (84%) | 30 (15%) | 2 (1%) | 15 | 54 |
| 34 | 1d | 206/209 (99%) | 181 (88%) | 21 (10%) | 4 (2%) | 8 | 40 |
| 34 | 2d | 206/209 (99%) | 189 (92%) | 16 (8%) | 1 (0%) | 29 | 68 |
| 35 | 1e | 146/162 (90%) | 127 (87%) | 17 (12%) | 2 (1%) | 11 | 46 |
| 35 | 2e | 146/162 (90%) | 127 (87%) | 19 (13%) | 0 | 100 | 100 |
| 36 | 1f | 98/101 (97%) | 92 (94%) | 6 (6%) | 0 | 100 | 100 |
| 36 | 2f | 98/101 (97%) | 92 (94%) | 6 (6%) | 0 | 100 | 100 |
| 37 | 1g | 153/156 (98%) | 135 (88%) | 14 (9%) | 4 (3%) | 5 | 33 |
| 37 | 2g | 153/156 (98%) | 135 (88%) | 14 (9%) | 4 (3%) | 5 | 33 |
| 38 | 1h | 135/138 (98%) | 125 (93%) | 10 (7%) | 0 | 100 | 100 |
| 38 | 2h | 135/138 (98%) | 118 (87%) | 16 (12%) | 1 (1%) | 22 | 61 |
| 39 | 1i | 125/128 (98%) | 106 (85%) | 19 (15%) | 0 | 100 | 100 |
| 39 | 2i | 125/128 (98%) | 104 (83%) | 21 (17%) | 0 | 100 | 100 |
| 40 | 1j | 95/105 (90%) | 82 (86%) | 9 (10%) | 4 (4%) | 3 | 23 |
| 40 | 2j | 94/105 (90%) | 78 (83%) | 15 (16%) | 1 (1%) | 14 | 52 |
| 41 | 1k | 112/129 (87%) | 101 (90%) | 9 (8%) | 2 (2%) | 8 | 41 |
| 41 | 2k | 112/129 (87%) | 98 (88%) | 12 (11%) | 2 (2%) | 8 | 41 |
| 42 | 1l | 119/132 (90%) | 109 (92%) | 9 (8%) | 1 (1%) | 19 | 58 |
| 42 | 2l | 119/132 (90%) | 97 (82%) | 19 (16%) | 3 (2%) | 5 | 34 |
| 43 | 1m | 116/126 (92%) | 100 (86%) | 16 (14%) | 0 | 100 | 100 |
| 43 | 2m | 120/126 (95%) | 104 (87%) | 14 (12%) | 2 (2%) | 9 | 42 |
| 44 | 1n | 58/61 (95%) | 49 (84%) | 8 (14%) | 1 (2%) | 9 | 42 |
| 44 | 2n | 58/61 (95%) | 50 (86%) | 7 (12%) | 1 (2%) | 9 | 42 |
| 45 | 1o | 86/89 (97%) | 79 (92%) | 5 (6%) | 2 (2%) | 6 | 36 |

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| Mol | Chain | Analysed | Favoured | Allowed | Outliers | Percentiles | |
|---|---|---|---|---|---|---|---|
| 45 | 2o | 86/89 (97%) | 78 (91%) | 4 (5%) | 4 (5%) | 2 | 20 |
| 46 | 1p | 80/88 (91%) | 66 (82%) | 12 (15%) | 2 (2%) | 5 | 34 |
| 46 | 2p | 80/88 (91%) | 71 (89%) | 8 (10%) | 1 (1%) | 12 | 48 |
| 47 | 1q | 97/105 (92%) | 84 (87%) | 13 (13%) | 0 | 100 | 100 |
| 47 | 2q | 97/105 (92%) | 84 (87%) | 11 (11%) | 2 (2%) | 7 | 38 |
| 48 | 1r | 66/88 (75%) | 64 (97%) | 2 (3%) | 0 | 100 | 100 |
| 48 | 2r | 66/88 (75%) | 62 (94%) | 3 (4%) | 1 (2%) | 10 | 45 |
| 49 | 1s | 81/93 (87%) | 68 (84%) | 9 (11%) | 4 (5%) | 2 | 19 |
| 49 | 2s | 81/93 (87%) | 65 (80%) | 14 (17%) | 2 (2%) | 5 | 34 |
| 50 | 1t | 94/106 (89%) | 82 (87%) | 7 (7%) | 5 (5%) | 2 | 17 |
| 50 | 2t | 94/106 (89%) | 81 (86%) | 10 (11%) | 3 (3%) | 4 | 29 |
| 51 | 1u | 21/27 (78%) | 18 (86%) | 3 (14%) | 0 | 100 | 100 |
| 51 | 2u | 21/27 (78%) | 19 (90%) | 2 (10%) | 0 | 100 | 100 |
| 52 | 1v | 724/758 (96%) | 593 (82%) | 105 (14%) | 26 (4%) | 3 | 26 |
| 52 | 2v | 724/758 (96%) | 602 (83%) | 97 (13%) | 25 (4%) | 3 | 27 |
| 53 | 1w | 183/185 (99%) | 159 (87%) | 16 (9%) | 8 (4%) | 2 | 21 |
| 53 | 2w | 183/185 (99%) | 165 (90%) | 13 (7%) | 5 (3%) | 5 | 33 |
| All | All | 12975/13718 (95%) | 11321 (87%) | 1394 (11%) | 260 (2%) | 7 | 39 |

All (260) Ramachandran outliers are listed below:

| Mol | Chain | Res | Type |
|---|---|---|---|
| 5 | 1F | 130 | ALA |
| 7 | 1H | 126 | PRO |
| 10 | 1P | 53 | GLY |
| 11 | 1Q | 16 | ARG |
| 16 | 1V | 97 | LYS |
| 20 | 1Z | 177 | PRO |
| 20 | 1Z | 184 | ALA |
| 20 | 1Z | 198 | LYS |
| 35 | 1e | 21 | ALA |
| 40 | 1j | 55 | LYS |
| 52 | 1v | -57 | GLU |
| 52 | 1v | 85 | PRO |
| 52 | 1v | 92 | ILE |
| 52 | 1v | 183 | MET |

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| Mol | Chain | Res | Type |
|---|---|---|---|
| 52 | 1v | 401 | SER |
| 52 | 1v | 472 | VAL |
| 53 | 1w | 61 | PRO |
| 5 | 2F | 130 | ALA |
| 7 | 2H | 29 | PRO |
| 7 | 2H | 126 | PRO |
| 19 | 2Y | 21 | LYS |
| 20 | 2Z | 182 | LYS |
| 20 | 2Z | 183 | LEU |
| 28 | 27 | 46 | VAL |
| 42 | 2l | 121 | GLY |
| 52 | 2v | -57 | GLU |
| 52 | 2v | 85 | PRO |
| 52 | 2v | 92 | ILE |
| 52 | 2v | 183 | MET |
| 52 | 2v | 472 | VAL |
| 3 | 1D | 169 | GLU |
| 4 | 1E | 113 | PHE |
| 5 | 1F | 54 | ARG |
| 12 | 1R | 3 | HIS |
| 12 | 1R | 23 | ASN |
| 16 | 1V | 79 | VAL |
| 20 | 1Z | 119 | GLU |
| 23 | 12 | 69 | ARG |
| 25 | 14 | 44 | THR |
| 25 | 14 | 45 | GLY |
| 25 | 14 | 53 | GLU |
| 32 | 1b | 22 | LYS |
| 37 | 1g | 79 | ARG |
| 45 | 1o | 17 | ARG |
| 46 | 1p | 53 | VAL |
| 49 | 1s | 63 | THR |
| 52 | 1v | 402 | ILE |
| 52 | 1v | 444 | PRO |
| 52 | 1v | 447 | GLY |
| 53 | 1w | 30 | THR |
| 53 | 1w | 84 | ARG |
| 53 | 1w | 97 | ASP |
| 3 | 2D | 3 | VAL |
| 6 | 2G | 126 | ASP |
| 8 | 2N | 8 | GLN |
| 10 | 2P | 38 | GLN |

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| Mol | Chain | Res | Type |
|---|---|---|---|
| 11 | 2Q | 27 | VAL |
| 13 | 2S | 94 | TYR |
| 14 | 2T | 56 | GLY |
| 16 | 2V | 79 | VAL |
| 17 | 2W | 98 | LYS |
| 20 | 2Z | 154 | ASP |
| 25 | 24 | 46 | GLN |
| 34 | 2d | 5 | ILE |
| 37 | 2g | 114 | ARG |
| 41 | 2k | 105 | VAL |
| 43 | 2m | 23 | TYR |
| 52 | 2v | 88 | VAL |
| 52 | 2v | 401 | SER |
| 52 | 2v | 605 | ILE |
| 53 | 2w | 85 | ASP |
| 3 | 1D | 144 | ALA |
| 3 | 1D | 206 | LEU |
| 4 | 1E | 52 | LEU |
| 10 | 1P | 58 | THR |
| 17 | 1W | 90 | ARG |
| 18 | 1X | 93 | GLU |
| 19 | 1Y | 54 | LYS |
| 25 | 14 | 57 | GLU |
| 32 | 1b | 8 | LYS |
| 32 | 1b | 36 | ARG |
| 32 | 1b | 231 | GLU |
| 33 | 1c | 98 | ASN |
| 40 | 1j | 78 | ASN |
| 45 | 1o | 23 | GLY |
| 49 | 1s | 35 | SER |
| 49 | 1s | 65 | ASN |
| 50 | 1t | 9 | ASN |
| 50 | 1t | 95 | ALA |
| 52 | 1v | 87 | HIS |
| 52 | 1v | 88 | VAL |
| 52 | 1v | 171 | GLU |
| 52 | 1v | 482 | ALA |
| 3 | 2D | 79 | VAL |
| 3 | 2D | 125 | ILE |
| 3 | 2D | 257 | LEU |
| 12 | 2R | 14 | SER |
| 15 | 2U | 5 | LYS |

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| Mol | Chain | Res | Type |
|---|---|---|---|
| 20 | 2Z | 135 | GLU |
| 22 | 21 | 3 | LYS |
| 25 | 24 | 61 | ARG |
| 32 | 2b | 8 | LYS |
| 32 | 2b | 16 | HIS |
| 32 | 2b | 17 | PHE |
| 32 | 2b | 95 | GLN |
| 32 | 2b | 150 | SER |
| 37 | 2g | 7 | ALA |
| 43 | 2m | 6 | GLY |
| 44 | 2n | 28 | GLY |
| 45 | 2o | 6 | GLU |
| 50 | 2t | 47 | GLY |
| 52 | 2v | 171 | GLU |
| 52 | 2v | 469 | GLU |
| 52 | 2v | 471 | LYS |
| 52 | 2v | 473 | ASP |
| 52 | 2v | 688 | ILE |
| 3 | 1D | 99 | ASP |
| 6 | 1G | 75 | LYS |
| 9 | 1O | 25 | LEU |
| 12 | 1R | 53 | HIS |
| 15 | 1U | 9 | VAL |
| 15 | 1U | 24 | TYR |
| 19 | 1Y | 53 | PRO |
| 20 | 1Z | 155 | LEU |
| 32 | 1b | 20 | GLU |
| 32 | 1b | 125 | PRO |
| 34 | 1d | 5 | ILE |
| 37 | 1g | 114 | ARG |
| 46 | 1p | 28 | ARG |
| 50 | 1t | 10 | LEU |
| 50 | 1t | 100 | ILE |
| 52 | 1v | 404 | VAL |
| 52 | 1v | 473 | ASP |
| 53 | 1w | 2 | THR |
| 3 | 2D | 31 | LYS |
| 3 | 2D | 80 | ALA |
| 4 | 2E | 52 | LEU |
| 5 | 2F | 169 | ASN |
| 6 | 2G | 47 | LYS |
| 6 | 2G | 116 | ASP |

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| Mol | Chain | Res | Type |
|---|---|---|---|
| 8 | 2N | 23 | LEU |
| 8 | 2N | 41 | ASP |
| 18 | 2X | 2 | LYS |
| 20 | 2Z | 155 | LEU |
| 20 | 2Z | 184 | ALA |
| 20 | 2Z | 198 | LYS |
| 22 | 21 | 45 | ASN |
| 32 | 2b | 125 | PRO |
| 32 | 2b | 231 | GLU |
| 33 | 2c | 71 | ALA |
| 37 | 2g | 4 | ARG |
| 41 | 2k | 49 | GLY |
| 42 | 2l | 107 | ALA |
| 45 | 2o | 17 | ARG |
| 45 | 2o | 88 | ARG |
| 49 | 2s | 12 | ASP |
| 50 | 2t | 102 | GLY |
| 52 | 2v | -25 | SER |
| 53 | 2w | 167 | GLU |
| 3 | 1D | 127 | VAL |
| 4 | 1E | 134 | ILE |
| 11 | 1Q | 13 | GLN |
| 12 | 1R | 59 | ASP |
| 17 | 1W | 5 | ALA |
| 20 | 1Z | 161 | VAL |
| 20 | 1Z | 197 | ILE |
| 23 | 12 | 32 | LEU |
| 23 | 12 | 68 | ARG |
| 24 | 13 | 16 | PRO |
| 25 | 14 | 56 | VAL |
| 33 | 1c | 66 | VAL |
| 37 | 1g | 80 | VAL |
| 37 | 1g | 131 | LYS |
| 40 | 1j | 56 | HIS |
| 40 | 1j | 77 | PRO |
| 42 | 1l | 74 | GLY |
| 49 | 1s | 66 | MET |
| 52 | 1v | 170 | ARG |
| 52 | 1v | 604 | PRO |
| 52 | 1v | 671 | MET |
| 4 | 2E | 41 | LYS |
| 5 | 2F | 23 | ASP |

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| Mol | Chain | Res | Type |
|---|---|---|---|
| 9 | 2O | 17 | ARG |
| 10 | 2P | 53 | GLY |
| 19 | 2Y | 58 | GLY |
| 20 | 2Z | 11 | GLU |
| 20 | 2Z | 157 | LEU |
| 20 | 2Z | 179 | ASP |
| 20 | 2Z | 197 | ILE |
| 21 | 20 | 33 | ALA |
| 27 | 26 | 3 | SER |
| 33 | 2c | 3 | ASN |
| 37 | 2g | 80 | VAL |
| 38 | 2h | 102 | ARG |
| 42 | 2l | 120 | TYR |
| 48 | 2r | 52 | PRO |
| 52 | 2v | 404 | VAL |
| 52 | 2v | 671 | MET |
| 4 | 1E | 100 | GLU |
| 18 | 1X | 45 | THR |
| 20 | 1Z | 191 | VAL |
| 25 | 14 | 62 | ARG |
| 32 | 1b | 17 | PHE |
| 33 | 1c | 3 | ASN |
| 33 | 1c | 99 | VAL |
| 34 | 1d | 73 | ARG |
| 44 | 1n | 14 | PRO |
| 52 | 1v | 324 | ARG |
| 52 | 1v | 640 | ALA |
| 52 | 1v | 684 | GLN |
| 13 | 2S | 84 | GLN |
| 19 | 2Y | 103 | GLY |
| 24 | 23 | 59 | VAL |
| 25 | 24 | 11 | PRO |
| 25 | 24 | 48 | ARG |
| 32 | 2b | 131 | PRO |
| 45 | 2o | 23 | GLY |
| 49 | 2s | 76 | PRO |
| 50 | 2t | 99 | LEU |
| 52 | 2v | 447 | GLY |
| 52 | 2v | 481 | VAL |
| 53 | 2w | 55 | ILE |
| 53 | 2w | 84 | ARG |
| 34 | 1d | 90 | GLY |

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| Mol | Chain | Res | Type |
|---|---|---|---|
| 41 | 1k | 49 | GLY |
| 41 | 1k | 105 | VAL |
| 52 | 1v | 477 | GLY |
| 20 | 2Z | 161 | VAL |
| 47 | 2q | 33 | GLY |
| 52 | 2v | 288 | PRO |
| 20 | 1Z | 157 | LEU |
| 52 | 1v | 598 | ASP |
| 53 | 1w | 31 | GLY |
| 6 | 2G | 177 | GLY |
| 52 | 2v | 402 | ILE |
| 52 | 2v | 477 | GLY |
| 7 | 1H | 55 | PRO |
| 18 | 1X | 94 | GLY |
| 29 | 18 | 28 | GLY |
| 34 | 1d | 69 | GLY |
| 35 | 1e | 85 | GLY |
| 50 | 1t | 47 | GLY |
| 52 | 1v | 502 | GLY |
| 52 | 1v | 503 | GLY |
| 6 | 2G | 127 | GLY |
| 20 | 2Z | 180 | VAL |
| 40 | 2j | 75 | ILE |
| 47 | 2q | 77 | VAL |
| 52 | 2v | 294 | PRO |
| 52 | 2v | 405 | PRO |
| 53 | 2w | 61 | PRO |
| 3 | 1D | 207 | GLY |
| 8 | 1N | 111 | PRO |
| 52 | 1v | 532 | GLY |
| 53 | 1w | 35 | PRO |
| 46 | 2p | 53 | VAL |
| 52 | 2v | 115 | GLU |
| 52 | 2v | 535 | PRO |
| 9 | 1O | 77 | ILE |
| 53 | 1w | 27 | GLY |

### 5.3.2 Protein sidechains (i)

In the following table, the Percentiles column shows the percent sidechain outliers of the chain as a percentile score with respect to all 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 | |
|---|---|---|---|---|---|---|
| 3 | 1D | 215/218 (99%) | 199 (93%) | 16 (7%) | 13 | 44 |
| 3 | 2D | 215/218 (99%) | 202 (94%) | 13 (6%) | 19 | 52 |
| 4 | 1E | 164/166 (99%) | 148 (90%) | 16 (10%) | 8 | 33 |
| 4 | 2E | 164/166 (99%) | 152 (93%) | 12 (7%) | 14 | 45 |
| 5 | 1F | 160/166 (96%) | 146 (91%) | 14 (9%) | 10 | 38 |
| 5 | 2F | 159/166 (96%) | 157 (99%) | 2 (1%) | 69 | 86 |
| 6 | 1G | 150/156 (96%) | 140 (93%) | 10 (7%) | 16 | 48 |
| 6 | 2G | 150/156 (96%) | 144 (96%) | 6 (4%) | 31 | 64 |
| 7 | 1H | 144/148 (97%) | 138 (96%) | 6 (4%) | 30 | 63 |
| 7 | 2H | 144/148 (97%) | 139 (96%) | 5 (4%) | 36 | 67 |
| 8 | 1N | 118/119 (99%) | 107 (91%) | 11 (9%) | 9 | 35 |
| 8 | 2N | 118/119 (99%) | 112 (95%) | 6 (5%) | 24 | 57 |
| 9 | 1O | 100/100 (100%) | 94 (94%) | 6 (6%) | 19 | 52 |
| 9 | 2O | 100/100 (100%) | 98 (98%) | 2 (2%) | 55 | 79 |
| 10 | 1P | 115/116 (99%) | 107 (93%) | 8 (7%) | 15 | 46 |
| 10 | 2P | 115/116 (99%) | 110 (96%) | 5 (4%) | 29 | 62 |
| 11 | 1Q | 111/111 (100%) | 106 (96%) | 5 (4%) | 27 | 61 |
| 11 | 2Q | 111/111 (100%) | 105 (95%) | 6 (5%) | 22 | 55 |
| 12 | 1R | 101/101 (100%) | 85 (84%) | 16 (16%) | 2 | 15 |
| 12 | 2R | 101/101 (100%) | 96 (95%) | 5 (5%) | 24 | 58 |
| 13 | 1S | 86/88 (98%) | 77 (90%) | 9 (10%) | 7 | 31 |
| 13 | 2S | 85/88 (97%) | 79 (93%) | 6 (7%) | 14 | 46 |
| 14 | 1T | 115/127 (91%) | 106 (92%) | 9 (8%) | 12 | 42 |
| 14 | 2T | 113/127 (89%) | 109 (96%) | 4 (4%) | 36 | 67 |
| 15 | 1U | 93/94 (99%) | 90 (97%) | 3 (3%) | 39 | 69 |
| 15 | 2U | 93/94 (99%) | 91 (98%) | 2 (2%) | 52 | 78 |
| 16 | 1V | 80/82 (98%) | 72 (90%) | 8 (10%) | 7 | 32 |
| 16 | 2V | 80/82 (98%) | 77 (96%) | 3 (4%) | 33 | 65 |
| 17 | 1W | 90/92 (98%) | 85 (94%) | 5 (6%) | 21 | 54 |
| 17 | 2W | 90/92 (98%) | 80 (89%) | 10 (11%) | 6 | 28 |

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| Mol | Chain | Analysed | Rotameric | Outliers | Percentiles | |
|---|---|---|---|---|---|---|
| 18 | 1X | 77/78 (99%) | 74 (96%) | 3 (4%) | 32 | 64 |
| 18 | 2X | 77/78 (99%) | 73 (95%) | 4 (5%) | 23 | 56 |
| 19 | 1Y | 85/91 (93%) | 77 (91%) | 8 (9%) | 8 | 35 |
| 19 | 2Y | 85/91 (93%) | 82 (96%) | 3 (4%) | 36 | 67 |
| 20 | 1Z | 167/179 (93%) | 150 (90%) | 17 (10%) | 7 | 32 |
| 20 | 2Z | 167/179 (93%) | 151 (90%) | 16 (10%) | 8 | 34 |
| 21 | 10 | 60/67 (90%) | 59 (98%) | 1 (2%) | 60 | 82 |
| 21 | 20 | 60/67 (90%) | 58 (97%) | 2 (3%) | 38 | 68 |
| 22 | 11 | 80/83 (96%) | 75 (94%) | 5 (6%) | 18 | 51 |
| 22 | 21 | 80/83 (96%) | 76 (95%) | 4 (5%) | 24 | 58 |
| 23 | 12 | 65/67 (97%) | 60 (92%) | 5 (8%) | 13 | 42 |
| 23 | 22 | 65/67 (97%) | 64 (98%) | 1 (2%) | 65 | 84 |
| 24 | 13 | 51/52 (98%) | 45 (88%) | 6 (12%) | 5 | 25 |
| 24 | 23 | 50/52 (96%) | 48 (96%) | 2 (4%) | 31 | 64 |
| 25 | 14 | 59/63 (94%) | 51 (86%) | 8 (14%) | 3 | 20 |
| 25 | 24 | 53/63 (84%) | 47 (89%) | 6 (11%) | 6 | 27 |
| 26 | 15 | 50/52 (96%) | 47 (94%) | 3 (6%) | 19 | 52 |
| 26 | 25 | 50/52 (96%) | 47 (94%) | 3 (6%) | 19 | 52 |
| 27 | 16 | 51/52 (98%) | 48 (94%) | 3 (6%) | 19 | 53 |
| 27 | 26 | 50/52 (96%) | 49 (98%) | 1 (2%) | 55 | 79 |
| 28 | 17 | 41/42 (98%) | 37 (90%) | 4 (10%) | 8 | 33 |
| 28 | 27 | 41/42 (98%) | 36 (88%) | 5 (12%) | 5 | 23 |
| 29 | 18 | 54/55 (98%) | 50 (93%) | 4 (7%) | 13 | 44 |
| 29 | 28 | 54/55 (98%) | 54 (100%) | 0 | 100 | 100 |
| 30 | 19 | 34/34 (100%) | 33 (97%) | 1 (3%) | 42 | 71 |
| 30 | 29 | 34/34 (100%) | 31 (91%) | 3 (9%) | 10 | 38 |
| 32 | 1b | 192/220 (87%) | 182 (95%) | 10 (5%) | 23 | 56 |
| 32 | 2b | 187/220 (85%) | 180 (96%) | 7 (4%) | 34 | 65 |
| 33 | 1c | 142/188 (76%) | 138 (97%) | 4 (3%) | 43 | 72 |
| 33 | 2c | 140/188 (74%) | 133 (95%) | 7 (5%) | 24 | 58 |
| 34 | 1d | 169/181 (93%) | 160 (95%) | 9 (5%) | 22 | 55 |

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| Mol | Chain | Analysed | Rotameric | Outliers | Percentiles | |
|---|---|---|---|---|---|---|
| 34 | 2d | 173/181 (96%) | 166 (96%) | 7 (4%) | 31 | 64 |
| 35 | 1e | 113/123 (92%) | 109 (96%) | 4 (4%) | 36 | 67 |
| 35 | 2e | 114/123 (93%) | 107 (94%) | 7 (6%) | 18 | 51 |
| 36 | 1f | 84/90 (93%) | 83 (99%) | 1 (1%) | 71 | 87 |
| 36 | 2f | 85/90 (94%) | 81 (95%) | 4 (5%) | 26 | 60 |
| 37 | 1g | 119/127 (94%) | 114 (96%) | 5 (4%) | 30 | 63 |
| 37 | 2g | 120/127 (94%) | 119 (99%) | 1 (1%) | 81 | 91 |
| 38 | 1h | 114/119 (96%) | 110 (96%) | 4 (4%) | 36 | 67 |
| 38 | 2h | 114/119 (96%) | 108 (95%) | 6 (5%) | 22 | 55 |
| 39 | 1i | 90/99 (91%) | 85 (94%) | 5 (6%) | 21 | 54 |
| 39 | 2i | 89/99 (90%) | 83 (93%) | 6 (7%) | 16 | 48 |
| 40 | 1j | 66/92 (72%) | 64 (97%) | 2 (3%) | 41 | 71 |
| 40 | 2j | 69/92 (75%) | 66 (96%) | 3 (4%) | 29 | 62 |
| 41 | 1k | 82/99 (83%) | 80 (98%) | 2 (2%) | 49 | 76 |
| 41 | 2k | 83/99 (84%) | 83 (100%) | 0 | 100 | 100 |
| 42 | 1l | 96/108 (89%) | 91 (95%) | 5 (5%) | 23 | 56 |
| 42 | 2l | 96/108 (89%) | 94 (98%) | 2 (2%) | 53 | 79 |
| 43 | 1m | 89/101 (88%) | 86 (97%) | 3 (3%) | 37 | 68 |
| 43 | 2m | 92/101 (91%) | 88 (96%) | 4 (4%) | 29 | 62 |
| 44 | 1n | 49/50 (98%) | 47 (96%) | 2 (4%) | 30 | 63 |
| 44 | 2n | 49/50 (98%) | 47 (96%) | 2 (4%) | 30 | 63 |
| 45 | 1o | 78/80 (98%) | 77 (99%) | 1 (1%) | 69 | 86 |
| 45 | 2o | 78/80 (98%) | 72 (92%) | 6 (8%) | 13 | 42 |
| 46 | 1p | 69/74 (93%) | 64 (93%) | 5 (7%) | 14 | 45 |
| 46 | 2p | 68/74 (92%) | 63 (93%) | 5 (7%) | 13 | 44 |
| 47 | 1q | 94/97 (97%) | 91 (97%) | 3 (3%) | 39 | 69 |
| 47 | 2q | 94/97 (97%) | 92 (98%) | 2 (2%) | 53 | 79 |
| 48 | 1r | 59/77 (77%) | 56 (95%) | 3 (5%) | 24 | 57 |
| 48 | 2r | 59/77 (77%) | 57 (97%) | 2 (3%) | 37 | 68 |
| 49 | 1s | 69/80 (86%) | 65 (94%) | 4 (6%) | 20 | 53 |
| 49 | 2s | 67/80 (84%) | 64 (96%) | 3 (4%) | 27 | 61 |

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| Mol | Chain | Analysed | Rotameric | Outliers | Percentiles | |
|---|---|---|---|---|---|---|
| 50 | 1t | 70/82 (85%) | 67 (96%) | 3 (4%) | 29 | 62 |
| 50 | 2t | 70/82 (85%) | 69 (99%) | 1 (1%) | 67 | 85 |
| 51 | 1u | 18/22 (82%) | 18 (100%) | 0 | 100 | 100 |
| 51 | 2u | 18/22 (82%) | 18 (100%) | 0 | 100 | 100 |
| 52 | 1v | 605/636 (95%) | 518 (86%) | 87 (14%) | 3 | 18 |
| 52 | 2v | 605/636 (95%) | 523 (86%) | 82 (14%) | 3 | 20 |
| 53 | 1w | 157/157 (100%) | 133 (85%) | 24 (15%) | 2 | 17 |
| 53 | 2w | 157/157 (100%) | 140 (89%) | 17 (11%) | 6 | 30 |
| All | All | 10671/11402 (94%) | 9964 (93%) | 707 (7%) | 16 | 49 |

All (707) residues with a non-rotameric sidechain are listed below:

| Mol | Chain | Res | Type |
|---|---|---|---|
| 3 | 1D | 14 | ARG |
| 3 | 1D | 15 | PHE |
| 3 | 1D | 35 | LYS |
| 3 | 1D | 50 | THR |
| 3 | 1D | 60 | ARG |
| 3 | 1D | 83 | GLU |
| 3 | 1D | 116 | GLN |
| 3 | 1D | 141 | VAL |
| 3 | 1D | 154 | LYS |
| 3 | 1D | 211 | ARG |
| 3 | 1D | 212 | SER |
| 3 | 1D | 221 | VAL |
| 3 | 1D | 229 | VAL |
| 3 | 1D | 242 | ARG |
| 3 | 1D | 254 | THR |
| 3 | 1D | 257 | LEU |
| 4 | 1E | 7 | VAL |
| 4 | 1E | 14 | ILE |
| 4 | 1E | 23 | VAL |
| 4 | 1E | 24 | THR |
| 4 | 1E | 73 | GLU |
| 4 | 1E | 75 | VAL |
| 4 | 1E | 97 | LYS |
| 4 | 1E | 103 | ASP |
| 4 | 1E | 104 | VAL |
| 4 | 1E | 117 | MET |

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| Mol | Chain | Res | Type |
|---|---|---|---|
| 4 | 1E | 119 | ARG |
| 4 | 1E | 140 | SER |
| 4 | 1E | 160 | TYR |
| 4 | 1E | 168 | MET |
| 4 | 1E | 178 | GLU |
| 4 | 1E | 184 | VAL |
| 5 | 1F | 19 | GLU |
| 5 | 1F | 54 | ARG |
| 5 | 1F | 57 | VAL |
| 5 | 1F | 70 | THR |
| 5 | 1F | 74 | ARG |
| 5 | 1F | 78 | ILE |
| 5 | 1F | 89 | VAL |
| 5 | 1F | 106 | ARG |
| 5 | 1F | 125 | LEU |
| 5 | 1F | 149 | ASP |
| 5 | 1F | 165 | ARG |
| 5 | 1F | 170 | LEU |
| 5 | 1F | 175 | THR |
| 5 | 1F | 183 | VAL |
| 6 | 1G | 3 | LEU |
| 6 | 1G | 7 | LEU |
| 6 | 1G | 28 | VAL |
| 6 | 1G | 43 | LEU |
| 6 | 1G | 59 | GLU |
| 6 | 1G | 64 | THR |
| 6 | 1G | 70 | VAL |
| 6 | 1G | 91 | ARG |
| 6 | 1G | 133 | LEU |
| 6 | 1G | 161 | THR |
| 7 | 1H | 2 | SER |
| 7 | 1H | 15 | VAL |
| 7 | 1H | 45 | VAL |
| 7 | 1H | 69 | ARG |
| 7 | 1H | 71 | LEU |
| 7 | 1H | 155 | SER |
| 8 | 1N | 32 | THR |
| 8 | 1N | 33 | LEU |
| 8 | 1N | 34 | LEU |
| 8 | 1N | 48 | MET |
| 8 | 1N | 55 | VAL |
| 8 | 1N | 61 | ARG |

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| Mol | Chain | Res | Type |
|---|---|---|---|
| 8 | 1N | 62 | VAL |
| 8 | 1N | 67 | LEU |
| 8 | 1N | 99 | LEU |
| 8 | 1N | 101 | HIS |
| 8 | 1N | 120 | LEU |
| 9 | 1O | 12 | ASP |
| 9 | 1O | 21 | CYS |
| 9 | 1O | 32 | TYR |
| 9 | 1O | 57 | VAL |
| 9 | 1O | 80 | ASP |
| 9 | 1O | 108 | GLU |
| 10 | 1P | 46 | LYS |
| 10 | 1P | 71 | VAL |
| 10 | 1P | 95 | VAL |
| 10 | 1P | 96 | THR |
| 10 | 1P | 98 | GLU |
| 10 | 1P | 112 | LEU |
| 10 | 1P | 133 | SER |
| 10 | 1P | 148 | LEU |
| 11 | 1Q | 14 | ARG |
| 11 | 1Q | 79 | LEU |
| 11 | 1Q | 85 | LYS |
| 11 | 1Q | 109 | VAL |
| 11 | 1Q | 110 | THR |
| 12 | 1R | 14 | SER |
| 12 | 1R | 24 | GLN |
| 12 | 1R | 29 | LEU |
| 12 | 1R | 34 | ILE |
| 12 | 1R | 36 | THR |
| 12 | 1R | 44 | LEU |
| 12 | 1R | 57 | ARG |
| 12 | 1R | 59 | ASP |
| 12 | 1R | 65 | LEU |
| 12 | 1R | 67 | LEU |
| 12 | 1R | 79 | LEU |
| 12 | 1R | 95 | THR |
| 12 | 1R | 99 | LYS |
| 12 | 1R | 100 | LEU |
| 12 | 1R | 102 | GLU |
| 12 | 1R | 114 | VAL |
| 13 | 1S | 8 | GLU |
| 13 | 1S | 19 | LYS |

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| Mol | Chain | Res | Type |
|---|---|---|---|
| 13 | 1S | 25 | ARG |
| 13 | 1S | 31 | SER |
| 13 | 1S | 36 | TYR |
| 13 | 1S | 49 | VAL |
| 13 | 1S | 50 | SER |
| 13 | 1S | 85 | VAL |
| 13 | 1S | 98 | VAL |
| 14 | 1T | 6 | LEU |
| 14 | 1T | 21 | GLU |
| 14 | 1T | 27 | THR |
| 14 | 1T | 28 | VAL |
| 14 | 1T | 53 | ARG |
| 14 | 1T | 96 | ARG |
| 14 | 1T | 106 | SER |
| 14 | 1T | 114 | LEU |
| 14 | 1T | 128 | GLU |
| 15 | 1U | 74 | LEU |
| 15 | 1U | 77 | SER |
| 15 | 1U | 97 | ASP |
| 16 | 1V | 13 | ARG |
| 16 | 1V | 33 | VAL |
| 16 | 1V | 52 | VAL |
| 16 | 1V | 62 | LEU |
| 16 | 1V | 72 | VAL |
| 16 | 1V | 82 | ARG |
| 16 | 1V | 95 | LEU |
| 16 | 1V | 98 | GLU |
| 17 | 1W | 1 | MET |
| 17 | 1W | 23 | LEU |
| 17 | 1W | 24 | ILE |
| 17 | 1W | 67 | ASP |
| 17 | 1W | 107 | LEU |
| 18 | 1X | 3 | THR |
| 18 | 1X | 35 | THR |
| 18 | 1X | 57 | LEU |
| 19 | 1Y | 12 | THR |
| 19 | 1Y | 31 | LEU |
| 19 | 1Y | 43 | ASN |
| 19 | 1Y | 55 | TYR |
| 19 | 1Y | 60 | PHE |
| 19 | 1Y | 72 | VAL |
| 19 | 1Y | 98 | VAL |

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| Mol | Chain | Res | Type |
|---|---|---|---|
| 19 | 1Y | 99 | CYS |
| 20 | 1Z | 33 | LEU |
| 20 | 1Z | 34 | ASN |
| 20 | 1Z | 41 | LEU |
| 20 | 1Z | 49 | ARG |
| 20 | 1Z | 56 | VAL |
| 20 | 1Z | 63 | ASP |
| 20 | 1Z | 78 | LYS |
| 20 | 1Z | 81 | ARG |
| 20 | 1Z | 87 | ASP |
| 20 | 1Z | 91 | LEU |
| 20 | 1Z | 123 | ASP |
| 20 | 1Z | 126 | VAL |
| 20 | 1Z | 136 | PHE |
| 20 | 1Z | 154 | ASP |
| 20 | 1Z | 156 | LYS |
| 20 | 1Z | 178 | GLU |
| 20 | 1Z | 180 | VAL |
| 21 | 10 | 36 | ILE |
| 22 | 11 | 14 | VAL |
| 22 | 11 | 30 | VAL |
| 22 | 11 | 35 | THR |
| 22 | 11 | 40 | ARG |
| 22 | 11 | 56 | GLN |
| 23 | 12 | 3 | LEU |
| 23 | 12 | 4 | SER |
| 23 | 12 | 32 | LEU |
| 23 | 12 | 33 | MET |
| 23 | 12 | 69 | ARG |
| 24 | 13 | 17 | LYS |
| 24 | 13 | 29 | ARG |
| 24 | 13 | 31 | LEU |
| 24 | 13 | 40 | THR |
| 24 | 13 | 56 | VAL |
| 24 | 13 | 60 | GLU |
| 25 | 14 | 16 | CYS |
| 25 | 14 | 33 | VAL |
| 25 | 14 | 46 | GLN |
| 25 | 14 | 49 | PHE |
| 25 | 14 | 52 | THR |
| 25 | 14 | 56 | VAL |
| 25 | 14 | 63 | TYR |

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| Mol | Chain | Res | Type |
|---|---|---|---|
| 25 | 14 | 67 | TYR |
| 26 | 15 | 16 | ARG |
| 26 | 15 | 19 | ARG |
| 26 | 15 | 40 | LYS |
| 27 | 16 | 6 | ARG |
| 27 | 16 | 13 | CYS |
| 27 | 16 | 51 | GLU |
| 28 | 17 | 1 | MET |
| 28 | 17 | 4 | THR |
| 28 | 17 | 41 | ARG |
| 28 | 17 | 43 | THR |
| 29 | 18 | 27 | THR |
| 29 | 18 | 31 | HIS |
| 29 | 18 | 34 | TRP |
| 29 | 18 | 37 | SER |
| 30 | 19 | 12 | ASP |
| 32 | 1b | 8 | LYS |
| 32 | 1b | 19 | HIS |
| 32 | 1b | 21 | ARG |
| 32 | 1b | 37 | ASN |
| 32 | 1b | 94 | ASN |
| 32 | 1b | 122 | PHE |
| 32 | 1b | 140 | HIS |
| 32 | 1b | 162 | ILE |
| 32 | 1b | 195 | ASP |
| 32 | 1b | 198 | ASP |
| 33 | 1c | 17 | ASP |
| 33 | 1c | 57 | ILE |
| 33 | 1c | 115 | LEU |
| 33 | 1c | 124 | ILE |
| 34 | 1d | 28 | SER |
| 34 | 1d | 59 | ARG |
| 34 | 1d | 108 | LEU |
| 34 | 1d | 134 | ASP |
| 34 | 1d | 135 | LEU |
| 34 | 1d | 170 | VAL |
| 34 | 1d | 188 | LEU |
| 34 | 1d | 190 | ASP |
| 34 | 1d | 204 | ILE |
| 35 | 1e | 10 | MET |
| 35 | 1e | 41 | VAL |
| 35 | 1e | 67 | VAL |

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| Mol | Chain | Res | Type |
|---|---|---|---|
| 35 | 1e | 81 | GLU |
| 36 | 1f | 15 | ASP |
| 37 | 1g | 10 | ARG |
| 37 | 1g | 16 | LEU |
| 37 | 1g | 35 | LYS |
| 37 | 1g | 111 | ARG |
| 37 | 1g | 113 | GLU |
| 38 | 1h | 52 | ASP |
| 38 | 1h | 99 | GLU |
| 38 | 1h | 104 | ARG |
| 38 | 1h | 133 | LEU |
| 39 | 1i | 17 | VAL |
| 39 | 1i | 31 | GLN |
| 39 | 1i | 65 | VAL |
| 39 | 1i | 92 | TYR |
| 39 | 1i | 128 | ARG |
| 40 | 1j | 8 | LEU |
| 40 | 1j | 49 | VAL |
| 41 | 1k | 51 | LYS |
| 41 | 1k | 80 | VAL |
| 42 | 1l | 6 | THR |
| 42 | 1l | 37 | CYS |
| 42 | 1l | 44 | THR |
| 42 | 1l | 67 | THR |
| 42 | 1l | 85 | ILE |
| 43 | 1m | 32 | GLU |
| 43 | 1m | 110 | ARG |
| 43 | 1m | 117 | VAL |
| 44 | 1n | 18 | VAL |
| 44 | 1n | 33 | VAL |
| 45 | 1o | 21 | ASP |
| 46 | 1p | 1 | MET |
| 46 | 1p | 16 | HIS |
| 46 | 1p | 20 | VAL |
| 46 | 1p | 60 | LEU |
| 46 | 1p | 74 | LEU |
| 47 | 1q | 9 | VAL |
| 47 | 1q | 59 | ILE |
| 47 | 1q | 92 | ARG |
| 48 | 1r | 30 | ASP |
| 48 | 1r | 31 | LEU |
| 48 | 1r | 76 | LEU |

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| Mol | Chain | Res | Type |
|---|---|---|---|
| 49 | 1s | 7 | LYS |
| 49 | 1s | 16 | LEU |
| 49 | 1s | 28 | LYS |
| 49 | 1s | 81 | ARG |
| 50 | 1t | 13 | LEU |
| 50 | 1t | 15 | ARG |
| 50 | 1t | 84 | LEU |
| 52 | 1v | -52 | VAL |
| 52 | 1v | -19 | GLU |
| 52 | 1v | -13 | GLN |
| 52 | 1v | -6 | ARG |
| 52 | 1v | -1 | GLU |
| 52 | 1v | 10 | LYS |
| 52 | 1v | 13 | ARG |
| 52 | 1v | 15 | ILE |
| 52 | 1v | 38 | ARG |
| 52 | 1v | 69 | VAL |
| 52 | 1v | 70 | THR |
| 52 | 1v | 72 | CYS |
| 52 | 1v | 75 | LYS |
| 52 | 1v | 89 | ASP |
| 52 | 1v | 91 | THR |
| 52 | 1v | 92 | ILE |
| 52 | 1v | 96 | ARG |
| 52 | 1v | 98 | MET |
| 52 | 1v | 102 | ASP |
| 52 | 1v | 112 | GLN |
| 52 | 1v | 114 | VAL |
| 52 | 1v | 130 | VAL |
| 52 | 1v | 132 | ARG |
| 52 | 1v | 139 | MET |
| 52 | 1v | 146 | LEU |
| 52 | 1v | 160 | ARG |
| 52 | 1v | 166 | LEU |
| 52 | 1v | 170 | ARG |
| 52 | 1v | 172 | ASP |
| 52 | 1v | 197 | ARG |
| 52 | 1v | 198 | GLU |
| 52 | 1v | 203 | GLU |
| 52 | 1v | 214 | GLU |
| 52 | 1v | 222 | ASP |
| 52 | 1v | 228 | MET |

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| Mol | Chain | Res | Type |
|---|---|---|---|
| 52 | 1v | 233 | GLU |
| 52 | 1v | 238 | THR |
| 52 | 1v | 252 | ASP |
| 52 | 1v | 260 | LEU |
| 52 | 1v | 264 | LEU |
| 52 | 1v | 279 | TYR |
| 52 | 1v | 284 | LEU |
| 52 | 1v | 286 | ILE |
| 52 | 1v | 289 | ILE |
| 52 | 1v | 297 | GLU |
| 52 | 1v | 328 | ILE |
| 52 | 1v | 329 | ARG |
| 52 | 1v | 344 | THR |
| 52 | 1v | 352 | VAL |
| 52 | 1v | 354 | ARG |
| 52 | 1v | 362 | HIS |
| 52 | 1v | 369 | LEU |
| 52 | 1v | 374 | LEU |
| 52 | 1v | 377 | VAL |
| 52 | 1v | 385 | THR |
| 52 | 1v | 399 | LEU |
| 52 | 1v | 402 | ILE |
| 52 | 1v | 409 | ILE |
| 52 | 1v | 418 | LYS |
| 52 | 1v | 420 | ASP |
| 52 | 1v | 421 | GLN |
| 52 | 1v | 422 | GLU |
| 52 | 1v | 446 | THR |
| 52 | 1v | 475 | ASN |
| 52 | 1v | 481 | VAL |
| 52 | 1v | 484 | ARG |
| 52 | 1v | 491 | VAL |
| 52 | 1v | 504 | ARG |
| 52 | 1v | 512 | ILE |
| 52 | 1v | 530 | VAL |
| 52 | 1v | 533 | VAL |
| 52 | 1v | 572 | TYR |
| 52 | 1v | 579 | GLU |
| 52 | 1v | 601 | ILE |
| 52 | 1v | 605 | ILE |
| 52 | 1v | 606 | MET |
| 52 | 1v | 614 | GLU |

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| Mol | Chain | Res | Type |
|---|---|---|---|
| 52 | 1v | 615 | GLU |
| 52 | 1v | 630 | GLN |
| 52 | 1v | 634 | MET |
| 52 | 1v | 641 | GLN |
| 52 | 1v | 644 | ARG |
| 52 | 1v | 646 | PHE |
| 52 | 1v | 647 | VAL |
| 52 | 1v | 670 | VAL |
| 52 | 1v | 681 | LYS |
| 52 | 1v | 682 | GLN |
| 53 | 1w | 1 | MET |
| 53 | 1w | 3 | LEU |
| 53 | 1w | 6 | LEU |
| 53 | 1w | 16 | LYS |
| 53 | 1w | 38 | LEU |
| 53 | 1w | 43 | VAL |
| 53 | 1w | 50 | VAL |
| 53 | 1w | 55 | ILE |
| 53 | 1w | 59 | THR |
| 53 | 1w | 81 | LYS |
| 53 | 1w | 85 | ASP |
| 53 | 1w | 88 | LEU |
| 53 | 1w | 99 | LEU |
| 53 | 1w | 101 | ILE |
| 53 | 1w | 106 | LEU |
| 53 | 1w | 107 | THR |
| 53 | 1w | 112 | LYS |
| 53 | 1w | 116 | ARG |
| 53 | 1w | 133 | ARG |
| 53 | 1w | 154 | THR |
| 53 | 1w | 155 | LYS |
| 53 | 1w | 156 | ARG |
| 53 | 1w | 173 | ASP |
| 53 | 1w | 174 | GLN |
| 3 | 2D | 27 | THR |
| 3 | 2D | 71 | ASP |
| 3 | 2D | 94 | LEU |
| 3 | 2D | 112 | GLN |
| 3 | 2D | 113 | VAL |
| 3 | 2D | 134 | ARG |
| 3 | 2D | 142 | VAL |
| 3 | 2D | 150 | LYS |

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| Mol | Chain | Res | Type |
|---|---|---|---|
| 3 | 2D | 169 | GLU |
| 3 | 2D | 229 | VAL |
| 3 | 2D | 242 | ARG |
| 3 | 2D | 263 | ARG |
| 3 | 2D | 276 | LYS |
| 4 | 2E | 7 | VAL |
| 4 | 2E | 19 | ARG |
| 4 | 2E | 21 | VAL |
| 4 | 2E | 24 | THR |
| 4 | 2E | 33 | VAL |
| 4 | 2E | 52 | LEU |
| 4 | 2E | 75 | VAL |
| 4 | 2E | 107 | THR |
| 4 | 2E | 119 | ARG |
| 4 | 2E | 184 | VAL |
| 4 | 2E | 195 | LEU |
| 4 | 2E | 201 | THR |
| 5 | 2F | 84 | VAL |
| 5 | 2F | 192 | LEU |
| 6 | 2G | 31 | VAL |
| 6 | 2G | 43 | LEU |
| 6 | 2G | 49 | ASP |
| 6 | 2G | 111 | LEU |
| 6 | 2G | 135 | LEU |
| 6 | 2G | 174 | GLU |
| 7 | 2H | 68 | THR |
| 7 | 2H | 69 | ARG |
| 7 | 2H | 71 | LEU |
| 7 | 2H | 129 | THR |
| 7 | 2H | 171 | LEU |
| 8 | 2N | 15 | LEU |
| 8 | 2N | 28 | THR |
| 8 | 2N | 34 | LEU |
| 8 | 2N | 58 | ASP |
| 8 | 2N | 87 | LEU |
| 8 | 2N | 96 | GLU |
| 9 | 2O | 24 | VAL |
| 9 | 2O | 53 | LYS |
| 10 | 2P | 7 | ARG |
| 10 | 2P | 71 | VAL |
| 10 | 2P | 87 | ASP |
| 10 | 2P | 95 | VAL |

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| Mol | Chain | Res | Type |
|---|---|---|---|
| 10 | 2P | 112 | LEU |
| 11 | 2Q | 1 | MET |
| 11 | 2Q | 16 | ARG |
| 11 | 2Q | 18 | LYS |
| 11 | 2Q | 21 | THR |
| 11 | 2Q | 109 | VAL |
| 11 | 2Q | 110 | THR |
| 12 | 2R | 8 | ARG |
| 12 | 2R | 28 | LEU |
| 12 | 2R | 29 | LEU |
| 12 | 2R | 81 | ASP |
| 12 | 2R | 100 | LEU |
| 13 | 2S | 8 | GLU |
| 13 | 2S | 25 | ARG |
| 13 | 2S | 58 | LEU |
| 13 | 2S | 69 | VAL |
| 13 | 2S | 85 | VAL |
| 13 | 2S | 110 | LEU |
| 14 | 2T | 40 | THR |
| 14 | 2T | 59 | THR |
| 14 | 2T | 95 | ARG |
| 14 | 2T | 96 | ARG |
| 15 | 2U | 45 | TYR |
| 15 | 2U | 78 | THR |
| 16 | 2V | 61 | VAL |
| 16 | 2V | 69 | LYS |
| 16 | 2V | 79 | VAL |
| 17 | 2W | 11 | ARG |
| 17 | 2W | 19 | LEU |
| 17 | 2W | 23 | LEU |
| 17 | 2W | 28 | SER |
| 17 | 2W | 60 | ASN |
| 17 | 2W | 63 | ASP |
| 17 | 2W | 94 | ASP |
| 17 | 2W | 100 | THR |
| 17 | 2W | 102 | HIS |
| 17 | 2W | 107 | LEU |
| 18 | 2X | 27 | THR |
| 18 | 2X | 35 | THR |
| 18 | 2X | 66 | LEU |
| 18 | 2X | 70 | LEU |
| 19 | 2Y | 49 | VAL |

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| Mol | Chain | Res | Type |
|---|---|---|---|
| 19 | 2Y | 72 | VAL |
| 19 | 2Y | 99 | CYS |
| 20 | 2Z | 18 | LEU |
| 20 | 2Z | 19 | ARG |
| 20 | 2Z | 31 | ARG |
| 20 | 2Z | 33 | LEU |
| 20 | 2Z | 56 | VAL |
| 20 | 2Z | 73 | GLN |
| 20 | 2Z | 78 | LYS |
| 20 | 2Z | 86 | VAL |
| 20 | 2Z | 116 | VAL |
| 20 | 2Z | 123 | ASP |
| 20 | 2Z | 139 | VAL |
| 20 | 2Z | 154 | ASP |
| 20 | 2Z | 156 | LYS |
| 20 | 2Z | 170 | THR |
| 20 | 2Z | 175 | VAL |
| 20 | 2Z | 179 | ASP |
| 21 | 20 | 10 | THR |
| 21 | 20 | 14 | ARG |
| 22 | 21 | 5 | CYS |
| 22 | 21 | 30 | VAL |
| 22 | 21 | 89 | GLU |
| 22 | 21 | 95 | LEU |
| 23 | 22 | 53 | LEU |
| 24 | 23 | 54 | VAL |
| 24 | 23 | 57 | GLU |
| 25 | 24 | 32 | TYR |
| 25 | 24 | 49 | PHE |
| 25 | 24 | 50 | VAL |
| 25 | 24 | 58 | ARG |
| 25 | 24 | 59 | PHE |
| 25 | 24 | 63 | TYR |
| 26 | 25 | 6 | VAL |
| 26 | 25 | 16 | ARG |
| 26 | 25 | 44 | THR |
| 27 | 26 | 6 | ARG |
| 28 | 27 | 4 | THR |
| 28 | 27 | 39 | ARG |
| 28 | 27 | 42 | LEU |
| 28 | 27 | 43 | THR |
| 28 | 27 | 47 | ARG |

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| Mol | Chain | Res | Type |
|---|---|---|---|
| 30 | 29 | 7 | VAL |
| 30 | 29 | 11 | CYS |
| 30 | 29 | 14 | CYS |
| 32 | 2b | 7 | VAL |
| 32 | 2b | 11 | LEU |
| 32 | 2b | 76 | GLN |
| 32 | 2b | 94 | ASN |
| 32 | 2b | 126 | GLU |
| 32 | 2b | 127 | ILE |
| 32 | 2b | 189 | ASP |
| 33 | 2c | 3 | ASN |
| 33 | 2c | 36 | ASP |
| 33 | 2c | 98 | ASN |
| 33 | 2c | 124 | ILE |
| 33 | 2c | 152 | ILE |
| 33 | 2c | 166 | GLU |
| 33 | 2c | 191 | THR |
| 34 | 2d | 5 | ILE |
| 34 | 2d | 31 | CYS |
| 34 | 2d | 59 | ARG |
| 34 | 2d | 86 | LYS |
| 34 | 2d | 107 | ARG |
| 34 | 2d | 141 | ARG |
| 34 | 2d | 150 | GLU |
| 35 | 2e | 10 | MET |
| 35 | 2e | 24 | ARG |
| 35 | 2e | 25 | ARG |
| 35 | 2e | 31 | LEU |
| 35 | 2e | 41 | VAL |
| 35 | 2e | 125 | SER |
| 35 | 2e | 147 | ASP |
| 36 | 2f | 19 | LEU |
| 36 | 2f | 46 | ARG |
| 36 | 2f | 70 | ASP |
| 36 | 2f | 72 | VAL |
| 37 | 2g | 79 | ARG |
| 38 | 2h | 2 | LEU |
| 38 | 2h | 39 | LEU |
| 38 | 2h | 51 | VAL |
| 38 | 2h | 83 | ILE |
| 38 | 2h | 112 | LEU |
| 38 | 2h | 114 | THR |

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| Mol | Chain | Res | Type |
|---|---|---|---|
| 39 | 2i | 53 | VAL |
| 39 | 2i | 65 | VAL |
| 39 | 2i | 89 | ASN |
| 39 | 2i | 93 | ARG |
| 39 | 2i | 102 | LEU |
| 39 | 2i | 108 | VAL |
| 40 | 2j | 9 | ARG |
| 40 | 2j | 55 | LYS |
| 40 | 2j | 74 | ILE |
| 42 | 2l | 6 | THR |
| 42 | 2l | 27 | LEU |
| 43 | 2m | 3 | ARG |
| 43 | 2m | 15 | VAL |
| 43 | 2m | 78 | ILE |
| 43 | 2m | 116 | THR |
| 44 | 2n | 41 | ARG |
| 44 | 2n | 44 | LEU |
| 45 | 2o | 7 | GLU |
| 45 | 2o | 28 | GLN |
| 45 | 2o | 39 | LEU |
| 45 | 2o | 70 | LEU |
| 45 | 2o | 72 | ARG |
| 45 | 2o | 83 | GLU |
| 46 | 2p | 2 | VAL |
| 46 | 2p | 20 | VAL |
| 46 | 2p | 25 | ARG |
| 46 | 2p | 52 | ASP |
| 46 | 2p | 67 | THR |
| 47 | 2q | 9 | VAL |
| 47 | 2q | 74 | LEU |
| 48 | 2r | 47 | THR |
| 48 | 2r | 76 | LEU |
| 49 | 2s | 33 | THR |
| 49 | 2s | 47 | HIS |
| 49 | 2s | 77 | THR |
| 50 | 2t | 84 | LEU |
| 52 | 2v | -65 | LYS |
| 52 | 2v | -58 | LEU |
| 52 | 2v | -26 | GLU |
| 52 | 2v | -10 | ARG |
| 52 | 2v | -9 | LEU |
| 52 | 2v | -6 | ARG |

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| Mol | Chain | Res | Type |
|---|---|---|---|
| 52 | 2v | 9 | LEU |
| 52 | 2v | 13 | ARG |
| 52 | 2v | 15 | ILE |
| 52 | 2v | 35 | TYR |
| 52 | 2v | 72 | CYS |
| 52 | 2v | 75 | LYS |
| 52 | 2v | 91 | THR |
| 52 | 2v | 92 | ILE |
| 52 | 2v | 102 | ASP |
| 52 | 2v | 112 | GLN |
| 52 | 2v | 114 | VAL |
| 52 | 2v | 119 | GLU |
| 52 | 2v | 121 | VAL |
| 52 | 2v | 132 | ARG |
| 52 | 2v | 146 | LEU |
| 52 | 2v | 152 | THR |
| 52 | 2v | 157 | LEU |
| 52 | 2v | 160 | ARG |
| 52 | 2v | 170 | ARG |
| 52 | 2v | 172 | ASP |
| 52 | 2v | 196 | ILE |
| 52 | 2v | 198 | GLU |
| 52 | 2v | 199 | ILE |
| 52 | 2v | 203 | GLU |
| 52 | 2v | 225 | GLU |
| 52 | 2v | 226 | ASN |
| 52 | 2v | 235 | GLU |
| 52 | 2v | 238 | THR |
| 52 | 2v | 260 | LEU |
| 52 | 2v | 264 | LEU |
| 52 | 2v | 286 | ILE |
| 52 | 2v | 290 | LYS |
| 52 | 2v | 298 | VAL |
| 52 | 2v | 312 | LEU |
| 52 | 2v | 328 | ILE |
| 52 | 2v | 329 | ARG |
| 52 | 2v | 334 | THR |
| 52 | 2v | 336 | THR |
| 52 | 2v | 344 | THR |
| 52 | 2v | 352 | VAL |
| 52 | 2v | 354 | ARG |
| 52 | 2v | 362 | HIS |

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| Mol | Chain | Res | Type |
|---|---|---|---|
| 52 | 2v | 373 | ASP |
| 52 | 2v | 374 | LEU |
| 52 | 2v | 377 | VAL |
| 52 | 2v | 381 | LYS |
| 52 | 2v | 402 | ILE |
| 52 | 2v | 403 | GLU |
| 52 | 2v | 406 | GLU |
| 52 | 2v | 408 | VAL |
| 52 | 2v | 422 | GLU |
| 52 | 2v | 437 | THR |
| 52 | 2v | 446 | THR |
| 52 | 2v | 473 | ASP |
| 52 | 2v | 475 | ASN |
| 52 | 2v | 484 | ARG |
| 52 | 2v | 485 | GLU |
| 52 | 2v | 488 | THR |
| 52 | 2v | 504 | ARG |
| 52 | 2v | 506 | GLN |
| 52 | 2v | 512 | ILE |
| 52 | 2v | 533 | VAL |
| 52 | 2v | 569 | ASP |
| 52 | 2v | 579 | GLU |
| 52 | 2v | 605 | ILE |
| 52 | 2v | 616 | TYR |
| 52 | 2v | 631 | ILE |
| 52 | 2v | 634 | MET |
| 52 | 2v | 641 | GLN |
| 52 | 2v | 644 | ARG |
| 52 | 2v | 647 | VAL |
| 52 | 2v | 670 | VAL |
| 52 | 2v | 678 | GLU |
| 52 | 2v | 681 | LYS |
| 52 | 2v | 683 | VAL |
| 52 | 2v | 689 | LYS |
| 53 | 2w | 6 | LEU |
| 53 | 2w | 9 | GLU |
| 53 | 2w | 13 | HIS |
| 53 | 2w | 16 | LYS |
| 53 | 2w | 29 | ARG |
| 53 | 2w | 32 | ARG |
| 53 | 2w | 34 | ASN |
| 53 | 2w | 52 | LEU |

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| Mol | Chain | Res | Type |
|---|---|---|---|
| 53 | 2w | 73 | GLN |
| 53 | 2w | 84 | ARG |
| 53 | 2w | 91 | ASN |
| 53 | 2w | 114 | LEU |
| 53 | 2w | 127 | VAL |
| 53 | 2w | 133 | ARG |
| 53 | 2w | 137 | LEU |
| 53 | 2w | 152 | ASP |
| 53 | 2w | 154 | THR |

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (123) such sidechains are listed below:

| Mol | Chain | Res | Type |
|---|---|---|---|
| 3 | 1D | 87 | ASN |
| 3 | 1D | 96 | HIS |
| 3 | 1D | 116 | GLN |
| 3 | 1D | 126 | GLN |
| 3 | 1D | 220 | HIS |
| 3 | 1D | 231 | HIS |
| 4 | 1E | 48 | GLN |
| 4 | 1E | 137 | HIS |
| 5 | 1F | 8 | GLN |
| 5 | 1F | 69 | HIS |
| 5 | 1F | 75 | HIS |
| 10 | 1P | 27 | HIS |
| 11 | 1Q | 12 | GLN |
| 11 | 1Q | 57 | HIS |
| 11 | 1Q | 123 | HIS |
| 13 | 1S | 61 | ASN |
| 14 | 1T | 43 | GLN |
| 16 | 1V | 80 | GLN |
| 18 | 1X | 31 | HIS |
| 20 | 1Z | 73 | GLN |
| 20 | 1Z | 121 | HIS |
| 22 | 11 | 56 | GLN |
| 24 | 13 | 32 | GLN |
| 26 | 15 | 23 | HIS |
| 33 | 1c | 170 | GLN |
| 34 | 1d | 160 | GLN |
| 34 | 1d | 161 | ASN |
| 35 | 1e | 78 | HIS |
| 37 | 1g | 13 | GLN |

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| Mol | Chain | Res | Type |
|---|---|---|---|
| 37 | 1g | 28 | ASN |
| 38 | 1h | 78 | GLN |
| 39 | 1i | 73 | GLN |
| 39 | 1i | 124 | GLN |
| 41 | 1k | 26 | ASN |
| 42 | 1l | 99 | HIS |
| 45 | 1o | 62 | GLN |
| 46 | 1p | 65 | GLN |
| 47 | 1q | 26 | GLN |
| 49 | 1s | 23 | ASN |
| 49 | 1s | 47 | HIS |
| 52 | 1v | -50 | GLN |
| 52 | 1v | 154 | GLN |
| 52 | 1v | 165 | GLN |
| 52 | 1v | 208 | GLN |
| 52 | 1v | 421 | GLN |
| 52 | 1v | 475 | ASN |
| 52 | 1v | 625 | ASN |
| 52 | 1v | 641 | GLN |
| 52 | 1v | 675 | HIS |
| 52 | 1v | 677 | GLN |
| 52 | 1v | 684 | GLN |
| 53 | 1w | 69 | GLN |
| 53 | 1w | 74 | ASN |
| 53 | 1w | 174 | GLN |
| 3 | 2D | 203 | ASN |
| 4 | 2E | 48 | GLN |
| 4 | 2E | 159 | HIS |
| 6 | 2G | 123 | ASN |
| 7 | 2H | 143 | GLN |
| 9 | 2O | 5 | GLN |
| 11 | 2Q | 57 | HIS |
| 11 | 2Q | 89 | ASN |
| 12 | 2R | 3 | HIS |
| 12 | 2R | 24 | GLN |
| 12 | 2R | 71 | GLN |
| 12 | 2R | 91 | GLN |
| 13 | 2S | 38 | GLN |
| 14 | 2T | 43 | GLN |
| 14 | 2T | 55 | ASN |
| 14 | 2T | 58 | ASN |
| 15 | 2U | 94 | ASN |

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| Mol | Chain | Res | Type |
|---|---|---|---|
| 17 | 2W | 60 | ASN |
| 20 | 2Z | 34 | ASN |
| 20 | 2Z | 73 | GLN |
| 22 | 21 | 47 | GLN |
| 22 | 21 | 56 | GLN |
| 23 | 22 | 47 | ASN |
| 24 | 23 | 19 | GLN |
| 24 | 23 | 32 | GLN |
| 26 | 25 | 22 | HIS |
| 28 | 27 | 6 | GLN |
| 30 | 29 | 20 | HIS |
| 32 | 2b | 94 | ASN |
| 32 | 2b | 140 | HIS |
| 32 | 2b | 212 | GLN |
| 33 | 2c | 6 | HIS |
| 33 | 2c | 102 | ASN |
| 34 | 2d | 116 | GLN |
| 34 | 2d | 125 | HIS |
| 35 | 2e | 73 | ASN |
| 35 | 2e | 78 | HIS |
| 36 | 2f | 32 | ASN |
| 37 | 2g | 28 | ASN |
| 37 | 2g | 37 | ASN |
| 37 | 2g | 64 | GLN |
| 37 | 2g | 68 | ASN |
| 37 | 2g | 106 | GLN |
| 37 | 2g | 109 | ASN |
| 39 | 2i | 89 | ASN |
| 40 | 2j | 62 | HIS |
| 43 | 2m | 12 | ASN |
| 43 | 2m | 106 | ASN |
| 45 | 2o | 28 | GLN |
| 45 | 2o | 46 | HIS |
| 46 | 2p | 76 | GLN |
| 49 | 2s | 47 | HIS |
| 52 | 2v | -50 | GLN |
| 52 | 2v | -13 | GLN |
| 52 | 2v | 7 | ASN |
| 52 | 2v | 77 | HIS |
| 52 | 2v | 208 | GLN |
| 52 | 2v | 426 | GLN |
| 52 | 2v | 448 | GLN |

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| Mol | Chain | Res | Type |
|---|---|---|---|
| 52 | 2v | 506 | GLN |
| 52 | 2v | 527 | ASN |
| 52 | 2v | 641 | GLN |
| 52 | 2v | 675 | HIS |
| 52 | 2v | 684 | GLN |
| 53 | 2w | 15 | GLN |
| 53 | 2w | 23 | HIS |
| 53 | 2w | 34 | ASN |
| 53 | 2w | 49 | HIS |
| 53 | 2w | 120 | GLN |

### 5.3.3 RNA (i)

| Mol | Chain | Analysed | Backbone Outliers | Pucker Outliers |
|---|---|---|---|---|
| 1 | 1A | 2862/2915 (98%) | 486 (16%) | 28 (0%) |
| 1 | 2A | 2789/2915 (95%) | 495 (17%) | 21 (0%) |
| 2 | 1B | 119/121 (98%) | 15 (12%) | 0 |
| 2 | 2B | 118/121 (97%) | 24 (20%) | 0 |
| 31 | 1a | 1492/1521 (98%) | 230 (15%) | 0 |
| 31 | 2a | 1498/1521 (98%) | 245 (16%) | 0 |
| 54 | 1x | 71/76 (93%) | 30 (42%) | 0 |
| 54 | 1y | 71/76 (93%) | 16 (22%) | 0 |
| 54 | 2x | 71/76 (93%) | 29 (40%) | 0 |
| 54 | 2y | 71/76 (93%) | 18 (25%) | 0 |
| 55 | 1z | 9/21 (42%) | 5 (55%) | 0 |
| 55 | 2z | 9/21 (42%) | 6 (66%) | 0 |
| All | All | 9180/9460 (97%) | 1599 (17%) | 49 (0%) |

All (1599) RNA backbone outliers are listed below:

| Mol | Chain | Res | Type |
|---|---|---|---|
| 1 | 1A | 12 | U |
| 1 | 1A | 13 | A |
| 1 | 1A | 15 | G |
| 1 | 1A | 27 | G |
| 1 | 1A | 34 | C |
| 1 | 1A | 37 | C |
| 1 | 1A | 45 | C |
| 1 | 1A | 51 | G |
| 1 | 1A | 55 | G |
| 1 | 1A | 58 | G |

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| Mol | Chain | Res | Type |
|---|---|---|---|
| 1 | 1A | 61 | G |
| 1 | 1A | 63 | U |
| 1 | 1A | 64 | A |
| 1 | 1A | 71 | A |
| 1 | 1A | 72 | U |
| 1 | 1A | 74 | A |
| 1 | 1A | 75 | G |
| 1 | 1A | 84 | A |
| 1 | 1A | 118 | A |
| 1 | 1A | 119 | A |
| 1 | 1A | 120 | U |
| 1 | 1A | 131 | G |
| 1 | 1A | 173 | G |
| 1 | 1A | 182 | A |
| 1 | 1A | 196 | A |
| 1 | 1A | 199 | A |
| 1 | 1A | 201 | C |
| 1 | 1A | 204 | A |
| 1 | 1A | 205 | G |
| 1 | 1A | 213 | A |
| 1 | 1A | 214 | G |
| 1 | 1A | 215 | G |
| 1 | 1A | 216 | A |
| 1 | 1A | 222 | A |
| 1 | 1A | 225 | A |
| 1 | 1A | 228 | A |
| 1 | 1A | 229 | A |
| 1 | 1A | 230 | U |
| 1 | 1A | 233 | A |
| 1 | 1A | 248 | G |
| 1 | 1A | 261 | G |
| 1 | 1A | 264 | C |
| 1 | 1A | 266 | G |
| 1 | 1A | 269 | U |
| 1 | 1A | 271(J) | C |
| 1 | 1A | 271(L) | U |
| 1 | 1A | 271(M) | G |
| 1 | 1A | 271(N) | U |
| 1 | 1A | 271(O) | C |
| 1 | 1A | 271(S) | G |
| 1 | 1A | 272(B) | G |
| 1 | 1A | 275 | G |

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| Mol | Chain | Res | Type |
|---|---|---|---|
| 1 | 1A | 279 | C |
| 1 | 1A | 311 | A |
| 1 | 1A | 317 | G |
| 1 | 1A | 325 | G |
| 1 | 1A | 329 | G |
| 1 | 1A | 330 | A |
| 1 | 1A | 331 | A |
| 1 | 1A | 352 | G |
| 1 | 1A | 353 | G |
| 1 | 1A | 362 | U |
| 1 | 1A | 363 | G |
| 1 | 1A | 371 | A |
| 1 | 1A | 372 | G |
| 1 | 1A | 386 | G |
| 1 | 1A | 396 | G |
| 1 | 1A | 405 | U |
| 1 | 1A | 411 | G |
| 1 | 1A | 428 | A |
| 1 | 1A | 444 | C |
| 1 | 1A | 448 | U |
| 1 | 1A | 456 | C |
| 1 | 1A | 457 | A |
| 1 | 1A | 471 | A |
| 1 | 1A | 481 | G |
| 1 | 1A | 494 | G |
| 1 | 1A | 504 | U |
| 1 | 1A | 505 | A |
| 1 | 1A | 509 | C |
| 1 | 1A | 513 | A |
| 1 | 1A | 528 | A |
| 1 | 1A | 530 | G |
| 1 | 1A | 531 | C |
| 1 | 1A | 532 | A |
| 1 | 1A | 533 | G |
| 1 | 1A | 536 | A |
| 1 | 1A | 545 | G |
| 1 | 1A | 549 | G |
| 1 | 1A | 556 | G |
| 1 | 1A | 563 | G |
| 1 | 1A | 564 | C |
| 1 | 1A | 566 | U |
| 1 | 1A | 573 | G |

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| Mol | Chain | Res | Type |
|---|---|---|---|
| 1 | 1A | 575 | A |
| 1 | 1A | 584 | C |
| 1 | 1A | 603 | A |
| 1 | 1A | 604 | G |
| 1 | 1A | 607 | U |
| 1 | 1A | 614(A) | U |
| 1 | 1A | 614(B) | G |
| 1 | 1A | 615 | G |
| 1 | 1A | 627 | A |
| 1 | 1A | 632 | A |
| 1 | 1A | 634 | C |
| 1 | 1A | 637 | A |
| 1 | 1A | 646 | A |
| 1 | 1A | 652(T) | C |
| 1 | 1A | 654 | A |
| 1 | 1A | 669 | G |
| 1 | 1A | 670 | A |
| 1 | 1A | 675 | A |
| 1 | 1A | 686 | G |
| 1 | 1A | 696 | G |
| 1 | 1A | 730 | C |
| 1 | 1A | 758 | C |
| 1 | 1A | 764 | A |
| 1 | 1A | 765 | G |
| 1 | 1A | 775 | G |
| 1 | 1A | 776 | G |
| 1 | 1A | 777 | A |
| 1 | 1A | 782 | A |
| 1 | 1A | 784 | A |
| 1 | 1A | 785 | G |
| 1 | 1A | 788 | A |
| 1 | 1A | 789 | A |
| 1 | 1A | 792 | G |
| 1 | 1A | 796 | C |
| 1 | 1A | 805 | G |
| 1 | 1A | 811 | U |
| 1 | 1A | 812 | C |
| 1 | 1A | 819 | A |
| 1 | 1A | 827 | U |
| 1 | 1A | 828 | U |
| 1 | 1A | 831 | G |
| 1 | 1A | 839 | U |

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| Mol | Chain | Res | Type |
|---|---|---|---|
| 1 | 1A | 859 | G |
| 1 | 1A | 860 | U |
| 1 | 1A | 876 | C |
| 1 | 1A | 880 | G |
| 1 | 1A | 884 | C |
| 1 | 1A | 885 | C |
| 1 | 1A | 886 | C |
| 1 | 1A | 887 | A |
| 1 | 1A | 889 | C |
| 1 | 1A | 890 | A |
| 1 | 1A | 896 | A |
| 1 | 1A | 897 | C |
| 1 | 1A | 898 | C |
| 1 | 1A | 900 | A |
| 1 | 1A | 907 | U |
| 1 | 1A | 910 | A |
| 1 | 1A | 914 | C |
| 1 | 1A | 915 | C |
| 1 | 1A | 919 | G |
| 1 | 1A | 932 | G |
| 1 | 1A | 938 | G |
| 1 | 1A | 945 | A |
| 1 | 1A | 946 | G |
| 1 | 1A | 957 | A |
| 1 | 1A | 959 | A |
| 1 | 1A | 961 | C |
| 1 | 1A | 974 | G |
| 1 | 1A | 975 | C |
| 1 | 1A | 980 | A |
| 1 | 1A | 983 | A |
| 1 | 1A | 995 | C |
| 1 | 1A | 996 | A |
| 1 | 1A | 1005 | C |
| 1 | 1A | 1012 | U |
| 1 | 1A | 1013 | C |
| 1 | 1A | 1021 | A |
| 1 | 1A | 1022 | G |
| 1 | 1A | 1023 | U |
| 1 | 1A | 1026 | U |
| 1 | 1A | 1033 | U |
| 1 | 1A | 1038 | C |
| 1 | 1A | 1041 | C |

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| Mol | Chain | Res | Type |
|---|---|---|---|
| 1 | 1A | 1044 | G |
| 1 | 1A | 1045 | A |
| 1 | 1A | 1046 | A |
| 1 | 1A | 1047 | G |
| 1 | 1A | 1048 | A |
| 1 | 1A | 1052 | C |
| 1 | 1A | 1054 | A |
| 1 | 1A | 1055 | G |
| 1 | 1A | 1058 | G |
| 1 | 1A | 1059 | G |
| 1 | 1A | 1063 | G |
| 1 | 1A | 1064 | C |
| 1 | 1A | 1068 | G |
| 1 | 1A | 1071 | G |
| 1 | 1A | 1073 | A |
| 1 | 1A | 1074 | G |
| 1 | 1A | 1075 | C |
| 1 | 1A | 1076 | C |
| 1 | 1A | 1078 | U |
| 1 | 1A | 1079 | C |
| 1 | 1A | 1083 | U |
| 1 | 1A | 1085 | A |
| 1 | 1A | 1088 | A |
| 1 | 1A | 1089 | G |
| 1 | 1A | 1090 | U |
| 1 | 1A | 1094 | U |
| 1 | 1A | 1101 | U |
| 1 | 1A | 1111 | A |
| 1 | 1A | 1112 | G |
| 1 | 1A | 1116 | C |
| 1 | 1A | 1126 | A |
| 1 | 1A | 1128 | A |
| 1 | 1A | 1130 | U |
| 1 | 1A | 1135 | C |
| 1 | 1A | 1136 | G |
| 1 | 1A | 1139 | G |
| 1 | 1A | 1143 | A |
| 1 | 1A | 1155 | A |
| 1 | 1A | 1171 | G |
| 1 | 1A | 1173 | G |
| 1 | 1A | 1174 | A |
| 1 | 1A | 1175 | U |

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| Mol | Chain | Res | Type |
|---|---|---|---|
| 1 | 1A | 1176 | G |
| 1 | 1A | 1177 | A |
| 1 | 1A | 1178 | C |
| 1 | 1A | 1210 | A |
| 1 | 1A | 1211 | U |
| 1 | 1A | 1220 | A |
| 1 | 1A | 1236 | G |
| 1 | 1A | 1237 | A |
| 1 | 1A | 1240 | U |
| 1 | 1A | 1244 | G |
| 1 | 1A | 1253 | A |
| 1 | 1A | 1254 | A |
| 1 | 1A | 1256 | G |
| 1 | 1A | 1271 | G |
| 1 | 1A | 1272 | A |
| 1 | 1A | 1273 | U |
| 1 | 1A | 1276 | A |
| 1 | 1A | 1281 | G |
| 1 | 1A | 1300 | U |
| 1 | 1A | 1301 | A |
| 1 | 1A | 1309 | G |
| 1 | 1A | 1313 | U |
| 1 | 1A | 1320 | C |
| 1 | 1A | 1321 | A |
| 1 | 1A | 1343 | G |
| 1 | 1A | 1352 | U |
| 1 | 1A | 1359 | A |
| 1 | 1A | 1360 | A |
| 1 | 1A | 1365 | A |
| 1 | 1A | 1373 | A |
| 1 | 1A | 1378 | A |
| 1 | 1A | 1380 | G |
| 1 | 1A | 1384 | A |
| 1 | 1A | 1385 | G |
| 1 | 1A | 1395 | A |
| 1 | 1A | 1396 | U |
| 1 | 1A | 1416 | G |
| 1 | 1A | 1417 | C |
| 1 | 1A | 1420 | U |
| 1 | 1A | 1421 | G |
| 1 | 1A | 1428 | C |
| 1 | 1A | 1445 | A |

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| Mol | Chain | Res | Type |
|---|---|---|---|
| 1 | 1A | 1450 | G |
| 1 | 1A | 1455 | G |
| 1 | 1A | 1467 | C |
| 1 | 1A | 1471 | A |
| 1 | 1A | 1482 | G |
| 1 | 1A | 1493 | C |
| 1 | 1A | 1509 | C |
| 1 | 1A | 1509(A) | A |
| 1 | 1A | 1514 | U |
| 1 | 1A | 1547 | C |
| 1 | 1A | 1554 | A |
| 1 | 1A | 1558 | A |
| 1 | 1A | 1565 | C |
| 1 | 1A | 1566 | A |
| 1 | 1A | 1569 | A |
| 1 | 1A | 1578 | U |
| 1 | 1A | 1580 | A |
| 1 | 1A | 1584 | C |
| 1 | 1A | 1586 | A |
| 1 | 1A | 1608 | A |
| 1 | 1A | 1609 | A |
| 1 | 1A | 1610 | A |
| 1 | 1A | 1613 | G |
| 1 | 1A | 1616 | A |
| 1 | 1A | 1639 | U |
| 1 | 1A | 1646 | C |
| 1 | 1A | 1647 | G |
| 1 | 1A | 1648 | C |
| 1 | 1A | 1654 | A |
| 1 | 1A | 1674 | G |
| 1 | 1A | 1696 | G |
| 1 | 1A | 1700 | A |
| 1 | 1A | 1722 | A |
| 1 | 1A | 1739 | U |
| 1 | 1A | 1746 | G |
| 1 | 1A | 1763 | G |
| 1 | 1A | 1764 | G |
| 1 | 1A | 1769 | G |
| 1 | 1A | 1773 | A |
| 1 | 1A | 1780 | A |
| 1 | 1A | 1791 | A |
| 1 | 1A | 1800 | C |

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| Mol | Chain | Res | Type |
|---|---|---|---|
| 1 | 1A | 1816 | G |
| 1 | 1A | 1821 | A |
| 1 | 1A | 1829 | A |
| 1 | 1A | 1839 | G |
| 1 | 1A | 1847 | A |
| 1 | 1A | 1877 | A |
| 1 | 1A | 1897 | G |
| 1 | 1A | 1900 | A |
| 1 | 1A | 1906 | G |
| 1 | 1A | 1912 | A |
| 1 | 1A | 1913 | A |
| 1 | 1A | 1914 | C |
| 1 | 1A | 1918 | A |
| 1 | 1A | 1927 | A |
| 1 | 1A | 1929 | G |
| 1 | 1A | 1930 | G |
| 1 | 1A | 1937 | A |
| 1 | 1A | 1938 | A |
| 1 | 1A | 1940 | U |
| 1 | 1A | 1955 | U |
| 1 | 1A | 1963 | U |
| 1 | 1A | 1967 | C |
| 1 | 1A | 1970 | A |
| 1 | 1A | 1971 | A |
| 1 | 1A | 1972 | A |
| 1 | 1A | 1993 | U |
| 1 | 1A | 1997 | G |
| 1 | 1A | 2013 | A |
| 1 | 1A | 2020 | A |
| 1 | 1A | 2023 | G |
| 1 | 1A | 2031 | A |
| 1 | 1A | 2032 | G |
| 1 | 1A | 2033 | A |
| 1 | 1A | 2039 | C |
| 1 | 1A | 2043 | C |
| 1 | 1A | 2055 | C |
| 1 | 1A | 2056 | G |
| 1 | 1A | 2060 | A |
| 1 | 1A | 2061 | G |
| 1 | 1A | 2062 | A |
| 1 | 1A | 2069 | G |
| 1 | 1A | 2078 | C |

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| Mol | Chain | Res | Type |
|---|---|---|---|
| 1 | 1A | 2093 | G |
| 1 | 1A | 2111 | C |
| 1 | 1A | 2113 | U |
| 1 | 1A | 2116 | G |
| 1 | 1A | 2118 | U |
| 1 | 1A | 2121 | G |
| 1 | 1A | 2122 | U |
| 1 | 1A | 2125 | G |
| 1 | 1A | 2126 | A |
| 1 | 1A | 2127 | G |
| 1 | 1A | 2130 | U |
| 1 | 1A | 2131 | G |
| 1 | 1A | 2132 | U |
| 1 | 1A | 2133 | G |
| 1 | 1A | 2134 | A |
| 1 | 1A | 2135 | A |
| 1 | 1A | 2140 | C |
| 1 | 1A | 2142 | C |
| 1 | 1A | 2144 | U |
| 1 | 1A | 2146 | C |
| 1 | 1A | 2147 | G |
| 1 | 1A | 2150 | U |
| 1 | 1A | 2151 | G |
| 1 | 1A | 2157 | G |
| 1 | 1A | 2158 | A |
| 1 | 1A | 2159 | G |
| 1 | 1A | 2165 | G |
| 1 | 1A | 2166 | G |
| 1 | 1A | 2167 | U |
| 1 | 1A | 2168 | G |
| 1 | 1A | 2169 | A |
| 1 | 1A | 2171 | A |
| 1 | 1A | 2172 | U |
| 1 | 1A | 2173 | A |
| 1 | 1A | 2181 | G |
| 1 | 1A | 2182 | G |
| 1 | 1A | 2184 | G |
| 1 | 1A | 2185 | C |
| 1 | 1A | 2192 | G |
| 1 | 1A | 2198 | A |
| 1 | 1A | 2206 | G |
| 1 | 1A | 2207 | G |

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| Mol | Chain | Res | Type |
|---|---|---|---|
| 1 | 1A | 2208 | A |
| 1 | 1A | 2219 | G |
| 1 | 1A | 2225 | A |
| 1 | 1A | 2238 | G |
| 1 | 1A | 2239 | G |
| 1 | 1A | 2278 | A |
| 1 | 1A | 2279 | G |
| 1 | 1A | 2283 | C |
| 1 | 1A | 2287 | A |
| 1 | 1A | 2288 | A |
| 1 | 1A | 2299 | G |
| 1 | 1A | 2305 | A |
| 1 | 1A | 2307 | G |
| 1 | 1A | 2308 | G |
| 1 | 1A | 2320 | A |
| 1 | 1A | 2325 | G |
| 1 | 1A | 2334 | G |
| 1 | 1A | 2336 | A |
| 1 | 1A | 2341 | G |
| 1 | 1A | 2347 | C |
| 1 | 1A | 2350 | C |
| 1 | 1A | 2358 | G |
| 1 | 1A | 2361 | A |
| 1 | 1A | 2383 | G |
| 1 | 1A | 2385 | C |
| 1 | 1A | 2391 | G |
| 1 | 1A | 2406 | U |
| 1 | 1A | 2410 | G |
| 1 | 1A | 2425 | A |
| 1 | 1A | 2429 | G |
| 1 | 1A | 2430 | A |
| 1 | 1A | 2434 | A |
| 1 | 1A | 2439 | A |
| 1 | 1A | 2441 | C |
| 1 | 1A | 2448 | A |
| 1 | 1A | 2468 | G |
| 1 | 1A | 2470 | G |
| 1 | 1A | 2474 | C |
| 1 | 1A | 2476 | A |
| 1 | 1A | 2482 | G |
| 1 | 1A | 2484 | G |
| 1 | 1A | 2490 | G |

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| Mol | Chain | Res | Type |
|---|---|---|---|
| 1 | 1A | 2491 | U |
| 1 | 1A | 2495 | G |
| 1 | 1A | 2502 | G |
| 1 | 1A | 2504 | U |
| 1 | 1A | 2505 | G |
| 1 | 1A | 2506 | U |
| 1 | 1A | 2518 | A |
| 1 | 1A | 2529 | G |
| 1 | 1A | 2554 | U |
| 1 | 1A | 2562 | U |
| 1 | 1A | 2566 | A |
| 1 | 1A | 2567 | G |
| 1 | 1A | 2573 | C |
| 1 | 1A | 2581 | G |
| 1 | 1A | 2585 | U |
| 1 | 1A | 2586 | C |
| 1 | 1A | 2601 | C |
| 1 | 1A | 2602 | A |
| 1 | 1A | 2603 | G |
| 1 | 1A | 2609 | U |
| 1 | 1A | 2611 | U |
| 1 | 1A | 2612 | C |
| 1 | 1A | 2615 | U |
| 1 | 1A | 2628 | C |
| 1 | 1A | 2629 | A |
| 1 | 1A | 2630 | G |
| 1 | 1A | 2641 | G |
| 1 | 1A | 2654 | A |
| 1 | 1A | 2663 | G |
| 1 | 1A | 2689 | U |
| 1 | 1A | 2690 | C |
| 1 | 1A | 2691 | C |
| 1 | 1A | 2702 | U |
| 1 | 1A | 2703 | C |
| 1 | 1A | 2712(A) | A |
| 1 | 1A | 2713 | A |
| 1 | 1A | 2726 | U |
| 1 | 1A | 2730 | C |
| 1 | 1A | 2733 | A |
| 1 | 1A | 2757 | A |
| 1 | 1A | 2758 | A |
| 1 | 1A | 2764 | A |

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| Mol | Chain | Res | Type |
|---|---|---|---|
| 1 | 1A | 2765 | A |
| 1 | 1A | 2766 | G |
| 1 | 1A | 2778 | A |
| 1 | 1A | 2790 | A |
| 1 | 1A | 2791 | C |
| 1 | 1A | 2802 | G |
| 1 | 1A | 2805 | G |
| 1 | 1A | 2818 | G |
| 1 | 1A | 2820 | A |
| 1 | 1A | 2821 | A |
| 1 | 1A | 2834 | G |
| 1 | 1A | 2872 | G |
| 1 | 1A | 2892 | A |
| 1 | 1A | 2894 | G |
| 2 | 1B | 2 | C |
| 2 | 1B | 5 | C |
| 2 | 1B | 13 | A |
| 2 | 1B | 33 | G |
| 2 | 1B | 35 | U |
| 2 | 1B | 42 | C |
| 2 | 1B | 44 | G |
| 2 | 1B | 45 | A |
| 2 | 1B | 56 | G |
| 2 | 1B | 73 | A |
| 2 | 1B | 84 | C |
| 2 | 1B | 85 | G |
| 2 | 1B | 106 | G |
| 2 | 1B | 110 | G |
| 2 | 1B | 120 | A |
| 31 | 1a | 9 | G |
| 31 | 1a | 32 | A |
| 31 | 1a | 39 | G |
| 31 | 1a | 47 | C |
| 31 | 1a | 48 | C |
| 31 | 1a | 50 | A |
| 31 | 1a | 51 | A |
| 31 | 1a | 61 | G |
| 31 | 1a | 79 | G |
| 31 | 1a | 91 | C |
| 31 | 1a | 98 | G |
| 31 | 1a | 101 | A |
| 31 | 1a | 116 | A |

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| Mol | Chain | Res | Type |
|---|---|---|---|
| 31 | 1a | 121 | C |
| 31 | 1a | 131 | C |
| 31 | 1a | 145 | G |
| 31 | 1a | 163 | C |
| 31 | 1a | 174 | C |
| 31 | 1a | 182 | U |
| 31 | 1a | 189 | G |
| 31 | 1a | 189(A) | C |
| 31 | 1a | 189(F) | U |
| 31 | 1a | 195 | A |
| 31 | 1a | 197 | A |
| 31 | 1a | 203 | U |
| 31 | 1a | 204 | U |
| 31 | 1a | 216 | G |
| 31 | 1a | 217 | C |
| 31 | 1a | 220 | G |
| 31 | 1a | 247 | G |
| 31 | 1a | 251 | G |
| 31 | 1a | 266 | G |
| 31 | 1a | 267 | C |
| 31 | 1a | 279 | A |
| 31 | 1a | 289 | G |
| 31 | 1a | 321 | A |
| 31 | 1a | 328 | C |
| 31 | 1a | 332 | G |
| 31 | 1a | 343 | U |
| 31 | 1a | 345 | C |
| 31 | 1a | 347 | G |
| 31 | 1a | 351 | G |
| 31 | 1a | 352 | C |
| 31 | 1a | 353 | A |
| 31 | 1a | 354 | G |
| 31 | 1a | 356 | A |
| 31 | 1a | 367 | U |
| 31 | 1a | 372 | C |
| 31 | 1a | 373 | A |
| 31 | 1a | 384 | G |
| 31 | 1a | 397 | A |
| 31 | 1a | 398 | C |
| 31 | 1a | 412 | A |
| 31 | 1a | 423 | G |
| 31 | 1a | 424 | G |

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| Mol | Chain | Res | Type |
|---|---|---|---|
| 31 | 1a | 429 | U |
| 31 | 1a | 430 | A |
| 31 | 1a | 439 | A |
| 31 | 1a | 441 | A |
| 31 | 1a | 442 | C |
| 31 | 1a | 452 | A |
| 31 | 1a | 461 | A |
| 31 | 1a | 470 | C |
| 31 | 1a | 485 | G |
| 31 | 1a | 496 | A |
| 31 | 1a | 498 | U |
| 31 | 1a | 505 | G |
| 31 | 1a | 509 | A |
| 31 | 1a | 510 | A |
| 31 | 1a | 511 | C |
| 31 | 1a | 518 | C |
| 31 | 1a | 519 | C |
| 31 | 1a | 531 | U |
| 31 | 1a | 532 | A |
| 31 | 1a | 547 | A |
| 31 | 1a | 559 | A |
| 31 | 1a | 561 | U |
| 31 | 1a | 562 | C |
| 31 | 1a | 564 | C |
| 31 | 1a | 572 | A |
| 31 | 1a | 573 | A |
| 31 | 1a | 576 | G |
| 31 | 1a | 577 | G |
| 31 | 1a | 596 | C |
| 31 | 1a | 630 | G |
| 31 | 1a | 634 | C |
| 31 | 1a | 641 | U |
| 31 | 1a | 653 | A |
| 31 | 1a | 665 | A |
| 31 | 1a | 688 | G |
| 31 | 1a | 695 | A |
| 31 | 1a | 721 | G |
| 31 | 1a | 723 | U |
| 31 | 1a | 731 | G |
| 31 | 1a | 734 | G |
| 31 | 1a | 749 | C |
| 31 | 1a | 755 | G |

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| Mol | Chain | Res | Type |
|---|---|---|---|
| 31 | 1a | 767 | A |
| 31 | 1a | 777 | A |
| 31 | 1a | 793 | U |
| 31 | 1a | 794 | A |
| 31 | 1a | 816 | A |
| 31 | 1a | 817 | C |
| 31 | 1a | 821 | G |
| 31 | 1a | 828 | A |
| 31 | 1a | 836 | G |
| 31 | 1a | 840 | C |
| 31 | 1a | 841 | U |
| 31 | 1a | 851 | G |
| 31 | 1a | 859 | A |
| 31 | 1a | 866 | C |
| 31 | 1a | 902 | G |
| 31 | 1a | 914 | A |
| 31 | 1a | 926 | G |
| 31 | 1a | 927 | G |
| 31 | 1a | 934 | C |
| 31 | 1a | 952 | U |
| 31 | 1a | 960 | U |
| 31 | 1a | 961 | U |
| 31 | 1a | 968 | A |
| 31 | 1a | 969 | A |
| 31 | 1a | 971 | G |
| 31 | 1a | 972 | C |
| 31 | 1a | 974 | A |
| 31 | 1a | 975 | A |
| 31 | 1a | 976 | G |
| 31 | 1a | 977 | A |
| 31 | 1a | 982 | U |
| 31 | 1a | 992 | U |
| 31 | 1a | 993 | G |
| 31 | 1a | 1000 | U |
| 31 | 1a | 1003 | G |
| 31 | 1a | 1005 | A |
| 31 | 1a | 1006 | C |
| 31 | 1a | 1020 | U |
| 31 | 1a | 1022 | G |
| 31 | 1a | 1025 | U |
| 31 | 1a | 1026 | G |
| 31 | 1a | 1027 | C |

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| Mol | Chain | Res | Type |
|---|---|---|---|
| 31 | 1a | 1029 | C |
| 31 | 1a | 1030(A) | G |
| 31 | 1a | 1031 | G |
| 31 | 1a | 1033 | G |
| 31 | 1a | 1037 | C |
| 31 | 1a | 1038 | C |
| 31 | 1a | 1039 | C |
| 31 | 1a | 1044 | A |
| 31 | 1a | 1050 | G |
| 31 | 1a | 1054 | C |
| 31 | 1a | 1055 | A |
| 31 | 1a | 1065 | U |
| 31 | 1a | 1066 | C |
| 31 | 1a | 1068 | G |
| 31 | 1a | 1081 | G |
| 31 | 1a | 1084 | G |
| 31 | 1a | 1094 | G |
| 31 | 1a | 1095 | U |
| 31 | 1a | 1101 | A |
| 31 | 1a | 1108 | G |
| 31 | 1a | 1122 | U |
| 31 | 1a | 1124 | G |
| 31 | 1a | 1125 | U |
| 31 | 1a | 1127 | G |
| 31 | 1a | 1134 | G |
| 31 | 1a | 1137 | C |
| 31 | 1a | 1138 | G |
| 31 | 1a | 1139 | G |
| 31 | 1a | 1146 | A |
| 31 | 1a | 1152 | A |
| 31 | 1a | 1159 | U |
| 31 | 1a | 1184 | G |
| 31 | 1a | 1186 | G |
| 31 | 1a | 1187 | G |
| 31 | 1a | 1196 | U |
| 31 | 1a | 1197 | G |
| 31 | 1a | 1200 | C |
| 31 | 1a | 1202 | G |
| 31 | 1a | 1212 | U |
| 31 | 1a | 1213 | A |
| 31 | 1a | 1220 | G |
| 31 | 1a | 1225 | A |

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| Mol | Chain | Res | Type |
|---|---|---|---|
| 31 | 1a | 1226 | C |
| 31 | 1a | 1227 | A |
| 31 | 1a | 1236 | A |
| 31 | 1a | 1238 | A |
| 31 | 1a | 1241 | G |
| 31 | 1a | 1256 | A |
| 31 | 1a | 1257 | U |
| 31 | 1a | 1258 | G |
| 31 | 1a | 1260 | C |
| 31 | 1a | 1268 | A |
| 31 | 1a | 1270 | C |
| 31 | 1a | 1278 | U |
| 31 | 1a | 1279 | A |
| 31 | 1a | 1280 | A |
| 31 | 1a | 1286 | A |
| 31 | 1a | 1287 | A |
| 31 | 1a | 1299 | A |
| 31 | 1a | 1300 | G |
| 31 | 1a | 1305 | G |
| 31 | 1a | 1320 | C |
| 31 | 1a | 1336 | C |
| 31 | 1a | 1346 | A |
| 31 | 1a | 1347 | G |
| 31 | 1a | 1353 | G |
| 31 | 1a | 1358 | U |
| 31 | 1a | 1363 | C |
| 31 | 1a | 1364 | U |
| 31 | 1a | 1370 | G |
| 31 | 1a | 1378 | C |
| 31 | 1a | 1398 | A |
| 31 | 1a | 1419 | G |
| 31 | 1a | 1442 | G |
| 31 | 1a | 1442(A) | G |
| 31 | 1a | 1446 | U |
| 31 | 1a | 1447 | A |
| 31 | 1a | 1452 | C |
| 31 | 1a | 1456 | G |
| 31 | 1a | 1487 | G |
| 31 | 1a | 1491 | G |
| 31 | 1a | 1492 | A |
| 31 | 1a | 1493 | A |
| 31 | 1a | 1494 | G |

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| Mol | Chain | Res | Type |
|---|---|---|---|
| 31 | 1a | 1499 | A |
| 31 | 1a | 1503 | A |
| 31 | 1a | 1504 | G |
| 31 | 1a | 1506 | U |
| 31 | 1a | 1517 | G |
| 31 | 1a | 1529 | G |
| 31 | 1a | 1530 | G |
| 54 | 1x | 2 | C |
| 54 | 1x | 3 | C |
| 54 | 1x | 4 | C |
| 54 | 1x | 5 | G |
| 54 | 1x | 8 | 4SU |
| 54 | 1x | 19 | G |
| 54 | 1x | 20 | U |
| 54 | 1x | 21 | A |
| 54 | 1x | 22 | G |
| 54 | 1x | 26 | A |
| 54 | 1x | 33 | U |
| 54 | 1x | 35 | A |
| 54 | 1x | 36 | A |
| 54 | 1x | 38 | A |
| 54 | 1x | 42 | C |
| 54 | 1x | 44 | G |
| 54 | 1x | 45 | U |
| 54 | 1x | 46 | 7MG |
| 54 | 1x | 47 | U |
| 54 | 1x | 48 | C |
| 54 | 1x | 52 | G |
| 54 | 1x | 57 | G |
| 54 | 1x | 59 | U |
| 54 | 1x | 60 | U |
| 54 | 1x | 65 | G |
| 54 | 1x | 69 | G |
| 54 | 1x | 70 | G |
| 54 | 1x | 71 | G |
| 54 | 1x | 75 | C |
| 54 | 1x | 76 | A |
| 54 | 1y | 2 | C |
| 54 | 1y | 5 | G |
| 54 | 1y | 9 | A |
| 54 | 1y | 13 | C |
| 54 | 1y | 14 | A |

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| Mol | Chain | Res | Type |
|---|---|---|---|
| 54 | 1y | 20 | U |
| 54 | 1y | 21 | A |
| 54 | 1y | 26 | A |
| 54 | 1y | 44 | G |
| 54 | 1y | 45 | U |
| 54 | 1y | 46 | 7MG |
| 54 | 1y | 47 | U |
| 54 | 1y | 48 | C |
| 54 | 1y | 49 | C |
| 54 | 1y | 59 | U |
| 54 | 1y | 60 | U |
| 55 | 1z | 13 | A |
| 55 | 1z | 15 | A |
| 55 | 1z | 19 | U |
| 55 | 1z | 20 | A |
| 55 | 1z | 21 | A |
| 1 | 2A | 12 | U |
| 1 | 2A | 14 | A |
| 1 | 2A | 15 | G |
| 1 | 2A | 27 | G |
| 1 | 2A | 34 | C |
| 1 | 2A | 35 | G |
| 1 | 2A | 45 | C |
| 1 | 2A | 49 | A |
| 1 | 2A | 50 | U |
| 1 | 2A | 51 | G |
| 1 | 2A | 71 | A |
| 1 | 2A | 74 | A |
| 1 | 2A | 75 | G |
| 1 | 2A | 84 | A |
| 1 | 2A | 90 | U |
| 1 | 2A | 98 | G |
| 1 | 2A | 100 | G |
| 1 | 2A | 102 | G |
| 1 | 2A | 118 | A |
| 1 | 2A | 120 | U |
| 1 | 2A | 125 | G |
| 1 | 2A | 139(A) | G |
| 1 | 2A | 154(A) | C |
| 1 | 2A | 157 | U |
| 1 | 2A | 173 | G |
| 1 | 2A | 181 | A |

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| Mol | Chain | Res | Type |
|---|---|---|---|
| 1 | 2A | 196 | A |
| 1 | 2A | 199 | A |
| 1 | 2A | 201 | C |
| 1 | 2A | 204 | A |
| 1 | 2A | 205 | G |
| 1 | 2A | 216 | A |
| 1 | 2A | 222 | A |
| 1 | 2A | 228 | A |
| 1 | 2A | 229 | A |
| 1 | 2A | 233 | A |
| 1 | 2A | 248 | G |
| 1 | 2A | 249 | C |
| 1 | 2A | 266 | G |
| 1 | 2A | 271(L) | U |
| 1 | 2A | 271(M) | G |
| 1 | 2A | 271(N) | U |
| 1 | 2A | 271(O) | C |
| 1 | 2A | 272(B) | G |
| 1 | 2A | 272(I) | U |
| 1 | 2A | 272(J) | C |
| 1 | 2A | 277 | C |
| 1 | 2A | 278 | A |
| 1 | 2A | 294 | A |
| 1 | 2A | 302 | C |
| 1 | 2A | 311 | A |
| 1 | 2A | 317 | G |
| 1 | 2A | 324 | A |
| 1 | 2A | 327 | G |
| 1 | 2A | 329 | G |
| 1 | 2A | 330 | A |
| 1 | 2A | 333 | G |
| 1 | 2A | 352 | G |
| 1 | 2A | 362 | U |
| 1 | 2A | 363 | G |
| 1 | 2A | 363(B) | G |
| 1 | 2A | 363(D) | G |
| 1 | 2A | 372 | G |
| 1 | 2A | 386 | G |
| 1 | 2A | 396 | G |
| 1 | 2A | 405 | U |
| 1 | 2A | 406 | G |
| 1 | 2A | 411 | G |

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| Mol | Chain | Res | Type |
|---|---|---|---|
| 1 | 2A | 422 | A |
| 1 | 2A | 435 | C |
| 1 | 2A | 444 | C |
| 1 | 2A | 448 | U |
| 1 | 2A | 449 | A |
| 1 | 2A | 454 | A |
| 1 | 2A | 457 | A |
| 1 | 2A | 480 | A |
| 1 | 2A | 481 | G |
| 1 | 2A | 504 | U |
| 1 | 2A | 505 | A |
| 1 | 2A | 509 | C |
| 1 | 2A | 529 | A |
| 1 | 2A | 530 | G |
| 1 | 2A | 531 | C |
| 1 | 2A | 532 | A |
| 1 | 2A | 533 | G |
| 1 | 2A | 563 | G |
| 1 | 2A | 568 | U |
| 1 | 2A | 573 | G |
| 1 | 2A | 574 | C |
| 1 | 2A | 575 | A |
| 1 | 2A | 599 | G |
| 1 | 2A | 603 | A |
| 1 | 2A | 604 | G |
| 1 | 2A | 607 | U |
| 1 | 2A | 610 | G |
| 1 | 2A | 614(B) | G |
| 1 | 2A | 615 | G |
| 1 | 2A | 616 | G |
| 1 | 2A | 627 | A |
| 1 | 2A | 632 | A |
| 1 | 2A | 634 | C |
| 1 | 2A | 637 | A |
| 1 | 2A | 645 | C |
| 1 | 2A | 651 | G |
| 1 | 2A | 652(B) | A |
| 1 | 2A | 652(C) | G |
| 1 | 2A | 668 | G |
| 1 | 2A | 669 | G |
| 1 | 2A | 675 | A |
| 1 | 2A | 686 | G |

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| Mol | Chain | Res | Type |
|---|---|---|---|
| 1 | 2A | 717 | G |
| 1 | 2A | 726 | G |
| 1 | 2A | 730 | C |
| 1 | 2A | 753 | C |
| 1 | 2A | 764 | A |
| 1 | 2A | 771 | G |
| 1 | 2A | 775 | G |
| 1 | 2A | 776 | G |
| 1 | 2A | 782 | A |
| 1 | 2A | 783 | A |
| 1 | 2A | 784 | A |
| 1 | 2A | 785 | G |
| 1 | 2A | 789 | A |
| 1 | 2A | 792 | G |
| 1 | 2A | 793 | A |
| 1 | 2A | 801 | G |
| 1 | 2A | 805 | G |
| 1 | 2A | 812 | C |
| 1 | 2A | 819 | A |
| 1 | 2A | 825 | C |
| 1 | 2A | 827 | U |
| 1 | 2A | 829 | A |
| 1 | 2A | 831 | G |
| 1 | 2A | 843 | G |
| 1 | 2A | 846 | C |
| 1 | 2A | 847 | U |
| 1 | 2A | 857 | C |
| 1 | 2A | 859 | G |
| 1 | 2A | 866 | A |
| 1 | 2A | 869 | G |
| 1 | 2A | 874 | G |
| 1 | 2A | 875 | G |
| 1 | 2A | 879 | G |
| 1 | 2A | 880 | G |
| 1 | 2A | 884 | C |
| 1 | 2A | 886 | C |
| 1 | 2A | 887 | A |
| 1 | 2A | 888 | C |
| 1 | 2A | 889 | C |
| 1 | 2A | 890 | A |
| 1 | 2A | 893 | C |
| 1 | 2A | 894 | C |

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| Mol | Chain | Res | Type |
|---|---|---|---|
| 1 | 2A | 895 | U |
| 1 | 2A | 896 | A |
| 1 | 2A | 897 | C |
| 1 | 2A | 900 | A |
| 1 | 2A | 901 | A |
| 1 | 2A | 907 | U |
| 1 | 2A | 910 | A |
| 1 | 2A | 915 | C |
| 1 | 2A | 917 | A |
| 1 | 2A | 932 | G |
| 1 | 2A | 941 | A |
| 1 | 2A | 945 | A |
| 1 | 2A | 946 | G |
| 1 | 2A | 953 | A |
| 1 | 2A | 957 | A |
| 1 | 2A | 958 | U |
| 1 | 2A | 959 | A |
| 1 | 2A | 961 | C |
| 1 | 2A | 973 | A |
| 1 | 2A | 974 | G |
| 1 | 2A | 975 | C |
| 1 | 2A | 975(A) | G |
| 1 | 2A | 980 | A |
| 1 | 2A | 983 | A |
| 1 | 2A | 996 | A |
| 1 | 2A | 997 | G |
| 1 | 2A | 1012 | U |
| 1 | 2A | 1013 | C |
| 1 | 2A | 1017 | G |
| 1 | 2A | 1020 | A |
| 1 | 2A | 1022 | G |
| 1 | 2A | 1023 | U |
| 1 | 2A | 1025 | G |
| 1 | 2A | 1033 | U |
| 1 | 2A | 1038 | C |
| 1 | 2A | 1039 | G |
| 1 | 2A | 1043 | C |
| 1 | 2A | 1114 | G |
| 1 | 2A | 1116 | C |
| 1 | 2A | 1125 | G |
| 1 | 2A | 1129 | A |
| 1 | 2A | 1130 | U |

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| Mol | Chain | Res | Type |
|---|---|---|---|
| 1 | 2A | 1132 | A |
| 1 | 2A | 1135 | C |
| 1 | 2A | 1136 | G |
| 1 | 2A | 1139 | G |
| 1 | 2A | 1143 | A |
| 1 | 2A | 1144 | G |
| 1 | 2A | 1169 | G |
| 1 | 2A | 1171 | G |
| 1 | 2A | 1187 | G |
| 1 | 2A | 1188 | U |
| 1 | 2A | 1210 | A |
| 1 | 2A | 1211 | U |
| 1 | 2A | 1212 | G |
| 1 | 2A | 1220 | A |
| 1 | 2A | 1237 | A |
| 1 | 2A | 1250 | G |
| 1 | 2A | 1252 | G |
| 1 | 2A | 1253 | A |
| 1 | 2A | 1256 | G |
| 1 | 2A | 1271 | G |
| 1 | 2A | 1272 | A |
| 1 | 2A | 1273 | U |
| 1 | 2A | 1300 | U |
| 1 | 2A | 1301 | A |
| 1 | 2A | 1313 | U |
| 1 | 2A | 1314 | C |
| 1 | 2A | 1321 | A |
| 1 | 2A | 1352 | U |
| 1 | 2A | 1359 | A |
| 1 | 2A | 1360 | A |
| 1 | 2A | 1365 | A |
| 1 | 2A | 1368 | G |
| 1 | 2A | 1378 | A |
| 1 | 2A | 1380 | G |
| 1 | 2A | 1384 | A |
| 1 | 2A | 1385 | G |
| 1 | 2A | 1386 | C |
| 1 | 2A | 1411 | C |
| 1 | 2A | 1416 | G |
| 1 | 2A | 1417 | C |
| 1 | 2A | 1420 | U |
| 1 | 2A | 1421 | G |

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| Mol | Chain | Res | Type |
|---|---|---|---|
| 1 | 2A | 1427 | A |
| 1 | 2A | 1428 | C |
| 1 | 2A | 1435 | G |
| 1 | 2A | 1437 | C |
| 1 | 2A | 1445 | A |
| 1 | 2A | 1449 | A |
| 1 | 2A | 1450 | G |
| 1 | 2A | 1455 | G |
| 1 | 2A | 1460 | A |
| 1 | 2A | 1467 | C |
| 1 | 2A | 1471 | A |
| 1 | 2A | 1482 | G |
| 1 | 2A | 1490 | A |
| 1 | 2A | 1493 | C |
| 1 | 2A | 1495 | A |
| 1 | 2A | 1496 | A |
| 1 | 2A | 1497 | U |
| 1 | 2A | 1507 | A |
| 1 | 2A | 1508 | A |
| 1 | 2A | 1509 | C |
| 1 | 2A | 1509(A) | A |
| 1 | 2A | 1531 | C |
| 1 | 2A | 1532 | C |
| 1 | 2A | 1533 | G |
| 1 | 2A | 1543 | C |
| 1 | 2A | 1546 | C |
| 1 | 2A | 1558 | A |
| 1 | 2A | 1566 | A |
| 1 | 2A | 1569 | A |
| 1 | 2A | 1578 | U |
| 1 | 2A | 1580 | A |
| 1 | 2A | 1584 | C |
| 1 | 2A | 1586 | A |
| 1 | 2A | 1602 | U |
| 1 | 2A | 1603 | A |
| 1 | 2A | 1608 | A |
| 1 | 2A | 1609 | A |
| 1 | 2A | 1610 | A |
| 1 | 2A | 1640 | C |
| 1 | 2A | 1646 | C |
| 1 | 2A | 1648 | C |
| 1 | 2A | 1654 | A |

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| Mol | Chain | Res | Type |
|---|---|---|---|
| 1 | 2A | 1674 | G |
| 1 | 2A | 1696 | G |
| 1 | 2A | 1698 | A |
| 1 | 2A | 1700 | A |
| 1 | 2A | 1701 | A |
| 1 | 2A | 1703 | G |
| 1 | 2A | 1721 | G |
| 1 | 2A | 1722 | A |
| 1 | 2A | 1740 | G |
| 1 | 2A | 1745(A) | C |
| 1 | 2A | 1746 | G |
| 1 | 2A | 1756 | G |
| 1 | 2A | 1758 | G |
| 1 | 2A | 1763 | G |
| 1 | 2A | 1764 | G |
| 1 | 2A | 1769 | G |
| 1 | 2A | 1773 | A |
| 1 | 2A | 1778 | U |
| 1 | 2A | 1780 | A |
| 1 | 2A | 1791 | A |
| 1 | 2A | 1800 | C |
| 1 | 2A | 1801 | G |
| 1 | 2A | 1809 | A |
| 1 | 2A | 1813 | G |
| 1 | 2A | 1816 | G |
| 1 | 2A | 1827 | C |
| 1 | 2A | 1835 | G |
| 1 | 2A | 1847 | A |
| 1 | 2A | 1848 | A |
| 1 | 2A | 1877 | A |
| 1 | 2A | 1878 | G |
| 1 | 2A | 1902 | C |
| 1 | 2A | 1912 | A |
| 1 | 2A | 1914 | C |
| 1 | 2A | 1915 | 5MU |
| 1 | 2A | 1916 | A |
| 1 | 2A | 1917 | PSU |
| 1 | 2A | 1918 | A |
| 1 | 2A | 1919 | A |
| 1 | 2A | 1920 | OMC |
| 1 | 2A | 1929 | G |
| 1 | 2A | 1930 | G |

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| Mol | Chain | Res | Type |
|---|---|---|---|
| 1 | 2A | 1934 | C |
| 1 | 2A | 1936 | A |
| 1 | 2A | 1955 | U |
| 1 | 2A | 1963 | U |
| 1 | 2A | 1964 | G |
| 1 | 2A | 1965 | C |
| 1 | 2A | 1967 | C |
| 1 | 2A | 1970 | A |
| 1 | 2A | 1971 | A |
| 1 | 2A | 1972 | A |
| 1 | 2A | 1984 | G |
| 1 | 2A | 1993 | U |
| 1 | 2A | 1997 | G |
| 1 | 2A | 2023 | G |
| 1 | 2A | 2027 | G |
| 1 | 2A | 2030 | A |
| 1 | 2A | 2031 | A |
| 1 | 2A | 2032 | G |
| 1 | 2A | 2033 | A |
| 1 | 2A | 2034 | U |
| 1 | 2A | 2043 | C |
| 1 | 2A | 2055 | C |
| 1 | 2A | 2056 | G |
| 1 | 2A | 2060 | A |
| 1 | 2A | 2061 | G |
| 1 | 2A | 2062 | A |
| 1 | 2A | 2069 | G |
| 1 | 2A | 2093 | G |
| 1 | 2A | 2096 | U |
| 1 | 2A | 2105 | C |
| 1 | 2A | 2108 | C |
| 1 | 2A | 2111 | C |
| 1 | 2A | 2112 | G |
| 1 | 2A | 2116 | G |
| 1 | 2A | 2119 | A |
| 1 | 2A | 2120 | G |
| 1 | 2A | 2122 | U |
| 1 | 2A | 2126 | A |
| 1 | 2A | 2127 | G |
| 1 | 2A | 2129 | C |
| 1 | 2A | 2131 | G |
| 1 | 2A | 2132 | U |

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| Mol | Chain | Res | Type |
|---|---|---|---|
| 1 | 2A | 2133 | G |
| 1 | 2A | 2134 | A |
| 1 | 2A | 2135 | A |
| 1 | 2A | 2136 | C |
| 1 | 2A | 2138 | C |
| 1 | 2A | 2140 | C |
| 1 | 2A | 2142 | C |
| 1 | 2A | 2146 | C |
| 1 | 2A | 2150 | U |
| 1 | 2A | 2156 | G |
| 1 | 2A | 2157 | G |
| 1 | 2A | 2161 | C |
| 1 | 2A | 2165 | G |
| 1 | 2A | 2166 | G |
| 1 | 2A | 2167 | U |
| 1 | 2A | 2168 | G |
| 1 | 2A | 2172 | U |
| 1 | 2A | 2174 | C |
| 1 | 2A | 2178 | C |
| 1 | 2A | 2192 | G |
| 1 | 2A | 2198 | A |
| 1 | 2A | 2206 | G |
| 1 | 2A | 2207 | G |
| 1 | 2A | 2208 | A |
| 1 | 2A | 2225 | A |
| 1 | 2A | 2238 | G |
| 1 | 2A | 2239 | G |
| 1 | 2A | 2275 | C |
| 1 | 2A | 2279 | G |
| 1 | 2A | 2283 | C |
| 1 | 2A | 2287 | A |
| 1 | 2A | 2291 | U |
| 1 | 2A | 2305 | A |
| 1 | 2A | 2308 | G |
| 1 | 2A | 2311 | A |
| 1 | 2A | 2319 | G |
| 1 | 2A | 2320 | A |
| 1 | 2A | 2325 | G |
| 1 | 2A | 2334 | G |
| 1 | 2A | 2336 | A |
| 1 | 2A | 2347 | C |
| 1 | 2A | 2350 | C |

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| Mol | Chain | Res | Type |
|---|---|---|---|
| 1 | 2A | 2352 | A |
| 1 | 2A | 2371 | G |
| 1 | 2A | 2376 | A |
| 1 | 2A | 2383 | G |
| 1 | 2A | 2385 | C |
| 1 | 2A | 2402 | C |
| 1 | 2A | 2403 | C |
| 1 | 2A | 2406 | U |
| 1 | 2A | 2410 | G |
| 1 | 2A | 2425 | A |
| 1 | 2A | 2427 | C |
| 1 | 2A | 2428 | G |
| 1 | 2A | 2429 | G |
| 1 | 2A | 2430 | A |
| 1 | 2A | 2435 | A |
| 1 | 2A | 2439 | A |
| 1 | 2A | 2441 | C |
| 1 | 2A | 2447 | G |
| 1 | 2A | 2448 | A |
| 1 | 2A | 2469 | A |
| 1 | 2A | 2474 | C |
| 1 | 2A | 2476 | A |
| 1 | 2A | 2478 | A |
| 1 | 2A | 2490 | G |
| 1 | 2A | 2491 | U |
| 1 | 2A | 2492 | U |
| 1 | 2A | 2502 | G |
| 1 | 2A | 2504 | U |
| 1 | 2A | 2505 | G |
| 1 | 2A | 2507 | C |
| 1 | 2A | 2518 | A |
| 1 | 2A | 2519 | U |
| 1 | 2A | 2520 | C |
| 1 | 2A | 2525 | G |
| 1 | 2A | 2529 | G |
| 1 | 2A | 2538 | C |
| 1 | 2A | 2554 | U |
| 1 | 2A | 2564 | A |
| 1 | 2A | 2566 | A |
| 1 | 2A | 2567 | G |
| 1 | 2A | 2573 | C |
| 1 | 2A | 2579 | C |

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| Mol | Chain | Res | Type |
|---|---|---|---|
| 1 | 2A | 2582 | G |
| 1 | 2A | 2585 | U |
| 1 | 2A | 2586 | C |
| 1 | 2A | 2601 | C |
| 1 | 2A | 2609 | U |
| 1 | 2A | 2611 | U |
| 1 | 2A | 2612 | C |
| 1 | 2A | 2615 | U |
| 1 | 2A | 2626 | C |
| 1 | 2A | 2629 | A |
| 1 | 2A | 2630 | G |
| 1 | 2A | 2634 | G |
| 1 | 2A | 2646 | C |
| 1 | 2A | 2654 | A |
| 1 | 2A | 2682 | U |
| 1 | 2A | 2689 | U |
| 1 | 2A | 2690 | C |
| 1 | 2A | 2691 | C |
| 1 | 2A | 2702 | U |
| 1 | 2A | 2712(A) | A |
| 1 | 2A | 2713 | A |
| 1 | 2A | 2714 | G |
| 1 | 2A | 2718 | G |
| 1 | 2A | 2726 | U |
| 1 | 2A | 2733 | A |
| 1 | 2A | 2739 | U |
| 1 | 2A | 2748 | A |
| 1 | 2A | 2751 | G |
| 1 | 2A | 2752 | C |
| 1 | 2A | 2757 | A |
| 1 | 2A | 2764 | A |
| 1 | 2A | 2765 | A |
| 1 | 2A | 2778 | A |
| 1 | 2A | 2789 | C |
| 1 | 2A | 2802 | G |
| 1 | 2A | 2807 | G |
| 1 | 2A | 2808 | U |
| 1 | 2A | 2818 | G |
| 1 | 2A | 2820 | A |
| 1 | 2A | 2821 | A |
| 1 | 2A | 2823 | A |
| 1 | 2A | 2833 | G |

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| Mol | Chain | Res | Type |
|---|---|---|---|
| 1 | 2A | 2835 | A |
| 1 | 2A | 2836 | U |
| 1 | 2A | 2872 | G |
| 1 | 2A | 2876 | G |
| 1 | 2A | 2880 | C |
| 1 | 2A | 2894 | G |
| 1 | 2A | 2897 | U |
| 2 | 2B | 2 | C |
| 2 | 2B | 8 | U |
| 2 | 2B | 13 | A |
| 2 | 2B | 16 | G |
| 2 | 2B | 20 | C |
| 2 | 2B | 24 | G |
| 2 | 2B | 30 | C |
| 2 | 2B | 42 | C |
| 2 | 2B | 53 | A |
| 2 | 2B | 63 | G |
| 2 | 2B | 66 | A |
| 2 | 2B | 67 | G |
| 2 | 2B | 72 | G |
| 2 | 2B | 73 | A |
| 2 | 2B | 74 | U |
| 2 | 2B | 75 | G |
| 2 | 2B | 85 | G |
| 2 | 2B | 88 | C |
| 2 | 2B | 89 | G |
| 2 | 2B | 106 | G |
| 2 | 2B | 108 | U |
| 2 | 2B | 110 | G |
| 2 | 2B | 112 | U |
| 2 | 2B | 114 | C |
| 31 | 2a | 9 | G |
| 31 | 2a | 32 | A |
| 31 | 2a | 39 | G |
| 31 | 2a | 47 | C |
| 31 | 2a | 48 | C |
| 31 | 2a | 49 | U |
| 31 | 2a | 50 | A |
| 31 | 2a | 51 | A |
| 31 | 2a | 52 | G |
| 31 | 2a | 54 | C |
| 31 | 2a | 66 | G |

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| Mol | Chain | Res | Type |
|---|---|---|---|
| 31 | 2a | 78 | G |
| 31 | 2a | 89 | C |
| 31 | 2a | 101 | A |
| 31 | 2a | 116 | A |
| 31 | 2a | 121 | C |
| 31 | 2a | 129(A) | G |
| 31 | 2a | 131 | C |
| 31 | 2a | 143 | A |
| 31 | 2a | 163 | C |
| 31 | 2a | 174 | C |
| 31 | 2a | 182 | U |
| 31 | 2a | 189(E) | U |
| 31 | 2a | 195 | A |
| 31 | 2a | 197 | A |
| 31 | 2a | 199 | G |
| 31 | 2a | 202 | U |
| 31 | 2a | 203 | U |
| 31 | 2a | 216 | G |
| 31 | 2a | 220 | G |
| 31 | 2a | 247 | G |
| 31 | 2a | 251 | G |
| 31 | 2a | 266 | G |
| 31 | 2a | 267 | C |
| 31 | 2a | 279 | A |
| 31 | 2a | 289 | G |
| 31 | 2a | 301 | G |
| 31 | 2a | 305 | G |
| 31 | 2a | 321 | A |
| 31 | 2a | 328 | C |
| 31 | 2a | 332 | G |
| 31 | 2a | 351 | G |
| 31 | 2a | 352 | C |
| 31 | 2a | 353 | A |
| 31 | 2a | 354 | G |
| 31 | 2a | 367 | U |
| 31 | 2a | 372 | C |
| 31 | 2a | 373 | A |
| 31 | 2a | 384 | G |
| 31 | 2a | 397 | A |
| 31 | 2a | 398 | C |
| 31 | 2a | 406 | G |
| 31 | 2a | 412 | A |

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| Mol | Chain | Res | Type |
|---|---|---|---|
| 31 | 2a | 421 | U |
| 31 | 2a | 424 | G |
| 31 | 2a | 429 | U |
| 31 | 2a | 439 | A |
| 31 | 2a | 442 | C |
| 31 | 2a | 452 | A |
| 31 | 2a | 454 | C |
| 31 | 2a | 470 | C |
| 31 | 2a | 485 | G |
| 31 | 2a | 496 | A |
| 31 | 2a | 498 | U |
| 31 | 2a | 505 | G |
| 31 | 2a | 507 | C |
| 31 | 2a | 508 | C |
| 31 | 2a | 509 | A |
| 31 | 2a | 510 | A |
| 31 | 2a | 511 | C |
| 31 | 2a | 518 | C |
| 31 | 2a | 527 | 7MG |
| 31 | 2a | 531 | U |
| 31 | 2a | 532 | A |
| 31 | 2a | 535 | A |
| 31 | 2a | 536 | C |
| 31 | 2a | 547 | A |
| 31 | 2a | 559 | A |
| 31 | 2a | 560 | U |
| 31 | 2a | 561 | U |
| 31 | 2a | 564 | C |
| 31 | 2a | 572 | A |
| 31 | 2a | 573 | A |
| 31 | 2a | 576 | G |
| 31 | 2a | 577 | G |
| 31 | 2a | 596 | C |
| 31 | 2a | 618 | C |
| 31 | 2a | 630 | G |
| 31 | 2a | 632 | A |
| 31 | 2a | 641 | U |
| 31 | 2a | 653 | A |
| 31 | 2a | 665 | A |
| 31 | 2a | 686 | U |
| 31 | 2a | 687 | A |
| 31 | 2a | 688 | G |

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| Mol | Chain | Res | Type |
|---|---|---|---|
| 31 | 2a | 731 | G |
| 31 | 2a | 749 | C |
| 31 | 2a | 755 | G |
| 31 | 2a | 777 | A |
| 31 | 2a | 790 | A |
| 31 | 2a | 793 | U |
| 31 | 2a | 794 | A |
| 31 | 2a | 816 | A |
| 31 | 2a | 817 | C |
| 31 | 2a | 821 | G |
| 31 | 2a | 828 | A |
| 31 | 2a | 840 | C |
| 31 | 2a | 841 | U |
| 31 | 2a | 848 | C |
| 31 | 2a | 853 | G |
| 31 | 2a | 859 | A |
| 31 | 2a | 872 | A |
| 31 | 2a | 873 | A |
| 31 | 2a | 889 | A |
| 31 | 2a | 900 | A |
| 31 | 2a | 902 | G |
| 31 | 2a | 914 | A |
| 31 | 2a | 927 | G |
| 31 | 2a | 931 | C |
| 31 | 2a | 932 | C |
| 31 | 2a | 934 | C |
| 31 | 2a | 935 | A |
| 31 | 2a | 960 | U |
| 31 | 2a | 961 | U |
| 31 | 2a | 968 | A |
| 31 | 2a | 969 | A |
| 31 | 2a | 971 | G |
| 31 | 2a | 974 | A |
| 31 | 2a | 975 | A |
| 31 | 2a | 976 | G |
| 31 | 2a | 977 | A |
| 31 | 2a | 992 | U |
| 31 | 2a | 993 | G |
| 31 | 2a | 997 | U |
| 31 | 2a | 1001(A) | G |
| 31 | 2a | 1002 | G |
| 31 | 2a | 1003 | G |

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| Mol | Chain | Res | Type |
|---|---|---|---|
| 31 | 2a | 1004 | A |
| 31 | 2a | 1005 | A |
| 31 | 2a | 1006 | C |
| 31 | 2a | 1007 | C |
| 31 | 2a | 1009 | G |
| 31 | 2a | 1022 | G |
| 31 | 2a | 1023 | G |
| 31 | 2a | 1025 | U |
| 31 | 2a | 1026 | G |
| 31 | 2a | 1027 | C |
| 31 | 2a | 1030 | C |
| 31 | 2a | 1030(A) | G |
| 31 | 2a | 1031 | G |
| 31 | 2a | 1033 | G |
| 31 | 2a | 1036 | G |
| 31 | 2a | 1038 | C |
| 31 | 2a | 1039 | C |
| 31 | 2a | 1040 | U |
| 31 | 2a | 1045 | C |
| 31 | 2a | 1051 | C |
| 31 | 2a | 1053 | G |
| 31 | 2a | 1065 | U |
| 31 | 2a | 1066 | C |
| 31 | 2a | 1068 | G |
| 31 | 2a | 1070 | U |
| 31 | 2a | 1077 | G |
| 31 | 2a | 1081 | G |
| 31 | 2a | 1094 | G |
| 31 | 2a | 1096 | C |
| 31 | 2a | 1098 | C |
| 31 | 2a | 1101 | A |
| 31 | 2a | 1117 | G |
| 31 | 2a | 1122 | U |
| 31 | 2a | 1125 | U |
| 31 | 2a | 1129 | C |
| 31 | 2a | 1137 | C |
| 31 | 2a | 1138 | G |
| 31 | 2a | 1139 | G |
| 31 | 2a | 1140 | C |
| 31 | 2a | 1146 | A |
| 31 | 2a | 1152 | A |
| 31 | 2a | 1159 | U |

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| Mol | Chain | Res | Type |
|---|---|---|---|
| 31 | 2a | 1160 | G |
| 31 | 2a | 1166 | G |
| 31 | 2a | 1172 | C |
| 31 | 2a | 1182 | G |
| 31 | 2a | 1184 | G |
| 31 | 2a | 1196 | U |
| 31 | 2a | 1197 | G |
| 31 | 2a | 1202 | G |
| 31 | 2a | 1211 | U |
| 31 | 2a | 1212 | U |
| 31 | 2a | 1213 | A |
| 31 | 2a | 1215 | G |
| 31 | 2a | 1226 | C |
| 31 | 2a | 1227 | A |
| 31 | 2a | 1236 | A |
| 31 | 2a | 1238 | A |
| 31 | 2a | 1256 | A |
| 31 | 2a | 1257 | U |
| 31 | 2a | 1258 | G |
| 31 | 2a | 1260 | C |
| 31 | 2a | 1263 | C |
| 31 | 2a | 1264 | C |
| 31 | 2a | 1268 | A |
| 31 | 2a | 1270 | C |
| 31 | 2a | 1272 | G |
| 31 | 2a | 1275 | A |
| 31 | 2a | 1279 | A |
| 31 | 2a | 1280 | A |
| 31 | 2a | 1287 | A |
| 31 | 2a | 1303 | C |
| 31 | 2a | 1320 | C |
| 31 | 2a | 1323 | G |
| 31 | 2a | 1331 | G |
| 31 | 2a | 1340 | A |
| 31 | 2a | 1346 | A |
| 31 | 2a | 1347 | G |
| 31 | 2a | 1353 | G |
| 31 | 2a | 1363 | C |
| 31 | 2a | 1364 | U |
| 31 | 2a | 1381 | U |
| 31 | 2a | 1386 | G |
| 31 | 2a | 1398 | A |

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| Mol | Chain | Res | Type |
|---|---|---|---|
| 31 | 2a | 1419 | G |
| 31 | 2a | 1442 | G |
| 31 | 2a | 1442(A) | G |
| 31 | 2a | 1442(B) | A |
| 31 | 2a | 1446 | U |
| 31 | 2a | 1447 | A |
| 31 | 2a | 1452 | C |
| 31 | 2a | 1456 | G |
| 31 | 2a | 1475 | G |
| 31 | 2a | 1487 | G |
| 31 | 2a | 1492 | A |
| 31 | 2a | 1493 | A |
| 31 | 2a | 1494 | G |
| 31 | 2a | 1495 | U |
| 31 | 2a | 1496 | C |
| 31 | 2a | 1503 | A |
| 31 | 2a | 1504 | G |
| 31 | 2a | 1506 | U |
| 31 | 2a | 1517 | G |
| 31 | 2a | 1520 | G |
| 31 | 2a | 1529 | G |
| 31 | 2a | 1530 | G |
| 31 | 2a | 1531 | A |
| 31 | 2a | 1532 | U |
| 54 | 2x | 3 | C |
| 54 | 2x | 4 | C |
| 54 | 2x | 5 | G |
| 54 | 2x | 8 | 4SU |
| 54 | 2x | 19 | G |
| 54 | 2x | 20 | U |
| 54 | 2x | 21 | A |
| 54 | 2x | 22 | G |
| 54 | 2x | 26 | A |
| 54 | 2x | 35 | A |
| 54 | 2x | 36 | A |
| 54 | 2x | 38 | A |
| 54 | 2x | 39 | PSU |
| 54 | 2x | 40 | C |
| 54 | 2x | 41 | C |
| 54 | 2x | 42 | C |
| 54 | 2x | 44 | G |
| 54 | 2x | 45 | U |

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| Mol | Chain | Res | Type |
|---|---|---|---|
| 54 | 2x | 46 | 7MG |
| 54 | 2x | 47 | U |
| 54 | 2x | 48 | C |
| 54 | 2x | 59 | U |
| 54 | 2x | 60 | U |
| 54 | 2x | 65 | G |
| 54 | 2x | 69 | G |
| 54 | 2x | 70 | G |
| 54 | 2x | 71 | G |
| 54 | 2x | 75 | C |
| 54 | 2x | 76 | A |
| 54 | 2y | 2 | C |
| 54 | 2y | 3 | C |
| 54 | 2y | 5 | G |
| 54 | 2y | 9 | A |
| 54 | 2y | 10 | G |
| 54 | 2y | 13 | C |
| 54 | 2y | 14 | A |
| 54 | 2y | 19 | G |
| 54 | 2y | 20 | U |
| 54 | 2y | 21 | A |
| 54 | 2y | 26 | A |
| 54 | 2y | 44 | G |
| 54 | 2y | 45 | U |
| 54 | 2y | 46 | 7MG |
| 54 | 2y | 47 | U |
| 54 | 2y | 48 | C |
| 54 | 2y | 59 | U |
| 54 | 2y | 60 | U |
| 55 | 2z | 13 | A |
| 55 | 2z | 15 | A |
| 55 | 2z | 18 | C |
| 55 | 2z | 19 | U |
| 55 | 2z | 20 | A |
| 55 | 2z | 21 | A |

All (49) RNA pucker outliers are listed below:

| Mol | Chain | Res | Type |
|---|---|---|---|
| 1 | 1A | 195 | A |
| 1 | 1A | 196 | A |
| 1 | 1A | 214 | G |

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| Mol | Chain | Res | Type |
|---|---|---|---|
| 1 | 1A | 266 | G |
| 1 | 1A | 271(K) | U |
| 1 | 1A | 278 | A |
| 1 | 1A | 548 | A |
| 1 | 1A | 764 | A |
| 1 | 1A | 859 | G |
| 1 | 1A | 895 | U |
| 1 | 1A | 960 | A |
| 1 | 1A | 1047 | G |
| 1 | 1A | 1065 | U |
| 1 | 1A | 1067 | A |
| 1 | 1A | 1174 | A |
| 1 | 1A | 1176 | G |
| 1 | 1A | 1210 | A |
| 1 | 1A | 1275 | A |
| 1 | 1A | 1379 | A |
| 1 | 1A | 1442 | G |
| 1 | 1A | 1508 | A |
| 1 | 1A | 1653 | G |
| 1 | 1A | 1992 | G |
| 1 | 1A | 2134 | A |
| 1 | 1A | 2181 | G |
| 1 | 1A | 2183 | C |
| 1 | 1A | 2439 | A |
| 1 | 1A | 2689 | U |
| 1 | 2A | 228 | A |
| 1 | 2A | 266 | G |
| 1 | 2A | 271(M) | G |
| 1 | 2A | 277 | C |
| 1 | 2A | 528 | A |
| 1 | 2A | 752 | A |
| 1 | 2A | 856 | C |
| 1 | 2A | 900 | A |
| 1 | 2A | 1187 | G |
| 1 | 2A | 1210 | A |
| 1 | 2A | 1379 | A |
| 1 | 2A | 1420 | U |
| 1 | 2A | 1442 | G |
| 1 | 2A | 1530 | C |
| 1 | 2A | 1653 | G |
| 1 | 2A | 1911 | PSU |
| 1 | 2A | 1992 | G |

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| Mol | Chain | Res | Type |
|---|---|---|---|
| 1 | 2A | 2119 | A |
| 1 | 2A | 2351 | G |
| 1 | 2A | 2689 | U |
| 1 | 2A | 2756 | U |

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

76 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 | $\#\|Z\| > 2$ |
| 54 | 7MG | 1y | 46 | 54 | 22,26,27 | 1.28 | 4 (18%) | 29,39,42 | 2.60 | 7 (24%) |
| 1 | 5MC | 1A | 1962 | 1 | 18,22,23 | 0.94 | 2 (11%) | 26,32,35 | 1.19 | 3 (11%) |
| 31 | PSU | 1a | 516 | 31,56 | 18,21,22 | 1.35 | 2 (11%) | 22,30,33 | 1.79 | 5 (22%) |
| 1 | PSU | 1A | 1911 | 1 | 18,21,22 | 1.36 | 4 (22%) | 22,30,33 | 1.74 | 4 (18%) |
| 1 | 5MC | 2A | 1942 | 1 | 18,22,23 | 0.94 | 2 (11%) | 26,32,35 | 1.17 | 3 (11%) |
| 1 | 5MU | 2A | 1939 | 1 | 19,22,23 | 1.37 | 5 (26%) | 28,32,35 | 2.19 | 6 (21%) |
| 1 | OMG | 1A | 2251 | 1,56 | 18,26,27 | 1.08 | 1 (5%) | 19,38,41 | 1.18 | 3 (15%) |
| 31 | 4OC | 1a | 1402 | 31 | 20,23,24 | 0.76 | 0 | 26,32,35 | 0.98 | 1 (3%) |
| 54 | 4SU | 1y | 8 | 54 | 18,21,22 | 1.83 | 5 (27%) | 26,30,33 | 2.21 | 5 (19%) |
| 54 | PSU | 1y | 55 | 54 | 18,21,22 | 1.31 | 2 (11%) | 22,30,33 | 1.95 | 3 (13%) |
| 54 | MIA | 2x | 37 | 54 | 18,24,32 | 1.10 | 2 (11%) | 18,35,47 | 1.31 | 2 (11%) |
| 31 | MA6 | 2a | 1518 | 31,56 | 19,26,27 | 0.94 | 1 (5%) | 18,38,41 | 1.80 | 6 (33%) |
| 54 | PSU | 2x | 39 | 54 | 18,21,22 | 1.29 | 2 (11%) | 22,30,33 | 2.08 | 4 (18%) |
| 1 | 5MC | 1A | 1942 | 1 | 18,22,23 | 0.93 | 2 (11%) | 26,32,35 | 1.35 | 4 (15%) |
| 54 | 5MU | 2x | 54 | 54 | 19,22,23 | 1.46 | 5 (26%) | 28,32,35 | 1.94 | 5 (17%) |
| 1 | 2MA | 1A | 2503 | 1,56 | 17,25,26 | 1.10 | 1 (5%) | 17,37,40 | 1.21 | 3 (17%) |
| 1 | 5MC | 2A | 1962 | 1 | 18,22,23 | 0.97 | 1 (5%) | 26,32,35 | 1.11 | 3 (11%) |
| 31 | MA6 | 1a | 1518 | 31 | 19,26,27 | 0.95 | 1 (5%) | 18,38,41 | 1.62 | 4 (22%) |
| 54 | PSU | 2y | 32 | 54 | 18,21,22 | 1.33 | 2 (11%) | 22,30,33 | 1.84 | 4 (18%) |

| Mol | Type | Chain | Res | Link | Bond lengths | | | Bond angles | | |
|---|---|---|---|---|---|---|---|---|---|---|
| | | | | | Counts | RMSZ | $\#\|Z\| > 2$ | Counts | RMSZ | $\#\|Z\| > 2$ |
| 1 | 2MA | 2A | 2503 | 1,56 | 17,25,26 | 1.02 | 1 (5%) | 17,37,40 | 1.04 | 2 (11%) |
| 54 | PSU | 2y | 39 | 54 | 18,21,22 | 1.33 | 2 (11%) | 22,30,33 | 1.81 | 3 (13%) |
| 1 | PSU | 2A | 1911 | 1,56 | 18,21,22 | 1.40 | 3 (16%) | 22,30,33 | 2.02 | 3 (13%) |
| 1 | PSU | 1A | 1917 | 1 | 18,21,22 | 1.40 | 2 (11%) | 22,30,33 | 1.92 | 4 (18%) |
| 31 | M2G | 2a | 966 | 31 | 20,27,28 | 1.48 | 3 (15%) | 22,40,43 | 0.92 | 2 (9%) |
| 1 | 5MU | 1A | 1915 | 1 | 19,22,23 | 1.41 | 5 (26%) | 28,32,35 | 2.11 | 6 (21%) |
| 1 | 2MU | 2A | 2552 | 1 | 19,22,24 | 1.25 | 4 (21%) | 26,31,36 | 1.82 | 5 (19%) |
| 54 | MIA | 1y | 37 | 31,54 | 18,24,32 | 1.10 | 2 (11%) | 18,35,47 | 1.26 | 2 (11%) |
| 1 | 2MU | 1A | 2552 | 1,56 | 19,22,24 | 1.30 | 3 (15%) | 26,31,36 | 1.95 | 3 (11%) |
| 31 | UR3 | 2a | 1498 | 31 | 19,22,23 | 1.03 | 2 (10%) | 26,32,35 | 1.46 | 1 (3%) |
| 31 | MA6 | 2a | 1519 | 31 | 19,26,27 | 1.00 | 1 (5%) | 18,38,41 | 1.70 | 5 (27%) |
| 54 | PSU | 1x | 55 | 54 | 18,21,22 | 1.33 | 2 (11%) | 22,30,33 | 1.95 | 4 (18%) |
| 54 | MIA | 1x | 37 | 54 | 18,24,32 | 1.16 | 2 (11%) | 18,35,47 | 1.34 | 2 (11%) |
| 54 | 7MG | 1x | 46 | 54 | 22,26,27 | 1.28 | 3 (13%) | 29,39,42 | 2.60 | 7 (24%) |
| 42 | 0TD | 1l | 92 | 42 | 7,9,10 | 4.64 | 1 (14%) | 6,11,13 | 4.72 | 2 (33%) |
| 54 | 5MU | 1x | 54 | 54 | 19,22,23 | 1.37 | 5 (26%) | 28,32,35 | 2.23 | 6 (21%) |
| 31 | 5MC | 1a | 1400 | 31 | 18,22,23 | 0.98 | 2 (11%) | 26,32,35 | 1.15 | 2 (7%) |
| 31 | 5MC | 1a | 1404 | 31 | 18,22,23 | 0.98 | 2 (11%) | 26,32,35 | 1.23 | 4 (15%) |
| 54 | PSU | 2x | 55 | 54 | 18,21,22 | 1.34 | 2 (11%) | 22,30,33 | 1.91 | 4 (18%) |
| 31 | 5MC | 1a | 1407 | 31 | 18,22,23 | 0.94 | 1 (5%) | 26,32,35 | 1.00 | 1 (3%) |
| 1 | 5MU | 2A | 1915 | 1,56 | 19,22,23 | 1.53 | 4 (21%) | 28,32,35 | 2.07 | 7 (25%) |
| 54 | 4SU | 2y | 8 | 54 | 18,21,22 | 1.74 | 4 (22%) | 26,30,33 | 2.07 | 4 (15%) |
| 54 | PSU | 1x | 32 | 54,56 | 18,21,22 | 1.38 | 2 (11%) | 22,30,33 | 1.85 | 3 (13%) |
| 54 | PSU | 1x | 39 | 54 | 18,21,22 | 1.42 | 3 (16%) | 22,30,33 | 1.86 | 4 (18%) |
| 31 | PSU | 2a | 516 | 31,56 | 18,21,22 | 1.32 | 2 (11%) | 22,30,33 | 1.82 | 3 (13%) |
| 54 | 7MG | 2x | 46 | 54 | 22,26,27 | 1.29 | 4 (18%) | 29,39,42 | 2.65 | 8 (27%) |
| 54 | PSU | 2y | 55 | 54 | 18,21,22 | 1.32 | 2 (11%) | 22,30,33 | 1.91 | 3 (13%) |
| 31 | 5MC | 2a | 1404 | 31 | 18,22,23 | 0.94 | 2 (11%) | 26,32,35 | 1.12 | 3 (11%) |
| 54 | 4SU | 2x | 8 | 54 | 18,21,22 | 1.65 | 4 (22%) | 26,30,33 | 2.21 | 4 (15%) |
| 42 | 0TD | 2l | 92 | 42 | 7,9,10 | 4.63 | 1 (14%) | 6,11,13 | 1.98 | 2 (33%) |
| 1 | OMC | 1A | 1920 | 1 | 19,22,23 | 0.83 | 0 | 26,31,34 | 1.16 | 3 (11%) |
| 31 | 7MG | 1a | 527 | 31,56 | 22,26,27 | 1.31 | 3 (13%) | 29,39,42 | 2.51 | 8 (27%) |
| 31 | 2MG | 1a | 1207 | 31 | 18,26,27 | 0.89 | 1 (5%) | 16,38,41 | 1.17 | 2 (12%) |
| 1 | PSU | 2A | 2605 | 1,56 | 18,21,22 | 1.37 | 2 (11%) | 22,30,33 | 2.14 | 4 (18%) |
| 54 | 7MG | 2y | 46 | 54 | 22,26,27 | 1.32 | 4 (18%) | 29,39,42 | 2.56 | 7 (24%) |

| Mol | Type | Chain | Res | Link | Bond lengths | | | Bond angles | | |
|---|---|---|---|---|---|---|---|---|---|---|
| | | | | | Counts | RMSZ | $\#\|Z\| > 2$ | Counts | RMSZ | $\#\|Z\| > 2$ |
| 54 | MIA | 2y | 37 | 54 | 18,24,32 | 1.06 | 2 (11%) | 18,35,47 | 1.33 | 2 (11%) |
| 31 | MA6 | 1a | 1519 | 31 | 19,26,27 | 1.05 | 1 (5%) | 18,38,41 | 1.59 | 4 (22%) |
| 1 | 5MU | 1A | 1939 | 1 | 19,22,23 | 1.49 | 5 (26%) | 28,32,35 | 2.11 | 7 (25%) |
| 31 | 5MC | 1a | 967 | 31 | 18,22,23 | 0.97 | 1 (5%) | 26,32,35 | 1.17 | 3 (11%) |
| 31 | 7MG | 2a | 527 | 31 | 22,26,27 | 1.36 | 3 (13%) | 29,39,42 | 2.48 | 7 (24%) |
| 1 | PSU | 2A | 1917 | 1,56 | 18,21,22 | 1.43 | 2 (11%) | 22,30,33 | 1.74 | 4 (18%) |
| 31 | M2G | 1a | 966 | 31 | 20,27,28 | 1.51 | 3 (15%) | 22,40,43 | 0.92 | 2 (9%) |
| 1 | OMG | 2A | 2251 | 1,56 | 18,26,27 | 0.98 | 1 (5%) | 19,38,41 | 0.99 | 2 (10%) |
| 31 | 2MG | 2a | 1207 | 31 | 18,26,27 | 0.88 | 1 (5%) | 16,38,41 | 1.17 | 2 (12%) |
| 31 | 4OC | 2a | 1402 | 31 | 20,23,24 | 0.79 | 0 | 26,32,35 | 1.03 | 1 (3%) |
| 31 | 5MC | 2a | 1407 | 31,56 | 18,22,23 | 0.96 | 1 (5%) | 26,32,35 | 1.05 | 2 (7%) |
| 54 | PSU | 1y | 32 | 54 | 18,21,22 | 1.35 | 2 (11%) | 22,30,33 | 1.72 | 3 (13%) |
| 54 | PSU | 2x | 32 | 54,56 | 18,21,22 | 1.35 | 2 (11%) | 22,30,33 | 1.93 | 4 (18%) |
| 54 | PSU | 1y | 39 | 54 | 18,21,22 | 1.33 | 2 (11%) | 22,30,33 | 1.97 | 4 (18%) |
| 54 | 5MU | 1y | 54 | 54 | 19,22,23 | 1.46 | 5 (26%) | 28,32,35 | 2.10 | 7 (25%) |
| 54 | 5MU | 2y | 54 | 54 | 19,22,23 | 1.44 | 5 (26%) | 28,32,35 | 2.09 | 6 (21%) |
| 31 | UR3 | 1a | 1498 | 31,56 | 19,22,23 | 1.04 | 2 (10%) | 26,32,35 | 1.45 | 3 (11%) |
| 31 | 5MC | 2a | 967 | 31 | 18,22,23 | 0.95 | 2 (11%) | 26,32,35 | 1.15 | 3 (11%) |
| 31 | 5MC | 2a | 1400 | 31 | 18,22,23 | 0.98 | 1 (5%) | 26,32,35 | 1.11 | 3 (11%) |
| 1 | PSU | 1A | 2605 | 1 | 18,21,22 | 1.42 | 2 (11%) | 22,30,33 | 1.96 | 4 (18%) |
| 1 | OMC | 2A | 1920 | 1 | 19,22,23 | 0.80 | 0 | 26,31,34 | 0.81 | 0 |
| 54 | 4SU | 1x | 8 | 54,56 | 18,21,22 | 1.61 | 4 (22%) | 26,30,33 | 2.39 | 8 (30%) |

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 |
|---|---|---|---|---|---|---|---|
| 54 | 7MG | 1y | 46 | 54 | - | 5/7/37/38 | 0/3/3/3 |
| 1 | 5MC | 1A | 1962 | 1 | - | 0/7/25/26 | 0/2/2/2 |
| 31 | PSU | 1a | 516 | 31,56 | - | 0/7/25/26 | 0/2/2/2 |
| 1 | PSU | 1A | 1911 | 1 | - | 0/7/25/26 | 0/2/2/2 |
| 1 | 5MC | 2A | 1942 | 1 | - | 0/7/25/26 | 0/2/2/2 |
| 1 | 5MU | 2A | 1939 | 1 | - | 0/7/25/26 | 0/2/2/2 |
| 1 | OMG | 1A | 2251 | 1,56 | - | 0/5/27/28 | 0/3/3/3 |
| 31 | 4OC | 1a | 1402 | 31 | - | 2/9/29/30 | 0/2/2/2 |

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| Mol | Type | Chain | Res | Link | Chirals | Torsions | Rings |
|---|---|---|---|---|---|---|---|
| 54 | 4SU | 1y | 8 | 54 | - | 0/7/25/26 | 0/2/2/2 |
| 54 | PSU | 1y | 55 | 54 | - | 0/7/25/26 | 0/2/2/2 |
| 54 | MIA | 2x | 37 | 54 | - | 3/3/25/34 | 0/3/3/3 |
| 31 | MA6 | 2a | 1518 | 31,56 | - | 1/7/29/30 | 0/3/3/3 |
| 54 | PSU | 2x | 39 | 54 | - | 2/7/25/26 | 0/2/2/2 |
| 1 | 5MC | 1A | 1942 | 1 | - | 0/7/25/26 | 0/2/2/2 |
| 54 | 5MU | 2x | 54 | 54 | - | 1/7/25/26 | 0/2/2/2 |
| 1 | 2MA | 1A | 2503 | 1,56 | - | 2/3/25/26 | 0/3/3/3 |
| 1 | 5MC | 2A | 1962 | 1 | - | 0/7/25/26 | 0/2/2/2 |
| 31 | MA6 | 1a | 1518 | 31 | - | 3/7/29/30 | 0/3/3/3 |
| 54 | PSU | 2y | 32 | 54 | - | 0/7/25/26 | 0/2/2/2 |
| 1 | 2MA | 2A | 2503 | 1,56 | - | 2/3/25/26 | 0/3/3/3 |
| 54 | PSU | 2y | 39 | 54 | - | 0/7/25/26 | 0/2/2/2 |
| 1 | PSU | 2A | 1911 | 1,56 | - | 1/7/25/26 | 0/2/2/2 |
| 1 | PSU | 1A | 1917 | 1 | - | 0/7/25/26 | 0/2/2/2 |
| 31 | M2G | 2a | 966 | 31 | - | 0/7/29/30 | 0/3/3/3 |
| 1 | 5MU | 1A | 1915 | 1 | - | 2/7/25/26 | 0/2/2/2 |
| 1 | 2MU | 2A | 2552 | 1 | - | 0/9/27/28 | 0/2/2/2 |
| 54 | MIA | 1y | 37 | 31,54 | - | 3/3/25/34 | 0/3/3/3 |
| 1 | 2MU | 1A | 2552 | 1,56 | - | 0/9/27/28 | 0/2/2/2 |
| 31 | UR3 | 2a | 1498 | 31 | - | 0/7/25/26 | 0/2/2/2 |
| 31 | MA6 | 2a | 1519 | 31 | - | 4/7/29/30 | 0/3/3/3 |
| 54 | PSU | 1x | 55 | 54 | - | 1/7/25/26 | 0/2/2/2 |
| 54 | MIA | 1x | 37 | 54 | - | 2/3/25/34 | 0/3/3/3 |
| 54 | 7MG | 1x | 46 | 54 | - | 1/7/37/38 | 0/3/3/3 |
| 42 | 0TD | 1l | 92 | 42 | - | 3/7/12/14 | - |
| 54 | 5MU | 1x | 54 | 54 | - | 2/7/25/26 | 0/2/2/2 |
| 31 | 5MC | 1a | 1400 | 31 | - | 0/7/25/26 | 0/2/2/2 |
| 31 | 5MC | 1a | 1404 | 31 | - | 0/7/25/26 | 0/2/2/2 |
| 54 | PSU | 2x | 55 | 54 | - | 2/7/25/26 | 0/2/2/2 |
| 31 | 5MC | 1a | 1407 | 31 | - | 0/7/25/26 | 0/2/2/2 |
| 1 | 5MU | 2A | 1915 | 1,56 | - | 0/7/25/26 | 0/2/2/2 |
| 54 | 4SU | 2y | 8 | 54 | - | 0/7/25/26 | 0/2/2/2 |
| 54 | PSU | 1x | 32 | 54,56 | - | 2/7/25/26 | 0/2/2/2 |
| 54 | PSU | 1x | 39 | 54 | - | 2/7/25/26 | 0/2/2/2 |
| 31 | PSU | 2a | 516 | 31,56 | - | 0/7/25/26 | 0/2/2/2 |
| 54 | 7MG | 2x | 46 | 54 | - | 1/7/37/38 | 0/3/3/3 |
| 54 | PSU | 2y | 55 | 54 | - | 0/7/25/26 | 0/2/2/2 |
| 31 | 5MC | 2a | 1404 | 31 | - | 0/7/25/26 | 0/2/2/2 |

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| Mol | Type | Chain | Res | Link | Chirals | Torsions | Rings |
|---|---|---|---|---|---|---|---|
| 54 | 4SU | 2x | 8 | 54 | - | 2/7/25/26 | 0/2/2/2 |
| 42 | 0TD | 2l | 92 | 42 | - | 2/7/12/14 | - |
| 1 | OMC | 1A | 1920 | 1 | - | 1/9/27/28 | 0/2/2/2 |
| 31 | 7MG | 1a | 527 | 31,56 | - | 2/7/37/38 | 0/3/3/3 |
| 31 | 2MG | 1a | 1207 | 31 | - | 0/5/27/28 | 0/3/3/3 |
| 1 | PSU | 2A | 2605 | 1,56 | - | 0/7/25/26 | 0/2/2/2 |
| 54 | 7MG | 2y | 46 | 54 | - | 4/7/37/38 | 0/3/3/3 |
| 54 | MIA | 2y | 37 | 54 | - | 3/3/25/34 | 0/3/3/3 |
| 31 | MA6 | 1a | 1519 | 31 | - | 3/7/29/30 | 0/3/3/3 |
| 1 | 5MU | 1A | 1939 | 1 | - | 1/7/25/26 | 0/2/2/2 |
| 31 | 5MC | 1a | 967 | 31 | - | 0/7/25/26 | 0/2/2/2 |
| 31 | 7MG | 2a | 527 | 31 | - | 2/7/37/38 | 0/3/3/3 |
| 1 | PSU | 2A | 1917 | 1,56 | - | 5/7/25/26 | 0/2/2/2 |
| 31 | M2G | 1a | 966 | 31 | - | 0/7/29/30 | 0/3/3/3 |
| 1 | OMG | 2A | 2251 | 1,56 | - | 0/5/27/28 | 0/3/3/3 |
| 31 | 2MG | 2a | 1207 | 31 | - | 1/5/27/28 | 0/3/3/3 |
| 31 | 4OC | 2a | 1402 | 31 | - | 2/9/29/30 | 0/2/2/2 |
| 31 | 5MC | 2a | 1407 | 31,56 | - | 0/7/25/26 | 0/2/2/2 |
| 54 | PSU | 1y | 32 | 54 | - | 0/7/25/26 | 0/2/2/2 |
| 54 | PSU | 2x | 32 | 54,56 | - | 0/7/25/26 | 0/2/2/2 |
| 54 | PSU | 1y | 39 | 54 | - | 0/7/25/26 | 0/2/2/2 |
| 54 | 5MU | 1y | 54 | 54 | - | 0/7/25/26 | 0/2/2/2 |
| 54 | 5MU | 2y | 54 | 54 | - | 0/7/25/26 | 0/2/2/2 |
| 31 | UR3 | 1a | 1498 | 31,56 | - | 0/7/25/26 | 0/2/2/2 |
| 31 | 5MC | 2a | 967 | 31 | - | 1/7/25/26 | 0/2/2/2 |
| 31 | 5MC | 2a | 1400 | 31 | - | 4/7/25/26 | 0/2/2/2 |
| 1 | PSU | 1A | 2605 | 1 | - | 0/7/25/26 | 0/2/2/2 |
| 1 | OMC | 2A | 1920 | 1 | - | 0/9/27/28 | 0/2/2/2 |
| 54 | 4SU | 1x | 8 | 54,56 | - | 4/7/25/26 | 0/2/2/2 |

All (177) bond length outliers are listed below:

| Mol | Chain | Res | Type | Atoms | Z | Observed(Å) | Ideal(Å) |
|---|---|---|---|---|---|---|---|
| 42 | 1l | 92 | 0TD | CB-SB | -11.95 | 1.70 | 1.82 |
| 42 | 2l | 92 | 0TD | CB-SB | -11.94 | 1.70 | 1.82 |
| 31 | 1a | 966 | M2G | C2-N3 | 4.83 | 1.36 | 1.30 |
| 31 | 2a | 966 | M2G | C2-N3 | 4.74 | 1.36 | 1.30 |
| 54 | 1y | 8 | 4SU | C4-S4 | -4.64 | 1.59 | 1.68 |
| 54 | 2y | 8 | 4SU | C4-S4 | -4.49 | 1.59 | 1.68 |
| 54 | 2x | 8 | 4SU | C4-S4 | -4.29 | 1.60 | 1.68 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(Å) | Ideal(Å) |
|---|---|---|---|---|---|---|---|
| 54 | 1x | 8 | 4SU | C4-S4 | -3.84 | 1.61 | 1.68 |
| 1 | 1A | 2605 | PSU | C6-C5 | 3.67 | 1.39 | 1.35 |
| 31 | 2a | 527 | 7MG | C4-N9 | -3.66 | 1.33 | 1.37 |
| 54 | 2y | 32 | PSU | C6-C5 | 3.63 | 1.39 | 1.35 |
| 54 | 2x | 55 | PSU | C6-C5 | 3.60 | 1.39 | 1.35 |
| 54 | 1y | 8 | 4SU | C4-N3 | -3.56 | 1.33 | 1.37 |
| 54 | 1y | 32 | PSU | C6-C5 | 3.55 | 1.39 | 1.35 |
| 1 | 2A | 1917 | PSU | C6-C5 | 3.45 | 1.39 | 1.35 |
| 54 | 1x | 32 | PSU | C6-C5 | 3.45 | 1.39 | 1.35 |
| 54 | 1x | 39 | PSU | C6-C5 | 3.42 | 1.39 | 1.35 |
| 54 | 1x | 55 | PSU | C6-C5 | 3.40 | 1.39 | 1.35 |
| 54 | 1x | 46 | 7MG | C4-N9 | -3.39 | 1.33 | 1.37 |
| 54 | 2y | 39 | PSU | C6-C5 | 3.39 | 1.39 | 1.35 |
| 54 | 2y | 8 | 4SU | C4-N3 | -3.38 | 1.34 | 1.37 |
| 31 | 1a | 516 | PSU | C6-C5 | 3.36 | 1.39 | 1.35 |
| 1 | 1A | 1917 | PSU | C6-C5 | 3.33 | 1.39 | 1.35 |
| 1 | 2A | 1911 | PSU | C6-C5 | 3.29 | 1.39 | 1.35 |
| 54 | 1y | 39 | PSU | C6-C5 | 3.25 | 1.39 | 1.35 |
| 1 | 1A | 2251 | OMG | C6-N1 | -3.23 | 1.33 | 1.37 |
| 54 | 2x | 32 | PSU | C6-C5 | 3.22 | 1.39 | 1.35 |
| 54 | 2y | 55 | PSU | C6-C5 | 3.21 | 1.39 | 1.35 |
| 54 | 1y | 55 | PSU | C6-C5 | 3.13 | 1.39 | 1.35 |
| 1 | 2A | 2605 | PSU | C4-N3 | -3.12 | 1.33 | 1.38 |
| 1 | 2A | 1915 | 5MU | C2-N1 | 3.11 | 1.43 | 1.38 |
| 54 | 2x | 39 | PSU | C6-C5 | 3.10 | 1.38 | 1.35 |
| 54 | 2x | 46 | 7MG | C4-N9 | -3.06 | 1.34 | 1.37 |
| 31 | 2a | 1400 | 5MC | C6-C5 | 3.05 | 1.39 | 1.34 |
| 54 | 1y | 46 | 7MG | C5-C4 | 3.04 | 1.48 | 1.38 |
| 31 | 2a | 516 | PSU | C6-C5 | 3.02 | 1.38 | 1.35 |
| 54 | 2y | 46 | 7MG | C5-C4 | 3.02 | 1.48 | 1.38 |
| 1 | 1A | 1911 | PSU | C6-C5 | 3.02 | 1.38 | 1.35 |
| 1 | 1A | 1939 | 5MU | C6-C5 | 3.01 | 1.39 | 1.34 |
| 31 | 1a | 527 | 7MG | C4-N9 | -2.98 | 1.34 | 1.37 |
| 1 | 2A | 1915 | 5MU | C6-C5 | 2.97 | 1.39 | 1.34 |
| 31 | 2a | 1407 | 5MC | C6-C5 | 2.96 | 1.39 | 1.34 |
| 1 | 2A | 1962 | 5MC | C6-C5 | 2.95 | 1.39 | 1.34 |
| 31 | 1a | 966 | M2G | C2-N2 | 2.92 | 1.40 | 1.35 |
| 31 | 1a | 527 | 7MG | C5-C4 | 2.91 | 1.47 | 1.38 |
| 54 | 2x | 46 | 7MG | C5-C4 | 2.91 | 1.47 | 1.38 |
| 1 | 1A | 2552 | 2MU | C4-N3 | -2.87 | 1.33 | 1.38 |
| 31 | 2a | 527 | 7MG | C5-C4 | 2.86 | 1.47 | 1.38 |
| 54 | 2x | 54 | 5MU | C6-C5 | 2.84 | 1.39 | 1.34 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(Å) | Ideal(Å) |
|---|---|---|---|---|---|---|---|
| 54 | 1x | 46 | 7MG | C5-C4 | 2.83 | 1.47 | 1.38 |
| 1 | 1A | 1915 | 5MU | C6-C5 | 2.83 | 1.39 | 1.34 |
| 54 | 2x | 8 | 4SU | C4-N3 | -2.83 | 1.34 | 1.37 |
| 54 | 1x | 37 | MIA | C2-N3 | 2.82 | 1.36 | 1.32 |
| 1 | 2A | 1939 | 5MU | C6-C5 | 2.81 | 1.39 | 1.34 |
| 31 | 1a | 967 | 5MC | C6-C5 | 2.81 | 1.39 | 1.34 |
| 54 | 1y | 54 | 5MU | C6-C5 | 2.80 | 1.39 | 1.34 |
| 54 | 2y | 54 | 5MU | C6-C5 | 2.80 | 1.39 | 1.34 |
| 1 | 1A | 1939 | 5MU | C4-N3 | -2.79 | 1.33 | 1.38 |
| 31 | 1a | 1400 | 5MC | C6-C5 | 2.78 | 1.39 | 1.34 |
| 54 | 1x | 54 | 5MU | C6-C5 | 2.77 | 1.39 | 1.34 |
| 31 | 2a | 966 | M2G | C2-N2 | 2.76 | 1.40 | 1.35 |
| 31 | 2a | 1519 | MA6 | C5-C4 | 2.75 | 1.48 | 1.40 |
| 54 | 1y | 54 | 5MU | C2-N1 | 2.74 | 1.42 | 1.38 |
| 54 | 1x | 37 | MIA | C5-C4 | 2.73 | 1.48 | 1.40 |
| 54 | 1x | 8 | 4SU | C2-N1 | 2.72 | 1.42 | 1.38 |
| 31 | 1a | 1404 | 5MC | C6-C5 | 2.72 | 1.39 | 1.34 |
| 1 | 1A | 1911 | PSU | C4-N3 | -2.71 | 1.33 | 1.38 |
| 1 | 2A | 1911 | PSU | C4-N3 | -2.69 | 1.33 | 1.38 |
| 54 | 1y | 8 | 4SU | C5-C4 | -2.69 | 1.39 | 1.42 |
| 31 | 1a | 1407 | 5MC | C6-C5 | 2.67 | 1.39 | 1.34 |
| 1 | 1A | 1915 | 5MU | C4-N3 | -2.67 | 1.33 | 1.38 |
| 54 | 2x | 37 | MIA | C5-C4 | 2.66 | 1.48 | 1.40 |
| 54 | 2y | 46 | 7MG | C4-N9 | -2.66 | 1.34 | 1.37 |
| 54 | 2y | 54 | 5MU | C2-N1 | 2.66 | 1.42 | 1.38 |
| 1 | 1A | 1917 | PSU | C4-N3 | -2.65 | 1.33 | 1.38 |
| 54 | 1x | 55 | PSU | C4-N3 | -2.65 | 1.33 | 1.38 |
| 31 | 1a | 1519 | MA6 | C5-C4 | 2.64 | 1.47 | 1.40 |
| 1 | 2A | 1915 | 5MU | C4-C5 | 2.64 | 1.49 | 1.44 |
| 1 | 2A | 2251 | OMG | C6-N1 | -2.64 | 1.33 | 1.37 |
| 1 | 2A | 1939 | 5MU | C4-N3 | -2.64 | 1.33 | 1.38 |
| 54 | 1x | 8 | 4SU | C4-N3 | -2.63 | 1.34 | 1.37 |
| 31 | 2a | 967 | 5MC | C6-C5 | 2.63 | 1.38 | 1.34 |
| 54 | 1y | 37 | MIA | C5-C4 | 2.63 | 1.47 | 1.40 |
| 1 | 2A | 1917 | PSU | C4-N3 | -2.63 | 1.34 | 1.38 |
| 54 | 2x | 54 | 5MU | C4-N3 | -2.63 | 1.34 | 1.38 |
| 1 | 1A | 2552 | 2MU | C5-C4 | 2.61 | 1.49 | 1.43 |
| 54 | 2x | 39 | PSU | C4-N3 | -2.61 | 1.34 | 1.38 |
| 54 | 1y | 39 | PSU | C4-N3 | -2.60 | 1.34 | 1.38 |
| 54 | 2x | 54 | 5MU | C2-N1 | 2.60 | 1.42 | 1.38 |
| 1 | 2A | 2605 | PSU | C6-C5 | 2.59 | 1.38 | 1.35 |
| 31 | 2a | 516 | PSU | C4-N3 | -2.59 | 1.34 | 1.38 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(Å) | Ideal(Å) |
|---|---|---|---|---|---|---|---|
| 54 | 2y | 55 | PSU | C4-N3 | -2.57 | 1.34 | 1.38 |
| 54 | 1x | 39 | PSU | C4-N3 | -2.56 | 1.34 | 1.38 |
| 54 | 1y | 37 | MIA | C2-N3 | 2.56 | 1.36 | 1.32 |
| 54 | 2x | 32 | PSU | C4-N3 | -2.56 | 1.34 | 1.38 |
| 54 | 2x | 37 | MIA | C2-N3 | 2.55 | 1.36 | 1.32 |
| 54 | 2y | 37 | MIA | C5-C4 | 2.55 | 1.47 | 1.40 |
| 1 | 2A | 1915 | 5MU | C4-N3 | -2.54 | 1.34 | 1.38 |
| 54 | 1y | 54 | 5MU | C4-N3 | -2.53 | 1.34 | 1.38 |
| 31 | 2a | 966 | M2G | C6-N1 | -2.53 | 1.34 | 1.37 |
| 54 | 1y | 54 | 5MU | C4-C5 | 2.53 | 1.49 | 1.44 |
| 54 | 1x | 32 | PSU | C4-N3 | -2.52 | 1.34 | 1.38 |
| 1 | 2A | 2552 | 2MU | C4-N3 | -2.52 | 1.34 | 1.38 |
| 1 | 2A | 1942 | 5MC | C6-C5 | 2.52 | 1.38 | 1.34 |
| 1 | 1A | 2605 | PSU | C4-N3 | -2.51 | 1.34 | 1.38 |
| 54 | 1x | 54 | 5MU | C4-N3 | -2.51 | 1.34 | 1.38 |
| 54 | 1y | 55 | PSU | C4-N3 | -2.51 | 1.34 | 1.38 |
| 31 | 2a | 1518 | MA6 | C5-C4 | 2.50 | 1.47 | 1.40 |
| 1 | 2A | 1939 | 5MU | C6-N1 | -2.49 | 1.33 | 1.38 |
| 54 | 2y | 54 | 5MU | C4-C5 | 2.48 | 1.48 | 1.44 |
| 54 | 2y | 37 | MIA | C2-N3 | 2.48 | 1.36 | 1.32 |
| 54 | 1y | 46 | 7MG | C4-N9 | -2.48 | 1.34 | 1.37 |
| 1 | 1A | 1962 | 5MC | C6-C5 | 2.47 | 1.38 | 1.34 |
| 31 | 1a | 1518 | MA6 | C5-C4 | 2.46 | 1.47 | 1.40 |
| 31 | 2a | 1404 | 5MC | C6-C5 | 2.44 | 1.38 | 1.34 |
| 54 | 1x | 8 | 4SU | C5-C4 | -2.43 | 1.39 | 1.42 |
| 31 | 1a | 516 | PSU | C4-N3 | -2.43 | 1.34 | 1.38 |
| 54 | 2x | 55 | PSU | C4-N3 | -2.43 | 1.34 | 1.38 |
| 1 | 2A | 1939 | 5MU | C4-C5 | 2.43 | 1.48 | 1.44 |
| 54 | 2y | 39 | PSU | C4-N3 | -2.42 | 1.34 | 1.38 |
| 54 | 2y | 8 | 4SU | C5-C4 | -2.41 | 1.39 | 1.42 |
| 1 | 1A | 1942 | 5MC | C6-N1 | -2.40 | 1.33 | 1.38 |
| 54 | 2y | 54 | 5MU | C4-N3 | -2.39 | 1.34 | 1.38 |
| 1 | 2A | 1942 | 5MC | C6-N1 | -2.39 | 1.34 | 1.38 |
| 1 | 1A | 1939 | 5MU | C2-N1 | 2.38 | 1.42 | 1.38 |
| 31 | 1a | 1207 | 2MG | C6-N1 | -2.38 | 1.34 | 1.37 |
| 31 | 1a | 966 | M2G | C6-N1 | -2.37 | 1.34 | 1.37 |
| 1 | 1A | 1942 | 5MC | C6-C5 | 2.36 | 1.38 | 1.34 |
| 54 | 1x | 54 | 5MU | C4-C5 | 2.35 | 1.48 | 1.44 |
| 54 | 1y | 32 | PSU | C4-N3 | -2.34 | 1.34 | 1.38 |
| 54 | 2y | 32 | PSU | C4-N3 | -2.34 | 1.34 | 1.38 |
| 31 | 1a | 1400 | 5MC | C6-N1 | -2.34 | 1.34 | 1.38 |
| 1 | 1A | 2503 | 2MA | C2-N3 | 2.34 | 1.36 | 1.31 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(Å) | Ideal(Å) |
|---|---|---|---|---|---|---|---|
| 54 | 2x | 54 | 5MU | C4-C5 | 2.32 | 1.48 | 1.44 |
| 31 | 1a | 1404 | 5MC | C6-N1 | -2.32 | 1.34 | 1.38 |
| 1 | 1A | 1915 | 5MU | C4-C5 | 2.30 | 1.48 | 1.44 |
| 31 | 2a | 967 | 5MC | C6-N1 | -2.30 | 1.34 | 1.38 |
| 31 | 2a | 1207 | 2MG | C6-N1 | -2.30 | 1.34 | 1.37 |
| 54 | 2x | 8 | 4SU | C5-C4 | -2.30 | 1.39 | 1.42 |
| 54 | 1x | 54 | 5MU | C2-N1 | 2.28 | 1.42 | 1.38 |
| 31 | 1a | 527 | 7MG | C6-N1 | -2.28 | 1.34 | 1.38 |
| 54 | 1y | 8 | 4SU | C2-N3 | -2.27 | 1.33 | 1.38 |
| 54 | 2y | 46 | 7MG | C6-N1 | -2.25 | 1.34 | 1.38 |
| 54 | 1x | 54 | 5MU | C6-N1 | -2.25 | 1.34 | 1.38 |
| 54 | 2x | 8 | 4SU | C2-N1 | 2.24 | 1.42 | 1.38 |
| 54 | 2y | 8 | 4SU | C2-N3 | -2.23 | 1.34 | 1.38 |
| 1 | 1A | 1939 | 5MU | C4-C5 | 2.23 | 1.48 | 1.44 |
| 31 | 2a | 527 | 7MG | C6-N1 | -2.23 | 1.34 | 1.38 |
| 1 | 2A | 2552 | 2MU | C2-N3 | -2.19 | 1.34 | 1.38 |
| 1 | 1A | 1915 | 5MU | C6-N1 | -2.18 | 1.34 | 1.38 |
| 54 | 1y | 54 | 5MU | C6-N1 | -2.18 | 1.34 | 1.38 |
| 31 | 2a | 1404 | 5MC | C6-N1 | -2.18 | 1.34 | 1.38 |
| 54 | 2y | 46 | 7MG | C8-N9 | 2.17 | 1.47 | 1.46 |
| 54 | 1y | 8 | 4SU | C2-N1 | 2.17 | 1.41 | 1.38 |
| 1 | 2A | 1939 | 5MU | C2-N3 | -2.16 | 1.34 | 1.38 |
| 1 | 2A | 2552 | 2MU | C5-C4 | 2.15 | 1.48 | 1.43 |
| 54 | 2y | 54 | 5MU | C6-N1 | -2.14 | 1.34 | 1.38 |
| 31 | 1a | 1498 | UR3 | C6-C5 | 2.14 | 1.40 | 1.35 |
| 31 | 2a | 1498 | UR3 | C2-N1 | 2.12 | 1.41 | 1.38 |
| 31 | 1a | 1498 | UR3 | C2-N1 | 2.11 | 1.41 | 1.38 |
| 1 | 2A | 2552 | 2MU | C2-N1 | 2.09 | 1.41 | 1.38 |
| 1 | 1A | 1915 | 5MU | C2-N3 | -2.08 | 1.34 | 1.38 |
| 54 | 2x | 46 | 7MG | C6-N1 | -2.08 | 1.35 | 1.38 |
| 1 | 2A | 1911 | PSU | C2-N1 | -2.07 | 1.33 | 1.36 |
| 54 | 1y | 46 | 7MG | C6-N1 | -2.07 | 1.35 | 1.38 |
| 1 | 1A | 1911 | PSU | C2-N1 | -2.06 | 1.33 | 1.36 |
| 54 | 2x | 54 | 5MU | C6-N1 | -2.06 | 1.34 | 1.38 |
| 1 | 1A | 1911 | PSU | C2-N3 | -2.06 | 1.34 | 1.37 |
| 54 | 1x | 46 | 7MG | C5-C6 | 2.05 | 1.48 | 1.43 |
| 54 | 1x | 39 | PSU | C4-C5 | 2.04 | 1.50 | 1.44 |
| 1 | 1A | 2552 | 2MU | C6-C5 | 2.03 | 1.39 | 1.35 |
| 31 | 2a | 1498 | UR3 | C6-C5 | 2.03 | 1.39 | 1.35 |
| 1 | 1A | 1939 | 5MU | C6-N1 | -2.02 | 1.34 | 1.38 |
| 1 | 2A | 2503 | 2MA | C2-N3 | 2.02 | 1.35 | 1.31 |
| 1 | 1A | 1962 | 5MC | C6-N1 | -2.01 | 1.34 | 1.38 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(Å) | Ideal(Å) |
|---|---|---|---|---|---|---|---|
| 54 | 2x | 46 | 7MG | C5-C6 | 2.01 | 1.48 | 1.43 |
| 54 | 1y | 46 | 7MG | C5-C6 | 2.01 | 1.48 | 1.43 |

All (289) bond angle outliers are listed below:

| Mol | Chain | Res | Type | Atoms | Z | Observed($^o$) | Ideal($^o$) |
|---|---|---|---|---|---|---|---|
| 42 | 1l | 92 | 0TD | CSB-SB-CB | -11.03 | 82.48 | 102.44 |
| 54 | 1y | 46 | 7MG | N9-C4-N3 | 9.13 | 139.12 | 125.47 |
| 54 | 2y | 46 | 7MG | N9-C4-N3 | 9.06 | 139.03 | 125.47 |
| 54 | 2x | 46 | 7MG | N9-C4-N3 | 8.86 | 138.72 | 125.47 |
| 31 | 1a | 527 | 7MG | N9-C4-N3 | 8.71 | 138.50 | 125.47 |
| 31 | 2a | 527 | 7MG | N9-C4-N3 | 8.47 | 138.13 | 125.47 |
| 54 | 1x | 46 | 7MG | N9-C4-N3 | 8.36 | 137.97 | 125.47 |
| 54 | 2x | 8 | 4SU | C4-N3-C2 | -6.94 | 120.60 | 127.34 |
| 54 | 1y | 8 | 4SU | C4-N3-C2 | -6.76 | 120.77 | 127.34 |
| 1 | 2A | 2605 | PSU | N1-C2-N3 | 6.69 | 122.71 | 115.13 |
| 1 | 1A | 2552 | 2MU | N3-C2-N1 | 6.49 | 123.50 | 114.89 |
| 1 | 2A | 1911 | PSU | N1-C2-N3 | 6.44 | 122.43 | 115.13 |
| 54 | 2y | 8 | 4SU | C4-N3-C2 | -6.40 | 121.12 | 127.34 |
| 54 | 1y | 39 | PSU | N1-C2-N3 | 6.29 | 122.26 | 115.13 |
| 54 | 1x | 8 | 4SU | C1'-N1-C2 | 6.23 | 128.85 | 117.57 |
| 54 | 1y | 8 | 4SU | C5-C4-N3 | 6.21 | 120.44 | 114.69 |
| 54 | 1x | 46 | 7MG | N9-C8-N7 | -6.12 | 94.63 | 103.38 |
| 54 | 2x | 32 | PSU | N1-C2-N3 | 6.06 | 122.00 | 115.13 |
| 31 | 2a | 1498 | UR3 | C4-N3-C2 | -6.02 | 118.89 | 124.56 |
| 54 | 1x | 55 | PSU | N1-C2-N3 | 6.02 | 121.95 | 115.13 |
| 54 | 1y | 55 | PSU | N1-C2-N3 | 5.98 | 121.91 | 115.13 |
| 1 | 1A | 1917 | PSU | N1-C2-N3 | 5.98 | 121.91 | 115.13 |
| 54 | 2x | 39 | PSU | N1-C2-N3 | 5.95 | 121.87 | 115.13 |
| 54 | 2y | 55 | PSU | N1-C2-N3 | 5.95 | 121.87 | 115.13 |
| 54 | 1x | 39 | PSU | N1-C2-N3 | 5.86 | 121.77 | 115.13 |
| 54 | 2y | 8 | 4SU | C5-C4-N3 | 5.83 | 120.10 | 114.69 |
| 31 | 1a | 1498 | UR3 | C4-N3-C2 | -5.83 | 119.07 | 124.56 |
| 54 | 2x | 55 | PSU | N1-C2-N3 | 5.81 | 121.72 | 115.13 |
| 54 | 2x | 8 | 4SU | C5-C4-N3 | 5.80 | 120.07 | 114.69 |
| 54 | 1x | 32 | PSU | N1-C2-N3 | 5.76 | 121.65 | 115.13 |
| 31 | 2a | 516 | PSU | N1-C2-N3 | 5.71 | 121.60 | 115.13 |
| 54 | 2y | 39 | PSU | N1-C2-N3 | 5.68 | 121.57 | 115.13 |
| 54 | 1y | 46 | 7MG | C5-C4-N3 | -5.66 | 117.34 | 128.13 |
| 54 | 2x | 46 | 7MG | C5-C4-N3 | -5.65 | 117.36 | 128.13 |
| 54 | 1x | 54 | 5MU | C4-N3-C2 | -5.64 | 120.05 | 127.35 |
| 1 | 1A | 2605 | PSU | N1-C2-N3 | 5.62 | 121.50 | 115.13 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed($^o$) | Ideal($^o$) |
|---|---|---|---|---|---|---|---|
| 54 | 1x | 8 | 4SU | C4-N3-C2 | -5.61 | 121.89 | 127.34 |
| 1 | 2A | 1917 | PSU | N1-C2-N3 | 5.58 | 121.45 | 115.13 |
| 54 | 2y | 32 | PSU | N1-C2-N3 | 5.54 | 121.40 | 115.13 |
| 31 | 2a | 527 | 7MG | N9-C8-N7 | -5.50 | 95.52 | 103.38 |
| 1 | 2A | 1939 | 5MU | C4-N3-C2 | -5.48 | 120.26 | 127.35 |
| 54 | 1x | 54 | 5MU | N3-C2-N1 | 5.44 | 122.11 | 114.89 |
| 54 | 2x | 46 | 7MG | N9-C8-N7 | -5.37 | 95.70 | 103.38 |
| 54 | 2y | 46 | 7MG | C5-C4-N3 | -5.37 | 117.90 | 128.13 |
| 54 | 1y | 32 | PSU | N1-C2-N3 | 5.36 | 121.20 | 115.13 |
| 1 | 1A | 1915 | 5MU | C4-N3-C2 | -5.33 | 120.44 | 127.35 |
| 54 | 1x | 46 | 7MG | C5-C4-N3 | -5.33 | 117.97 | 128.13 |
| 31 | 1a | 527 | 7MG | C5-C4-N3 | -5.30 | 118.03 | 128.13 |
| 1 | 2A | 1939 | 5MU | N3-C2-N1 | 5.23 | 121.83 | 114.89 |
| 54 | 2y | 46 | 7MG | N9-C8-N7 | -5.22 | 95.91 | 103.38 |
| 54 | 2y | 54 | 5MU | C4-N3-C2 | -5.20 | 120.62 | 127.35 |
| 31 | 1a | 516 | PSU | N1-C2-N3 | 5.17 | 120.99 | 115.13 |
| 54 | 1y | 54 | 5MU | C4-N3-C2 | -5.16 | 120.67 | 127.35 |
| 31 | 1a | 527 | 7MG | N9-C8-N7 | -5.14 | 96.03 | 103.38 |
| 54 | 1y | 46 | 7MG | N9-C8-N7 | -5.14 | 96.03 | 103.38 |
| 31 | 2a | 527 | 7MG | C5-C4-N3 | -5.08 | 118.44 | 128.13 |
| 1 | 2A | 1915 | 5MU | C4-N3-C2 | -5.06 | 120.80 | 127.35 |
| 1 | 1A | 1911 | PSU | N1-C2-N3 | 5.06 | 120.86 | 115.13 |
| 1 | 2A | 1915 | 5MU | N3-C2-N1 | 5.03 | 121.56 | 114.89 |
| 1 | 1A | 1939 | 5MU | C4-N3-C2 | -5.03 | 120.84 | 127.35 |
| 54 | 1y | 54 | 5MU | N3-C2-N1 | 4.98 | 121.51 | 114.89 |
| 1 | 1A | 1939 | 5MU | C5-C6-N1 | -4.98 | 118.21 | 123.34 |
| 1 | 1A | 1915 | 5MU | N3-C2-N1 | 4.95 | 121.46 | 114.89 |
| 1 | 1A | 1939 | 5MU | N3-C2-N1 | 4.94 | 121.45 | 114.89 |
| 54 | 2y | 54 | 5MU | N3-C2-N1 | 4.94 | 121.44 | 114.89 |
| 1 | 1A | 1915 | 5MU | C5-C4-N3 | 4.89 | 119.48 | 115.31 |
| 54 | 2x | 54 | 5MU | N3-C2-N1 | 4.73 | 121.17 | 114.89 |
| 54 | 2x | 54 | 5MU | C4-N3-C2 | -4.72 | 121.23 | 127.35 |
| 1 | 2A | 2552 | 2MU | N3-C2-N1 | 4.67 | 121.09 | 114.89 |
| 1 | 2A | 2605 | PSU | C4-N3-C2 | -4.59 | 119.73 | 126.34 |
| 54 | 2x | 46 | 7MG | C2-N3-C4 | 4.58 | 120.45 | 112.30 |
| 1 | 1A | 2552 | 2MU | C4-N3-C2 | -4.55 | 120.57 | 126.58 |
| 54 | 1x | 8 | 4SU | C5-C4-N3 | 4.51 | 118.87 | 114.69 |
| 54 | 1y | 46 | 7MG | C2-N3-C4 | 4.50 | 120.31 | 112.30 |
| 54 | 1y | 54 | 5MU | C5-C4-N3 | 4.45 | 119.11 | 115.31 |
| 1 | 2A | 2552 | 2MU | C4-N3-C2 | -4.44 | 120.73 | 126.58 |
| 54 | 2y | 54 | 5MU | C5-C4-N3 | 4.41 | 119.08 | 115.31 |
| 1 | 2A | 1915 | 5MU | C5-C4-N3 | 4.38 | 119.05 | 115.31 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed($^o$) | Ideal($^o$) |
|---|---|---|---|---|---|---|---|
| 1 | 2A | 1939 | 5MU | C5-C4-N3 | 4.34 | 119.01 | 115.31 |
| 1 | 2A | 1939 | 5MU | C5-C6-N1 | -4.29 | 118.92 | 123.34 |
| 31 | 1a | 527 | 7MG | C2-N3-C4 | 4.27 | 119.91 | 112.30 |
| 54 | 1x | 54 | 5MU | C5-C4-N3 | 4.27 | 118.95 | 115.31 |
| 54 | 2y | 46 | 7MG | C2-N3-C4 | 4.24 | 119.84 | 112.30 |
| 54 | 1x | 46 | 7MG | C2-N3-C4 | 4.23 | 119.83 | 112.30 |
| 54 | 1x | 54 | 5MU | O4-C4-C5 | -4.19 | 120.05 | 124.90 |
| 54 | 1y | 39 | PSU | C4-N3-C2 | -4.17 | 120.33 | 126.34 |
| 54 | 1x | 55 | PSU | C4-N3-C2 | -4.15 | 120.35 | 126.34 |
| 1 | 2A | 1911 | PSU | O2-C2-N1 | -4.11 | 118.27 | 122.79 |
| 31 | 2a | 527 | 7MG | C2-N3-C4 | 4.11 | 119.61 | 112.30 |
| 54 | 1x | 8 | 4SU | N3-C2-N1 | 4.10 | 120.33 | 114.89 |
| 54 | 2x | 8 | 4SU | N3-C2-N1 | 4.06 | 120.28 | 114.89 |
| 1 | 1A | 1917 | PSU | C4-N3-C2 | -4.06 | 120.48 | 126.34 |
| 1 | 2A | 1911 | PSU | C4-N3-C2 | -4.03 | 120.53 | 126.34 |
| 1 | 1A | 1915 | 5MU | O4-C4-C5 | -4.03 | 120.23 | 124.90 |
| 54 | 2x | 54 | 5MU | C5-C4-N3 | 4.02 | 118.74 | 115.31 |
| 1 | 2A | 2605 | PSU | O2-C2-N1 | -4.00 | 118.39 | 122.79 |
| 31 | 1a | 1400 | 5MC | C5-C6-N1 | -3.98 | 119.24 | 123.34 |
| 1 | 1A | 2605 | PSU | C4-N3-C2 | -3.97 | 120.62 | 126.34 |
| 54 | 1y | 55 | PSU | O2-C2-N1 | -3.97 | 118.42 | 122.79 |
| 54 | 2x | 39 | PSU | C4-N3-C2 | -3.95 | 120.64 | 126.34 |
| 54 | 2y | 54 | 5MU | O4-C4-C5 | -3.94 | 120.34 | 124.90 |
| 54 | 2y | 55 | PSU | C4-N3-C2 | -3.92 | 120.69 | 126.34 |
| 1 | 2A | 1939 | 5MU | O2-C2-N1 | -3.90 | 117.60 | 122.79 |
| 54 | 2x | 55 | PSU | C4-N3-C2 | -3.89 | 120.74 | 126.34 |
| 54 | 1y | 55 | PSU | C4-N3-C2 | -3.88 | 120.74 | 126.34 |
| 54 | 2y | 8 | 4SU | N3-C2-N1 | 3.85 | 120.00 | 114.89 |
| 54 | 2x | 32 | PSU | C4-N3-C2 | -3.84 | 120.81 | 126.34 |
| 1 | 1A | 1915 | 5MU | C5-C6-N1 | -3.83 | 119.40 | 123.34 |
| 54 | 2x | 32 | PSU | O2-C2-N1 | -3.82 | 118.59 | 122.79 |
| 54 | 1y | 8 | 4SU | N3-C2-N1 | 3.81 | 119.95 | 114.89 |
| 54 | 1x | 54 | 5MU | C5-C6-N1 | -3.80 | 119.42 | 123.34 |
| 31 | 2a | 516 | PSU | C4-N3-C2 | -3.79 | 120.87 | 126.34 |
| 54 | 1y | 54 | 5MU | O4-C4-C5 | -3.76 | 120.55 | 124.90 |
| 54 | 2y | 55 | PSU | O2-C2-N1 | -3.75 | 118.67 | 122.79 |
| 54 | 2y | 32 | PSU | C4-N3-C2 | -3.74 | 120.94 | 126.34 |
| 54 | 2x | 8 | 4SU | C5-C4-S4 | -3.74 | 119.65 | 124.47 |
| 54 | 2y | 39 | PSU | C4-N3-C2 | -3.73 | 120.96 | 126.34 |
| 1 | 2A | 1915 | 5MU | O4-C4-C5 | -3.73 | 120.58 | 124.90 |
| 31 | 1a | 516 | PSU | C4-N3-C2 | -3.71 | 121.00 | 126.34 |
| 31 | 2a | 1519 | MA6 | N1-C6-N6 | 3.69 | 120.94 | 117.06 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed($^o$) | Ideal($^o$) |
|---|---|---|---|---|---|---|---|
| 1 | 1A | 1939 | 5MU | C5-C4-N3 | 3.67 | 118.44 | 115.31 |
| 1 | 2A | 1939 | 5MU | O4-C4-C5 | -3.65 | 120.67 | 124.90 |
| 1 | 1A | 1942 | 5MC | C5-C6-N1 | -3.61 | 119.62 | 123.34 |
| 54 | 1x | 32 | PSU | O2-C2-N1 | -3.61 | 118.81 | 122.79 |
| 54 | 1x | 32 | PSU | C4-N3-C2 | -3.60 | 121.15 | 126.34 |
| 54 | 2x | 55 | PSU | O2-C2-N1 | -3.56 | 118.87 | 122.79 |
| 54 | 1y | 8 | 4SU | C5-C4-S4 | -3.56 | 119.88 | 124.47 |
| 31 | 1a | 1519 | MA6 | C4-C5-N7 | -3.56 | 105.69 | 109.40 |
| 54 | 2x | 54 | 5MU | C5-C6-N1 | -3.56 | 119.68 | 123.34 |
| 31 | 1a | 1404 | 5MC | C5-C6-N1 | -3.55 | 119.68 | 123.34 |
| 54 | 2y | 37 | MIA | N3-C2-N1 | -3.53 | 123.17 | 128.68 |
| 54 | 2x | 54 | 5MU | O4-C4-C5 | -3.52 | 120.82 | 124.90 |
| 54 | 2x | 39 | PSU | C3'-C2'-C1' | 3.49 | 105.70 | 101.64 |
| 31 | 2a | 1518 | MA6 | C9-N6-C6 | -3.48 | 108.97 | 119.51 |
| 1 | 1A | 2552 | 2MU | O2-C2-N1 | -3.48 | 118.16 | 122.79 |
| 54 | 2x | 37 | MIA | N3-C2-N1 | -3.47 | 123.25 | 128.68 |
| 1 | 1A | 1962 | 5MC | C5-C6-N1 | -3.47 | 119.77 | 123.34 |
| 1 | 2A | 1917 | PSU | O2-C2-N1 | -3.46 | 118.98 | 122.79 |
| 54 | 1x | 39 | PSU | C4-N3-C2 | -3.46 | 121.36 | 126.34 |
| 54 | 1y | 39 | PSU | O2-C2-N1 | -3.45 | 118.99 | 122.79 |
| 54 | 1x | 8 | 4SU | C1'-N1-C6 | -3.44 | 113.33 | 120.84 |
| 1 | 2A | 1915 | 5MU | C5-C6-N1 | -3.44 | 119.80 | 123.34 |
| 1 | 1A | 1939 | 5MU | O4-C4-C5 | -3.43 | 120.93 | 124.90 |
| 54 | 2x | 39 | PSU | O2-C2-N1 | -3.41 | 119.04 | 122.79 |
| 54 | 1y | 32 | PSU | C4-N3-C2 | -3.39 | 121.45 | 126.34 |
| 31 | 1a | 1518 | MA6 | N3-C2-N1 | -3.38 | 123.39 | 128.68 |
| 54 | 1x | 39 | PSU | O2-C2-N1 | -3.37 | 119.08 | 122.79 |
| 54 | 1y | 37 | MIA | N3-C2-N1 | -3.36 | 123.42 | 128.68 |
| 1 | 1A | 1939 | 5MU | O2-C2-N1 | -3.36 | 118.32 | 122.79 |
| 54 | 1x | 54 | 5MU | O2-C2-N1 | -3.36 | 118.32 | 122.79 |
| 31 | 2a | 516 | PSU | O2-C2-N1 | -3.35 | 119.10 | 122.79 |
| 1 | 1A | 1911 | PSU | C4-N3-C2 | -3.32 | 121.55 | 126.34 |
| 54 | 2y | 54 | 5MU | C5-C6-N1 | -3.31 | 119.93 | 123.34 |
| 54 | 1y | 54 | 5MU | C5-C6-N1 | -3.31 | 119.94 | 123.34 |
| 54 | 1x | 8 | 4SU | C5-C4-S4 | -3.30 | 120.22 | 124.47 |
| 31 | 1a | 1518 | MA6 | C9-N6-C6 | -3.29 | 109.55 | 119.51 |
| 31 | 2a | 1400 | 5MC | C5-C6-N1 | -3.28 | 119.97 | 123.34 |
| 1 | 1A | 2605 | PSU | C6-C5-C4 | -3.20 | 115.96 | 118.20 |
| 31 | 2a | 1518 | MA6 | C4-C5-N7 | -3.16 | 106.10 | 109.40 |
| 31 | 2a | 1404 | 5MC | C5-C6-N1 | -3.16 | 120.09 | 123.34 |
| 54 | 2x | 46 | 7MG | C5-C6-N1 | 3.14 | 116.53 | 110.99 |
| 54 | 1x | 37 | MIA | N3-C2-N1 | -3.14 | 123.77 | 128.68 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed($^o$) | Ideal($^o$) |
|---|---|---|---|---|---|---|---|
| 54 | 1x | 55 | PSU | O2-C2-N1 | -3.12 | 119.35 | 122.79 |
| 1 | 1A | 1911 | PSU | O2-C2-N1 | -3.11 | 119.37 | 122.79 |
| 31 | 1a | 1518 | MA6 | C4-C5-N7 | -3.10 | 106.17 | 109.40 |
| 31 | 2a | 1519 | MA6 | C9-N6-C6 | -3.08 | 110.17 | 119.51 |
| 54 | 2y | 32 | PSU | O2-C2-N1 | -3.07 | 119.41 | 122.79 |
| 54 | 2y | 8 | 4SU | C5-C4-S4 | -3.06 | 120.52 | 124.47 |
| 42 | 2l | 92 | 0TD | CSB-SB-CB | -3.05 | 96.92 | 102.44 |
| 1 | 2A | 2552 | 2MU | C5-C4-N3 | 3.04 | 119.39 | 114.84 |
| 31 | 2a | 1518 | MA6 | C10-N6-C6 | -3.03 | 110.33 | 119.51 |
| 31 | 2a | 1519 | MA6 | C4-C5-N7 | -3.03 | 106.24 | 109.40 |
| 31 | 1a | 967 | 5MC | C5-C6-N1 | -3.03 | 120.22 | 123.34 |
| 54 | 2y | 39 | PSU | O2-C2-N1 | -3.01 | 119.48 | 122.79 |
| 1 | 1A | 2605 | PSU | O2-C2-N1 | -3.00 | 119.49 | 122.79 |
| 1 | 1A | 1911 | PSU | C6-C5-C4 | -2.99 | 116.10 | 118.20 |
| 54 | 1y | 32 | PSU | O2-C2-N1 | -2.99 | 119.50 | 122.79 |
| 31 | 2a | 1518 | MA6 | N3-C2-N1 | -2.99 | 124.01 | 128.68 |
| 31 | 1a | 1519 | MA6 | N3-C2-N1 | -2.98 | 124.02 | 128.68 |
| 1 | 1A | 1917 | PSU | O2-C2-N1 | -2.98 | 119.51 | 122.79 |
| 31 | 2a | 967 | 5MC | C5-C6-N1 | -2.97 | 120.28 | 123.34 |
| 1 | 2A | 1962 | 5MC | C5-C6-N1 | -2.96 | 120.29 | 123.34 |
| 1 | 2A | 2552 | 2MU | O4-C4-C5 | -2.95 | 119.98 | 125.16 |
| 1 | 1A | 1915 | 5MU | O2-C2-N1 | -2.92 | 118.90 | 122.79 |
| 54 | 1x | 37 | MIA | C4-C5-N7 | -2.92 | 106.36 | 109.40 |
| 1 | 1A | 1920 | OMC | C1'-N1-C2 | 2.92 | 124.94 | 118.42 |
| 1 | 2A | 1942 | 5MC | C5-C6-N1 | -2.92 | 120.34 | 123.34 |
| 1 | 2A | 1917 | PSU | C4-N3-C2 | -2.90 | 122.16 | 126.34 |
| 31 | 2a | 1518 | MA6 | N1-C6-N6 | 2.89 | 120.10 | 117.06 |
| 54 | 1y | 46 | 7MG | C5-C6-N1 | 2.87 | 116.04 | 110.99 |
| 31 | 2a | 967 | 5MC | C5-C4-N3 | -2.87 | 118.58 | 121.67 |
| 31 | 1a | 1519 | MA6 | C9-N6-C6 | -2.81 | 111.00 | 119.51 |
| 42 | 2l | 92 | 0TD | OD2-CG-CB | 2.78 | 119.16 | 113.15 |
| 54 | 1x | 8 | 4SU | O2-C2-N3 | -2.77 | 116.34 | 121.50 |
| 31 | 1a | 527 | 7MG | C5-C6-N1 | 2.75 | 115.84 | 110.99 |
| 31 | 2a | 1400 | 5MC | C5-C4-N3 | -2.73 | 118.73 | 121.67 |
| 31 | 2a | 1407 | 5MC | C5-C6-N1 | -2.70 | 120.56 | 123.34 |
| 1 | 1A | 2503 | 2MA | C3'-C2'-C1' | 2.70 | 105.05 | 100.98 |
| 31 | 1a | 516 | PSU | O2-C2-N1 | -2.70 | 119.82 | 122.79 |
| 31 | 1a | 1407 | 5MC | C5-C4-N3 | -2.68 | 118.78 | 121.67 |
| 54 | 1x | 46 | 7MG | N2-C2-N3 | -2.67 | 114.54 | 119.73 |
| 54 | 2y | 46 | 7MG | C5-C6-N1 | 2.66 | 115.69 | 110.99 |
| 1 | 1A | 1942 | 5MC | C5-C4-N3 | -2.66 | 118.80 | 121.67 |
| 1 | 2A | 2503 | 2MA | C5-C6-N1 | 2.66 | 118.62 | 114.02 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed($^o$) | Ideal($^o$) |
|---|---|---|---|---|---|---|---|
| 1 | 1A | 1942 | 5MC | CM5-C5-C6 | -2.66 | 119.30 | 122.85 |
| 31 | 2a | 1407 | 5MC | C5-C4-N3 | -2.65 | 118.82 | 121.67 |
| 31 | 2a | 1404 | 5MC | C5-C4-N3 | -2.62 | 118.85 | 121.67 |
| 31 | 2a | 527 | 7MG | C5-C6-N1 | 2.62 | 115.60 | 110.99 |
| 31 | 2a | 1518 | MA6 | C10-N6-C9 | -2.61 | 107.72 | 116.12 |
| 54 | 1x | 46 | 7MG | C5-C6-N1 | 2.60 | 115.57 | 110.99 |
| 54 | 2y | 37 | MIA | C4-C5-N7 | -2.60 | 106.69 | 109.40 |
| 1 | 1A | 1942 | 5MC | O2-C2-N3 | -2.59 | 118.12 | 122.33 |
| 54 | 1x | 39 | PSU | C6-C5-C4 | -2.59 | 116.39 | 118.20 |
| 42 | 1l | 92 | 0TD | OD2-CG-CB | 2.57 | 118.70 | 113.15 |
| 1 | 1A | 2251 | OMG | C5-C6-N1 | 2.57 | 118.48 | 113.95 |
| 31 | 2a | 1519 | MA6 | C10-N6-C6 | -2.56 | 111.77 | 119.51 |
| 54 | 1y | 37 | MIA | C4-C5-N7 | -2.54 | 106.75 | 109.40 |
| 31 | 1a | 1207 | 2MG | C8-N7-C5 | 2.54 | 107.83 | 102.99 |
| 1 | 2A | 2503 | 2MA | C8-N7-C5 | 2.53 | 107.81 | 102.99 |
| 54 | 2y | 46 | 7MG | C5-C4-N9 | -2.53 | 103.06 | 106.35 |
| 1 | 2A | 2605 | PSU | C5-C6-N1 | -2.53 | 118.32 | 122.11 |
| 54 | 1x | 8 | 4SU | C6-N1-C2 | -2.52 | 117.77 | 120.99 |
| 1 | 2A | 2552 | 2MU | C2'-C1'-N1 | -2.52 | 109.34 | 114.22 |
| 31 | 1a | 1400 | 5MC | C5-C4-N3 | -2.47 | 119.00 | 121.67 |
| 1 | 2A | 1942 | 5MC | C5-C4-N3 | -2.46 | 119.02 | 121.67 |
| 31 | 1a | 516 | PSU | C6-C5-C4 | -2.46 | 116.48 | 118.20 |
| 54 | 2x | 37 | MIA | C4-C5-N7 | -2.44 | 106.86 | 109.40 |
| 31 | 1a | 1402 | 4OC | CM4-N4-C4 | -2.42 | 117.72 | 122.45 |
| 31 | 1a | 967 | 5MC | O2-C2-N3 | -2.42 | 118.39 | 122.33 |
| 31 | 2a | 1519 | MA6 | N3-C2-N1 | -2.41 | 124.92 | 128.68 |
| 31 | 1a | 1519 | MA6 | N1-C6-N6 | 2.40 | 119.58 | 117.06 |
| 31 | 1a | 967 | 5MC | C5-C4-N3 | -2.40 | 119.09 | 121.67 |
| 1 | 1A | 1939 | 5MU | C6-C5-C4 | 2.37 | 120.02 | 118.03 |
| 31 | 2a | 1207 | 2MG | C8-N7-C5 | 2.37 | 107.51 | 102.99 |
| 31 | 1a | 1207 | 2MG | C5-C6-N1 | 2.36 | 118.13 | 113.95 |
| 54 | 1y | 54 | 5MU | C1'-N1-C2 | 2.36 | 121.84 | 117.57 |
| 1 | 1A | 2503 | 2MA | C8-N7-C5 | 2.33 | 107.43 | 102.99 |
| 31 | 1a | 1404 | 5MC | O2-C2-N3 | -2.33 | 118.54 | 122.33 |
| 31 | 1a | 1518 | MA6 | C10-N6-C9 | -2.32 | 108.64 | 116.12 |
| 31 | 2a | 1207 | 2MG | C5-C6-N1 | 2.32 | 118.05 | 113.95 |
| 54 | 2x | 46 | 7MG | O6-C6-C5 | -2.32 | 121.86 | 127.54 |
| 31 | 1a | 1498 | UR3 | C6-N1-C2 | -2.32 | 119.72 | 121.79 |
| 1 | 1A | 1920 | OMC | O2-C2-N3 | -2.30 | 118.59 | 122.33 |
| 31 | 2a | 527 | 7MG | O6-C6-C5 | -2.29 | 121.91 | 127.54 |
| 54 | 2y | 54 | 5MU | C1'-N1-C2 | 2.29 | 121.71 | 117.57 |
| 1 | 2A | 1962 | 5MC | O2-C2-N3 | -2.28 | 118.63 | 122.33 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed($^o$) | Ideal($^o$) |
|---|---|---|---|---|---|---|---|
| 54 | 2y | 32 | PSU | C6-C5-C4 | -2.27 | 116.61 | 118.20 |
| 1 | 1A | 2503 | 2MA | C5-C6-N1 | 2.27 | 117.94 | 114.02 |
| 31 | 2a | 527 | 7MG | C5-C4-N9 | -2.26 | 103.41 | 106.35 |
| 31 | 1a | 966 | M2G | C8-N7-C5 | 2.26 | 107.29 | 102.99 |
| 54 | 1y | 46 | 7MG | O6-C6-C5 | -2.25 | 122.01 | 127.54 |
| 1 | 2A | 1942 | 5MC | O2-C2-N3 | -2.25 | 118.67 | 122.33 |
| 31 | 2a | 1402 | 4OC | C6-C5-C4 | 2.25 | 119.71 | 116.96 |
| 31 | 1a | 1498 | UR3 | C3U-N3-C2 | 2.23 | 121.23 | 117.31 |
| 31 | 1a | 527 | 7MG | C5-C4-N9 | -2.23 | 103.45 | 106.35 |
| 31 | 1a | 527 | 7MG | O6-C6-C5 | -2.23 | 122.08 | 127.54 |
| 31 | 2a | 1404 | 5MC | CM5-C5-C6 | -2.23 | 119.88 | 122.85 |
| 31 | 1a | 516 | PSU | O4'-C1'-C2' | 2.22 | 108.28 | 105.14 |
| 31 | 1a | 966 | M2G | C5-C6-N1 | 2.22 | 117.88 | 113.95 |
| 1 | 1A | 1917 | PSU | O4'-C1'-C2' | 2.22 | 108.27 | 105.14 |
| 1 | 1A | 2251 | OMG | C2-N1-C6 | -2.21 | 121.03 | 125.10 |
| 1 | 1A | 1962 | 5MC | O2-C2-N3 | -2.19 | 118.77 | 122.33 |
| 54 | 2x | 32 | PSU | O4'-C1'-C2' | 2.18 | 108.22 | 105.14 |
| 1 | 2A | 1915 | 5MU | O2-C2-N3 | -2.18 | 117.45 | 121.50 |
| 54 | 1y | 46 | 7MG | C5-C4-N9 | -2.17 | 103.54 | 106.35 |
| 54 | 1x | 46 | 7MG | O6-C6-C5 | -2.16 | 122.25 | 127.54 |
| 54 | 2x | 46 | 7MG | C2-N1-C6 | -2.15 | 121.17 | 125.10 |
| 31 | 1a | 1404 | 5MC | C5-C4-N3 | -2.15 | 119.35 | 121.67 |
| 1 | 1A | 1920 | OMC | N4-C4-N3 | 2.14 | 121.73 | 117.97 |
| 1 | 2A | 1962 | 5MC | C5-C4-N3 | -2.13 | 119.37 | 121.67 |
| 54 | 2y | 46 | 7MG | O6-C6-C5 | -2.13 | 122.33 | 127.54 |
| 31 | 1a | 527 | 7MG | CM7-N7-C5 | 2.12 | 131.87 | 126.40 |
| 31 | 2a | 967 | 5MC | C1'-N1-C6 | -2.11 | 117.61 | 121.12 |
| 31 | 2a | 966 | M2G | C8-N7-C5 | 2.11 | 107.01 | 102.99 |
| 31 | 1a | 1404 | 5MC | CM5-C5-C6 | -2.09 | 120.05 | 122.85 |
| 1 | 1A | 2251 | OMG | CM2-O2'-C2' | -2.08 | 109.07 | 114.52 |
| 1 | 2A | 2251 | OMG | C5-C6-N1 | 2.07 | 117.62 | 113.95 |
| 1 | 2A | 2251 | OMG | C8-N7-C5 | 2.07 | 106.94 | 102.99 |
| 31 | 2a | 1400 | 5MC | O2-C2-N3 | -2.06 | 118.98 | 122.33 |
| 54 | 1y | 8 | 4SU | C1'-N1-C2 | 2.05 | 121.29 | 117.57 |
| 1 | 2A | 1915 | 5MU | C1'-N1-C2 | 2.05 | 121.28 | 117.57 |
| 31 | 2a | 966 | M2G | C5-C6-N1 | 2.05 | 117.57 | 113.95 |
| 54 | 1y | 54 | 5MU | C5M-C5-C4 | 2.04 | 121.01 | 118.77 |
| 54 | 1x | 55 | PSU | O4'-C1'-C2' | 2.04 | 108.02 | 105.14 |
| 54 | 2x | 46 | 7MG | CM7-N7-C5 | 2.04 | 131.66 | 126.40 |
| 54 | 1y | 39 | PSU | C5-C6-N1 | -2.03 | 119.06 | 122.11 |
| 54 | 2x | 55 | PSU | C6-C5-C4 | -2.03 | 116.78 | 118.20 |
| 1 | 2A | 1917 | PSU | O4'-C1'-C2' | 2.02 | 108.00 | 105.14 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed($^o$) | Ideal($^o$) |
|---|---|---|---|---|---|---|---|
| 1 | 1A | 1962 | 5MC | C5-C4-N3 | -2.02 | 119.50 | 121.67 |

There are no chirality outliers.

All (84) torsion outliers are listed below:

| Mol | Chain | Res | Type | Atoms |
|---|---|---|---|---|
| 42 | 1l | 92 | 0TD | CA-CB-SB-CSB |
| 42 | 1l | 92 | 0TD | CG-CB-SB-CSB |
| 1 | 2A | 1917 | PSU | C2'-C1'-C5-C4 |
| 1 | 2A | 1917 | PSU | C2'-C1'-C5-C6 |
| 31 | 2a | 527 | 7MG | C3'-C4'-C5'-O5' |
| 31 | 2a | 1207 | 2MG | N3-C2-N2-CM2 |
| 31 | 1a | 1402 | 4OC | O4'-C4'-C5'-O5' |
| 31 | 2a | 1402 | 4OC | O4'-C4'-C5'-O5' |
| 31 | 1a | 1518 | MA6 | C5-C6-N6-C9 |
| 31 | 1a | 1518 | MA6 | C5-C6-N6-C10 |
| 31 | 1a | 1519 | MA6 | C5-C6-N6-C10 |
| 31 | 2a | 1519 | MA6 | O4'-C4'-C5'-O5' |
| 31 | 2a | 1519 | MA6 | C3'-C4'-C5'-O5' |
| 54 | 1x | 37 | MIA | C3'-C4'-C5'-O5' |
| 54 | 1y | 37 | MIA | C3'-C4'-C5'-O5' |
| 54 | 2y | 37 | MIA | C3'-C4'-C5'-O5' |
| 54 | 1x | 39 | PSU | C2'-C1'-C5-C4 |
| 54 | 1x | 39 | PSU | C2'-C1'-C5-C6 |
| 54 | 2x | 39 | PSU | C3'-C4'-C5'-O5' |
| 54 | 1y | 46 | 7MG | C4'-C5'-O5'-P |
| 54 | 1y | 46 | 7MG | C3'-C4'-C5'-O5' |
| 54 | 2y | 46 | 7MG | C4'-C5'-O5'-P |
| 54 | 2y | 46 | 7MG | C3'-C4'-C5'-O5' |
| 54 | 2y | 46 | 7MG | C2'-C1'-N9-C8 |
| 54 | 2x | 55 | PSU | C2'-C1'-C5-C6 |
| 54 | 2x | 55 | PSU | O4'-C1'-C5-C6 |
| 54 | 1x | 8 | 4SU | C2'-C1'-N1-C6 |
| 54 | 1x | 8 | 4SU | C2'-C1'-N1-C2 |
| 1 | 1A | 2503 | 2MA | O4'-C4'-C5'-O5' |
| 1 | 1A | 2503 | 2MA | C3'-C4'-C5'-O5' |
| 31 | 1a | 1402 | 4OC | C3'-C4'-C5'-O5' |
| 31 | 2a | 1402 | 4OC | C3'-C4'-C5'-O5' |
| 54 | 1x | 37 | MIA | O4'-C4'-C5'-O5' |
| 54 | 2x | 37 | MIA | O4'-C4'-C5'-O5' |
| 54 | 2x | 37 | MIA | C3'-C4'-C5'-O5' |
| 31 | 2a | 527 | 7MG | O4'-C4'-C5'-O5' |

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| Mol | Chain | Res | Type | Atoms |
|---|---|---|---|---|
| 54 | 1y | 37 | MIA | O4'-C4'-C5'-O5' |
| 31 | 1a | 1518 | MA6 | N1-C6-N6-C9 |
| 31 | 2a | 1400 | 5MC | C2'-C1'-N1-C6 |
| 31 | 1a | 1519 | MA6 | O4'-C4'-C5'-O5' |
| 1 | 2A | 1917 | PSU | C3'-C4'-C5'-O5' |
| 54 | 2y | 37 | MIA | O4'-C4'-C5'-O5' |
| 54 | 2x | 37 | MIA | C4'-C5'-O5'-P |
| 54 | 1x | 46 | 7MG | C4'-C5'-O5'-P |
| 31 | 1a | 527 | 7MG | C3'-C4'-C5'-O5' |
| 54 | 2x | 39 | PSU | O4'-C4'-C5'-O5' |
| 54 | 1y | 46 | 7MG | O4'-C4'-C5'-O5' |
| 54 | 2y | 46 | 7MG | O4'-C4'-C5'-O5' |
| 54 | 1x | 54 | 5MU | C3'-C4'-C5'-O5' |
| 1 | 1A | 1915 | 5MU | C3'-C4'-C5'-O5' |
| 54 | 2x | 8 | 4SU | O4'-C4'-C5'-O5' |
| 31 | 2a | 1400 | 5MC | C2'-C1'-N1-C2 |
| 31 | 2a | 1400 | 5MC | O4'-C1'-N1-C6 |
| 54 | 1y | 46 | 7MG | C2'-C1'-N9-C8 |
| 1 | 2A | 1917 | PSU | O4'-C4'-C5'-O5' |
| 54 | 2x | 8 | 4SU | C3'-C4'-C5'-O5' |
| 42 | 2l | 92 | 0TD | CG-CB-SB-CSB |
| 54 | 1x | 54 | 5MU | O4'-C4'-C5'-O5' |
| 42 | 2l | 92 | 0TD | SB-CB-CG-OD1 |
| 1 | 2A | 2503 | 2MA | O4'-C4'-C5'-O5' |
| 31 | 1a | 527 | 7MG | O4'-C4'-C5'-O5' |
| 1 | 2A | 1917 | PSU | C4'-C5'-O5'-P |
| 31 | 2a | 1400 | 5MC | O4'-C1'-N1-C2 |
| 31 | 2a | 1518 | MA6 | C5-C6-N6-C10 |
| 31 | 2a | 1519 | MA6 | C5-C6-N6-C10 |
| 54 | 1y | 37 | MIA | C4'-C5'-O5'-P |
| 54 | 2x | 46 | 7MG | C4'-C5'-O5'-P |
| 1 | 2A | 2503 | 2MA | C4'-C5'-O5'-P |
| 54 | 2y | 37 | MIA | C4'-C5'-O5'-P |
| 31 | 1a | 1519 | MA6 | C3'-C4'-C5'-O5' |
| 54 | 2x | 54 | 5MU | C3'-C4'-C5'-O5' |
| 54 | 1x | 8 | 4SU | C3'-C4'-C5'-O5' |
| 31 | 2a | 1519 | MA6 | C4'-C5'-O5'-P |
| 54 | 1x | 32 | PSU | O4'-C1'-C5-C4 |
| 54 | 1x | 55 | PSU | O4'-C1'-C5-C4 |
| 31 | 2a | 967 | 5MC | O4'-C4'-C5'-O5' |
| 54 | 1y | 46 | 7MG | O4'-C1'-N9-C8 |
| 1 | 1A | 1920 | OMC | C2'-C1'-N1-C2 |

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| Mol | Chain | Res | Type | Atoms |
|---|---|---|---|---|
| 1 | 1A | 1915 | 5MU | O4'-C4'-C5'-O5' |
| 1 | 1A | 1939 | 5MU | O4'-C4'-C5'-O5' |
| 54 | 1x | 8 | 4SU | O4'-C4'-C5'-O5' |
| 1 | 2A | 1911 | PSU | O4'-C1'-C5-C6 |
| 54 | 1x | 32 | PSU | O4'-C1'-C5-C6 |
| 42 | 1l | 92 | 0TD | SB-CB-CG-OD1 |

There are no ring outliers.

No monomer is involved in short contacts.

## 5.5 Carbohydrates (i)

There are no monosaccharides in this entry.

## 5.6 Ligand geometry (i)

Of 2890 ligands modelled in this entry, 2886 are monoatomic - leaving 4 for Mogul analysis.

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

| Mol | Type | Chain | Res | Link | Bond lengths | | | Bond angles | | |
|---|---|---|---|---|---|---|---|---|---|---|
| | | | | | Counts | RMSZ | $\#\|Z\| > 2$ | Counts | RMSZ | $\#\|Z\| > 2$ |
| 58 | SF4 | 1d | 304 | 34 | 0,12,12 | - | - | - | | |
| 58 | SF4 | 2d | 303 | 34 | 0,12,12 | - | - | - | | |
| 59 | GDP | 1v | 704 | 56 | 24,30,30 | 1.00 | 1 (4%) | 30,47,47 | 1.38 | 3 (10%) |
| 59 | GDP | 2v | 704 | - | 24,30,30 | 0.98 | 1 (4%) | 30,47,47 | 1.35 | 4 (13%) |

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 |
|---|---|---|---|---|---|---|---|
| 58 | SF4 | 1d | 304 | 34 | - | - | 0/6/5/5 |
| 58 | SF4 | 2d | 303 | 34 | - | - | 0/6/5/5 |

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| Mol | Type | Chain | Res | Link | Chirals | Torsions | Rings |
|---|---|---|---|---|---|---|---|
| 59 | GDP | 1v | 704 | 56 | - | 0/12/32/32 | 0/3/3/3 |
| 59 | GDP | 2v | 704 | - | - | 5/12/32/32 | 0/3/3/3 |

All (2) bond length outliers are listed below:

| Mol | Chain | Res | Type | Atoms | Z | Observed(Å) | Ideal(Å) |
|---|---|---|---|---|---|---|---|
| 59 | 1v | 704 | GDP | C6-N1 | -2.48 | 1.34 | 1.37 |
| 59 | 2v | 704 | GDP | C6-N1 | -2.34 | 1.34 | 1.37 |

All (7) bond angle outliers are listed below:

| Mol | Chain | Res | Type | Atoms | Z | Observed($^o$) | Ideal($^o$) |
|---|---|---|---|---|---|---|---|
| 59 | 1v | 704 | GDP | PA-O3A-PB | -4.50 | 117.38 | 132.83 |
| 59 | 2v | 704 | GDP | PA-O3A-PB | -4.37 | 117.83 | 132.83 |
| 59 | 1v | 704 | GDP | C3'-C2'-C1' | 3.23 | 105.84 | 100.98 |
| 59 | 2v | 704 | GDP | C3'-C2'-C1' | 2.86 | 105.28 | 100.98 |
| 59 | 1v | 704 | GDP | C8-N7-C5 | 2.48 | 107.71 | 102.99 |
| 59 | 2v | 704 | GDP | C8-N7-C5 | 2.34 | 107.45 | 102.99 |
| 59 | 2v | 704 | GDP | C5-C6-N1 | 2.03 | 117.54 | 113.95 |

There are no chirality outliers.

All (5) torsion outliers are listed below:

| Mol | Chain | Res | Type | Atoms |
|---|---|---|---|---|
| 59 | 2v | 704 | GDP | C5'-O5'-PA-O1A |
| 59 | 2v | 704 | GDP | O4'-C4'-C5'-O5' |
| 59 | 2v | 704 | GDP | C3'-C4'-C5'-O5' |
| 59 | 2v | 704 | GDP | C5'-O5'-PA-O3A |
| 59 | 2v | 704 | GDP | C5'-O5'-PA-O2A |

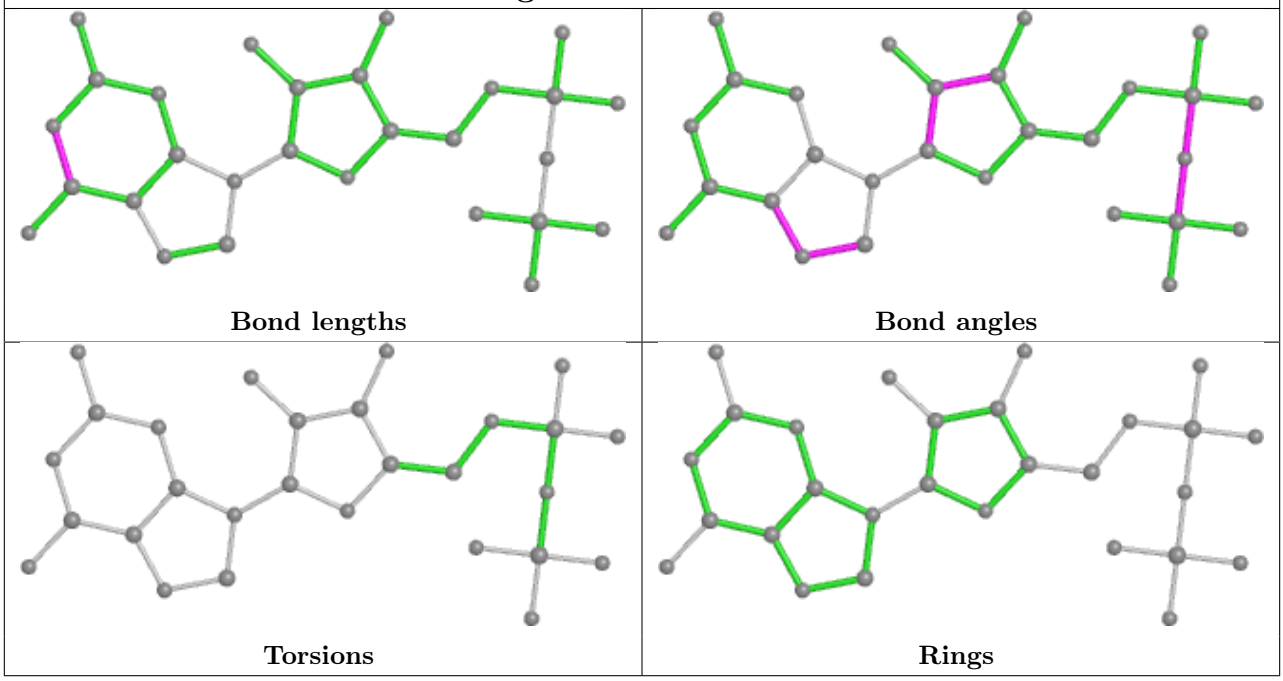
There are no ring outliers.

No monomer is involved in short contacts.

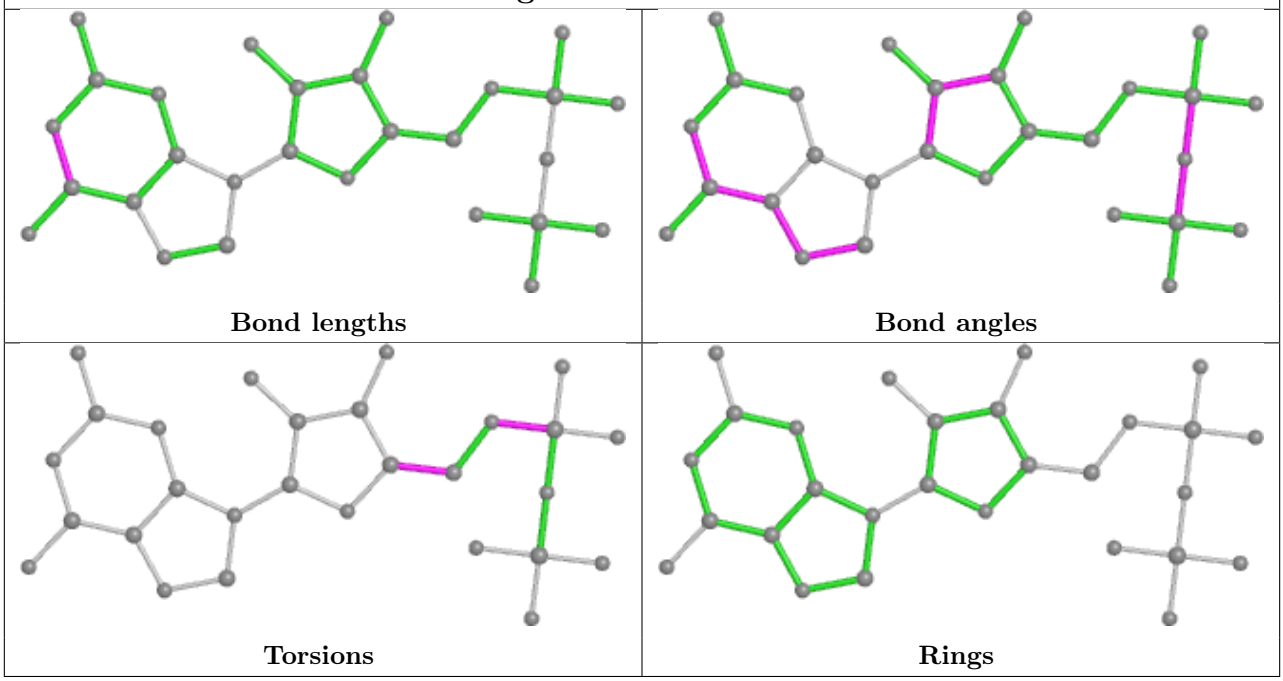
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. 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 GDP 1v 704**




**Ligand GDP 2v 704**




## 5.7 Other polymers (i)

There are no such residues in this entry.

## 5.8 Polymer linkage issues (i)

There are no chain breaks in this entry.

# 6 Fit of model and data (i)

## 6.1 Protein, DNA and RNA chains (i)

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 | 1A | 2860/2915 (98%) | 0.13 | 44 (1%) | 73 | 68 | 54, 75, 190, 283 | 0 |
| 1 | 2A | 2789/2915 (95%) | 0.15 | 130 (4%) | 31 | 28 | 84, 119, 191, 306 | 0 |
| 2 | 1B | 120/121 (99%) | -0.11 | 0 | 100 | 100 | 71, 95, 113, 126 | 0 |
| 2 | 2B | 120/121 (99%) | -0.59 | 1 (0%) | 86 | 81 | 132, 165, 184, 198 | 0 |
| 3 | 1D | 275/276 (99%) | 0.62 | 17 (6%) | 20 | 18 | 62, 80, 92, 98 | 0 |
| 3 | 2D | 275/276 (99%) | 0.64 | 31 (11%) | 5 | 6 | 89, 102, 117, 121 | 0 |
| 4 | 1E | 204/206 (99%) | 1.16 | 60 (29%) | 0 | 0 | 60, 81, 94, 100 | 0 |
| 4 | 2E | 204/206 (99%) | 0.08 | 7 (3%) | 45 | 40 | 96, 125, 137, 142 | 0 |
| 5 | 1F | 203/210 (96%) | 0.03 | 8 (3%) | 39 | 35 | 55, 82, 100, 109 | 0 |
| 5 | 2F | 203/210 (96%) | 0.43 | 16 (7%) | 12 | 13 | 94, 141, 155, 160 | 0 |
| 6 | 1G | 181/182 (99%) | -0.34 | 2 (1%) | 80 | 75 | 105, 135, 158, 175 | 0 |
| 6 | 2G | 181/182 (99%) | 1.76 | 62 (34%) | 0 | 0 | 175, 205, 219, 227 | 0 |
| 7 | 1H | 174/180 (96%) | -0.18 | 0 | 100 | 100 | 80, 88, 97, 101 | 0 |
| 7 | 2H | 174/180 (96%) | 1.16 | 38 (21%) | 0 | 0 | 150, 166, 181, 184 | 0 |
| 8 | 1N | 140/140 (100%) | 0.25 | 4 (2%) | 51 | 45 | 64, 73, 84, 90 | 0 |
| 8 | 2N | 140/140 (100%) | 1.05 | 26 (18%) | 1 | 1 | 113, 128, 139, 141 | 0 |
| 9 | 1O | 122/122 (100%) | 2.10 | 65 (53%) | 0 | 0 | 74, 85, 96, 100 | 0 |
| 9 | 2O | 122/122 (100%) | 2.04 | 60 (49%) | 0 | 0 | 108, 121, 131, 132 | 0 |
| 10 | 1P | 149/150 (99%) | 0.04 | 4 (2%) | 54 | 48 | 55, 82, 104, 111 | 0 |
| 10 | 2P | 149/150 (99%) | 1.18 | 39 (26%) | 0 | 0 | 102, 134, 149, 151 | 0 |
| 11 | 1Q | 141/141 (100%) | 0.03 | 0 | 100 | 100 | 64, 79, 89, 101 | 0 |
| 11 | 2Q | 141/141 (100%) | 1.50 | 45 (31%) | 0 | 0 | 108, 134, 150, 153 | 0 |
| 12 | 1R | 118/118 (100%) | 0.56 | 4 (3%) | 45 | 40 | 64, 72, 81, 84 | 0 |
| 12 | 2R | 118/118 (100%) | 0.03 | 2 (1%) | 70 | 64 | 96, 112, 122, 126 | 0 |

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| Mol | Chain | Analysed | <RSRZ> | #RSRZ>2 | OWAB(Å$^2$) | Q<0.9 |
|---|---|---|---|---|---|---|
| 13 | 1S | 110/112 (98%) | -0.44 | 0 100 100 | 83, 90, 97, 100 | 0 |
| 13 | 2S | 110/112 (98%) | -0.02 | 2 (1%) 68 62 | 147, 159, 166, 168 | 0 |
| 14 | 1T | 131/146 (89%) | 1.52 | 47 (35%) 0 0 | 79, 89, 111, 118 | 0 |
| 14 | 2T | 131/146 (89%) | 0.70 | 22 (16%) 1 2 | 120, 128, 143, 148 | 0 |
| 15 | 1U | 116/118 (98%) | 0.30 | 2 (1%) 70 64 | 58, 65, 73, 75 | 0 |
| 15 | 2U | 116/118 (98%) | 0.44 | 7 (6%) 21 19 | 105, 125, 137, 139 | 0 |
| 16 | 1V | 101/101 (100%) | 0.06 | 1 (0%) 82 77 | 55, 74, 81, 83 | 0 |
| 16 | 2V | 101/101 (100%) | 0.67 | 12 (11%) 4 5 | 106, 138, 144, 148 | 0 |
| 17 | 1W | 112/113 (99%) | 0.95 | 8 (7%) 16 15 | 60, 65, 81, 91 | 0 |
| 17 | 2W | 112/113 (99%) | 0.16 | 0 100 100 | 88, 99, 107, 117 | 0 |
| 18 | 1X | 95/96 (98%) | 0.04 | 2 (2%) 63 58 | 71, 76, 84, 88 | 0 |
| 18 | 2X | 95/96 (98%) | -0.44 | 0 100 100 | 102, 110, 118, 129 | 0 |
| 19 | 1Y | 107/110 (97%) | -0.15 | 1 (0%) 84 79 | 78, 83, 90, 101 | 0 |
| 19 | 2Y | 107/110 (97%) | 0.69 | 12 (11%) 5 6 | 118, 137, 145, 147 | 0 |
| 20 | 1Z | 204/206 (99%) | -0.22 | 1 (0%) 91 88 | 83, 99, 113, 123 | 0 |
| 20 | 2Z | 204/206 (99%) | 1.05 | 41 (20%) 1 1 | 127, 157, 174, 179 | 0 |
| 21 | 10 | 75/85 (88%) | -0.01 | 1 (1%) 77 71 | 68, 74, 81, 85 | 0 |
| 21 | 20 | 75/85 (88%) | 1.34 | 25 (33%) 0 0 | 118, 129, 139, 144 | 0 |
| 22 | 11 | 97/98 (98%) | 0.82 | 15 (15%) 2 2 | 67, 82, 107, 111 | 0 |
| 22 | 21 | 97/98 (98%) | 1.73 | 41 (42%) 0 0 | 106, 124, 149, 156 | 0 |
| 23 | 12 | 70/72 (97%) | -0.04 | 0 100 100 | 82, 87, 97, 104 | 0 |
| 23 | 22 | 70/72 (97%) | -0.23 | 1 (1%) 75 69 | 119, 132, 140, 141 | 0 |
| 24 | 13 | 59/60 (98%) | 0.47 | 2 (3%) 45 40 | 63, 71, 83, 90 | 0 |
| 24 | 23 | 59/60 (98%) | 1.08 | 10 (16%) 1 2 | 122, 130, 133, 135 | 0 |
| 25 | 14 | 69/71 (97%) | -0.77 | 0 100 100 | 123, 162, 237, 238 | 0 |
| 25 | 24 | 69/71 (97%) | 0.80 | 14 (20%) 1 1 | 195, 221, 254, 255 | 0 |
| 26 | 15 | 59/60 (98%) | 0.96 | 8 (13%) 3 4 | 57, 73, 77, 79 | 0 |
| 26 | 25 | 59/60 (98%) | -0.11 | 0 100 100 | 92, 114, 120, 121 | 0 |
| 27 | 16 | 53/54 (98%) | 0.12 | 1 (1%) 66 61 | 74, 80, 83, 85 | 0 |
| 27 | 26 | 53/54 (98%) | 3.26 | 40 (75%) 0 0 | 123, 130, 134, 147 | 0 |
| 28 | 17 | 48/49 (97%) | 0.70 | 2 (4%) 36 32 | 60, 63, 71, 73 | 0 |

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| Mol | Chain | Analysed | <RSRZ> | #RSRZ>2 | | | OWAB(Å$^2$) | Q<0.9 |
|---|---|---|---|---|---|---|---|---|
| 28 | 27 | 48/49 (97%) | 0.31 | 2 (4%) | 36 | 32 | 85, 96, 100, 101 | 0 |
| 29 | 18 | 64/65 (98%) | 0.77 | 4 (6%) | 20 | 18 | 63, 70, 76, 78 | 0 |
| 29 | 28 | 64/65 (98%) | 2.62 | 39 (60%) | 0 | 0 | 114, 119, 128, 133 | 0 |
| 30 | 19 | 37/37 (100%) | 0.01 | 0 | 100 | 100 | 77, 79, 81, 83 | 0 |
| 30 | 29 | 37/37 (100%) | 1.11 | 8 (21%) | 0 | 1 | 133, 141, 149, 152 | 0 |
| 31 | 1a | 1487/1521 (97%) | -0.04 | 89 (5%) | 21 | 19 | 90, 142, 235, 306 | 0 |
| 31 | 2a | 1491/1521 (98%) | 0.13 | 102 (6%) | 17 | 16 | 117, 163, 259, 294 | 0 |
| 32 | 1b | 231/256 (90%) | 0.07 | 9 (3%) | 39 | 35 | 157, 172, 189, 196 | 0 |
| 32 | 2b | 231/256 (90%) | 0.04 | 9 (3%) | 39 | 35 | 185, 199, 223, 234 | 0 |
| 33 | 1c | 206/239 (86%) | 3.16 | 130 (63%) | 0 | 0 | 185, 200, 218, 220 | 0 |
| 33 | 2c | 206/239 (86%) | 2.58 | 112 (54%) | 0 | 0 | 216, 231, 246, 248 | 0 |
| 34 | 1d | 208/209 (99%) | 0.47 | 19 (9%) | 9 | 9 | 137, 149, 154, 155 | 0 |
| 34 | 2d | 208/209 (99%) | 0.34 | 23 (11%) | 5 | 6 | 140, 164, 167, 169 | 0 |
| 35 | 1e | 148/162 (91%) | 0.78 | 23 (15%) | 2 | 2 | 127, 141, 148, 153 | 0 |
| 35 | 2e | 148/162 (91%) | 1.65 | 51 (34%) | 0 | 0 | 157, 171, 185, 190 | 0 |
| 36 | 1f | 100/101 (99%) | 0.04 | 0 | 100 | 100 | 132, 138, 147, 153 | 0 |
| 36 | 2f | 100/101 (99%) | -0.20 | 0 | 100 | 100 | 143, 148, 155, 160 | 0 |
| 37 | 1g | 155/156 (99%) | 2.48 | 69 (44%) | 0 | 0 | 175, 205, 212, 215 | 0 |
| 37 | 2g | 155/156 (99%) | 5.37 | 114 (73%) | 0 | 0 | 201, 227, 234, 238 | 0 |
| 38 | 1h | 137/138 (99%) | 0.35 | 5 (3%) | 42 | 38 | 125, 138, 147, 157 | 0 |
| 38 | 2h | 137/138 (99%) | 0.28 | 10 (7%) | 15 | 15 | 153, 163, 173, 185 | 0 |
| 39 | 1i | 127/128 (99%) | 1.06 | 31 (24%) | 0 | 0 | 182, 221, 226, 229 | 0 |
| 39 | 2i | 127/128 (99%) | 1.12 | 33 (25%) | 0 | 0 | 213, 246, 251, 252 | 0 |
| 40 | 1j | 97/105 (92%) | 2.31 | 43 (44%) | 0 | 0 | 199, 222, 226, 227 | 0 |
| 40 | 2j | 96/105 (91%) | 0.87 | 24 (25%) | 0 | 0 | 229, 244, 251, 252 | 0 |
| 41 | 1k | 114/129 (88%) | 1.75 | 45 (39%) | 0 | 0 | 116, 144, 150, 157 | 0 |
| 41 | 2k | 114/129 (88%) | 2.40 | 61 (53%) | 0 | 0 | 134, 161, 170, 176 | 0 |
| 42 | 1l | 121/132 (91%) | 0.75 | 17 (14%) | 2 | 3 | 116, 130, 138, 140 | 0 |
| 42 | 2l | 121/132 (91%) | 2.09 | 53 (43%) | 0 | 0 | 144, 153, 162, 166 | 0 |
| 43 | 1m | 118/126 (93%) | 0.26 | 12 (10%) | 6 | 7 | 201, 226, 227, 229 | 0 |
| 43 | 2m | 122/126 (96%) | 1.52 | 29 (23%) | 0 | 0 | 222, 242, 245, 247 | 0 |

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| Mol | Chain | Analysed | <RSRZ> | #RSRZ>2 | OWAB(Å$^2$) | Q<0.9 |
|---|---|---|---|---|---|---|
| 44 | 1n | 60/61 (98%) | 2.59 | 32 (53%) 0 0 | 207, 215, 227, 228 | 0 |
| 44 | 2n | 60/61 (98%) | 2.32 | 31 (51%) 0 0 | 234, 239, 249, 250 | 0 |
| 45 | 1o | 88/89 (98%) | -0.30 | 0 100 100 | 116, 128, 133, 135 | 0 |
| 45 | 2o | 88/89 (98%) | 0.28 | 5 (5%) 23 21 | 136, 148, 153, 154 | 0 |
| 46 | 1p | 82/88 (93%) | 0.28 | 5 (6%) 21 19 | 135, 146, 154, 159 | 0 |
| 46 | 2p | 82/88 (93%) | 0.37 | 2 (2%) 59 53 | 152, 160, 168, 176 | 0 |
| 47 | 1q | 99/105 (94%) | -0.12 | 1 (1%) 82 77 | 116, 125, 131, 134 | 0 |
| 47 | 2q | 99/105 (94%) | 2.08 | 48 (48%) 0 0 | 138, 151, 155, 156 | 0 |
| 48 | 1r | 68/88 (77%) | 0.24 | 1 (1%) 73 68 | 133, 139, 143, 147 | 0 |
| 48 | 2r | 68/88 (77%) | 0.45 | 8 (11%) 4 5 | 147, 154, 159, 160 | 0 |
| 49 | 1s | 83/93 (89%) | 0.18 | 11 (13%) 3 4 | 213, 234, 238, 239 | 0 |
| 49 | 2s | 83/93 (89%) | 1.29 | 22 (26%) 0 0 | 235, 252, 255, 255 | 0 |
| 50 | 1t | 96/106 (90%) | -0.01 | 3 (3%) 49 43 | 136, 144, 148, 149 | 0 |
| 50 | 2t | 96/106 (90%) | 0.11 | 3 (3%) 49 43 | 152, 157, 163, 165 | 0 |
| 51 | 1u | 23/27 (85%) | -0.38 | 0 100 100 | 217, 220, 226, 227 | 0 |
| 51 | 2u | 23/27 (85%) | 0.39 | 5 (21%) 0 0 | 239, 242, 244, 244 | 0 |
| 52 | 1v | 728/758 (96%) | 0.35 | 86 (11%) 4 5 | 30, 144, 211, 217 | 0 |
| 52 | 2v | 728/758 (96%) | 1.46 | 232 (31%) 0 0 | 30, 197, 259, 264 | 0 |
| 53 | 1w | 185/185 (100%) | 0.59 | 14 (7%) 13 14 | 87, 118, 158, 166 | 0 |
| 53 | 2w | 185/185 (100%) | 3.44 | 103 (55%) 0 0 | 123, 157, 206, 217 | 0 |
| 54 | 1x | 67/76 (88%) | 2.28 | 36 (53%) 0 0 | 91, 195, 204, 206 | 0 |
| 54 | 1y | 67/76 (88%) | 1.57 | 23 (34%) 0 0 | 74, 212, 238, 247 | 0 |
| 54 | 2x | 67/76 (88%) | 10.21 | 66 (98%) 0 0 | 124, 232, 243, 245 | 0 |
| 54 | 2y | 67/76 (88%) | 4.02 | 53 (79%) 0 0 | 118, 252, 277, 282 | 0 |
| 55 | 1z | 10/21 (47%) | 3.36 | 9 (90%) 0 0 | 150, 157, 164, 164 | 0 |
| 55 | 2z | 10/21 (47%) | 2.57 | 3 (30%) 0 0 | 181, 185, 203, 204 | 0 |
| All | All | 22334/23178 (96%) | 0.60 | 2951 (13%) 3 4 | 30, 134, 241, 306 | 0 |

All (2951) RSRZ outliers are listed below:

| Mol | Chain | Res | Type | RSRZ |
|---|---|---|---|---|
| 37 | 2g | 91 | VAL | 20.4 |
| 37 | 2g | 85 | TYR | 18.2 |

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| Mol | Chain | Res | Type | RSRZ |
|---|---|---|---|---|
| 54 | 2x | 62 | C | 18.2 |
| 37 | 2g | 84 | ASN | 18.2 |
| 52 | 2v | 501 | THR | 17.2 |
| 54 | 2x | 48 | C | 17.1 |
| 37 | 2g | 86 | GLN | 16.9 |
| 37 | 2g | 78 | ARG | 16.8 |
| 37 | 2g | 83 | ALA | 16.4 |
| 43 | 2m | 123 | ALA | 16.3 |
| 37 | 2g | 90 | GLU | 16.3 |
| 53 | 2w | 32 | ARG | 16.1 |
| 40 | 1j | 62 | HIS | 15.9 |
| 37 | 2g | 89 | MET | 15.7 |
| 37 | 2g | 76 | ARG | 15.6 |
| 37 | 2g | 74 | GLU | 15.4 |
| 1 | 2A | 2140 | C | 15.4 |
| 43 | 2m | 119 | GLY | 15.3 |
| 54 | 2x | 49 | C | 15.1 |
| 37 | 2g | 77 | SER | 14.9 |
| 54 | 2x | 22 | G | 14.7 |
| 54 | 2x | 61 | C | 14.7 |
| 54 | 2x | 72 | C | 14.7 |
| 43 | 2m | 120 | LYS | 14.6 |
| 37 | 2g | 152 | ALA | 14.5 |
| 54 | 2x | 59 | U | 14.5 |
| 49 | 2s | 84 | GLY | 14.5 |
| 43 | 2m | 124 | PRO | 14.5 |
| 54 | 2x | 44 | G | 14.4 |
| 54 | 2x | 69 | G | 14.4 |
| 54 | 2x | 21 | A | 14.3 |
| 54 | 2x | 47 | U | 14.0 |
| 54 | 2x | 19 | G | 14.0 |
| 52 | 2v | 413 | ILE | 13.9 |
| 54 | 2x | 12 | U | 13.9 |
| 54 | 2x | 13 | C | 13.6 |
| 54 | 2x | 7 | A | 13.6 |
| 54 | 2x | 70 | G | 13.5 |
| 54 | 2x | 11 | C | 13.3 |
| 37 | 2g | 148 | ASN | 13.2 |
| 37 | 2g | 153 | HIS | 13.1 |
| 54 | 2x | 3 | C | 13.1 |
| 37 | 2g | 156 | TRP | 12.9 |
| 54 | 2x | 64 | A | 12.9 |

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| Mol | Chain | Res | Type | RSRZ |
|---|---|---|---|---|
| 54 | 2x | 74 | C | 12.9 |
| 54 | 2x | 65 | G | 12.9 |
| 54 | 2x | 5 | G | 12.7 |
| 54 | 2x | 57 | G | 12.7 |
| 33 | 1c | 156 | ARG | 12.6 |
| 54 | 2x | 71 | G | 12.6 |
| 52 | 1v | 502 | GLY | 12.5 |
| 31 | 2a | 1030(B) | C | 12.5 |
| 37 | 2g | 82 | GLY | 12.5 |
| 37 | 2g | 88 | PRO | 12.4 |
| 37 | 1g | 74 | GLU | 12.2 |
| 54 | 2x | 20 | U | 12.2 |
| 54 | 2y | 62 | C | 12.2 |
| 54 | 2x | 27 | G | 12.1 |
| 33 | 2c | 79 | ARG | 12.1 |
| 54 | 2x | 56 | C | 12.0 |
| 54 | 2y | 61 | C | 12.0 |
| 37 | 1g | 77 | SER | 11.9 |
| 39 | 2i | 56 | LEU | 11.8 |
| 53 | 2w | 45 | TYR | 11.8 |
| 53 | 2w | 40 | HIS | 11.7 |
| 54 | 2x | 63 | G | 11.7 |
| 54 | 2x | 52 | G | 11.7 |
| 54 | 2x | 24 | G | 11.6 |
| 53 | 2w | 71 | TRP | 11.5 |
| 37 | 2g | 144 | MET | 11.2 |
| 37 | 2g | 71 | PRO | 11.2 |
| 37 | 1g | 85 | TYR | 11.2 |
| 37 | 2g | 72 | ARG | 11.0 |
| 40 | 1j | 47 | PHE | 11.0 |
| 53 | 2w | 70 | SER | 10.9 |
| 20 | 2Z | 204 | GLU | 10.8 |
| 52 | 2v | 414 | GLU | 10.7 |
| 54 | 2x | 58 | A | 10.6 |
| 54 | 2x | 51 | U | 10.4 |
| 53 | 2w | 41 | LEU | 10.3 |
| 37 | 2g | 70 | LYS | 10.3 |
| 37 | 2g | 87 | VAL | 10.3 |
| 37 | 2g | 81 | GLY | 10.3 |
| 54 | 2x | 28 | G | 10.3 |
| 39 | 1i | 121 | ARG | 10.2 |
| 54 | 2x | 75 | C | 10.2 |

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| Mol | Chain | Res | Type | RSRZ |
|---|---|---|---|---|
| 53 | 2w | 93 | SER | 10.1 |
| 33 | 2c | 81 | GLY | 10.1 |
| 52 | 1v | 501 | THR | 10.1 |
| 43 | 2m | 122 | LYS | 10.1 |
| 53 | 2w | 44 | GLU | 10.1 |
| 37 | 2g | 73 | MET | 10.1 |
| 37 | 2g | 145 | ALA | 10.0 |
| 52 | 2v | 471 | LYS | 10.0 |
| 54 | 2x | 43 | C | 10.0 |
| 37 | 2g | 149 | ARG | 10.0 |
| 53 | 2w | 74 | ASN | 9.9 |
| 33 | 1c | 190 | ARG | 9.9 |
| 37 | 1g | 78 | ARG | 9.9 |
| 33 | 1c | 155 | GLY | 9.9 |
| 52 | 2v | 454 | MET | 9.9 |
| 52 | 2v | 500 | GLN | 9.9 |
| 54 | 2x | 50 | U | 9.9 |
| 54 | 2y | 1 | G | 9.8 |
| 40 | 2j | 47 | PHE | 9.8 |
| 52 | 2v | 442 | THR | 9.8 |
| 1 | 2A | 2132 | U | 9.7 |
| 53 | 2w | 100 | TYR | 9.7 |
| 53 | 2w | 72 | ASP | 9.7 |
| 54 | 2x | 73 | A | 9.7 |
| 27 | 26 | 54 | ILE | 9.7 |
| 33 | 2c | 103 | VAL | 9.7 |
| 54 | 2x | 6 | G | 9.6 |
| 37 | 2g | 75 | VAL | 9.6 |
| 1 | 2A | 2139 | C | 9.6 |
| 42 | 2l | 68 | ALA | 9.6 |
| 22 | 21 | 2 | SER | 9.6 |
| 54 | 2x | 9 | A | 9.6 |
| 54 | 2x | 23 | A | 9.6 |
| 33 | 2c | 80 | GLY | 9.6 |
| 37 | 2g | 101 | LEU | 9.5 |
| 54 | 2x | 45 | U | 9.5 |
| 54 | 2x | 53 | G | 9.5 |
| 37 | 2g | 139 | GLU | 9.4 |
| 37 | 1g | 144 | MET | 9.4 |
| 37 | 2g | 155 | ARG | 9.4 |
| 54 | 2x | 1 | G | 9.4 |
| 6 | 2G | 87 | PRO | 9.3 |

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| Mol | Chain | Res | Type | RSRZ |
|---|---|---|---|---|
| 37 | 2g | 154 | TYR | 9.3 |
| 55 | 2z | 21 | A | 9.3 |
| 53 | 2w | 87 | ASP | 9.3 |
| 53 | 2w | 73 | GLN | 9.2 |
| 53 | 2w | 97 | ASP | 9.2 |
| 53 | 2w | 43 | VAL | 9.2 |
| 1 | 2A | 2153 | G | 9.2 |
| 54 | 2x | 60 | U | 9.1 |
| 1 | 2A | 2154 | G | 9.1 |
| 37 | 2g | 80 | VAL | 9.1 |
| 37 | 1g | 153 | HIS | 9.0 |
| 52 | 2v | 453 | GLY | 9.0 |
| 40 | 1j | 60 | ARG | 9.0 |
| 37 | 2g | 151 | TYR | 8.9 |
| 53 | 2w | 46 | TYR | 8.9 |
| 53 | 2w | 90 | LEU | 8.9 |
| 33 | 1c | 161 | GLU | 8.9 |
| 37 | 2g | 103 | TRP | 8.9 |
| 6 | 2G | 88 | ILE | 8.8 |
| 33 | 2c | 78 | GLY | 8.7 |
| 1 | 2A | 888 | C | 8.7 |
| 35 | 2e | 9 | LYS | 8.6 |
| 52 | 2v | 452 | SER | 8.6 |
| 6 | 2G | 138 | GLN | 8.6 |
| 37 | 2g | 54 | THR | 8.6 |
| 54 | 2x | 66 | U | 8.5 |
| 20 | 2Z | 203 | GLU | 8.5 |
| 37 | 1g | 86 | GLN | 8.5 |
| 43 | 2m | 118 | ALA | 8.4 |
| 39 | 1i | 128 | ARG | 8.4 |
| 54 | 2x | 18 | G | 8.4 |
| 43 | 2m | 121 | LYS | 8.4 |
| 44 | 1n | 34 | TYR | 8.4 |
| 1 | 2A | 2152 | G | 8.4 |
| 53 | 2w | 38 | LEU | 8.4 |
| 54 | 2x | 76 | A | 8.3 |
| 37 | 2g | 137 | LYS | 8.3 |
| 52 | 2v | 427 | ALA | 8.3 |
| 53 | 2w | 99 | LEU | 8.3 |
| 53 | 2w | 58 | VAL | 8.2 |
| 6 | 2G | 41 | GLN | 8.2 |
| 52 | 2v | 522 | GLY | 8.2 |

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| Mol | Chain | Res | Type | RSRZ |
|---|---|---|---|---|
| 33 | 2c | 76 | VAL | 8.2 |
| 52 | 2v | 597 | GLY | 8.2 |
| 37 | 2g | 104 | LEU | 8.2 |
| 40 | 1j | 61 | GLU | 8.2 |
| 54 | 2y | 6 | G | 8.2 |
| 52 | 2v | 467 | LYS | 8.1 |
| 52 | 2v | 598 | ASP | 8.0 |
| 37 | 2g | 97 | GLN | 8.0 |
| 43 | 2m | 94 | ARG | 8.0 |
| 40 | 1j | 96 | ILE | 8.0 |
| 1 | 2A | 2141 | G | 8.0 |
| 37 | 1g | 76 | ARG | 8.0 |
| 47 | 2q | 24 | GLU | 8.0 |
| 52 | 2v | 477 | GLY | 7.9 |
| 52 | 2v | 578 | SER | 7.9 |
| 27 | 26 | 25 | LYS | 7.9 |
| 52 | 2v | 472 | VAL | 7.9 |
| 37 | 1g | 73 | MET | 7.8 |
| 49 | 2s | 81 | ARG | 7.8 |
| 54 | 2x | 68 | C | 7.8 |
| 40 | 2j | 61 | GLU | 7.8 |
| 33 | 1c | 66 | VAL | 7.8 |
| 1 | 2A | 2156 | G | 7.7 |
| 33 | 1c | 157 | ILE | 7.7 |
| 37 | 1g | 82 | GLY | 7.7 |
| 33 | 2c | 188 | LEU | 7.7 |
| 52 | 2v | 466 | LEU | 7.7 |
| 37 | 2g | 79 | ARG | 7.7 |
| 52 | 2v | 456 | GLU | 7.6 |
| 43 | 2m | 117 | VAL | 7.6 |
| 54 | 1x | 44 | G | 7.6 |
| 53 | 2w | 83 | ILE | 7.6 |
| 52 | 2v | 475 | ASN | 7.6 |
| 53 | 2w | 42 | LYS | 7.6 |
| 53 | 2w | 102 | ASN | 7.6 |
| 25 | 24 | 54 | GLY | 7.5 |
| 54 | 2x | 4 | C | 7.5 |
| 41 | 2k | 49 | GLY | 7.5 |
| 7 | 2H | 24 | VAL | 7.5 |
| 52 | 2v | 426 | GLN | 7.5 |
| 37 | 2g | 96 | GLN | 7.5 |
| 53 | 2w | 56 | ALA | 7.5 |

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| Mol | Chain | Res | Type | RSRZ |
|---|---|---|---|---|
| 37 | 2g | 69 | VAL | 7.5 |
| 33 | 1c | 131 | ARG | 7.4 |
| 33 | 2c | 71 | ALA | 7.4 |
| 35 | 2e | 10 | MET | 7.4 |
| 54 | 2x | 2 | C | 7.4 |
| 33 | 1c | 59 | ARG | 7.4 |
| 20 | 2Z | 201 | LYS | 7.4 |
| 54 | 2x | 25 | C | 7.4 |
| 53 | 2w | 91 | ASN | 7.3 |
| 52 | 2v | 561 | VAL | 7.3 |
| 40 | 1j | 63 | PHE | 7.3 |
| 52 | 2v | 609 | GLU | 7.3 |
| 33 | 2c | 72 | LYS | 7.2 |
| 33 | 2c | 89 | GLU | 7.2 |
| 54 | 2x | 29 | G | 7.2 |
| 7 | 2H | 25 | LYS | 7.2 |
| 54 | 2x | 10 | G | 7.2 |
| 37 | 2g | 140 | ASP | 7.2 |
| 37 | 1g | 156 | TRP | 7.2 |
| 52 | 2v | 687 | LEU | 7.1 |
| 37 | 1g | 89 | MET | 7.1 |
| 53 | 2w | 89 | GLY | 7.1 |
| 1 | 2A | 2115 | G | 7.1 |
| 53 | 2w | 86 | SER | 7.1 |
| 37 | 2g | 146 | GLU | 7.1 |
| 53 | 2w | 1 | MET | 7.1 |
| 42 | 2l | 94 | PRO | 7.1 |
| 33 | 2c | 86 | VAL | 7.1 |
| 37 | 2g | 141 | VAL | 7.0 |
| 22 | 1l | 2 | SER | 7.0 |
| 52 | 2v | 656 | ALA | 7.0 |
| 54 | 2x | 67 | C | 7.0 |
| 37 | 1g | 84 | ASN | 7.0 |
| 29 | 2S | 12 | LYS | 7.0 |
| 39 | 1i | 127 | LYS | 7.0 |
| 54 | 2y | 63 | G | 7.0 |
| 33 | 1c | 58 | GLU | 7.0 |
| 35 | 2e | 8 | GLU | 7.0 |
| 41 | 2k | 77 | MET | 7.0 |
| 41 | 2k | 16 | SER | 6.9 |
| 47 | 2q | 9 | VAL | 6.9 |
| 54 | 2x | 26 | A | 6.9 |

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| Mol | Chain | Res | Type | RSRZ |
|---|---|---|---|---|
| 54 | 2x | 36 | A | 6.9 |
| 52 | 2v | 595 | GLN | 6.9 |
| 33 | 1c | 201 | TYR | 6.9 |
| 52 | 2v | 441 | SER | 6.9 |
| 37 | 1g | 88 | PRO | 6.9 |
| 52 | 2v | 556 | ILE | 6.9 |
| 53 | 2w | 98 | ALA | 6.9 |
| 6 | 2G | 155 | MET | 6.9 |
| 1 | 2A | 2146 | C | 6.9 |
| 27 | 26 | 23 | THR | 6.9 |
| 52 | 2v | 428 | LEU | 6.8 |
| 54 | 2x | 38 | A | 6.8 |
| 47 | 2q | 59 | ILE | 6.8 |
| 37 | 2g | 129 | GLU | 6.8 |
| 42 | 2l | 67 | THR | 6.8 |
| 33 | 1c | 56 | ASP | 6.8 |
| 52 | 2v | 488 | THR | 6.8 |
| 44 | 2n | 44 | LEU | 6.8 |
| 52 | 2v | 409 | ILE | 6.8 |
| 33 | 2c | 44 | GLU | 6.7 |
| 52 | 2v | 502 | GLY | 6.7 |
| 33 | 1c | 103 | VAL | 6.7 |
| 1 | 2A | 2131 | G | 6.7 |
| 52 | 1v | 503 | GLY | 6.7 |
| 52 | 2v | 653 | PHE | 6.7 |
| 37 | 2g | 16 | LEU | 6.7 |
| 20 | 2Z | 191 | VAL | 6.7 |
| 6 | 2G | 81 | LYS | 6.7 |
| 37 | 2g | 142 | GLU | 6.7 |
| 42 | 2l | 33 | ARG | 6.7 |
| 6 | 2G | 45 | GLU | 6.6 |
| 52 | 2v | 567 | LEU | 6.6 |
| 33 | 2c | 45 | LYS | 6.6 |
| 37 | 2g | 68 | ASN | 6.6 |
| 53 | 2w | 47 | GLY | 6.6 |
| 27 | 26 | 53 | LYS | 6.6 |
| 52 | 2v | 412 | ALA | 6.6 |
| 33 | 1c | 170 | GLN | 6.6 |
| 54 | 2y | 41 | C | 6.6 |
| 53 | 2w | 96 | GLY | 6.6 |
| 33 | 1c | 164 | ARG | 6.6 |
| 37 | 1g | 90 | GLU | 6.6 |

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| Mol | Chain | Res | Type | RSRZ |
|---|---|---|---|---|
| 52 | 2v | 469 | GLU | 6.6 |
| 54 | 2y | 5 | G | 6.6 |
| 37 | 2g | 132 | GLY | 6.6 |
| 33 | 1c | 57 | ILE | 6.6 |
| 33 | 1c | 55 | VAL | 6.6 |
| 53 | 2w | 146 | GLU | 6.6 |
| 54 | 2x | 15 | G | 6.6 |
| 53 | 2w | 69 | GLN | 6.6 |
| 54 | 2y | 3 | C | 6.6 |
| 40 | 1j | 46 | ARG | 6.5 |
| 52 | 2v | 594 | VAL | 6.5 |
| 33 | 1c | 54 | ARG | 6.5 |
| 52 | 2v | 670 | VAL | 6.5 |
| 53 | 2w | 39 | LEU | 6.5 |
| 54 | 2y | 64 | A | 6.5 |
| 6 | 2G | 135 | LEU | 6.5 |
| 52 | 2v | 444 | PRO | 6.5 |
| 53 | 2w | 55 | ILE | 6.5 |
| 47 | 2q | 23 | VAL | 6.5 |
| 52 | 2v | 417 | THR | 6.5 |
| 47 | 2q | 25 | ARG | 6.5 |
| 54 | 2y | 18 | G | 6.5 |
| 6 | 2G | 72 | ARG | 6.4 |
| 6 | 2G | 43 | LEU | 6.4 |
| 33 | 2c | 75 | VAL | 6.4 |
| 30 | 29 | 15 | LYS | 6.4 |
| 33 | 1c | 162 | GLN | 6.4 |
| 33 | 2c | 85 | ARG | 6.4 |
| 6 | 2G | 157 | ILE | 6.4 |
| 20 | 2Z | 79 | ARG | 6.4 |
| 44 | 2n | 26 | ARG | 6.4 |
| 53 | 2w | 143 | LEU | 6.4 |
| 1 | 2A | 2138 | C | 6.4 |
| 52 | 2v | 474 | ALA | 6.4 |
| 53 | 2w | 79 | ILE | 6.4 |
| 37 | 1g | 142 | GLU | 6.3 |
| 40 | 1j | 53 | PRO | 6.3 |
| 53 | 2w | 76 | LEU | 6.3 |
| 52 | 1v | 417 | THR | 6.3 |
| 53 | 2w | 101 | ILE | 6.3 |
| 35 | 2e | 120 | THR | 6.3 |
| 37 | 2g | 26 | PHE | 6.3 |

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| Mol | Chain | Res | Type | RSRZ |
|---|---|---|---|---|
| 10 | 2P | 50 | ARG | 6.3 |
| 33 | 1c | 191 | THR | 6.3 |
| 40 | 2j | 63 | PHE | 6.3 |
| 52 | 2v | 455 | GLY | 6.3 |
| 33 | 1c | 130 | VAL | 6.3 |
| 37 | 1g | 154 | TYR | 6.3 |
| 33 | 1c | 154 | SER | 6.3 |
| 39 | 1i | 122 | ALA | 6.2 |
| 1 | 2A | 2175 | C | 6.2 |
| 25 | 24 | 8 | LYS | 6.2 |
| 16 | 2V | 1 | MET | 6.2 |
| 37 | 1g | 75 | VAL | 6.2 |
| 37 | 2g | 130 | GLY | 6.2 |
| 37 | 2g | 58 | PRO | 6.2 |
| 49 | 2s | 59 | PRO | 6.1 |
| 1 | 2A | 2157 | G | 6.1 |
| 1 | 2A | 2155 | G | 6.1 |
| 29 | 28 | 4 | MET | 6.1 |
| 33 | 2c | 77 | ILE | 6.1 |
| 33 | 1c | 189 | ALA | 6.1 |
| 44 | 2n | 58 | LYS | 6.1 |
| 37 | 2g | 143 | ARG | 6.1 |
| 37 | 2g | 133 | GLY | 6.1 |
| 37 | 1g | 79 | ARG | 6.1 |
| 52 | 2v | 599 | PRO | 6.1 |
| 9 | 2O | 1 | MET | 6.0 |
| 33 | 2c | 87 | LEU | 6.0 |
| 52 | 2v | 548 | GLU | 6.0 |
| 52 | 2v | 425 | SER | 6.0 |
| 52 | 2v | 503 | GLY | 6.0 |
| 1 | 1A | 2141 | G | 6.0 |
| 52 | 2v | 465 | ARG | 6.0 |
| 41 | 1k | 88 | GLY | 6.0 |
| 44 | 1n | 58 | LYS | 6.0 |
| 53 | 2w | 57 | THR | 6.0 |
| 33 | 1c | 4 | LYS | 6.0 |
| 27 | 26 | 27 | LYS | 6.0 |
| 41 | 2k | 13 | GLN | 6.0 |
| 52 | 2v | 580 | MET | 6.0 |
| 52 | 2v | 612 | THR | 6.0 |
| 39 | 2i | 57 | GLY | 5.9 |
| 39 | 2i | 115 | GLY | 5.9 |

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| Mol | Chain | Res | Type | RSRZ |
|---|---|---|---|---|
| 52 | 1v | 512 | ILE | 5.9 |
| 20 | 2Z | 78 | LYS | 5.9 |
| 52 | 2v | 496 | LYS | 5.9 |
| 34 | 2d | 168 | ARG | 5.9 |
| 33 | 1c | 68 | VAL | 5.9 |
| 52 | 2v | 632 | LEU | 5.9 |
| 29 | 28 | 13 | ARG | 5.9 |
| 40 | 2j | 56 | HIS | 5.9 |
| 54 | 2x | 14 | A | 5.9 |
| 33 | 1c | 166 | GLU | 5.9 |
| 37 | 2g | 93 | PRO | 5.9 |
| 8 | 2N | 140 | VAL | 5.9 |
| 33 | 2c | 90 | GLU | 5.8 |
| 39 | 2i | 52 | ALA | 5.8 |
| 44 | 1n | 26 | ARG | 5.8 |
| 53 | 2w | 92 | PRO | 5.8 |
| 52 | 2v | 415 | PRO | 5.8 |
| 54 | 2y | 60 | U | 5.8 |
| 53 | 2w | 33 | ALA | 5.8 |
| 33 | 1c | 183 | ASP | 5.8 |
| 33 | 1c | 160 | ALA | 5.8 |
| 37 | 2g | 138 | LYS | 5.8 |
| 38 | 2h | 129 | VAL | 5.8 |
| 1 | 2A | 2151 | G | 5.8 |
| 54 | 2y | 4 | C | 5.8 |
| 54 | 2y | 65 | G | 5.8 |
| 37 | 1g | 83 | ALA | 5.7 |
| 52 | 2v | 430 | ARG | 5.7 |
| 33 | 2c | 49 | SER | 5.7 |
| 33 | 2c | 28 | GLN | 5.7 |
| 52 | 2v | 610 | VAL | 5.7 |
| 37 | 2g | 61 | VAL | 5.7 |
| 47 | 2q | 100 | LYS | 5.7 |
| 31 | 1a | 1030(B) | C | 5.7 |
| 6 | 2G | 86 | MET | 5.7 |
| 53 | 2w | 110 | ARG | 5.7 |
| 37 | 1g | 148 | ASN | 5.7 |
| 33 | 1c | 52 | LEU | 5.7 |
| 52 | 1v | 505 | GLY | 5.7 |
| 47 | 2q | 26 | GLN | 5.7 |
| 41 | 2k | 14 | VAL | 5.7 |
| 37 | 2g | 150 | ALA | 5.6 |

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| Mol | Chain | Res | Type | RSRZ |
|---|---|---|---|---|
| 39 | 1i | 116 | LYS | 5.6 |
| 41 | 2k | 90 | GLY | 5.6 |
| 33 | 2c | 82 | GLU | 5.6 |
| 37 | 1g | 101 | LEU | 5.6 |
| 33 | 1c | 85 | ARG | 5.6 |
| 51 | 2u | 2 | GLY | 5.6 |
| 52 | 1v | 510 | VAL | 5.6 |
| 33 | 1c | 159 | GLY | 5.6 |
| 33 | 2c | 156 | ARG | 5.6 |
| 1 | 2A | 2106 | G | 5.6 |
| 52 | 2v | 585 | ALA | 5.6 |
| 1 | 2A | 2133 | G | 5.6 |
| 10 | 2P | 76 | LYS | 5.6 |
| 52 | 2v | 449 | THR | 5.6 |
| 33 | 1c | 65 | ALA | 5.6 |
| 44 | 2n | 22 | THR | 5.6 |
| 54 | 1y | 47 | U | 5.6 |
| 52 | 2v | 630 | GLN | 5.6 |
| 52 | 2v | 554 | PRO | 5.6 |
| 41 | 1k | 89 | ALA | 5.6 |
| 52 | 2v | 489 | LYS | 5.6 |
| 52 | 2v | 576 | ASP | 5.6 |
| 53 | 2w | 85 | ASP | 5.6 |
| 1 | 2A | 2104 | G | 5.5 |
| 33 | 1c | 127 | ARG | 5.5 |
| 40 | 1j | 48 | THR | 5.5 |
| 49 | 1s | 82 | GLY | 5.5 |
| 53 | 2w | 113 | ASP | 5.5 |
| 37 | 1g | 141 | VAL | 5.5 |
| 43 | 1m | 94 | ARG | 5.5 |
| 35 | 2e | 89 | ILE | 5.5 |
| 1 | 2A | 2105 | C | 5.5 |
| 37 | 2g | 65 | ALA | 5.5 |
| 52 | 1v | 499 | ARG | 5.5 |
| 54 | 2y | 53 | G | 5.5 |
| 35 | 2e | 118 | ILE | 5.5 |
| 52 | 2v | 525 | PHE | 5.5 |
| 41 | 2k | 15 | ALA | 5.5 |
| 14 | 2T | 39 | ARG | 5.5 |
| 41 | 2k | 98 | LEU | 5.5 |
| 52 | 2v | 665 | GLY | 5.5 |
| 6 | 2G | 90 | LEU | 5.5 |

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| Mol | Chain | Res | Type | RSRZ |
|---|---|---|---|---|
| 27 | 26 | 26 | ASN | 5.5 |
| 54 | 2y | 42 | C | 5.5 |
| 43 | 2m | 116 | THR | 5.4 |
| 41 | 1k | 50 | TYR | 5.4 |
| 31 | 2a | 1030(A) | G | 5.4 |
| 33 | 1c | 165 | THR | 5.4 |
| 42 | 2l | 18 | VAL | 5.4 |
| 43 | 2m | 110 | ARG | 5.4 |
| 52 | 2v | 544 | LYS | 5.4 |
| 40 | 1j | 59 | SER | 5.4 |
| 10 | 2P | 46 | LYS | 5.4 |
| 33 | 2c | 41 | GLY | 5.4 |
| 37 | 2g | 136 | LYS | 5.4 |
| 31 | 1a | 901 | A | 5.4 |
| 6 | 2G | 39 | ILE | 5.4 |
| 33 | 1c | 15 | THR | 5.4 |
| 9 | 1O | 41 | ALA | 5.4 |
| 33 | 1c | 105 | GLU | 5.4 |
| 22 | 21 | 36 | GLY | 5.4 |
| 41 | 2k | 79 | SER | 5.4 |
| 33 | 1c | 138 | VAL | 5.4 |
| 33 | 1c | 153 | VAL | 5.4 |
| 33 | 1c | 195 | VAL | 5.4 |
| 53 | 2w | 34 | ASN | 5.4 |
| 33 | 1c | 67 | THR | 5.4 |
| 52 | 2v | 589 | ALA | 5.4 |
| 42 | 2l | 66 | VAL | 5.4 |
| 54 | 2y | 72 | C | 5.4 |
| 29 | 28 | 10 | ALA | 5.3 |
| 41 | 2k | 17 | GLY | 5.3 |
| 22 | 21 | 38 | SER | 5.3 |
| 52 | 2v | 543 | GLN | 5.3 |
| 33 | 2c | 91 | LEU | 5.3 |
| 35 | 2e | 109 | ILE | 5.3 |
| 52 | 1v | 594 | VAL | 5.3 |
| 9 | 2O | 84 | ALA | 5.3 |
| 37 | 2g | 134 | ALA | 5.3 |
| 53 | 2w | 52 | LEU | 5.3 |
| 1 | 2A | 2145 | C | 5.3 |
| 52 | 1v | 509 | HIS | 5.3 |
| 53 | 2w | 37 | LEU | 5.3 |
| 52 | 2v | 642 | VAL | 5.3 |

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| Mol | Chain | Res | Type | RSRZ |
|---|---|---|---|---|
| 52 | 2v | 510 | VAL | 5.3 |
| 52 | 2v | 635 | GLU | 5.3 |
| 37 | 1g | 18 | TYR | 5.3 |
| 31 | 2a | 956 | U | 5.3 |
| 40 | 1j | 72 | VAL | 5.3 |
| 37 | 2g | 100 | ALA | 5.3 |
| 33 | 1c | 102 | ASN | 5.3 |
| 54 | 1x | 24 | G | 5.3 |
| 52 | 2v | 499 | ARG | 5.3 |
| 22 | 21 | 66 | HIS | 5.3 |
| 1 | 1A | 2152 | G | 5.3 |
| 54 | 2y | 15 | G | 5.3 |
| 54 | 2y | 27 | G | 5.3 |
| 44 | 1n | 37 | PHE | 5.3 |
| 10 | 2P | 59 | LEU | 5.2 |
| 52 | 2v | 673 | PHE | 5.2 |
| 21 | 10 | 10 | THR | 5.2 |
| 52 | 2v | 408 | VAL | 5.2 |
| 39 | 2i | 51 | ARG | 5.2 |
| 10 | 2P | 108 | LYS | 5.2 |
| 1 | 2A | 887 | A | 5.2 |
| 32 | 1b | 233 | SER | 5.2 |
| 35 | 2e | 88 | LYS | 5.2 |
| 9 | 2O | 20 | MET | 5.2 |
| 33 | 2c | 37 | GLN | 5.2 |
| 37 | 1g | 69 | VAL | 5.2 |
| 5 | 2F | 87 | GLY | 5.2 |
| 43 | 2m | 113 | PRO | 5.2 |
| 35 | 2e | 130 | ASN | 5.2 |
| 55 | 2z | 19 | U | 5.1 |
| 42 | 2l | 23 | LYS | 5.1 |
| 42 | 2l | 56 | ALA | 5.1 |
| 10 | 2P | 72 | PRO | 5.1 |
| 54 | 2y | 19 | G | 5.1 |
| 20 | 2Z | 200 | GLY | 5.1 |
| 53 | 2w | 109 | GLU | 5.1 |
| 9 | 2O | 101 | PRO | 5.1 |
| 43 | 1m | 118 | ALA | 5.1 |
| 55 | 1z | 19 | U | 5.1 |
| 53 | 2w | 95 | LYS | 5.1 |
| 37 | 2g | 24 | THR | 5.1 |
| 1 | 2A | 229 | A | 5.1 |

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| Mol | Chain | Res | Type | RSRZ |
|---|---|---|---|---|
| 1 | 2A | 2129 | C | 5.1 |
| 33 | 1c | 101 | LEU | 5.1 |
| 1 | 1A | 2602 | A | 5.1 |
| 37 | 1g | 143 | ARG | 5.1 |
| 54 | 2y | 40 | C | 5.1 |
| 1 | 2A | 2119 | A | 5.1 |
| 33 | 2c | 31 | HIS | 5.1 |
| 33 | 1c | 7 | PRO | 5.1 |
| 37 | 1g | 72 | ARG | 5.1 |
| 33 | 2c | 189 | ALA | 5.1 |
| 40 | 1j | 50 | ILE | 5.1 |
| 39 | 2i | 53 | VAL | 5.1 |
| 44 | 1n | 25 | VAL | 5.1 |
| 33 | 1c | 158 | GLY | 5.1 |
| 33 | 2c | 84 | ILE | 5.1 |
| 42 | 2l | 14 | GLY | 5.1 |
| 6 | 2G | 73 | ALA | 5.0 |
| 7 | 2H | 89 | ILE | 5.0 |
| 52 | 1v | 413 | ILE | 5.0 |
| 40 | 1j | 8 | LEU | 5.0 |
| 42 | 2l | 22 | SER | 5.0 |
| 33 | 2c | 55 | VAL | 5.0 |
| 54 | 2y | 7 | A | 5.0 |
| 54 | 1x | 1 | G | 5.0 |
| 35 | 2e | 81 | GLU | 5.0 |
| 55 | 2z | 20 | A | 5.0 |
| 9 | 2O | 22 | ILE | 5.0 |
| 1 | 2A | 2174 | C | 5.0 |
| 47 | 2q | 71 | PHE | 5.0 |
| 40 | 2j | 46 | ARG | 5.0 |
| 33 | 2c | 68 | VAL | 5.0 |
| 53 | 2w | 50 | VAL | 5.0 |
| 37 | 2g | 99 | LEU | 5.0 |
| 37 | 2g | 123 | GLU | 5.0 |
| 33 | 1c | 8 | ILE | 5.0 |
| 37 | 1g | 145 | ALA | 5.0 |
| 41 | 2k | 97 | ALA | 5.0 |
| 52 | 2v | 562 | ASP | 5.0 |
| 6 | 2G | 52 | ILE | 5.0 |
| 33 | 1c | 150 | LYS | 5.0 |
| 31 | 1a | 1030(C) | G | 5.0 |
| 14 | 1T | 45 | PHE | 5.0 |

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| Mol | Chain | Res | Type | RSRZ |
|---|---|---|---|---|
| 27 | 26 | 28 | ARG | 5.0 |
| 54 | 2y | 43 | C | 5.0 |
| 52 | 1v | 506 | GLN | 5.0 |
| 49 | 2s | 82 | GLY | 5.0 |
| 52 | 2v | 463 | VAL | 5.0 |
| 31 | 2a | 1488 | G | 5.0 |
| 54 | 1x | 74 | C | 5.0 |
| 33 | 2c | 66 | VAL | 4.9 |
| 33 | 2c | 74 | GLY | 4.9 |
| 40 | 1j | 64 | GLU | 4.9 |
| 44 | 1n | 49 | HIS | 4.9 |
| 9 | 2O | 64 | ARG | 4.9 |
| 37 | 1g | 97 | GLN | 4.9 |
| 47 | 2q | 58 | GLU | 4.9 |
| 27 | 26 | 52 | VAL | 4.9 |
| 53 | 2w | 153 | GLU | 4.9 |
| 37 | 1g | 100 | ALA | 4.9 |
| 22 | 11 | 22 | GLY | 4.9 |
| 37 | 1g | 87 | VAL | 4.9 |
| 53 | 2w | 48 | ALA | 4.9 |
| 6 | 2G | 74 | LYS | 4.9 |
| 54 | 2y | 2 | C | 4.9 |
| 33 | 1c | 75 | VAL | 4.9 |
| 52 | 1v | 87 | HIS | 4.9 |
| 33 | 1c | 202 | ILE | 4.9 |
| 24 | 13 | 60 | GLU | 4.9 |
| 44 | 1n | 30 | ALA | 4.9 |
| 53 | 2w | 78 | ALA | 4.9 |
| 17 | 1W | 112 | GLY | 4.9 |
| 37 | 1g | 149 | ARG | 4.9 |
| 54 | 2y | 44 | G | 4.9 |
| 8 | 2N | 16 | ILE | 4.9 |
| 4 | 1E | 143 | ASN | 4.9 |
| 31 | 1a | 1397 | C | 4.9 |
| 54 | 2x | 42 | C | 4.9 |
| 48 | 2r | 22 | VAL | 4.9 |
| 53 | 2w | 82 | ALA | 4.8 |
| 14 | 1T | 46 | GLU | 4.8 |
| 33 | 2c | 101 | LEU | 4.8 |
| 22 | 21 | 6 | GLU | 4.8 |
| 37 | 2g | 126 | ASP | 4.8 |
| 1 | 2A | 2107 | C | 4.8 |

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| Mol | Chain | Res | Type | RSRZ |
|---|---|---|---|---|
| 1 | 2A | 1913 | A | 4.8 |
| 1 | 1A | 2132 | U | 4.8 |
| 44 | 1n | 29 | ARG | 4.8 |
| 41 | 2k | 36 | ASP | 4.8 |
| 54 | 1y | 13 | C | 4.8 |
| 55 | 1z | 21 | A | 4.8 |
| 53 | 2w | 59 | THR | 4.8 |
| 33 | 1c | 53 | ALA | 4.8 |
| 53 | 2w | 63 | PRO | 4.8 |
| 6 | 2G | 152 | LEU | 4.8 |
| 20 | 2Z | 23 | LYS | 4.8 |
| 27 | 26 | 34 | LEU | 4.8 |
| 6 | 2G | 80 | PHE | 4.8 |
| 37 | 2g | 53 | LYS | 4.8 |
| 52 | 2v | 464 | ASP | 4.8 |
| 22 | 21 | 37 | ILE | 4.8 |
| 54 | 2y | 73 | A | 4.8 |
| 40 | 1j | 49 | VAL | 4.8 |
| 40 | 1j | 58 | ASP | 4.8 |
| 47 | 2q | 21 | VAL | 4.8 |
| 1 | 1A | 2151 | G | 4.8 |
| 14 | 2T | 46 | GLU | 4.8 |
| 33 | 1c | 129 | ALA | 4.8 |
| 37 | 2g | 147 | ALA | 4.8 |
| 39 | 1i | 110 | GLU | 4.8 |
| 49 | 2s | 61 | TYR | 4.7 |
| 1 | 2A | 2117 | A | 4.7 |
| 45 | 2o | 89 | GLY | 4.7 |
| 52 | 2v | 470 | PHE | 4.7 |
| 33 | 2c | 39 | ILE | 4.7 |
| 33 | 2c | 131 | ARG | 4.7 |
| 37 | 2g | 18 | TYR | 4.7 |
| 49 | 1s | 81 | ARG | 4.7 |
| 6 | 2G | 159 | VAL | 4.7 |
| 52 | 2v | 542 | VAL | 4.7 |
| 11 | 2Q | 17 | LEU | 4.7 |
| 47 | 2q | 43 | LEU | 4.7 |
| 6 | 2G | 134 | GLY | 4.7 |
| 27 | 26 | 8 | LYS | 4.7 |
| 29 | 28 | 9 | GLY | 4.7 |
| 49 | 2s | 58 | VAL | 4.7 |
| 52 | 1v | 524 | GLU | 4.7 |

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| Mol | Chain | Res | Type | RSRZ |
|---|---|---|---|---|
| 1 | 2A | 2123 | G | 4.7 |
| 6 | 2G | 144 | ILE | 4.7 |
| 14 | 1T | 84 | GLN | 4.7 |
| 33 | 1c | 128 | PHE | 4.7 |
| 27 | 26 | 50 | ARG | 4.7 |
| 33 | 2c | 88 | ARG | 4.7 |
| 52 | 2v | 650 | ALA | 4.7 |
| 53 | 2w | 88 | LEU | 4.7 |
| 24 | 23 | 60 | GLU | 4.7 |
| 37 | 2g | 10 | ARG | 4.7 |
| 44 | 1n | 39 | LEU | 4.7 |
| 14 | 2T | 45 | PHE | 4.7 |
| 35 | 2e | 106 | PRO | 4.7 |
| 54 | 2x | 33 | U | 4.7 |
| 21 | 20 | 10 | THR | 4.7 |
| 54 | 1y | 44 | G | 4.7 |
| 37 | 1g | 99 | LEU | 4.7 |
| 6 | 2G | 82 | LEU | 4.6 |
| 9 | 1O | 120 | GLU | 4.6 |
| 52 | 2v | 457 | LEU | 4.6 |
| 52 | 2v | 689 | LYS | 4.6 |
| 20 | 2Z | 5 | LEU | 4.6 |
| 37 | 2g | 20 | ASP | 4.6 |
| 42 | 2l | 20 | LYS | 4.6 |
| 37 | 2g | 64 | GLN | 4.6 |
| 47 | 2q | 98 | LEU | 4.6 |
| 6 | 2G | 147 | ASP | 4.6 |
| 29 | 28 | 29 | LYS | 4.6 |
| 22 | 21 | 27 | GLU | 4.6 |
| 7 | 2H | 26 | VAL | 4.6 |
| 27 | 26 | 22 | ALA | 4.6 |
| 37 | 2g | 57 | GLU | 4.6 |
| 7 | 2H | 105 | LEU | 4.6 |
| 10 | 2P | 45 | LEU | 4.6 |
| 37 | 2g | 17 | VAL | 4.6 |
| 52 | 2v | 579 | GLU | 4.6 |
| 7 | 2H | 162 | ILE | 4.6 |
| 33 | 1c | 39 | ILE | 4.6 |
| 33 | 1c | 142 | MET | 4.6 |
| 39 | 2i | 95 | LYS | 4.6 |
| 42 | 1l | 89 | ARG | 4.6 |
| 52 | 2v | 547 | GLU | 4.6 |

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| Mol | Chain | Res | Type | RSRZ |
|---|---|---|---|---|
| 6 | 2G | 83 | ARG | 4.6 |
| 9 | 2O | 102 | VAL | 4.6 |
| 10 | 2P | 149 | GLU | 4.6 |
| 52 | 2v | 93 | GLU | 4.6 |
| 29 | 28 | 61 | LEU | 4.6 |
| 3 | 2D | 5 | LYS | 4.6 |
| 52 | 1v | 523 | PHE | 4.6 |
| 54 | 2x | 30 | G | 4.6 |
| 44 | 1n | 55 | GLY | 4.6 |
| 31 | 1a | 935 | A | 4.6 |
| 52 | 2v | 592 | GLU | 4.6 |
| 33 | 1c | 188 | LEU | 4.6 |
| 6 | 2G | 63 | ILE | 4.6 |
| 37 | 2g | 21 | VAL | 4.6 |
| 39 | 1i | 115 | GLY | 4.6 |
| 37 | 2g | 27 | ILE | 4.5 |
| 22 | 11 | 23 | LYS | 4.5 |
| 39 | 2i | 54 | ASP | 4.5 |
| 29 | 28 | 3 | LYS | 4.5 |
| 52 | 1v | 471 | LYS | 4.5 |
| 9 | 1O | 26 | LYS | 4.5 |
| 15 | 2U | 72 | HIS | 4.5 |
| 41 | 2k | 40 | ILE | 4.5 |
| 41 | 1k | 51 | LYS | 4.5 |
| 11 | 2Q | 97 | VAL | 4.5 |
| 37 | 2g | 105 | VAL | 4.5 |
| 42 | 2l | 31 | PRO | 4.5 |
| 31 | 1a | 1035 | A | 4.5 |
| 53 | 2w | 81 | LYS | 4.5 |
| 43 | 2m | 93 | ARG | 4.5 |
| 49 | 1s | 83 | HIS | 4.5 |
| 9 | 2O | 83 | ALA | 4.5 |
| 54 | 2y | 49 | C | 4.5 |
| 26 | 15 | 60 | VAL | 4.5 |
| 1 | 2A | 1118 | C | 4.5 |
| 7 | 2H | 33 | LEU | 4.5 |
| 22 | 21 | 22 | GLY | 4.5 |
| 37 | 2g | 62 | PHE | 4.5 |
| 37 | 1g | 146 | GLU | 4.5 |
| 42 | 2l | 93 | LEU | 4.5 |
| 52 | 2v | 484 | ARG | 4.5 |
| 6 | 2G | 47 | LYS | 4.5 |

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| Mol | Chain | Res | Type | RSRZ |
|---|---|---|---|---|
| 41 | 2k | 50 | TYR | 4.5 |
| 47 | 2q | 22 | LEU | 4.5 |
| 4 | 1E | 142 | GLY | 4.5 |
| 43 | 2m | 111 | LYS | 4.5 |
| 33 | 2c | 157 | ILE | 4.5 |
| 6 | 2G | 141 | PHE | 4.5 |
| 9 | 1O | 59 | LYS | 4.5 |
| 37 | 2g | 131 | LYS | 4.5 |
| 34 | 2d | 68 | TYR | 4.4 |
| 33 | 1c | 5 | ILE | 4.4 |
| 47 | 2q | 38 | ARG | 4.4 |
| 1 | 2A | 2179 | C | 4.4 |
| 1 | 2A | 2185 | C | 4.4 |
| 33 | 1c | 28 | GLN | 4.4 |
| 33 | 1c | 38 | ARG | 4.4 |
| 39 | 1i | 125 | TYR | 4.4 |
| 3 | 2D | 231 | HIS | 4.4 |
| 34 | 2d | 102 | ASP | 4.4 |
| 33 | 2c | 155 | GLY | 4.4 |
| 54 | 1y | 14 | A | 4.4 |
| 19 | 2Y | 64 | GLU | 4.4 |
| 37 | 1g | 134 | ALA | 4.4 |
| 4 | 2E | 126 | PRO | 4.4 |
| 37 | 1g | 155 | ARG | 4.4 |
| 44 | 1n | 35 | ARG | 4.4 |
| 47 | 2q | 37 | LYS | 4.4 |
| 27 | 26 | 20 | ASN | 4.4 |
| 1 | 2A | 2142 | C | 4.4 |
| 40 | 1j | 89 | ASP | 4.4 |
| 41 | 2k | 99 | GLN | 4.4 |
| 6 | 2G | 75 | LYS | 4.4 |
| 11 | 2Q | 98 | LYS | 4.4 |
| 22 | 21 | 25 | LYS | 4.4 |
| 37 | 2g | 29 | LYS | 4.4 |
| 7 | 2H | 169 | VAL | 4.4 |
| 33 | 1c | 64 | VAL | 4.4 |
| 37 | 1g | 91 | VAL | 4.4 |
| 41 | 2k | 35 | PRO | 4.4 |
| 39 | 1i | 95 | LYS | 4.4 |
| 52 | 1v | -50 | GLN | 4.4 |
| 11 | 2Q | 10 | ARG | 4.4 |
| 33 | 1c | 199 | LYS | 4.4 |

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| Mol | Chain | Res | Type | RSRZ |
|---|---|---|---|---|
| 53 | 2w | 53 | ASN | 4.4 |
| 47 | 2q | 36 | ILE | 4.4 |
| 52 | 1v | 487 | ILE | 4.4 |
| 52 | 2v | 669 | PHE | 4.4 |
| 41 | 2k | 92 | GLU | 4.4 |
| 44 | 2n | 25 | VAL | 4.4 |
| 39 | 1i | 111 | ARG | 4.4 |
| 22 | 21 | 16 | ASN | 4.4 |
| 40 | 1j | 44 | VAL | 4.4 |
| 53 | 2w | 35 | PRO | 4.4 |
| 54 | 2y | 67 | C | 4.4 |
| 42 | 2l | 26 | ALA | 4.4 |
| 52 | 2v | 429 | ALA | 4.4 |
| 10 | 2P | 60 | MET | 4.4 |
| 52 | 2v | 590 | ILE | 4.4 |
| 33 | 1c | 76 | VAL | 4.4 |
| 54 | 1x | 76 | A | 4.4 |
| 10 | 2P | 51 | PHE | 4.4 |
| 31 | 1a | 1056 | U | 4.4 |
| 35 | 2e | 91 | LEU | 4.4 |
| 42 | 2l | 95 | GLY | 4.4 |
| 33 | 2c | 64 | VAL | 4.4 |
| 52 | 1v | 89 | ASP | 4.4 |
| 1 | 2A | 2181 | G | 4.4 |
| 54 | 2y | 57 | G | 4.4 |
| 54 | 2y | 58 | A | 4.3 |
| 1 | 2A | 1924 | C | 4.3 |
| 52 | 2v | 591 | LYS | 4.3 |
| 1 | 1A | 2153 | G | 4.3 |
| 31 | 2a | 1030(C) | G | 4.3 |
| 52 | 2v | 649 | LEU | 4.3 |
| 33 | 2c | 164 | ARG | 4.3 |
| 35 | 1e | 18 | ARG | 4.3 |
| 31 | 2a | 1349 | A | 4.3 |
| 9 | 2O | 65 | THR | 4.3 |
| 49 | 2s | 49 | ILE | 4.3 |
| 6 | 2G | 142 | PRO | 4.3 |
| 24 | 23 | 2 | PRO | 4.3 |
| 33 | 2c | 152 | ILE | 4.3 |
| 47 | 2q | 7 | THR | 4.3 |
| 1 | 2A | 1914 | C | 4.3 |
| 39 | 2i | 103 | THR | 4.3 |

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| Mol | Chain | Res | Type | RSRZ |
|---|---|---|---|---|
| 40 | 1j | 10 | GLY | 4.3 |
| 52 | 2v | 584 | ILE | 4.3 |
| 42 | 2l | 16 | GLU | 4.3 |
| 37 | 1g | 140 | ASP | 4.3 |
| 33 | 1c | 89 | GLU | 4.3 |
| 40 | 1j | 97 | GLU | 4.3 |
| 33 | 1c | 91 | LEU | 4.3 |
| 42 | 2l | 21 | LYS | 4.3 |
| 52 | 2v | 583 | LYS | 4.3 |
| 52 | 2v | 636 | PRO | 4.3 |
| 53 | 2w | 94 | ASN | 4.3 |
| 1 | 2A | 1925 | C | 4.3 |
| 31 | 1a | 1384 | C | 4.3 |
| 3 | 2D | 276 | LYS | 4.3 |
| 47 | 2q | 42 | TYR | 4.3 |
| 10 | 2P | 67 | MET | 4.3 |
| 31 | 2a | 957 | U | 4.3 |
| 52 | 1v | 563 | ILE | 4.3 |
| 43 | 1m | 119 | GLY | 4.3 |
| 21 | 20 | 70 | GLN | 4.2 |
| 7 | 2H | 103 | LEU | 4.2 |
| 6 | 2G | 145 | THR | 4.2 |
| 42 | 2l | 65 | GLU | 4.2 |
| 33 | 1c | 167 | TRP | 4.2 |
| 27 | 26 | 5 | VAL | 4.2 |
| 54 | 2x | 31 | A | 4.2 |
| 49 | 2s | 56 | GLN | 4.2 |
| 54 | 2y | 74 | C | 4.2 |
| 14 | 2T | 50 | ILE | 4.2 |
| 40 | 2j | 62 | HIS | 4.2 |
| 52 | 2v | 573 | HIS | 4.2 |
| 55 | 1z | 13 | A | 4.2 |
| 55 | 1z | 20 | A | 4.2 |
| 33 | 1c | 104 | GLN | 4.2 |
| 33 | 2c | 40 | ARG | 4.2 |
| 33 | 1c | 99 | VAL | 4.2 |
| 7 | 2H | 17 | VAL | 4.2 |
| 53 | 2w | 68 | VAL | 4.2 |
| 37 | 2g | 28 | ASN | 4.2 |
| 54 | 2y | 75 | C | 4.2 |
| 41 | 2k | 91 | ARG | 4.2 |
| 37 | 1g | 71 | PRO | 4.2 |

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| Mol | Chain | Res | Type | RSRZ |
|---|---|---|---|---|
| 41 | 2k | 32 | ILE | 4.2 |
| 33 | 2c | 83 | ARG | 4.2 |
| 31 | 1a | 1209 | C | 4.2 |
| 33 | 1c | 163 | ALA | 4.2 |
| 6 | 2G | 62 | LEU | 4.2 |
| 14 | 1T | 85 | LYS | 4.2 |
| 10 | 2P | 47 | ASP | 4.2 |
| 42 | 2l | 15 | ARG | 4.2 |
| 52 | 2v | 528 | ALA | 4.2 |
| 54 | 1x | 13 | C | 4.2 |
| 54 | 1y | 12 | U | 4.2 |
| 6 | 2G | 44 | GLY | 4.2 |
| 31 | 2a | 1168 | A | 4.2 |
| 54 | 1x | 15 | G | 4.2 |
| 49 | 1s | 56 | GLN | 4.2 |
| 41 | 1k | 31 | THR | 4.2 |
| 27 | 26 | 24 | GLU | 4.2 |
| 29 | 28 | 8 | LYS | 4.2 |
| 52 | 2v | 686 | LYS | 4.2 |
| 35 | 1e | 24 | ARG | 4.2 |
| 31 | 1a | 1050 | G | 4.1 |
| 9 | 2O | 45 | GLU | 4.1 |
| 33 | 2c | 73 | PRO | 4.1 |
| 14 | 2T | 67 | SER | 4.1 |
| 6 | 2G | 70 | VAL | 4.1 |
| 52 | 2v | 604 | PRO | 4.1 |
| 54 | 1x | 22 | G | 4.1 |
| 14 | 1T | 22 | PHE | 4.1 |
| 8 | 2N | 51 | PHE | 4.1 |
| 35 | 1e | 25 | ARG | 4.1 |
| 54 | 2y | 47 | U | 4.1 |
| 27 | 26 | 2 | ALA | 4.1 |
| 52 | 1v | 476 | VAL | 4.1 |
| 50 | 2t | 9 | ASN | 4.1 |
| 24 | 23 | 53 | LEU | 4.1 |
| 27 | 26 | 9 | LEU | 4.1 |
| 41 | 1k | 87 | THR | 4.1 |
| 52 | 1v | -32 | LEU | 4.1 |
| 52 | 2v | 683 | VAL | 4.1 |
| 54 | 1x | 75 | C | 4.1 |
| 9 | 1O | 17 | ARG | 4.1 |
| 33 | 2c | 153 | VAL | 4.1 |

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| Mol | Chain | Res | Type | RSRZ |
|---|---|---|---|---|
| 41 | 2k | 104 | GLN | 4.1 |
| 53 | 2w | 5 | GLU | 4.1 |
| 1 | 2A | 2112 | G | 4.1 |
| 31 | 1a | 811 | C | 4.1 |
| 4 | 1E | 157 | ALA | 4.1 |
| 35 | 2e | 104 | ALA | 4.1 |
| 53 | 2w | 138 | ASP | 4.1 |
| 6 | 2G | 84 | LYS | 4.1 |
| 29 | 28 | 14 | VAL | 4.1 |
| 34 | 1d | 181 | MET | 4.1 |
| 35 | 2e | 33 | VAL | 4.1 |
| 44 | 1n | 50 | LYS | 4.1 |
| 11 | 2Q | 40 | ALA | 4.1 |
| 1 | 2A | 2113 | U | 4.1 |
| 31 | 2a | 955 | U | 4.1 |
| 34 | 1d | 7 | PRO | 4.1 |
| 8 | 2N | 52 | VAL | 4.1 |
| 44 | 2n | 45 | ARG | 4.1 |
| 11 | 2Q | 75 | THR | 4.1 |
| 44 | 1n | 61 | TRP | 4.1 |
| 54 | 2y | 26 | A | 4.1 |
| 35 | 2e | 75 | THR | 4.1 |
| 10 | 2P | 68 | GLN | 4.0 |
| 14 | 1T | 29 | ARG | 4.0 |
| 37 | 1g | 138 | LYS | 4.0 |
| 9 | 2O | 41 | ALA | 4.0 |
| 35 | 2e | 108 | ALA | 4.0 |
| 41 | 2k | 101 | SER | 4.0 |
| 53 | 2w | 49 | HIS | 4.0 |
| 52 | 2v | 476 | VAL | 4.0 |
| 31 | 2a | 1203 | C | 4.0 |
| 37 | 1g | 151 | TYR | 4.0 |
| 35 | 2e | 6 | PHE | 4.0 |
| 41 | 1k | 13 | GLN | 4.0 |
| 22 | 21 | 39 | LYS | 4.0 |
| 29 | 28 | 26 | LYS | 4.0 |
| 37 | 2g | 22 | LEU | 4.0 |
| 49 | 1s | 59 | PRO | 4.0 |
| 41 | 2k | 94 | ALA | 4.0 |
| 31 | 1a | 1028 | C | 4.0 |
| 33 | 1c | 49 | SER | 4.0 |
| 35 | 2e | 76 | ILE | 4.0 |

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| Mol | Chain | Res | Type | RSRZ |
|---|---|---|---|---|
| 49 | 2s | 47 | HIS | 4.0 |
| 53 | 2w | 80 | GLU | 4.0 |
| 44 | 1n | 36 | PHE | 4.0 |
| 1 | 2A | 2159 | G | 4.0 |
| 27 | 26 | 6 | ARG | 4.0 |
| 33 | 1c | 141 | VAL | 4.0 |
| 37 | 1g | 80 | VAL | 4.0 |
| 52 | 2v | 684 | GLN | 4.0 |
| 53 | 2w | 147 | LEU | 4.0 |
| 44 | 2n | 54 | PRO | 4.0 |
| 40 | 1j | 71 | LEU | 4.0 |
| 54 | 1y | 23 | A | 4.0 |
| 54 | 1y | 20 | U | 4.0 |
| 1 | 2A | 2186 | G | 4.0 |
| 53 | 2w | 84 | ARG | 4.0 |
| 9 | 2O | 5 | GLN | 4.0 |
| 37 | 1g | 131 | LYS | 4.0 |
| 37 | 1g | 135 | VAL | 4.0 |
| 53 | 2w | 114 | LEU | 4.0 |
| 33 | 2c | 63 | ASN | 4.0 |
| 33 | 2c | 108 | ASN | 4.0 |
| 4 | 1E | 158 | GLY | 4.0 |
| 31 | 2a | 890 | G | 4.0 |
| 27 | 26 | 4 | GLU | 4.0 |
| 33 | 2c | 104 | GLN | 4.0 |
| 31 | 1a | 1045 | C | 4.0 |
| 35 | 2e | 87 | SER | 4.0 |
| 9 | 2O | 9 | GLU | 4.0 |
| 37 | 2g | 128 | ALA | 4.0 |
| 4 | 1E | 6 | GLY | 4.0 |
| 33 | 2c | 102 | ASN | 4.0 |
| 1 | 2A | 2184 | G | 3.9 |
| 16 | 2V | 53 | GLU | 3.9 |
| 41 | 2k | 19 | ALA | 4.0 |
| 31 | 1a | 1049 | U | 3.9 |
| 41 | 2k | 78 | GLN | 3.9 |
| 37 | 2g | 135 | VAL | 3.9 |
| 31 | 1a | 1044 | A | 3.9 |
| 43 | 2m | 95 | GLY | 3.9 |
| 29 | 28 | 11 | LYS | 3.9 |
| 42 | 2l | 91 | LYS | 3.9 |
| 52 | 2v | 678 | GLU | 3.9 |

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| Mol | Chain | Res | Type | RSRZ |
|---|---|---|---|---|
| 54 | 1y | 27 | G | 3.9 |
| 41 | 1k | 90 | GLY | 3.9 |
| 51 | 2u | 3 | LYS | 3.9 |
| 31 | 2a | 1028 | C | 3.9 |
| 42 | 2l | 64 | TYR | 3.9 |
| 29 | 28 | 25 | MET | 3.9 |
| 1 | 2A | 2147 | G | 3.9 |
| 7 | 2H | 36 | PRO | 3.9 |
| 9 | 1O | 68 | GLU | 3.9 |
| 9 | 2O | 33 | ALA | 3.9 |
| 33 | 1c | 29 | TYR | 3.9 |
| 42 | 1l | 64 | TYR | 3.9 |
| 52 | 2v | 655 | TYR | 3.9 |
| 52 | 2v | 681 | LYS | 3.9 |
| 14 | 1T | 86 | ILE | 3.9 |
| 54 | 1x | 72 | C | 3.9 |
| 31 | 2a | 1517 | G | 3.9 |
| 6 | 2G | 64 | THR | 3.9 |
| 37 | 2g | 23 | VAL | 3.9 |
| 33 | 1c | 193 | TYR | 3.9 |
| 33 | 2c | 54 | ARG | 3.9 |
| 7 | 2H | 35 | VAL | 3.9 |
| 33 | 1c | 196 | LEU | 3.9 |
| 44 | 2n | 11 | LYS | 3.9 |
| 10 | 2P | 49 | ARG | 3.9 |
| 31 | 2a | 787 | A | 3.9 |
| 6 | 2G | 146 | TYR | 3.9 |
| 48 | 2r | 87 | ARG | 3.9 |
| 39 | 2i | 94 | ALA | 3.9 |
| 52 | 2v | 421 | GLN | 3.9 |
| 9 | 1O | 95 | GLY | 3.9 |
| 25 | 24 | 31 | ILE | 3.9 |
| 34 | 1d | 110 | PHE | 3.9 |
| 6 | 2G | 40 | ASN | 3.9 |
| 52 | 2v | 495 | GLY | 3.9 |
| 54 | 1x | 11 | C | 3.9 |
| 6 | 1G | 87 | PRO | 3.9 |
| 9 | 1O | 19 | ILE | 3.9 |
| 1 | 2A | 2585 | U | 3.9 |
| 40 | 2j | 64 | GLU | 3.9 |
| 31 | 1a | 1202 | G | 3.9 |
| 42 | 2l | 24 | VAL | 3.9 |

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| Mol | Chain | Res | Type | RSRZ |
|---|---|---|---|---|
| 52 | 2v | 555 | LEU | 3.9 |
| 4 | 1E | 115 | GLY | 3.8 |
| 33 | 1c | 184 | TYR | 3.8 |
| 53 | 2w | 30 | THR | 3.8 |
| 44 | 1n | 2 | ALA | 3.8 |
| 54 | 1y | 24 | G | 3.8 |
| 29 | 28 | 2 | PRO | 3.8 |
| 7 | 2H | 130 | ARG | 3.8 |
| 22 | 11 | 21 | ARG | 3.8 |
| 29 | 28 | 7 | HIS | 3.8 |
| 4 | 2E | 124 | GLY | 3.8 |
| 27 | 26 | 7 | ILE | 3.8 |
| 52 | 2v | 459 | LEU | 3.8 |
| 22 | 21 | 60 | PHE | 3.8 |
| 33 | 2c | 65 | ALA | 3.8 |
| 40 | 1j | 66 | ARG | 3.8 |
| 1 | 2A | 2143 | C | 3.8 |
| 54 | 2y | 52 | G | 3.8 |
| 37 | 1g | 16 | LEU | 3.8 |
| 52 | 1v | 565 | VAL | 3.8 |
| 9 | 2O | 42 | SER | 3.8 |
| 47 | 2q | 99 | SER | 3.8 |
| 11 | 2Q | 6 | ARG | 3.8 |
| 41 | 2k | 54 | ARG | 3.8 |
| 29 | 28 | 50 | LEU | 3.8 |
| 38 | 2h | 112 | LEU | 3.8 |
| 52 | 2v | 624 | LEU | 3.8 |
| 54 | 2y | 20 | U | 3.8 |
| 33 | 2c | 207 | VAL | 3.8 |
| 44 | 1n | 44 | LEU | 3.8 |
| 6 | 2G | 133 | LEU | 3.8 |
| 10 | 2P | 62 | LEU | 3.8 |
| 35 | 2e | 128 | PRO | 3.8 |
| 10 | 2P | 79 | ARG | 3.8 |
| 44 | 2n | 2 | ALA | 3.8 |
| 33 | 1c | 32 | LEU | 3.8 |
| 31 | 2a | 1029 | C | 3.8 |
| 40 | 1j | 73 | ASP | 3.8 |
| 7 | 2H | 104 | GLU | 3.8 |
| 52 | 1v | 489 | LYS | 3.8 |
| 53 | 2w | 139 | LYS | 3.8 |
| 7 | 2H | 90 | LYS | 3.8 |

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| Mol | Chain | Res | Type | RSRZ |
|---|---|---|---|---|
| 52 | 2v | 524 | GLU | 3.8 |
| 9 | 2O | 15 | GLY | 3.8 |
| 17 | 1W | 92 | ARG | 3.8 |
| 4 | 1E | 124 | GLY | 3.8 |
| 14 | 1T | 38 | ASN | 3.8 |
| 10 | 2P | 77 | ARG | 3.8 |
| 37 | 2g | 67 | GLU | 3.8 |
| 1 | 2A | 384 | U | 3.8 |
| 20 | 2Z | 7 | ALA | 3.8 |
| 35 | 2e | 122 | GLU | 3.8 |
| 37 | 2g | 66 | VAL | 3.7 |
| 52 | 1v | 470 | PHE | 3.7 |
| 31 | 2a | 1257 | U | 3.7 |
| 7 | 2H | 82 | GLY | 3.7 |
| 14 | 1T | 47 | GLY | 3.7 |
| 52 | 2v | 526 | VAL | 3.7 |
| 52 | 2v | 574 | GLU | 3.7 |
| 43 | 2m | 6 | GLY | 3.7 |
| 20 | 2Z | 80 | ARG | 3.7 |
| 33 | 2c | 120 | VAL | 3.7 |
| 47 | 2q | 11 | VAL | 3.7 |
| 33 | 2c | 21 | ARG | 3.7 |
| 47 | 2q | 74 | LEU | 3.7 |
| 9 | 2O | 46 | ALA | 3.7 |
| 33 | 2c | 60 | ALA | 3.7 |
| 39 | 2i | 15 | ALA | 3.7 |
| 35 | 2e | 121 | LYS | 3.7 |
| 9 | 1O | 63 | VAL | 3.7 |
| 42 | 1l | 98 | TYR | 3.7 |
| 3 | 2D | 226 | MET | 3.7 |
| 4 | 1E | 151 | TYR | 3.7 |
| 22 | 21 | 28 | GLY | 3.7 |
| 52 | 2v | 577 | SER | 3.7 |
| 1 | 2A | 2158 | A | 3.7 |
| 10 | 2P | 64 | LYS | 3.7 |
| 33 | 2c | 56 | ASP | 3.7 |
| 1 | 1A | 2140 | C | 3.7 |
| 39 | 2i | 7 | THR | 3.7 |
| 42 | 2l | 19 | ARG | 3.7 |
| 52 | 2v | 676 | TYR | 3.7 |
| 9 | 1O | 22 | ILE | 3.7 |
| 33 | 1c | 168 | ALA | 3.7 |

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| Mol | Chain | Res | Type | RSRZ |
|---|---|---|---|---|
| 44 | 1n | 17 | LYS | 3.7 |
| 19 | 2Y | 42 | VAL | 3.7 |
| 44 | 1n | 31 | ARG | 3.7 |
| 52 | 2v | 407 | PRO | 3.7 |
| 31 | 2a | 912 | C | 3.7 |
| 33 | 1c | 144 | SER | 3.7 |
| 44 | 2n | 50 | LYS | 3.7 |
| 37 | 1g | 150 | ALA | 3.7 |
| 54 | 2y | 24 | G | 3.7 |
| 39 | 1i | 81 | ILE | 3.7 |
| 9 | 1O | 5 | GLN | 3.7 |
| 42 | 1l | 26 | ALA | 3.7 |
| 27 | 26 | 51 | GLU | 3.7 |
| 40 | 1j | 95 | GLU | 3.7 |
| 52 | 1v | 468 | ARG | 3.7 |
| 54 | 1x | 25 | C | 3.7 |
| 1 | 2A | 250 | G | 3.7 |
| 54 | 2y | 28 | G | 3.7 |
| 3 | 1D | 2 | ALA | 3.7 |
| 44 | 2n | 10 | ALA | 3.7 |
| 37 | 1g | 132 | GLY | 3.7 |
| 4 | 1E | 138 | PRO | 3.7 |
| 50 | 1t | 55 | ILE | 3.7 |
| 33 | 1c | 198 | VAL | 3.7 |
| 11 | 2Q | 104 | PHE | 3.7 |
| 31 | 1a | 1383 | C | 3.7 |
| 33 | 1c | 200 | ALA | 3.7 |
| 39 | 2i | 121 | ARG | 3.7 |
| 52 | 2v | 523 | PHE | 3.7 |
| 52 | 2v | 634 | MET | 3.6 |
| 5 | 2F | 131 | GLY | 3.6 |
| 37 | 1g | 96 | GLN | 3.6 |
| 33 | 1c | 98 | ASN | 3.6 |
| 42 | 2l | 57 | LYS | 3.6 |
| 49 | 2s | 63 | THR | 3.6 |
| 33 | 1c | 126 | ARG | 3.6 |
| 52 | 2v | 416 | LYS | 3.6 |
| 39 | 2i | 58 | HIS | 3.6 |
| 9 | 1O | 21 | CYS | 3.6 |
| 49 | 2s | 29 | ARG | 3.6 |
| 39 | 2i | 93 | ARG | 3.6 |
| 54 | 1x | 70 | G | 3.6 |

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| Mol | Chain | Res | Type | RSRZ |
|---|---|---|---|---|
| 52 | 2v | 566 | THR | 3.6 |
| 8 | 1N | 83 | LYS | 3.6 |
| 14 | 1T | 105 | LEU | 3.6 |
| 52 | 2v | 575 | VAL | 3.6 |
| 1 | 2A | 2180 | U | 3.6 |
| 1 | 2A | 2602 | A | 3.6 |
| 31 | 1a | 1043 | C | 3.6 |
| 53 | 2w | 54 | GLN | 3.6 |
| 9 | 1O | 82 | ASN | 3.6 |
| 49 | 2s | 60 | VAL | 3.6 |
| 52 | 1v | 514 | VAL | 3.6 |
| 9 | 1O | 1 | MET | 3.6 |
| 37 | 2g | 8 | GLU | 3.6 |
| 37 | 2g | 92 | SER | 3.6 |
| 52 | 2v | 611 | THR | 3.6 |
| 20 | 2Z | 6 | LYS | 3.6 |
| 26 | 15 | 2 | ALA | 3.6 |
| 37 | 2g | 25 | ALA | 3.6 |
| 33 | 2c | 38 | ARG | 3.6 |
| 40 | 1j | 70 | ARG | 3.6 |
| 22 | 21 | 30 | VAL | 3.6 |
| 33 | 2c | 158 | GLY | 3.6 |
| 33 | 1c | 87 | LEU | 3.6 |
| 40 | 1j | 11 | PHE | 3.6 |
| 52 | 2v | 420 | ASP | 3.6 |
| 52 | 2v | 652 | MET | 3.6 |
| 8 | 2N | 53 | VAL | 3.6 |
| 52 | 2v | 447 | GLY | 3.6 |
| 31 | 1a | 1195 | C | 3.6 |
| 52 | 1v | 504 | ARG | 3.6 |
| 41 | 2k | 80 | VAL | 3.6 |
| 52 | 2v | 478 | LYS | 3.6 |
| 52 | 2v | 521 | SER | 3.6 |
| 37 | 2g | 127 | ALA | 3.6 |
| 53 | 2w | 75 | ALA | 3.6 |
| 39 | 1i | 7 | THR | 3.6 |
| 52 | 2v | 490 | PRO | 3.6 |
| 37 | 2g | 11 | GLN | 3.6 |
| 44 | 2n | 20 | ALA | 3.6 |
| 33 | 1c | 6 | HIS | 3.6 |
| 37 | 2g | 98 | SER | 3.6 |
| 49 | 2s | 83 | HIS | 3.6 |

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| Mol | Chain | Res | Type | RSRZ |
|---|---|---|---|---|
| 1 | 2A | 2110 | G | 3.6 |
| 43 | 2m | 114 | ARG | 3.6 |
| 50 | 1t | 9 | ASN | 3.6 |
| 8 | 2N | 128 | HIS | 3.6 |
| 52 | 2v | 571 | SER | 3.6 |
| 43 | 2m | 7 | VAL | 3.6 |
| 33 | 2c | 13 | GLY | 3.6 |
| 40 | 1j | 65 | LEU | 3.6 |
| 52 | 2v | 473 | ASP | 3.6 |
| 5 | 1F | 69 | HIS | 3.5 |
| 9 | 1O | 18 | LYS | 3.5 |
| 52 | 1v | 571 | SER | 3.5 |
| 54 | 2y | 68 | C | 3.5 |
| 52 | 2v | 514 | VAL | 3.5 |
| 9 | 1O | 64 | ARG | 3.5 |
| 34 | 2d | 164 | ALA | 3.5 |
| 37 | 1g | 127 | ALA | 3.5 |
| 8 | 2N | 8 | GLN | 3.5 |
| 26 | 15 | 59 | GLU | 3.5 |
| 33 | 1c | 33 | LEU | 3.5 |
| 52 | 1v | 426 | GLN | 3.5 |
| 1 | 2A | 2286 | A | 3.5 |
| 29 | 28 | 30 | ARG | 3.5 |
| 42 | 2l | 71 | PRO | 3.5 |
| 52 | 1v | -28 | ALA | 3.5 |
| 42 | 2l | 98 | TYR | 3.5 |
| 47 | 2q | 60 | ILE | 3.5 |
| 29 | 28 | 62 | LEU | 3.5 |
| 35 | 2e | 119 | LEU | 3.5 |
| 52 | 1v | 527 | ASN | 3.5 |
| 20 | 2Z | 202 | GLU | 3.5 |
| 22 | 21 | 21 | ARG | 3.5 |
| 33 | 1c | 44 | GLU | 3.5 |
| 54 | 1y | 6 | G | 3.5 |
| 7 | 2H | 88 | LEU | 3.5 |
| 17 | 1W | 94 | ASP | 3.5 |
| 37 | 2g | 12 | LEU | 3.5 |
| 8 | 2N | 12 | ARG | 3.5 |
| 33 | 1c | 151 | VAL | 3.5 |
| 37 | 2g | 59 | LEU | 3.5 |
| 9 | 1O | 104 | ARG | 3.5 |
| 15 | 2U | 88 | ILE | 3.5 |

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| Mol | Chain | Res | Type | RSRZ |
|---|---|---|---|---|
| 29 | 28 | 47 | LYS | 3.5 |
| 41 | 1k | 25 | TYR | 3.5 |
| 53 | 1w | 29 | ARG | 3.5 |
| 6 | 2G | 85 | GLY | 3.5 |
| 52 | 2v | 461 | ILE | 3.5 |
| 37 | 1g | 139 | GLU | 3.5 |
| 40 | 1j | 4 | ILE | 3.5 |
| 11 | 2Q | 1 | MET | 3.5 |
| 39 | 2i | 128 | ARG | 3.5 |
| 31 | 1a | 1203 | C | 3.5 |
| 8 | 2N | 15 | LEU | 3.5 |
| 4 | 1E | 125 | GLY | 3.5 |
| 14 | 2T | 62 | THR | 3.5 |
| 32 | 1b | 148 | TYR | 3.5 |
| 16 | 2V | 5 | VAL | 3.5 |
| 27 | 26 | 10 | LEU | 3.5 |
| 31 | 1a | 1194 | U | 3.5 |
| 14 | 1T | 32 | TYR | 3.5 |
| 29 | 28 | 44 | LYS | 3.5 |
| 33 | 2c | 199 | LYS | 3.5 |
| 44 | 1n | 33 | VAL | 3.5 |
| 44 | 1n | 41 | ARG | 3.5 |
| 6 | 2G | 89 | GLY | 3.5 |
| 35 | 2e | 24 | ARG | 3.5 |
| 49 | 2s | 30 | LEU | 3.5 |
| 54 | 1x | 26 | A | 3.5 |
| 14 | 1T | 43 | GLN | 3.5 |
| 52 | 1v | -47 | ASP | 3.5 |
| 9 | 2O | 120 | GLU | 3.5 |
| 9 | 1O | 107 | ARG | 3.5 |
| 37 | 1g | 104 | LEU | 3.5 |
| 52 | 2v | 644 | ARG | 3.5 |
| 1 | 2A | 382 | G | 3.5 |
| 4 | 1E | 123 | ALA | 3.5 |
| 54 | 1x | 34 | G | 3.5 |
| 9 | 2O | 38 | VAL | 3.5 |
| 33 | 2c | 48 | TYR | 3.5 |
| 33 | 2c | 201 | TYR | 3.5 |
| 49 | 1s | 76 | PRO | 3.4 |
| 33 | 1c | 37 | GLN | 3.4 |
| 4 | 1E | 153 | GLY | 3.4 |
| 33 | 1c | 69 | HIS | 3.4 |

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| Mol | Chain | Res | Type | RSRZ |
|---|---|---|---|---|
| 33 | 2c | 109 | PRO | 3.4 |
| 33 | 2c | 151 | VAL | 3.4 |
| 39 | 1i | 113 | LYS | 3.4 |
| 40 | 1j | 52 | GLY | 3.4 |
| 35 | 2e | 11 | ILE | 3.4 |
| 47 | 2q | 68 | ARG | 3.4 |
| 29 | 28 | 51 | ALA | 3.4 |
| 22 | 21 | 47 | GLN | 3.4 |
| 35 | 1e | 14 | ARG | 3.4 |
| 42 | 2l | 78 | GLN | 3.4 |
| 31 | 2a | 913 | A | 3.4 |
| 1 | 2A | 886 | C | 3.4 |
| 42 | 2l | 25 | PRO | 3.4 |
| 52 | 2v | 540 | PRO | 3.4 |
| 3 | 2D | 230 | ASP | 3.4 |
| 52 | 2v | 593 | ALA | 3.4 |
| 7 | 2H | 18 | GLU | 3.4 |
| 1 | 1A | 2062 | A | 3.4 |
| 9 | 2O | 3 | GLN | 3.4 |
| 11 | 2Q | 12 | GLN | 3.4 |
| 37 | 2g | 50 | ILE | 3.4 |
| 1 | 2A | 1922 | G | 3.4 |
| 1 | 2A | 2188 | C | 3.4 |
| 31 | 1a | 1512 | U | 3.4 |
| 3 | 2D | 166 | GLN | 3.4 |
| 33 | 1c | 152 | ILE | 3.4 |
| 39 | 1i | 77 | ILE | 3.4 |
| 4 | 1E | 155 | LYS | 3.4 |
| 41 | 2k | 71 | LYS | 3.4 |
| 22 | 21 | 17 | SER | 3.4 |
| 41 | 1k | 42 | TRP | 3.4 |
| 31 | 2a | 996 | A | 3.4 |
| 54 | 1x | 40 | C | 3.4 |
| 54 | 1x | 45 | U | 3.4 |
| 41 | 2k | 57 | THR | 3.4 |
| 52 | 1v | -64 | VAL | 3.4 |
| 33 | 2c | 22 | TRP | 3.4 |
| 9 | 1O | 122 | LEU | 3.4 |
| 21 | 20 | 21 | LEU | 3.4 |
| 1 | 2A | 226 | G | 3.4 |
| 22 | 21 | 33 | LYS | 3.4 |
| 6 | 2G | 46 | ALA | 3.4 |

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| Mol | Chain | Res | Type | RSRZ |
|---|---|---|---|---|
| 6 | 2G | 79 | ASN | 3.4 |
| 41 | 2k | 52 | GLY | 3.4 |
| 20 | 2Z | 176 | PRO | 3.4 |
| 25 | 24 | 11 | PRO | 3.4 |
| 37 | 2g | 56 | GLN | 3.4 |
| 42 | 2l | 83 | VAL | 3.4 |
| 53 | 2w | 77 | LYS | 3.4 |
| 8 | 2N | 54 | VAL | 3.4 |
| 43 | 2m | 90 | LEU | 3.4 |
| 44 | 2n | 52 | GLN | 3.4 |
| 52 | 2v | 483 | TYR | 3.4 |
| 1 | 2A | 2284 | C | 3.4 |
| 10 | 2P | 111 | ARG | 3.4 |
| 40 | 2j | 55 | LYS | 3.4 |
| 14 | 1T | 109 | GLU | 3.4 |
| 43 | 2m | 87 | TYR | 3.4 |
| 35 | 2e | 15 | ARG | 3.4 |
| 22 | 21 | 34 | THR | 3.4 |
| 52 | 2v | 560 | VAL | 3.4 |
| 4 | 1E | 154 | LYS | 3.4 |
| 35 | 2e | 31 | LEU | 3.4 |
| 42 | 2l | 13 | LYS | 3.4 |
| 52 | 2v | 462 | ILE | 3.4 |
| 33 | 1c | 79 | ARG | 3.4 |
| 52 | 2v | 637 | ARG | 3.4 |
| 10 | 2P | 109 | GLY | 3.3 |
| 22 | 11 | 36 | GLY | 3.3 |
| 52 | 2v | 468 | ARG | 3.3 |
| 14 | 1T | 83 | ILE | 3.3 |
| 27 | 26 | 21 | TYR | 3.3 |
| 46 | 1p | 4 | ILE | 3.3 |
| 14 | 1T | 87 | ASP | 3.3 |
| 10 | 2P | 44 | GLY | 3.3 |
| 44 | 2n | 41 | ARG | 3.3 |
| 20 | 2Z | 55 | HIS | 3.3 |
| 47 | 1q | 100 | LYS | 3.3 |
| 31 | 1a | 1214 | C | 3.3 |
| 6 | 2G | 102 | PHE | 3.3 |
| 9 | 2O | 14 | THR | 3.3 |
| 35 | 2e | 29 | GLY | 3.3 |
| 53 | 2w | 31 | GLY | 3.3 |
| 42 | 2l | 52 | LEU | 3.3 |

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| Mol | Chain | Res | Type | RSRZ |
|---|---|---|---|---|
| 22 | 21 | 10 | LYS | 3.3 |
| 26 | 15 | 3 | LYS | 3.3 |
| 31 | 2a | 250 | A | 3.3 |
| 33 | 2c | 70 | VAL | 3.3 |
| 9 | 2O | 56 | ASP | 3.3 |
| 31 | 2a | 84 | U | 3.3 |
| 37 | 2g | 122 | HIS | 3.3 |
| 41 | 2k | 43 | SER | 3.3 |
| 37 | 2g | 94 | ARG | 3.3 |
| 40 | 1j | 5 | ARG | 3.3 |
| 11 | 2Q | 33 | GLY | 3.3 |
| 37 | 1g | 81 | GLY | 3.3 |
| 37 | 2g | 102 | ARG | 3.3 |
| 6 | 2G | 131 | TYR | 3.3 |
| 11 | 2Q | 25 | ASP | 3.3 |
| 33 | 1c | 9 | GLY | 3.3 |
| 1 | 2A | 1039 | G | 3.3 |
| 29 | 28 | 46 | ARG | 3.3 |
| 52 | 2v | 588 | MET | 3.3 |
| 7 | 2H | 168 | PRO | 3.3 |
| 48 | 2r | 84 | LYS | 3.3 |
| 52 | 2v | 613 | PRO | 3.3 |
| 4 | 1E | 137 | HIS | 3.3 |
| 41 | 2k | 118 | GLY | 3.3 |
| 1 | 2A | 245 | G | 3.3 |
| 9 | 1O | 86 | ILE | 3.3 |
| 4 | 1E | 140 | SER | 3.3 |
| 41 | 2k | 41 | THR | 3.3 |
| 17 | 1W | 90 | ARG | 3.3 |
| 30 | 29 | 12 | ASP | 3.3 |
| 35 | 2e | 77 | PRO | 3.3 |
| 35 | 2e | 129 | ILE | 3.3 |
| 37 | 1g | 17 | VAL | 3.3 |
| 53 | 2w | 105 | PRO | 3.3 |
| 22 | 11 | 34 | THR | 3.3 |
| 29 | 28 | 65 | GLU | 3.3 |
| 33 | 2c | 27 | LYS | 3.3 |
| 41 | 2k | 96 | ARG | 3.3 |
| 1 | 2A | 251 | A | 3.3 |
| 4 | 1E | 129 | HIS | 3.3 |
| 17 | 1W | 111 | HIS | 3.3 |
| 31 | 2a | 1378 | C | 3.3 |

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| Mol | Chain | Res | Type | RSRZ |
|---|---|---|---|---|
| 33 | 1c | 204 | LEU | 3.3 |
| 33 | 2c | 93 | LYS | 3.3 |
| 11 | 2Q | 90 | VAL | 3.3 |
| 41 | 1k | 30 | VAL | 3.3 |
| 21 | 20 | 76 | GLY | 3.2 |
| 41 | 2k | 51 | LYS | 3.2 |
| 6 | 2G | 78 | SER | 3.2 |
| 41 | 1k | 32 | ILE | 3.2 |
| 1 | 1A | 2586 | C | 3.2 |
| 33 | 2c | 67 | THR | 3.2 |
| 9 | 2O | 60 | ALA | 3.2 |
| 10 | 2P | 39 | LYS | 3.2 |
| 22 | 21 | 40 | ARG | 3.2 |
| 44 | 1n | 59 | ALA | 3.2 |
| 52 | 1v | 599 | PRO | 3.2 |
| 53 | 2w | 29 | ARG | 3.2 |
| 32 | 2b | 197 | VAL | 3.2 |
| 1 | 2A | 2144 | U | 3.2 |
| 9 | 2O | 39 | ILE | 3.2 |
| 53 | 2w | 156 | ARG | 3.2 |
| 6 | 2G | 148 | MET | 3.2 |
| 41 | 2k | 110 | ASP | 3.2 |
| 3 | 1D | 184 | LYS | 3.2 |
| 37 | 2g | 124 | LEU | 3.2 |
| 37 | 2g | 95 | ARG | 3.2 |
| 44 | 1n | 32 | SER | 3.2 |
| 22 | 21 | 64 | ALA | 3.2 |
| 52 | 2v | 627 | ARG | 3.2 |
| 53 | 1w | 46 | TYR | 3.2 |
| 33 | 1c | 35 | GLU | 3.2 |
| 52 | 2v | 181 | LEU | 3.2 |
| 6 | 2G | 54 | GLU | 3.2 |
| 29 | 28 | 43 | GLN | 3.2 |
| 35 | 2e | 45 | PHE | 3.2 |
| 37 | 2g | 14 | PRO | 3.2 |
| 22 | 11 | 33 | LYS | 3.2 |
| 47 | 2q | 40 | LYS | 3.2 |
| 52 | 2v | 144 | ALA | 3.2 |
| 14 | 1T | 76 | PHE | 3.2 |
| 31 | 2a | 1350 | A | 3.2 |
| 41 | 2k | 108 | ILE | 3.2 |
| 44 | 2n | 3 | ARG | 3.2 |

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| Mol | Chain | Res | Type | RSRZ |
|---|---|---|---|---|
| 4 | 1E | 18 | ASP | 3.2 |
| 52 | 1v | 569 | ASP | 3.2 |
| 52 | 2v | 347 | GLY | 3.2 |
| 4 | 1E | 141 | ILE | 3.2 |
| 41 | 1k | 29 | ILE | 3.2 |
| 44 | 2n | 7 | ILE | 3.2 |
| 54 | 2y | 51 | U | 3.2 |
| 34 | 1d | 115 | ARG | 3.2 |
| 52 | 2v | 559 | PRO | 3.2 |
| 1 | 2A | 2176 | A | 3.2 |
| 11 | 2Q | 89 | ASN | 3.2 |
| 11 | 2Q | 93 | TYR | 3.2 |
| 33 | 2c | 25 | GLY | 3.2 |
| 10 | 2P | 75 | ILE | 3.2 |
| 34 | 1d | 5 | ILE | 3.2 |
| 42 | 2l | 77 | LEU | 3.2 |
| 31 | 1a | 1029 | C | 3.2 |
| 54 | 1y | 3 | C | 3.2 |
| 21 | 2O | 31 | VAL | 3.2 |
| 9 | 1O | 20 | MET | 3.2 |
| 9 | 2O | 100 | GLY | 3.2 |
| 11 | 2Q | 108 | GLY | 3.2 |
| 9 | 2O | 97 | ARG | 3.2 |
| 52 | 2v | 643 | ILE | 3.2 |
| 31 | 2a | 941 | G | 3.2 |
| 53 | 2w | 154 | THR | 3.2 |
| 5 | 2F | 154 | VAL | 3.2 |
| 33 | 1c | 71 | ALA | 3.2 |
| 30 | 29 | 26 | ILE | 3.2 |
| 31 | 2a | 571 | U | 3.2 |
| 34 | 2d | 49 | ARG | 3.2 |
| 40 | 1j | 51 | ARG | 3.2 |
| 12 | 1R | 5 | LYS | 3.2 |
| 53 | 2w | 107 | THR | 3.2 |
| 7 | 2H | 159 | GLU | 3.2 |
| 20 | 2Z | 155 | LEU | 3.2 |
| 33 | 1c | 77 | ILE | 3.2 |
| 29 | 28 | 24 | ALA | 3.2 |
| 37 | 1g | 66 | VAL | 3.2 |
| 55 | 1z | 16 | U | 3.2 |
| 5 | 1F | 72 | ARG | 3.2 |
| 8 | 2N | 117 | PHE | 3.2 |

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| Mol | Chain | Res | Type | RSRZ |
|---|---|---|---|---|
| 33 | 1c | 169 | ALA | 3.2 |
| 52 | 2v | 536 | LYS | 3.2 |
| 25 | 24 | 27 | THR | 3.2 |
| 42 | 2l | 99 | HIS | 3.2 |
| 53 | 2w | 160 | GLU | 3.2 |
| 1 | 2A | 246 | C | 3.2 |
| 25 | 24 | 66 | SER | 3.2 |
| 31 | 2a | 562 | C | 3.2 |
| 3 | 2D | 223 | GLY | 3.2 |
| 9 | 2O | 17 | ARG | 3.2 |
| 35 | 1e | 40 | ARG | 3.2 |
| 41 | 2k | 62 | GLN | 3.1 |
| 11 | 2Q | 19 | GLY | 3.1 |
| 1 | 2A | 2182 | G | 3.1 |
| 27 | 26 | 35 | GLU | 3.1 |
| 31 | 2a | 998 | G | 3.1 |
| 11 | 2Q | 130 | LYS | 3.1 |
| 22 | 11 | 20 | ARG | 3.1 |
| 33 | 1c | 50 | ALA | 3.1 |
| 26 | 15 | 7 | PRO | 3.1 |
| 39 | 1i | 99 | LEU | 3.1 |
| 52 | 2v | 516 | PRO | 3.1 |
| 4 | 1E | 159 | HIS | 3.1 |
| 14 | 1T | 28 | VAL | 3.1 |
| 44 | 1n | 18 | VAL | 3.1 |
| 54 | 2y | 66 | U | 3.1 |
| 33 | 1c | 192 | THR | 3.1 |
| 52 | 1v | -29 | LEU | 3.1 |
| 31 | 2a | 887 | G | 3.1 |
| 22 | 21 | 23 | LYS | 3.1 |
| 9 | 2O | 57 | VAL | 3.1 |
| 40 | 1j | 92 | THR | 3.1 |
| 44 | 2n | 35 | ARG | 3.1 |
| 31 | 2a | 1035 | A | 3.1 |
| 9 | 2O | 10 | VAL | 3.1 |
| 16 | 2V | 64 | HIS | 3.1 |
| 7 | 2H | 27 | LYS | 3.1 |
| 34 | 2d | 165 | MET | 3.1 |
| 9 | 1O | 40 | VAL | 3.1 |
| 40 | 1j | 54 | PHE | 3.1 |
| 27 | 26 | 3 | SER | 3.1 |
| 40 | 2j | 49 | VAL | 3.1 |

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| Mol | Chain | Res | Type | RSRZ |
|---|---|---|---|---|
| 44 | 1n | 27 | CYS | 3.1 |
| 35 | 2e | 21 | ALA | 3.1 |
| 55 | 1z | 15 | A | 3.1 |
| 41 | 2k | 31 | THR | 3.1 |
| 52 | 2v | 617 | MET | 3.1 |
| 31 | 2a | 4 | U | 3.1 |
| 33 | 1c | 2 | GLY | 3.1 |
| 33 | 1c | 19 | GLU | 3.1 |
| 34 | 2d | 163 | GLU | 3.1 |
| 52 | 2v | 641 | GLN | 3.1 |
| 41 | 1k | 98 | LEU | 3.1 |
| 38 | 2h | 86 | ILE | 3.1 |
| 46 | 1p | 36 | ILE | 3.1 |
| 33 | 1c | 70 | VAL | 3.1 |
| 9 | 1O | 3 | GLN | 3.1 |
| 31 | 1a | 1342 | C | 3.1 |
| 31 | 1a | 1359 | C | 3.1 |
| 42 | 2l | 49 | ASN | 3.1 |
| 52 | 2v | 581 | ALA | 3.1 |
| 54 | 2y | 71 | G | 3.1 |
| 15 | 2U | 108 | GLU | 3.1 |
| 44 | 1n | 3 | ARG | 3.1 |
| 37 | 1g | 137 | LYS | 3.1 |
| 4 | 1E | 122 | PHE | 3.1 |
| 4 | 1E | 187 | ALA | 3.1 |
| 2 | 2B | 91 | C | 3.1 |
| 54 | 2x | 40 | C | 3.1 |
| 20 | 2Z | 76 | LEU | 3.1 |
| 31 | 1a | 1057 | G | 3.1 |
| 11 | 2Q | 38 | GLU | 3.1 |
| 1 | 1A | 888 | C | 3.1 |
| 31 | 2a | 788 | U | 3.1 |
| 40 | 1j | 6 | ILE | 3.1 |
| 14 | 2T | 70 | VAL | 3.1 |
| 49 | 2s | 79 | THR | 3.1 |
| 41 | 1k | 49 | GLY | 3.1 |
| 52 | 1v | -46 | VAL | 3.1 |
| 52 | 2v | 432 | ALA | 3.1 |
| 31 | 1a | 898 | G | 3.1 |
| 9 | 1O | 84 | ALA | 3.1 |
| 9 | 1O | 96 | THR | 3.1 |
| 35 | 2e | 105 | VAL | 3.1 |

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| Mol | Chain | Res | Type | RSRZ |
|---|---|---|---|---|
| 4 | 1E | 128 | SER | 3.1 |
| 25 | 24 | 30 | GLU | 3.1 |
| 31 | 1a | 1205 | U | 3.1 |
| 53 | 1w | 71 | TRP | 3.1 |
| 14 | 1T | 30 | VAL | 3.1 |
| 27 | 26 | 17 | LYS | 3.1 |
| 9 | 1O | 54 | GLU | 3.1 |
| 10 | 2P | 58 | THR | 3.1 |
| 31 | 2a | 959 | A | 3.1 |
| 41 | 1k | 43 | SER | 3.1 |
| 9 | 2O | 86 | ILE | 3.1 |
| 9 | 2O | 16 | ALA | 3.0 |
| 52 | 2v | 504 | ARG | 3.0 |
| 53 | 2w | 157 | ALA | 3.0 |
| 55 | 1z | 17 | U | 3.0 |
| 33 | 2c | 110 | ASN | 3.0 |
| 52 | 2v | 437 | THR | 3.0 |
| 49 | 1s | 49 | ILE | 3.0 |
| 52 | 1v | 541 | ALA | 3.0 |
| 9 | 1O | 45 | GLU | 3.0 |
| 53 | 2w | 66 | LEU | 3.0 |
| 54 | 1x | 38 | A | 3.0 |
| 27 | 26 | 18 | ARG | 3.0 |
| 47 | 2q | 27 | PHE | 3.0 |
| 14 | 1T | 33 | LYS | 3.0 |
| 47 | 2q | 95 | TYR | 3.0 |
| 10 | 2P | 73 | GLY | 3.0 |
| 33 | 2c | 107 | GLN | 3.0 |
| 12 | 2R | 69 | ASP | 3.0 |
| 39 | 2i | 28 | VAL | 3.0 |
| 41 | 2k | 81 | ASP | 3.0 |
| 33 | 2c | 182 | ILE | 3.0 |
| 1 | 2A | 2137 | C | 3.0 |
| 31 | 2a | 1209 | C | 3.0 |
| 52 | 2v | 440 | VAL | 3.0 |
| 20 | 2Z | 192 | ALA | 3.0 |
| 37 | 1g | 98 | SER | 3.0 |
| 8 | 2N | 138 | LEU | 3.0 |
| 41 | 2k | 76 | GLY | 3.0 |
| 11 | 2Q | 39 | PRO | 3.0 |
| 1 | 2A | 1912 | A | 3.0 |
| 11 | 2Q | 131 | ILE | 3.0 |

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| Mol | Chain | Res | Type | RSRZ |
|---|---|---|---|---|
| 31 | 1a | 1055 | A | 3.0 |
| 33 | 1c | 20 | SER | 3.0 |
| 39 | 1i | 19 | LEU | 3.0 |
| 21 | 20 | 17 | GLN | 3.0 |
| 52 | 1v | 560 | VAL | 3.0 |
| 5 | 1F | 70 | THR | 3.0 |
| 19 | 2Y | 59 | GLY | 3.0 |
| 31 | 2a | 793 | U | 3.0 |
| 25 | 24 | 14 | ILE | 3.0 |
| 31 | 2a | 938 | A | 3.0 |
| 33 | 1c | 82 | GLU | 3.0 |
| 35 | 1e | 89 | ILE | 3.0 |
| 54 | 1y | 7 | A | 3.0 |
| 39 | 1i | 123 | PRO | 3.0 |
| 3 | 2D | 2 | ALA | 3.0 |
| 6 | 2G | 34 | LEU | 3.0 |
| 52 | 2v | 451 | ILE | 3.0 |
| 1 | 2A | 1032 | A | 3.0 |
| 3 | 1D | 222 | ARG | 3.0 |
| 14 | 1T | 64 | ARG | 3.0 |
| 34 | 1d | 144 | ASP | 3.0 |
| 54 | 2x | 35 | A | 3.0 |
| 29 | 28 | 36 | LYS | 3.0 |
| 52 | 2v | 513 | LYS | 3.0 |
| 1 | 2A | 2103 | C | 3.0 |
| 31 | 1a | 1385 | G | 3.0 |
| 31 | 1a | 1511 | G | 3.0 |
| 21 | 20 | 46 | LYS | 3.0 |
| 33 | 2c | 130 | VAL | 3.0 |
| 1 | 2A | 227 | A | 3.0 |
| 19 | 2Y | 83 | THR | 3.0 |
| 31 | 1a | 974 | A | 3.0 |
| 31 | 2a | 1227 | A | 3.0 |
| 33 | 2c | 43 | LEU | 3.0 |
| 47 | 2q | 32 | TYR | 3.0 |
| 42 | 2l | 89 | ARG | 3.0 |
| 9 | 2O | 2 | ILE | 3.0 |
| 1 | 2A | 2124 | G | 3.0 |
| 31 | 1a | 769 | G | 3.0 |
| 10 | 2P | 63 | PRO | 3.0 |
| 20 | 2Z | 22 | GLY | 3.0 |
| 34 | 2d | 3 | ARG | 3.0 |

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| Mol | Chain | Res | Type | RSRZ |
|---|---|---|---|---|
| 33 | 2c | 57 | ILE | 3.0 |
| 43 | 2m | 4 | ILE | 3.0 |
| 5 | 2F | 77 | ASP | 3.0 |
| 8 | 2N | 17 | ASP | 3.0 |
| 52 | 2v | 443 | HIS | 3.0 |
| 52 | 2v | 671 | MET | 3.0 |
| 27 | 26 | 33 | LYS | 3.0 |
| 32 | 2b | 196 | LEU | 3.0 |
| 35 | 2e | 113 | ALA | 3.0 |
| 49 | 1s | 79 | THR | 3.0 |
| 49 | 2s | 48 | THR | 3.0 |
| 52 | 1v | 429 | ALA | 3.0 |
| 52 | 1v | 511 | LYS | 3.0 |
| 1 | 2A | 1119 | C | 3.0 |
| 24 | 23 | 34 | GLU | 3.0 |
| 1 | 1A | 275 | G | 3.0 |
| 41 | 1k | 126 | ARG | 3.0 |
| 45 | 2o | 88 | ARG | 3.0 |
| 29 | 28 | 27 | THR | 3.0 |
| 41 | 1k | 47 | VAL | 3.0 |
| 41 | 2k | 82 | VAL | 3.0 |
| 54 | 1y | 26 | A | 3.0 |
| 1 | 2A | 2109 | U | 3.0 |
| 33 | 1c | 10 | PHE | 3.0 |
| 33 | 1c | 21 | ARG | 3.0 |
| 1 | 1A | 2551 | C | 2.9 |
| 31 | 2a | 1403 | C | 2.9 |
| 47 | 2q | 12 | SER | 2.9 |
| 40 | 1j | 98 | ILE | 2.9 |
| 49 | 2s | 62 | ILE | 2.9 |
| 53 | 2w | 103 | ILE | 2.9 |
| 1 | 2A | 242 | G | 2.9 |
| 1 | 2A | 2125 | G | 2.9 |
| 40 | 2j | 65 | LEU | 2.9 |
| 52 | 2v | 418 | LYS | 2.9 |
| 4 | 1E | 121 | ASN | 2.9 |
| 47 | 2q | 94 | ASN | 2.9 |
| 3 | 1D | 230 | ASP | 2.9 |
| 4 | 1E | 194 | GLY | 2.9 |
| 33 | 1c | 146 | ALA | 2.9 |
| 1 | 2A | 2130 | U | 2.9 |
| 14 | 1T | 1 | MET | 2.9 |

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| Mol | Chain | Res | Type | RSRZ |
|---|---|---|---|---|
| 20 | 2Z | 194 | PRO | 2.9 |
| 22 | 21 | 44 | PRO | 2.9 |
| 41 | 2k | 106 | LYS | 2.9 |
| 1 | 2A | 252 | G | 2.9 |
| 31 | 2a | 1489 | G | 2.9 |
| 1 | 2A | 383 | U | 2.9 |
| 21 | 20 | 79 | VAL | 2.9 |
| 9 | 1O | 2 | ILE | 2.9 |
| 9 | 1O | 44 | LYS | 2.9 |
| 42 | 1l | 28 | LYS | 2.9 |
| 14 | 1T | 21 | GLU | 2.9 |
| 52 | 2v | 680 | PRO | 2.9 |
| 48 | 2r | 56 | THR | 2.9 |
| 22 | 21 | 15 | ALA | 2.9 |
| 37 | 2g | 2 | ALA | 2.9 |
| 52 | 2v | 419 | ALA | 2.9 |
| 42 | 2l | 102 | ARG | 2.9 |
| 54 | 1x | 59 | U | 2.9 |
| 54 | 2y | 69 | G | 2.9 |
| 34 | 2d | 93 | PHE | 2.9 |
| 39 | 2i | 49 | PRO | 2.9 |
| 22 | 21 | 63 | ALA | 2.9 |
| 29 | 28 | 45 | GLY | 2.9 |
| 35 | 2e | 86 | ALA | 2.9 |
| 31 | 1a | 934 | C | 2.9 |
| 31 | 2a | 121 | C | 2.9 |
| 41 | 2k | 93 | GLN | 2.9 |
| 37 | 1g | 61 | VAL | 2.9 |
| 42 | 1l | 25 | PRO | 2.9 |
| 31 | 1a | 965 | A | 2.9 |
| 35 | 1e | 17 | ALA | 2.9 |
| 1 | 2A | 2121 | G | 2.9 |
| 33 | 2c | 32 | LEU | 2.9 |
| 39 | 1i | 120 | ARG | 2.9 |
| 47 | 2q | 6 | LEU | 2.9 |
| 3 | 1D | 181 | GLU | 2.9 |
| 52 | 2v | 422 | GLU | 2.9 |
| 54 | 2y | 22 | G | 2.9 |
| 52 | 2v | 587 | SER | 2.9 |
| 4 | 1E | 131 | ALA | 2.9 |
| 54 | 1y | 40 | C | 2.9 |
| 11 | 2Q | 48 | GLU | 2.9 |

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| Mol | Chain | Res | Type | RSRZ |
|---|---|---|---|---|
| 4 | 2E | 127 | ASP | 2.9 |
| 27 | 26 | 29 | ASN | 2.9 |
| 11 | 2Q | 50 | ALA | 2.9 |
| 1 | 2A | 1907 | G | 2.9 |
| 22 | 21 | 26 | ARG | 2.9 |
| 33 | 2c | 183 | ASP | 2.9 |
| 43 | 2m | 112 | GLY | 2.9 |
| 42 | 2l | 32 | PHE | 2.9 |
| 8 | 2N | 14 | VAL | 2.9 |
| 37 | 2g | 9 | VAL | 2.9 |
| 47 | 2q | 73 | VAL | 2.9 |
| 52 | 1v | -65 | LYS | 2.9 |
| 3 | 2D | 174 | ILE | 2.9 |
| 22 | 21 | 7 | ILE | 2.9 |
| 20 | 2Z | 107 | THR | 2.9 |
| 44 | 1n | 56 | VAL | 2.9 |
| 54 | 1x | 31 | A | 2.9 |
| 38 | 2h | 100 | ILE | 2.9 |
| 44 | 2n | 23 | ARG | 2.9 |
| 31 | 2a | 888 | G | 2.9 |
| 52 | 2v | 361 | ASN | 2.9 |
| 1 | 1A | 790 | C | 2.9 |
| 38 | 2h | 99 | GLU | 2.9 |
| 52 | 2v | 608 | VAL | 2.9 |
| 54 | 1y | 45 | U | 2.9 |
| 1 | 2A | 255 | A | 2.9 |
| 11 | 2Q | 99 | PRO | 2.9 |
| 3 | 1D | 226 | MET | 2.9 |
| 52 | 2v | 445 | GLU | 2.9 |
| 40 | 2j | 67 | THR | 2.9 |
| 9 | 2O | 95 | GLY | 2.9 |
| 43 | 2m | 5 | ALA | 2.9 |
| 52 | 2v | 505 | GLY | 2.9 |
| 52 | 2v | 300 | GLU | 2.9 |
| 37 | 2g | 120 | ILE | 2.9 |
| 6 | 2G | 42 | GLY | 2.9 |
| 42 | 1l | 68 | ALA | 2.9 |
| 42 | 2l | 53 | ARG | 2.9 |
| 31 | 2a | 786 | G | 2.9 |
| 37 | 1g | 147 | ALA | 2.9 |
| 52 | 2v | 520 | GLY | 2.8 |
| 41 | 2k | 109 | VAL | 2.8 |

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| Mol | Chain | Res | Type | RSRZ |
|---|---|---|---|---|
| 52 | 1v | 414 | GLU | 2.8 |
| 10 | 2P | 70 | GLN | 2.8 |
| 52 | 2v | 438 | PHE | 2.8 |
| 51 | 2u | 4 | GLY | 2.8 |
| 5 | 2F | 175 | THR | 2.8 |
| 54 | 2y | 12 | U | 2.8 |
| 22 | 11 | 27 | GLU | 2.8 |
| 27 | 26 | 11 | LEU | 2.8 |
| 31 | 1a | 1048 | G | 2.8 |
| 54 | 1y | 43 | C | 2.8 |
| 42 | 2l | 30 | ALA | 2.8 |
| 31 | 2a | 696 | A | 2.8 |
| 20 | 2Z | 193 | GLU | 2.8 |
| 4 | 1E | 15 | PHE | 2.8 |
| 14 | 2T | 99 | LEU | 2.8 |
| 31 | 2a | 1427 | U | 2.8 |
| 42 | 1l | 99 | HIS | 2.8 |
| 33 | 1c | 181 | ASN | 2.8 |
| 54 | 1x | 62 | C | 2.8 |
| 1 | 1A | 748 | G | 2.8 |
| 54 | 1x | 10 | G | 2.8 |
| 1 | 2A | 2134 | A | 2.8 |
| 33 | 2c | 146 | ALA | 2.8 |
| 33 | 1c | 132 | ARG | 2.8 |
| 9 | 2O | 21 | CYS | 2.8 |
| 34 | 2d | 4 | TYR | 2.8 |
| 31 | 1a | 984 | C | 2.8 |
| 31 | 2a | 962 | C | 2.8 |
| 39 | 2i | 55 | ALA | 2.8 |
| 42 | 2l | 80 | HIS | 2.8 |
| 1 | 2A | 247 | G | 2.8 |
| 1 | 2A | 257 | A | 2.8 |
| 31 | 2a | 570 | G | 2.8 |
| 35 | 2e | 12 | LEU | 2.8 |
| 54 | 1y | 22 | G | 2.8 |
| 54 | 2y | 34 | G | 2.8 |
| 14 | 2T | 38 | ASN | 2.8 |
| 9 | 2O | 58 | VAL | 2.8 |
| 43 | 2m | 109 | THR | 2.8 |
| 52 | 2v | 538 | TYR | 2.8 |
| 4 | 1E | 132 | HIS | 2.8 |
| 9 | 2O | 44 | LYS | 2.8 |

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| Mol | Chain | Res | Type | RSRZ |
|---|---|---|---|---|
| 33 | 1c | 178 | LEU | 2.8 |
| 6 | 2G | 150 | ASP | 2.8 |
| 37 | 1g | 103 | TRP | 2.8 |
| 41 | 1k | 40 | ILE | 2.8 |
| 41 | 2k | 84 | VAL | 2.8 |
| 52 | 1v | 412 | ALA | 2.8 |
| 1 | 2A | 2114 | A | 2.8 |
| 4 | 1E | 145 | LYS | 2.8 |
| 3 | 2D | 6 | PHE | 2.8 |
| 7 | 2H | 34 | GLU | 2.8 |
| 43 | 1m | 90 | LEU | 2.8 |
| 3 | 2D | 54 | ARG | 2.8 |
| 29 | 28 | 55 | ALA | 2.8 |
| 33 | 1c | 73 | PRO | 2.8 |
| 43 | 1m | 100 | GLY | 2.8 |
| 11 | 2Q | 18 | LYS | 2.8 |
| 38 | 1h | 109 | ILE | 2.8 |
| 35 | 2e | 40 | ARG | 2.8 |
| 14 | 1T | 35 | LYS | 2.8 |
| 52 | 1v | 416 | LYS | 2.8 |
| 53 | 2w | 51 | PRO | 2.8 |
| 1 | 2A | 2148 | G | 2.8 |
| 31 | 2a | 1050 | G | 2.8 |
| 33 | 1c | 34 | LEU | 2.8 |
| 38 | 1h | 15 | ASN | 2.8 |
| 53 | 2w | 145 | LYS | 2.8 |
| 1 | 2A | 2178 | C | 2.8 |
| 12 | 2R | 111 | LEU | 2.8 |
| 4 | 1E | 116 | VAL | 2.8 |
| 17 | 1W | 1 | MET | 2.8 |
| 41 | 1k | 83 | ILE | 2.8 |
| 52 | 2v | 105 | ILE | 2.8 |
| 43 | 1m | 87 | TYR | 2.8 |
| 35 | 2e | 28 | PHE | 2.8 |
| 39 | 1i | 37 | PHE | 2.8 |
| 9 | 1O | 98 | VAL | 2.8 |
| 11 | 2Q | 96 | VAL | 2.8 |
| 14 | 1T | 62 | THR | 2.8 |
| 21 | 20 | 12 | ASN | 2.8 |
| 39 | 1i | 17 | VAL | 2.8 |
| 49 | 1s | 60 | VAL | 2.8 |
| 49 | 2s | 51 | VAL | 2.8 |

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| Mol | Chain | Res | Type | RSRZ |
|---|---|---|---|---|
| 53 | 1w | 32 | ARG | 2.8 |
| 31 | 2a | 89 | C | 2.8 |
| 35 | 2e | 92 | LYS | 2.8 |
| 47 | 2q | 41 | LYS | 2.8 |
| 41 | 1k | 19 | ALA | 2.8 |
| 4 | 1E | 189 | PRO | 2.8 |
| 22 | 21 | 41 | ARG | 2.8 |
| 29 | 28 | 5 | LYS | 2.8 |
| 44 | 1n | 22 | THR | 2.8 |
| 5 | 2F | 181 | LEU | 2.8 |
| 37 | 2g | 121 | ALA | 2.8 |
| 52 | 2v | 458 | HIS | 2.8 |
| 3 | 2D | 52 | ARG | 2.8 |
| 10 | 2P | 95 | VAL | 2.8 |
| 37 | 1g | 70 | LYS | 2.8 |
| 31 | 1a | 968 | A | 2.8 |
| 33 | 1c | 47 | LEU | 2.8 |
| 7 | 2H | 21 | PRO | 2.7 |
| 33 | 1c | 140 | ARG | 2.7 |
| 35 | 1e | 41 | VAL | 2.7 |
| 29 | 28 | 64 | TYR | 2.7 |
| 1 | 1A | 1667 | G | 2.7 |
| 31 | 2a | 1164 | G | 2.7 |
| 31 | 2a | 891 | U | 2.7 |
| 1 | 1A | 2142 | C | 2.7 |
| 3 | 2D | 4 | LYS | 2.7 |
| 6 | 2G | 48 | GLU | 2.7 |
| 31 | 2a | 1344 | C | 2.7 |
| 52 | 1v | 88 | VAL | 2.7 |
| 35 | 2e | 93 | PRO | 2.7 |
| 31 | 2a | 1377 | A | 2.7 |
| 13 | 2S | 82 | ILE | 2.7 |
| 14 | 2T | 40 | THR | 2.7 |
| 33 | 2c | 26 | LYS | 2.7 |
| 11 | 2Q | 103 | MET | 2.7 |
| 19 | 2Y | 82 | PRO | 2.7 |
| 52 | 2v | 479 | PRO | 2.7 |
| 31 | 2a | 1222 | G | 2.7 |
| 14 | 1T | 74 | ARG | 2.7 |
| 16 | 2V | 14 | VAL | 2.7 |
| 31 | 2a | 1335 | C | 2.7 |
| 38 | 2h | 95 | VAL | 2.7 |

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| Mol | Chain | Res | Type | RSRZ |
|---|---|---|---|---|
| 54 | 1x | 61 | C | 2.7 |
| 20 | 2Z | 38 | TYR | 2.7 |
| 29 | 28 | 63 | PRO | 2.7 |
| 39 | 1i | 117 | HIS | 2.7 |
| 37 | 1g | 130 | GLY | 2.7 |
| 9 | 2O | 43 | VAL | 2.7 |
| 31 | 1a | 1196 | U | 2.7 |
| 12 | 1R | 1 | MET | 2.7 |
| 19 | 1Y | 1 | MET | 2.7 |
| 40 | 1j | 15 | THR | 2.7 |
| 1 | 2A | 264 | C | 2.7 |
| 1 | 2A | 2313 | C | 2.7 |
| 49 | 1s | 74 | PHE | 2.7 |
| 9 | 1O | 121 | VAL | 2.7 |
| 38 | 2h | 84 | ARG | 2.7 |
| 52 | 2v | 645 | ALA | 2.7 |
| 35 | 2e | 110 | LEU | 2.7 |
| 3 | 2D | 55 | GLY | 2.7 |
| 4 | 1E | 149 | ARG | 2.7 |
| 7 | 2H | 23 | ARG | 2.7 |
| 27 | 26 | 37 | ARG | 2.7 |
| 40 | 1j | 45 | ARG | 2.7 |
| 43 | 2m | 92 | HIS | 2.7 |
| 33 | 2c | 50 | ALA | 2.7 |
| 33 | 2c | 163 | ALA | 2.7 |
| 9 | 1O | 39 | ILE | 2.7 |
| 10 | 2P | 126 | VAL | 2.7 |
| 11 | 2Q | 109 | VAL | 2.7 |
| 1 | 2A | 2116 | G | 2.7 |
| 31 | 2a | 954 | G | 2.7 |
| 31 | 2a | 1026 | G | 2.7 |
| 20 | 2Z | 74 | VAL | 2.7 |
| 44 | 2n | 59 | ALA | 2.7 |
| 6 | 2G | 176 | LEU | 2.7 |
| 34 | 1d | 11 | LEU | 2.7 |
| 5 | 1F | 66 | PRO | 2.7 |
| 53 | 2w | 12 | SER | 2.7 |
| 31 | 2a | 555 | C | 2.7 |
| 54 | 1x | 4 | C | 2.7 |
| 31 | 1a | 958 | A | 2.7 |
| 52 | 2v | 507 | TYR | 2.7 |
| 21 | 20 | 13 | GLY | 2.7 |

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| Mol | Chain | Res | Type | RSRZ |
|---|---|---|---|---|
| 35 | 2e | 134 | ALA | 2.7 |
| 44 | 1n | 7 | ILE | 2.7 |
| 47 | 2q | 8 | GLY | 2.7 |
| 14 | 1T | 77 | PRO | 2.7 |
| 52 | 2v | 631 | ILE | 2.7 |
| 8 | 2N | 70 | LYS | 2.7 |
| 9 | 2O | 111 | PHE | 2.7 |
| 14 | 1T | 27 | THR | 2.7 |
| 31 | 2a | 889 | A | 2.7 |
| 54 | 2y | 14 | A | 2.7 |
| 42 | 2l | 58 | VAL | 2.7 |
| 3 | 2D | 195 | ALA | 2.7 |
| 33 | 1c | 81 | GLY | 2.7 |
| 46 | 1p | 19 | ILE | 2.7 |
| 20 | 2Z | 83 | PRO | 2.7 |
| 51 | 2u | 14 | TRP | 2.7 |
| 21 | 20 | 41 | ARG | 2.7 |
| 35 | 2e | 123 | LEU | 2.7 |
| 52 | 2v | 91 | THR | 2.7 |
| 10 | 2P | 71 | VAL | 2.7 |
| 52 | 2v | 625 | ASN | 2.7 |
| 1 | 2A | 254 | G | 2.7 |
| 37 | 1g | 126 | ASP | 2.7 |
| 52 | 2v | 558 | PHE | 2.7 |
| 12 | 1R | 115 | GLU | 2.7 |
| 52 | 2v | 660 | ARG | 2.7 |
| 53 | 1w | 41 | LEU | 2.7 |
| 9 | 1O | 83 | ALA | 2.7 |
| 29 | 28 | 58 | ILE | 2.7 |
| 31 | 1a | 532 | A | 2.7 |
| 31 | 2a | 937 | A | 2.7 |
| 1 | 1A | 2513 | G | 2.7 |
| 5 | 2F | 148 | LEU | 2.6 |
| 20 | 2Z | 44 | PHE | 2.7 |
| 34 | 2d | 118 | ARG | 2.6 |
| 54 | 2x | 34 | G | 2.7 |
| 52 | 2v | 436 | PRO | 2.6 |
| 6 | 2G | 151 | ALA | 2.6 |
| 33 | 2c | 53 | ALA | 2.6 |
| 52 | 1v | 591 | LYS | 2.6 |
| 4 | 1E | 119 | ARG | 2.6 |
| 35 | 1e | 91 | LEU | 2.6 |

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| Mol | Chain | Res | Type | RSRZ |
|---|---|---|---|---|
| 27 | 26 | 48 | VAL | 2.6 |
| 44 | 2n | 8 | GLU | 2.6 |
| 30 | 29 | 1 | MET | 2.6 |
| 34 | 1d | 102 | ASP | 2.6 |
| 42 | 1l | 97 | ARG | 2.6 |
| 43 | 1m | 48 | LEU | 2.6 |
| 52 | 1v | 472 | VAL | 2.6 |
| 19 | 2Y | 4 | LYS | 2.6 |
| 31 | 2a | 1078 | U | 2.6 |
| 39 | 2i | 98 | PRO | 2.6 |
| 52 | 2v | 511 | LYS | 2.6 |
| 20 | 2Z | 150 | LEU | 2.6 |
| 21 | 20 | 14 | ARG | 2.6 |
| 44 | 1n | 28 | GLY | 2.6 |
| 31 | 1a | 900 | A | 2.6 |
| 44 | 2n | 57 | ARG | 2.6 |
| 8 | 2N | 62 | VAL | 2.6 |
| 24 | 23 | 38 | GLU | 2.6 |
| 53 | 2w | 67 | VAL | 2.6 |
| 6 | 2G | 76 | SER | 2.6 |
| 24 | 23 | 8 | LEU | 2.6 |
| 34 | 2d | 167 | GLY | 2.6 |
| 40 | 2j | 66 | ARG | 2.6 |
| 22 | 21 | 62 | VAL | 2.6 |
| 34 | 1d | 125 | HIS | 2.6 |
| 4 | 1E | 133 | LYS | 2.6 |
| 11 | 2Q | 137 | TYR | 2.6 |
| 27 | 26 | 12 | GLU | 2.6 |
| 52 | 2v | 563 | ILE | 2.6 |
| 5 | 1F | 67 | GLN | 2.6 |
| 33 | 2c | 62 | ASP | 2.6 |
| 3 | 2D | 237 | GLU | 2.6 |
| 4 | 1E | 113 | PHE | 2.6 |
| 11 | 2Q | 51 | ARG | 2.6 |
| 31 | 2a | 1202 | G | 2.6 |
| 33 | 2c | 52 | LEU | 2.6 |
| 33 | 2c | 160 | ALA | 2.6 |
| 52 | 2v | 535 | PRO | 2.6 |
| 14 | 1T | 31 | SER | 2.6 |
| 31 | 1a | 936 | C | 2.6 |
| 33 | 2c | 195 | VAL | 2.6 |
| 15 | 2U | 106 | PHE | 2.6 |

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| Mol | Chain | Res | Type | RSRZ |
|---|---|---|---|---|
| 20 | 2Z | 81 | ARG | 2.6 |
| 33 | 1c | 145 | GLY | 2.6 |
| 7 | 2H | 115 | VAL | 2.6 |
| 9 | 1O | 85 | VAL | 2.6 |
| 13 | 2S | 28 | VAL | 2.6 |
| 19 | 2Y | 43 | ASN | 2.6 |
| 7 | 2H | 119 | GLU | 2.6 |
| 9 | 1O | 28 | SER | 2.6 |
| 9 | 1O | 78 | ARG | 2.6 |
| 30 | 29 | 9 | ARG | 2.6 |
| 31 | 2a | 916 | G | 2.6 |
| 31 | 2a | 1036 | G | 2.6 |
| 35 | 2e | 84 | PHE | 2.6 |
| 40 | 1j | 87 | THR | 2.6 |
| 1 | 2A | 2108 | C | 2.6 |
| 29 | 28 | 59 | LYS | 2.6 |
| 43 | 1m | 45 | VAL | 2.6 |
| 31 | 2a | 279 | A | 2.6 |
| 11 | 2Q | 68 | ILE | 2.6 |
| 1 | 1A | 2585 | U | 2.6 |
| 6 | 2G | 156 | ASP | 2.6 |
| 7 | 2H | 137 | ASP | 2.6 |
| 21 | 20 | 71 | ASP | 2.6 |
| 3 | 1D | 276 | LYS | 2.6 |
| 34 | 1d | 8 | VAL | 2.6 |
| 40 | 2j | 53 | PRO | 2.6 |
| 10 | 2P | 74 | GLU | 2.6 |
| 54 | 2y | 11 | C | 2.6 |
| 4 | 1E | 193 | GLY | 2.6 |
| 8 | 2N | 84 | LYS | 2.6 |
| 9 | 2O | 12 | ASP | 2.6 |
| 31 | 2a | 1030(D) | A | 2.6 |
| 33 | 1c | 62 | ASP | 2.6 |
| 52 | 1v | 513 | LYS | 2.6 |
| 41 | 2k | 18 | ARG | 2.6 |
| 52 | 2v | 677 | GLN | 2.6 |
| 33 | 1c | 171 | GLY | 2.6 |
| 52 | 2v | 423 | LYS | 2.6 |
| 1 | 2A | 1765 | C | 2.6 |
| 31 | 2a | 1487 | G | 2.6 |
| 1 | 2A | 1690 | A | 2.6 |
| 14 | 2T | 68 | TYR | 2.6 |

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| Mol | Chain | Res | Type | RSRZ |
|---|---|---|---|---|
| 4 | 2E | 133 | LYS | 2.6 |
| 31 | 1a | 1030(D) | A | 2.6 |
| 52 | 1v | 677 | GLN | 2.6 |
| 6 | 2G | 161 | THR | 2.6 |
| 22 | 11 | 37 | ILE | 2.6 |
| 35 | 1e | 19 | MET | 2.6 |
| 21 | 20 | 22 | GLY | 2.6 |
| 31 | 2a | 240 | C | 2.6 |
| 1 | 1A | 652(U) | G | 2.6 |
| 31 | 1a | 1030(A) | G | 2.6 |
| 31 | 2a | 1034 | G | 2.6 |
| 31 | 2a | 1408 | A | 2.6 |
| 3 | 2D | 181 | GLU | 2.6 |
| 4 | 1E | 8 | LYS | 2.6 |
| 14 | 2T | 82 | LEU | 2.6 |
| 9 | 1O | 58 | VAL | 2.6 |
| 33 | 2c | 198 | VAL | 2.6 |
| 39 | 2i | 16 | ARG | 2.6 |
| 39 | 2i | 106 | ALA | 2.6 |
| 35 | 1e | 26 | PHE | 2.6 |
| 9 | 2O | 122 | LEU | 2.5 |
| 30 | 29 | 24 | TYR | 2.5 |
| 42 | 2l | 84 | LEU | 2.5 |
| 27 | 26 | 30 | THR | 2.5 |
| 1 | 1A | 1792 | G | 2.5 |
| 31 | 1a | 1193 | G | 2.5 |
| 5 | 2F | 82 | ILE | 2.5 |
| 24 | 23 | 26 | LEU | 2.5 |
| 41 | 2k | 95 | ILE | 2.5 |
| 9 | 2O | 32 | TYR | 2.5 |
| 47 | 2q | 10 | VAL | 2.5 |
| 3 | 2D | 234 | GLY | 2.5 |
| 41 | 1k | 68 | ALA | 2.5 |
| 31 | 2a | 71 | C | 2.5 |
| 52 | 1v | 493 | VAL | 2.5 |
| 54 | 1y | 4 | C | 2.5 |
| 25 | 24 | 51 | ASP | 2.5 |
| 9 | 1O | 53 | LYS | 2.5 |
| 9 | 1O | 111 | PHE | 2.5 |
| 14 | 2T | 83 | ILE | 2.5 |
| 39 | 1i | 118 | LYS | 2.5 |
| 46 | 1p | 35 | LYS | 2.5 |

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| Mol | Chain | Res | Type | RSRZ |
|---|---|---|---|---|
| 52 | 2v | 512 | ILE | 2.5 |
| 7 | 2H | 80 | SER | 2.5 |
| 52 | 2v | 434 | GLU | 2.5 |
| 11 | 2Q | 23 | GLY | 2.5 |
| 14 | 2T | 71 | GLY | 2.5 |
| 15 | 1U | 117 | GLN | 2.5 |
| 16 | 2V | 54 | GLY | 2.5 |
| 21 | 20 | 47 | PRO | 2.5 |
| 28 | 17 | 48 | LYS | 2.5 |
| 32 | 2b | 163 | PHE | 2.5 |
| 35 | 1e | 92 | LYS | 2.5 |
| 53 | 1w | 73 | GLN | 2.5 |
| 1 | 2A | 393 | C | 2.5 |
| 14 | 1T | 99 | LEU | 2.5 |
| 39 | 2i | 50 | LEU | 2.5 |
| 47 | 2q | 20 | THR | 2.5 |
| 31 | 1a | 790 | A | 2.5 |
| 35 | 2e | 90 | VAL | 2.5 |
| 4 | 1E | 136 | ARG | 2.5 |
| 22 | 21 | 65 | SER | 2.5 |
| 39 | 2i | 88 | TYR | 2.5 |
| 5 | 1F | 75 | HIS | 2.5 |
| 33 | 1c | 137 | ALA | 2.5 |
| 52 | 2v | 541 | ALA | 2.5 |
| 41 | 1k | 108 | ILE | 2.5 |
| 33 | 2c | 106 | VAL | 2.5 |
| 52 | 1v | 526 | VAL | 2.5 |
| 4 | 2E | 125 | GLY | 2.5 |
| 5 | 2F | 52 | LYS | 2.5 |
| 20 | 2Z | 62 | PRO | 2.5 |
| 22 | 21 | 24 | ALA | 2.5 |
| 54 | 1y | 61 | C | 2.5 |
| 34 | 1d | 126 | ILE | 2.5 |
| 32 | 1b | 96 | ARG | 2.5 |
| 1 | 2A | 2127 | G | 2.5 |
| 3 | 2D | 184 | LYS | 2.5 |
| 23 | 22 | 1 | MET | 2.5 |
| 16 | 2V | 73 | SER | 2.5 |
| 54 | 1x | 27 | G | 2.5 |
| 52 | 1v | 539 | ILE | 2.5 |
| 5 | 2F | 56 | GLU | 2.5 |
| 9 | 1O | 94 | ARG | 2.5 |

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| Mol | Chain | Res | Type | RSRZ |
|---|---|---|---|---|
| 25 | 24 | 23 | GLU | 2.5 |
| 9 | 2O | 34 | THR | 2.5 |
| 22 | 21 | 48 | LYS | 2.5 |
| 40 | 2j | 92 | THR | 2.5 |
| 47 | 2q | 4 | LYS | 2.5 |
| 30 | 29 | 37 | GLY | 2.5 |
| 31 | 2a | 695 | A | 2.5 |
| 43 | 1m | 95 | GLY | 2.5 |
| 33 | 2c | 34 | LEU | 2.5 |
| 3 | 1D | 273 | ARG | 2.5 |
| 16 | 2V | 12 | TYR | 2.5 |
| 1 | 2A | 386 | G | 2.5 |
| 31 | 1a | 698 | G | 2.5 |
| 4 | 1E | 5 | LEU | 2.5 |
| 14 | 1T | 80 | SER | 2.5 |
| 21 | 20 | 59 | LEU | 2.5 |
| 27 | 26 | 42 | TRP | 2.5 |
| 30 | 29 | 16 | VAL | 2.5 |
| 21 | 20 | 72 | ARG | 2.5 |
| 1 | 1A | 2143 | C | 2.5 |
| 1 | 1A | 2571 | C | 2.5 |
| 3 | 2D | 233 | HIS | 2.5 |
| 52 | 2v | 497 | PHE | 2.5 |
| 52 | 2v | 568 | TYR | 2.5 |
| 53 | 1w | 146 | GLU | 2.5 |
| 33 | 2c | 175 | LEU | 2.5 |
| 41 | 1k | 28 | THR | 2.5 |
| 41 | 1k | 57 | THR | 2.5 |
| 41 | 1k | 97 | ALA | 2.5 |
| 42 | 2l | 121 | GLY | 2.5 |
| 52 | 1v | 447 | GLY | 2.5 |
| 33 | 1c | 134 | ILE | 2.5 |
| 52 | 2v | 529 | ILE | 2.5 |
| 22 | 21 | 11 | ARG | 2.5 |
| 27 | 26 | 44 | ARG | 2.5 |
| 9 | 1O | 81 | ASP | 2.5 |
| 33 | 2c | 145 | GLY | 2.5 |
| 41 | 1k | 22 | HIS | 2.5 |
| 9 | 2O | 52 | VAL | 2.5 |
| 22 | 21 | 18 | ILE | 2.5 |
| 22 | 21 | 20 | ARG | 2.5 |
| 41 | 1k | 14 | VAL | 2.5 |

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| Mol | Chain | Res | Type | RSRZ |
|---|---|---|---|---|
| 31 | 1a | 970 | C | 2.5 |
| 31 | 2a | 1298 | C | 2.5 |
| 41 | 2k | 87 | THR | 2.5 |
| 9 | 1O | 42 | SER | 2.5 |
| 55 | 1z | 12 | A | 2.5 |
| 15 | 2U | 47 | TYR | 2.5 |
| 9 | 1O | 33 | ALA | 2.5 |
| 42 | 2l | 103 | GLY | 2.5 |
| 11 | 2Q | 77 | LYS | 2.5 |
| 14 | 1T | 65 | LYS | 2.5 |
| 33 | 2c | 17 | ASP | 2.5 |
| 34 | 1d | 118 | ARG | 2.5 |
| 41 | 2k | 48 | ILE | 2.5 |
| 47 | 2q | 5 | VAL | 2.5 |
| 1 | 2A | 1117 | G | 2.5 |
| 8 | 2N | 44 | PRO | 2.5 |
| 8 | 2N | 139 | GLU | 2.5 |
| 1 | 2A | 2586 | C | 2.5 |
| 54 | 1y | 36 | A | 2.5 |
| 10 | 2P | 124 | LYS | 2.5 |
| 35 | 1e | 88 | LYS | 2.5 |
| 4 | 1E | 147 | PRO | 2.5 |
| 37 | 1g | 62 | PHE | 2.5 |
| 39 | 1i | 114 | TYR | 2.5 |
| 29 | 28 | 60 | LEU | 2.5 |
| 10 | 2P | 107 | LYS | 2.5 |
| 38 | 2h | 109 | ILE | 2.5 |
| 39 | 2i | 116 | LYS | 2.5 |
| 42 | 2l | 17 | LYS | 2.5 |
| 52 | 1v | 440 | VAL | 2.5 |
| 53 | 2w | 118 | VAL | 2.5 |
| 21 | 20 | 69 | PHE | 2.5 |
| 52 | 2v | 582 | PHE | 2.5 |
| 27 | 26 | 32 | ASN | 2.4 |
| 31 | 1a | 972 | C | 2.4 |
| 31 | 2a | 1051 | C | 2.4 |
| 41 | 1k | 33 | THR | 2.4 |
| 41 | 2k | 39 | PRO | 2.4 |
| 43 | 2m | 66 | LEU | 2.4 |
| 49 | 2s | 53 | ASN | 2.4 |
| 52 | 1v | 448 | GLN | 2.4 |
| 7 | 2H | 107 | VAL | 2.4 |

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| Mol | Chain | Res | Type | RSRZ |
|---|---|---|---|---|
| 11 | 2Q | 106 | VAL | 2.4 |
| 14 | 2T | 72 | VAL | 2.4 |
| 20 | 2Z | 82 | ARG | 2.4 |
| 33 | 1c | 149 | ALA | 2.4 |
| 41 | 2k | 72 | ALA | 2.4 |
| 52 | 2v | 531 | GLY | 2.4 |
| 8 | 2N | 72 | TYR | 2.4 |
| 52 | 2v | 515 | GLU | 2.4 |
| 14 | 2T | 48 | ILE | 2.4 |
| 26 | 15 | 6 | VAL | 2.4 |
| 52 | 1v | 425 | SER | 2.4 |
| 1 | 2A | 2111 | C | 2.4 |
| 31 | 1a | 926 | G | 2.4 |
| 31 | 1a | 1210 | C | 2.4 |
| 9 | 2O | 8 | LEU | 2.4 |
| 33 | 1c | 12 | LEU | 2.4 |
| 34 | 2d | 67 | ILE | 2.4 |
| 53 | 1w | 83 | ILE | 2.4 |
| 8 | 2N | 9 | VAL | 2.4 |
| 14 | 1T | 54 | ARG | 2.4 |
| 52 | 1v | 609 | GLU | 2.4 |
| 1 | 2A | 171 | G | 2.4 |
| 1 | 2A | 194 | G | 2.4 |
| 31 | 2a | 953 | G | 2.4 |
| 41 | 2k | 38 | ASN | 2.4 |
| 5 | 2F | 155 | LEU | 2.4 |
| 14 | 1T | 73 | GLU | 2.4 |
| 22 | 11 | 26 | ARG | 2.4 |
| 41 | 1k | 63 | LEU | 2.4 |
| 52 | 2v | 157 | LEU | 2.4 |
| 33 | 1c | 31 | HIS | 2.4 |
| 39 | 2i | 41 | VAL | 2.4 |
| 37 | 1g | 152 | ALA | 2.4 |
| 52 | 2v | 654 | GLY | 2.4 |
| 37 | 2g | 15 | ASP | 2.4 |
| 52 | 2v | 410 | ASP | 2.4 |
| 11 | 2Q | 91 | GLU | 2.4 |
| 22 | 21 | 43 | TYR | 2.4 |
| 31 | 2a | 884 | U | 2.4 |
| 35 | 2e | 107 | ARG | 2.4 |
| 37 | 1g | 129 | GLU | 2.4 |
| 41 | 2k | 59 | TYR | 2.4 |

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| Mol | Chain | Res | Type | RSRZ |
|---|---|---|---|---|
| 47 | 2q | 34 | LYS | 2.4 |
| 52 | 1v | 491 | VAL | 2.4 |
| 5 | 1F | 71 | GLY | 2.4 |
| 41 | 2k | 56 | GLY | 2.4 |
| 52 | 2v | 487 | ILE | 2.4 |
| 54 | 1x | 41 | C | 2.4 |
| 31 | 2a | 1131 | G | 2.4 |
| 52 | 1v | 500 | GLN | 2.4 |
| 9 | 1O | 8 | LEU | 2.4 |
| 35 | 1e | 120 | THR | 2.4 |
| 51 | 2u | 5 | ASP | 2.4 |
| 14 | 2T | 96 | ARG | 2.4 |
| 27 | 26 | 19 | ARG | 2.4 |
| 40 | 1j | 43 | ARG | 2.4 |
| 8 | 2N | 81 | GLY | 2.4 |
| 29 | 18 | 4 | MET | 2.4 |
| 41 | 1k | 21 | ILE | 2.4 |
| 40 | 1j | 56 | HIS | 2.4 |
| 1 | 1A | 2440 | C | 2.4 |
| 19 | 2Y | 35 | TYR | 2.4 |
| 33 | 2c | 127 | ARG | 2.4 |
| 38 | 1h | 46 | LYS | 2.4 |
| 52 | 1v | 655 | TYR | 2.4 |
| 18 | 1X | 1 | MET | 2.4 |
| 33 | 2c | 200 | ALA | 2.4 |
| 16 | 2V | 20 | LEU | 2.4 |
| 34 | 2d | 169 | LYS | 2.4 |
| 1 | 2A | 2118 | U | 2.4 |
| 4 | 1E | 14 | ILE | 2.4 |
| 20 | 2Z | 169 | GLU | 2.4 |
| 43 | 1m | 84 | ILE | 2.4 |
| 52 | 2v | 168 | ILE | 2.4 |
| 53 | 1w | 86 | SER | 2.4 |
| 33 | 2c | 147 | LYS | 2.4 |
| 1 | 1A | 1990 | C | 2.4 |
| 1 | 2A | 896 | A | 2.4 |
| 22 | 21 | 19 | GLN | 2.4 |
| 24 | 23 | 6 | VAL | 2.4 |
| 31 | 1a | 1344 | C | 2.4 |
| 33 | 2c | 42 | LEU | 2.4 |
| 35 | 1e | 141 | GLN | 2.4 |
| 54 | 1x | 36 | A | 2.4 |

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| Mol | Chain | Res | Type | RSRZ |
|---|---|---|---|---|
| 54 | 1x | 73 | A | 2.4 |
| 6 | 2G | 137 | GLU | 2.4 |
| 32 | 2b | 97 | TRP | 2.4 |
| 52 | 2v | 498 | ILE | 2.4 |
| 53 | 2w | 161 | ILE | 2.4 |
| 42 | 2l | 51 | ALA | 2.4 |
| 32 | 1b | 232 | PRO | 2.4 |
| 39 | 2i | 125 | TYR | 2.4 |
| 44 | 1n | 52 | GLN | 2.4 |
| 11 | 2Q | 105 | GLU | 2.4 |
| 14 | 1T | 57 | PHE | 2.4 |
| 37 | 1g | 30 | ILE | 2.4 |
| 1 | 1A | 652(T) | C | 2.4 |
| 1 | 1A | 1656 | C | 2.4 |
| 25 | 24 | 64 | GLY | 2.4 |
| 9 | 2O | 96 | THR | 2.4 |
| 31 | 1a | 1201 | A | 2.4 |
| 52 | 2v | 564 | LYS | 2.4 |
| 52 | 2v | 633 | GLY | 2.4 |
| 20 | 2Z | 195 | GLU | 2.4 |
| 33 | 2c | 58 | GLU | 2.4 |
| 52 | 2v | 494 | GLU | 2.4 |
| 29 | 28 | 52 | LYS | 2.4 |
| 31 | 1a | 1521 | G | 2.4 |
| 31 | 2a | 895 | G | 2.4 |
| 54 | 1x | 63 | G | 2.4 |
| 15 | 1U | 28 | ARG | 2.4 |
| 24 | 23 | 4 | LEU | 2.4 |
| 39 | 1i | 93 | ARG | 2.4 |
| 40 | 2j | 59 | SER | 2.4 |
| 41 | 1k | 82 | VAL | 2.4 |
| 29 | 28 | 16 | ILE | 2.4 |
| 31 | 1a | 915 | A | 2.4 |
| 31 | 1a | 1208 | C | 2.4 |
| 31 | 2a | 915 | A | 2.4 |
| 45 | 2o | 46 | HIS | 2.4 |
| 47 | 2q | 96 | GLU | 2.4 |
| 53 | 2w | 135 | GLU | 2.4 |
| 43 | 1m | 104 | ARG | 2.4 |
| 7 | 2H | 131 | VAL | 2.4 |
| 3 | 2D | 275 | LYS | 2.4 |
| 34 | 2d | 70 | ILE | 2.4 |

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| Mol | Chain | Res | Type | RSRZ |
|---|---|---|---|---|
| 25 | 24 | 9 | LEU | 2.4 |
| 33 | 2c | 159 | GLY | 2.4 |
| 35 | 1e | 43 | LEU | 2.4 |
| 39 | 2i | 102 | LEU | 2.4 |
| 52 | 2v | 143 | GLY | 2.4 |
| 41 | 1k | 65 | ALA | 2.4 |
| 34 | 2d | 166 | LYS | 2.4 |
| 52 | 1v | 93 | GLU | 2.3 |
| 21 | 20 | 80 | HIS | 2.3 |
| 33 | 1c | 78 | GLY | 2.3 |
| 42 | 1l | 27 | LEU | 2.3 |
| 42 | 2l | 27 | LEU | 2.3 |
| 53 | 2w | 184 | LEU | 2.3 |
| 1 | 1A | 2125 | G | 2.3 |
| 46 | 2p | 36 | ILE | 2.3 |
| 9 | 1O | 101 | PRO | 2.3 |
| 1 | 2A | 412 | A | 2.3 |
| 6 | 2G | 120 | LEU | 2.3 |
| 21 | 20 | 75 | LEU | 2.3 |
| 31 | 1a | 1349 | A | 2.3 |
| 37 | 1g | 65 | ALA | 2.3 |
| 1 | 2A | 2128 | C | 2.3 |
| 17 | 1W | 101 | SER | 2.3 |
| 31 | 1a | 957 | U | 2.3 |
| 53 | 2w | 180 | GLU | 2.3 |
| 9 | 1O | 25 | LEU | 2.3 |
| 52 | 2v | 539 | ILE | 2.3 |
| 54 | 1x | 30 | G | 2.3 |
| 31 | 1a | 1350 | A | 2.3 |
| 11 | 2Q | 81 | VAL | 2.3 |
| 31 | 1a | 817 | C | 2.3 |
| 31 | 2a | 789 | U | 2.3 |
| 40 | 2j | 42 | THR | 2.3 |
| 42 | 1l | 87 | GLY | 2.3 |
| 52 | 2v | 506 | GLN | 2.3 |
| 14 | 1T | 78 | LEU | 2.3 |
| 4 | 1E | 117 | MET | 2.3 |
| 3 | 1D | 17 | THR | 2.3 |
| 5 | 2F | 53 | THR | 2.3 |
| 20 | 2Z | 118 | GLN | 2.3 |
| 21 | 20 | 19 | LYS | 2.3 |
| 42 | 2l | 54 | LYS | 2.3 |

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| Mol | Chain | Res | Type | RSRZ |
|---|---|---|---|---|
| 43 | 2m | 103 | THR | 2.3 |
| 52 | 2v | 104 | ALA | 2.3 |
| 1 | 2A | 1764 | G | 2.3 |
| 3 | 2D | 217 | ARG | 2.3 |
| 14 | 1T | 52 | ILE | 2.3 |
| 31 | 1a | 1061 | G | 2.3 |
| 31 | 1a | 1343 | G | 2.3 |
| 31 | 2a | 286 | G | 2.3 |
| 35 | 1e | 143 | ARG | 2.3 |
| 52 | 1v | -63 | ILE | 2.3 |
| 54 | 1x | 23 | A | 2.3 |
| 32 | 1b | 165 | VAL | 2.3 |
| 53 | 1w | 158 | GLU | 2.3 |
| 19 | 2Y | 5 | MET | 2.3 |
| 6 | 2G | 98 | ARG | 2.3 |
| 9 | 2O | 81 | ASP | 2.3 |
| 10 | 2P | 48 | PRO | 2.3 |
| 29 | 18 | 13 | ARG | 2.3 |
| 7 | 2H | 161 | GLY | 2.3 |
| 9 | 2O | 18 | LYS | 2.3 |
| 40 | 1j | 69 | ASN | 2.3 |
| 52 | 2v | 679 | VAL | 2.3 |
| 52 | 1v | -66 | MET | 2.3 |
| 52 | 2v | 667 | GLY | 2.3 |
| 22 | 11 | 24 | ALA | 2.3 |
| 1 | 1A | 2139 | C | 2.3 |
| 9 | 2O | 47 | ILE | 2.3 |
| 15 | 2U | 36 | ARG | 2.3 |
| 31 | 1a | 902 | G | 2.3 |
| 31 | 2a | 1375 | A | 2.3 |
| 33 | 1c | 136 | GLN | 2.3 |
| 42 | 2l | 86 | ARG | 2.3 |
| 52 | 1v | -40 | ARG | 2.3 |
| 53 | 2w | 61 | PRO | 2.3 |
| 54 | 2y | 36 | A | 2.3 |
| 54 | 1y | 62 | C | 2.3 |
| 3 | 1D | 5 | LYS | 2.3 |
| 14 | 2T | 73 | GLU | 2.3 |
| 52 | 2v | 346 | LYS | 2.3 |
| 52 | 2v | 672 | PHE | 2.3 |
| 9 | 1O | 87 | ILE | 2.3 |
| 14 | 1T | 51 | ARG | 2.3 |

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| Mol | Chain | Res | Type | RSRZ |
|---|---|---|---|---|
| 25 | 24 | 69 | LYS | 2.3 |
| 28 | 27 | 46 | VAL | 2.3 |
| 29 | 18 | 50 | LEU | 2.3 |
| 33 | 1c | 175 | LEU | 2.3 |
| 42 | 1l | 38 | THR | 2.3 |
| 42 | 1l | 91 | LYS | 2.3 |
| 1 | 2A | 2310 | A | 2.3 |
| 16 | 1V | 101 | GLY | 2.3 |
| 1 | 1A | 1657 | C | 2.3 |
| 4 | 1E | 1 | MET | 2.3 |
| 31 | 1a | 1520 | G | 2.3 |
| 31 | 2a | 796 | C | 2.3 |
| 31 | 2a | 1226 | C | 2.3 |
| 41 | 1k | 91 | ARG | 2.3 |
| 47 | 2q | 92 | ARG | 2.3 |
| 54 | 1y | 15 | G | 2.3 |
| 54 | 2y | 56 | C | 2.3 |
| 12 | 1R | 113 | LEU | 2.3 |
| 34 | 2d | 176 | LEU | 2.3 |
| 41 | 2k | 34 | ASP | 2.3 |
| 42 | 2l | 104 | VAL | 2.3 |
| 44 | 2n | 34 | TYR | 2.3 |
| 8 | 2N | 136 | GLU | 2.3 |
| 34 | 1d | 156 | GLU | 2.3 |
| 52 | 1v | 492 | ASP | 2.3 |
| 11 | 2Q | 100 | GLY | 2.3 |
| 52 | 1v | -31 | ALA | 2.3 |
| 14 | 1T | 50 | ILE | 2.3 |
| 8 | 1N | 84 | LYS | 2.3 |
| 10 | 1P | 59 | LEU | 2.3 |
| 20 | 2Z | 41 | LEU | 2.3 |
| 31 | 1a | 781 | A | 2.3 |
| 4 | 1E | 103 | ASP | 2.3 |
| 31 | 2a | 784 | C | 2.3 |
| 33 | 1c | 74 | GLY | 2.3 |
| 41 | 1k | 41 | THR | 2.3 |
| 3 | 2D | 224 | ALA | 2.3 |
| 4 | 1E | 135 | HIS | 2.3 |
| 14 | 1T | 79 | HIS | 2.3 |
| 9 | 2O | 113 | LYS | 2.3 |
| 11 | 2Q | 78 | PRO | 2.3 |
| 33 | 2c | 170 | GLN | 2.3 |

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| Mol | Chain | Res | Type | RSRZ |
|---|---|---|---|---|
| 39 | 1i | 85 | LEU | 2.3 |
| 44 | 2n | 53 | LEU | 2.3 |
| 52 | 1v | 595 | GLN | 2.3 |
| 4 | 1E | 144 | ARG | 2.3 |
| 32 | 1b | 152 | PHE | 2.3 |
| 39 | 1i | 101 | PHE | 2.3 |
| 35 | 2e | 138 | ALA | 2.3 |
| 1 | 2A | 2388 | A | 2.3 |
| 31 | 1a | 1213 | A | 2.3 |
| 47 | 2q | 88 | TYR | 2.3 |
| 53 | 2w | 28 | LEU | 2.3 |
| 31 | 1a | 999 | C | 2.3 |
| 31 | 2a | 241 | C | 2.3 |
| 31 | 2a | 701 | C | 2.3 |
| 31 | 2a | 1208 | C | 2.3 |
| 3 | 1D | 15 | PHE | 2.3 |
| 40 | 2j | 45 | ARG | 2.3 |
| 1 | 1A | 2506 | U | 2.3 |
| 7 | 2H | 151 | ILE | 2.3 |
| 52 | 2v | 621 | ILE | 2.3 |
| 40 | 1j | 94 | VAL | 2.3 |
| 54 | 2y | 45 | U | 2.3 |
| 14 | 1T | 3 | ARG | 2.3 |
| 34 | 2d | 110 | PHE | 2.3 |
| 52 | 2v | 603 | GLU | 2.3 |
| 9 | 1O | 103 | ALA | 2.3 |
| 1 | 1A | 652(S) | C | 2.3 |
| 1 | 1A | 1675 | C | 2.3 |
| 32 | 2b | 108 | ILE | 2.3 |
| 53 | 2w | 129 | ILE | 2.3 |
| 27 | 26 | 39 | TYR | 2.3 |
| 33 | 2c | 165 | THR | 2.3 |
| 41 | 2k | 25 | TYR | 2.3 |
| 1 | 1A | 2793 | G | 2.2 |
| 37 | 2g | 4 | ARG | 2.2 |
| 4 | 1E | 11 | MET | 2.2 |
| 4 | 1E | 118 | LYS | 2.2 |
| 4 | 1E | 156 | MET | 2.2 |
| 10 | 2P | 69 | GLY | 2.2 |
| 39 | 1i | 6 | GLY | 2.2 |
| 9 | 1O | 11 | ALA | 2.2 |
| 35 | 1e | 76 | ILE | 2.2 |

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| Mol | Chain | Res | Type | RSRZ |
|---|---|---|---|---|
| 3 | 1D | 168 | ARG | 2.2 |
| 44 | 2n | 37 | PHE | 2.2 |
| 44 | 2n | 46 | GLU | 2.2 |
| 53 | 2w | 158 | GLU | 2.2 |
| 32 | 2b | 232 | PRO | 2.2 |
| 52 | 2v | 629 | GLY | 2.2 |
| 11 | 2Q | 132 | VAL | 2.2 |
| 27 | 16 | 2 | ALA | 2.2 |
| 33 | 2c | 61 | ALA | 2.2 |
| 45 | 2o | 38 | ARG | 2.2 |
| 31 | 1a | 954 | G | 2.2 |
| 34 | 2d | 98 | GLU | 2.2 |
| 53 | 2w | 2 | THR | 2.2 |
| 3 | 1D | 231 | HIS | 2.2 |
| 35 | 1e | 70 | PRO | 2.2 |
| 44 | 2n | 49 | HIS | 2.2 |
| 22 | 21 | 5 | CYS | 2.2 |
| 41 | 1k | 95 | ILE | 2.2 |
| 41 | 2k | 73 | MET | 2.2 |
| 47 | 2q | 56 | VAL | 2.2 |
| 52 | 2v | 659 | LEU | 2.2 |
| 9 | 1O | 23 | ARG | 2.2 |
| 9 | 2O | 49 | ARG | 2.2 |
| 31 | 1a | 1531 | A | 2.2 |
| 52 | 2v | 572 | TYR | 2.2 |
| 47 | 2q | 69 | LYS | 2.2 |
| 1 | 1A | 2511 | U | 2.2 |
| 41 | 2k | 88 | GLY | 2.2 |
| 44 | 2n | 13 | THR | 2.2 |
| 53 | 1w | 154 | THR | 2.2 |
| 25 | 24 | 22 | ILE | 2.2 |
| 4 | 1E | 120 | TRP | 2.2 |
| 14 | 1T | 41 | ARG | 2.2 |
| 1 | 1A | 2505 | G | 2.2 |
| 1 | 2A | 1989 | G | 2.2 |
| 31 | 2a | 1475 | G | 2.2 |
| 31 | 2a | 1516 | G | 2.2 |
| 47 | 2q | 67 | LYS | 2.2 |
| 32 | 1b | 72 | GLY | 2.2 |
| 1 | 2A | 2169 | A | 2.2 |
| 6 | 2G | 97 | ASP | 2.2 |
| 31 | 1a | 983 | A | 2.2 |

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| Mol | Chain | Res | Type | RSRZ |
|---|---|---|---|---|
| 40 | 2j | 94 | VAL | 2.2 |
| 50 | 1t | 71 | THR | 2.2 |
| 1 | 2A | 387 | U | 2.2 |
| 9 | 1O | 108 | GLU | 2.2 |
| 52 | 2v | 400 | GLU | 2.2 |
| 52 | 1v | 475 | ASN | 2.2 |
| 33 | 1c | 118 | GLN | 2.2 |
| 52 | 1v | 543 | GLN | 2.2 |
| 52 | 2v | 549 | ALA | 2.2 |
| 52 | 2v | 565 | VAL | 2.2 |
| 33 | 2c | 10 | PHE | 2.2 |
| 44 | 2n | 15 | LYS | 2.2 |
| 54 | 2y | 10 | G | 2.2 |
| 16 | 2V | 94 | LEU | 2.2 |
| 24 | 23 | 47 | VAL | 2.2 |
| 31 | 1a | 814 | A | 2.2 |
| 31 | 1a | 697 | U | 2.2 |
| 38 | 1h | 111 | ILE | 2.2 |
| 14 | 2T | 22 | PHE | 2.2 |
| 31 | 1a | 1226 | C | 2.2 |
| 33 | 2c | 123 | GLN | 2.2 |
| 39 | 2i | 82 | ALA | 2.2 |
| 4 | 2E | 128 | SER | 2.2 |
| 33 | 2c | 51 | GLY | 2.2 |
| 9 | 2O | 94 | ARG | 2.2 |
| 41 | 2k | 100 | ALA | 2.2 |
| 52 | 1v | 525 | PHE | 2.2 |
| 31 | 2a | 1497 | G | 2.2 |
| 3 | 2D | 169 | GLU | 2.2 |
| 3 | 2D | 194 | GLY | 2.2 |
| 14 | 2T | 36 | GLU | 2.2 |
| 35 | 2e | 82 | VAL | 2.2 |
| 44 | 2n | 56 | VAL | 2.2 |
| 52 | 2v | 433 | GLU | 2.2 |
| 52 | 2v | 450 | ILE | 2.2 |
| 41 | 1k | 69 | ALA | 2.2 |
| 41 | 1k | 75 | TYR | 2.2 |
| 3 | 2D | 206 | LEU | 2.2 |
| 10 | 2P | 57 | THR | 2.2 |
| 43 | 2m | 97 | PRO | 2.2 |
| 14 | 1T | 48 | ILE | 2.2 |
| 32 | 2b | 115 | LEU | 2.2 |

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| Mol | Chain | Res | Type | RSRZ |
|---|---|---|---|---|
| 33 | 2c | 6 | HIS | 2.2 |
| 46 | 1p | 34 | GLU | 2.2 |
| 49 | 2s | 77 | THR | 2.2 |
| 33 | 2c | 59 | ARG | 2.2 |
| 31 | 1a | 1368 | G | 2.2 |
| 31 | 2a | 782 | A | 2.2 |
| 31 | 2a | 1342 | C | 2.2 |
| 41 | 2k | 111 | ASP | 2.2 |
| 42 | 2l | 55 | VAL | 2.2 |
| 47 | 2q | 53 | LEU | 2.2 |
| 48 | 1r | 31 | LEU | 2.2 |
| 55 | 1z | 18 | C | 2.2 |
| 52 | 2v | 86 | GLY | 2.2 |
| 1 | 2A | 2099 | U | 2.2 |
| 8 | 1N | 140 | VAL | 2.2 |
| 33 | 2c | 18 | TRP | 2.2 |
| 43 | 1m | 15 | VAL | 2.2 |
| 52 | 2v | 389 | LEU | 2.2 |
| 54 | 2y | 50 | U | 2.2 |
| 6 | 1G | 144 | ILE | 2.2 |
| 14 | 2T | 65 | LYS | 2.2 |
| 19 | 2Y | 46 | LYS | 2.2 |
| 31 | 1a | 1513 | A | 2.2 |
| 40 | 2j | 48 | THR | 2.2 |
| 41 | 1k | 45 | GLY | 2.2 |
| 52 | 1v | -34 | ARG | 2.2 |
| 52 | 2v | 508 | GLY | 2.2 |
| 41 | 1k | 64 | ALA | 2.2 |
| 41 | 2k | 65 | ALA | 2.2 |
| 42 | 1l | 22 | SER | 2.2 |
| 31 | 2a | 1214 | C | 2.2 |
| 3 | 2D | 261 | LYS | 2.2 |
| 4 | 1E | 152 | LYS | 2.2 |
| 9 | 2O | 98 | VAL | 2.2 |
| 9 | 2O | 106 | LEU | 2.2 |
| 37 | 2g | 13 | GLN | 2.2 |
| 41 | 1k | 109 | VAL | 2.2 |
| 48 | 2r | 26 | LEU | 2.2 |
| 52 | 1v | 608 | VAL | 2.2 |
| 24 | 13 | 2 | PRO | 2.2 |
| 32 | 1b | 202 | PRO | 2.2 |
| 8 | 2N | 127 | ASP | 2.2 |

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| Mol | Chain | Res | Type | RSRZ |
|---|---|---|---|---|
| 9 | 1O | 56 | ASP | 2.2 |
| 9 | 1O | 65 | THR | 2.2 |
| 47 | 2q | 97 | SER | 2.2 |
| 9 | 1O | 32 | TYR | 2.2 |
| 52 | 1v | 538 | TYR | 2.2 |
| 33 | 1c | 206 | GLU | 2.2 |
| 35 | 1e | 80 | ILE | 2.2 |
| 39 | 2i | 6 | GLY | 2.2 |
| 28 | 27 | 1 | MET | 2.2 |
| 31 | 1a | 998 | G | 2.2 |
| 31 | 2a | 812 | C | 2.2 |
| 54 | 2y | 13 | C | 2.2 |
| 9 | 1O | 97 | ARG | 2.2 |
| 29 | 18 | 26 | LYS | 2.2 |
| 37 | 1g | 95 | ARG | 2.2 |
| 42 | 2l | 39 | VAL | 2.2 |
| 9 | 1O | 27 | GLY | 2.1 |
| 1 | 1A | 752 | A | 2.1 |
| 7 | 2H | 57 | ASP | 2.1 |
| 14 | 2T | 74 | ARG | 2.1 |
| 27 | 26 | 14 | THR | 2.1 |
| 33 | 2c | 4 | LYS | 2.1 |
| 34 | 1d | 112 | VAL | 2.1 |
| 38 | 2h | 73 | ASP | 2.1 |
| 48 | 2r | 21 | LYS | 2.1 |
| 53 | 2w | 144 | ALA | 2.1 |
| 9 | 2O | 121 | VAL | 2.1 |
| 11 | 2Q | 76 | LYS | 2.1 |
| 14 | 1T | 100 | TYR | 2.1 |
| 26 | 15 | 58 | LEU | 2.1 |
| 33 | 2c | 111 | LEU | 2.1 |
| 38 | 1h | 112 | LEU | 2.1 |
| 53 | 1w | 156 | ARG | 2.1 |
| 10 | 2P | 42 | SER | 2.1 |
| 33 | 1c | 18 | TRP | 2.1 |
| 39 | 1i | 74 | ILE | 2.1 |
| 43 | 2m | 78 | ILE | 2.1 |
| 50 | 2t | 55 | ILE | 2.1 |
| 52 | 1v | 529 | ILE | 2.1 |
| 19 | 2Y | 58 | GLY | 2.1 |
| 1 | 1A | 1669 | A | 2.1 |
| 20 | 2Z | 59 | LEU | 2.1 |

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| Mol | Chain | Res | Type | RSRZ |
|---|---|---|---|---|
| 22 | 11 | 25 | LYS | 2.1 |
| 22 | 21 | 4 | VAL | 2.1 |
| 42 | 1l | 47 | LYS | 2.1 |
| 1 | 2A | 201 | C | 2.1 |
| 7 | 2H | 72 | ILE | 2.1 |
| 31 | 2a | 248 | C | 2.1 |
| 1 | 2A | 958 | U | 2.1 |
| 1 | 2A | 2167 | U | 2.1 |
| 4 | 2E | 130 | GLY | 2.1 |
| 11 | 2Q | 138 | ASP | 2.1 |
| 31 | 2a | 926 | G | 2.1 |
| 48 | 2r | 62 | GLU | 2.1 |
| 54 | 1x | 29 | G | 2.1 |
| 3 | 2D | 245 | PRO | 2.1 |
| 4 | 1E | 114 | ALA | 2.1 |
| 4 | 1E | 104 | VAL | 2.1 |
| 37 | 2g | 44 | TYR | 2.1 |
| 39 | 2i | 79 | LEU | 2.1 |
| 52 | 1v | -48 | VAL | 2.1 |
| 44 | 2n | 61 | TRP | 2.1 |
| 5 | 2F | 81 | PRO | 2.1 |
| 35 | 1e | 119 | LEU | 2.1 |
| 52 | 2v | 550 | MET | 2.1 |
| 19 | 2Y | 40 | GLU | 2.1 |
| 4 | 1E | 127 | ASP | 2.1 |
| 35 | 2e | 16 | THR | 2.1 |
| 20 | 2Z | 39 | VAL | 2.1 |
| 46 | 2p | 18 | ARG | 2.1 |
| 1 | 1A | 1938 | A | 2.1 |
| 1 | 2A | 204 | A | 2.1 |
| 4 | 1E | 160 | TYR | 2.1 |
| 52 | 2v | 255 | ILE | 2.1 |
| 35 | 2e | 47 | LYS | 2.1 |
| 52 | 1v | -45 | LYS | 2.1 |
| 52 | 1v | 494 | GLU | 2.1 |
| 5 | 1F | 74 | ARG | 2.1 |
| 14 | 1T | 103 | ARG | 2.1 |
| 28 | 17 | 47 | ARG | 2.1 |
| 31 | 2a | 1049 | U | 2.1 |
| 34 | 1d | 66 | ARG | 2.1 |
| 54 | 1x | 60 | U | 2.1 |
| 50 | 2t | 12 | ALA | 2.1 |

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| Mol | Chain | Res | Type | RSRZ |
|---|---|---|---|---|
| 29 | 28 | 33 | ASN | 2.1 |
| 52 | 1v | 582 | PHE | 2.1 |
| 7 | 2H | 167 | GLU | 2.1 |
| 37 | 2g | 55 | GLY | 2.1 |
| 5 | 2F | 167 | ALA | 2.1 |
| 7 | 2H | 171 | LEU | 2.1 |
| 35 | 1e | 48 | ALA | 2.1 |
| 39 | 1i | 119 | ALA | 2.1 |
| 5 | 2F | 83 | PHE | 2.1 |
| 31 | 1a | 1341 | U | 2.1 |
| 41 | 1k | 27 | ASN | 2.1 |
| 1 | 1A | 886 | C | 2.1 |
| 44 | 1n | 15 | LYS | 2.1 |
| 3 | 2D | 235 | GLY | 2.1 |
| 16 | 2V | 42 | GLY | 2.1 |
| 3 | 1D | 37 | LEU | 2.1 |
| 11 | 2Q | 37 | LEU | 2.1 |
| 14 | 1T | 114 | LEU | 2.1 |
| 40 | 2j | 70 | ARG | 2.1 |
| 1 | 2A | 381 | G | 2.1 |
| 1 | 2A | 2396 | G | 2.1 |
| 8 | 1N | 109 | LYS | 2.1 |
| 9 | 1O | 37 | ASP | 2.1 |
| 11 | 2Q | 129 | THR | 2.1 |
| 31 | 1a | 953 | G | 2.1 |
| 35 | 2e | 13 | ILE | 2.1 |
| 40 | 2j | 89 | ASP | 2.1 |
| 42 | 2l | 45 | PRO | 2.1 |
| 31 | 2a | 1044 | A | 2.1 |
| 33 | 1c | 16 | ARG | 2.1 |
| 34 | 1d | 183 | GLY | 2.1 |
| 44 | 1n | 20 | ALA | 2.1 |
| 9 | 1O | 7 | TYR | 2.1 |
| 31 | 1a | 1051 | C | 2.1 |
| 33 | 2c | 14 | ILE | 2.1 |
| 40 | 1j | 91 | PRO | 2.1 |
| 4 | 1E | 196 | VAL | 2.1 |
| 18 | 1X | 92 | LEU | 2.1 |
| 34 | 1d | 148 | VAL | 2.1 |
| 39 | 1i | 106 | ALA | 2.1 |
| 52 | 1v | 427 | ALA | 2.1 |
| 31 | 1a | 1034 | G | 2.1 |

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| Mol | Chain | Res | Type | RSRZ |
|---|---|---|---|---|
| 20 | 2Z | 121 | HIS | 2.1 |
| 31 | 1a | 1358 | U | 2.1 |
| 4 | 1E | 146 | THR | 2.1 |
| 9 | 2O | 23 | ARG | 2.1 |
| 10 | 2P | 94 | GLU | 2.1 |
| 34 | 1d | 168 | ARG | 2.1 |
| 53 | 2w | 148 | HIS | 2.1 |
| 44 | 2n | 14 | PRO | 2.1 |
| 9 | 2O | 13 | ASN | 2.1 |
| 52 | 2v | 527 | ASN | 2.1 |
| 10 | 2P | 110 | TYR | 2.1 |
| 26 | 15 | 8 | LYS | 2.1 |
| 22 | 11 | 19 | GLN | 2.1 |
| 7 | 2H | 133 | VAL | 2.1 |
| 14 | 1T | 40 | THR | 2.1 |
| 22 | 21 | 29 | GLY | 2.1 |
| 33 | 2c | 46 | GLU | 2.1 |
| 35 | 1e | 22 | GLY | 2.1 |
| 37 | 1g | 59 | LEU | 2.1 |
| 39 | 1i | 100 | GLY | 2.1 |
| 42 | 1l | 29 | GLY | 2.1 |
| 1 | 2A | 1918 | A | 2.1 |
| 1 | 2A | 2120 | G | 2.1 |
| 4 | 1E | 192 | ASN | 2.1 |
| 33 | 1c | 72 | LYS | 2.1 |
| 53 | 1w | 42 | LYS | 2.1 |
| 9 | 2O | 7 | TYR | 2.1 |
| 1 | 2A | 253 | C | 2.1 |
| 1 | 2A | 2177 | C | 2.1 |
| 8 | 2N | 11 | PRO | 2.1 |
| 9 | 2O | 4 | PRO | 2.1 |
| 14 | 1T | 82 | LEU | 2.1 |
| 29 | 28 | 54 | GLU | 2.1 |
| 8 | 2N | 1 | MET | 2.1 |
| 10 | 1P | 29 | LYS | 2.1 |
| 21 | 20 | 15 | ASP | 2.1 |
| 37 | 2g | 60 | LYS | 2.1 |
| 52 | 2v | 546 | ILE | 2.1 |
| 52 | 1v | -56 | ASN | 2.1 |
| 52 | 2v | 666 | ARG | 2.1 |
| 1 | 2A | 2189 | U | 2.1 |
| 21 | 20 | 38 | VAL | 2.1 |

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| Mol | Chain | Res | Type | RSRZ |
|---|---|---|---|---|
| 3 | 1D | 237 | GLU | 2.1 |
| 7 | 2H | 62 | LYS | 2.0 |
| 9 | 1O | 66 | LYS | 2.0 |
| 11 | 2Q | 15 | GLY | 2.1 |
| 16 | 2V | 35 | LEU | 2.1 |
| 34 | 2d | 101 | LEU | 2.1 |
| 34 | 2d | 135 | LEU | 2.1 |
| 54 | 1x | 12 | U | 2.1 |
| 52 | 1v | 90 | PHE | 2.1 |
| 20 | 2Z | 170 | THR | 2.0 |
| 31 | 1a | 1047 | G | 2.0 |
| 52 | 1v | 490 | PRO | 2.0 |
| 37 | 2g | 125 | MET | 2.0 |
| 53 | 1w | 55 | ILE | 2.0 |
| 54 | 1y | 5 | G | 2.0 |
| 41 | 1k | 54 | ARG | 2.0 |
| 31 | 1a | 1501 | C | 2.0 |
| 31 | 1a | 1514 | C | 2.0 |
| 32 | 1b | 93 | VAL | 2.0 |
| 9 | 1O | 79 | PHE | 2.0 |
| 9 | 1O | 113 | LYS | 2.0 |
| 9 | 2O | 55 | GLY | 2.0 |
| 22 | 11 | 84 | GLY | 2.0 |
| 52 | 2v | 545 | GLY | 2.0 |
| 4 | 1E | 126 | PRO | 2.0 |
| 9 | 1O | 60 | ALA | 2.0 |
| 9 | 1O | 93 | PRO | 2.0 |
| 17 | 1W | 89 | ALA | 2.0 |
| 39 | 2i | 61 | ALA | 2.0 |
| 47 | 2q | 30 | PRO | 2.0 |
| 9 | 1O | 12 | ASP | 2.0 |
| 34 | 2d | 27 | TYR | 2.0 |
| 38 | 2h | 93 | VAL | 2.0 |
| 10 | 1P | 44 | GLY | 2.0 |
| 15 | 2U | 89 | GLU | 2.0 |
| 34 | 1d | 200 | GLU | 2.0 |
| 1 | 1A | 2049 | G | 2.0 |
| 31 | 1a | 1206 | G | 2.0 |
| 31 | 2a | 80 | G | 2.0 |
| 31 | 2a | 1031 | G | 2.0 |
| 1 | 1A | 2129 | C | 2.0 |
| 3 | 1D | 239 | ARG | 2.0 |

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| Mol | Chain | Res | Type | RSRZ |
|---|---|---|---|---|
| 53 | 2w | 150 | SER | 2.0 |
| 1 | 2A | 1923 | U | 2.0 |
| 9 | 1O | 80 | ASP | 2.0 |
| 20 | 2Z | 36 | LYS | 2.0 |
| 32 | 2b | 220 | ASP | 2.0 |
| 40 | 2j | 58 | ASP | 2.0 |
| 45 | 2o | 47 | LYS | 2.0 |
| 40 | 2j | 98 | ILE | 2.0 |
| 41 | 1k | 77 | MET | 2.0 |
| 49 | 2s | 78 | ARG | 2.0 |
| 53 | 2w | 64 | ARG | 2.0 |
| 49 | 1s | 58 | VAL | 2.0 |
| 54 | 1x | 14 | A | 2.0 |
| 10 | 1P | 51 | PHE | 2.0 |
| 6 | 2G | 177 | GLY | 2.0 |
| 1 | 2A | 385 | C | 2.0 |
| 1 | 2A | 1904 | G | 2.0 |
| 1 | 2A | 2165 | G | 2.0 |
| 3 | 2D | 247 | ALA | 2.0 |
| 31 | 2a | 1045 | C | 2.0 |
| 31 | 2a | 1526 | G | 2.0 |
| 39 | 2i | 87 | GLN | 2.0 |
| 20 | 2Z | 53 | ILE | 2.0 |
| 34 | 2d | 5 | ILE | 2.0 |
| 42 | 1l | 30 | ALA | 2.0 |
| 4 | 1E | 203 | LYS | 2.0 |
| 1 | 1A | 676 | A | 2.0 |
| 9 | 2O | 103 | ALA | 2.0 |
| 20 | 2Z | 124 | ILE | 2.0 |
| 31 | 1a | 959 | A | 2.0 |
| 40 | 2j | 60 | ARG | 2.0 |
| 52 | 1v | 473 | ASP | 2.0 |
| 5 | 2F | 156 | LEU | 2.0 |
| 32 | 2b | 139 | LYS | 2.0 |
| 41 | 1k | 122 | LYS | 2.0 |
| 1 | 1A | 745 | G | 2.0 |
| 1 | 1A | 2146 | C | 2.0 |
| 20 | 1Z | 10 | ARG | 2.0 |
| 21 | 20 | 44 | ARG | 2.0 |
| 21 | 20 | 74 | ARG | 2.0 |
| 31 | 1a | 973 | G | 2.0 |
| 31 | 2a | 1491 | G | 2.0 |

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| Mol | Chain | Res | Type | RSRZ |
|---|---|---|---|---|
| 33 | 1c | 30 | ARG | 2.0 |
| 48 | 2r | 55 | ARG | 2.0 |
| 54 | 1x | 18 | G | 2.0 |
| 3 | 1D | 3 | VAL | 2.0 |
| 3 | 2D | 53 | PHE | 2.0 |
| 33 | 1c | 111 | LEU | 2.0 |
| 49 | 2s | 66 | MET | 2.0 |
| 47 | 2q | 70 | ARG | 2.0 |
| 52 | 1v | 552 | SER | 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 |
|---|---|---|---|---|---|---|---|---|
| 54 | PSU | 2x | 55 | 20/21 | 0.34 | 1.03 | 240,240,240,240 | 0 |
| 54 | PSU | 2y | 32 | 20/21 | 0.50 | 0.37 | 220,220,220,220 | 0 |
| 54 | 7MG | 1x | 46 | 24/25 | 0.52 | 0.32 | 203,203,203,203 | 0 |
| 54 | PSU | 2y | 55 | 20/21 | 0.52 | 0.47 | 279,279,279,279 | 0 |
| 54 | 5MU | 2x | 54 | 21/22 | 0.54 | 0.72 | 237,237,237,237 | 0 |
| 54 | 4SU | 2x | 8 | 20/21 | 0.61 | 1.10 | 239,239,239,239 | 0 |
| 54 | 5MU | 2y | 54 | 21/22 | 0.62 | 0.74 | 276,276,276,276 | 0 |
| 54 | 7MG | 2y | 46 | 24/25 | 0.65 | 0.39 | 261,261,261,261 | 0 |
| 54 | 7MG | 2x | 46 | 24/25 | 0.66 | 1.03 | 241,241,241,241 | 0 |
| 54 | 4SU | 1x | 8 | 20/21 | 0.66 | 0.35 | 199,199,199,199 | 0 |
| 54 | PSU | 1y | 32 | 20/21 | 0.66 | 0.43 | 188,188,188,188 | 0 |
| 54 | PSU | 1x | 55 | 20/21 | 0.68 | 0.32 | 194,194,194,194 | 0 |
| 54 | 5MU | 1y | 54 | 21/22 | 0.69 | 0.17 | 236,236,236,236 | 0 |
| 54 | MIA | 2y | 37 | 22/30 | 0.69 | 0.39 | 208,208,208,208 | 0 |
| 1 | PSU | 2A | 1911 | 20/21 | 0.73 | 0.25 | 158,158,158,158 | 0 |
| 54 | PSU | 1y | 55 | 20/21 | 0.73 | 0.14 | 240,240,240,240 | 0 |
| 54 | 4SU | 2y | 8 | 20/21 | 0.74 | 0.32 | 259,259,259,259 | 0 |
| 54 | PSU | 2x | 32 | 20/21 | 0.75 | 0.66 | 214,214,214,214 | 0 |
| 31 | 5MC | 2a | 967 | 21/22 | 0.76 | 0.15 | 216,216,216,216 | 0 |
| 54 | MIA | 2x | 37 | 22/30 | 0.78 | 0.72 | 192,192,192,192 | 0 |
| 54 | MIA | 1y | 37 | 22/30 | 0.79 | 0.32 | 175,175,175,175 | 0 |
| 54 | PSU | 2y | 39 | 20/21 | 0.79 | 0.67 | 212,212,212,212 | 0 |
| 54 | 5MU | 1x | 54 | 21/22 | 0.80 | 0.32 | 193,193,193,193 | 0 |

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| Mol | Type | Chain | Res | Atoms | RSCC | RSR | B-factors(Å$^2$) | Q<0.9 |
|---|---|---|---|---|---|---|---|---|
| 1 | PSU | 1A | 1911 | 20/21 | 0.80 | 0.29 | 130,130,130,130 | 0 |
| 54 | MIA | 1x | 37 | 22/30 | 0.81 | 0.50 | 163,163,163,163 | 0 |
| 54 | PSU | 1x | 32 | 20/21 | 0.81 | 0.65 | 184,184,184,184 | 0 |
| 54 | PSU | 2x | 39 | 20/21 | 0.82 | 0.99 | 204,204,204,204 | 0 |
| 54 | 7MG | 1y | 46 | 24/25 | 0.82 | 0.33 | 222,222,222,222 | 0 |
| 54 | 4SU | 1y | 8 | 20/21 | 0.82 | 0.34 | 217,217,217,217 | 0 |
| 31 | 2MG | 1a | 1207 | 24/25 | 0.83 | 0.31 | 209,209,209,209 | 0 |
| 54 | PSU | 1x | 39 | 20/21 | 0.83 | 0.39 | 173,173,173,173 | 0 |
| 31 | 5MC | 2a | 1404 | 21/22 | 0.84 | 0.35 | 156,156,156,156 | 0 |
| 1 | 5MU | 2A | 1915 | 21/22 | 0.84 | 0.36 | 169,169,169,169 | 0 |
| 1 | PSU | 2A | 1917 | 20/21 | 0.84 | 0.30 | 164,164,164,164 | 0 |
| 31 | 4OC | 2a | 1402 | 22/23 | 0.84 | 0.28 | 165,165,165,165 | 0 |
| 31 | PSU | 1a | 516 | 20/21 | 0.85 | 0.15 | 144,144,144,144 | 0 |
| 31 | 5MC | 1a | 967 | 21/22 | 0.85 | 0.41 | 188,188,188,188 | 0 |
| 31 | 5MC | 2a | 1407 | 21/22 | 0.85 | 0.41 | 157,157,157,157 | 0 |
| 31 | MA6 | 2a | 1518 | 24/25 | 0.86 | 0.48 | 149,149,149,149 | 0 |
| 31 | 2MG | 2a | 1207 | 24/25 | 0.86 | 0.23 | 232,232,232,232 | 0 |
| 31 | 5MC | 1a | 1407 | 21/22 | 0.87 | 0.24 | 129,129,129,129 | 0 |
| 1 | PSU | 1A | 1917 | 20/21 | 0.87 | 0.15 | 138,138,138,138 | 0 |
| 31 | M2G | 1a | 966 | 25/26 | 0.88 | 0.37 | 184,184,184,184 | 0 |
| 31 | UR3 | 2a | 1498 | 21/22 | 0.89 | 0.34 | 158,158,158,158 | 0 |
| 31 | PSU | 2a | 516 | 20/21 | 0.89 | 0.14 | 166,166,166,166 | 0 |
| 31 | MA6 | 2a | 1519 | 24/25 | 0.89 | 0.54 | 148,148,148,148 | 0 |
| 31 | 7MG | 2a | 527 | 24/25 | 0.90 | 0.18 | 155,155,155,155 | 0 |
| 31 | 5MC | 2a | 1400 | 21/22 | 0.90 | 0.44 | 182,182,182,182 | 0 |
| 1 | OMC | 2A | 1920 | 21/22 | 0.90 | 0.32 | 153,153,153,153 | 0 |
| 42 | 0TD | 2l | 92 | 10/11 | 0.90 | 0.66 | 155,155,155,155 | 0 |
| 42 | 0TD | 1l | 92 | 10/11 | 0.90 | 0.36 | 132,132,132,132 | 0 |
| 31 | 7MG | 1a | 527 | 24/25 | 0.90 | 0.21 | 133,133,133,133 | 0 |
| 31 | M2G | 2a | 966 | 25/26 | 0.91 | 0.19 | 211,211,211,211 | 0 |
| 1 | PSU | 1A | 2605 | 20/21 | 0.91 | 0.33 | 69,69,69,69 | 0 |
| 1 | 5MU | 1A | 1915 | 21/22 | 0.91 | 0.17 | 142,142,142,142 | 0 |
| 54 | PSU | 1y | 39 | 20/21 | 0.91 | 0.34 | 177,177,177,177 | 0 |
| 31 | 5MC | 1a | 1404 | 21/22 | 0.91 | 0.27 | 126,126,126,126 | 0 |
| 1 | 2MA | 1A | 2503 | 23/24 | 0.91 | 0.39 | 58,58,58,58 | 0 |
| 1 | PSU | 2A | 2605 | 20/21 | 0.92 | 0.26 | 95,95,95,95 | 0 |
| 1 | 2MU | 2A | 2552 | 21/23 | 0.92 | 0.25 | 105,105,105,105 | 0 |
| 1 | OMG | 2A | 2251 | 24/25 | 0.92 | 0.18 | 106,106,106,106 | 0 |
| 1 | 5MU | 1A | 1939 | 21/22 | 0.93 | 0.24 | 74,74,74,74 | 0 |
| 1 | 5MC | 2A | 1962 | 21/22 | 0.93 | 0.15 | 112,112,112,112 | 0 |
| 1 | OMC | 1A | 1920 | 21/22 | 0.93 | 0.27 | 126,126,126,126 | 0 |
| 31 | 4OC | 1a | 1402 | 22/23 | 0.93 | 0.22 | 134,134,134,134 | 0 |

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| Mol | Type | Chain | Res | Atoms | RSCC | RSR | B-factors(Å$^2$) | Q<0.9 |
|---|---|---|---|---|---|---|---|---|
| 1 | 5MU | 2A | 1939 | 21/22 | 0.94 | 0.23 | 101,101,101,101 | 0 |
| 31 | UR3 | 1a | 1498 | 21/22 | 0.94 | 0.25 | 133,133,133,133 | 0 |
| 1 | 5MC | 1A | 1962 | 21/22 | 0.94 | 0.21 | 81,81,81,81 | 0 |
| 1 | 2MU | 1A | 2552 | 21/23 | 0.95 | 0.28 | 71,71,71,71 | 0 |
| 1 | OMG | 1A | 2251 | 24/25 | 0.95 | 0.25 | 62,62,62,62 | 0 |
| 31 | 5MC | 1a | 1400 | 21/22 | 0.95 | 0.25 | 153,153,153,153 | 0 |
| 1 | 2MA | 2A | 2503 | 23/24 | 0.95 | 0.22 | 95,95,95,95 | 0 |
| 31 | MA6 | 1a | 1518 | 24/25 | 0.95 | 0.28 | 123,123,123,123 | 0 |
| 31 | MA6 | 1a | 1519 | 24/25 | 0.96 | 0.27 | 122,122,122,122 | 0 |
| 1 | 5MC | 1A | 1942 | 21/22 | 0.96 | 0.24 | 81,81,81,81 | 0 |
| 1 | 5MC | 2A | 1942 | 21/22 | 0.96 | 0.17 | 112,112,112,112 | 0 |

## 6.3 Carbohydrates (i)

There are no monosaccharides 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 |
|---|---|---|---|---|---|---|---|---|
| 56 | MG | 2A | 3246 | 1/1 | -0.24 | 0.56 | 153,153,153,153 | 0 |
| 56 | MG | 2g | 202 | 1/1 | -0.23 | 0.63 | 185,185,185,185 | 0 |
| 56 | MG | 2a | 1801 | 1/1 | -0.17 | 0.39 | 215,215,215,215 | 0 |
| 56 | MG | 2a | 1763 | 1/1 | -0.14 | 0.14 | 240,240,240,240 | 0 |
| 56 | MG | 2a | 1766 | 1/1 | -0.13 | 0.46 | 261,261,261,261 | 0 |
| 56 | MG | 2a | 1767 | 1/1 | -0.10 | 0.38 | 276,276,276,276 | 0 |
| 56 | MG | 2a | 1765 | 1/1 | -0.08 | 0.28 | 250,250,250,250 | 0 |
| 56 | MG | 1a | 1854 | 1/1 | -0.07 | 0.67 | 229,229,229,229 | 0 |
| 56 | MG | 2A | 3252 | 1/1 | -0.07 | 0.40 | 127,127,127,127 | 0 |
| 56 | MG | 2a | 1684 | 1/1 | -0.04 | 0.77 | 161,161,161,161 | 0 |
| 56 | MG | 2x | 108 | 1/1 | -0.02 | 0.66 | 245,245,245,245 | 0 |
| 56 | MG | 2m | 202 | 1/1 | -0.01 | 0.66 | 230,230,230,230 | 0 |
| 56 | MG | 2A | 3122 | 1/1 | 0.01 | 1.52 | 117,117,117,117 | 0 |
| 56 | MG | 2x | 105 | 1/1 | 0.03 | 2.65 | 237,237,237,237 | 0 |
| 56 | MG | 2a | 1828 | 1/1 | 0.06 | 0.71 | 163,163,163,163 | 0 |
| 56 | MG | 1a | 1730 | 1/1 | 0.09 | 0.52 | 162,162,162,162 | 0 |

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| Mol | Type | Chain | Res | Atoms | RSCC | RSR | B-factors(Å$^2$) | Q<0.9 |
|---|---|---|---|---|---|---|---|---|
| 56 | MG | 2a | 1785 | 1/1 | 0.15 | 1.07 | 228,228,228,228 | 0 |
| 56 | MG | 1a | 1670 | 1/1 | 0.16 | 0.41 | 137,137,137,137 | 0 |
| 56 | MG | 2A | 3184 | 1/1 | 0.16 | 0.70 | 135,135,135,135 | 0 |
| 56 | MG | 2Q | 202 | 1/1 | 0.17 | 0.41 | 132,132,132,132 | 0 |
| 56 | MG | 2r | 301 | 1/1 | 0.19 | 0.52 | 139,139,139,139 | 0 |
| 56 | MG | 2a | 1602 | 1/1 | 0.19 | 0.41 | 151,151,151,151 | 0 |
| 56 | MG | 2p | 102 | 1/1 | 0.19 | 0.70 | 148,148,148,148 | 0 |
| 56 | MG | 2a | 1714 | 1/1 | 0.20 | 0.67 | 143,143,143,143 | 0 |
| 56 | MG | 1a | 1823 | 1/1 | 0.20 | 0.26 | 211,211,211,211 | 0 |
| 56 | MG | 2y | 106 | 1/1 | 0.20 | 0.70 | 263,263,263,263 | 0 |
| 56 | MG | 2A | 3245 | 1/1 | 0.21 | 0.64 | 111,111,111,111 | 0 |
| 56 | MG | 2i | 202 | 1/1 | 0.21 | 0.20 | 255,255,255,255 | 0 |
| 56 | MG | 2A | 3681 | 1/1 | 0.22 | 0.42 | 119,119,119,119 | 0 |
| 56 | MG | 2g | 203 | 1/1 | 0.22 | 0.25 | 214,214,214,214 | 0 |
| 56 | MG | 2A | 3517 | 1/1 | 0.22 | 0.42 | 132,132,132,132 | 0 |
| 56 | MG | 2g | 201 | 1/1 | 0.23 | 0.23 | 229,229,229,229 | 0 |
| 56 | MG | 2a | 1761 | 1/1 | 0.26 | 0.31 | 210,210,210,210 | 0 |
| 56 | MG | 2A | 3552 | 1/1 | 0.26 | 0.51 | 105,105,105,105 | 0 |
| 56 | MG | 1a | 1637 | 1/1 | 0.27 | 0.23 | 119,119,119,119 | 0 |
| 56 | MG | 2a | 1706 | 1/1 | 0.28 | 0.48 | 150,150,150,150 | 0 |
| 56 | MG | 2A | 3830 | 1/1 | 0.28 | 0.73 | 125,125,125,125 | 0 |
| 56 | MG | 2a | 1664 | 1/1 | 0.28 | 0.48 | 150,150,150,150 | 0 |
| 56 | MG | 1a | 1899 | 1/1 | 0.28 | 0.26 | 149,149,149,149 | 0 |
| 56 | MG | 2a | 1659 | 1/1 | 0.29 | 0.33 | 117,117,117,117 | 0 |
| 56 | MG | 1b | 305 | 1/1 | 0.29 | 0.60 | 166,166,166,166 | 0 |
| 56 | MG | 2a | 1674 | 1/1 | 0.29 | 0.88 | 127,127,127,127 | 0 |
| 56 | MG | 2A | 3597 | 1/1 | 0.30 | 0.18 | 120,120,120,120 | 0 |
| 56 | MG | 2a | 1887 | 1/1 | 0.30 | 0.66 | 134,134,134,134 | 0 |
| 56 | MG | 1a | 1782 | 1/1 | 0.30 | 0.36 | 127,127,127,127 | 0 |
| 56 | MG | 1a | 1685 | 1/1 | 0.31 | 0.54 | 173,173,173,173 | 0 |
| 56 | MG | 2a | 1800 | 1/1 | 0.31 | 0.18 | 220,220,220,220 | 0 |
| 56 | MG | 1A | 4503 | 1/1 | 0.31 | 0.56 | 102,102,102,102 | 0 |
| 56 | MG | 1a | 1803 | 1/1 | 0.32 | 0.74 | 125,125,125,125 | 0 |
| 56 | MG | 2a | 1760 | 1/1 | 0.33 | 0.21 | 220,220,220,220 | 0 |
| 56 | MG | 2l | 204 | 1/1 | 0.34 | 0.50 | 136,136,136,136 | 0 |
| 56 | MG | 2l | 206 | 1/1 | 0.34 | 0.53 | 145,145,145,145 | 0 |
| 56 | MG | 2A | 3629 | 1/1 | 0.34 | 0.61 | 114,114,114,114 | 0 |
| 56 | MG | 1a | 1768 | 1/1 | 0.34 | 0.51 | 122,122,122,122 | 0 |
| 56 | MG | 2a | 1661 | 1/1 | 0.35 | 0.33 | 145,145,145,145 | 0 |
| 56 | MG | 2a | 1677 | 1/1 | 0.35 | 0.26 | 166,166,166,166 | 0 |
| 56 | MG | 2B | 208 | 1/1 | 0.36 | 0.93 | 135,135,135,135 | 0 |

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| Mol | Type | Chain | Res | Atoms | RSCC | RSR | B-factors(Å$^2$) | Q<0.9 |
|---|---|---|---|---|---|---|---|---|
| 56 | MG | 2a | 1899 | 1/1 | 0.36 | 0.59 | 125,125,125,125 | 0 |
| 56 | MG | 2a | 1669 | 1/1 | 0.37 | 0.70 | 140,140,140,140 | 0 |
| 56 | MG | 2A | 3071 | 1/1 | 0.37 | 0.68 | 129,129,129,129 | 0 |
| 56 | MG | 2Q | 206 | 1/1 | 0.37 | 0.45 | 118,118,118,118 | 0 |
| 56 | MG | 2A | 3692 | 1/1 | 0.38 | 0.41 | 133,133,133,133 | 0 |
| 56 | MG | 1s | 103 | 1/1 | 0.39 | 0.23 | 203,203,203,203 | 0 |
| 56 | MG | 2A | 3390 | 1/1 | 0.40 | 0.21 | 116,116,116,116 | 0 |
| 56 | MG | 2Z | 401 | 1/1 | 0.40 | 0.44 | 142,142,142,142 | 0 |
| 56 | MG | 2A | 3387 | 1/1 | 0.41 | 0.33 | 123,123,123,123 | 0 |
| 56 | MG | 2A | 3574 | 1/1 | 0.41 | 0.56 | 253,253,253,253 | 0 |
| 56 | MG | 2A | 3795 | 1/1 | 0.41 | 0.38 | 109,109,109,109 | 0 |
| 56 | MG | 1a | 1681 | 1/1 | 0.41 | 0.30 | 158,158,158,158 | 0 |
| 56 | MG | 1x | 301 | 1/1 | 0.41 | 0.22 | 193,193,193,193 | 0 |
| 56 | MG | 2A | 3639 | 1/1 | 0.41 | 0.44 | 118,118,118,118 | 0 |
| 56 | MG | 2T | 302 | 1/1 | 0.42 | 0.33 | 124,124,124,124 | 0 |
| 56 | MG | 2a | 1844 | 1/1 | 0.42 | 0.29 | 238,238,238,238 | 0 |
| 56 | MG | 1q | 201 | 1/1 | 0.42 | 0.83 | 115,115,115,115 | 0 |
| 56 | MG | 2A | 3083 | 1/1 | 0.42 | 1.40 | 115,115,115,115 | 0 |
| 56 | MG | 2A | 3022 | 1/1 | 0.43 | 0.41 | 126,126,126,126 | 0 |
| 56 | MG | 2a | 1776 | 1/1 | 0.43 | 0.48 | 197,197,197,197 | 0 |
| 56 | MG | 1a | 1669 | 1/1 | 0.43 | 0.46 | 124,124,124,124 | 0 |
| 56 | MG | 2a | 1709 | 1/1 | 0.44 | 0.59 | 156,156,156,156 | 0 |
| 56 | MG | 1A | 4516 | 1/1 | 0.44 | 0.87 | 118,118,118,118 | 0 |
| 56 | MG | 2A | 3680 | 1/1 | 0.44 | 0.24 | 114,114,114,114 | 0 |
| 56 | MG | 1a | 1671 | 1/1 | 0.44 | 0.22 | 139,139,139,139 | 0 |
| 56 | MG | 1a | 1776 | 1/1 | 0.44 | 0.52 | 122,122,122,122 | 0 |
| 56 | MG | 2a | 1686 | 1/1 | 0.44 | 0.32 | 150,150,150,150 | 0 |
| 56 | MG | 1a | 1777 | 1/1 | 0.44 | 0.49 | 128,128,128,128 | 0 |
| 56 | MG | 1a | 1725 | 1/1 | 0.45 | 0.33 | 117,117,117,117 | 0 |
| 56 | MG | 1a | 1843 | 1/1 | 0.45 | 0.48 | 281,281,281,281 | 0 |
| 56 | MG | 2B | 217 | 1/1 | 0.45 | 0.34 | 177,177,177,177 | 0 |
| 56 | MG | 1a | 1908 | 1/1 | 0.45 | 0.84 | 131,131,131,131 | 0 |
| 56 | MG | 2m | 203 | 1/1 | 0.45 | 0.10 | 238,238,238,238 | 0 |
| 56 | MG | 2A | 3536 | 1/1 | 0.46 | 0.78 | 123,123,123,123 | 0 |
| 56 | MG | 2A | 3097 | 1/1 | 0.46 | 0.53 | 99,99,99,99 | 0 |
| 56 | MG | 2A | 3248 | 1/1 | 0.46 | 0.51 | 123,123,123,123 | 0 |
| 56 | MG | 2a | 1607 | 1/1 | 0.46 | 0.60 | 142,142,142,142 | 0 |
| 56 | MG | 2B | 227 | 1/1 | 0.46 | 0.39 | 132,132,132,132 | 0 |
| 56 | MG | 1a | 1910 | 1/1 | 0.46 | 0.50 | 127,127,127,127 | 0 |
| 56 | MG | 2A | 3531 | 1/1 | 0.46 | 0.28 | 138,138,138,138 | 0 |
| 56 | MG | 1A | 4307 | 1/1 | 0.47 | 0.52 | 96,96,96,96 | 0 |

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| Mol | Type | Chain | Res | Atoms | RSCC | RSR | B-factors(Å$^2$) | Q<0.9 |
|---|---|---|---|---|---|---|---|---|
| 56 | MG | 23 | 103 | 1/1 | 0.47 | 0.41 | 112,112,112,112 | 0 |
| 56 | MG | 2e | 202 | 1/1 | 0.47 | 0.21 | 153,153,153,153 | 0 |
| 56 | MG | 2A | 3538 | 1/1 | 0.47 | 0.21 | 134,134,134,134 | 0 |
| 56 | MG | 2A | 3631 | 1/1 | 0.47 | 0.37 | 113,113,113,113 | 0 |
| 56 | MG | 2s | 102 | 1/1 | 0.47 | 0.42 | 247,247,247,247 | 0 |
| 56 | MG | 2u | 103 | 1/1 | 0.47 | 0.20 | 238,238,238,238 | 0 |
| 56 | MG | 2a | 1654 | 1/1 | 0.47 | 0.35 | 132,132,132,132 | 0 |
| 56 | MG | 1A | 4518 | 1/1 | 0.47 | 0.91 | 122,122,122,122 | 0 |
| 56 | MG | 1A | 4052 | 1/1 | 0.47 | 0.59 | 92,92,92,92 | 0 |
| 56 | MG | 1n | 102 | 1/1 | 0.48 | 0.32 | 210,210,210,210 | 0 |
| 56 | MG | 2A | 3087 | 1/1 | 0.48 | 0.37 | 121,121,121,121 | 0 |
| 56 | MG | 1A | 4054 | 1/1 | 0.48 | 0.81 | 95,95,95,95 | 0 |
| 56 | MG | 2A | 3770 | 1/1 | 0.48 | 0.76 | 87,87,87,87 | 0 |
| 56 | MG | 2B | 224 | 1/1 | 0.48 | 0.20 | 128,128,128,128 | 0 |
| 56 | MG | 2a | 1716 | 1/1 | 0.48 | 0.95 | 135,135,135,135 | 0 |
| 56 | MG | 1n | 101 | 1/1 | 0.49 | 0.20 | 207,207,207,207 | 0 |
| 56 | MG | 1a | 1906 | 1/1 | 0.49 | 0.44 | 121,121,121,121 | 0 |
| 56 | MG | 2a | 1668 | 1/1 | 0.49 | 1.01 | 151,151,151,151 | 0 |
| 56 | MG | 2A | 3116 | 1/1 | 0.49 | 1.38 | 127,127,127,127 | 0 |
| 56 | MG | 1A | 4060 | 1/1 | 0.49 | 0.56 | 72,72,72,72 | 0 |
| 56 | MG | 2A | 3385 | 1/1 | 0.49 | 0.36 | 120,120,120,120 | 0 |
| 56 | MG | 2y | 101 | 1/1 | 0.49 | 0.52 | 154,154,154,154 | 0 |
| 56 | MG | 1g | 302 | 1/1 | 0.49 | 0.33 | 194,194,194,194 | 0 |
| 56 | MG | 2F | 303 | 1/1 | 0.50 | 0.57 | 126,126,126,126 | 0 |
| 56 | MG | 1a | 1900 | 1/1 | 0.50 | 0.30 | 134,134,134,134 | 0 |
| 56 | MG | 2A | 3016 | 1/1 | 0.50 | 0.95 | 118,118,118,118 | 0 |
| 56 | MG | 2A | 3556 | 1/1 | 0.50 | 0.59 | 96,96,96,96 | 0 |
| 56 | MG | 2u | 101 | 1/1 | 0.50 | 0.69 | 221,221,221,221 | 0 |
| 56 | MG | 2y | 109 | 1/1 | 0.50 | 0.27 | 247,247,247,247 | 0 |
| 56 | MG | 2B | 232 | 1/1 | 0.51 | 0.52 | 144,144,144,144 | 0 |
| 56 | MG | 1A | 4889 | 1/1 | 0.51 | 0.51 | 61,61,61,61 | 0 |
| 56 | MG | 2a | 1786 | 1/1 | 0.52 | 0.53 | 234,234,234,234 | 0 |
| 56 | MG | 2a | 1909 | 1/1 | 0.52 | 0.22 | 225,225,225,225 | 0 |
| 56 | MG | 2A | 3282 | 1/1 | 0.52 | 0.37 | 107,107,107,107 | 0 |
| 56 | MG | 1B | 223 | 1/1 | 0.52 | 0.57 | 97,97,97,97 | 0 |
| 56 | MG | 2a | 1627 | 1/1 | 0.52 | 0.51 | 153,153,153,153 | 0 |
| 56 | MG | 1A | 4790 | 1/1 | 0.52 | 0.48 | 99,99,99,99 | 0 |
| 56 | MG | 1A | 4891 | 1/1 | 0.52 | 0.34 | 109,109,109,109 | 0 |
| 56 | MG | 2A | 3421 | 1/1 | 0.53 | 0.26 | 146,146,146,146 | 0 |
| 56 | MG | 2A | 3562 | 1/1 | 0.53 | 0.40 | 90,90,90,90 | 0 |
| 56 | MG | 1a | 1706 | 1/1 | 0.53 | 0.65 | 103,103,103,103 | 0 |

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| Mol | Type | Chain | Res | Atoms | RSCC | RSR | B-factors(Å$^2$) | Q<0.9 |
|---|---|---|---|---|---|---|---|---|
| 56 | MG | 2A | 3579 | 1/1 | 0.53 | 0.68 | 115,115,115,115 | 0 |
| 56 | MG | 2A | 3590 | 1/1 | 0.53 | 0.29 | 171,171,171,171 | 0 |
| 56 | MG | 1a | 1634 | 1/1 | 0.53 | 0.60 | 117,117,117,117 | 0 |
| 56 | MG | 2a | 1794 | 1/1 | 0.54 | 0.67 | 168,168,168,168 | 0 |
| 56 | MG | 1A | 4809 | 1/1 | 0.54 | 0.99 | 58,58,58,58 | 0 |
| 56 | MG | 1A | 4282 | 1/1 | 0.54 | 0.51 | 69,69,69,69 | 0 |
| 56 | MG | 2a | 1826 | 1/1 | 0.54 | 0.52 | 162,162,162,162 | 0 |
| 56 | MG | 2A | 3817 | 1/1 | 0.54 | 0.21 | 139,139,139,139 | 0 |
| 56 | MG | 1A | 4756 | 1/1 | 0.54 | 0.75 | 106,106,106,106 | 0 |
| 56 | MG | 2A | 3833 | 1/1 | 0.54 | 0.22 | 111,111,111,111 | 0 |
| 56 | MG | 2m | 201 | 1/1 | 0.54 | 0.89 | 166,166,166,166 | 0 |
| 56 | MG | 1A | 5014 | 1/1 | 0.54 | 0.42 | 71,71,71,71 | 0 |
| 56 | MG | 1A | 4048 | 1/1 | 0.54 | 0.66 | 103,103,103,103 | 0 |
| 56 | MG | 2i | 204 | 1/1 | 0.55 | 0.48 | 241,241,241,241 | 0 |
| 56 | MG | 1a | 1682 | 1/1 | 0.55 | 0.62 | 197,197,197,197 | 0 |
| 56 | MG | 2a | 1735 | 1/1 | 0.55 | 0.43 | 132,132,132,132 | 0 |
| 56 | MG | 1a | 1895 | 1/1 | 0.55 | 0.38 | 121,121,121,121 | 0 |
| 56 | MG | 2a | 1789 | 1/1 | 0.55 | 0.35 | 233,233,233,233 | 0 |
| 56 | MG | 2B | 201 | 1/1 | 0.55 | 0.37 | 115,115,115,115 | 0 |
| 56 | MG | 2h | 202 | 1/1 | 0.55 | 0.11 | 180,180,180,180 | 0 |
| 56 | MG | 2a | 1768 | 1/1 | 0.55 | 0.43 | 260,260,260,260 | 0 |
| 56 | MG | 1A | 4259 | 1/1 | 0.56 | 0.46 | 61,61,61,61 | 0 |
| 56 | MG | 2A | 3206 | 1/1 | 0.56 | 0.48 | 120,120,120,120 | 0 |
| 56 | MG | 1A | 4452 | 1/1 | 0.56 | 0.29 | 64,64,64,64 | 0 |
| 56 | MG | 2a | 1636 | 1/1 | 0.56 | 0.38 | 150,150,150,150 | 0 |
| 56 | MG | 2x | 103 | 1/1 | 0.56 | 0.57 | 192,192,192,192 | 0 |
| 56 | MG | 23 | 102 | 1/1 | 0.57 | 0.34 | 124,124,124,124 | 0 |
| 56 | MG | 2A | 3502 | 1/1 | 0.57 | 0.46 | 104,104,104,104 | 0 |
| 56 | MG | 2O | 301 | 1/1 | 0.57 | 0.15 | 136,136,136,136 | 0 |
| 56 | MG | 1A | 4038 | 1/1 | 0.57 | 0.58 | 81,81,81,81 | 0 |
| 56 | MG | 2o | 301 | 1/1 | 0.57 | 0.67 | 118,118,118,118 | 0 |
| 56 | MG | 2A | 3832 | 1/1 | 0.57 | 0.27 | 121,121,121,121 | 0 |
| 56 | MG | 2A | 3284 | 1/1 | 0.57 | 0.43 | 97,97,97,97 | 0 |
| 56 | MG | 2A | 3137 | 1/1 | 0.57 | 0.42 | 134,134,134,134 | 0 |
| 56 | MG | 1a | 1709 | 1/1 | 0.58 | 0.32 | 107,107,107,107 | 0 |
| 56 | MG | 2A | 3403 | 1/1 | 0.58 | 0.61 | 219,219,219,219 | 0 |
| 56 | MG | 1a | 1780 | 1/1 | 0.58 | 0.83 | 124,124,124,124 | 0 |
| 56 | MG | 1a | 1731 | 1/1 | 0.58 | 0.26 | 136,136,136,136 | 0 |
| 56 | MG | 2g | 206 | 1/1 | 0.58 | 0.53 | 216,216,216,216 | 0 |
| 56 | MG | 2A | 3329 | 1/1 | 0.59 | 0.51 | 87,87,87,87 | 0 |
| 56 | MG | 2a | 1885 | 1/1 | 0.59 | 0.32 | 162,162,162,162 | 0 |

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| Mol | Type | Chain | Res | Atoms | RSCC | RSR | B-factors(Å$^2$) | Q<0.9 |
|---|---|---|---|---|---|---|---|---|
| 56 | MG | 1A | 4519 | 1/1 | 0.59 | 0.66 | 94,94,94,94 | 0 |
| 56 | MG | 1a | 1792 | 1/1 | 0.59 | 0.62 | 105,105,105,105 | 0 |
| 56 | MG | 1b | 301 | 1/1 | 0.59 | 0.18 | 165,165,165,165 | 0 |
| 56 | MG | 2A | 3762 | 1/1 | 0.59 | 0.23 | 124,124,124,124 | 0 |
| 56 | MG | 2a | 1617 | 1/1 | 0.60 | 0.44 | 127,127,127,127 | 0 |
| 56 | MG | 2a | 1624 | 1/1 | 0.60 | 0.38 | 137,137,137,137 | 0 |
| 56 | MG | 1A | 4301 | 1/1 | 0.60 | 0.81 | 102,102,102,102 | 0 |
| 56 | MG | 1A | 4323 | 1/1 | 0.60 | 0.76 | 85,85,85,85 | 0 |
| 56 | MG | 2a | 1722 | 1/1 | 0.60 | 0.81 | 141,141,141,141 | 0 |
| 56 | MG | 2A | 3257 | 1/1 | 0.60 | 0.48 | 87,87,87,87 | 0 |
| 56 | MG | 2a | 1737 | 1/1 | 0.60 | 0.29 | 132,132,132,132 | 0 |
| 56 | MG | 2a | 1753 | 1/1 | 0.60 | 0.46 | 138,138,138,138 | 0 |
| 56 | MG | 2a | 1758 | 1/1 | 0.60 | 0.54 | 205,205,205,205 | 0 |
| 56 | MG | 2A | 3030 | 1/1 | 0.60 | 0.96 | 97,97,97,97 | 0 |
| 56 | MG | 2a | 1893 | 1/1 | 0.60 | 0.82 | 123,123,123,123 | 0 |
| 56 | MG | 1A | 4723 | 1/1 | 0.60 | 0.37 | 77,77,77,77 | 0 |
| 56 | MG | 2B | 205 | 1/1 | 0.60 | 0.35 | 119,119,119,119 | 0 |
| 56 | MG | 2v | 703 | 1/1 | 0.60 | 0.25 | 154,154,154,154 | 0 |
| 56 | MG | 2A | 3761 | 1/1 | 0.60 | 0.37 | 126,126,126,126 | 0 |
| 56 | MG | 2B | 216 | 1/1 | 0.60 | 0.44 | 174,174,174,174 | 0 |
| 56 | MG | 1s | 102 | 1/1 | 0.60 | 0.07 | 229,229,229,229 | 0 |
| 56 | MG | 28 | 101 | 1/1 | 0.60 | 1.11 | 109,109,109,109 | 0 |
| 56 | MG | 1a | 1835 | 1/1 | 0.60 | 0.07 | 221,221,221,221 | 0 |
| 56 | MG | 1A | 4343 | 1/1 | 0.60 | 0.29 | 71,71,71,71 | 0 |
| 56 | MG | 2A | 3350 | 1/1 | 0.61 | 0.45 | 104,104,104,104 | 0 |
| 56 | MG | 2A | 3402 | 1/1 | 0.61 | 0.44 | 112,112,112,112 | 0 |
| 56 | MG | 2a | 1756 | 1/1 | 0.61 | 0.35 | 205,205,205,205 | 0 |
| 56 | MG | 2a | 1868 | 1/1 | 0.61 | 0.35 | 144,144,144,144 | 0 |
| 56 | MG | 2A | 3735 | 1/1 | 0.61 | 0.52 | 101,101,101,101 | 0 |
| 56 | MG | 1a | 1653 | 1/1 | 0.61 | 0.34 | 119,119,119,119 | 0 |
| 56 | MG | 1m | 201 | 1/1 | 0.61 | 0.63 | 216,216,216,216 | 0 |
| 56 | MG | 2x | 106 | 1/1 | 0.62 | 0.26 | 211,211,211,211 | 0 |
| 56 | MG | 1a | 1615 | 1/1 | 0.62 | 0.61 | 92,92,92,92 | 0 |
| 56 | MG | 2a | 1913 | 1/1 | 0.62 | 0.24 | 246,246,246,246 | 0 |
| 56 | MG | 2B | 230 | 1/1 | 0.62 | 0.59 | 151,151,151,151 | 0 |
| 56 | MG | 1a | 1913 | 1/1 | 0.62 | 0.40 | 97,97,97,97 | 0 |
| 56 | MG | 2v | 701 | 1/1 | 0.63 | 0.45 | 171,171,171,171 | 0 |
| 56 | MG | 2a | 1666 | 1/1 | 0.63 | 0.43 | 133,133,133,133 | 0 |
| 56 | MG | 2A | 3193 | 1/1 | 0.63 | 0.59 | 107,107,107,107 | 0 |
| 56 | MG | 28 | 104 | 1/1 | 0.63 | 0.17 | 110,110,110,110 | 0 |
| 56 | MG | 2F | 302 | 1/1 | 0.63 | 0.33 | 90,90,90,90 | 0 |

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| Mol | Type | Chain | Res | Atoms | RSCC | RSR | B-factors(Å$^2$) | Q<0.9 |
|---|---|---|---|---|---|---|---|---|
| 56 | MG | 2a | 1780 | 1/1 | 0.63 | 0.46 | 211,211,211,211 | 0 |
| 56 | MG | 1a | 1875 | 1/1 | 0.63 | 0.63 | 118,118,118,118 | 0 |
| 56 | MG | 2A | 3020 | 1/1 | 0.63 | 0.68 | 103,103,103,103 | 0 |
| 56 | MG | 1o | 101 | 1/1 | 0.63 | 0.38 | 113,113,113,113 | 0 |
| 56 | MG | 2A | 3546 | 1/1 | 0.64 | 0.40 | 97,97,97,97 | 0 |
| 56 | MG | 2a | 1734 | 1/1 | 0.64 | 0.29 | 127,127,127,127 | 0 |
| 56 | MG | 2A | 3208 | 1/1 | 0.64 | 0.25 | 118,118,118,118 | 0 |
| 56 | MG | 2A | 3763 | 1/1 | 0.64 | 0.36 | 133,133,133,133 | 0 |
| 56 | MG | 1A | 4550 | 1/1 | 0.64 | 0.62 | 89,89,89,89 | 0 |
| 56 | MG | 2l | 202 | 1/1 | 0.64 | 0.27 | 150,150,150,150 | 0 |
| 56 | MG | 2a | 1754 | 1/1 | 0.64 | 0.56 | 148,148,148,148 | 0 |
| 56 | MG | 2A | 3529 | 1/1 | 0.64 | 0.47 | 118,118,118,118 | 0 |
| 56 | MG | 2A | 3566 | 1/1 | 0.64 | 0.36 | 114,114,114,114 | 0 |
| 56 | MG | 1A | 4138 | 1/1 | 0.64 | 0.36 | 72,72,72,72 | 0 |
| 56 | MG | 2A | 3689 | 1/1 | 0.64 | 0.27 | 161,161,161,161 | 0 |
| 56 | MG | 2A | 3112 | 1/1 | 0.64 | 0.97 | 136,136,136,136 | 0 |
| 56 | MG | 2A | 3440 | 1/1 | 0.64 | 0.61 | 99,99,99,99 | 0 |
| 56 | MG | 2A | 3383 | 1/1 | 0.65 | 0.40 | 100,100,100,100 | 0 |
| 56 | MG | 2A | 3583 | 1/1 | 0.65 | 1.00 | 122,122,122,122 | 0 |
| 56 | MG | 2A | 3831 | 1/1 | 0.65 | 0.35 | 128,128,128,128 | 0 |
| 56 | MG | 2A | 3423 | 1/1 | 0.65 | 0.16 | 130,130,130,130 | 0 |
| 56 | MG | 2A | 3724 | 1/1 | 0.65 | 0.43 | 91,91,91,91 | 0 |
| 56 | MG | 2a | 1771 | 1/1 | 0.65 | 0.25 | 178,178,178,178 | 0 |
| 56 | MG | 2a | 1773 | 1/1 | 0.65 | 0.32 | 228,228,228,228 | 0 |
| 56 | MG | 1a | 1649 | 1/1 | 0.65 | 0.74 | 105,105,105,105 | 0 |
| 56 | MG | 2A | 3802 | 1/1 | 0.65 | 0.36 | 108,108,108,108 | 0 |
| 56 | MG | 1a | 1684 | 1/1 | 0.66 | 0.91 | 202,202,202,202 | 0 |
| 56 | MG | 2A | 3612 | 1/1 | 0.66 | 0.43 | 136,136,136,136 | 0 |
| 56 | MG | 2a | 1710 | 1/1 | 0.66 | 1.10 | 131,131,131,131 | 0 |
| 56 | MG | 2a | 1711 | 1/1 | 0.66 | 0.37 | 149,149,149,149 | 0 |
| 56 | MG | 1A | 4291 | 1/1 | 0.66 | 0.59 | 71,71,71,71 | 0 |
| 56 | MG | 2A | 3094 | 1/1 | 0.66 | 0.55 | 113,113,113,113 | 0 |
| 56 | MG | 1D | 308 | 1/1 | 0.66 | 0.72 | 77,77,77,77 | 0 |
| 56 | MG | 1A | 4662 | 1/1 | 0.66 | 0.61 | 87,87,87,87 | 0 |
| 56 | MG | 2x | 104 | 1/1 | 0.66 | 0.41 | 219,219,219,219 | 0 |
| 56 | MG | 1A | 4678 | 1/1 | 0.66 | 0.52 | 86,86,86,86 | 0 |
| 56 | MG | 2A | 3577 | 1/1 | 0.66 | 0.40 | 143,143,143,143 | 0 |
| 56 | MG | 2A | 3027 | 1/1 | 0.66 | 1.06 | 123,123,123,123 | 0 |
| 56 | MG | 1A | 4806 | 1/1 | 0.66 | 0.31 | 73,73,73,73 | 0 |
| 56 | MG | 1B | 205 | 1/1 | 0.66 | 0.41 | 87,87,87,87 | 0 |
| 56 | MG | 2A | 3758 | 1/1 | 0.66 | 0.09 | 211,211,211,211 | 0 |

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| Mol | Type | Chain | Res | Atoms | RSCC | RSR | B-factors(Å$^2$) | Q<0.9 |
|---|---|---|---|---|---|---|---|---|
| 56 | MG | 2A | 3076 | 1/1 | 0.67 | 0.93 | 113,113,113,113 | 0 |
| 56 | MG | 2A | 3461 | 1/1 | 0.67 | 0.41 | 111,111,111,111 | 0 |
| 56 | MG | 1u | 101 | 1/1 | 0.67 | 0.29 | 211,211,211,211 | 0 |
| 56 | MG | 1a | 1765 | 1/1 | 0.67 | 0.72 | 125,125,125,125 | 0 |
| 56 | MG | 2a | 1732 | 1/1 | 0.67 | 0.43 | 110,110,110,110 | 0 |
| 56 | MG | 2a | 1634 | 1/1 | 0.67 | 0.44 | 120,120,120,120 | 0 |
| 56 | MG | 2A | 3351 | 1/1 | 0.67 | 0.49 | 146,146,146,146 | 0 |
| 56 | MG | 1a | 1845 | 1/1 | 0.67 | 0.46 | 234,234,234,234 | 0 |
| 56 | MG | 2E | 302 | 1/1 | 0.67 | 0.28 | 96,96,96,96 | 0 |
| 56 | MG | 1A | 4699 | 1/1 | 0.67 | 0.48 | 75,75,75,75 | 0 |
| 56 | MG | 2A | 3614 | 1/1 | 0.67 | 0.40 | 102,102,102,102 | 0 |
| 56 | MG | 2A | 3615 | 1/1 | 0.67 | 0.60 | 138,138,138,138 | 0 |
| 56 | MG | 2A | 3808 | 1/1 | 0.67 | 0.55 | 173,173,173,173 | 0 |
| 56 | MG | 2A | 3537 | 1/1 | 0.67 | 0.17 | 73,73,73,73 | 0 |
| 56 | MG | 1A | 4027 | 1/1 | 0.67 | 0.68 | 62,62,62,62 | 0 |
| 56 | MG | 1a | 1810 | 1/1 | 0.67 | 0.98 | 100,100,100,100 | 0 |
| 56 | MG | 2A | 3645 | 1/1 | 0.67 | 0.30 | 116,116,116,116 | 0 |
| 56 | MG | 2c | 301 | 1/1 | 0.67 | 0.17 | 225,225,225,225 | 0 |
| 56 | MG | 1A | 4861 | 1/1 | 0.67 | 0.63 | 85,85,85,85 | 0 |
| 56 | MG | 2a | 1697 | 1/1 | 0.67 | 0.24 | 136,136,136,136 | 0 |
| 56 | MG | 2A | 3136 | 1/1 | 0.67 | 0.50 | 110,110,110,110 | 0 |
| 56 | MG | 2A | 3263 | 1/1 | 0.67 | 0.67 | 89,89,89,89 | 0 |
| 56 | MG | 2g | 204 | 1/1 | 0.67 | 0.28 | 216,216,216,216 | 0 |
| 56 | MG | 1A | 5035 | 1/1 | 0.67 | 0.57 | 68,68,68,68 | 0 |
| 56 | MG | 2y | 108 | 1/1 | 0.67 | 0.33 | 245,245,245,245 | 0 |
| 56 | MG | 2h | 201 | 1/1 | 0.67 | 0.14 | 179,179,179,179 | 0 |
| 56 | MG | 1a | 1807 | 1/1 | 0.68 | 0.36 | 100,100,100,100 | 0 |
| 56 | MG | 2a | 1921 | 1/1 | 0.68 | 0.50 | 152,152,152,152 | 0 |
| 56 | MG | 1A | 4970 | 1/1 | 0.68 | 0.35 | 89,89,89,89 | 0 |
| 56 | MG | 2A | 3205 | 1/1 | 0.68 | 0.26 | 122,122,122,122 | 0 |
| 56 | MG | 2A | 3828 | 1/1 | 0.68 | 0.44 | 126,126,126,126 | 0 |
| 56 | MG | 2a | 1798 | 1/1 | 0.68 | 0.35 | 239,239,239,239 | 0 |
| 56 | MG | 1D | 306 | 1/1 | 0.68 | 1.01 | 69,69,69,69 | 0 |
| 56 | MG | 1A | 4973 | 1/1 | 0.68 | 0.49 | 80,80,80,80 | 0 |
| 56 | MG | 2a | 1805 | 1/1 | 0.68 | 0.89 | 114,114,114,114 | 0 |
| 56 | MG | 1A | 4535 | 1/1 | 0.68 | 0.49 | 77,77,77,77 | 0 |
| 56 | MG | 1A | 4288 | 1/1 | 0.68 | 0.71 | 74,74,74,74 | 0 |
| 56 | MG | 1A | 5055 | 1/1 | 0.68 | 0.26 | 133,133,133,133 | 0 |
| 56 | MG | 1a | 1863 | 1/1 | 0.68 | 0.66 | 215,215,215,215 | 0 |
| 56 | MG | 1a | 1794 | 1/1 | 0.68 | 0.93 | 84,84,84,84 | 0 |
| 56 | MG | 2A | 3407 | 1/1 | 0.68 | 0.18 | 117,117,117,117 | 0 |

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| Mol | Type | Chain | Res | Atoms | RSCC | RSR | B-factors(Å$^2$) | Q<0.9 |
|---|---|---|---|---|---|---|---|---|
| 56 | MG | 2y | 103 | 1/1 | 0.68 | 0.59 | 223,223,223,223 | 0 |
| 56 | MG | 1A | 4691 | 1/1 | 0.68 | 0.33 | 81,81,81,81 | 0 |
| 56 | MG | 2B | 221 | 1/1 | 0.68 | 0.55 | 122,122,122,122 | 0 |
| 56 | MG | 1a | 1805 | 1/1 | 0.68 | 1.08 | 140,140,140,140 | 0 |
| 56 | MG | 2a | 1625 | 1/1 | 0.69 | 0.52 | 148,148,148,148 | 0 |
| 56 | MG | 1a | 1738 | 1/1 | 0.69 | 0.41 | 148,148,148,148 | 0 |
| 56 | MG | 1a | 1739 | 1/1 | 0.69 | 0.25 | 144,144,144,144 | 0 |
| 56 | MG | 2a | 1812 | 1/1 | 0.69 | 0.30 | 126,126,126,126 | 0 |
| 56 | MG | 1A | 4859 | 1/1 | 0.69 | 0.29 | 72,72,72,72 | 0 |
| 56 | MG | 2A | 3449 | 1/1 | 0.69 | 0.61 | 84,84,84,84 | 0 |
| 56 | MG | 1a | 1656 | 1/1 | 0.69 | 0.33 | 102,102,102,102 | 0 |
| 56 | MG | 2A | 3464 | 1/1 | 0.69 | 1.00 | 129,129,129,129 | 0 |
| 56 | MG | 1a | 1704 | 1/1 | 0.69 | 0.55 | 125,125,125,125 | 0 |
| 56 | MG | 1a | 1831 | 1/1 | 0.69 | 0.40 | 152,152,152,152 | 0 |
| 56 | MG | 2P | 203 | 1/1 | 0.69 | 0.67 | 113,113,113,113 | 0 |
| 56 | MG | 1A | 4600 | 1/1 | 0.69 | 0.58 | 78,78,78,78 | 0 |
| 56 | MG | 1B | 206 | 1/1 | 0.69 | 0.21 | 71,71,71,71 | 0 |
| 56 | MG | 2A | 3388 | 1/1 | 0.69 | 0.31 | 117,117,117,117 | 0 |
| 56 | MG | 2A | 3389 | 1/1 | 0.69 | 0.71 | 117,117,117,117 | 0 |
| 56 | MG | 2A | 3643 | 1/1 | 0.69 | 0.36 | 131,131,131,131 | 0 |
| 56 | MG | 1A | 4747 | 1/1 | 0.69 | 0.80 | 84,84,84,84 | 0 |
| 56 | MG | 2A | 3395 | 1/1 | 0.69 | 0.30 | 128,128,128,128 | 0 |
| 56 | MG | 2A | 3397 | 1/1 | 0.69 | 0.48 | 189,189,189,189 | 0 |
| 56 | MG | 2A | 3555 | 1/1 | 0.69 | 0.77 | 107,107,107,107 | 0 |
| 56 | MG | 1a | 1645 | 1/1 | 0.69 | 0.26 | 127,127,127,127 | 0 |
| 56 | MG | 1d | 301 | 1/1 | 0.69 | 0.77 | 128,128,128,128 | 0 |
| 56 | MG | 2a | 1622 | 1/1 | 0.69 | 0.50 | 156,156,156,156 | 0 |
| 56 | MG | 2a | 1718 | 1/1 | 0.69 | 0.65 | 136,136,136,136 | 0 |
| 56 | MG | 1A | 4633 | 1/1 | 0.69 | 0.43 | 71,71,71,71 | 0 |
| 56 | MG | 1a | 1909 | 1/1 | 0.70 | 0.57 | 136,136,136,136 | 0 |
| 56 | MG | 2A | 3476 | 1/1 | 0.70 | 0.47 | 116,116,116,116 | 0 |
| 56 | MG | 2A | 3798 | 1/1 | 0.70 | 0.50 | 98,98,98,98 | 0 |
| 56 | MG | 1y | 105 | 1/1 | 0.70 | 0.29 | 180,180,180,180 | 0 |
| 56 | MG | 2A | 3199 | 1/1 | 0.70 | 0.29 | 111,111,111,111 | 0 |
| 56 | MG | 2A | 3398 | 1/1 | 0.70 | 0.40 | 155,155,155,155 | 0 |
| 56 | MG | 2A | 3091 | 1/1 | 0.70 | 0.68 | 112,112,112,112 | 0 |
| 56 | MG | 1O | 204 | 1/1 | 0.70 | 2.09 | 87,87,87,87 | 0 |
| 56 | MG | 2A | 3717 | 1/1 | 0.70 | 0.29 | 108,108,108,108 | 0 |
| 56 | MG | 1A | 4285 | 1/1 | 0.70 | 0.51 | 62,62,62,62 | 0 |
| 56 | MG | 2a | 1910 | 1/1 | 0.70 | 0.19 | 240,240,240,240 | 0 |
| 56 | MG | 1a | 1915 | 1/1 | 0.70 | 0.19 | 134,134,134,134 | 0 |

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| Mol | Type | Chain | Res | Atoms | RSCC | RSR | B-factors(Å$^2$) | Q<0.9 |
|---|---|---|---|---|---|---|---|---|
| 56 | MG | 1A | 4303 | 1/1 | 0.70 | 0.28 | 87,87,87,87 | 0 |
| 56 | MG | 1A | 4706 | 1/1 | 0.70 | 0.44 | 68,68,68,68 | 0 |
| 56 | MG | 1a | 1786 | 1/1 | 0.70 | 0.37 | 119,119,119,119 | 0 |
| 56 | MG | 1A | 4714 | 1/1 | 0.70 | 0.61 | 99,99,99,99 | 0 |
| 56 | MG | 2A | 3647 | 1/1 | 0.71 | 0.86 | 108,108,108,108 | 0 |
| 56 | MG | 2A | 3675 | 1/1 | 0.71 | 0.57 | 123,123,123,123 | 0 |
| 56 | MG | 2A | 3826 | 1/1 | 0.71 | 0.57 | 114,114,114,114 | 0 |
| 56 | MG | 1a | 1884 | 1/1 | 0.71 | 0.39 | 122,122,122,122 | 0 |
| 56 | MG | 1a | 1814 | 1/1 | 0.71 | 0.27 | 158,158,158,158 | 0 |
| 56 | MG | 12 | 101 | 1/1 | 0.71 | 0.50 | 84,84,84,84 | 0 |
| 56 | MG | 1a | 1611 | 1/1 | 0.71 | 0.34 | 99,99,99,99 | 0 |
| 56 | MG | 2A | 3412 | 1/1 | 0.71 | 0.27 | 105,105,105,105 | 0 |
| 56 | MG | 2A | 3591 | 1/1 | 0.71 | 0.52 | 191,191,191,191 | 0 |
| 56 | MG | 1A | 4639 | 1/1 | 0.71 | 0.45 | 71,71,71,71 | 0 |
| 56 | MG | 1a | 1629 | 1/1 | 0.71 | 0.81 | 101,101,101,101 | 0 |
| 56 | MG | 2a | 1673 | 1/1 | 0.71 | 0.88 | 167,167,167,167 | 0 |
| 56 | MG | 2g | 205 | 1/1 | 0.71 | 0.22 | 211,211,211,211 | 0 |
| 56 | MG | 1a | 1844 | 1/1 | 0.71 | 0.37 | 270,270,270,270 | 0 |
| 56 | MG | 2a | 1676 | 1/1 | 0.71 | 0.45 | 163,163,163,163 | 0 |
| 56 | MG | 2A | 3548 | 1/1 | 0.71 | 0.25 | 104,104,104,104 | 0 |
| 56 | MG | 1A | 4888 | 1/1 | 0.71 | 0.43 | 69,69,69,69 | 0 |
| 56 | MG | 1A | 4935 | 1/1 | 0.71 | 0.35 | 67,67,67,67 | 0 |
| 56 | MG | 1a | 1672 | 1/1 | 0.71 | 0.28 | 99,99,99,99 | 0 |
| 56 | MG | 1A | 5033 | 1/1 | 0.71 | 0.80 | 68,68,68,68 | 0 |
| 56 | MG | 2A | 3477 | 1/1 | 0.71 | 0.49 | 126,126,126,126 | 0 |
| 56 | MG | 1a | 1763 | 1/1 | 0.72 | 0.58 | 109,109,109,109 | 0 |
| 56 | MG | 20 | 101 | 1/1 | 0.72 | 0.39 | 128,128,128,128 | 0 |
| 56 | MG | 2A | 3151 | 1/1 | 0.72 | 0.54 | 97,97,97,97 | 0 |
| 56 | MG | 2A | 3155 | 1/1 | 0.72 | 0.50 | 100,100,100,100 | 0 |
| 56 | MG | 2A | 3337 | 1/1 | 0.72 | 0.49 | 91,91,91,91 | 0 |
| 56 | MG | 2A | 3173 | 1/1 | 0.72 | 0.38 | 87,87,87,87 | 0 |
| 56 | MG | 2A | 3472 | 1/1 | 0.72 | 0.51 | 99,99,99,99 | 0 |
| 56 | MG | 19 | 101 | 1/1 | 0.72 | 0.28 | 71,71,71,71 | 0 |
| 56 | MG | 2a | 1609 | 1/1 | 0.72 | 0.93 | 138,138,138,138 | 0 |
| 56 | MG | 2x | 102 | 1/1 | 0.72 | 1.07 | 107,107,107,107 | 0 |
| 56 | MG | 1a | 1860 | 1/1 | 0.72 | 0.11 | 214,214,214,214 | 0 |
| 56 | MG | 2A | 3811 | 1/1 | 0.72 | 0.32 | 115,115,115,115 | 0 |
| 56 | MG | 2A | 3613 | 1/1 | 0.72 | 0.24 | 122,122,122,122 | 0 |
| 56 | MG | 1A | 4604 | 1/1 | 0.72 | 0.28 | 67,67,67,67 | 0 |
| 56 | MG | 2A | 3719 | 1/1 | 0.72 | 0.47 | 134,134,134,134 | 0 |
| 56 | MG | 1a | 1707 | 1/1 | 0.72 | 0.20 | 125,125,125,125 | 0 |

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| Mol | Type | Chain | Res | Atoms | RSCC | RSR | B-factors(Å$^2$) | Q<0.9 |
|---|---|---|---|---|---|---|---|---|
| 56 | MG | 2A | 3272 | 1/1 | 0.72 | 0.54 | 81,81,81,81 | 0 |
| 56 | MG | 2A | 3752 | 1/1 | 0.72 | 0.39 | 117,117,117,117 | 0 |
| 56 | MG | 2A | 3754 | 1/1 | 0.72 | 0.16 | 121,121,121,121 | 0 |
| 56 | MG | 2A | 3572 | 1/1 | 0.72 | 0.53 | 182,182,182,182 | 0 |
| 56 | MG | 2a | 1639 | 1/1 | 0.73 | 0.28 | 141,141,141,141 | 0 |
| 56 | MG | 2a | 1648 | 1/1 | 0.73 | 0.74 | 124,124,124,124 | 0 |
| 56 | MG | 1A | 4178 | 1/1 | 0.73 | 0.21 | 60,60,60,60 | 0 |
| 56 | MG | 2a | 1657 | 1/1 | 0.73 | 0.32 | 138,138,138,138 | 0 |
| 56 | MG | 2A | 3111 | 1/1 | 0.73 | 0.72 | 137,137,137,137 | 0 |
| 56 | MG | 2A | 3486 | 1/1 | 0.73 | 0.44 | 141,141,141,141 | 0 |
| 56 | MG | 2A | 3611 | 1/1 | 0.73 | 0.29 | 141,141,141,141 | 0 |
| 56 | MG | 1a | 1859 | 1/1 | 0.73 | 0.27 | 207,207,207,207 | 0 |
| 56 | MG | 2A | 3509 | 1/1 | 0.73 | 0.33 | 93,93,93,93 | 0 |
| 56 | MG | 2A | 3025 | 1/1 | 0.73 | 1.33 | 118,118,118,118 | 0 |
| 56 | MG | 1A | 4354 | 1/1 | 0.73 | 0.45 | 62,62,62,62 | 0 |
| 56 | MG | 2A | 3624 | 1/1 | 0.73 | 0.64 | 156,156,156,156 | 0 |
| 56 | MG | 1A | 4012 | 1/1 | 0.73 | 0.81 | 71,71,71,71 | 0 |
| 56 | MG | 2A | 3066 | 1/1 | 0.73 | 0.32 | 125,125,125,125 | 0 |
| 56 | MG | 2Z | 404 | 1/1 | 0.73 | 0.26 | 132,132,132,132 | 0 |
| 56 | MG | 1A | 4521 | 1/1 | 0.73 | 0.57 | 79,79,79,79 | 0 |
| 56 | MG | 2A | 3073 | 1/1 | 0.73 | 0.27 | 127,127,127,127 | 0 |
| 56 | MG | 2a | 1703 | 1/1 | 0.73 | 0.34 | 157,157,157,157 | 0 |
| 56 | MG | 2A | 3160 | 1/1 | 0.73 | 1.40 | 103,103,103,103 | 0 |
| 56 | MG | 1A | 5053 | 1/1 | 0.73 | 0.25 | 275,275,275,275 | 0 |
| 56 | MG | 2A | 3327 | 1/1 | 0.73 | 0.77 | 91,91,91,91 | 0 |
| 56 | MG | 13 | 301 | 1/1 | 0.73 | 0.45 | 65,65,65,65 | 0 |
| 56 | MG | 2a | 1606 | 1/1 | 0.73 | 0.72 | 137,137,137,137 | 0 |
| 56 | MG | 2A | 3333 | 1/1 | 0.73 | 0.26 | 98,98,98,98 | 0 |
| 56 | MG | 2a | 1845 | 1/1 | 0.73 | 0.20 | 229,229,229,229 | 0 |
| 56 | MG | 2a | 1608 | 1/1 | 0.73 | 0.81 | 135,135,135,135 | 0 |
| 56 | MG | 2a | 1873 | 1/1 | 0.73 | 0.18 | 157,157,157,157 | 0 |
| 56 | MG | 2A | 3428 | 1/1 | 0.73 | 0.18 | 166,166,166,166 | 0 |
| 56 | MG | 2A | 3191 | 1/1 | 0.73 | 0.47 | 92,92,92,92 | 0 |
| 56 | MG | 1A | 4927 | 1/1 | 0.73 | 0.49 | 87,87,87,87 | 0 |
| 56 | MG | 2A | 3451 | 1/1 | 0.73 | 0.43 | 99,99,99,99 | 0 |
| 56 | MG | 1A | 4330 | 1/1 | 0.73 | 0.31 | 77,77,77,77 | 0 |
| 56 | MG | 2a | 1748 | 1/1 | 0.73 | 0.64 | 114,114,114,114 | 0 |
| 56 | MG | 2A | 3372 | 1/1 | 0.73 | 0.25 | 107,107,107,107 | 0 |
| 56 | MG | 1A | 4549 | 1/1 | 0.73 | 0.62 | 125,125,125,125 | 0 |
| 56 | MG | 2A | 3753 | 1/1 | 0.73 | 0.35 | 97,97,97,97 | 0 |
| 56 | MG | 1A | 4742 | 1/1 | 0.74 | 0.38 | 73,73,73,73 | 0 |

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| Mol | Type | Chain | Res | Atoms | RSCC | RSR | B-factors(Å$^2$) | Q<0.9 |
|---|---|---|---|---|---|---|---|---|
| 56 | MG | 2a | 1623 | 1/1 | 0.74 | 0.22 | 182,182,182,182 | 0 |
| 56 | MG | 2A | 3521 | 1/1 | 0.74 | 0.71 | 105,105,105,105 | 0 |
| 56 | MG | 2a | 1713 | 1/1 | 0.74 | 0.92 | 143,143,143,143 | 0 |
| 56 | MG | 1A | 4304 | 1/1 | 0.74 | 0.63 | 81,81,81,81 | 0 |
| 56 | MG | 1a | 1864 | 1/1 | 0.74 | 0.39 | 211,211,211,211 | 0 |
| 56 | MG | 2a | 1804 | 1/1 | 0.74 | 0.37 | 107,107,107,107 | 0 |
| 56 | MG | 2A | 3617 | 1/1 | 0.74 | 0.38 | 102,102,102,102 | 0 |
| 56 | MG | 2A | 3283 | 1/1 | 0.74 | 0.44 | 108,108,108,108 | 0 |
| 56 | MG | 1A | 5012 | 1/1 | 0.74 | 0.34 | 115,115,115,115 | 0 |
| 56 | MG | 1A | 4197 | 1/1 | 0.74 | 0.52 | 94,94,94,94 | 0 |
| 56 | MG | 1a | 1834 | 1/1 | 0.74 | 0.29 | 210,210,210,210 | 0 |
| 56 | MG | 1A | 4788 | 1/1 | 0.74 | 0.76 | 107,107,107,107 | 0 |
| 56 | MG | 2a | 1658 | 1/1 | 0.74 | 0.35 | 122,122,122,122 | 0 |
| 56 | MG | 2r | 302 | 1/1 | 0.74 | 0.25 | 149,149,149,149 | 0 |
| 56 | MG | 1A | 4715 | 1/1 | 0.74 | 0.27 | 90,90,90,90 | 0 |
| 56 | MG | 2A | 3431 | 1/1 | 0.74 | 0.82 | 93,93,93,93 | 0 |
| 56 | MG | 2A | 3346 | 1/1 | 0.74 | 0.36 | 102,102,102,102 | 0 |
| 56 | MG | 2A | 3077 | 1/1 | 0.74 | 0.70 | 108,108,108,108 | 0 |
| 56 | MG | 1A | 4677 | 1/1 | 0.74 | 0.78 | 102,102,102,102 | 0 |
| 56 | MG | 2w | 202 | 1/1 | 0.74 | 0.46 | 88,88,88,88 | 0 |
| 56 | MG | 1a | 1687 | 1/1 | 0.74 | 0.36 | 118,118,118,118 | 0 |
| 56 | MG | 2a | 1671 | 1/1 | 0.74 | 0.41 | 173,173,173,173 | 0 |
| 56 | MG | 1a | 1853 | 1/1 | 0.74 | 0.20 | 225,225,225,225 | 0 |
| 56 | MG | 1A | 4733 | 1/1 | 0.74 | 0.15 | 82,82,82,82 | 0 |
| 56 | MG | 1a | 1856 | 1/1 | 0.74 | 0.69 | 227,227,227,227 | 0 |
| 56 | MG | 1y | 106 | 1/1 | 0.74 | 0.27 | 173,173,173,173 | 0 |
| 56 | MG | 1a | 1857 | 1/1 | 0.74 | 0.20 | 211,211,211,211 | 0 |
| 56 | MG | 2A | 3018 | 1/1 | 0.74 | 0.42 | 124,124,124,124 | 0 |
| 56 | MG | 2A | 3508 | 1/1 | 0.74 | 0.28 | 97,97,97,97 | 0 |
| 56 | MG | 2a | 1610 | 1/1 | 0.74 | 0.38 | 141,141,141,141 | 0 |
| 56 | MG | 1A | 4960 | 1/1 | 0.74 | 0.46 | 91,91,91,91 | 0 |
| 56 | MG | 2A | 3789 | 1/1 | 0.75 | 0.61 | 97,97,97,97 | 0 |
| 56 | MG | 2A | 3028 | 1/1 | 0.75 | 0.82 | 133,133,133,133 | 0 |
| 56 | MG | 2h | 203 | 1/1 | 0.75 | 1.01 | 144,144,144,144 | 0 |
| 56 | MG | 1a | 1912 | 1/1 | 0.75 | 1.11 | 131,131,131,131 | 0 |
| 56 | MG | 1A | 4948 | 1/1 | 0.75 | 0.70 | 62,62,62,62 | 0 |
| 56 | MG | 2A | 3408 | 1/1 | 0.75 | 0.26 | 129,129,129,129 | 0 |
| 56 | MG | 2A | 3582 | 1/1 | 0.75 | 0.71 | 106,106,106,106 | 0 |
| 56 | MG | 1A | 4768 | 1/1 | 0.75 | 0.31 | 65,65,65,65 | 0 |
| 56 | MG | 1A | 4538 | 1/1 | 0.75 | 0.84 | 83,83,83,83 | 0 |
| 56 | MG | 1a | 1796 | 1/1 | 0.75 | 0.36 | 105,105,105,105 | 0 |

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| Mol | Type | Chain | Res | Atoms | RSCC | RSR | B-factors(Å$^2$) | Q<0.9 |
|---|---|---|---|---|---|---|---|---|
| 56 | MG | 2Z | 403 | 1/1 | 0.75 | 0.90 | 130,130,130,130 | 0 |
| 56 | MG | 2A | 3706 | 1/1 | 0.75 | 0.33 | 94,94,94,94 | 0 |
| 56 | MG | 2A | 3593 | 1/1 | 0.75 | 0.12 | 129,129,129,129 | 0 |
| 56 | MG | 23 | 101 | 1/1 | 0.75 | 0.72 | 104,104,104,104 | 0 |
| 56 | MG | 1a | 1688 | 1/1 | 0.75 | 0.67 | 131,131,131,131 | 0 |
| 56 | MG | 1A | 4202 | 1/1 | 0.75 | 0.61 | 95,95,95,95 | 0 |
| 56 | MG | 1A | 4182 | 1/1 | 0.75 | 0.30 | 58,58,58,58 | 0 |
| 56 | MG | 2A | 3176 | 1/1 | 0.75 | 0.99 | 114,114,114,114 | 0 |
| 56 | MG | 1A | 4900 | 1/1 | 0.75 | 0.33 | 81,81,81,81 | 0 |
| 56 | MG | 2B | 215 | 1/1 | 0.75 | 0.25 | 164,164,164,164 | 0 |
| 56 | MG | 1A | 4134 | 1/1 | 0.75 | 0.71 | 72,72,72,72 | 0 |
| 56 | MG | 1A | 4762 | 1/1 | 0.75 | 0.49 | 71,71,71,71 | 0 |
| 56 | MG | 2A | 3470 | 1/1 | 0.75 | 0.61 | 104,104,104,104 | 0 |
| 56 | MG | 2d | 301 | 1/1 | 0.75 | 0.51 | 147,147,147,147 | 0 |
| 56 | MG | 2A | 3299 | 1/1 | 0.75 | 0.56 | 91,91,91,91 | 0 |
| 56 | MG | 2f | 302 | 1/1 | 0.75 | 0.26 | 143,143,143,143 | 0 |
| 56 | MG | 2a | 1688 | 1/1 | 0.75 | 0.48 | 153,153,153,153 | 0 |
| 56 | MG | 2A | 3307 | 1/1 | 0.75 | 1.09 | 92,92,92,92 | 0 |
| 56 | MG | 2a | 1618 | 1/1 | 0.75 | 0.31 | 145,145,145,145 | 0 |
| 56 | MG | 2a | 1620 | 1/1 | 0.75 | 0.52 | 151,151,151,151 | 0 |
| 56 | MG | 10 | 101 | 1/1 | 0.75 | 0.43 | 64,64,64,64 | 0 |
| 56 | MG | 2A | 3783 | 1/1 | 0.75 | 0.79 | 139,139,139,139 | 0 |
| 56 | MG | 2z | 103 | 1/1 | 0.75 | 1.01 | 179,179,179,179 | 0 |
| 56 | MG | 1Z | 305 | 1/1 | 0.76 | 0.35 | 72,72,72,72 | 0 |
| 56 | MG | 1a | 1742 | 1/1 | 0.76 | 0.54 | 106,106,106,106 | 0 |
| 56 | MG | 2a | 1791 | 1/1 | 0.76 | 0.50 | 239,239,239,239 | 0 |
| 56 | MG | 2a | 1792 | 1/1 | 0.76 | 0.08 | 250,250,250,250 | 0 |
| 56 | MG | 1a | 1751 | 1/1 | 0.76 | 0.28 | 131,131,131,131 | 0 |
| 56 | MG | 1a | 1837 | 1/1 | 0.76 | 0.28 | 226,226,226,226 | 0 |
| 56 | MG | 1a | 1752 | 1/1 | 0.76 | 0.44 | 128,128,128,128 | 0 |
| 56 | MG | 1A | 4884 | 1/1 | 0.76 | 0.42 | 84,84,84,84 | 0 |
| 56 | MG | 2a | 1628 | 1/1 | 0.76 | 0.41 | 161,161,161,161 | 0 |
| 56 | MG | 1A | 4764 | 1/1 | 0.76 | 0.52 | 64,64,64,64 | 0 |
| 56 | MG | 1A | 4767 | 1/1 | 0.76 | 0.32 | 80,80,80,80 | 0 |
| 56 | MG | 1A | 4428 | 1/1 | 0.76 | 1.28 | 59,59,59,59 | 0 |
| 56 | MG | 1A | 4780 | 1/1 | 0.76 | 0.14 | 76,76,76,76 | 0 |
| 56 | MG | 1A | 4546 | 1/1 | 0.76 | 0.57 | 104,104,104,104 | 0 |
| 56 | MG | 1A | 4006 | 1/1 | 0.76 | 0.37 | 59,59,59,59 | 0 |
| 56 | MG | 2a | 1854 | 1/1 | 0.76 | 0.13 | 286,286,286,286 | 0 |
| 56 | MG | 2A | 3539 | 1/1 | 0.76 | 0.17 | 125,125,125,125 | 0 |
| 56 | MG | 1A | 4746 | 1/1 | 0.76 | 0.29 | 76,76,76,76 | 0 |

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| Mol | Type | Chain | Res | Atoms | RSCC | RSR | B-factors(Å$^2$) | Q<0.9 |
|---|---|---|---|---|---|---|---|---|
| 56 | MG | 2a | 1881 | 1/1 | 0.76 | 0.40 | 171,171,171,171 | 0 |
| 56 | MG | 1B | 212 | 1/1 | 0.76 | 0.62 | 87,87,87,87 | 0 |
| 56 | MG | 1a | 1642 | 1/1 | 0.76 | 0.64 | 112,112,112,112 | 0 |
| 56 | MG | 1A | 4609 | 1/1 | 0.76 | 0.39 | 70,70,70,70 | 0 |
| 56 | MG | 1a | 1708 | 1/1 | 0.76 | 0.13 | 108,108,108,108 | 0 |
| 56 | MG | 2A | 3319 | 1/1 | 0.76 | 0.64 | 87,87,87,87 | 0 |
| 56 | MG | 1A | 4966 | 1/1 | 0.76 | 0.48 | 83,83,83,83 | 0 |
| 56 | MG | 1a | 1898 | 1/1 | 0.76 | 1.10 | 108,108,108,108 | 0 |
| 56 | MG | 2a | 1918 | 1/1 | 0.76 | 0.58 | 138,138,138,138 | 0 |
| 56 | MG | 1A | 4622 | 1/1 | 0.76 | 0.38 | 115,115,115,115 | 0 |
| 56 | MG | 1A | 4721 | 1/1 | 0.76 | 0.27 | 82,82,82,82 | 0 |
| 56 | MG | 1a | 1901 | 1/1 | 0.76 | 0.22 | 113,113,113,113 | 0 |
| 56 | MG | 2e | 201 | 1/1 | 0.76 | 0.52 | 122,122,122,122 | 0 |
| 56 | MG | 1a | 1659 | 1/1 | 0.76 | 0.24 | 118,118,118,118 | 0 |
| 56 | MG | 1a | 1820 | 1/1 | 0.76 | 0.32 | 205,205,205,205 | 0 |
| 56 | MG | 2A | 3738 | 1/1 | 0.76 | 0.29 | 96,96,96,96 | 0 |
| 56 | MG | 2B | 218 | 1/1 | 0.76 | 0.44 | 171,171,171,171 | 0 |
| 56 | MG | 1P | 202 | 1/1 | 0.76 | 0.70 | 60,60,60,60 | 0 |
| 56 | MG | 2A | 3107 | 1/1 | 0.77 | 0.45 | 166,166,166,166 | 0 |
| 56 | MG | 2a | 1675 | 1/1 | 0.77 | 0.32 | 166,166,166,166 | 0 |
| 56 | MG | 2D | 301 | 1/1 | 0.77 | 0.33 | 74,74,74,74 | 0 |
| 56 | MG | 1a | 1621 | 1/1 | 0.77 | 0.81 | 97,97,97,97 | 0 |
| 56 | MG | 1A | 5052 | 1/1 | 0.77 | 0.39 | 267,267,267,267 | 0 |
| 56 | MG | 1A | 4373 | 1/1 | 0.77 | 0.42 | 64,64,64,64 | 0 |
| 56 | MG | 1a | 1852 | 1/1 | 0.77 | 0.53 | 224,224,224,224 | 0 |
| 56 | MG | 1A | 4075 | 1/1 | 0.77 | 0.58 | 83,83,83,83 | 0 |
| 56 | MG | 2a | 1769 | 1/1 | 0.77 | 0.31 | 269,269,269,269 | 0 |
| 56 | MG | 1a | 1812 | 1/1 | 0.77 | 0.33 | 88,88,88,88 | 0 |
| 56 | MG | 1A | 4242 | 1/1 | 0.77 | 0.38 | 71,71,71,71 | 0 |
| 56 | MG | 10 | 104 | 1/1 | 0.77 | 0.42 | 79,79,79,79 | 0 |
| 56 | MG | 1A | 4895 | 1/1 | 0.77 | 1.00 | 59,59,59,59 | 0 |
| 56 | MG | 1A | 4329 | 1/1 | 0.77 | 0.31 | 73,73,73,73 | 0 |
| 56 | MG | 2B | 203 | 1/1 | 0.77 | 0.54 | 131,131,131,131 | 0 |
| 56 | MG | 2B | 204 | 1/1 | 0.77 | 0.25 | 130,130,130,130 | 0 |
| 56 | MG | 2a | 1790 | 1/1 | 0.77 | 0.13 | 249,249,249,249 | 0 |
| 56 | MG | 20 | 104 | 1/1 | 0.77 | 0.14 | 122,122,122,122 | 0 |
| 56 | MG | 2A | 3174 | 1/1 | 0.77 | 0.38 | 109,109,109,109 | 0 |
| 56 | MG | 1a | 1833 | 1/1 | 0.77 | 0.28 | 201,201,201,201 | 0 |
| 56 | MG | 1A | 4736 | 1/1 | 0.77 | 0.28 | 61,61,61,61 | 0 |
| 56 | MG | 2A | 3482 | 1/1 | 0.77 | 0.49 | 117,117,117,117 | 0 |
| 56 | MG | 2A | 3305 | 1/1 | 0.77 | 0.69 | 128,128,128,128 | 0 |

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| Mol | Type | Chain | Res | Atoms | RSCC | RSR | B-factors(Å$^2$) | Q<0.9 |
|---|---|---|---|---|---|---|---|---|
| 56 | MG | 1a | 1867 | 1/1 | 0.77 | 0.11 | 227,227,227,227 | 0 |
| 56 | MG | 1A | 4647 | 1/1 | 0.77 | 0.34 | 68,68,68,68 | 0 |
| 56 | MG | 1A | 4361 | 1/1 | 0.77 | 0.25 | 84,84,84,84 | 0 |
| 56 | MG | 2A | 3204 | 1/1 | 0.77 | 0.55 | 111,111,111,111 | 0 |
| 56 | MG | 2A | 3801 | 1/1 | 0.77 | 0.13 | 128,128,128,128 | 0 |
| 56 | MG | 2a | 1757 | 1/1 | 0.77 | 0.28 | 211,211,211,211 | 0 |
| 56 | MG | 1A | 4689 | 1/1 | 0.78 | 0.26 | 89,89,89,89 | 0 |
| 56 | MG | 1A | 4297 | 1/1 | 0.78 | 0.39 | 99,99,99,99 | 0 |
| 56 | MG | 2a | 1912 | 1/1 | 0.78 | 0.42 | 137,137,137,137 | 0 |
| 56 | MG | 1a | 1911 | 1/1 | 0.78 | 0.78 | 105,105,105,105 | 0 |
| 56 | MG | 1a | 1705 | 1/1 | 0.78 | 0.36 | 122,122,122,122 | 0 |
| 56 | MG | 1A | 4068 | 1/1 | 0.78 | 0.73 | 84,84,84,84 | 0 |
| 56 | MG | 2A | 3695 | 1/1 | 0.78 | 0.62 | 84,84,84,84 | 0 |
| 56 | MG | 2A | 3131 | 1/1 | 0.78 | 1.02 | 130,130,130,130 | 0 |
| 56 | MG | 2A | 3416 | 1/1 | 0.78 | 0.37 | 114,114,114,114 | 0 |
| 56 | MG | 2A | 3021 | 1/1 | 0.78 | 0.96 | 112,112,112,112 | 0 |
| 56 | MG | 1A | 4500 | 1/1 | 0.78 | 0.39 | 69,69,69,69 | 0 |
| 56 | MG | 2A | 3146 | 1/1 | 0.78 | 0.61 | 87,87,87,87 | 0 |
| 56 | MG | 2A | 3302 | 1/1 | 0.78 | 0.53 | 100,100,100,100 | 0 |
| 56 | MG | 2a | 1651 | 1/1 | 0.78 | 0.14 | 142,142,142,142 | 0 |
| 56 | MG | 2A | 3739 | 1/1 | 0.78 | 0.69 | 103,103,103,103 | 0 |
| 56 | MG | 2A | 3747 | 1/1 | 0.78 | 0.25 | 107,107,107,107 | 0 |
| 56 | MG | 2A | 3576 | 1/1 | 0.78 | 0.38 | 151,151,151,151 | 0 |
| 56 | MG | 1a | 1606 | 1/1 | 0.78 | 0.15 | 115,115,115,115 | 0 |
| 56 | MG | 2A | 3442 | 1/1 | 0.78 | 0.38 | 108,108,108,108 | 0 |
| 56 | MG | 1B | 214 | 1/1 | 0.78 | 0.48 | 69,69,69,69 | 0 |
| 56 | MG | 2h | 204 | 1/1 | 0.78 | 0.13 | 164,164,164,164 | 0 |
| 56 | MG | 1a | 1865 | 1/1 | 0.78 | 0.08 | 224,224,224,224 | 0 |
| 56 | MG | 2A | 3161 | 1/1 | 0.78 | 1.06 | 100,100,100,100 | 0 |
| 56 | MG | 1g | 301 | 1/1 | 0.78 | 0.21 | 186,186,186,186 | 0 |
| 56 | MG | 1A | 4985 | 1/1 | 0.78 | 0.99 | 73,73,73,73 | 0 |
| 56 | MG | 2T | 301 | 1/1 | 0.78 | 0.20 | 124,124,124,124 | 0 |
| 56 | MG | 2A | 3781 | 1/1 | 0.78 | 0.20 | 80,80,80,80 | 0 |
| 56 | MG | 1A | 4579 | 1/1 | 0.78 | 0.34 | 56,56,56,56 | 0 |
| 56 | MG | 2A | 3338 | 1/1 | 0.78 | 0.37 | 86,86,86,86 | 0 |
| 56 | MG | 2A | 3181 | 1/1 | 0.78 | 0.32 | 114,114,114,114 | 0 |
| 56 | MG | 2a | 1683 | 1/1 | 0.78 | 0.82 | 158,158,158,158 | 0 |
| 56 | MG | 2q | 201 | 1/1 | 0.78 | 0.57 | 124,124,124,124 | 0 |
| 56 | MG | 1A | 4009 | 1/1 | 0.78 | 0.79 | 79,79,79,79 | 0 |
| 56 | MG | 2A | 3800 | 1/1 | 0.78 | 0.87 | 151,151,151,151 | 0 |
| 56 | MG | 1a | 1840 | 1/1 | 0.78 | 0.09 | 237,237,237,237 | 0 |
| 56 | MG | 2a | 1696 | 1/1 | 0.78 | 0.35 | 161,161,161,161 | 0 |

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| Mol | Type | Chain | Res | Atoms | RSCC | RSR | B-factors(Å$^2$) | Q<0.9 |
|---|---|---|---|---|---|---|---|---|
| 56 | MG | 1A | 4121 | 1/1 | 0.78 | 0.49 | 81,81,81,81 | 0 |
| 56 | MG | 2a | 1821 | 1/1 | 0.78 | 0.20 | 143,143,143,143 | 0 |
| 56 | MG | 2a | 1824 | 1/1 | 0.78 | 0.37 | 158,158,158,158 | 0 |
| 56 | MG | 1A | 4933 | 1/1 | 0.78 | 0.65 | 102,102,102,102 | 0 |
| 56 | MG | 2A | 3084 | 1/1 | 0.78 | 0.50 | 115,115,115,115 | 0 |
| 56 | MG | 1A | 4540 | 1/1 | 0.78 | 0.35 | 77,77,77,77 | 0 |
| 56 | MG | 1a | 1850 | 1/1 | 0.78 | 0.76 | 113,113,113,113 | 0 |
| 56 | MG | 2a | 1604 | 1/1 | 0.78 | 0.18 | 148,148,148,148 | 0 |
| 56 | MG | 1a | 1745 | 1/1 | 0.78 | 0.52 | 122,122,122,122 | 0 |
| 56 | MG | 2A | 3244 | 1/1 | 0.78 | 0.24 | 104,104,104,104 | 0 |
| 56 | MG | 1A | 4765 | 1/1 | 0.78 | 0.67 | 60,60,60,60 | 0 |
| 56 | MG | 2A | 3105 | 1/1 | 0.78 | 0.53 | 155,155,155,155 | 0 |
| 56 | MG | 2A | 3661 | 1/1 | 0.78 | 0.27 | 105,105,105,105 | 0 |
| 56 | MG | 2A | 3834 | 1/1 | 0.78 | 0.14 | 115,115,115,115 | 0 |
| 56 | MG | 2a | 1733 | 1/1 | 0.78 | 0.18 | 125,125,125,125 | 0 |
| 56 | MG | 2a | 1905 | 1/1 | 0.78 | 0.97 | 218,218,218,218 | 0 |
| 56 | MG | 1A | 4950 | 1/1 | 0.79 | 0.22 | 61,61,61,61 | 0 |
| 56 | MG | 1A | 4047 | 1/1 | 0.79 | 0.44 | 69,69,69,69 | 0 |
| 56 | MG | 1a | 1686 | 1/1 | 0.79 | 0.18 | 116,116,116,116 | 0 |
| 56 | MG | 1A | 4464 | 1/1 | 0.79 | 0.43 | 66,66,66,66 | 0 |
| 56 | MG | 2A | 3194 | 1/1 | 0.79 | 0.17 | 109,109,109,109 | 0 |
| 56 | MG | 1a | 1622 | 1/1 | 0.79 | 0.98 | 99,99,99,99 | 0 |
| 56 | MG | 2A | 3465 | 1/1 | 0.79 | 0.64 | 129,129,129,129 | 0 |
| 56 | MG | 1A | 4153 | 1/1 | 0.79 | 0.29 | 55,55,55,55 | 0 |
| 56 | MG | 2a | 1745 | 1/1 | 0.79 | 0.16 | 162,162,162,162 | 0 |
| 56 | MG | 1A | 4667 | 1/1 | 0.79 | 0.24 | 75,75,75,75 | 0 |
| 56 | MG | 2a | 1663 | 1/1 | 0.79 | 0.79 | 143,143,143,143 | 0 |
| 56 | MG | 1A | 4327 | 1/1 | 0.79 | 0.31 | 66,66,66,66 | 0 |
| 56 | MG | 2A | 3841 | 1/1 | 0.79 | 0.32 | 146,146,146,146 | 0 |
| 56 | MG | 1A | 5006 | 1/1 | 0.79 | 0.81 | 74,74,74,74 | 0 |
| 56 | MG | 2a | 1876 | 1/1 | 0.79 | 0.32 | 147,147,147,147 | 0 |
| 56 | MG | 27 | 101 | 1/1 | 0.79 | 0.63 | 90,90,90,90 | 0 |
| 56 | MG | 1y | 101 | 1/1 | 0.79 | 0.33 | 87,87,87,87 | 0 |
| 56 | MG | 1A | 4511 | 1/1 | 0.79 | 0.39 | 68,68,68,68 | 0 |
| 56 | MG | 1A | 4772 | 1/1 | 0.79 | 0.46 | 70,70,70,70 | 0 |
| 56 | MG | 1P | 203 | 1/1 | 0.79 | 0.23 | 68,68,68,68 | 0 |
| 56 | MG | 2a | 1901 | 1/1 | 0.79 | 0.90 | 171,171,171,171 | 0 |
| 56 | MG | 1Q | 201 | 1/1 | 0.79 | 0.44 | 70,70,70,70 | 0 |
| 56 | MG | 2A | 3512 | 1/1 | 0.79 | 0.42 | 94,94,94,94 | 0 |
| 56 | MG | 2A | 3019 | 1/1 | 0.79 | 0.90 | 112,112,112,112 | 0 |
| 56 | MG | 1A | 4681 | 1/1 | 0.79 | 0.25 | 67,67,67,67 | 0 |

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| Mol | Type | Chain | Res | Atoms | RSCC | RSR | B-factors(Å$^2$) | Q<0.9 |
|---|---|---|---|---|---|---|---|---|
| 56 | MG | 1A | 4616 | 1/1 | 0.79 | 0.23 | 86,86,86,86 | 0 |
| 56 | MG | 1A | 5051 | 1/1 | 0.79 | 0.20 | 192,192,192,192 | 0 |
| 56 | MG | 1b | 304 | 1/1 | 0.79 | 0.44 | 173,173,173,173 | 0 |
| 56 | MG | 1A | 4036 | 1/1 | 0.79 | 0.72 | 76,76,76,76 | 0 |
| 56 | MG | 2a | 1700 | 1/1 | 0.79 | 0.73 | 140,140,140,140 | 0 |
| 56 | MG | 2x | 107 | 1/1 | 0.79 | 1.42 | 131,131,131,131 | 0 |
| 56 | MG | 1A | 4042 | 1/1 | 0.79 | 0.29 | 58,58,58,58 | 0 |
| 56 | MG | 1d | 305 | 1/1 | 0.79 | 0.26 | 142,142,142,142 | 0 |
| 56 | MG | 2A | 3034 | 1/1 | 0.79 | 0.86 | 100,100,100,100 | 0 |
| 56 | MG | 2A | 3057 | 1/1 | 0.79 | 0.73 | 96,96,96,96 | 0 |
| 56 | MG | 1A | 5054 | 1/1 | 0.79 | 0.30 | 142,142,142,142 | 0 |
| 56 | MG | 1A | 4750 | 1/1 | 0.79 | 0.37 | 68,68,68,68 | 0 |
| 56 | MG | 2A | 3805 | 1/1 | 0.79 | 0.26 | 100,100,100,100 | 0 |
| 57 | ZN | 2Y | 203 | 1/1 | 0.79 | 0.08 | 153,153,153,153 | 0 |
| 56 | MG | 2a | 1682 | 1/1 | 0.80 | 0.66 | 131,131,131,131 | 0 |
| 56 | MG | 1A | 4822 | 1/1 | 0.80 | 0.61 | 82,82,82,82 | 0 |
| 56 | MG | 1R | 203 | 1/1 | 0.80 | 0.90 | 52,52,52,52 | 0 |
| 56 | MG | 2A | 3133 | 1/1 | 0.80 | 1.15 | 143,143,143,143 | 0 |
| 56 | MG | 2A | 3732 | 1/1 | 0.80 | 0.32 | 95,95,95,95 | 0 |
| 56 | MG | 1Z | 301 | 1/1 | 0.80 | 0.39 | 80,80,80,80 | 0 |
| 56 | MG | 1A | 4192 | 1/1 | 0.80 | 0.37 | 68,68,68,68 | 0 |
| 56 | MG | 2A | 3142 | 1/1 | 0.80 | 1.06 | 102,102,102,102 | 0 |
| 56 | MG | 2B | 213 | 1/1 | 0.80 | 0.26 | 151,151,151,151 | 0 |
| 56 | MG | 2A | 3745 | 1/1 | 0.80 | 0.44 | 112,112,112,112 | 0 |
| 56 | MG | 2A | 3143 | 1/1 | 0.80 | 0.35 | 89,89,89,89 | 0 |
| 56 | MG | 1A | 4404 | 1/1 | 0.80 | 0.55 | 70,70,70,70 | 0 |
| 56 | MG | 2i | 203 | 1/1 | 0.80 | 0.12 | 234,234,234,234 | 0 |
| 56 | MG | 2A | 3608 | 1/1 | 0.80 | 0.21 | 111,111,111,111 | 0 |
| 56 | MG | 1A | 4962 | 1/1 | 0.80 | 0.53 | 69,69,69,69 | 0 |
| 56 | MG | 2a | 1808 | 1/1 | 0.80 | 0.56 | 102,102,102,102 | 0 |
| 56 | MG | 1a | 1666 | 1/1 | 0.80 | 0.32 | 116,116,116,116 | 0 |
| 56 | MG | 1A | 4275 | 1/1 | 0.80 | 0.33 | 65,65,65,65 | 0 |
| 56 | MG | 1A | 4514 | 1/1 | 0.80 | 0.46 | 81,81,81,81 | 0 |
| 56 | MG | 2a | 1719 | 1/1 | 0.80 | 0.13 | 151,151,151,151 | 0 |
| 56 | MG | 2A | 3168 | 1/1 | 0.80 | 0.61 | 90,90,90,90 | 0 |
| 56 | MG | 2A | 3768 | 1/1 | 0.80 | 0.30 | 90,90,90,90 | 0 |
| 56 | MG | 1A | 4621 | 1/1 | 0.80 | 0.55 | 114,114,114,114 | 0 |
| 56 | MG | 2F | 301 | 1/1 | 0.80 | 0.27 | 133,133,133,133 | 0 |
| 56 | MG | 2a | 1860 | 1/1 | 0.80 | 0.47 | 153,153,153,153 | 0 |
| 56 | MG | 1A | 4126 | 1/1 | 0.80 | 0.40 | 78,78,78,78 | 0 |
| 56 | MG | 1A | 4294 | 1/1 | 0.80 | 0.36 | 84,84,84,84 | 0 |
| 56 | MG | 2A | 3312 | 1/1 | 0.80 | 0.33 | 129,129,129,129 | 0 |

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| Mol | Type | Chain | Res | Atoms | RSCC | RSR | B-factors(Å$^2$) | Q<0.9 |
|---|---|---|---|---|---|---|---|---|
| 56 | MG | 2A | 3632 | 1/1 | 0.80 | 0.77 | 110,110,110,110 | 0 |
| 56 | MG | 2A | 3637 | 1/1 | 0.80 | 0.45 | 88,88,88,88 | 0 |
| 56 | MG | 1A | 4696 | 1/1 | 0.80 | 0.26 | 72,72,72,72 | 0 |
| 56 | MG | 1D | 307 | 1/1 | 0.80 | 0.16 | 99,99,99,99 | 0 |
| 56 | MG | 2A | 3550 | 1/1 | 0.80 | 0.21 | 104,104,104,104 | 0 |
| 56 | MG | 2A | 3188 | 1/1 | 0.80 | 0.27 | 103,103,103,103 | 0 |
| 56 | MG | 1a | 1819 | 1/1 | 0.80 | 0.34 | 204,204,204,204 | 0 |
| 56 | MG | 1A | 4917 | 1/1 | 0.80 | 1.15 | 62,62,62,62 | 0 |
| 56 | MG | 1A | 4485 | 1/1 | 0.80 | 0.19 | 61,61,61,61 | 0 |
| 56 | MG | 1a | 1829 | 1/1 | 0.80 | 0.11 | 194,194,194,194 | 0 |
| 56 | MG | 1A | 4700 | 1/1 | 0.80 | 0.25 | 79,79,79,79 | 0 |
| 56 | MG | 2A | 3573 | 1/1 | 0.80 | 0.23 | 282,282,282,282 | 0 |
| 56 | MG | 2A | 3023 | 1/1 | 0.80 | 0.77 | 120,120,120,120 | 0 |
| 56 | MG | 1A | 4520 | 1/1 | 0.80 | 0.49 | 75,75,75,75 | 0 |
| 56 | MG | 2A | 3713 | 1/1 | 0.80 | 0.19 | 112,112,112,112 | 0 |
| 56 | MG | 2a | 1678 | 1/1 | 0.80 | 0.41 | 167,167,167,167 | 0 |
| 56 | MG | 2a | 1775 | 1/1 | 0.80 | 0.30 | 208,208,208,208 | 0 |
| 56 | MG | 1a | 1601 | 1/1 | 0.81 | 0.22 | 73,73,73,73 | 0 |
| 56 | MG | 1A | 4626 | 1/1 | 0.81 | 0.49 | 95,95,95,95 | 0 |
| 56 | MG | 2a | 1635 | 1/1 | 0.81 | 0.12 | 147,147,147,147 | 0 |
| 56 | MG | 2a | 1796 | 1/1 | 0.81 | 0.41 | 111,111,111,111 | 0 |
| 56 | MG | 1a | 1677 | 1/1 | 0.81 | 0.52 | 157,157,157,157 | 0 |
| 56 | MG | 2A | 3242 | 1/1 | 0.81 | 0.21 | 106,106,106,106 | 0 |
| 56 | MG | 1A | 5020 | 1/1 | 0.81 | 0.57 | 69,69,69,69 | 0 |
| 56 | MG | 2a | 1649 | 1/1 | 0.81 | 0.30 | 143,143,143,143 | 0 |
| 56 | MG | 1A | 4395 | 1/1 | 0.81 | 0.43 | 63,63,63,63 | 0 |
| 56 | MG | 2a | 1729 | 1/1 | 0.81 | 0.28 | 124,124,124,124 | 0 |
| 56 | MG | 1A | 4942 | 1/1 | 0.81 | 0.18 | 79,79,79,79 | 0 |
| 56 | MG | 1a | 1827 | 1/1 | 0.81 | 0.24 | 190,190,190,190 | 0 |
| 56 | MG | 1a | 1828 | 1/1 | 0.81 | 0.34 | 175,175,175,175 | 0 |
| 56 | MG | 2l | 201 | 1/1 | 0.81 | 0.48 | 132,132,132,132 | 0 |
| 56 | MG | 2A | 3487 | 1/1 | 0.81 | 0.23 | 145,145,145,145 | 0 |
| 56 | MG | 2A | 3062 | 1/1 | 0.81 | 0.31 | 85,85,85,85 | 0 |
| 56 | MG | 1A | 4881 | 1/1 | 0.81 | 0.40 | 82,82,82,82 | 0 |
| 56 | MG | 2a | 1746 | 1/1 | 0.81 | 0.37 | 120,120,120,120 | 0 |
| 56 | MG | 1A | 4697 | 1/1 | 0.81 | 0.87 | 68,68,68,68 | 0 |
| 56 | MG | 1A | 4584 | 1/1 | 0.81 | 0.39 | 105,105,105,105 | 0 |
| 56 | MG | 1A | 4730 | 1/1 | 0.81 | 0.69 | 71,71,71,71 | 0 |
| 56 | MG | 2a | 1869 | 1/1 | 0.81 | 0.50 | 151,151,151,151 | 0 |
| 56 | MG | 2A | 3609 | 1/1 | 0.81 | 0.15 | 132,132,132,132 | 0 |
| 56 | MG | 1a | 1699 | 1/1 | 0.81 | 0.31 | 118,118,118,118 | 0 |
| 56 | MG | 2a | 1672 | 1/1 | 0.81 | 0.38 | 181,181,181,181 | 0 |

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| Mol | Type | Chain | Res | Atoms | RSCC | RSR | B-factors(Å$^2$) | Q<0.9 |
|---|---|---|---|---|---|---|---|---|
| 56 | MG | 2A | 3742 | 1/1 | 0.81 | 0.45 | 91,91,91,91 | 0 |
| 56 | MG | 2A | 3528 | 1/1 | 0.81 | 0.25 | 106,106,106,106 | 0 |
| 56 | MG | 1V | 201 | 1/1 | 0.81 | 0.42 | 74,74,74,74 | 0 |
| 56 | MG | 2A | 3751 | 1/1 | 0.81 | 0.12 | 101,101,101,101 | 0 |
| 56 | MG | 1A | 4374 | 1/1 | 0.81 | 0.40 | 94,94,94,94 | 0 |
| 56 | MG | 2a | 1904 | 1/1 | 0.81 | 0.26 | 245,245,245,245 | 0 |
| 56 | MG | 1A | 5059 | 1/1 | 0.81 | 0.45 | 86,86,86,86 | 0 |
| 56 | MG | 2a | 1906 | 1/1 | 0.81 | 0.22 | 240,240,240,240 | 0 |
| 56 | MG | 1A | 4495 | 1/1 | 0.81 | 0.61 | 78,78,78,78 | 0 |
| 56 | MG | 1A | 4712 | 1/1 | 0.81 | 0.30 | 76,76,76,76 | 0 |
| 56 | MG | 1A | 4916 | 1/1 | 0.81 | 0.22 | 73,73,73,73 | 0 |
| 56 | MG | 2A | 3101 | 1/1 | 0.81 | 0.59 | 133,133,133,133 | 0 |
| 56 | MG | 1A | 4834 | 1/1 | 0.81 | 0.53 | 72,72,72,72 | 0 |
| 56 | MG | 17 | 103 | 1/1 | 0.81 | 0.56 | 73,73,73,73 | 0 |
| 56 | MG | 1A | 4848 | 1/1 | 0.81 | 0.33 | 74,74,74,74 | 0 |
| 56 | MG | 2A | 3640 | 1/1 | 0.81 | 0.36 | 127,127,127,127 | 0 |
| 56 | MG | 2A | 3642 | 1/1 | 0.81 | 0.33 | 132,132,132,132 | 0 |
| 56 | MG | 1a | 1809 | 1/1 | 0.81 | 0.31 | 127,127,127,127 | 0 |
| 56 | MG | 2y | 110 | 1/1 | 0.81 | 0.40 | 248,248,248,248 | 0 |
| 56 | MG | 2A | 3340 | 1/1 | 0.81 | 0.69 | 75,75,75,75 | 0 |
| 56 | MG | 2f | 304 | 1/1 | 0.81 | 0.77 | 137,137,137,137 | 0 |
| 56 | MG | 29 | 101 | 1/1 | 0.82 | 0.20 | 130,130,130,130 | 0 |
| 56 | MG | 2a | 1782 | 1/1 | 0.82 | 1.08 | 205,205,205,205 | 0 |
| 56 | MG | 2a | 1783 | 1/1 | 0.82 | 1.14 | 174,174,174,174 | 0 |
| 56 | MG | 1S | 202 | 1/1 | 0.82 | 1.27 | 92,92,92,92 | 0 |
| 56 | MG | 1A | 4524 | 1/1 | 0.82 | 0.35 | 74,74,74,74 | 0 |
| 56 | MG | 1A | 4862 | 1/1 | 0.82 | 0.65 | 74,74,74,74 | 0 |
| 56 | MG | 2a | 1695 | 1/1 | 0.82 | 0.77 | 146,146,146,146 | 0 |
| 56 | MG | 1a | 1735 | 1/1 | 0.82 | 0.57 | 150,150,150,150 | 0 |
| 56 | MG | 2A | 3347 | 1/1 | 0.82 | 0.28 | 99,99,99,99 | 0 |
| 56 | MG | 1A | 4453 | 1/1 | 0.82 | 0.21 | 66,66,66,66 | 0 |
| 56 | MG | 1A | 4163 | 1/1 | 0.82 | 0.19 | 57,57,57,57 | 0 |
| 56 | MG | 2A | 3358 | 1/1 | 0.82 | 0.16 | 97,97,97,97 | 0 |
| 56 | MG | 2a | 1799 | 1/1 | 0.82 | 0.26 | 238,238,238,238 | 0 |
| 56 | MG | 1B | 202 | 1/1 | 0.82 | 0.18 | 114,114,114,114 | 0 |
| 56 | MG | 1B | 203 | 1/1 | 0.82 | 0.50 | 95,95,95,95 | 0 |
| 56 | MG | 1A | 4785 | 1/1 | 0.82 | 1.19 | 70,70,70,70 | 0 |
| 56 | MG | 2k | 201 | 1/1 | 0.82 | 0.21 | 158,158,158,158 | 0 |
| 56 | MG | 1a | 1674 | 1/1 | 0.82 | 0.19 | 134,134,134,134 | 0 |
| 56 | MG | 1A | 4402 | 1/1 | 0.82 | 0.15 | 73,73,73,73 | 0 |
| 56 | MG | 1A | 4710 | 1/1 | 0.82 | 0.34 | 73,73,73,73 | 0 |
| 56 | MG | 2B | 223 | 1/1 | 0.82 | 0.17 | 129,129,129,129 | 0 |

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| Mol | Type | Chain | Res | Atoms | RSCC | RSR | B-factors(Å$^2$) | Q<0.9 |
|---|---|---|---|---|---|---|---|---|
| 56 | MG | 1A | 4802 | 1/1 | 0.82 | 0.40 | 73,73,73,73 | 0 |
| 56 | MG | 2A | 3393 | 1/1 | 0.82 | 0.29 | 132,132,132,132 | 0 |
| 56 | MG | 2a | 1723 | 1/1 | 0.82 | 1.05 | 118,118,118,118 | 0 |
| 56 | MG | 1a | 1771 | 1/1 | 0.82 | 0.35 | 135,135,135,135 | 0 |
| 56 | MG | 1A | 4997 | 1/1 | 0.82 | 0.15 | 80,80,80,80 | 0 |
| 56 | MG | 1A | 4087 | 1/1 | 0.82 | 0.32 | 69,69,69,69 | 0 |
| 56 | MG | 2q | 202 | 1/1 | 0.82 | 0.37 | 149,149,149,149 | 0 |
| 56 | MG | 2A | 3269 | 1/1 | 0.82 | 0.40 | 94,94,94,94 | 0 |
| 56 | MG | 2E | 303 | 1/1 | 0.82 | 0.29 | 81,81,81,81 | 0 |
| 56 | MG | 2A | 3635 | 1/1 | 0.82 | 0.31 | 103,103,103,103 | 0 |
| 56 | MG | 2A | 3773 | 1/1 | 0.82 | 0.22 | 115,115,115,115 | 0 |
| 56 | MG | 1A | 4010 | 1/1 | 0.82 | 0.48 | 73,73,73,73 | 0 |
| 56 | MG | 1a | 1916 | 1/1 | 0.82 | 0.41 | 146,146,146,146 | 0 |
| 56 | MG | 2A | 3785 | 1/1 | 0.82 | 0.34 | 119,119,119,119 | 0 |
| 56 | MG | 1A | 4820 | 1/1 | 0.82 | 0.45 | 72,72,72,72 | 0 |
| 56 | MG | 1A | 4920 | 1/1 | 0.82 | 0.33 | 61,61,61,61 | 0 |
| 56 | MG | 2A | 3414 | 1/1 | 0.82 | 0.52 | 117,117,117,117 | 0 |
| 56 | MG | 1O | 205 | 1/1 | 0.82 | 0.34 | 112,112,112,112 | 0 |
| 56 | MG | 1A | 4040 | 1/1 | 0.82 | 0.16 | 93,93,93,93 | 0 |
| 56 | MG | 2A | 3654 | 1/1 | 0.82 | 1.27 | 115,115,115,115 | 0 |
| 56 | MG | 1A | 4562 | 1/1 | 0.82 | 0.40 | 65,65,65,65 | 0 |
| 56 | MG | 2A | 3673 | 1/1 | 0.82 | 0.80 | 133,133,133,133 | 0 |
| 56 | MG | 1a | 1798 | 1/1 | 0.82 | 0.45 | 118,118,118,118 | 0 |
| 56 | MG | 1a | 1802 | 1/1 | 0.82 | 0.58 | 142,142,142,142 | 0 |
| 56 | MG | 1A | 4631 | 1/1 | 0.82 | 0.39 | 70,70,70,70 | 0 |
| 56 | MG | 1R | 201 | 1/1 | 0.82 | 0.54 | 68,68,68,68 | 0 |
| 56 | MG | 2A | 3446 | 1/1 | 0.82 | 0.85 | 84,84,84,84 | 0 |
| 56 | MG | 1a | 1646 | 1/1 | 0.82 | 0.80 | 116,116,116,116 | 0 |
| 56 | MG | 2z | 102 | 1/1 | 0.82 | 0.14 | 175,175,175,175 | 0 |
| 56 | MG | 2a | 1680 | 1/1 | 0.82 | 0.42 | 162,162,162,162 | 0 |
| 56 | MG | 1A | 4505 | 1/1 | 0.82 | 0.40 | 92,92,92,92 | 0 |
| 56 | MG | 1v | 701 | 1/1 | 0.83 | 0.74 | 117,117,117,117 | 0 |
| 56 | MG | 2a | 1647 | 1/1 | 0.83 | 0.37 | 139,139,139,139 | 0 |
| 56 | MG | 1A | 4763 | 1/1 | 0.83 | 0.26 | 69,69,69,69 | 0 |
| 56 | MG | 1A | 4165 | 1/1 | 0.83 | 0.40 | 56,56,56,56 | 0 |
| 56 | MG | 1A | 4858 | 1/1 | 0.83 | 1.08 | 58,58,58,58 | 0 |
| 56 | MG | 1a | 1734 | 1/1 | 0.83 | 0.74 | 147,147,147,147 | 0 |
| 56 | MG | 2A | 3015 | 1/1 | 0.83 | 0.69 | 112,112,112,112 | 0 |
| 56 | MG | 2A | 3106 | 1/1 | 0.83 | 0.40 | 170,170,170,170 | 0 |
| 56 | MG | 1a | 1801 | 1/1 | 0.83 | 0.35 | 105,105,105,105 | 0 |
| 56 | MG | 1T | 204 | 1/1 | 0.83 | 0.28 | 115,115,115,115 | 0 |
| 56 | MG | 1a | 1623 | 1/1 | 0.83 | 0.13 | 100,100,100,100 | 0 |

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| Mol | Type | Chain | Res | Atoms | RSCC | RSR | B-factors(Å$^2$) | Q<0.9 |
|---|---|---|---|---|---|---|---|---|
| 56 | MG | 2A | 3214 | 1/1 | 0.83 | 0.35 | 93,93,93,93 | 0 |
| 56 | MG | 2A | 3497 | 1/1 | 0.83 | 0.59 | 79,79,79,79 | 0 |
| 56 | MG | 2A | 3767 | 1/1 | 0.83 | 0.64 | 93,93,93,93 | 0 |
| 56 | MG | 2A | 3367 | 1/1 | 0.83 | 0.34 | 92,92,92,92 | 0 |
| 56 | MG | 2A | 3217 | 1/1 | 0.83 | 0.30 | 91,91,91,91 | 0 |
| 56 | MG | 2Q | 201 | 1/1 | 0.83 | 0.26 | 126,126,126,126 | 0 |
| 56 | MG | 2A | 3221 | 1/1 | 0.83 | 0.20 | 114,114,114,114 | 0 |
| 56 | MG | 2A | 3224 | 1/1 | 0.83 | 0.22 | 119,119,119,119 | 0 |
| 56 | MG | 1A | 5024 | 1/1 | 0.83 | 0.27 | 55,55,55,55 | 0 |
| 56 | MG | 1A | 4703 | 1/1 | 0.83 | 0.55 | 64,64,64,64 | 0 |
| 56 | MG | 2V | 201 | 1/1 | 0.83 | 0.34 | 129,129,129,129 | 0 |
| 56 | MG | 1a | 1917 | 1/1 | 0.83 | 0.24 | 128,128,128,128 | 0 |
| 56 | MG | 2A | 3793 | 1/1 | 0.83 | 0.45 | 116,116,116,116 | 0 |
| 56 | MG | 1a | 1636 | 1/1 | 0.83 | 0.19 | 120,120,120,120 | 0 |
| 56 | MG | 1A | 4094 | 1/1 | 0.83 | 0.29 | 68,68,68,68 | 0 |
| 56 | MG | 20 | 103 | 1/1 | 0.83 | 0.48 | 97,97,97,97 | 0 |
| 56 | MG | 2A | 3532 | 1/1 | 0.83 | 0.24 | 118,118,118,118 | 0 |
| 56 | MG | 2A | 3533 | 1/1 | 0.83 | 0.41 | 124,124,124,124 | 0 |
| 56 | MG | 2A | 3249 | 1/1 | 0.83 | 0.32 | 128,128,128,128 | 0 |
| 56 | MG | 1A | 5036 | 1/1 | 0.83 | 0.20 | 72,72,72,72 | 0 |
| 56 | MG | 2A | 3649 | 1/1 | 0.83 | 0.57 | 110,110,110,110 | 0 |
| 56 | MG | 1A | 4130 | 1/1 | 0.83 | 0.49 | 58,58,58,58 | 0 |
| 56 | MG | 1A | 4219 | 1/1 | 0.83 | 0.44 | 61,61,61,61 | 0 |
| 56 | MG | 2A | 3823 | 1/1 | 0.83 | 0.41 | 95,95,95,95 | 0 |
| 56 | MG | 2A | 3664 | 1/1 | 0.83 | 0.31 | 112,112,112,112 | 0 |
| 56 | MG | 2A | 3672 | 1/1 | 0.83 | 0.11 | 120,120,120,120 | 0 |
| 56 | MG | 2A | 3264 | 1/1 | 0.83 | 0.59 | 81,81,81,81 | 0 |
| 56 | MG | 1a | 1767 | 1/1 | 0.83 | 0.29 | 133,133,133,133 | 0 |
| 56 | MG | 2a | 1838 | 1/1 | 0.83 | 0.06 | 244,244,244,244 | 0 |
| 56 | MG | 1a | 1822 | 1/1 | 0.83 | 0.11 | 215,215,215,215 | 0 |
| 56 | MG | 2A | 3152 | 1/1 | 0.83 | 0.25 | 96,96,96,96 | 0 |
| 56 | MG | 2a | 1849 | 1/1 | 0.83 | 0.13 | 142,142,142,142 | 0 |
| 56 | MG | 2a | 1853 | 1/1 | 0.83 | 0.41 | 269,269,269,269 | 0 |
| 56 | MG | 1A | 4812 | 1/1 | 0.83 | 0.30 | 72,72,72,72 | 0 |
| 56 | MG | 2a | 1857 | 1/1 | 0.83 | 0.19 | 145,145,145,145 | 0 |
| 56 | MG | 2a | 1612 | 1/1 | 0.83 | 0.32 | 141,141,141,141 | 0 |
| 56 | MG | 1A | 4987 | 1/1 | 0.83 | 0.42 | 62,62,62,62 | 0 |
| 56 | MG | 2A | 3842 | 1/1 | 0.83 | 0.25 | 99,99,99,99 | 0 |
| 56 | MG | 2A | 3292 | 1/1 | 0.83 | 0.75 | 79,79,79,79 | 0 |
| 56 | MG | 2A | 3298 | 1/1 | 0.83 | 0.58 | 94,94,94,94 | 0 |
| 56 | MG | 2A | 3424 | 1/1 | 0.83 | 0.35 | 142,142,142,142 | 0 |
| 56 | MG | 1a | 1775 | 1/1 | 0.83 | 0.32 | 131,131,131,131 | 0 |

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| Mol | Type | Chain | Res | Atoms | RSCC | RSR | B-factors(Å$^2$) | Q<0.9 |
|---|---|---|---|---|---|---|---|---|
| 56 | MG | 2B | 207 | 1/1 | 0.83 | 1.03 | 161,161,161,161 | 0 |
| 56 | MG | 18 | 102 | 1/1 | 0.83 | 0.33 | 66,66,66,66 | 0 |
| 56 | MG | 2a | 1894 | 1/1 | 0.83 | 0.47 | 151,151,151,151 | 0 |
| 56 | MG | 1A | 4988 | 1/1 | 0.83 | 0.50 | 79,79,79,79 | 0 |
| 56 | MG | 1a | 1662 | 1/1 | 0.83 | 0.37 | 123,123,123,123 | 0 |
| 56 | MG | 1A | 4776 | 1/1 | 0.83 | 0.65 | 96,96,96,96 | 0 |
| 56 | MG | 2a | 1749 | 1/1 | 0.83 | 0.39 | 115,115,115,115 | 0 |
| 56 | MG | 1A | 4305 | 1/1 | 0.83 | 0.58 | 82,82,82,82 | 0 |
| 57 | ZN | 24 | 102 | 1/1 | 0.83 | 0.08 | 230,230,230,230 | 0 |
| 56 | MG | 2A | 3222 | 1/1 | 0.84 | 0.54 | 112,112,112,112 | 0 |
| 56 | MG | 1A | 4265 | 1/1 | 0.84 | 0.37 | 61,61,61,61 | 0 |
| 56 | MG | 2A | 3381 | 1/1 | 0.84 | 0.23 | 98,98,98,98 | 0 |
| 56 | MG | 2N | 201 | 1/1 | 0.84 | 0.48 | 113,113,113,113 | 0 |
| 56 | MG | 1a | 1770 | 1/1 | 0.84 | 0.42 | 101,101,101,101 | 0 |
| 56 | MG | 1A | 4396 | 1/1 | 0.84 | 0.26 | 72,72,72,72 | 0 |
| 56 | MG | 1T | 205 | 1/1 | 0.84 | 0.30 | 109,109,109,109 | 0 |
| 56 | MG | 2f | 301 | 1/1 | 0.84 | 0.70 | 138,138,138,138 | 0 |
| 56 | MG | 1A | 4610 | 1/1 | 0.84 | 0.19 | 60,60,60,60 | 0 |
| 56 | MG | 2A | 3516 | 1/1 | 0.84 | 0.67 | 82,82,82,82 | 0 |
| 56 | MG | 2a | 1779 | 1/1 | 0.84 | 0.53 | 183,183,183,183 | 0 |
| 56 | MG | 1a | 1626 | 1/1 | 0.84 | 0.68 | 98,98,98,98 | 0 |
| 56 | MG | 1A | 4013 | 1/1 | 0.84 | 0.36 | 81,81,81,81 | 0 |
| 56 | MG | 1A | 4403 | 1/1 | 0.84 | 0.36 | 62,62,62,62 | 0 |
| 56 | MG | 2Y | 201 | 1/1 | 0.84 | 0.75 | 113,113,113,113 | 0 |
| 56 | MG | 2A | 3255 | 1/1 | 0.84 | 0.21 | 126,126,126,126 | 0 |
| 56 | MG | 1a | 1784 | 1/1 | 0.84 | 0.67 | 124,124,124,124 | 0 |
| 56 | MG | 1a | 1869 | 1/1 | 0.84 | 0.09 | 226,226,226,226 | 0 |
| 56 | MG | 2A | 3399 | 1/1 | 0.84 | 0.43 | 194,194,194,194 | 0 |
| 56 | MG | 1a | 1678 | 1/1 | 0.84 | 0.21 | 162,162,162,162 | 0 |
| 56 | MG | 2i | 201 | 1/1 | 0.84 | 0.58 | 245,245,245,245 | 0 |
| 56 | MG | 1i | 201 | 1/1 | 0.84 | 0.38 | 212,212,212,212 | 0 |
| 56 | MG | 2A | 3043 | 1/1 | 0.84 | 0.27 | 113,113,113,113 | 0 |
| 56 | MG | 1l | 301 | 1/1 | 0.84 | 0.63 | 133,133,133,133 | 0 |
| 56 | MG | 2a | 1691 | 1/1 | 0.84 | 0.55 | 139,139,139,139 | 0 |
| 56 | MG | 2A | 3825 | 1/1 | 0.84 | 1.48 | 97,97,97,97 | 0 |
| 56 | MG | 2A | 3058 | 1/1 | 0.84 | 0.24 | 85,85,85,85 | 0 |
| 56 | MG | 1a | 1832 | 1/1 | 0.84 | 0.18 | 189,189,189,189 | 0 |
| 56 | MG | 2a | 1699 | 1/1 | 0.84 | 0.41 | 138,138,138,138 | 0 |
| 56 | MG | 1A | 4334 | 1/1 | 0.84 | 0.28 | 73,73,73,73 | 0 |
| 56 | MG | 2A | 3418 | 1/1 | 0.84 | 0.48 | 117,117,117,117 | 0 |
| 56 | MG | 1A | 4175 | 1/1 | 0.84 | 0.27 | 60,60,60,60 | 0 |
| 56 | MG | 1O | 203 | 1/1 | 0.84 | 0.25 | 87,87,87,87 | 0 |

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| Mol | Type | Chain | Res | Atoms | RSCC | RSR | B-factors(Å$^2$) | Q<0.9 |
|---|---|---|---|---|---|---|---|---|
| 56 | MG | 1A | 4435 | 1/1 | 0.84 | 0.20 | 65,65,65,65 | 0 |
| 56 | MG | 1s | 101 | 1/1 | 0.84 | 1.12 | 216,216,216,216 | 0 |
| 56 | MG | 2A | 3078 | 1/1 | 0.84 | 0.24 | 119,119,119,119 | 0 |
| 56 | MG | 2A | 3082 | 1/1 | 0.84 | 0.30 | 126,126,126,126 | 0 |
| 56 | MG | 1A | 4698 | 1/1 | 0.84 | 0.76 | 70,70,70,70 | 0 |
| 56 | MG | 1a | 1902 | 1/1 | 0.84 | 0.56 | 135,135,135,135 | 0 |
| 56 | MG | 1a | 1903 | 1/1 | 0.84 | 0.47 | 121,121,121,121 | 0 |
| 56 | MG | 2A | 3196 | 1/1 | 0.84 | 0.52 | 92,92,92,92 | 0 |
| 56 | MG | 1A | 4921 | 1/1 | 0.84 | 0.26 | 71,71,71,71 | 0 |
| 56 | MG | 2v | 702 | 1/1 | 0.84 | 0.11 | 183,183,183,183 | 0 |
| 56 | MG | 2B | 209 | 1/1 | 0.84 | 0.45 | 77,77,77,77 | 0 |
| 56 | MG | 2A | 3462 | 1/1 | 0.84 | 0.76 | 104,104,104,104 | 0 |
| 56 | MG | 1A | 4191 | 1/1 | 0.84 | 0.17 | 67,67,67,67 | 0 |
| 56 | MG | 1a | 1754 | 1/1 | 0.84 | 0.29 | 100,100,100,100 | 0 |
| 56 | MG | 2A | 3466 | 1/1 | 0.84 | 0.80 | 129,129,129,129 | 0 |
| 56 | MG | 2A | 3099 | 1/1 | 0.84 | 0.14 | 152,152,152,152 | 0 |
| 56 | MG | 2B | 220 | 1/1 | 0.84 | 0.16 | 140,140,140,140 | 0 |
| 56 | MG | 2A | 3598 | 1/1 | 0.84 | 0.16 | 121,121,121,121 | 0 |
| 56 | MG | 2A | 3605 | 1/1 | 0.84 | 0.19 | 105,105,105,105 | 0 |
| 56 | MG | 2a | 1637 | 1/1 | 0.84 | 0.32 | 146,146,146,146 | 0 |
| 56 | MG | 2A | 3607 | 1/1 | 0.84 | 0.16 | 127,127,127,127 | 0 |
| 56 | MG | 2a | 1900 | 1/1 | 0.84 | 0.42 | 174,174,174,174 | 0 |
| 56 | MG | 2B | 225 | 1/1 | 0.84 | 0.18 | 132,132,132,132 | 0 |
| 56 | MG | 1A | 4314 | 1/1 | 0.84 | 0.46 | 107,107,107,107 | 0 |
| 56 | MG | 2A | 3755 | 1/1 | 0.84 | 0.12 | 130,130,130,130 | 0 |
| 56 | MG | 2A | 3473 | 1/1 | 0.84 | 0.63 | 131,131,131,131 | 0 |
| 56 | MG | 1A | 4300 | 1/1 | 0.84 | 0.49 | 90,90,90,90 | 0 |
| 56 | MG | 2A | 3008 | 1/1 | 0.84 | 0.58 | 94,94,94,94 | 0 |
| 56 | MG | 1A | 4287 | 1/1 | 0.84 | 0.58 | 50,50,50,50 | 0 |
| 56 | MG | 2a | 1879 | 1/1 | 0.85 | 0.53 | 150,150,150,150 | 0 |
| 56 | MG | 2A | 3493 | 1/1 | 0.85 | 0.54 | 134,134,134,134 | 0 |
| 56 | MG | 2a | 1884 | 1/1 | 0.85 | 0.31 | 168,168,168,168 | 0 |
| 56 | MG | 2A | 3044 | 1/1 | 0.85 | 0.37 | 107,107,107,107 | 0 |
| 56 | MG | 2a | 1886 | 1/1 | 0.85 | 0.38 | 147,147,147,147 | 0 |
| 56 | MG | 2A | 3342 | 1/1 | 0.85 | 0.20 | 86,86,86,86 | 0 |
| 56 | MG | 2A | 3183 | 1/1 | 0.85 | 0.47 | 124,124,124,124 | 0 |
| 56 | MG | 1A | 4624 | 1/1 | 0.85 | 0.44 | 118,118,118,118 | 0 |
| 56 | MG | 2a | 1727 | 1/1 | 0.85 | 0.34 | 124,124,124,124 | 0 |
| 56 | MG | 1A | 4053 | 1/1 | 0.85 | 0.85 | 112,112,112,112 | 0 |
| 56 | MG | 1A | 4860 | 1/1 | 0.85 | 0.27 | 59,59,59,59 | 0 |
| 56 | MG | 1a | 1673 | 1/1 | 0.85 | 0.23 | 117,117,117,117 | 0 |
| 56 | MG | 1a | 1839 | 1/1 | 0.85 | 0.18 | 146,146,146,146 | 0 |

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| Mol | Type | Chain | Res | Atoms | RSCC | RSR | B-factors(Å$^2$) | Q<0.9 |
|---|---|---|---|---|---|---|---|---|
| 56 | MG | 2a | 1614 | 1/1 | 0.85 | 0.24 | 165,165,165,165 | 0 |
| 56 | MG | 1B | 204 | 1/1 | 0.85 | 0.43 | 93,93,93,93 | 0 |
| 56 | MG | 2a | 1738 | 1/1 | 0.85 | 0.62 | 138,138,138,138 | 0 |
| 56 | MG | 1A | 4014 | 1/1 | 0.85 | 0.68 | 87,87,87,87 | 0 |
| 56 | MG | 2A | 3201 | 1/1 | 0.85 | 0.38 | 115,115,115,115 | 0 |
| 56 | MG | 2A | 3203 | 1/1 | 0.85 | 0.35 | 124,124,124,124 | 0 |
| 56 | MG | 1A | 4431 | 1/1 | 0.85 | 0.29 | 72,72,72,72 | 0 |
| 56 | MG | 1A | 4867 | 1/1 | 0.85 | 0.28 | 58,58,58,58 | 0 |
| 56 | MG | 1A | 4875 | 1/1 | 0.85 | 0.22 | 71,71,71,71 | 0 |
| 56 | MG | 1B | 220 | 1/1 | 0.85 | 0.27 | 79,79,79,79 | 0 |
| 56 | MG | 1a | 1781 | 1/1 | 0.85 | 0.67 | 110,110,110,110 | 0 |
| 56 | MG | 2a | 1632 | 1/1 | 0.85 | 0.17 | 137,137,137,137 | 0 |
| 56 | MG | 2A | 3086 | 1/1 | 0.85 | 0.32 | 119,119,119,119 | 0 |
| 56 | MG | 1A | 4532 | 1/1 | 0.85 | 0.27 | 45,45,45,45 | 0 |
| 56 | MG | 2B | 212 | 1/1 | 0.85 | 0.47 | 156,156,156,156 | 0 |
| 56 | MG | 1A | 4640 | 1/1 | 0.85 | 0.33 | 69,69,69,69 | 0 |
| 56 | MG | 1A | 4644 | 1/1 | 0.85 | 0.34 | 65,65,65,65 | 0 |
| 56 | MG | 1A | 4798 | 1/1 | 0.85 | 0.35 | 62,62,62,62 | 0 |
| 56 | MG | 2A | 3243 | 1/1 | 0.85 | 0.26 | 109,109,109,109 | 0 |
| 56 | MG | 2A | 3098 | 1/1 | 0.85 | 0.25 | 159,159,159,159 | 0 |
| 56 | MG | 2A | 3565 | 1/1 | 0.85 | 0.28 | 102,102,102,102 | 0 |
| 56 | MG | 2A | 3737 | 1/1 | 0.85 | 0.53 | 100,100,100,100 | 0 |
| 56 | MG | 1A | 4037 | 1/1 | 0.85 | 0.70 | 89,89,89,89 | 0 |
| 56 | MG | 1a | 1627 | 1/1 | 0.85 | 0.38 | 95,95,95,95 | 0 |
| 56 | MG | 2a | 1777 | 1/1 | 0.85 | 0.68 | 117,117,117,117 | 0 |
| 56 | MG | 1A | 4894 | 1/1 | 0.85 | 0.47 | 63,63,63,63 | 0 |
| 56 | MG | 2A | 3743 | 1/1 | 0.85 | 0.43 | 83,83,83,83 | 0 |
| 56 | MG | 2a | 1781 | 1/1 | 0.85 | 0.23 | 230,230,230,230 | 0 |
| 56 | MG | 1a | 1630 | 1/1 | 0.85 | 0.84 | 108,108,108,108 | 0 |
| 56 | MG | 1A | 4804 | 1/1 | 0.85 | 1.06 | 89,89,89,89 | 0 |
| 56 | MG | 1A | 4298 | 1/1 | 0.85 | 0.51 | 76,76,76,76 | 0 |
| 56 | MG | 2D | 302 | 1/1 | 0.85 | 0.31 | 80,80,80,80 | 0 |
| 56 | MG | 1a | 1872 | 1/1 | 0.85 | 0.10 | 195,195,195,195 | 0 |
| 56 | MG | 2A | 3262 | 1/1 | 0.85 | 0.73 | 73,73,73,73 | 0 |
| 56 | MG | 2A | 3115 | 1/1 | 0.85 | 0.56 | 135,135,135,135 | 0 |
| 56 | MG | 2A | 3430 | 1/1 | 0.85 | 0.62 | 73,73,73,73 | 0 |
| 56 | MG | 1a | 1804 | 1/1 | 0.85 | 0.41 | 130,130,130,130 | 0 |
| 56 | MG | 2A | 3759 | 1/1 | 0.85 | 0.42 | 232,232,232,232 | 0 |
| 56 | MG | 2a | 1797 | 1/1 | 0.85 | 0.17 | 238,238,238,238 | 0 |
| 56 | MG | 1A | 4707 | 1/1 | 0.85 | 0.31 | 73,73,73,73 | 0 |
| 56 | MG | 1a | 1890 | 1/1 | 0.85 | 0.16 | 218,218,218,218 | 0 |
| 56 | MG | 1a | 1893 | 1/1 | 0.85 | 0.30 | 98,98,98,98 | 0 |

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| Mol | Type | Chain | Res | Atoms | RSCC | RSR | B-factors(Å$^2$) | Q<0.9 |
|---|---|---|---|---|---|---|---|---|
| 56 | MG | 1A | 5027 | 1/1 | 0.85 | 0.75 | 63,63,63,63 | 0 |
| 56 | MG | 1a | 1644 | 1/1 | 0.85 | 0.71 | 120,120,120,120 | 0 |
| 56 | MG | 1A | 4184 | 1/1 | 0.85 | 0.45 | 61,61,61,61 | 0 |
| 56 | MG | 1A | 4818 | 1/1 | 0.85 | 0.32 | 69,69,69,69 | 0 |
| 56 | MG | 2A | 3777 | 1/1 | 0.85 | 0.45 | 100,100,100,100 | 0 |
| 56 | MG | 1A | 4711 | 1/1 | 0.85 | 0.27 | 78,78,78,78 | 0 |
| 56 | MG | 1a | 1737 | 1/1 | 0.85 | 0.59 | 74,74,74,74 | 0 |
| 56 | MG | 2a | 1693 | 1/1 | 0.85 | 0.28 | 141,141,141,141 | 0 |
| 56 | MG | 1A | 4461 | 1/1 | 0.85 | 0.26 | 78,78,78,78 | 0 |
| 56 | MG | 2A | 3154 | 1/1 | 0.85 | 0.93 | 92,92,92,92 | 0 |
| 56 | MG | 2A | 3791 | 1/1 | 0.85 | 0.36 | 93,93,93,93 | 0 |
| 56 | MG | 1a | 1654 | 1/1 | 0.85 | 0.52 | 120,120,120,120 | 0 |
| 56 | MG | 2a | 1847 | 1/1 | 0.85 | 0.26 | 160,160,160,160 | 0 |
| 56 | MG | 1A | 4932 | 1/1 | 0.85 | 0.30 | 153,153,153,153 | 0 |
| 56 | MG | 1A | 4832 | 1/1 | 0.85 | 0.68 | 71,71,71,71 | 0 |
| 56 | MG | 2a | 1705 | 1/1 | 0.85 | 0.38 | 150,150,150,150 | 0 |
| 56 | MG | 1a | 1747 | 1/1 | 0.85 | 0.34 | 149,149,149,149 | 0 |
| 56 | MG | 1A | 4274 | 1/1 | 0.85 | 0.68 | 51,51,51,51 | 0 |
| 56 | MG | 1A | 4356 | 1/1 | 0.85 | 0.33 | 75,75,75,75 | 0 |
| 56 | MG | 2A | 3633 | 1/1 | 0.85 | 0.28 | 110,110,110,110 | 0 |
| 56 | MG | 1A | 5058 | 1/1 | 0.85 | 0.49 | 100,100,100,100 | 0 |
| 56 | MG | 28 | 106 | 1/1 | 0.85 | 0.24 | 79,79,79,79 | 0 |
| 57 | ZN | 1n | 103 | 1/1 | 0.85 | 0.09 | 212,212,212,212 | 0 |
| 56 | MG | 2a | 1877 | 1/1 | 0.85 | 0.33 | 151,151,151,151 | 0 |
| 56 | MG | 2a | 1878 | 1/1 | 0.85 | 0.55 | 115,115,115,115 | 0 |
| 57 | ZN | 2n | 501 | 1/1 | 0.85 | 0.11 | 239,239,239,239 | 0 |
| 56 | MG | 2A | 3634 | 1/1 | 0.86 | 0.34 | 104,104,104,104 | 0 |
| 56 | MG | 2P | 201 | 1/1 | 0.86 | 0.37 | 100,100,100,100 | 0 |
| 56 | MG | 1A | 4444 | 1/1 | 0.86 | 0.27 | 76,76,76,76 | 0 |
| 56 | MG | 2A | 3519 | 1/1 | 0.86 | 0.20 | 91,91,91,91 | 0 |
| 56 | MG | 1Q | 202 | 1/1 | 0.86 | 0.11 | 67,67,67,67 | 0 |
| 56 | MG | 1A | 4908 | 1/1 | 0.86 | 0.23 | 64,64,64,64 | 0 |
| 56 | MG | 2A | 3113 | 1/1 | 0.86 | 0.69 | 140,140,140,140 | 0 |
| 56 | MG | 1A | 4915 | 1/1 | 0.86 | 0.28 | 85,85,85,85 | 0 |
| 56 | MG | 1A | 4226 | 1/1 | 0.86 | 0.40 | 81,81,81,81 | 0 |
| 56 | MG | 2A | 3646 | 1/1 | 0.86 | 0.51 | 110,110,110,110 | 0 |
| 56 | MG | 1A | 4316 | 1/1 | 0.86 | 0.63 | 85,85,85,85 | 0 |
| 56 | MG | 2A | 3017 | 1/1 | 0.86 | 0.29 | 111,111,111,111 | 0 |
| 56 | MG | 2A | 3251 | 1/1 | 0.86 | 0.18 | 123,123,123,123 | 0 |
| 56 | MG | 1A | 5044 | 1/1 | 0.86 | 0.83 | 52,52,52,52 | 0 |
| 56 | MG | 1a | 1824 | 1/1 | 0.86 | 0.30 | 213,213,213,213 | 0 |
| 56 | MG | 2A | 3541 | 1/1 | 0.86 | 0.64 | 123,123,123,123 | 0 |

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| Mol | Type | Chain | Res | Atoms | RSCC | RSR | B-factors(Å$^2$) | Q<0.9 |
|---|---|---|---|---|---|---|---|---|
| 56 | MG | 1a | 1826 | 1/1 | 0.86 | 0.13 | 196,196,196,196 | 0 |
| 56 | MG | 1A | 4548 | 1/1 | 0.86 | 0.82 | 131,131,131,131 | 0 |
| 56 | MG | 1A | 4144 | 1/1 | 0.86 | 0.38 | 65,65,65,65 | 0 |
| 56 | MG | 1A | 4051 | 1/1 | 0.86 | 0.80 | 100,100,100,100 | 0 |
| 56 | MG | 2A | 3683 | 1/1 | 0.86 | 0.28 | 102,102,102,102 | 0 |
| 56 | MG | 1a | 1758 | 1/1 | 0.86 | 0.14 | 111,111,111,111 | 0 |
| 56 | MG | 2A | 3690 | 1/1 | 0.86 | 0.16 | 159,159,159,159 | 0 |
| 56 | MG | 2A | 3270 | 1/1 | 0.86 | 0.48 | 98,98,98,98 | 0 |
| 56 | MG | 29 | 102 | 1/1 | 0.86 | 0.27 | 128,128,128,128 | 0 |
| 56 | MG | 1A | 4841 | 1/1 | 0.86 | 0.48 | 103,103,103,103 | 0 |
| 56 | MG | 1A | 4638 | 1/1 | 0.86 | 0.32 | 66,66,66,66 | 0 |
| 56 | MG | 1A | 4551 | 1/1 | 0.86 | 0.40 | 69,69,69,69 | 0 |
| 56 | MG | 1A | 4425 | 1/1 | 0.86 | 0.14 | 78,78,78,78 | 0 |
| 56 | MG | 1A | 4490 | 1/1 | 0.86 | 0.34 | 89,89,89,89 | 0 |
| 56 | MG | 1A | 4581 | 1/1 | 0.86 | 0.29 | 61,61,61,61 | 0 |
| 56 | MG | 1A | 4778 | 1/1 | 0.86 | 0.19 | 71,71,71,71 | 0 |
| 56 | MG | 2a | 1822 | 1/1 | 0.86 | 0.27 | 167,167,167,167 | 0 |
| 56 | MG | 1A | 4650 | 1/1 | 0.86 | 0.42 | 63,63,63,63 | 0 |
| 56 | MG | 1A | 4659 | 1/1 | 0.86 | 0.39 | 87,87,87,87 | 0 |
| 56 | MG | 1b | 306 | 1/1 | 0.86 | 0.16 | 186,186,186,186 | 0 |
| 56 | MG | 1B | 211 | 1/1 | 0.86 | 0.64 | 82,82,82,82 | 0 |
| 56 | MG | 2a | 1839 | 1/1 | 0.86 | 0.08 | 241,241,241,241 | 0 |
| 56 | MG | 2B | 214 | 1/1 | 0.86 | 0.25 | 145,145,145,145 | 0 |
| 56 | MG | 1A | 4492 | 1/1 | 0.86 | 0.30 | 69,69,69,69 | 0 |
| 56 | MG | 1A | 4882 | 1/1 | 0.86 | 0.35 | 82,82,82,82 | 0 |
| 56 | MG | 1a | 1783 | 1/1 | 0.86 | 0.25 | 135,135,135,135 | 0 |
| 56 | MG | 1A | 4214 | 1/1 | 0.86 | 0.29 | 61,61,61,61 | 0 |
| 56 | MG | 2a | 1731 | 1/1 | 0.86 | 0.36 | 103,103,103,103 | 0 |
| 56 | MG | 1A | 4602 | 1/1 | 0.86 | 0.29 | 54,54,54,54 | 0 |
| 56 | MG | 1A | 4526 | 1/1 | 0.86 | 0.32 | 54,54,54,54 | 0 |
| 56 | MG | 1m | 202 | 1/1 | 0.86 | 0.07 | 211,211,211,211 | 0 |
| 56 | MG | 1A | 4993 | 1/1 | 0.86 | 0.17 | 85,85,85,85 | 0 |
| 56 | MG | 1A | 4890 | 1/1 | 0.86 | 0.60 | 114,114,114,114 | 0 |
| 56 | MG | 1E | 303 | 1/1 | 0.86 | 0.61 | 62,62,62,62 | 0 |
| 56 | MG | 2a | 1741 | 1/1 | 0.86 | 0.60 | 174,174,174,174 | 0 |
| 56 | MG | 1F | 301 | 1/1 | 0.86 | 0.35 | 76,76,76,76 | 0 |
| 56 | MG | 1A | 4531 | 1/1 | 0.86 | 0.34 | 68,68,68,68 | 0 |
| 56 | MG | 2a | 1643 | 1/1 | 0.86 | 0.20 | 144,144,144,144 | 0 |
| 56 | MG | 2A | 3355 | 1/1 | 0.86 | 0.26 | 89,89,89,89 | 0 |
| 56 | MG | 2A | 3207 | 1/1 | 0.86 | 0.32 | 123,123,123,123 | 0 |
| 56 | MG | 2D | 306 | 1/1 | 0.86 | 1.03 | 101,101,101,101 | 0 |
| 56 | MG | 1a | 1712 | 1/1 | 0.86 | 0.49 | 114,114,114,114 | 0 |

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| Mol | Type | Chain | Res | Atoms | RSCC | RSR | B-factors(Å$^2$) | Q<0.9 |
|---|---|---|---|---|---|---|---|---|
| 56 | MG | 2a | 1653 | 1/1 | 0.86 | 0.36 | 141,141,141,141 | 0 |
| 56 | MG | 1A | 4170 | 1/1 | 0.86 | 0.52 | 61,61,61,61 | 0 |
| 56 | MG | 1A | 4311 | 1/1 | 0.86 | 0.59 | 101,101,101,101 | 0 |
| 56 | MG | 2z | 101 | 1/1 | 0.86 | 0.33 | 177,177,177,177 | 0 |
| 56 | MG | 2A | 3382 | 1/1 | 0.86 | 0.30 | 101,101,101,101 | 0 |
| 56 | MG | 2a | 1762 | 1/1 | 0.86 | 0.14 | 235,235,235,235 | 0 |
| 56 | MG | 1A | 5015 | 1/1 | 0.86 | 0.52 | 89,89,89,89 | 0 |
| 56 | MG | 2a | 1764 | 1/1 | 0.86 | 0.33 | 270,270,270,270 | 0 |
| 56 | MG | 1A | 4899 | 1/1 | 0.86 | 0.39 | 68,68,68,68 | 0 |
| 56 | MG | 2a | 1907 | 1/1 | 0.86 | 0.23 | 256,256,256,256 | 0 |
| 56 | MG | 1A | 4417 | 1/1 | 0.87 | 0.36 | 52,52,52,52 | 0 |
| 56 | MG | 1a | 1692 | 1/1 | 0.87 | 0.24 | 129,129,129,129 | 0 |
| 56 | MG | 2a | 1665 | 1/1 | 0.87 | 0.24 | 139,139,139,139 | 0 |
| 56 | MG | 1b | 307 | 1/1 | 0.87 | 0.06 | 164,164,164,164 | 0 |
| 56 | MG | 1O | 201 | 1/1 | 0.87 | 0.48 | 82,82,82,82 | 0 |
| 56 | MG | 2A | 3185 | 1/1 | 0.87 | 0.45 | 95,95,95,95 | 0 |
| 56 | MG | 2A | 3332 | 1/1 | 0.87 | 0.28 | 97,97,97,97 | 0 |
| 56 | MG | 1A | 4136 | 1/1 | 0.87 | 0.66 | 92,92,92,92 | 0 |
| 56 | MG | 1A | 4779 | 1/1 | 0.87 | 0.23 | 68,68,68,68 | 0 |
| 56 | MG | 2Q | 204 | 1/1 | 0.87 | 0.54 | 118,118,118,118 | 0 |
| 56 | MG | 1A | 4119 | 1/1 | 0.87 | 0.41 | 74,74,74,74 | 0 |
| 56 | MG | 1A | 5042 | 1/1 | 0.87 | 0.23 | 77,77,77,77 | 0 |
| 56 | MG | 1a | 1795 | 1/1 | 0.87 | 0.47 | 107,107,107,107 | 0 |
| 56 | MG | 1A | 4636 | 1/1 | 0.87 | 0.35 | 64,64,64,64 | 0 |
| 56 | MG | 1a | 1641 | 1/1 | 0.87 | 0.22 | 124,124,124,124 | 0 |
| 56 | MG | 2A | 3492 | 1/1 | 0.87 | 0.35 | 120,120,120,120 | 0 |
| 56 | MG | 1A | 4866 | 1/1 | 0.87 | 0.34 | 69,69,69,69 | 0 |
| 56 | MG | 1a | 1723 | 1/1 | 0.87 | 0.45 | 118,118,118,118 | 0 |
| 56 | MG | 1A | 4003 | 1/1 | 0.87 | 0.50 | 53,53,53,53 | 0 |
| 56 | MG | 1A | 4390 | 1/1 | 0.87 | 0.31 | 82,82,82,82 | 0 |
| 56 | MG | 2a | 1793 | 1/1 | 0.87 | 0.20 | 251,251,251,251 | 0 |
| 56 | MG | 1A | 4956 | 1/1 | 0.87 | 0.25 | 71,71,71,71 | 0 |
| 56 | MG | 1a | 1647 | 1/1 | 0.87 | 0.73 | 118,118,118,118 | 0 |
| 56 | MG | 2A | 3373 | 1/1 | 0.87 | 0.39 | 93,93,93,93 | 0 |
| 56 | MG | 1A | 4743 | 1/1 | 0.87 | 0.16 | 74,74,74,74 | 0 |
| 56 | MG | 2A | 3100 | 1/1 | 0.87 | 0.22 | 152,152,152,152 | 0 |
| 56 | MG | 1A | 4799 | 1/1 | 0.87 | 0.47 | 87,87,87,87 | 0 |
| 56 | MG | 2A | 3523 | 1/1 | 0.87 | 0.28 | 100,100,100,100 | 0 |
| 56 | MG | 2A | 3524 | 1/1 | 0.87 | 0.32 | 103,103,103,103 | 0 |
| 56 | MG | 2A | 3526 | 1/1 | 0.87 | 0.09 | 106,106,106,106 | 0 |
| 56 | MG | 1A | 4436 | 1/1 | 0.87 | 0.25 | 64,64,64,64 | 0 |
| 56 | MG | 2l | 203 | 1/1 | 0.87 | 0.56 | 129,129,129,129 | 0 |

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| Mol | Type | Chain | Res | Atoms | RSCC | RSR | B-factors(Å$^2$) | Q<0.9 |
|---|---|---|---|---|---|---|---|---|
| 56 | MG | 1A | 4032 | 1/1 | 0.87 | 0.25 | 55,55,55,55 | 0 |
| 56 | MG | 2A | 3233 | 1/1 | 0.87 | 0.31 | 101,101,101,101 | 0 |
| 56 | MG | 2A | 3666 | 1/1 | 0.87 | 0.37 | 101,101,101,101 | 0 |
| 56 | MG | 1a | 1894 | 1/1 | 0.87 | 0.72 | 132,132,132,132 | 0 |
| 56 | MG | 2A | 3109 | 1/1 | 0.87 | 0.23 | 137,137,137,137 | 0 |
| 56 | MG | 1y | 104 | 1/1 | 0.87 | 0.31 | 99,99,99,99 | 0 |
| 56 | MG | 1W | 201 | 1/1 | 0.87 | 0.30 | 72,72,72,72 | 0 |
| 56 | MG | 1A | 4155 | 1/1 | 0.87 | 0.37 | 60,60,60,60 | 0 |
| 56 | MG | 1A | 4024 | 1/1 | 0.87 | 0.46 | 78,78,78,78 | 0 |
| 56 | MG | 2A | 3010 | 1/1 | 0.87 | 1.10 | 88,88,88,88 | 0 |
| 56 | MG | 2A | 3545 | 1/1 | 0.87 | 0.23 | 97,97,97,97 | 0 |
| 56 | MG | 1A | 4986 | 1/1 | 0.87 | 0.77 | 64,64,64,64 | 0 |
| 56 | MG | 1A | 4759 | 1/1 | 0.87 | 0.38 | 74,74,74,74 | 0 |
| 56 | MG | 2A | 3549 | 1/1 | 0.87 | 0.50 | 96,96,96,96 | 0 |
| 56 | MG | 1A | 4655 | 1/1 | 0.87 | 0.54 | 82,82,82,82 | 0 |
| 56 | MG | 1a | 1757 | 1/1 | 0.87 | 0.61 | 107,107,107,107 | 0 |
| 56 | MG | 2a | 1866 | 1/1 | 0.87 | 0.26 | 138,138,138,138 | 0 |
| 56 | MG | 1a | 1905 | 1/1 | 0.87 | 0.75 | 108,108,108,108 | 0 |
| 56 | MG | 1A | 4656 | 1/1 | 0.87 | 0.42 | 80,80,80,80 | 0 |
| 56 | MG | 1A | 4455 | 1/1 | 0.87 | 0.27 | 75,75,75,75 | 0 |
| 56 | MG | 2A | 3417 | 1/1 | 0.87 | 0.22 | 117,117,117,117 | 0 |
| 56 | MG | 1B | 219 | 1/1 | 0.87 | 0.15 | 77,77,77,77 | 0 |
| 56 | MG | 1A | 4824 | 1/1 | 0.87 | 0.21 | 81,81,81,81 | 0 |
| 56 | MG | 1B | 221 | 1/1 | 0.87 | 0.57 | 98,98,98,98 | 0 |
| 56 | MG | 1A | 4459 | 1/1 | 0.87 | 0.17 | 72,72,72,72 | 0 |
| 56 | MG | 2a | 1883 | 1/1 | 0.87 | 0.41 | 131,131,131,131 | 0 |
| 56 | MG | 2a | 1752 | 1/1 | 0.87 | 0.25 | 134,134,134,134 | 0 |
| 56 | MG | 1A | 4101 | 1/1 | 0.87 | 0.53 | 45,45,45,45 | 0 |
| 56 | MG | 1A | 4671 | 1/1 | 0.87 | 0.47 | 65,65,65,65 | 0 |
| 56 | MG | 2A | 3287 | 1/1 | 0.87 | 0.73 | 104,104,104,104 | 0 |
| 56 | MG | 2A | 3432 | 1/1 | 0.87 | 0.67 | 93,93,93,93 | 0 |
| 56 | MG | 1A | 4357 | 1/1 | 0.87 | 0.37 | 78,78,78,78 | 0 |
| 56 | MG | 2A | 3584 | 1/1 | 0.87 | 0.12 | 114,114,114,114 | 0 |
| 56 | MG | 1A | 4850 | 1/1 | 0.87 | 0.37 | 76,76,76,76 | 0 |
| 57 | ZN | 14 | 501 | 1/1 | 0.87 | 0.07 | 172,172,172,172 | 0 |
| 56 | MG | 2A | 3169 | 1/1 | 0.87 | 0.65 | 81,81,81,81 | 0 |
| 56 | MG | 1a | 1842 | 1/1 | 0.87 | 0.11 | 78,78,78,78 | 0 |
| 56 | MG | 2E | 305 | 1/1 | 0.87 | 0.14 | 121,121,121,121 | 0 |
| 56 | MG | 1E | 305 | 1/1 | 0.87 | 0.91 | 69,69,69,69 | 0 |
| 59 | GDP | 2v | 704 | 28/28 | 0.87 | 0.19 | 186,186,186,186 | 0 |
| 56 | MG | 2A | 3715 | 1/1 | 0.88 | 0.22 | 109,109,109,109 | 0 |
| 56 | MG | 1A | 4336 | 1/1 | 0.88 | 0.23 | 62,62,62,62 | 0 |

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| Mol | Type | Chain | Res | Atoms | RSCC | RSR | B-factors(Å$^2$) | Q<0.9 |
|---|---|---|---|---|---|---|---|---|
| 56 | MG | 1A | 4929 | 1/1 | 0.88 | 0.44 | 201,201,201,201 | 0 |
| 56 | MG | 1A | 4243 | 1/1 | 0.88 | 0.55 | 65,65,65,65 | 0 |
| 56 | MG | 1A | 4676 | 1/1 | 0.88 | 0.76 | 101,101,101,101 | 0 |
| 56 | MG | 2a | 1875 | 1/1 | 0.88 | 0.64 | 154,154,154,154 | 0 |
| 56 | MG | 1A | 4603 | 1/1 | 0.88 | 0.34 | 67,67,67,67 | 0 |
| 56 | MG | 1a | 1604 | 1/1 | 0.88 | 0.24 | 98,98,98,98 | 0 |
| 56 | MG | 1A | 4753 | 1/1 | 0.88 | 0.26 | 62,62,62,62 | 0 |
| 56 | MG | 1a | 1607 | 1/1 | 0.88 | 0.33 | 86,86,86,86 | 0 |
| 56 | MG | 1a | 1609 | 1/1 | 0.88 | 0.19 | 88,88,88,88 | 0 |
| 56 | MG | 2Q | 205 | 1/1 | 0.88 | 1.05 | 129,129,129,129 | 0 |
| 56 | MG | 2A | 3362 | 1/1 | 0.88 | 0.12 | 99,99,99,99 | 0 |
| 56 | MG | 2A | 3364 | 1/1 | 0.88 | 0.39 | 84,84,84,84 | 0 |
| 56 | MG | 1A | 4257 | 1/1 | 0.88 | 0.45 | 64,64,64,64 | 0 |
| 56 | MG | 2A | 3371 | 1/1 | 0.88 | 0.18 | 113,113,113,113 | 0 |
| 56 | MG | 2a | 1889 | 1/1 | 0.88 | 0.97 | 127,127,127,127 | 0 |
| 56 | MG | 2a | 1892 | 1/1 | 0.88 | 0.74 | 142,142,142,142 | 0 |
| 56 | MG | 2A | 3035 | 1/1 | 0.88 | 0.45 | 116,116,116,116 | 0 |
| 56 | MG | 1A | 4679 | 1/1 | 0.88 | 0.15 | 80,80,80,80 | 0 |
| 56 | MG | 2A | 3376 | 1/1 | 0.88 | 0.27 | 99,99,99,99 | 0 |
| 56 | MG | 1A | 4761 | 1/1 | 0.88 | 0.28 | 74,74,74,74 | 0 |
| 56 | MG | 2a | 1726 | 1/1 | 0.88 | 0.46 | 108,108,108,108 | 0 |
| 56 | MG | 2a | 1902 | 1/1 | 0.88 | 0.54 | 248,248,248,248 | 0 |
| 56 | MG | 2a | 1903 | 1/1 | 0.88 | 0.67 | 246,246,246,246 | 0 |
| 56 | MG | 2A | 3051 | 1/1 | 0.88 | 1.54 | 104,104,104,104 | 0 |
| 56 | MG | 1a | 1817 | 1/1 | 0.88 | 0.22 | 148,148,148,148 | 0 |
| 56 | MG | 1A | 4605 | 1/1 | 0.88 | 0.29 | 64,64,64,64 | 0 |
| 56 | MG | 2A | 3197 | 1/1 | 0.88 | 0.18 | 93,93,93,93 | 0 |
| 56 | MG | 1A | 4682 | 1/1 | 0.88 | 0.99 | 116,116,116,116 | 0 |
| 56 | MG | 2A | 3064 | 1/1 | 0.88 | 0.36 | 75,75,75,75 | 0 |
| 56 | MG | 1A | 4045 | 1/1 | 0.88 | 0.35 | 68,68,68,68 | 0 |
| 56 | MG | 2A | 3769 | 1/1 | 0.88 | 0.59 | 90,90,90,90 | 0 |
| 56 | MG | 1A | 4085 | 1/1 | 0.88 | 0.30 | 67,67,67,67 | 0 |
| 56 | MG | 1A | 4863 | 1/1 | 0.88 | 0.35 | 62,62,62,62 | 0 |
| 56 | MG | 2A | 3776 | 1/1 | 0.88 | 0.41 | 97,97,97,97 | 0 |
| 56 | MG | 1D | 302 | 1/1 | 0.88 | 0.34 | 57,57,57,57 | 0 |
| 56 | MG | 1a | 1631 | 1/1 | 0.88 | 0.35 | 126,126,126,126 | 0 |
| 56 | MG | 2a | 1603 | 1/1 | 0.88 | 0.22 | 151,151,151,151 | 0 |
| 56 | MG | 1a | 1919 | 1/1 | 0.88 | 0.52 | 144,144,144,144 | 0 |
| 56 | MG | 2A | 3401 | 1/1 | 0.88 | 0.12 | 89,89,89,89 | 0 |
| 56 | MG | 2f | 303 | 1/1 | 0.88 | 0.35 | 135,135,135,135 | 0 |
| 56 | MG | 1A | 4086 | 1/1 | 0.88 | 0.37 | 68,68,68,68 | 0 |
| 56 | MG | 2a | 1755 | 1/1 | 0.88 | 0.10 | 168,168,168,168 | 0 |

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| Mol | Type | Chain | Res | Atoms | RSCC | RSR | B-factors(Å$^2$) | Q<0.9 |
|---|---|---|---|---|---|---|---|---|
| 56 | MG | 1A | 4371 | 1/1 | 0.88 | 0.29 | 74,74,74,74 | 0 |
| 56 | MG | 2A | 3220 | 1/1 | 0.88 | 0.27 | 115,115,115,115 | 0 |
| 56 | MG | 2A | 3794 | 1/1 | 0.88 | 0.25 | 113,113,113,113 | 0 |
| 56 | MG | 1A | 4874 | 1/1 | 0.88 | 0.67 | 87,87,87,87 | 0 |
| 56 | MG | 1A | 4199 | 1/1 | 0.88 | 0.22 | 218,218,218,218 | 0 |
| 56 | MG | 2a | 1615 | 1/1 | 0.88 | 0.30 | 145,145,145,145 | 0 |
| 56 | MG | 1A | 4200 | 1/1 | 0.88 | 0.23 | 69,69,69,69 | 0 |
| 56 | MG | 2A | 3232 | 1/1 | 0.88 | 0.36 | 95,95,95,95 | 0 |
| 56 | MG | 2A | 3090 | 1/1 | 0.88 | 0.20 | 110,110,110,110 | 0 |
| 56 | MG | 1A | 4375 | 1/1 | 0.88 | 0.31 | 65,65,65,65 | 0 |
| 56 | MG | 1A | 5004 | 1/1 | 0.88 | 0.37 | 89,89,89,89 | 0 |
| 56 | MG | 2A | 3096 | 1/1 | 0.88 | 0.36 | 98,98,98,98 | 0 |
| 56 | MG | 1A | 4386 | 1/1 | 0.88 | 0.15 | 64,64,64,64 | 0 |
| 56 | MG | 1A | 4887 | 1/1 | 0.88 | 0.31 | 67,67,67,67 | 0 |
| 56 | MG | 2A | 3247 | 1/1 | 0.88 | 0.44 | 113,113,113,113 | 0 |
| 56 | MG | 2a | 1630 | 1/1 | 0.88 | 0.66 | 123,123,123,123 | 0 |
| 56 | MG | 1A | 4034 | 1/1 | 0.88 | 0.63 | 69,69,69,69 | 0 |
| 56 | MG | 1A | 4783 | 1/1 | 0.88 | 0.47 | 70,70,70,70 | 0 |
| 56 | MG | 2l | 205 | 1/1 | 0.88 | 0.27 | 148,148,148,148 | 0 |
| 56 | MG | 2A | 3250 | 1/1 | 0.88 | 0.59 | 158,158,158,158 | 0 |
| 56 | MG | 1a | 1760 | 1/1 | 0.88 | 0.23 | 114,114,114,114 | 0 |
| 56 | MG | 2A | 3102 | 1/1 | 0.88 | 0.24 | 144,144,144,144 | 0 |
| 56 | MG | 1A | 4393 | 1/1 | 0.88 | 0.33 | 84,84,84,84 | 0 |
| 56 | MG | 1A | 4151 | 1/1 | 0.88 | 0.32 | 60,60,60,60 | 0 |
| 56 | MG | 2p | 101 | 1/1 | 0.88 | 0.12 | 154,154,154,154 | 0 |
| 56 | MG | 1a | 1657 | 1/1 | 0.88 | 0.24 | 106,106,106,106 | 0 |
| 56 | MG | 1A | 4320 | 1/1 | 0.88 | 0.80 | 91,91,91,91 | 0 |
| 56 | MG | 1a | 1661 | 1/1 | 0.88 | 0.22 | 117,117,117,117 | 0 |
| 56 | MG | 1A | 4129 | 1/1 | 0.88 | 0.17 | 58,58,58,58 | 0 |
| 56 | MG | 1A | 4642 | 1/1 | 0.88 | 0.30 | 67,67,67,67 | 0 |
| 56 | MG | 2A | 3468 | 1/1 | 0.88 | 0.59 | 85,85,85,85 | 0 |
| 56 | MG | 1A | 4221 | 1/1 | 0.88 | 0.63 | 71,71,71,71 | 0 |
| 56 | MG | 1a | 1858 | 1/1 | 0.88 | 0.09 | 210,210,210,210 | 0 |
| 56 | MG | 2A | 3119 | 1/1 | 0.88 | 0.68 | 113,113,113,113 | 0 |
| 56 | MG | 2A | 3120 | 1/1 | 0.88 | 0.62 | 120,120,120,120 | 0 |
| 56 | MG | 2A | 3285 | 1/1 | 0.88 | 0.25 | 101,101,101,101 | 0 |
| 56 | MG | 1T | 201 | 1/1 | 0.88 | 0.34 | 66,66,66,66 | 0 |
| 56 | MG | 2A | 3658 | 1/1 | 0.88 | 0.66 | 112,112,112,112 | 0 |
| 56 | MG | 2A | 3289 | 1/1 | 0.88 | 0.25 | 107,107,107,107 | 0 |
| 56 | MG | 1A | 5041 | 1/1 | 0.88 | 0.26 | 79,79,79,79 | 0 |
| 56 | MG | 2A | 3132 | 1/1 | 0.88 | 0.28 | 141,141,141,141 | 0 |
| 56 | MG | 1A | 4905 | 1/1 | 0.88 | 0.26 | 65,65,65,65 | 0 |

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| Mol | Type | Chain | Res | Atoms | RSCC | RSR | B-factors(Å$^2$) | Q<0.9 |
|---|---|---|---|---|---|---|---|---|
| 56 | MG | 1A | 4559 | 1/1 | 0.88 | 0.40 | 60,60,60,60 | 0 |
| 56 | MG | 1A | 5047 | 1/1 | 0.88 | 0.32 | 89,89,89,89 | 0 |
| 56 | MG | 1A | 4039 | 1/1 | 0.88 | 0.16 | 79,79,79,79 | 0 |
| 56 | MG | 2A | 3308 | 1/1 | 0.88 | 0.76 | 100,100,100,100 | 0 |
| 56 | MG | 1A | 4507 | 1/1 | 0.88 | 0.30 | 106,106,106,106 | 0 |
| 56 | MG | 2B | 228 | 1/1 | 0.88 | 0.17 | 145,145,145,145 | 0 |
| 56 | MG | 2a | 1837 | 1/1 | 0.88 | 0.10 | 240,240,240,240 | 0 |
| 56 | MG | 1a | 1791 | 1/1 | 0.88 | 0.25 | 116,116,116,116 | 0 |
| 56 | MG | 1A | 4228 | 1/1 | 0.88 | 0.52 | 109,109,109,109 | 0 |
| 56 | MG | 2a | 1840 | 1/1 | 0.88 | 0.09 | 228,228,228,228 | 0 |
| 56 | MG | 2a | 1681 | 1/1 | 0.88 | 0.36 | 165,165,165,165 | 0 |
| 56 | MG | 1A | 4190 | 1/1 | 0.88 | 0.29 | 68,68,68,68 | 0 |
| 56 | MG | 2A | 3693 | 1/1 | 0.88 | 0.46 | 86,86,86,86 | 0 |
| 56 | MG | 2A | 3153 | 1/1 | 0.88 | 0.69 | 80,80,80,80 | 0 |
| 56 | MG | 2A | 3699 | 1/1 | 0.88 | 0.43 | 107,107,107,107 | 0 |
| 56 | MG | 1A | 4587 | 1/1 | 0.88 | 0.33 | 72,72,72,72 | 0 |
| 56 | MG | 1a | 1891 | 1/1 | 0.88 | 0.21 | 89,89,89,89 | 0 |
| 56 | MG | 1a | 1871 | 1/1 | 0.89 | 0.10 | 199,199,199,199 | 0 |
| 56 | MG | 2A | 3339 | 1/1 | 0.89 | 0.55 | 72,72,72,72 | 0 |
| 56 | MG | 2A | 3697 | 1/1 | 0.89 | 0.70 | 128,128,128,128 | 0 |
| 56 | MG | 2a | 1862 | 1/1 | 0.89 | 0.77 | 155,155,155,155 | 0 |
| 56 | MG | 2A | 3698 | 1/1 | 0.89 | 0.34 | 108,108,108,108 | 0 |
| 56 | MG | 1E | 308 | 1/1 | 0.89 | 0.50 | 68,68,68,68 | 0 |
| 56 | MG | 2E | 304 | 1/1 | 0.89 | 0.34 | 71,71,71,71 | 0 |
| 56 | MG | 2A | 3704 | 1/1 | 0.89 | 0.28 | 95,95,95,95 | 0 |
| 56 | MG | 1A | 4445 | 1/1 | 0.89 | 0.16 | 73,73,73,73 | 0 |
| 56 | MG | 1A | 4447 | 1/1 | 0.89 | 0.24 | 65,65,65,65 | 0 |
| 56 | MG | 1A | 4450 | 1/1 | 0.89 | 0.16 | 75,75,75,75 | 0 |
| 56 | MG | 1A | 4999 | 1/1 | 0.89 | 0.79 | 62,62,62,62 | 0 |
| 56 | MG | 2A | 3718 | 1/1 | 0.89 | 0.54 | 129,129,129,129 | 0 |
| 56 | MG | 2A | 3032 | 1/1 | 0.89 | 0.79 | 108,108,108,108 | 0 |
| 56 | MG | 2A | 3720 | 1/1 | 0.89 | 0.10 | 122,122,122,122 | 0 |
| 56 | MG | 1A | 5002 | 1/1 | 0.89 | 0.81 | 61,61,61,61 | 0 |
| 56 | MG | 1P | 201 | 1/1 | 0.89 | 0.46 | 53,53,53,53 | 0 |
| 56 | MG | 1A | 4383 | 1/1 | 0.89 | 0.26 | 65,65,65,65 | 0 |
| 56 | MG | 1A | 4186 | 1/1 | 0.89 | 0.47 | 59,59,59,59 | 0 |
| 56 | MG | 2a | 1888 | 1/1 | 0.89 | 0.32 | 136,136,136,136 | 0 |
| 56 | MG | 1a | 1788 | 1/1 | 0.89 | 1.09 | 118,118,118,118 | 0 |
| 56 | MG | 2A | 3369 | 1/1 | 0.89 | 0.14 | 84,84,84,84 | 0 |
| 56 | MG | 1A | 4132 | 1/1 | 0.89 | 0.56 | 61,61,61,61 | 0 |
| 56 | MG | 2A | 3198 | 1/1 | 0.89 | 0.53 | 100,100,100,100 | 0 |
| 56 | MG | 2a | 1897 | 1/1 | 0.89 | 1.12 | 153,153,153,153 | 0 |

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| Mol | Type | Chain | Res | Atoms | RSCC | RSR | B-factors(Å$^2$) | Q<0.9 |
|---|---|---|---|---|---|---|---|---|
| 56 | MG | 1A | 4116 | 1/1 | 0.89 | 0.16 | 65,65,65,65 | 0 |
| 56 | MG | 2A | 3374 | 1/1 | 0.89 | 0.17 | 102,102,102,102 | 0 |
| 56 | MG | 2Z | 402 | 1/1 | 0.89 | 1.17 | 120,120,120,120 | 0 |
| 56 | MG | 1A | 4629 | 1/1 | 0.89 | 0.24 | 71,71,71,71 | 0 |
| 56 | MG | 1A | 4349 | 1/1 | 0.89 | 0.32 | 54,54,54,54 | 0 |
| 56 | MG | 2a | 1730 | 1/1 | 0.89 | 0.14 | 127,127,127,127 | 0 |
| 56 | MG | 1a | 1904 | 1/1 | 0.89 | 0.57 | 83,83,83,83 | 0 |
| 56 | MG | 1A | 5021 | 1/1 | 0.89 | 0.20 | 81,81,81,81 | 0 |
| 56 | MG | 2A | 3558 | 1/1 | 0.89 | 0.78 | 93,93,93,93 | 0 |
| 56 | MG | 1A | 4350 | 1/1 | 0.89 | 0.39 | 68,68,68,68 | 0 |
| 56 | MG | 1A | 5025 | 1/1 | 0.89 | 0.33 | 75,75,75,75 | 0 |
| 56 | MG | 2a | 1736 | 1/1 | 0.89 | 0.30 | 137,137,137,137 | 0 |
| 56 | MG | 1a | 1680 | 1/1 | 0.89 | 0.14 | 155,155,155,155 | 0 |
| 56 | MG | 26 | 101 | 1/1 | 0.89 | 0.93 | 121,121,121,121 | 0 |
| 56 | MG | 2a | 1740 | 1/1 | 0.89 | 0.11 | 143,143,143,143 | 0 |
| 56 | MG | 26 | 103 | 1/1 | 0.89 | 0.57 | 119,119,119,119 | 0 |
| 56 | MG | 2a | 1744 | 1/1 | 0.89 | 0.64 | 95,95,95,95 | 0 |
| 56 | MG | 2d | 302 | 1/1 | 0.89 | 0.13 | 164,164,164,164 | 0 |
| 56 | MG | 2d | 304 | 1/1 | 0.89 | 0.28 | 161,161,161,161 | 0 |
| 56 | MG | 1A | 4892 | 1/1 | 0.89 | 0.53 | 72,72,72,72 | 0 |
| 56 | MG | 2A | 3216 | 1/1 | 0.89 | 0.11 | 100,100,100,100 | 0 |
| 56 | MG | 1U | 201 | 1/1 | 0.89 | 0.24 | 61,61,61,61 | 0 |
| 56 | MG | 1A | 4545 | 1/1 | 0.89 | 0.23 | 65,65,65,65 | 0 |
| 56 | MG | 1A | 4481 | 1/1 | 0.89 | 0.53 | 78,78,78,78 | 0 |
| 56 | MG | 1A | 4398 | 1/1 | 0.89 | 0.23 | 75,75,75,75 | 0 |
| 56 | MG | 1A | 4240 | 1/1 | 0.89 | 0.24 | 60,60,60,60 | 0 |
| 56 | MG | 2A | 3229 | 1/1 | 0.89 | 0.58 | 73,73,73,73 | 0 |
| 56 | MG | 2A | 3230 | 1/1 | 0.89 | 0.23 | 87,87,87,87 | 0 |
| 56 | MG | 2A | 3780 | 1/1 | 0.89 | 0.30 | 90,90,90,90 | 0 |
| 56 | MG | 2A | 3088 | 1/1 | 0.89 | 0.21 | 72,72,72,72 | 0 |
| 56 | MG | 1A | 4491 | 1/1 | 0.89 | 0.40 | 86,86,86,86 | 0 |
| 56 | MG | 1a | 1918 | 1/1 | 0.89 | 0.52 | 142,142,142,142 | 0 |
| 56 | MG | 1a | 1691 | 1/1 | 0.89 | 0.47 | 117,117,117,117 | 0 |
| 56 | MG | 1A | 4318 | 1/1 | 0.89 | 0.59 | 81,81,81,81 | 0 |
| 56 | MG | 2A | 3599 | 1/1 | 0.89 | 0.26 | 122,122,122,122 | 0 |
| 56 | MG | 1a | 1694 | 1/1 | 0.89 | 0.43 | 125,125,125,125 | 0 |
| 56 | MG | 2A | 3606 | 1/1 | 0.89 | 0.23 | 137,137,137,137 | 0 |
| 56 | MG | 1A | 4645 | 1/1 | 0.89 | 0.31 | 66,66,66,66 | 0 |
| 56 | MG | 1A | 5050 | 1/1 | 0.89 | 0.24 | 173,173,173,173 | 0 |
| 56 | MG | 1A | 4279 | 1/1 | 0.89 | 0.31 | 64,64,64,64 | 0 |
| 56 | MG | 2a | 1770 | 1/1 | 0.89 | 0.41 | 237,237,237,237 | 0 |
| 56 | MG | 1A | 4406 | 1/1 | 0.89 | 0.48 | 56,56,56,56 | 0 |

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| Mol | Type | Chain | Res | Atoms | RSCC | RSR | B-factors(Å$^2$) | Q<0.9 |
|---|---|---|---|---|---|---|---|---|
| 56 | MG | 1A | 4566 | 1/1 | 0.89 | 0.25 | 58,58,58,58 | 0 |
| 56 | MG | 2a | 1774 | 1/1 | 0.89 | 0.25 | 220,220,220,220 | 0 |
| 56 | MG | 1A | 4568 | 1/1 | 0.89 | 0.34 | 56,56,56,56 | 0 |
| 56 | MG | 2a | 1626 | 1/1 | 0.89 | 0.44 | 157,157,157,157 | 0 |
| 56 | MG | 1A | 4359 | 1/1 | 0.89 | 0.17 | 71,71,71,71 | 0 |
| 56 | MG | 1a | 1710 | 1/1 | 0.89 | 0.34 | 115,115,115,115 | 0 |
| 56 | MG | 1A | 4580 | 1/1 | 0.89 | 0.21 | 64,64,64,64 | 0 |
| 56 | MG | 1A | 4322 | 1/1 | 0.89 | 0.54 | 85,85,85,85 | 0 |
| 56 | MG | 1A | 4135 | 1/1 | 0.89 | 0.21 | 78,78,78,78 | 0 |
| 56 | MG | 1A | 4673 | 1/1 | 0.89 | 0.53 | 94,94,94,94 | 0 |
| 56 | MG | 1a | 1613 | 1/1 | 0.89 | 0.19 | 91,91,91,91 | 0 |
| 56 | MG | 1A | 4940 | 1/1 | 0.89 | 0.29 | 55,55,55,55 | 0 |
| 56 | MG | 2A | 3460 | 1/1 | 0.89 | 0.86 | 106,106,106,106 | 0 |
| 56 | MG | 1A | 4854 | 1/1 | 0.89 | 0.27 | 81,81,81,81 | 0 |
| 56 | MG | 2s | 101 | 1/1 | 0.89 | 0.26 | 250,250,250,250 | 0 |
| 56 | MG | 2A | 3277 | 1/1 | 0.89 | 0.16 | 88,88,88,88 | 0 |
| 56 | MG | 2A | 3281 | 1/1 | 0.89 | 0.32 | 104,104,104,104 | 0 |
| 56 | MG | 1A | 4855 | 1/1 | 0.89 | 0.20 | 59,59,59,59 | 0 |
| 56 | MG | 1B | 208 | 1/1 | 0.89 | 0.34 | 94,94,94,94 | 0 |
| 56 | MG | 2a | 1795 | 1/1 | 0.89 | 0.37 | 111,111,111,111 | 0 |
| 56 | MG | 1B | 209 | 1/1 | 0.89 | 0.51 | 89,89,89,89 | 0 |
| 56 | MG | 1A | 4857 | 1/1 | 0.89 | 0.68 | 61,61,61,61 | 0 |
| 56 | MG | 2a | 1656 | 1/1 | 0.89 | 0.09 | 145,145,145,145 | 0 |
| 56 | MG | 1A | 4954 | 1/1 | 0.89 | 0.26 | 62,62,62,62 | 0 |
| 56 | MG | 1A | 4509 | 1/1 | 0.89 | 0.24 | 62,62,62,62 | 0 |
| 56 | MG | 2A | 3648 | 1/1 | 0.89 | 0.42 | 137,137,137,137 | 0 |
| 56 | MG | 1A | 4217 | 1/1 | 0.89 | 0.26 | 59,59,59,59 | 0 |
| 56 | MG | 2A | 3650 | 1/1 | 0.89 | 0.20 | 115,115,115,115 | 0 |
| 56 | MG | 1A | 4432 | 1/1 | 0.89 | 0.20 | 95,95,95,95 | 0 |
| 56 | MG | 1A | 4244 | 1/1 | 0.89 | 0.40 | 51,51,51,51 | 0 |
| 56 | MG | 1A | 4968 | 1/1 | 0.89 | 0.69 | 82,82,82,82 | 0 |
| 56 | MG | 2A | 3147 | 1/1 | 0.89 | 0.43 | 82,82,82,82 | 0 |
| 56 | MG | 1a | 1640 | 1/1 | 0.89 | 0.39 | 115,115,115,115 | 0 |
| 56 | MG | 1A | 4080 | 1/1 | 0.89 | 0.36 | 55,55,55,55 | 0 |
| 56 | MG | 2A | 3310 | 1/1 | 0.89 | 0.57 | 117,117,117,117 | 0 |
| 56 | MG | 1D | 303 | 1/1 | 0.89 | 0.60 | 82,82,82,82 | 0 |
| 56 | MG | 2B | 222 | 1/1 | 0.89 | 0.23 | 133,133,133,133 | 0 |
| 56 | MG | 2A | 3678 | 1/1 | 0.89 | 0.38 | 100,100,100,100 | 0 |
| 56 | MG | 1a | 1764 | 1/1 | 0.89 | 0.35 | 121,121,121,121 | 0 |
| 56 | MG | 1A | 4380 | 1/1 | 0.89 | 0.29 | 56,56,56,56 | 0 |
| 56 | MG | 1A | 4984 | 1/1 | 0.89 | 0.25 | 87,87,87,87 | 0 |
| 56 | MG | 1A | 4684 | 1/1 | 0.89 | 0.56 | 52,52,52,52 | 0 |

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| Mol | Type | Chain | Res | Atoms | RSCC | RSR | B-factors(Å$^2$) | Q<0.9 |
|---|---|---|---|---|---|---|---|---|
| 56 | MG | 1A | 4687 | 1/1 | 0.89 | 0.20 | 88,88,88,88 | 0 |
| 56 | MG | 1A | 4868 | 1/1 | 0.89 | 0.17 | 62,62,62,62 | 0 |
| 56 | MG | 1A | 4321 | 1/1 | 0.90 | 0.36 | 102,102,102,102 | 0 |
| 56 | MG | 2A | 3684 | 1/1 | 0.90 | 0.22 | 94,94,94,94 | 0 |
| 56 | MG | 1A | 4098 | 1/1 | 0.90 | 0.28 | 53,53,53,53 | 0 |
| 56 | MG | 2a | 1856 | 1/1 | 0.90 | 0.22 | 147,147,147,147 | 0 |
| 56 | MG | 2A | 3192 | 1/1 | 0.90 | 0.13 | 99,99,99,99 | 0 |
| 56 | MG | 2A | 3055 | 1/1 | 0.90 | 0.29 | 102,102,102,102 | 0 |
| 56 | MG | 1A | 4100 | 1/1 | 0.90 | 0.34 | 66,66,66,66 | 0 |
| 56 | MG | 1A | 4586 | 1/1 | 0.90 | 0.21 | 73,73,73,73 | 0 |
| 56 | MG | 2a | 1867 | 1/1 | 0.90 | 0.51 | 79,79,79,79 | 0 |
| 56 | MG | 1a | 1619 | 1/1 | 0.90 | 0.39 | 95,95,95,95 | 0 |
| 56 | MG | 2D | 303 | 1/1 | 0.90 | 0.22 | 109,109,109,109 | 0 |
| 56 | MG | 2a | 1870 | 1/1 | 0.90 | 0.21 | 108,108,108,108 | 0 |
| 56 | MG | 2a | 1872 | 1/1 | 0.90 | 0.58 | 120,120,120,120 | 0 |
| 56 | MG | 2A | 3530 | 1/1 | 0.90 | 0.13 | 133,133,133,133 | 0 |
| 56 | MG | 1A | 4886 | 1/1 | 0.90 | 0.52 | 67,67,67,67 | 0 |
| 56 | MG | 1A | 4066 | 1/1 | 0.90 | 0.34 | 98,98,98,98 | 0 |
| 56 | MG | 2a | 1698 | 1/1 | 0.90 | 0.39 | 118,118,118,118 | 0 |
| 56 | MG | 2A | 3067 | 1/1 | 0.90 | 0.32 | 123,123,123,123 | 0 |
| 56 | MG | 1A | 4589 | 1/1 | 0.90 | 0.29 | 79,79,79,79 | 0 |
| 56 | MG | 1A | 4131 | 1/1 | 0.90 | 0.34 | 56,56,56,56 | 0 |
| 56 | MG | 2A | 3075 | 1/1 | 0.90 | 0.08 | 142,142,142,142 | 0 |
| 56 | MG | 1a | 1719 | 1/1 | 0.90 | 0.98 | 102,102,102,102 | 0 |
| 56 | MG | 2a | 1707 | 1/1 | 0.90 | 0.18 | 85,85,85,85 | 0 |
| 56 | MG | 2A | 3540 | 1/1 | 0.90 | 0.28 | 148,148,148,148 | 0 |
| 56 | MG | 1A | 4529 | 1/1 | 0.90 | 0.91 | 68,68,68,68 | 0 |
| 56 | MG | 1A | 4660 | 1/1 | 0.90 | 0.68 | 84,84,84,84 | 0 |
| 56 | MG | 2A | 3727 | 1/1 | 0.90 | 0.60 | 90,90,90,90 | 0 |
| 56 | MG | 2a | 1890 | 1/1 | 0.90 | 0.31 | 125,125,125,125 | 0 |
| 56 | MG | 2A | 3377 | 1/1 | 0.90 | 0.50 | 116,116,116,116 | 0 |
| 56 | MG | 1A | 4661 | 1/1 | 0.90 | 0.61 | 80,80,80,80 | 0 |
| 56 | MG | 1E | 302 | 1/1 | 0.90 | 0.19 | 59,59,59,59 | 0 |
| 56 | MG | 1A | 4154 | 1/1 | 0.90 | 0.17 | 68,68,68,68 | 0 |
| 56 | MG | 1b | 303 | 1/1 | 0.90 | 0.08 | 166,166,166,166 | 0 |
| 56 | MG | 1A | 4811 | 1/1 | 0.90 | 0.81 | 63,63,63,63 | 0 |
| 56 | MG | 1A | 4376 | 1/1 | 0.90 | 0.28 | 61,61,61,61 | 0 |
| 56 | MG | 2A | 3744 | 1/1 | 0.90 | 0.16 | 105,105,105,105 | 0 |
| 56 | MG | 1A | 4377 | 1/1 | 0.90 | 0.29 | 80,80,80,80 | 0 |
| 56 | MG | 1H | 201 | 1/1 | 0.90 | 0.24 | 69,69,69,69 | 0 |
| 56 | MG | 1A | 5019 | 1/1 | 0.90 | 0.47 | 75,75,75,75 | 0 |
| 56 | MG | 1A | 4606 | 1/1 | 0.90 | 0.33 | 67,67,67,67 | 0 |

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| Mol | Type | Chain | Res | Atoms | RSCC | RSR | B-factors(Å$^2$) | Q<0.9 |
|---|---|---|---|---|---|---|---|---|
| 56 | MG | 2A | 3571 | 1/1 | 0.90 | 0.29 | 172,172,172,172 | 0 |
| 56 | MG | 1A | 4050 | 1/1 | 0.90 | 0.69 | 100,100,100,100 | 0 |
| 56 | MG | 20 | 102 | 1/1 | 0.90 | 0.46 | 116,116,116,116 | 0 |
| 56 | MG | 2a | 1911 | 1/1 | 0.90 | 0.10 | 140,140,140,140 | 0 |
| 56 | MG | 1A | 4224 | 1/1 | 0.90 | 0.37 | 64,64,64,64 | 0 |
| 56 | MG | 1A | 4748 | 1/1 | 0.90 | 0.36 | 90,90,90,90 | 0 |
| 56 | MG | 21 | 101 | 1/1 | 0.90 | 0.18 | 110,110,110,110 | 0 |
| 56 | MG | 1A | 4543 | 1/1 | 0.90 | 0.39 | 83,83,83,83 | 0 |
| 56 | MG | 1a | 1651 | 1/1 | 0.90 | 0.17 | 121,121,121,121 | 0 |
| 56 | MG | 1A | 5031 | 1/1 | 0.90 | 0.28 | 88,88,88,88 | 0 |
| 56 | MG | 2A | 3104 | 1/1 | 0.90 | 0.35 | 53,53,53,53 | 0 |
| 56 | MG | 1A | 4835 | 1/1 | 0.90 | 0.23 | 63,63,63,63 | 0 |
| 56 | MG | 2a | 1747 | 1/1 | 0.90 | 0.20 | 122,122,122,122 | 0 |
| 56 | MG | 1a | 1761 | 1/1 | 0.90 | 0.36 | 112,112,112,112 | 0 |
| 56 | MG | 1A | 4752 | 1/1 | 0.90 | 0.34 | 63,63,63,63 | 0 |
| 56 | MG | 1p | 101 | 1/1 | 0.90 | 0.18 | 143,143,143,143 | 0 |
| 56 | MG | 1A | 4925 | 1/1 | 0.90 | 0.17 | 72,72,72,72 | 0 |
| 56 | MG | 2A | 3774 | 1/1 | 0.90 | 0.46 | 116,116,116,116 | 0 |
| 56 | MG | 2A | 3595 | 1/1 | 0.90 | 0.09 | 147,147,147,147 | 0 |
| 56 | MG | 1a | 1658 | 1/1 | 0.90 | 0.20 | 114,114,114,114 | 0 |
| 56 | MG | 1A | 4847 | 1/1 | 0.90 | 0.37 | 72,72,72,72 | 0 |
| 56 | MG | 2A | 3260 | 1/1 | 0.90 | 0.33 | 78,78,78,78 | 0 |
| 56 | MG | 1A | 4499 | 1/1 | 0.90 | 1.38 | 59,59,59,59 | 0 |
| 56 | MG | 2A | 3425 | 1/1 | 0.90 | 0.38 | 102,102,102,102 | 0 |
| 56 | MG | 1A | 4385 | 1/1 | 0.90 | 0.50 | 55,55,55,55 | 0 |
| 56 | MG | 1a | 1664 | 1/1 | 0.90 | 0.34 | 115,115,115,115 | 0 |
| 56 | MG | 1A | 4757 | 1/1 | 0.90 | 0.88 | 119,119,119,119 | 0 |
| 56 | MG | 2A | 3121 | 1/1 | 0.90 | 0.43 | 125,125,125,125 | 0 |
| 56 | MG | 1A | 4501 | 1/1 | 0.90 | 0.35 | 71,71,71,71 | 0 |
| 56 | MG | 2A | 3797 | 1/1 | 0.90 | 0.36 | 97,97,97,97 | 0 |
| 56 | MG | 1A | 4625 | 1/1 | 0.90 | 0.56 | 118,118,118,118 | 0 |
| 56 | MG | 1U | 203 | 1/1 | 0.90 | 0.27 | 64,64,64,64 | 0 |
| 56 | MG | 1a | 1866 | 1/1 | 0.90 | 0.20 | 224,224,224,224 | 0 |
| 56 | MG | 2k | 202 | 1/1 | 0.90 | 0.18 | 124,124,124,124 | 0 |
| 56 | MG | 2A | 3006 | 1/1 | 0.90 | 0.62 | 101,101,101,101 | 0 |
| 56 | MG | 2A | 3456 | 1/1 | 0.90 | 0.40 | 83,83,83,83 | 0 |
| 56 | MG | 2A | 3806 | 1/1 | 0.90 | 0.26 | 114,114,114,114 | 0 |
| 56 | MG | 1A | 4160 | 1/1 | 0.90 | 0.21 | 50,50,50,50 | 0 |
| 56 | MG | 2A | 3009 | 1/1 | 0.90 | 0.61 | 94,94,94,94 | 0 |
| 56 | MG | 1A | 4943 | 1/1 | 0.90 | 0.51 | 61,61,61,61 | 0 |
| 56 | MG | 2A | 3821 | 1/1 | 0.90 | 0.28 | 89,89,89,89 | 0 |
| 56 | MG | 2A | 3288 | 1/1 | 0.90 | 0.47 | 102,102,102,102 | 0 |

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| Mol | Type | Chain | Res | Atoms | RSCC | RSR | B-factors(Å$^2$) | Q<0.9 |
|---|---|---|---|---|---|---|---|---|
| 56 | MG | 1A | 4947 | 1/1 | 0.90 | 0.25 | 71,71,71,71 | 0 |
| 56 | MG | 1A | 4628 | 1/1 | 0.90 | 0.26 | 77,77,77,77 | 0 |
| 56 | MG | 2A | 3297 | 1/1 | 0.90 | 0.80 | 80,80,80,80 | 0 |
| 56 | MG | 1A | 4949 | 1/1 | 0.90 | 0.29 | 69,69,69,69 | 0 |
| 56 | MG | 1a | 1880 | 1/1 | 0.90 | 0.15 | 125,125,125,125 | 0 |
| 56 | MG | 1a | 1882 | 1/1 | 0.90 | 0.29 | 87,87,87,87 | 0 |
| 56 | MG | 2A | 3474 | 1/1 | 0.90 | 0.62 | 125,125,125,125 | 0 |
| 56 | MG | 2a | 1645 | 1/1 | 0.90 | 0.15 | 124,124,124,124 | 0 |
| 56 | MG | 2A | 3644 | 1/1 | 0.90 | 0.16 | 155,155,155,155 | 0 |
| 56 | MG | 2A | 3835 | 1/1 | 0.90 | 0.31 | 121,121,121,121 | 0 |
| 56 | MG | 2A | 3836 | 1/1 | 0.90 | 0.30 | 205,205,205,205 | 0 |
| 56 | MG | 2u | 102 | 1/1 | 0.90 | 0.12 | 241,241,241,241 | 0 |
| 56 | MG | 2a | 1650 | 1/1 | 0.90 | 0.37 | 136,136,136,136 | 0 |
| 56 | MG | 1A | 4008 | 1/1 | 0.90 | 0.28 | 71,71,71,71 | 0 |
| 56 | MG | 1a | 1790 | 1/1 | 0.90 | 0.48 | 87,87,87,87 | 0 |
| 56 | MG | 2A | 3850 | 1/1 | 0.90 | 0.23 | 109,109,109,109 | 0 |
| 56 | MG | 2A | 3478 | 1/1 | 0.90 | 0.52 | 127,127,127,127 | 0 |
| 56 | MG | 2A | 3157 | 1/1 | 0.90 | 0.36 | 102,102,102,102 | 0 |
| 56 | MG | 11 | 101 | 1/1 | 0.90 | 0.84 | 87,87,87,87 | 0 |
| 56 | MG | 1A | 5060 | 1/1 | 0.90 | 0.52 | 64,64,64,64 | 0 |
| 56 | MG | 1A | 4239 | 1/1 | 0.90 | 0.22 | 56,56,56,56 | 0 |
| 56 | MG | 2a | 1806 | 1/1 | 0.90 | 0.23 | 116,116,116,116 | 0 |
| 56 | MG | 2a | 1807 | 1/1 | 0.90 | 0.26 | 122,122,122,122 | 0 |
| 56 | MG | 1A | 4955 | 1/1 | 0.90 | 0.31 | 72,72,72,72 | 0 |
| 56 | MG | 1A | 4449 | 1/1 | 0.90 | 0.23 | 79,79,79,79 | 0 |
| 56 | MG | 2A | 3500 | 1/1 | 0.90 | 0.33 | 93,93,93,93 | 0 |
| 56 | MG | 1A | 4061 | 1/1 | 0.90 | 0.41 | 71,71,71,71 | 0 |
| 56 | MG | 2A | 3671 | 1/1 | 0.90 | 0.23 | 85,85,85,85 | 0 |
| 56 | MG | 2A | 3504 | 1/1 | 0.90 | 0.30 | 134,134,134,134 | 0 |
| 56 | MG | 1A | 4451 | 1/1 | 0.90 | 0.22 | 70,70,70,70 | 0 |
| 56 | MG | 1A | 4198 | 1/1 | 0.90 | 0.51 | 98,98,98,98 | 0 |
| 56 | MG | 2A | 3676 | 1/1 | 0.90 | 0.61 | 125,125,125,125 | 0 |
| 56 | MG | 2B | 219 | 1/1 | 0.90 | 0.51 | 77,77,77,77 | 0 |
| 56 | MG | 2A | 3677 | 1/1 | 0.90 | 0.73 | 115,115,115,115 | 0 |
| 56 | MG | 2a | 1841 | 1/1 | 0.90 | 0.36 | 224,224,224,224 | 0 |
| 56 | MG | 2a | 1843 | 1/1 | 0.90 | 0.37 | 253,253,253,253 | 0 |
| 56 | MG | 1A | 4702 | 1/1 | 0.90 | 0.97 | 58,58,58,58 | 0 |
| 56 | MG | 2A | 3038 | 1/1 | 0.90 | 0.67 | 69,69,69,69 | 0 |
| 56 | MG | 1A | 4123 | 1/1 | 0.90 | 0.40 | 77,77,77,77 | 0 |
| 56 | MG | 2A | 3236 | 1/1 | 0.91 | 0.48 | 96,96,96,96 | 0 |
| 56 | MG | 1A | 5062 | 1/1 | 0.91 | 0.57 | 87,87,87,87 | 0 |
| 56 | MG | 1B | 201 | 1/1 | 0.91 | 1.00 | 106,106,106,106 | 0 |

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| Mol | Type | Chain | Res | Atoms | RSCC | RSR | B-factors(Å$^2$) | Q<0.9 |
|---|---|---|---|---|---|---|---|---|
| 56 | MG | 1A | 4957 | 1/1 | 0.91 | 0.33 | 79,79,79,79 | 0 |
| 56 | MG | 2A | 3708 | 1/1 | 0.91 | 0.32 | 100,100,100,100 | 0 |
| 56 | MG | 2A | 3712 | 1/1 | 0.91 | 0.49 | 92,92,92,92 | 0 |
| 56 | MG | 1A | 4011 | 1/1 | 0.91 | 0.36 | 70,70,70,70 | 0 |
| 56 | MG | 2a | 1690 | 1/1 | 0.91 | 0.40 | 155,155,155,155 | 0 |
| 56 | MG | 2A | 3394 | 1/1 | 0.91 | 0.07 | 131,131,131,131 | 0 |
| 56 | MG | 1a | 1683 | 1/1 | 0.91 | 0.39 | 83,83,83,83 | 0 |
| 56 | MG | 1a | 1873 | 1/1 | 0.91 | 0.08 | 214,214,214,214 | 0 |
| 56 | MG | 1A | 4230 | 1/1 | 0.91 | 0.17 | 102,102,102,102 | 0 |
| 56 | MG | 2A | 3551 | 1/1 | 0.91 | 0.22 | 104,104,104,104 | 0 |
| 56 | MG | 1A | 4120 | 1/1 | 0.91 | 0.56 | 79,79,79,79 | 0 |
| 56 | MG | 2A | 3400 | 1/1 | 0.91 | 0.39 | 225,225,225,225 | 0 |
| 56 | MG | 1A | 4879 | 1/1 | 0.91 | 0.28 | 77,77,77,77 | 0 |
| 56 | MG | 1A | 4585 | 1/1 | 0.91 | 0.30 | 65,65,65,65 | 0 |
| 56 | MG | 2A | 3736 | 1/1 | 0.91 | 0.60 | 108,108,108,108 | 0 |
| 56 | MG | 2A | 3560 | 1/1 | 0.91 | 0.31 | 95,95,95,95 | 0 |
| 56 | MG | 1A | 4784 | 1/1 | 0.91 | 0.31 | 87,87,87,87 | 0 |
| 56 | MG | 2A | 3564 | 1/1 | 0.91 | 0.15 | 102,102,102,102 | 0 |
| 56 | MG | 1a | 1690 | 1/1 | 0.91 | 0.14 | 124,124,124,124 | 0 |
| 56 | MG | 1A | 4708 | 1/1 | 0.91 | 0.34 | 70,70,70,70 | 0 |
| 56 | MG | 2a | 1712 | 1/1 | 0.91 | 0.67 | 148,148,148,148 | 0 |
| 56 | MG | 1A | 4460 | 1/1 | 0.91 | 0.13 | 77,77,77,77 | 0 |
| 56 | MG | 1B | 213 | 1/1 | 0.91 | 0.71 | 88,88,88,88 | 0 |
| 56 | MG | 1A | 4368 | 1/1 | 0.91 | 0.18 | 63,63,63,63 | 0 |
| 56 | MG | 2a | 1717 | 1/1 | 0.91 | 0.24 | 143,143,143,143 | 0 |
| 56 | MG | 1B | 216 | 1/1 | 0.91 | 0.45 | 69,69,69,69 | 0 |
| 56 | MG | 2A | 3575 | 1/1 | 0.91 | 0.46 | 70,70,70,70 | 0 |
| 56 | MG | 1A | 4463 | 1/1 | 0.91 | 0.26 | 62,62,62,62 | 0 |
| 56 | MG | 2A | 3419 | 1/1 | 0.91 | 0.47 | 135,135,135,135 | 0 |
| 56 | MG | 2a | 1896 | 1/1 | 0.91 | 0.56 | 98,98,98,98 | 0 |
| 56 | MG | 2A | 3420 | 1/1 | 0.91 | 0.33 | 121,121,121,121 | 0 |
| 56 | MG | 2A | 3581 | 1/1 | 0.91 | 0.18 | 116,116,116,116 | 0 |
| 56 | MG | 1A | 4652 | 1/1 | 0.91 | 0.45 | 84,84,84,84 | 0 |
| 56 | MG | 1A | 4592 | 1/1 | 0.91 | 0.18 | 90,90,90,90 | 0 |
| 56 | MG | 1A | 4370 | 1/1 | 0.91 | 0.25 | 61,61,61,61 | 0 |
| 56 | MG | 2A | 3150 | 1/1 | 0.91 | 0.40 | 105,105,105,105 | 0 |
| 56 | MG | 2A | 3765 | 1/1 | 0.91 | 0.13 | 120,120,120,120 | 0 |
| 56 | MG | 1A | 4472 | 1/1 | 0.91 | 0.40 | 54,54,54,54 | 0 |
| 56 | MG | 1A | 4724 | 1/1 | 0.91 | 0.29 | 80,80,80,80 | 0 |
| 56 | MG | 1A | 5003 | 1/1 | 0.91 | 0.27 | 65,65,65,65 | 0 |
| 56 | MG | 1a | 1718 | 1/1 | 0.91 | 0.79 | 107,107,107,107 | 0 |
| 56 | MG | 24 | 101 | 1/1 | 0.91 | 0.11 | 73,73,73,73 | 0 |

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| Mol | Type | Chain | Res | Atoms | RSCC | RSR | B-factors(Å$^2$) | Q<0.9 |
|---|---|---|---|---|---|---|---|---|
| 56 | MG | 2A | 3037 | 1/1 | 0.91 | 0.81 | 104,104,104,104 | 0 |
| 56 | MG | 2A | 3156 | 1/1 | 0.91 | 0.40 | 100,100,100,100 | 0 |
| 56 | MG | 1A | 4072 | 1/1 | 0.91 | 0.21 | 63,63,63,63 | 0 |
| 56 | MG | 2A | 3448 | 1/1 | 0.91 | 0.83 | 78,78,78,78 | 0 |
| 56 | MG | 2a | 1920 | 1/1 | 0.91 | 0.19 | 222,222,222,222 | 0 |
| 56 | MG | 2A | 3040 | 1/1 | 0.91 | 0.34 | 116,116,116,116 | 0 |
| 56 | MG | 28 | 105 | 1/1 | 0.91 | 0.40 | 119,119,119,119 | 0 |
| 56 | MG | 2A | 3041 | 1/1 | 0.91 | 0.34 | 117,117,117,117 | 0 |
| 56 | MG | 2A | 3782 | 1/1 | 0.91 | 0.61 | 139,139,139,139 | 0 |
| 56 | MG | 1A | 4028 | 1/1 | 0.91 | 0.34 | 58,58,58,58 | 0 |
| 56 | MG | 1A | 4487 | 1/1 | 0.91 | 0.12 | 75,75,75,75 | 0 |
| 56 | MG | 2A | 3300 | 1/1 | 0.91 | 0.91 | 96,96,96,96 | 0 |
| 56 | MG | 1A | 4901 | 1/1 | 0.91 | 0.21 | 61,61,61,61 | 0 |
| 56 | MG | 1A | 4665 | 1/1 | 0.91 | 0.62 | 78,78,78,78 | 0 |
| 56 | MG | 1A | 5016 | 1/1 | 0.91 | 0.71 | 81,81,81,81 | 0 |
| 56 | MG | 1A | 4097 | 1/1 | 0.91 | 0.23 | 57,57,57,57 | 0 |
| 56 | MG | 1A | 4608 | 1/1 | 0.91 | 0.26 | 70,70,70,70 | 0 |
| 56 | MG | 2A | 3626 | 1/1 | 0.91 | 0.13 | 158,158,158,158 | 0 |
| 56 | MG | 2A | 3627 | 1/1 | 0.91 | 0.19 | 165,165,165,165 | 0 |
| 56 | MG | 1A | 4831 | 1/1 | 0.91 | 0.88 | 109,109,109,109 | 0 |
| 56 | MG | 1A | 4429 | 1/1 | 0.91 | 0.49 | 54,54,54,54 | 0 |
| 56 | MG | 2A | 3324 | 1/1 | 0.91 | 0.34 | 87,87,87,87 | 0 |
| 56 | MG | 1A | 4203 | 1/1 | 0.91 | 0.21 | 61,61,61,61 | 0 |
| 56 | MG | 2a | 1619 | 1/1 | 0.91 | 0.08 | 68,68,68,68 | 0 |
| 56 | MG | 1A | 4613 | 1/1 | 0.91 | 0.21 | 70,70,70,70 | 0 |
| 56 | MG | 2a | 1621 | 1/1 | 0.91 | 0.25 | 162,162,162,162 | 0 |
| 56 | MG | 2h | 205 | 1/1 | 0.91 | 0.46 | 152,152,152,152 | 0 |
| 56 | MG | 2A | 3809 | 1/1 | 0.91 | 0.72 | 86,86,86,86 | 0 |
| 56 | MG | 1A | 4078 | 1/1 | 0.91 | 0.41 | 66,66,66,66 | 0 |
| 56 | MG | 2a | 1772 | 1/1 | 0.91 | 0.51 | 70,70,70,70 | 0 |
| 56 | MG | 1A | 4845 | 1/1 | 0.91 | 0.52 | 68,68,68,68 | 0 |
| 56 | MG | 2A | 3818 | 1/1 | 0.91 | 0.21 | 136,136,136,136 | 0 |
| 56 | MG | 2A | 3335 | 1/1 | 0.91 | 0.31 | 97,97,97,97 | 0 |
| 56 | MG | 2A | 3483 | 1/1 | 0.91 | 0.87 | 106,106,106,106 | 0 |
| 56 | MG | 2A | 3484 | 1/1 | 0.91 | 0.47 | 119,119,119,119 | 0 |
| 56 | MG | 2a | 1778 | 1/1 | 0.91 | 0.85 | 162,162,162,162 | 0 |
| 56 | MG | 1a | 1836 | 1/1 | 0.91 | 0.07 | 225,225,225,225 | 0 |
| 56 | MG | 1A | 4497 | 1/1 | 0.91 | 0.21 | 69,69,69,69 | 0 |
| 56 | MG | 2a | 1633 | 1/1 | 0.91 | 0.37 | 125,125,125,125 | 0 |
| 56 | MG | 2A | 3490 | 1/1 | 0.91 | 0.60 | 76,76,76,76 | 0 |
| 56 | MG | 2A | 3491 | 1/1 | 0.91 | 0.64 | 133,133,133,133 | 0 |
| 56 | MG | 2a | 1784 | 1/1 | 0.91 | 0.42 | 90,90,90,90 | 0 |

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| Mol | Type | Chain | Res | Atoms | RSCC | RSR | B-factors(Å$^2$) | Q<0.9 |
|---|---|---|---|---|---|---|---|---|
| 56 | MG | 1A | 4754 | 1/1 | 0.91 | 0.28 | 62,62,62,62 | 0 |
| 56 | MG | 1a | 1755 | 1/1 | 0.91 | 0.32 | 100,100,100,100 | 0 |
| 56 | MG | 2a | 1787 | 1/1 | 0.91 | 0.23 | 231,231,231,231 | 0 |
| 56 | MG | 2a | 1788 | 1/1 | 0.91 | 0.25 | 229,229,229,229 | 0 |
| 56 | MG | 1A | 5040 | 1/1 | 0.91 | 0.21 | 78,78,78,78 | 0 |
| 56 | MG | 1A | 4185 | 1/1 | 0.91 | 0.26 | 62,62,62,62 | 0 |
| 56 | MG | 2A | 3202 | 1/1 | 0.91 | 0.32 | 114,114,114,114 | 0 |
| 56 | MG | 1A | 4064 | 1/1 | 0.91 | 0.30 | 69,69,69,69 | 0 |
| 56 | MG | 1A | 4273 | 1/1 | 0.91 | 0.29 | 69,69,69,69 | 0 |
| 56 | MG | 2A | 3844 | 1/1 | 0.91 | 0.58 | 107,107,107,107 | 0 |
| 56 | MG | 1A | 4082 | 1/1 | 0.91 | 0.19 | 58,58,58,58 | 0 |
| 56 | MG | 2A | 3089 | 1/1 | 0.91 | 0.36 | 122,122,122,122 | 0 |
| 56 | MG | 2A | 3667 | 1/1 | 0.91 | 0.34 | 93,93,93,93 | 0 |
| 56 | MG | 1A | 4688 | 1/1 | 0.91 | 0.28 | 65,65,65,65 | 0 |
| 56 | MG | 1A | 4946 | 1/1 | 0.91 | 0.16 | 52,52,52,52 | 0 |
| 56 | MG | 2B | 206 | 1/1 | 0.91 | 0.72 | 103,103,103,103 | 0 |
| 56 | MG | 1a | 1766 | 1/1 | 0.91 | 0.34 | 129,129,129,129 | 0 |
| 56 | MG | 2a | 1803 | 1/1 | 0.91 | 0.22 | 127,127,127,127 | 0 |
| 56 | MG | 2A | 3095 | 1/1 | 0.91 | 0.29 | 106,106,106,106 | 0 |
| 56 | MG | 2A | 3522 | 1/1 | 0.91 | 0.49 | 98,98,98,98 | 0 |
| 56 | MG | 2a | 1662 | 1/1 | 0.91 | 0.14 | 150,150,150,150 | 0 |
| 56 | MG | 1A | 4026 | 1/1 | 0.91 | 0.29 | 69,69,69,69 | 0 |
| 56 | MG | 1A | 4117 | 1/1 | 0.91 | 0.38 | 73,73,73,73 | 0 |
| 56 | MG | 1A | 4308 | 1/1 | 0.91 | 0.68 | 98,98,98,98 | 0 |
| 56 | MG | 1A | 4280 | 1/1 | 0.91 | 0.43 | 55,55,55,55 | 0 |
| 56 | MG | 2y | 105 | 1/1 | 0.91 | 0.07 | 262,262,262,262 | 0 |
| 56 | MG | 2a | 1667 | 1/1 | 0.91 | 0.21 | 151,151,151,151 | 0 |
| 56 | MG | 1A | 5056 | 1/1 | 0.91 | 0.11 | 137,137,137,137 | 0 |
| 56 | MG | 1A | 4635 | 1/1 | 0.91 | 0.40 | 68,68,68,68 | 0 |
| 56 | MG | 2a | 1827 | 1/1 | 0.91 | 1.19 | 122,122,122,122 | 0 |
| 56 | MG | 2a | 1670 | 1/1 | 0.91 | 0.14 | 163,163,163,163 | 0 |
| 56 | MG | 2A | 3685 | 1/1 | 0.91 | 0.22 | 109,109,109,109 | 0 |
| 56 | MG | 2A | 3686 | 1/1 | 0.91 | 0.23 | 107,107,107,107 | 0 |
| 56 | MG | 2A | 3379 | 1/1 | 0.91 | 0.13 | 101,101,101,101 | 0 |
| 56 | MG | 1A | 4576 | 1/1 | 0.91 | 0.48 | 55,55,55,55 | 0 |
| 56 | MG | 1A | 4312 | 1/1 | 0.91 | 1.07 | 115,115,115,115 | 0 |
| 56 | MG | 2A | 3534 | 1/1 | 0.91 | 0.18 | 133,133,133,133 | 0 |
| 56 | MG | 1v | 702 | 1/1 | 0.91 | 0.68 | 91,91,91,91 | 0 |
| 56 | MG | 2A | 3235 | 1/1 | 0.91 | 0.37 | 97,97,97,97 | 0 |
| 60 | K | 2A | 3001 | 1/1 | 0.91 | 0.95 | 108,108,108,108 | 0 |
| 56 | MG | 1A | 4961 | 1/1 | 0.92 | 0.14 | 100,100,100,100 | 0 |
| 56 | MG | 2a | 1846 | 1/1 | 0.92 | 0.26 | 225,225,225,225 | 0 |

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| Mol | Type | Chain | Res | Atoms | RSCC | RSR | B-factors(Å$^2$) | Q<0.9 |
|---|---|---|---|---|---|---|---|---|
| 56 | MG | 1B | 207 | 1/1 | 0.92 | 0.61 | 88,88,88,88 | 0 |
| 56 | MG | 2A | 3130 | 1/1 | 0.92 | 0.86 | 136,136,136,136 | 0 |
| 56 | MG | 1A | 4235 | 1/1 | 0.92 | 0.29 | 57,57,57,57 | 0 |
| 56 | MG | 1A | 4488 | 1/1 | 0.92 | 0.48 | 85,85,85,85 | 0 |
| 56 | MG | 1t | 201 | 1/1 | 0.92 | 0.15 | 42,42,42,42 | 0 |
| 56 | MG | 2A | 3134 | 1/1 | 0.92 | 0.69 | 83,83,83,83 | 0 |
| 56 | MG | 2a | 1859 | 1/1 | 0.92 | 0.15 | 160,160,160,160 | 0 |
| 56 | MG | 2A | 3135 | 1/1 | 0.92 | 0.20 | 105,105,105,105 | 0 |
| 56 | MG | 2a | 1861 | 1/1 | 0.92 | 0.08 | 153,153,153,153 | 0 |
| 56 | MG | 2A | 3309 | 1/1 | 0.92 | 0.22 | 108,108,108,108 | 0 |
| 56 | MG | 2a | 1865 | 1/1 | 0.92 | 0.14 | 119,119,119,119 | 0 |
| 56 | MG | 1a | 1724 | 1/1 | 0.92 | 0.21 | 126,126,126,126 | 0 |
| 56 | MG | 1A | 4112 | 1/1 | 0.92 | 0.22 | 59,59,59,59 | 0 |
| 56 | MG | 2B | 229 | 1/1 | 0.92 | 0.17 | 150,150,150,150 | 0 |
| 56 | MG | 1A | 4149 | 1/1 | 0.92 | 0.66 | 59,59,59,59 | 0 |
| 56 | MG | 2B | 231 | 1/1 | 0.92 | 0.24 | 152,152,152,152 | 0 |
| 56 | MG | 1A | 4972 | 1/1 | 0.92 | 0.19 | 77,77,77,77 | 0 |
| 56 | MG | 1a | 1732 | 1/1 | 0.92 | 0.59 | 144,144,144,144 | 0 |
| 56 | MG | 2a | 1874 | 1/1 | 0.92 | 0.51 | 155,155,155,155 | 0 |
| 56 | MG | 1A | 4328 | 1/1 | 0.92 | 0.42 | 55,55,55,55 | 0 |
| 56 | MG | 1a | 1624 | 1/1 | 0.92 | 0.19 | 102,102,102,102 | 0 |
| 56 | MG | 1A | 4981 | 1/1 | 0.92 | 0.20 | 57,57,57,57 | 0 |
| 56 | MG | 2a | 1704 | 1/1 | 0.92 | 0.20 | 160,160,160,160 | 0 |
| 56 | MG | 2A | 3003 | 1/1 | 0.92 | 0.38 | 108,108,108,108 | 0 |
| 56 | MG | 1A | 4035 | 1/1 | 0.92 | 0.46 | 73,73,73,73 | 0 |
| 56 | MG | 2a | 1882 | 1/1 | 0.92 | 0.11 | 163,163,163,163 | 0 |
| 56 | MG | 2A | 3007 | 1/1 | 0.92 | 0.74 | 98,98,98,98 | 0 |
| 56 | MG | 1A | 4693 | 1/1 | 0.92 | 0.29 | 67,67,67,67 | 0 |
| 56 | MG | 1a | 1740 | 1/1 | 0.92 | 0.20 | 151,151,151,151 | 0 |
| 56 | MG | 1A | 4695 | 1/1 | 0.92 | 0.25 | 74,74,74,74 | 0 |
| 56 | MG | 2A | 3343 | 1/1 | 0.92 | 0.38 | 89,89,89,89 | 0 |
| 56 | MG | 1A | 4774 | 1/1 | 0.92 | 0.32 | 68,68,68,68 | 0 |
| 56 | MG | 1A | 4063 | 1/1 | 0.92 | 0.31 | 64,64,64,64 | 0 |
| 56 | MG | 2A | 3164 | 1/1 | 0.92 | 0.42 | 97,97,97,97 | 0 |
| 56 | MG | 1A | 4777 | 1/1 | 0.92 | 0.23 | 68,68,68,68 | 0 |
| 56 | MG | 1A | 4333 | 1/1 | 0.92 | 0.09 | 83,83,83,83 | 0 |
| 56 | MG | 2A | 3725 | 1/1 | 0.92 | 0.41 | 79,79,79,79 | 0 |
| 56 | MG | 2a | 1721 | 1/1 | 0.92 | 0.39 | 145,145,145,145 | 0 |
| 56 | MG | 2Q | 203 | 1/1 | 0.92 | 0.61 | 107,107,107,107 | 0 |
| 56 | MG | 2A | 3726 | 1/1 | 0.92 | 0.20 | 91,91,91,91 | 0 |
| 56 | MG | 2a | 1724 | 1/1 | 0.92 | 0.51 | 141,141,141,141 | 0 |
| 56 | MG | 1a | 1639 | 1/1 | 0.92 | 0.31 | 112,112,112,112 | 0 |

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| Mol | Type | Chain | Res | Atoms | RSCC | RSR | B-factors(Å$^2$) | Q<0.9 |
|---|---|---|---|---|---|---|---|---|
| 56 | MG | 2A | 3729 | 1/1 | 0.92 | 0.30 | 83,83,83,83 | 0 |
| 56 | MG | 1a | 1862 | 1/1 | 0.92 | 0.23 | 215,215,215,215 | 0 |
| 56 | MG | 2A | 3733 | 1/1 | 0.92 | 0.27 | 77,77,77,77 | 0 |
| 56 | MG | 1A | 4015 | 1/1 | 0.92 | 0.83 | 63,63,63,63 | 0 |
| 56 | MG | 2A | 3179 | 1/1 | 0.92 | 0.74 | 139,139,139,139 | 0 |
| 56 | MG | 2A | 3542 | 1/1 | 0.92 | 0.15 | 110,110,110,110 | 0 |
| 56 | MG | 1A | 4379 | 1/1 | 0.92 | 0.74 | 95,95,95,95 | 0 |
| 56 | MG | 1A | 4560 | 1/1 | 0.92 | 0.17 | 59,59,59,59 | 0 |
| 56 | MG | 1A | 4701 | 1/1 | 0.92 | 0.34 | 68,68,68,68 | 0 |
| 56 | MG | 1A | 4502 | 1/1 | 0.92 | 0.44 | 70,70,70,70 | 0 |
| 56 | MG | 1A | 4786 | 1/1 | 0.92 | 0.17 | 63,63,63,63 | 0 |
| 56 | MG | 2a | 1739 | 1/1 | 0.92 | 0.39 | 151,151,151,151 | 0 |
| 56 | MG | 1A | 4637 | 1/1 | 0.92 | 0.12 | 68,68,68,68 | 0 |
| 56 | MG | 1a | 1648 | 1/1 | 0.92 | 0.41 | 135,135,135,135 | 0 |
| 56 | MG | 2b | 303 | 1/1 | 0.92 | 0.95 | 185,185,185,185 | 0 |
| 56 | MG | 20 | 106 | 1/1 | 0.92 | 0.07 | 128,128,128,128 | 0 |
| 56 | MG | 2A | 3750 | 1/1 | 0.92 | 0.16 | 104,104,104,104 | 0 |
| 56 | MG | 2A | 3553 | 1/1 | 0.92 | 0.15 | 106,106,106,106 | 0 |
| 56 | MG | 1A | 4310 | 1/1 | 0.92 | 0.68 | 73,73,73,73 | 0 |
| 56 | MG | 1a | 1874 | 1/1 | 0.92 | 0.32 | 196,196,196,196 | 0 |
| 56 | MG | 1A | 4504 | 1/1 | 0.92 | 0.19 | 92,92,92,92 | 0 |
| 56 | MG | 1a | 1879 | 1/1 | 0.92 | 0.20 | 97,97,97,97 | 0 |
| 56 | MG | 1A | 4897 | 1/1 | 0.92 | 1.03 | 66,66,66,66 | 0 |
| 56 | MG | 1A | 4337 | 1/1 | 0.92 | 0.28 | 59,59,59,59 | 0 |
| 56 | MG | 2A | 3760 | 1/1 | 0.92 | 0.28 | 133,133,133,133 | 0 |
| 56 | MG | 1A | 4506 | 1/1 | 0.92 | 0.49 | 96,96,96,96 | 0 |
| 56 | MG | 1a | 1774 | 1/1 | 0.92 | 0.46 | 139,139,139,139 | 0 |
| 56 | MG | 2A | 3046 | 1/1 | 0.92 | 0.29 | 91,91,91,91 | 0 |
| 56 | MG | 2A | 3391 | 1/1 | 0.92 | 0.12 | 122,122,122,122 | 0 |
| 56 | MG | 1A | 4339 | 1/1 | 0.92 | 0.21 | 59,59,59,59 | 0 |
| 56 | MG | 1A | 4340 | 1/1 | 0.92 | 0.20 | 57,57,57,57 | 0 |
| 56 | MG | 1A | 4341 | 1/1 | 0.92 | 0.21 | 48,48,48,48 | 0 |
| 56 | MG | 1a | 1779 | 1/1 | 0.92 | 0.58 | 122,122,122,122 | 0 |
| 56 | MG | 2A | 3061 | 1/1 | 0.92 | 0.84 | 92,92,92,92 | 0 |
| 56 | MG | 1A | 4911 | 1/1 | 0.92 | 0.24 | 62,62,62,62 | 0 |
| 56 | MG | 2A | 3063 | 1/1 | 0.92 | 0.19 | 83,83,83,83 | 0 |
| 56 | MG | 1A | 4247 | 1/1 | 0.92 | 0.31 | 49,49,49,49 | 0 |
| 56 | MG | 1A | 4719 | 1/1 | 0.92 | 0.12 | 89,89,89,89 | 0 |
| 56 | MG | 1R | 202 | 1/1 | 0.92 | 0.62 | 56,56,56,56 | 0 |
| 56 | MG | 1A | 4348 | 1/1 | 0.92 | 0.38 | 62,62,62,62 | 0 |
| 56 | MG | 2A | 3072 | 1/1 | 0.92 | 0.19 | 133,133,133,133 | 0 |
| 56 | MG | 1S | 201 | 1/1 | 0.92 | 0.58 | 74,74,74,74 | 0 |

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| Mol | Type | Chain | Res | Atoms | RSCC | RSR | B-factors(Å$^2$) | Q<0.9 |
|---|---|---|---|---|---|---|---|---|
| 56 | MG | 1A | 5037 | 1/1 | 0.92 | 0.11 | 78,78,78,78 | 0 |
| 56 | MG | 1A | 4290 | 1/1 | 0.92 | 0.58 | 70,70,70,70 | 0 |
| 56 | MG | 1A | 4821 | 1/1 | 0.92 | 0.21 | 73,73,73,73 | 0 |
| 56 | MG | 1A | 4313 | 1/1 | 0.92 | 0.44 | 50,50,50,50 | 0 |
| 56 | MG | 2A | 3080 | 1/1 | 0.92 | 0.05 | 127,127,127,127 | 0 |
| 56 | MG | 1A | 4657 | 1/1 | 0.92 | 0.26 | 84,84,84,84 | 0 |
| 56 | MG | 1A | 4193 | 1/1 | 0.92 | 0.15 | 64,64,64,64 | 0 |
| 56 | MG | 1A | 4594 | 1/1 | 0.92 | 0.31 | 64,64,64,64 | 0 |
| 56 | MG | 1a | 1797 | 1/1 | 0.92 | 0.33 | 85,85,85,85 | 0 |
| 56 | MG | 1A | 4833 | 1/1 | 0.92 | 0.64 | 70,70,70,70 | 0 |
| 56 | MG | 1W | 202 | 1/1 | 0.92 | 0.22 | 55,55,55,55 | 0 |
| 56 | MG | 1A | 4598 | 1/1 | 0.92 | 0.57 | 59,59,59,59 | 0 |
| 56 | MG | 1Z | 302 | 1/1 | 0.92 | 0.77 | 98,98,98,98 | 0 |
| 56 | MG | 1A | 4142 | 1/1 | 0.92 | 0.18 | 66,66,66,66 | 0 |
| 56 | MG | 2q | 204 | 1/1 | 0.92 | 0.61 | 141,141,141,141 | 0 |
| 56 | MG | 2A | 3439 | 1/1 | 0.92 | 0.45 | 56,56,56,56 | 0 |
| 56 | MG | 2A | 3816 | 1/1 | 0.92 | 0.40 | 121,121,121,121 | 0 |
| 56 | MG | 1A | 4837 | 1/1 | 0.92 | 0.19 | 57,57,57,57 | 0 |
| 56 | MG | 2A | 3441 | 1/1 | 0.92 | 0.19 | 109,109,109,109 | 0 |
| 56 | MG | 2t | 201 | 1/1 | 0.92 | 0.31 | 159,159,159,159 | 0 |
| 56 | MG | 1o | 102 | 1/1 | 0.92 | 0.36 | 69,69,69,69 | 0 |
| 56 | MG | 2A | 3628 | 1/1 | 0.92 | 0.53 | 119,119,119,119 | 0 |
| 56 | MG | 2A | 3444 | 1/1 | 0.92 | 0.30 | 99,99,99,99 | 0 |
| 56 | MG | 2A | 3254 | 1/1 | 0.92 | 0.09 | 122,122,122,122 | 0 |
| 56 | MG | 2A | 3447 | 1/1 | 0.92 | 0.53 | 87,87,87,87 | 0 |
| 56 | MG | 1A | 4664 | 1/1 | 0.92 | 0.18 | 73,73,73,73 | 0 |
| 56 | MG | 1A | 4180 | 1/1 | 0.92 | 0.38 | 48,48,48,48 | 0 |
| 56 | MG | 2A | 3258 | 1/1 | 0.92 | 0.45 | 75,75,75,75 | 0 |
| 56 | MG | 2A | 3259 | 1/1 | 0.92 | 0.50 | 82,82,82,82 | 0 |
| 56 | MG | 1A | 4525 | 1/1 | 0.92 | 0.70 | 104,104,104,104 | 0 |
| 56 | MG | 1A | 4749 | 1/1 | 0.92 | 0.31 | 77,77,77,77 | 0 |
| 56 | MG | 1A | 4156 | 1/1 | 0.92 | 0.30 | 54,54,54,54 | 0 |
| 56 | MG | 2A | 3839 | 1/1 | 0.92 | 0.20 | 139,139,139,139 | 0 |
| 56 | MG | 2A | 3463 | 1/1 | 0.92 | 0.60 | 67,67,67,67 | 0 |
| 56 | MG | 1b | 309 | 1/1 | 0.92 | 0.27 | 171,171,171,171 | 0 |
| 56 | MG | 2y | 102 | 1/1 | 0.92 | 0.20 | 73,73,73,73 | 0 |
| 56 | MG | 1a | 1697 | 1/1 | 0.92 | 0.25 | 142,142,142,142 | 0 |
| 56 | MG | 1d | 303 | 1/1 | 0.92 | 0.49 | 151,151,151,151 | 0 |
| 56 | MG | 1A | 4527 | 1/1 | 0.92 | 0.43 | 76,76,76,76 | 0 |
| 56 | MG | 2y | 107 | 1/1 | 0.92 | 0.57 | 207,207,207,207 | 0 |
| 56 | MG | 1a | 1821 | 1/1 | 0.92 | 0.15 | 202,202,202,202 | 0 |
| 56 | MG | 1a | 1701 | 1/1 | 0.92 | 0.08 | 153,153,153,153 | 0 |

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| Mol | Type | Chain | Res | Atoms | RSCC | RSR | B-factors(Å$^2$) | Q<0.9 |
|---|---|---|---|---|---|---|---|---|
| 56 | MG | 1A | 4412 | 1/1 | 0.92 | 0.32 | 62,62,62,62 | 0 |
| 56 | MG | 1A | 4530 | 1/1 | 0.92 | 0.32 | 68,68,68,68 | 0 |
| 56 | MG | 1A | 4484 | 1/1 | 0.92 | 0.34 | 60,60,60,60 | 0 |
| 56 | MG | 2a | 1834 | 1/1 | 0.92 | 0.13 | 161,161,161,161 | 0 |
| 56 | MG | 1a | 1605 | 1/1 | 0.92 | 0.24 | 89,89,89,89 | 0 |
| 56 | MG | 1A | 4157 | 1/1 | 0.92 | 0.40 | 52,52,52,52 | 0 |
| 56 | MG | 2A | 3481 | 1/1 | 0.92 | 0.43 | 112,112,112,112 | 0 |
| 56 | MG | 1A | 4486 | 1/1 | 0.92 | 0.32 | 67,67,67,67 | 0 |
| 57 | ZN | 26 | 102 | 1/1 | 0.92 | 0.07 | 130,130,130,130 | 0 |
| 56 | MG | 1a | 1830 | 1/1 | 0.92 | 0.10 | 194,194,194,194 | 0 |
| 56 | MG | 2A | 3291 | 1/1 | 0.92 | 0.34 | 75,75,75,75 | 0 |
| 56 | MG | 1a | 1608 | 1/1 | 0.92 | 0.36 | 69,69,69,69 | 0 |
| 56 | MG | 2a | 1814 | 1/1 | 0.93 | 0.23 | 142,142,142,142 | 0 |
| 56 | MG | 1A | 4233 | 1/1 | 0.93 | 0.22 | 65,65,65,65 | 0 |
| 56 | MG | 1A | 4296 | 1/1 | 0.93 | 0.84 | 82,82,82,82 | 0 |
| 56 | MG | 2A | 3366 | 1/1 | 0.93 | 0.57 | 82,82,82,82 | 0 |
| 56 | MG | 1A | 4575 | 1/1 | 0.93 | 0.24 | 56,56,56,56 | 0 |
| 56 | MG | 1A | 4234 | 1/1 | 0.93 | 0.34 | 59,59,59,59 | 0 |
| 56 | MG | 1A | 4059 | 1/1 | 0.93 | 0.36 | 72,72,72,72 | 0 |
| 56 | MG | 2a | 1829 | 1/1 | 0.93 | 0.18 | 147,147,147,147 | 0 |
| 56 | MG | 2A | 3004 | 1/1 | 0.93 | 0.83 | 93,93,93,93 | 0 |
| 56 | MG | 2A | 3162 | 1/1 | 0.93 | 0.30 | 102,102,102,102 | 0 |
| 56 | MG | 2A | 3569 | 1/1 | 0.93 | 0.21 | 96,96,96,96 | 0 |
| 56 | MG | 2A | 3570 | 1/1 | 0.93 | 0.16 | 167,167,167,167 | 0 |
| 56 | MG | 2A | 3005 | 1/1 | 0.93 | 0.87 | 102,102,102,102 | 0 |
| 56 | MG | 1A | 4299 | 1/1 | 0.93 | 0.32 | 95,95,95,95 | 0 |
| 56 | MG | 1Y | 301 | 1/1 | 0.93 | 0.14 | 85,85,85,85 | 0 |
| 56 | MG | 2A | 3170 | 1/1 | 0.93 | 0.48 | 90,90,90,90 | 0 |
| 56 | MG | 2a | 1652 | 1/1 | 0.93 | 0.11 | 142,142,142,142 | 0 |
| 56 | MG | 1A | 4238 | 1/1 | 0.93 | 0.28 | 59,59,59,59 | 0 |
| 56 | MG | 1A | 5023 | 1/1 | 0.93 | 0.28 | 58,58,58,58 | 0 |
| 56 | MG | 1a | 1841 | 1/1 | 0.93 | 0.23 | 231,231,231,231 | 0 |
| 56 | MG | 2a | 1851 | 1/1 | 0.93 | 0.09 | 145,145,145,145 | 0 |
| 56 | MG | 2a | 1852 | 1/1 | 0.93 | 0.27 | 45,45,45,45 | 0 |
| 56 | MG | 2A | 3012 | 1/1 | 0.93 | 0.51 | 108,108,108,108 | 0 |
| 56 | MG | 1A | 4583 | 1/1 | 0.93 | 0.27 | 56,56,56,56 | 0 |
| 56 | MG | 1A | 4405 | 1/1 | 0.93 | 0.13 | 71,71,71,71 | 0 |
| 56 | MG | 1A | 4669 | 1/1 | 0.93 | 0.50 | 89,89,89,89 | 0 |
| 56 | MG | 1A | 4124 | 1/1 | 0.93 | 0.21 | 76,76,76,76 | 0 |
| 56 | MG | 2A | 3588 | 1/1 | 0.93 | 0.09 | 127,127,127,127 | 0 |
| 56 | MG | 1A | 4672 | 1/1 | 0.93 | 0.54 | 67,67,67,67 | 0 |
| 56 | MG | 1A | 4077 | 1/1 | 0.93 | 0.24 | 78,78,78,78 | 0 |

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| Mol | Type | Chain | Res | Atoms | RSCC | RSR | B-factors(Å$^2$) | Q<0.9 |
|---|---|---|---|---|---|---|---|---|
| 56 | MG | 1A | 4065 | 1/1 | 0.93 | 0.81 | 67,67,67,67 | 0 |
| 56 | MG | 2A | 3594 | 1/1 | 0.93 | 0.12 | 74,74,74,74 | 0 |
| 56 | MG | 17 | 101 | 1/1 | 0.93 | 0.40 | 58,58,58,58 | 0 |
| 56 | MG | 1a | 1855 | 1/1 | 0.93 | 0.81 | 230,230,230,230 | 0 |
| 56 | MG | 1A | 4049 | 1/1 | 0.93 | 0.43 | 97,97,97,97 | 0 |
| 56 | MG | 1A | 4081 | 1/1 | 0.93 | 0.29 | 57,57,57,57 | 0 |
| 56 | MG | 2A | 3604 | 1/1 | 0.93 | 0.15 | 110,110,110,110 | 0 |
| 56 | MG | 1A | 4106 | 1/1 | 0.93 | 0.33 | 50,50,50,50 | 0 |
| 56 | MG | 1a | 1733 | 1/1 | 0.93 | 0.12 | 149,149,149,149 | 0 |
| 56 | MG | 1A | 4775 | 1/1 | 0.93 | 0.32 | 78,78,78,78 | 0 |
| 56 | MG | 1a | 1861 | 1/1 | 0.93 | 0.25 | 216,216,216,216 | 0 |
| 56 | MG | 1A | 4133 | 1/1 | 0.93 | 0.37 | 58,58,58,58 | 0 |
| 56 | MG | 1A | 4108 | 1/1 | 0.93 | 0.34 | 52,52,52,52 | 0 |
| 56 | MG | 2A | 3411 | 1/1 | 0.93 | 0.34 | 100,100,100,100 | 0 |
| 56 | MG | 1A | 4433 | 1/1 | 0.93 | 0.15 | 79,79,79,79 | 0 |
| 56 | MG | 2A | 3413 | 1/1 | 0.93 | 0.17 | 126,126,126,126 | 0 |
| 56 | MG | 2A | 3039 | 1/1 | 0.93 | 0.65 | 80,80,80,80 | 0 |
| 56 | MG | 2A | 3415 | 1/1 | 0.93 | 0.28 | 124,124,124,124 | 0 |
| 56 | MG | 1A | 4022 | 1/1 | 0.93 | 0.78 | 111,111,111,111 | 0 |
| 56 | MG | 2A | 3625 | 1/1 | 0.93 | 0.55 | 146,146,146,146 | 0 |
| 56 | MG | 1A | 4363 | 1/1 | 0.93 | 0.13 | 72,72,72,72 | 0 |
| 56 | MG | 2A | 3042 | 1/1 | 0.93 | 0.34 | 112,112,112,112 | 0 |
| 56 | MG | 2A | 3215 | 1/1 | 0.93 | 0.21 | 100,100,100,100 | 0 |
| 56 | MG | 1A | 4781 | 1/1 | 0.93 | 0.45 | 81,81,81,81 | 0 |
| 56 | MG | 1a | 1744 | 1/1 | 0.93 | 0.28 | 132,132,132,132 | 0 |
| 56 | MG | 2A | 3218 | 1/1 | 0.93 | 0.16 | 103,103,103,103 | 0 |
| 56 | MG | 1a | 1870 | 1/1 | 0.93 | 0.14 | 220,220,220,220 | 0 |
| 56 | MG | 2B | 211 | 1/1 | 0.93 | 0.56 | 88,88,88,88 | 0 |
| 56 | MG | 2A | 3048 | 1/1 | 0.93 | 0.20 | 88,88,88,88 | 0 |
| 56 | MG | 2a | 1702 | 1/1 | 0.93 | 0.41 | 156,156,156,156 | 0 |
| 56 | MG | 1A | 4912 | 1/1 | 0.93 | 0.41 | 57,57,57,57 | 0 |
| 56 | MG | 2A | 3636 | 1/1 | 0.93 | 0.21 | 125,125,125,125 | 0 |
| 56 | MG | 2A | 3052 | 1/1 | 0.93 | 0.15 | 103,103,103,103 | 0 |
| 56 | MG | 2A | 3226 | 1/1 | 0.93 | 0.19 | 100,100,100,100 | 0 |
| 56 | MG | 1A | 4367 | 1/1 | 0.93 | 0.33 | 56,56,56,56 | 0 |
| 56 | MG | 2A | 3056 | 1/1 | 0.93 | 0.74 | 107,107,107,107 | 0 |
| 56 | MG | 1A | 4690 | 1/1 | 0.93 | 0.15 | 83,83,83,83 | 0 |
| 56 | MG | 1A | 4267 | 1/1 | 0.93 | 0.38 | 63,63,63,63 | 0 |
| 56 | MG | 1a | 1753 | 1/1 | 0.93 | 0.21 | 115,115,115,115 | 0 |
| 56 | MG | 1a | 1878 | 1/1 | 0.93 | 0.16 | 105,105,105,105 | 0 |
| 56 | MG | 2A | 3239 | 1/1 | 0.93 | 0.26 | 108,108,108,108 | 0 |
| 56 | MG | 1A | 4083 | 1/1 | 0.93 | 0.17 | 58,58,58,58 | 0 |

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| Mol | Type | Chain | Res | Atoms | RSCC | RSR | B-factors(Å$^2$) | Q<0.9 |
|---|---|---|---|---|---|---|---|---|
| 56 | MG | 1A | 4694 | 1/1 | 0.93 | 0.36 | 70,70,70,70 | 0 |
| 56 | MG | 2a | 1914 | 1/1 | 0.93 | 0.12 | 242,242,242,242 | 0 |
| 56 | MG | 2a | 1915 | 1/1 | 0.93 | 0.09 | 123,123,123,123 | 0 |
| 56 | MG | 1A | 4923 | 1/1 | 0.93 | 0.22 | 66,66,66,66 | 0 |
| 56 | MG | 1a | 1883 | 1/1 | 0.93 | 0.30 | 124,124,124,124 | 0 |
| 56 | MG | 2A | 3655 | 1/1 | 0.93 | 0.55 | 117,117,117,117 | 0 |
| 56 | MG | 2b | 301 | 1/1 | 0.93 | 0.08 | 199,199,199,199 | 0 |
| 56 | MG | 2b | 302 | 1/1 | 0.93 | 0.14 | 196,196,196,196 | 0 |
| 56 | MG | 1A | 4448 | 1/1 | 0.93 | 0.44 | 78,78,78,78 | 0 |
| 56 | MG | 2A | 3660 | 1/1 | 0.93 | 0.34 | 147,147,147,147 | 0 |
| 56 | MG | 2A | 3458 | 1/1 | 0.93 | 0.44 | 90,90,90,90 | 0 |
| 56 | MG | 1a | 1625 | 1/1 | 0.93 | 0.39 | 80,80,80,80 | 0 |
| 56 | MG | 1A | 4926 | 1/1 | 0.93 | 0.40 | 76,76,76,76 | 0 |
| 56 | MG | 1A | 4797 | 1/1 | 0.93 | 0.40 | 78,78,78,78 | 0 |
| 56 | MG | 1A | 4069 | 1/1 | 0.93 | 0.31 | 72,72,72,72 | 0 |
| 56 | MG | 2E | 301 | 1/1 | 0.93 | 0.19 | 91,91,91,91 | 0 |
| 56 | MG | 1A | 4372 | 1/1 | 0.93 | 0.30 | 57,57,57,57 | 0 |
| 56 | MG | 1a | 1896 | 1/1 | 0.93 | 0.19 | 114,114,114,114 | 0 |
| 56 | MG | 1A | 4071 | 1/1 | 0.93 | 0.19 | 77,77,77,77 | 0 |
| 56 | MG | 1A | 4619 | 1/1 | 0.93 | 0.25 | 103,103,103,103 | 0 |
| 56 | MG | 1A | 4143 | 1/1 | 0.93 | 0.20 | 62,62,62,62 | 0 |
| 56 | MG | 1A | 4941 | 1/1 | 0.93 | 0.20 | 61,61,61,61 | 0 |
| 56 | MG | 1A | 4222 | 1/1 | 0.93 | 0.28 | 70,70,70,70 | 0 |
| 56 | MG | 1A | 4623 | 1/1 | 0.93 | 0.30 | 85,85,85,85 | 0 |
| 56 | MG | 1A | 4223 | 1/1 | 0.93 | 0.13 | 70,70,70,70 | 0 |
| 56 | MG | 1A | 4457 | 1/1 | 0.93 | 0.18 | 81,81,81,81 | 0 |
| 56 | MG | 2a | 1742 | 1/1 | 0.93 | 0.59 | 148,148,148,148 | 0 |
| 56 | MG | 2P | 202 | 1/1 | 0.93 | 0.56 | 127,127,127,127 | 0 |
| 56 | MG | 1B | 215 | 1/1 | 0.93 | 0.33 | 65,65,65,65 | 0 |
| 56 | MG | 2A | 3480 | 1/1 | 0.93 | 0.31 | 132,132,132,132 | 0 |
| 56 | MG | 1A | 4058 | 1/1 | 0.93 | 0.68 | 67,67,67,67 | 0 |
| 56 | MG | 2A | 3093 | 1/1 | 0.93 | 0.35 | 96,96,96,96 | 0 |
| 56 | MG | 1B | 218 | 1/1 | 0.93 | 0.41 | 61,61,61,61 | 0 |
| 56 | MG | 1A | 4324 | 1/1 | 0.93 | 0.80 | 78,78,78,78 | 0 |
| 56 | MG | 2A | 3279 | 1/1 | 0.93 | 0.58 | 80,80,80,80 | 0 |
| 56 | MG | 2S | 201 | 1/1 | 0.93 | 0.17 | 87,87,87,87 | 0 |
| 56 | MG | 1A | 4537 | 1/1 | 0.93 | 0.47 | 66,66,66,66 | 0 |
| 56 | MG | 2A | 3489 | 1/1 | 0.93 | 0.49 | 53,53,53,53 | 0 |
| 56 | MG | 1A | 4326 | 1/1 | 0.93 | 0.32 | 67,67,67,67 | 0 |
| 56 | MG | 1A | 4381 | 1/1 | 0.93 | 0.17 | 72,72,72,72 | 0 |
| 56 | MG | 1B | 224 | 1/1 | 0.93 | 0.50 | 83,83,83,83 | 0 |
| 56 | MG | 1B | 226 | 1/1 | 0.93 | 0.31 | 64,64,64,64 | 0 |

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| Mol | Type | Chain | Res | Atoms | RSCC | RSR | B-factors(Å$^2$) | Q<0.9 |
|---|---|---|---|---|---|---|---|---|
| 56 | MG | 1a | 1655 | 1/1 | 0.93 | 0.18 | 120,120,120,120 | 0 |
| 56 | MG | 1A | 4542 | 1/1 | 0.93 | 0.21 | 56,56,56,56 | 0 |
| 56 | MG | 1A | 4286 | 1/1 | 0.93 | 0.22 | 71,71,71,71 | 0 |
| 56 | MG | 2A | 3503 | 1/1 | 0.93 | 0.37 | 103,103,103,103 | 0 |
| 56 | MG | 1A | 4148 | 1/1 | 0.93 | 0.22 | 64,64,64,64 | 0 |
| 56 | MG | 2A | 3505 | 1/1 | 0.93 | 0.32 | 129,129,129,129 | 0 |
| 56 | MG | 1A | 4090 | 1/1 | 0.93 | 0.36 | 55,55,55,55 | 0 |
| 56 | MG | 2A | 3721 | 1/1 | 0.93 | 0.29 | 118,118,118,118 | 0 |
| 56 | MG | 1A | 4722 | 1/1 | 0.93 | 0.39 | 75,75,75,75 | 0 |
| 56 | MG | 1A | 4965 | 1/1 | 0.93 | 0.23 | 66,66,66,66 | 0 |
| 56 | MG | 1A | 4840 | 1/1 | 0.93 | 0.21 | 71,71,71,71 | 0 |
| 56 | MG | 1a | 1799 | 1/1 | 0.93 | 0.16 | 113,113,113,113 | 0 |
| 56 | MG | 25 | 101 | 1/1 | 0.93 | 0.39 | 45,45,45,45 | 0 |
| 56 | MG | 1a | 1800 | 1/1 | 0.93 | 0.10 | 119,119,119,119 | 0 |
| 56 | MG | 1A | 4547 | 1/1 | 0.93 | 0.38 | 129,129,129,129 | 0 |
| 56 | MG | 1A | 4482 | 1/1 | 0.93 | 0.17 | 61,61,61,61 | 0 |
| 56 | MG | 2A | 3734 | 1/1 | 0.93 | 0.32 | 108,108,108,108 | 0 |
| 56 | MG | 1A | 4725 | 1/1 | 0.93 | 0.17 | 73,73,73,73 | 0 |
| 56 | MG | 1A | 4726 | 1/1 | 0.93 | 0.44 | 79,79,79,79 | 0 |
| 56 | MG | 1A | 4980 | 1/1 | 0.93 | 1.06 | 59,59,59,59 | 0 |
| 56 | MG | 1A | 4727 | 1/1 | 0.93 | 0.30 | 82,82,82,82 | 0 |
| 56 | MG | 2A | 3125 | 1/1 | 0.93 | 0.19 | 81,81,81,81 | 0 |
| 56 | MG | 2A | 3126 | 1/1 | 0.93 | 0.25 | 138,138,138,138 | 0 |
| 56 | MG | 1A | 4387 | 1/1 | 0.93 | 0.22 | 81,81,81,81 | 0 |
| 56 | MG | 1A | 4643 | 1/1 | 0.93 | 0.22 | 64,64,64,64 | 0 |
| 56 | MG | 2A | 3331 | 1/1 | 0.93 | 0.48 | 91,91,91,91 | 0 |
| 56 | MG | 2A | 3746 | 1/1 | 0.93 | 0.24 | 93,93,93,93 | 0 |
| 56 | MG | 1A | 4734 | 1/1 | 0.93 | 0.21 | 64,64,64,64 | 0 |
| 56 | MG | 2A | 3535 | 1/1 | 0.93 | 0.11 | 141,141,141,141 | 0 |
| 56 | MG | 1A | 4389 | 1/1 | 0.93 | 0.11 | 78,78,78,78 | 0 |
| 56 | MG | 1A | 4739 | 1/1 | 0.93 | 0.17 | 74,74,74,74 | 0 |
| 56 | MG | 2a | 1613 | 1/1 | 0.93 | 0.25 | 147,147,147,147 | 0 |
| 56 | MG | 1A | 4189 | 1/1 | 0.93 | 0.26 | 60,60,60,60 | 0 |
| 56 | MG | 1A | 4231 | 1/1 | 0.93 | 0.10 | 72,72,72,72 | 0 |
| 56 | MG | 1A | 4394 | 1/1 | 0.93 | 0.26 | 60,60,60,60 | 0 |
| 56 | MG | 2A | 3756 | 1/1 | 0.93 | 0.31 | 137,137,137,137 | 0 |
| 56 | MG | 1A | 4561 | 1/1 | 0.93 | 0.21 | 57,57,57,57 | 0 |
| 56 | MG | 1A | 4864 | 1/1 | 0.93 | 0.19 | 75,75,75,75 | 0 |
| 56 | MG | 2A | 3544 | 1/1 | 0.93 | 0.22 | 108,108,108,108 | 0 |
| 56 | MG | 2A | 3144 | 1/1 | 0.93 | 0.33 | 65,65,65,65 | 0 |
| 56 | MG | 2A | 3344 | 1/1 | 0.93 | 0.23 | 91,91,91,91 | 0 |
| 56 | MG | 1A | 4865 | 1/1 | 0.93 | 0.33 | 64,64,64,64 | 0 |

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| Mol | Type | Chain | Res | Atoms | RSCC | RSR | B-factors(Å$^2$) | Q<0.9 |
|---|---|---|---|---|---|---|---|---|
| 56 | MG | 1A | 5005 | 1/1 | 0.93 | 0.25 | 86,86,86,86 | 0 |
| 56 | MG | 1a | 1689 | 1/1 | 0.93 | 0.13 | 133,133,133,133 | 0 |
| 56 | MG | 1A | 4489 | 1/1 | 0.93 | 0.11 | 75,75,75,75 | 0 |
| 56 | MG | 1T | 203 | 1/1 | 0.93 | 0.76 | 62,62,62,62 | 0 |
| 56 | MG | 2a | 1809 | 1/1 | 0.93 | 0.24 | 122,122,122,122 | 0 |
| 56 | MG | 1A | 5007 | 1/1 | 0.93 | 0.19 | 92,92,92,92 | 0 |
| 56 | MG | 2A | 3513 | 1/1 | 0.94 | 0.19 | 85,85,85,85 | 0 |
| 56 | MG | 1A | 4663 | 1/1 | 0.94 | 0.31 | 89,89,89,89 | 0 |
| 56 | MG | 2A | 3301 | 1/1 | 0.94 | 0.34 | 96,96,96,96 | 0 |
| 56 | MG | 1A | 4936 | 1/1 | 0.94 | 0.18 | 61,61,61,61 | 0 |
| 56 | MG | 2A | 3520 | 1/1 | 0.94 | 0.19 | 91,91,91,91 | 0 |
| 56 | MG | 1a | 1602 | 1/1 | 0.94 | 0.38 | 77,77,77,77 | 0 |
| 56 | MG | 2A | 3306 | 1/1 | 0.94 | 0.30 | 85,85,85,85 | 0 |
| 56 | MG | 2a | 1611 | 1/1 | 0.94 | 0.21 | 143,143,143,143 | 0 |
| 56 | MG | 1A | 4738 | 1/1 | 0.94 | 0.19 | 70,70,70,70 | 0 |
| 56 | MG | 2A | 3740 | 1/1 | 0.94 | 0.47 | 88,88,88,88 | 0 |
| 56 | MG | 1y | 102 | 1/1 | 0.94 | 0.44 | 123,123,123,123 | 0 |
| 56 | MG | 1A | 4278 | 1/1 | 0.94 | 0.41 | 65,65,65,65 | 0 |
| 56 | MG | 2a | 1817 | 1/1 | 0.94 | 0.12 | 133,133,133,133 | 0 |
| 56 | MG | 1A | 4836 | 1/1 | 0.94 | 0.29 | 58,58,58,58 | 0 |
| 56 | MG | 1A | 4466 | 1/1 | 0.94 | 0.24 | 56,56,56,56 | 0 |
| 56 | MG | 2A | 3138 | 1/1 | 0.94 | 0.49 | 118,118,118,118 | 0 |
| 56 | MG | 2A | 3139 | 1/1 | 0.94 | 0.20 | 102,102,102,102 | 0 |
| 56 | MG | 2A | 3141 | 1/1 | 0.94 | 0.27 | 96,96,96,96 | 0 |
| 56 | MG | 2A | 3328 | 1/1 | 0.94 | 0.18 | 91,91,91,91 | 0 |
| 56 | MG | 1z | 101 | 1/1 | 0.94 | 0.19 | 151,151,151,151 | 0 |
| 56 | MG | 1A | 4467 | 1/1 | 0.94 | 0.42 | 57,57,57,57 | 0 |
| 56 | MG | 1A | 4528 | 1/1 | 0.94 | 0.34 | 73,73,73,73 | 0 |
| 56 | MG | 2A | 3145 | 1/1 | 0.94 | 0.68 | 100,100,100,100 | 0 |
| 56 | MG | 1A | 4844 | 1/1 | 0.94 | 0.35 | 77,77,77,77 | 0 |
| 56 | MG | 2A | 3336 | 1/1 | 0.94 | 0.44 | 95,95,95,95 | 0 |
| 56 | MG | 1A | 4409 | 1/1 | 0.94 | 0.21 | 56,56,56,56 | 0 |
| 56 | MG | 2a | 1842 | 1/1 | 0.94 | 0.16 | 196,196,196,196 | 0 |
| 56 | MG | 2A | 3148 | 1/1 | 0.94 | 0.74 | 76,76,76,76 | 0 |
| 56 | MG | 1A | 4473 | 1/1 | 0.94 | 0.40 | 46,46,46,46 | 0 |
| 56 | MG | 2A | 3543 | 1/1 | 0.94 | 0.16 | 100,100,100,100 | 0 |
| 56 | MG | 1a | 1617 | 1/1 | 0.94 | 0.41 | 79,79,79,79 | 0 |
| 56 | MG | 1A | 4477 | 1/1 | 0.94 | 0.30 | 71,71,71,71 | 0 |
| 56 | MG | 1A | 4849 | 1/1 | 0.94 | 0.14 | 84,84,84,84 | 0 |
| 56 | MG | 2a | 1850 | 1/1 | 0.94 | 0.16 | 154,154,154,154 | 0 |
| 56 | MG | 2A | 3547 | 1/1 | 0.94 | 0.25 | 104,104,104,104 | 0 |
| 56 | MG | 2a | 1640 | 1/1 | 0.94 | 0.36 | 143,143,143,143 | 0 |

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| Mol | Type | Chain | Res | Atoms | RSCC | RSR | B-factors(Å$^2$) | Q<0.9 |
|---|---|---|---|---|---|---|---|---|
| 56 | MG | 1A | 4479 | 1/1 | 0.94 | 0.31 | 71,71,71,71 | 0 |
| 56 | MG | 1A | 4141 | 1/1 | 0.94 | 0.29 | 63,63,63,63 | 0 |
| 56 | MG | 1A | 4958 | 1/1 | 0.94 | 0.31 | 95,95,95,95 | 0 |
| 56 | MG | 2A | 3349 | 1/1 | 0.94 | 0.20 | 104,104,104,104 | 0 |
| 56 | MG | 2a | 1858 | 1/1 | 0.94 | 0.29 | 149,149,149,149 | 0 |
| 56 | MG | 2A | 3775 | 1/1 | 0.94 | 0.19 | 114,114,114,114 | 0 |
| 56 | MG | 1A | 4959 | 1/1 | 0.94 | 0.49 | 102,102,102,102 | 0 |
| 56 | MG | 1A | 4414 | 1/1 | 0.94 | 0.36 | 66,66,66,66 | 0 |
| 56 | MG | 2A | 3779 | 1/1 | 0.94 | 0.37 | 98,98,98,98 | 0 |
| 56 | MG | 1A | 4306 | 1/1 | 0.94 | 0.19 | 97,97,97,97 | 0 |
| 56 | MG | 1A | 4021 | 1/1 | 0.94 | 0.55 | 76,76,76,76 | 0 |
| 56 | MG | 2A | 3359 | 1/1 | 0.94 | 0.33 | 84,84,84,84 | 0 |
| 56 | MG | 2A | 3559 | 1/1 | 0.94 | 0.33 | 91,91,91,91 | 0 |
| 56 | MG | 2A | 3360 | 1/1 | 0.94 | 0.38 | 78,78,78,78 | 0 |
| 56 | MG | 2A | 3561 | 1/1 | 0.94 | 0.36 | 88,88,88,88 | 0 |
| 56 | MG | 2a | 1871 | 1/1 | 0.94 | 0.33 | 134,134,134,134 | 0 |
| 56 | MG | 2A | 3361 | 1/1 | 0.94 | 0.29 | 94,94,94,94 | 0 |
| 56 | MG | 1A | 4241 | 1/1 | 0.94 | 0.47 | 66,66,66,66 | 0 |
| 56 | MG | 2A | 3363 | 1/1 | 0.94 | 0.39 | 85,85,85,85 | 0 |
| 56 | MG | 2A | 3166 | 1/1 | 0.94 | 0.69 | 85,85,85,85 | 0 |
| 56 | MG | 2A | 3567 | 1/1 | 0.94 | 0.13 | 104,104,104,104 | 0 |
| 56 | MG | 2A | 3365 | 1/1 | 0.94 | 0.38 | 90,90,90,90 | 0 |
| 56 | MG | 1A | 4309 | 1/1 | 0.94 | 0.46 | 79,79,79,79 | 0 |
| 56 | MG | 1A | 4685 | 1/1 | 0.94 | 0.51 | 70,70,70,70 | 0 |
| 56 | MG | 2a | 1880 | 1/1 | 0.94 | 0.17 | 158,158,158,158 | 0 |
| 56 | MG | 2A | 3024 | 1/1 | 0.94 | 0.74 | 123,123,123,123 | 0 |
| 56 | MG | 2A | 3171 | 1/1 | 0.94 | 0.46 | 88,88,88,88 | 0 |
| 56 | MG | 1A | 4544 | 1/1 | 0.94 | 0.19 | 77,77,77,77 | 0 |
| 56 | MG | 1A | 4107 | 1/1 | 0.94 | 0.27 | 52,52,52,52 | 0 |
| 56 | MG | 1a | 1762 | 1/1 | 0.94 | 0.42 | 103,103,103,103 | 0 |
| 56 | MG | 2A | 3178 | 1/1 | 0.94 | 0.48 | 116,116,116,116 | 0 |
| 56 | MG | 2A | 3814 | 1/1 | 0.94 | 0.31 | 128,128,128,128 | 0 |
| 56 | MG | 2A | 3578 | 1/1 | 0.94 | 0.49 | 135,135,135,135 | 0 |
| 56 | MG | 2A | 3029 | 1/1 | 0.94 | 0.82 | 105,105,105,105 | 0 |
| 56 | MG | 1A | 4378 | 1/1 | 0.94 | 0.27 | 83,83,83,83 | 0 |
| 56 | MG | 2A | 3380 | 1/1 | 0.94 | 0.12 | 93,93,93,93 | 0 |
| 56 | MG | 1A | 4975 | 1/1 | 0.94 | 0.17 | 76,76,76,76 | 0 |
| 56 | MG | 1A | 4976 | 1/1 | 0.94 | 0.24 | 77,77,77,77 | 0 |
| 56 | MG | 1a | 1877 | 1/1 | 0.94 | 0.15 | 106,106,106,106 | 0 |
| 56 | MG | 2A | 3186 | 1/1 | 0.94 | 0.35 | 105,105,105,105 | 0 |
| 56 | MG | 2A | 3829 | 1/1 | 0.94 | 0.17 | 113,113,113,113 | 0 |
| 56 | MG | 2A | 3036 | 1/1 | 0.94 | 0.66 | 76,76,76,76 | 0 |

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| Mol | Type | Chain | Res | Atoms | RSCC | RSR | B-factors(Å$^2$) | Q<0.9 |
|---|---|---|---|---|---|---|---|---|
| 56 | MG | 2a | 1689 | 1/1 | 0.94 | 0.23 | 156,156,156,156 | 0 |
| 56 | MG | 1A | 4074 | 1/1 | 0.94 | 0.33 | 78,78,78,78 | 0 |
| 56 | MG | 1D | 305 | 1/1 | 0.94 | 0.30 | 81,81,81,81 | 0 |
| 56 | MG | 1A | 4183 | 1/1 | 0.94 | 0.14 | 63,63,63,63 | 0 |
| 56 | MG | 1a | 1881 | 1/1 | 0.94 | 0.11 | 151,151,151,151 | 0 |
| 56 | MG | 1A | 4692 | 1/1 | 0.94 | 0.54 | 61,61,61,61 | 0 |
| 56 | MG | 1A | 4627 | 1/1 | 0.94 | 0.37 | 80,80,80,80 | 0 |
| 56 | MG | 2a | 1908 | 1/1 | 0.94 | 0.16 | 230,230,230,230 | 0 |
| 56 | MG | 2A | 3603 | 1/1 | 0.94 | 0.13 | 103,103,103,103 | 0 |
| 56 | MG | 1a | 1772 | 1/1 | 0.94 | 0.05 | 136,136,136,136 | 0 |
| 56 | MG | 1a | 1885 | 1/1 | 0.94 | 0.11 | 128,128,128,128 | 0 |
| 56 | MG | 2A | 3200 | 1/1 | 0.94 | 0.19 | 109,109,109,109 | 0 |
| 56 | MG | 2A | 3845 | 1/1 | 0.94 | 0.82 | 85,85,85,85 | 0 |
| 56 | MG | 1a | 1889 | 1/1 | 0.94 | 0.18 | 153,153,153,153 | 0 |
| 56 | MG | 1A | 4773 | 1/1 | 0.94 | 0.28 | 68,68,68,68 | 0 |
| 56 | MG | 1A | 4227 | 1/1 | 0.94 | 0.20 | 86,86,86,86 | 0 |
| 56 | MG | 1a | 1892 | 1/1 | 0.94 | 0.42 | 117,117,117,117 | 0 |
| 56 | MG | 1E | 304 | 1/1 | 0.94 | 0.20 | 71,71,71,71 | 0 |
| 56 | MG | 1a | 1652 | 1/1 | 0.94 | 0.25 | 117,117,117,117 | 0 |
| 56 | MG | 1A | 4439 | 1/1 | 0.94 | 0.24 | 80,80,80,80 | 0 |
| 56 | MG | 1A | 4441 | 1/1 | 0.94 | 0.44 | 78,78,78,78 | 0 |
| 56 | MG | 2A | 3212 | 1/1 | 0.94 | 0.11 | 93,93,93,93 | 0 |
| 56 | MG | 2A | 3622 | 1/1 | 0.94 | 0.45 | 137,137,137,137 | 0 |
| 56 | MG | 2a | 1715 | 1/1 | 0.94 | 0.36 | 147,147,147,147 | 0 |
| 56 | MG | 2A | 3213 | 1/1 | 0.94 | 0.35 | 88,88,88,88 | 0 |
| 56 | MG | 2A | 3060 | 1/1 | 0.94 | 0.52 | 85,85,85,85 | 0 |
| 56 | MG | 1a | 1897 | 1/1 | 0.94 | 0.90 | 124,124,124,124 | 0 |
| 56 | MG | 1A | 4632 | 1/1 | 0.94 | 0.67 | 66,66,66,66 | 0 |
| 56 | MG | 1A | 4883 | 1/1 | 0.94 | 0.22 | 59,59,59,59 | 0 |
| 56 | MG | 1H | 202 | 1/1 | 0.94 | 0.39 | 76,76,76,76 | 0 |
| 56 | MG | 2A | 3630 | 1/1 | 0.94 | 0.39 | 102,102,102,102 | 0 |
| 56 | MG | 2A | 3065 | 1/1 | 0.94 | 0.22 | 117,117,117,117 | 0 |
| 56 | MG | 1A | 4442 | 1/1 | 0.94 | 0.15 | 75,75,75,75 | 0 |
| 56 | MG | 1A | 4033 | 1/1 | 0.94 | 0.26 | 70,70,70,70 | 0 |
| 56 | MG | 2A | 3069 | 1/1 | 0.94 | 0.23 | 149,149,149,149 | 0 |
| 56 | MG | 2A | 3225 | 1/1 | 0.94 | 0.58 | 113,113,113,113 | 0 |
| 56 | MG | 1A | 4007 | 1/1 | 0.94 | 0.22 | 64,64,64,64 | 0 |
| 56 | MG | 2A | 3227 | 1/1 | 0.94 | 0.20 | 94,94,94,94 | 0 |
| 56 | MG | 1a | 1789 | 1/1 | 0.94 | 0.20 | 111,111,111,111 | 0 |
| 56 | MG | 1A | 4317 | 1/1 | 0.94 | 0.70 | 106,106,106,106 | 0 |
| 56 | MG | 1A | 4292 | 1/1 | 0.94 | 0.42 | 96,96,96,96 | 0 |
| 56 | MG | 1a | 1907 | 1/1 | 0.94 | 0.35 | 117,117,117,117 | 0 |

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| Mol | Type | Chain | Res | Atoms | RSCC | RSR | B-factors(Å$^2$) | Q<0.9 |
|---|---|---|---|---|---|---|---|---|
| 56 | MG | 1A | 4263 | 1/1 | 0.94 | 0.56 | 51,51,51,51 | 0 |
| 56 | MG | 1A | 5011 | 1/1 | 0.94 | 0.32 | 77,77,77,77 | 0 |
| 56 | MG | 1A | 4264 | 1/1 | 0.94 | 0.39 | 61,61,61,61 | 0 |
| 56 | MG | 2A | 3443 | 1/1 | 0.94 | 0.18 | 111,111,111,111 | 0 |
| 56 | MG | 1A | 4057 | 1/1 | 0.94 | 0.75 | 63,63,63,63 | 0 |
| 56 | MG | 1Q | 203 | 1/1 | 0.94 | 0.41 | 50,50,50,50 | 0 |
| 56 | MG | 2a | 1743 | 1/1 | 0.94 | 0.70 | 151,151,151,151 | 0 |
| 56 | MG | 1A | 4360 | 1/1 | 0.94 | 0.12 | 88,88,88,88 | 0 |
| 56 | MG | 1a | 1914 | 1/1 | 0.94 | 0.19 | 193,193,193,193 | 0 |
| 56 | MG | 1A | 4166 | 1/1 | 0.94 | 0.40 | 34,34,34,34 | 0 |
| 56 | MG | 2A | 3450 | 1/1 | 0.94 | 0.60 | 85,85,85,85 | 0 |
| 56 | MG | 1A | 4896 | 1/1 | 0.94 | 1.29 | 61,61,61,61 | 0 |
| 56 | MG | 1A | 4454 | 1/1 | 0.94 | 0.27 | 78,78,78,78 | 0 |
| 56 | MG | 1A | 4646 | 1/1 | 0.94 | 0.28 | 69,69,69,69 | 0 |
| 56 | MG | 2A | 3459 | 1/1 | 0.94 | 0.47 | 98,98,98,98 | 0 |
| 56 | MG | 1A | 4582 | 1/1 | 0.94 | 0.18 | 65,65,65,65 | 0 |
| 56 | MG | 1A | 4648 | 1/1 | 0.94 | 0.29 | 66,66,66,66 | 0 |
| 56 | MG | 1A | 4902 | 1/1 | 0.94 | 0.62 | 63,63,63,63 | 0 |
| 56 | MG | 1A | 5026 | 1/1 | 0.94 | 0.29 | 70,70,70,70 | 0 |
| 56 | MG | 1A | 4649 | 1/1 | 0.94 | 0.21 | 65,65,65,65 | 0 |
| 56 | MG | 2a | 1759 | 1/1 | 0.94 | 0.15 | 218,218,218,218 | 0 |
| 56 | MG | 1A | 4805 | 1/1 | 0.94 | 0.83 | 95,95,95,95 | 0 |
| 56 | MG | 1A | 4909 | 1/1 | 0.94 | 0.20 | 59,59,59,59 | 0 |
| 56 | MG | 2A | 3467 | 1/1 | 0.94 | 0.37 | 79,79,79,79 | 0 |
| 56 | MG | 1A | 4720 | 1/1 | 0.94 | 0.25 | 79,79,79,79 | 0 |
| 56 | MG | 1A | 4807 | 1/1 | 0.94 | 0.32 | 58,58,58,58 | 0 |
| 56 | MG | 1A | 4512 | 1/1 | 0.94 | 0.28 | 73,73,73,73 | 0 |
| 56 | MG | 1A | 5038 | 1/1 | 0.94 | 0.44 | 70,70,70,70 | 0 |
| 56 | MG | 1A | 4651 | 1/1 | 0.94 | 0.43 | 88,88,88,88 | 0 |
| 56 | MG | 2A | 3266 | 1/1 | 0.94 | 0.46 | 86,86,86,86 | 0 |
| 56 | MG | 2A | 3687 | 1/1 | 0.94 | 0.28 | 118,118,118,118 | 0 |
| 56 | MG | 2A | 3267 | 1/1 | 0.94 | 0.28 | 99,99,99,99 | 0 |
| 56 | MG | 1Z | 303 | 1/1 | 0.94 | 0.29 | 42,42,42,42 | 0 |
| 56 | MG | 2A | 3479 | 1/1 | 0.94 | 0.30 | 122,122,122,122 | 0 |
| 56 | MG | 1Z | 304 | 1/1 | 0.94 | 0.56 | 64,64,64,64 | 0 |
| 56 | MG | 2A | 3271 | 1/1 | 0.94 | 0.24 | 113,113,113,113 | 0 |
| 56 | MG | 1A | 4268 | 1/1 | 0.94 | 0.41 | 65,65,65,65 | 0 |
| 56 | MG | 2A | 3273 | 1/1 | 0.94 | 0.33 | 70,70,70,70 | 0 |
| 56 | MG | 2A | 3108 | 1/1 | 0.94 | 0.08 | 139,139,139,139 | 0 |
| 56 | MG | 2A | 3701 | 1/1 | 0.94 | 0.25 | 93,93,93,93 | 0 |
| 56 | MG | 20 | 105 | 1/1 | 0.94 | 0.06 | 126,126,126,126 | 0 |
| 56 | MG | 1a | 1700 | 1/1 | 0.94 | 0.16 | 161,161,161,161 | 0 |

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| Mol | Type | Chain | Res | Atoms | RSCC | RSR | B-factors(Å$^2$) | Q<0.9 |
|---|---|---|---|---|---|---|---|---|
| 56 | MG | 2A | 3280 | 1/1 | 0.94 | 0.30 | 89,89,89,89 | 0 |
| 56 | MG | 2y | 104 | 1/1 | 0.94 | 0.13 | 248,248,248,248 | 0 |
| 56 | MG | 1A | 4815 | 1/1 | 0.94 | 0.52 | 77,77,77,77 | 0 |
| 56 | MG | 1a | 1703 | 1/1 | 0.94 | 0.10 | 149,149,149,149 | 0 |
| 56 | MG | 1A | 4816 | 1/1 | 0.94 | 0.33 | 75,75,75,75 | 0 |
| 56 | MG | 10 | 103 | 1/1 | 0.94 | 0.39 | 72,72,72,72 | 0 |
| 56 | MG | 1A | 4456 | 1/1 | 0.94 | 0.13 | 80,80,80,80 | 0 |
| 56 | MG | 1A | 4365 | 1/1 | 0.94 | 0.30 | 58,58,58,58 | 0 |
| 56 | MG | 1A | 4016 | 1/1 | 0.94 | 0.23 | 68,68,68,68 | 0 |
| 56 | MG | 1A | 4218 | 1/1 | 0.94 | 0.31 | 58,58,58,58 | 0 |
| 56 | MG | 1A | 4369 | 1/1 | 0.94 | 0.25 | 61,61,61,61 | 0 |
| 56 | MG | 28 | 102 | 1/1 | 0.94 | 0.78 | 119,119,119,119 | 0 |
| 56 | MG | 28 | 103 | 1/1 | 0.94 | 0.53 | 115,115,115,115 | 0 |
| 56 | MG | 2A | 3722 | 1/1 | 0.94 | 0.11 | 128,128,128,128 | 0 |
| 56 | MG | 2A | 3123 | 1/1 | 0.94 | 0.23 | 133,133,133,133 | 0 |
| 56 | MG | 2A | 3295 | 1/1 | 0.94 | 0.27 | 97,97,97,97 | 0 |
| 56 | MG | 1A | 4593 | 1/1 | 0.94 | 0.39 | 65,65,65,65 | 0 |
| 56 | MG | 1A | 4173 | 1/1 | 0.94 | 0.14 | 57,57,57,57 | 0 |
| 56 | MG | 2A | 3129 | 1/1 | 0.94 | 0.74 | 101,101,101,101 | 0 |
| 56 | MG | 2A | 3103 | 1/1 | 0.95 | 0.58 | 79,79,79,79 | 0 |
| 56 | MG | 1A | 4118 | 1/1 | 0.95 | 0.62 | 82,82,82,82 | 0 |
| 56 | MG | 1A | 4846 | 1/1 | 0.95 | 0.22 | 74,74,74,74 | 0 |
| 56 | MG | 2X | 201 | 1/1 | 0.95 | 0.23 | 108,108,108,108 | 0 |
| 56 | MG | 1b | 302 | 1/1 | 0.95 | 0.32 | 165,165,165,165 | 0 |
| 56 | MG | 2Y | 202 | 1/1 | 0.95 | 0.13 | 137,137,137,137 | 0 |
| 56 | MG | 2A | 3275 | 1/1 | 0.95 | 0.30 | 83,83,83,83 | 0 |
| 56 | MG | 1B | 222 | 1/1 | 0.95 | 0.19 | 91,91,91,91 | 0 |
| 56 | MG | 2A | 3278 | 1/1 | 0.95 | 0.33 | 86,86,86,86 | 0 |
| 56 | MG | 1A | 4401 | 1/1 | 0.95 | 0.22 | 78,78,78,78 | 0 |
| 56 | MG | 2A | 3691 | 1/1 | 0.95 | 0.26 | 165,165,165,165 | 0 |
| 56 | MG | 1A | 4745 | 1/1 | 0.95 | 0.22 | 81,81,81,81 | 0 |
| 56 | MG | 1A | 4137 | 1/1 | 0.95 | 0.15 | 102,102,102,102 | 0 |
| 56 | MG | 1A | 4601 | 1/1 | 0.95 | 0.13 | 102,102,102,102 | 0 |
| 56 | MG | 1A | 4232 | 1/1 | 0.95 | 0.28 | 64,64,64,64 | 0 |
| 56 | MG | 1A | 4963 | 1/1 | 0.95 | 0.43 | 78,78,78,78 | 0 |
| 56 | MG | 1A | 4964 | 1/1 | 0.95 | 0.38 | 67,67,67,67 | 0 |
| 56 | MG | 2A | 3700 | 1/1 | 0.95 | 0.20 | 113,113,113,113 | 0 |
| 56 | MG | 2A | 3488 | 1/1 | 0.95 | 0.42 | 115,115,115,115 | 0 |
| 56 | MG | 1A | 4670 | 1/1 | 0.95 | 0.26 | 71,71,71,71 | 0 |
| 56 | MG | 1e | 301 | 1/1 | 0.95 | 0.50 | 140,140,140,140 | 0 |
| 56 | MG | 2A | 3707 | 1/1 | 0.95 | 0.25 | 100,100,100,100 | 0 |
| 56 | MG | 1a | 1660 | 1/1 | 0.95 | 0.30 | 119,119,119,119 | 0 |

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| Mol | Type | Chain | Res | Atoms | RSCC | RSR | B-factors(Å$^2$) | Q<0.9 |
|---|---|---|---|---|---|---|---|---|
| 56 | MG | 2A | 3709 | 1/1 | 0.95 | 0.23 | 93,93,93,93 | 0 |
| 56 | MG | 1A | 4046 | 1/1 | 0.95 | 0.28 | 68,68,68,68 | 0 |
| 56 | MG | 1A | 4751 | 1/1 | 0.95 | 0.25 | 71,71,71,71 | 0 |
| 56 | MG | 2A | 3294 | 1/1 | 0.95 | 0.42 | 91,91,91,91 | 0 |
| 56 | MG | 1A | 4030 | 1/1 | 0.95 | 0.25 | 58,58,58,58 | 0 |
| 56 | MG | 2A | 3501 | 1/1 | 0.95 | 0.20 | 104,104,104,104 | 0 |
| 56 | MG | 2a | 1815 | 1/1 | 0.95 | 0.13 | 85,85,85,85 | 0 |
| 56 | MG | 2a | 1816 | 1/1 | 0.95 | 0.14 | 156,156,156,156 | 0 |
| 56 | MG | 1A | 4462 | 1/1 | 0.95 | 0.27 | 74,74,74,74 | 0 |
| 56 | MG | 2a | 1819 | 1/1 | 0.95 | 0.18 | 150,150,150,150 | 0 |
| 56 | MG | 2A | 3128 | 1/1 | 0.95 | 0.42 | 130,130,130,130 | 0 |
| 56 | MG | 1a | 1667 | 1/1 | 0.95 | 0.13 | 132,132,132,132 | 0 |
| 56 | MG | 1A | 4284 | 1/1 | 0.95 | 0.36 | 65,65,65,65 | 0 |
| 56 | MG | 2A | 3506 | 1/1 | 0.95 | 0.16 | 149,149,149,149 | 0 |
| 56 | MG | 1A | 4319 | 1/1 | 0.95 | 0.37 | 68,68,68,68 | 0 |
| 56 | MG | 1A | 4411 | 1/1 | 0.95 | 0.23 | 50,50,50,50 | 0 |
| 56 | MG | 1A | 4977 | 1/1 | 0.95 | 0.32 | 78,78,78,78 | 0 |
| 56 | MG | 2A | 3728 | 1/1 | 0.95 | 0.21 | 83,83,83,83 | 0 |
| 56 | MG | 1a | 1813 | 1/1 | 0.95 | 0.30 | 91,91,91,91 | 0 |
| 56 | MG | 1A | 4978 | 1/1 | 0.95 | 0.19 | 60,60,60,60 | 0 |
| 56 | MG | 1A | 4168 | 1/1 | 0.95 | 0.42 | 50,50,50,50 | 0 |
| 56 | MG | 1A | 4612 | 1/1 | 0.95 | 0.15 | 62,62,62,62 | 0 |
| 56 | MG | 1A | 4236 | 1/1 | 0.95 | 0.67 | 55,55,55,55 | 0 |
| 56 | MG | 1A | 4683 | 1/1 | 0.95 | 0.32 | 55,55,55,55 | 0 |
| 56 | MG | 2A | 3317 | 1/1 | 0.95 | 0.36 | 81,81,81,81 | 0 |
| 56 | MG | 1A | 4415 | 1/1 | 0.95 | 0.15 | 74,74,74,74 | 0 |
| 56 | MG | 2a | 1616 | 1/1 | 0.95 | 0.10 | 139,139,139,139 | 0 |
| 56 | MG | 2A | 3321 | 1/1 | 0.95 | 0.52 | 86,86,86,86 | 0 |
| 56 | MG | 2A | 3323 | 1/1 | 0.95 | 0.46 | 89,89,89,89 | 0 |
| 56 | MG | 2A | 3527 | 1/1 | 0.95 | 0.18 | 111,111,111,111 | 0 |
| 56 | MG | 1A | 4618 | 1/1 | 0.95 | 0.19 | 95,95,95,95 | 0 |
| 56 | MG | 1A | 4766 | 1/1 | 0.95 | 0.23 | 56,56,56,56 | 0 |
| 56 | MG | 1A | 4989 | 1/1 | 0.95 | 0.23 | 73,73,73,73 | 0 |
| 56 | MG | 1A | 4990 | 1/1 | 0.95 | 0.21 | 64,64,64,64 | 0 |
| 56 | MG | 2A | 3330 | 1/1 | 0.95 | 0.20 | 97,97,97,97 | 0 |
| 56 | MG | 2a | 1855 | 1/1 | 0.95 | 0.07 | 88,88,88,88 | 0 |
| 56 | MG | 1A | 4992 | 1/1 | 0.95 | 0.37 | 70,70,70,70 | 0 |
| 56 | MG | 1A | 4876 | 1/1 | 0.95 | 0.26 | 80,80,80,80 | 0 |
| 56 | MG | 1A | 4686 | 1/1 | 0.95 | 0.14 | 93,93,93,93 | 0 |
| 56 | MG | 1A | 4475 | 1/1 | 0.95 | 0.16 | 58,58,58,58 | 0 |
| 56 | MG | 2a | 1629 | 1/1 | 0.95 | 0.28 | 187,187,187,187 | 0 |
| 56 | MG | 2A | 3002 | 1/1 | 0.95 | 0.64 | 99,99,99,99 | 0 |

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| Mol | Type | Chain | Res | Atoms | RSCC | RSR | B-factors(Å$^2$) | Q<0.9 |
|---|---|---|---|---|---|---|---|---|
| 56 | MG | 1A | 4416 | 1/1 | 0.95 | 0.32 | 57,57,57,57 | 0 |
| 56 | MG | 2a | 1863 | 1/1 | 0.95 | 0.14 | 162,162,162,162 | 0 |
| 56 | MG | 1A | 4478 | 1/1 | 0.95 | 0.24 | 71,71,71,71 | 0 |
| 56 | MG | 1A | 4169 | 1/1 | 0.95 | 0.20 | 57,57,57,57 | 0 |
| 56 | MG | 1A | 4885 | 1/1 | 0.95 | 0.55 | 92,92,92,92 | 0 |
| 56 | MG | 2A | 3341 | 1/1 | 0.95 | 0.24 | 86,86,86,86 | 0 |
| 56 | MG | 1A | 4419 | 1/1 | 0.95 | 0.18 | 55,55,55,55 | 0 |
| 56 | MG | 1a | 1698 | 1/1 | 0.95 | 0.21 | 120,120,120,120 | 0 |
| 56 | MG | 2A | 3159 | 1/1 | 0.95 | 0.39 | 100,100,100,100 | 0 |
| 56 | MG | 2a | 1641 | 1/1 | 0.95 | 0.33 | 146,146,146,146 | 0 |
| 56 | MG | 1a | 1838 | 1/1 | 0.95 | 0.09 | 231,231,231,231 | 0 |
| 56 | MG | 1A | 4422 | 1/1 | 0.95 | 0.26 | 52,52,52,52 | 0 |
| 56 | MG | 2a | 1646 | 1/1 | 0.95 | 0.97 | 120,120,120,120 | 0 |
| 56 | MG | 2A | 3348 | 1/1 | 0.95 | 0.51 | 90,90,90,90 | 0 |
| 56 | MG | 1A | 4483 | 1/1 | 0.95 | 0.19 | 66,66,66,66 | 0 |
| 56 | MG | 2A | 3014 | 1/1 | 0.95 | 0.59 | 108,108,108,108 | 0 |
| 56 | MG | 1A | 4084 | 1/1 | 0.95 | 0.43 | 61,61,61,61 | 0 |
| 56 | MG | 2A | 3167 | 1/1 | 0.95 | 0.75 | 99,99,99,99 | 0 |
| 56 | MG | 1a | 1702 | 1/1 | 0.95 | 0.22 | 181,181,181,181 | 0 |
| 56 | MG | 2A | 3554 | 1/1 | 0.95 | 0.27 | 89,89,89,89 | 0 |
| 56 | MG | 1A | 4172 | 1/1 | 0.95 | 0.33 | 58,58,58,58 | 0 |
| 56 | MG | 2A | 3778 | 1/1 | 0.95 | 0.34 | 97,97,97,97 | 0 |
| 56 | MG | 1A | 4020 | 1/1 | 0.95 | 0.23 | 73,73,73,73 | 0 |
| 56 | MG | 1A | 4630 | 1/1 | 0.95 | 0.52 | 56,56,56,56 | 0 |
| 56 | MG | 2A | 3172 | 1/1 | 0.95 | 0.28 | 91,91,91,91 | 0 |
| 56 | MG | 1a | 1848 | 1/1 | 0.95 | 0.26 | 178,178,178,178 | 0 |
| 56 | MG | 1a | 1849 | 1/1 | 0.95 | 0.60 | 149,149,149,149 | 0 |
| 56 | MG | 2A | 3175 | 1/1 | 0.95 | 0.33 | 58,58,58,58 | 0 |
| 56 | MG | 2A | 3787 | 1/1 | 0.95 | 0.47 | 125,125,125,125 | 0 |
| 56 | MG | 2A | 3563 | 1/1 | 0.95 | 0.29 | 90,90,90,90 | 0 |
| 56 | MG | 1A | 4893 | 1/1 | 0.95 | 0.24 | 65,65,65,65 | 0 |
| 56 | MG | 2a | 1895 | 1/1 | 0.95 | 0.32 | 156,156,156,156 | 0 |
| 56 | MG | 2A | 3792 | 1/1 | 0.95 | 0.50 | 130,130,130,130 | 0 |
| 56 | MG | 1A | 4430 | 1/1 | 0.95 | 0.18 | 61,61,61,61 | 0 |
| 56 | MG | 2a | 1898 | 1/1 | 0.95 | 0.20 | 160,160,160,160 | 0 |
| 56 | MG | 1A | 4209 | 1/1 | 0.95 | 0.29 | 55,55,55,55 | 0 |
| 56 | MG | 1A | 5022 | 1/1 | 0.95 | 0.84 | 122,122,122,122 | 0 |
| 56 | MG | 2A | 3026 | 1/1 | 0.95 | 0.52 | 117,117,117,117 | 0 |
| 56 | MG | 1A | 4212 | 1/1 | 0.95 | 0.28 | 51,51,51,51 | 0 |
| 56 | MG | 1A | 4634 | 1/1 | 0.95 | 0.30 | 59,59,59,59 | 0 |
| 56 | MG | 1a | 1715 | 1/1 | 0.95 | 0.20 | 123,123,123,123 | 0 |
| 56 | MG | 1A | 4787 | 1/1 | 0.95 | 0.16 | 64,64,64,64 | 0 |

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| Mol | Type | Chain | Res | Atoms | RSCC | RSR | B-factors(Å$^2$) | Q<0.9 |
|---|---|---|---|---|---|---|---|---|
| 56 | MG | 1A | 4023 | 1/1 | 0.95 | 0.85 | 110,110,110,110 | 0 |
| 56 | MG | 1A | 4434 | 1/1 | 0.95 | 0.22 | 58,58,58,58 | 0 |
| 56 | MG | 1A | 5028 | 1/1 | 0.95 | 0.20 | 70,70,70,70 | 0 |
| 56 | MG | 1A | 4704 | 1/1 | 0.95 | 0.12 | 77,77,77,77 | 0 |
| 56 | MG | 2A | 3810 | 1/1 | 0.95 | 0.45 | 145,145,145,145 | 0 |
| 56 | MG | 1a | 1727 | 1/1 | 0.95 | 0.10 | 127,127,127,127 | 0 |
| 56 | MG | 1a | 1728 | 1/1 | 0.95 | 0.47 | 143,143,143,143 | 0 |
| 56 | MG | 2A | 3815 | 1/1 | 0.95 | 0.09 | 136,136,136,136 | 0 |
| 56 | MG | 1a | 1729 | 1/1 | 0.95 | 0.14 | 143,143,143,143 | 0 |
| 56 | MG | 2a | 1687 | 1/1 | 0.95 | 0.31 | 162,162,162,162 | 0 |
| 56 | MG | 2a | 1916 | 1/1 | 0.95 | 0.20 | 63,63,63,63 | 0 |
| 56 | MG | 1A | 4903 | 1/1 | 0.95 | 0.13 | 61,61,61,61 | 0 |
| 56 | MG | 1A | 5034 | 1/1 | 0.95 | 1.03 | 67,67,67,67 | 0 |
| 56 | MG | 1a | 1868 | 1/1 | 0.95 | 0.62 | 214,214,214,214 | 0 |
| 56 | MG | 2A | 3822 | 1/1 | 0.95 | 0.34 | 91,91,91,91 | 0 |
| 56 | MG | 2a | 1692 | 1/1 | 0.95 | 0.22 | 149,149,149,149 | 0 |
| 56 | MG | 2A | 3585 | 1/1 | 0.95 | 0.68 | 114,114,114,114 | 0 |
| 56 | MG | 2a | 1694 | 1/1 | 0.95 | 0.31 | 146,146,146,146 | 0 |
| 56 | MG | 2A | 3824 | 1/1 | 0.95 | 0.19 | 99,99,99,99 | 0 |
| 56 | MG | 2A | 3586 | 1/1 | 0.95 | 0.07 | 120,120,120,120 | 0 |
| 56 | MG | 2A | 3587 | 1/1 | 0.95 | 0.06 | 123,123,123,123 | 0 |
| 56 | MG | 16 | 101 | 1/1 | 0.95 | 0.09 | 72,72,72,72 | 0 |
| 56 | MG | 2A | 3392 | 1/1 | 0.95 | 0.22 | 124,124,124,124 | 0 |
| 56 | MG | 1A | 4705 | 1/1 | 0.95 | 0.34 | 72,72,72,72 | 0 |
| 56 | MG | 1A | 4146 | 1/1 | 0.95 | 0.25 | 59,59,59,59 | 0 |
| 56 | MG | 1A | 4331 | 1/1 | 0.95 | 0.15 | 73,73,73,73 | 0 |
| 56 | MG | 2A | 3050 | 1/1 | 0.95 | 0.13 | 93,93,93,93 | 0 |
| 56 | MG | 1A | 4910 | 1/1 | 0.95 | 0.20 | 55,55,55,55 | 0 |
| 56 | MG | 1A | 4437 | 1/1 | 0.95 | 0.24 | 64,64,64,64 | 0 |
| 56 | MG | 2A | 3211 | 1/1 | 0.95 | 0.29 | 94,94,94,94 | 0 |
| 56 | MG | 2A | 3837 | 1/1 | 0.95 | 0.15 | 68,68,68,68 | 0 |
| 56 | MG | 2A | 3838 | 1/1 | 0.95 | 0.14 | 44,44,44,44 | 0 |
| 56 | MG | 2A | 3601 | 1/1 | 0.95 | 0.24 | 101,101,101,101 | 0 |
| 56 | MG | 1A | 4563 | 1/1 | 0.95 | 0.38 | 68,68,68,68 | 0 |
| 56 | MG | 1A | 4565 | 1/1 | 0.95 | 0.15 | 58,58,58,58 | 0 |
| 56 | MG | 2A | 3843 | 1/1 | 0.95 | 0.37 | 76,76,76,76 | 0 |
| 56 | MG | 1A | 4250 | 1/1 | 0.95 | 0.14 | 64,64,64,64 | 0 |
| 56 | MG | 1A | 4253 | 1/1 | 0.95 | 0.64 | 54,54,54,54 | 0 |
| 56 | MG | 2A | 3847 | 1/1 | 0.95 | 0.24 | 91,91,91,91 | 0 |
| 56 | MG | 2A | 3849 | 1/1 | 0.95 | 0.20 | 153,153,153,153 | 0 |
| 56 | MG | 2A | 3059 | 1/1 | 0.95 | 0.10 | 88,88,88,88 | 0 |
| 56 | MG | 2A | 3853 | 1/1 | 0.95 | 0.69 | 84,84,84,84 | 0 |

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| Mol | Type | Chain | Res | Atoms | RSCC | RSR | B-factors(Å$^2$) | Q<0.9 |
|---|---|---|---|---|---|---|---|---|
| 56 | MG | 2A | 3410 | 1/1 | 0.95 | 0.25 | 108,108,108,108 | 0 |
| 56 | MG | 1A | 5049 | 1/1 | 0.95 | 0.65 | 72,72,72,72 | 0 |
| 56 | MG | 1a | 1746 | 1/1 | 0.95 | 0.12 | 154,154,154,154 | 0 |
| 56 | MG | 1A | 4079 | 1/1 | 0.95 | 0.40 | 58,58,58,58 | 0 |
| 56 | MG | 1a | 1748 | 1/1 | 0.95 | 0.17 | 145,145,145,145 | 0 |
| 56 | MG | 2a | 1728 | 1/1 | 0.95 | 0.21 | 79,79,79,79 | 0 |
| 56 | MG | 1a | 1749 | 1/1 | 0.95 | 0.31 | 134,134,134,134 | 0 |
| 56 | MG | 2A | 3223 | 1/1 | 0.95 | 0.10 | 118,118,118,118 | 0 |
| 56 | MG | 1A | 4443 | 1/1 | 0.95 | 0.28 | 75,75,75,75 | 0 |
| 56 | MG | 2B | 210 | 1/1 | 0.95 | 0.42 | 70,70,70,70 | 0 |
| 56 | MG | 2A | 3618 | 1/1 | 0.95 | 0.12 | 149,149,149,149 | 0 |
| 56 | MG | 1A | 4578 | 1/1 | 0.95 | 0.19 | 59,59,59,59 | 0 |
| 56 | MG | 1a | 1612 | 1/1 | 0.95 | 0.25 | 94,94,94,94 | 0 |
| 56 | MG | 1A | 4924 | 1/1 | 0.95 | 0.13 | 71,71,71,71 | 0 |
| 56 | MG | 2p | 103 | 1/1 | 0.95 | 0.50 | 152,152,152,152 | 0 |
| 56 | MG | 2A | 3070 | 1/1 | 0.95 | 0.31 | 156,156,156,156 | 0 |
| 56 | MG | 1A | 4181 | 1/1 | 0.95 | 0.37 | 45,45,45,45 | 0 |
| 56 | MG | 1A | 4261 | 1/1 | 0.95 | 0.14 | 63,63,63,63 | 0 |
| 56 | MG | 1A | 4819 | 1/1 | 0.95 | 0.38 | 119,119,119,119 | 0 |
| 56 | MG | 2A | 3426 | 1/1 | 0.95 | 0.25 | 93,93,93,93 | 0 |
| 56 | MG | 1a | 1620 | 1/1 | 0.95 | 0.19 | 98,98,98,98 | 0 |
| 56 | MG | 2A | 3429 | 1/1 | 0.95 | 0.21 | 117,117,117,117 | 0 |
| 56 | MG | 1A | 4055 | 1/1 | 0.95 | 0.36 | 86,86,86,86 | 0 |
| 56 | MG | 2A | 3238 | 1/1 | 0.95 | 0.25 | 108,108,108,108 | 0 |
| 56 | MG | 1A | 4930 | 1/1 | 0.95 | 0.39 | 110,110,110,110 | 0 |
| 56 | MG | 2A | 3434 | 1/1 | 0.95 | 0.29 | 95,95,95,95 | 0 |
| 56 | MG | 2B | 226 | 1/1 | 0.95 | 0.09 | 132,132,132,132 | 0 |
| 56 | MG | 2A | 3437 | 1/1 | 0.95 | 0.17 | 97,97,97,97 | 0 |
| 56 | MG | 2A | 3241 | 1/1 | 0.95 | 0.59 | 124,124,124,124 | 0 |
| 56 | MG | 1A | 4931 | 1/1 | 0.95 | 0.27 | 125,125,125,125 | 0 |
| 56 | MG | 1A | 4110 | 1/1 | 0.95 | 0.22 | 54,54,54,54 | 0 |
| 56 | MG | 1A | 4091 | 1/1 | 0.95 | 0.32 | 58,58,58,58 | 0 |
| 56 | MG | 1A | 4823 | 1/1 | 0.95 | 0.48 | 74,74,74,74 | 0 |
| 56 | MG | 1A | 4653 | 1/1 | 0.95 | 0.28 | 88,88,88,88 | 0 |
| 56 | MG | 2A | 3085 | 1/1 | 0.95 | 0.13 | 118,118,118,118 | 0 |
| 56 | MG | 1A | 4937 | 1/1 | 0.95 | 0.17 | 58,58,58,58 | 0 |
| 56 | MG | 1A | 4938 | 1/1 | 0.95 | 0.32 | 69,69,69,69 | 0 |
| 56 | MG | 1A | 4828 | 1/1 | 0.95 | 0.21 | 80,80,80,80 | 0 |
| 56 | MG | 1A | 4266 | 1/1 | 0.95 | 0.20 | 58,58,58,58 | 0 |
| 56 | MG | 2A | 3652 | 1/1 | 0.95 | 0.12 | 124,124,124,124 | 0 |
| 56 | MG | 1A | 4728 | 1/1 | 0.95 | 0.18 | 76,76,76,76 | 0 |
| 56 | MG | 2A | 3453 | 1/1 | 0.95 | 0.53 | 74,74,74,74 | 0 |

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| Mol | Type | Chain | Res | Atoms | RSCC | RSR | B-factors(Å$^2$) | Q<0.9 |
|---|---|---|---|---|---|---|---|---|
| 56 | MG | 2A | 3253 | 1/1 | 0.95 | 0.20 | 128,128,128,128 | 0 |
| 56 | MG | 1A | 4510 | 1/1 | 0.95 | 0.12 | 69,69,69,69 | 0 |
| 56 | MG | 2A | 3092 | 1/1 | 0.95 | 0.33 | 118,118,118,118 | 0 |
| 56 | MG | 2F | 304 | 1/1 | 0.95 | 0.15 | 135,135,135,135 | 0 |
| 56 | MG | 1a | 1638 | 1/1 | 0.95 | 0.43 | 117,117,117,117 | 0 |
| 56 | MG | 1A | 4732 | 1/1 | 0.95 | 0.21 | 56,56,56,56 | 0 |
| 56 | MG | 1A | 4113 | 1/1 | 0.95 | 0.32 | 55,55,55,55 | 0 |
| 56 | MG | 2A | 3668 | 1/1 | 0.95 | 0.38 | 91,91,91,91 | 0 |
| 56 | MG | 1A | 4114 | 1/1 | 0.95 | 0.25 | 56,56,56,56 | 0 |
| 56 | MG | 1A | 4093 | 1/1 | 0.95 | 0.31 | 62,62,62,62 | 0 |
| 56 | MG | 1A | 4737 | 1/1 | 0.95 | 0.16 | 76,76,76,76 | 0 |
| 56 | MG | 1A | 4953 | 1/1 | 0.95 | 0.19 | 60,60,60,60 | 0 |
| 56 | MG | 1A | 4515 | 1/1 | 0.95 | 0.33 | 70,70,70,70 | 0 |
| 57 | ZN | 29 | 103 | 1/1 | 0.95 | 0.05 | 143,143,143,143 | 0 |
| 56 | MG | 1A | 4018 | 1/1 | 0.95 | 0.47 | 68,68,68,68 | 0 |
| 59 | GDP | 1v | 704 | 28/28 | 0.95 | 0.18 | 117,117,117,117 | 0 |
| 56 | MG | 2A | 3469 | 1/1 | 0.95 | 0.28 | 115,115,115,115 | 0 |
| 56 | MG | 1a | 1787 | 1/1 | 0.95 | 0.39 | 124,124,124,124 | 0 |
| 56 | MG | 1A | 4315 | 1/1 | 0.96 | 0.43 | 111,111,111,111 | 0 |
| 56 | MG | 1b | 308 | 1/1 | 0.96 | 0.23 | 162,162,162,162 | 0 |
| 56 | MG | 2a | 1810 | 1/1 | 0.96 | 0.42 | 129,129,129,129 | 0 |
| 56 | MG | 2a | 1811 | 1/1 | 0.96 | 0.15 | 129,129,129,129 | 0 |
| 56 | MG | 1a | 1818 | 1/1 | 0.96 | 0.07 | 186,186,186,186 | 0 |
| 56 | MG | 1A | 4408 | 1/1 | 0.96 | 0.37 | 57,57,57,57 | 0 |
| 56 | MG | 1d | 302 | 1/1 | 0.96 | 0.17 | 149,149,149,149 | 0 |
| 56 | MG | 1A | 4791 | 1/1 | 0.96 | 0.43 | 73,73,73,73 | 0 |
| 56 | MG | 1a | 1603 | 1/1 | 0.96 | 0.17 | 98,98,98,98 | 0 |
| 56 | MG | 2A | 3766 | 1/1 | 0.96 | 0.73 | 66,66,66,66 | 0 |
| 56 | MG | 1A | 4969 | 1/1 | 0.96 | 0.23 | 63,63,63,63 | 0 |
| 56 | MG | 1e | 302 | 1/1 | 0.96 | 0.16 | 147,147,147,147 | 0 |
| 56 | MG | 2A | 3231 | 1/1 | 0.96 | 0.23 | 95,95,95,95 | 0 |
| 56 | MG | 1A | 4795 | 1/1 | 0.96 | 0.17 | 79,79,79,79 | 0 |
| 56 | MG | 2A | 3771 | 1/1 | 0.96 | 0.22 | 101,101,101,101 | 0 |
| 56 | MG | 2A | 3772 | 1/1 | 0.96 | 0.10 | 98,98,98,98 | 0 |
| 56 | MG | 1A | 4019 | 1/1 | 0.96 | 0.49 | 77,77,77,77 | 0 |
| 56 | MG | 2a | 1832 | 1/1 | 0.96 | 0.10 | 138,138,138,138 | 0 |
| 56 | MG | 2A | 3234 | 1/1 | 0.96 | 0.20 | 103,103,103,103 | 0 |
| 56 | MG | 2a | 1835 | 1/1 | 0.96 | 0.27 | 152,152,152,152 | 0 |
| 56 | MG | 1a | 1825 | 1/1 | 0.96 | 0.26 | 214,214,214,214 | 0 |
| 56 | MG | 1A | 4364 | 1/1 | 0.96 | 0.40 | 72,72,72,72 | 0 |
| 56 | MG | 1A | 4095 | 1/1 | 0.96 | 0.32 | 62,62,62,62 | 0 |
| 56 | MG | 2A | 3404 | 1/1 | 0.96 | 0.18 | 135,135,135,135 | 0 |

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| Mol | Type | Chain | Res | Atoms | RSCC | RSR | B-factors(Å$^2$) | Q<0.9 |
|---|---|---|---|---|---|---|---|---|
| 56 | MG | 2A | 3405 | 1/1 | 0.96 | 0.28 | 130,130,130,130 | 0 |
| 56 | MG | 1A | 4031 | 1/1 | 0.96 | 0.17 | 56,56,56,56 | 0 |
| 56 | MG | 2A | 3240 | 1/1 | 0.96 | 0.30 | 120,120,120,120 | 0 |
| 56 | MG | 1A | 4588 | 1/1 | 0.96 | 0.26 | 79,79,79,79 | 0 |
| 56 | MG | 1a | 1714 | 1/1 | 0.96 | 0.28 | 118,118,118,118 | 0 |
| 56 | MG | 2A | 3784 | 1/1 | 0.96 | 0.35 | 110,110,110,110 | 0 |
| 56 | MG | 1A | 4522 | 1/1 | 0.96 | 0.24 | 76,76,76,76 | 0 |
| 56 | MG | 2A | 3786 | 1/1 | 0.96 | 0.18 | 123,123,123,123 | 0 |
| 56 | MG | 1A | 4590 | 1/1 | 0.96 | 0.78 | 71,71,71,71 | 0 |
| 56 | MG | 2A | 3788 | 1/1 | 0.96 | 0.23 | 124,124,124,124 | 0 |
| 56 | MG | 1A | 4523 | 1/1 | 0.96 | 0.38 | 68,68,68,68 | 0 |
| 56 | MG | 1a | 1721 | 1/1 | 0.96 | 0.12 | 134,134,134,134 | 0 |
| 56 | MG | 1B | 217 | 1/1 | 0.96 | 0.23 | 71,71,71,71 | 0 |
| 56 | MG | 1a | 1618 | 1/1 | 0.96 | 0.31 | 94,94,94,94 | 0 |
| 56 | MG | 2A | 3110 | 1/1 | 0.96 | 0.19 | 189,189,189,189 | 0 |
| 56 | MG | 1A | 4982 | 1/1 | 0.96 | 0.13 | 54,54,54,54 | 0 |
| 56 | MG | 1A | 4204 | 1/1 | 0.96 | 0.14 | 64,64,64,64 | 0 |
| 56 | MG | 1A | 4115 | 1/1 | 0.96 | 0.24 | 62,62,62,62 | 0 |
| 56 | MG | 1A | 4595 | 1/1 | 0.96 | 0.37 | 62,62,62,62 | 0 |
| 56 | MG | 1A | 4898 | 1/1 | 0.96 | 0.29 | 60,60,60,60 | 0 |
| 56 | MG | 2A | 3117 | 1/1 | 0.96 | 0.23 | 134,134,134,134 | 0 |
| 56 | MG | 2A | 3803 | 1/1 | 0.96 | 0.19 | 112,112,112,112 | 0 |
| 56 | MG | 2a | 1864 | 1/1 | 0.96 | 0.32 | 161,161,161,161 | 0 |
| 56 | MG | 2A | 3256 | 1/1 | 0.96 | 0.25 | 92,92,92,92 | 0 |
| 56 | MG | 2A | 3427 | 1/1 | 0.96 | 0.36 | 95,95,95,95 | 0 |
| 56 | MG | 1x | 302 | 1/1 | 0.96 | 0.10 | 45,45,45,45 | 0 |
| 56 | MG | 1A | 4596 | 1/1 | 0.96 | 0.10 | 65,65,65,65 | 0 |
| 56 | MG | 1A | 4211 | 1/1 | 0.96 | 0.36 | 57,57,57,57 | 0 |
| 56 | MG | 1B | 225 | 1/1 | 0.96 | 0.37 | 92,92,92,92 | 0 |
| 56 | MG | 2A | 3813 | 1/1 | 0.96 | 0.17 | 126,126,126,126 | 0 |
| 56 | MG | 1A | 4179 | 1/1 | 0.96 | 0.14 | 60,60,60,60 | 0 |
| 56 | MG | 1a | 1846 | 1/1 | 0.96 | 0.78 | 193,193,193,193 | 0 |
| 56 | MG | 2A | 3435 | 1/1 | 0.96 | 0.44 | 97,97,97,97 | 0 |
| 56 | MG | 2A | 3610 | 1/1 | 0.96 | 0.71 | 114,114,114,114 | 0 |
| 56 | MG | 1a | 1628 | 1/1 | 0.96 | 0.35 | 101,101,101,101 | 0 |
| 56 | MG | 2A | 3127 | 1/1 | 0.96 | 0.37 | 135,135,135,135 | 0 |
| 56 | MG | 1D | 301 | 1/1 | 0.96 | 0.28 | 65,65,65,65 | 0 |
| 56 | MG | 2A | 3268 | 1/1 | 0.96 | 0.25 | 94,94,94,94 | 0 |
| 56 | MG | 1A | 4420 | 1/1 | 0.96 | 0.24 | 50,50,50,50 | 0 |
| 56 | MG | 1A | 4421 | 1/1 | 0.96 | 0.13 | 58,58,58,58 | 0 |
| 56 | MG | 1a | 1632 | 1/1 | 0.96 | 0.18 | 118,118,118,118 | 0 |
| 56 | MG | 2A | 3619 | 1/1 | 0.96 | 0.20 | 133,133,133,133 | 0 |

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| Mol | Type | Chain | Res | Atoms | RSCC | RSR | B-factors(Å$^2$) | Q<0.9 |
|---|---|---|---|---|---|---|---|---|
| 56 | MG | 2A | 3621 | 1/1 | 0.96 | 0.61 | 95,95,95,95 | 0 |
| 56 | MG | 1A | 4067 | 1/1 | 0.96 | 0.33 | 86,86,86,86 | 0 |
| 56 | MG | 1a | 1743 | 1/1 | 0.96 | 0.25 | 139,139,139,139 | 0 |
| 56 | MG | 1A | 4424 | 1/1 | 0.96 | 0.17 | 61,61,61,61 | 0 |
| 56 | MG | 1A | 4740 | 1/1 | 0.96 | 0.14 | 79,79,79,79 | 0 |
| 56 | MG | 1A | 4099 | 1/1 | 0.96 | 0.12 | 69,69,69,69 | 0 |
| 56 | MG | 1E | 301 | 1/1 | 0.96 | 0.18 | 57,57,57,57 | 0 |
| 56 | MG | 1A | 4825 | 1/1 | 0.96 | 0.16 | 92,92,92,92 | 0 |
| 56 | MG | 2A | 3454 | 1/1 | 0.96 | 0.17 | 90,90,90,90 | 0 |
| 56 | MG | 1A | 4245 | 1/1 | 0.96 | 0.23 | 52,52,52,52 | 0 |
| 56 | MG | 2A | 3457 | 1/1 | 0.96 | 0.46 | 93,93,93,93 | 0 |
| 56 | MG | 2A | 3140 | 1/1 | 0.96 | 0.29 | 101,101,101,101 | 0 |
| 56 | MG | 1A | 4829 | 1/1 | 0.96 | 0.25 | 74,74,74,74 | 0 |
| 56 | MG | 1A | 4830 | 1/1 | 0.96 | 0.28 | 76,76,76,76 | 0 |
| 56 | MG | 1A | 5009 | 1/1 | 0.96 | 0.25 | 72,72,72,72 | 0 |
| 56 | MG | 1A | 4675 | 1/1 | 0.96 | 0.23 | 104,104,104,104 | 0 |
| 56 | MG | 1A | 4536 | 1/1 | 0.96 | 1.13 | 115,115,115,115 | 0 |
| 56 | MG | 1a | 1756 | 1/1 | 0.96 | 0.20 | 109,109,109,109 | 0 |
| 56 | MG | 2A | 3641 | 1/1 | 0.96 | 0.26 | 127,127,127,127 | 0 |
| 56 | MG | 1A | 5013 | 1/1 | 0.96 | 0.55 | 38,38,38,38 | 0 |
| 56 | MG | 2a | 1701 | 1/1 | 0.96 | 0.24 | 146,146,146,146 | 0 |
| 56 | MG | 1A | 4246 | 1/1 | 0.96 | 0.20 | 51,51,51,51 | 0 |
| 56 | MG | 2B | 202 | 1/1 | 0.96 | 0.19 | 137,137,137,137 | 0 |
| 56 | MG | 1a | 1650 | 1/1 | 0.96 | 0.23 | 123,123,123,123 | 0 |
| 56 | MG | 1A | 4922 | 1/1 | 0.96 | 0.18 | 67,67,67,67 | 0 |
| 56 | MG | 1A | 4005 | 1/1 | 0.96 | 0.21 | 65,65,65,65 | 0 |
| 56 | MG | 1A | 4249 | 1/1 | 0.96 | 0.18 | 52,52,52,52 | 0 |
| 56 | MG | 2a | 1708 | 1/1 | 0.96 | 0.24 | 152,152,152,152 | 0 |
| 56 | MG | 1A | 4541 | 1/1 | 0.96 | 0.32 | 56,56,56,56 | 0 |
| 56 | MG | 1A | 4062 | 1/1 | 0.96 | 0.41 | 72,72,72,72 | 0 |
| 56 | MG | 1A | 4838 | 1/1 | 0.96 | 0.38 | 73,73,73,73 | 0 |
| 56 | MG | 2A | 3651 | 1/1 | 0.96 | 0.14 | 118,118,118,118 | 0 |
| 56 | MG | 2a | 1917 | 1/1 | 0.96 | 0.14 | 86,86,86,86 | 0 |
| 56 | MG | 2A | 3475 | 1/1 | 0.96 | 0.60 | 111,111,111,111 | 0 |
| 56 | MG | 2a | 1919 | 1/1 | 0.96 | 0.12 | 155,155,155,155 | 0 |
| 56 | MG | 2A | 3031 | 1/1 | 0.96 | 0.53 | 103,103,103,103 | 0 |
| 56 | MG | 2A | 3158 | 1/1 | 0.96 | 0.40 | 107,107,107,107 | 0 |
| 56 | MG | 2A | 3657 | 1/1 | 0.96 | 0.12 | 103,103,103,103 | 0 |
| 56 | MG | 1A | 4105 | 1/1 | 0.96 | 0.37 | 46,46,46,46 | 0 |
| 56 | MG | 2A | 3033 | 1/1 | 0.96 | 0.75 | 107,107,107,107 | 0 |
| 56 | MG | 1A | 4158 | 1/1 | 0.96 | 0.35 | 58,58,58,58 | 0 |
| 56 | MG | 2A | 3663 | 1/1 | 0.96 | 0.19 | 95,95,95,95 | 0 |

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| Mol | Type | Chain | Res | Atoms | RSCC | RSR | B-factors(Å$^2$) | Q<0.9 |
|---|---|---|---|---|---|---|---|---|
| 56 | MG | 1a | 1769 | 1/1 | 0.96 | 0.20 | 131,131,131,131 | 0 |
| 56 | MG | 2A | 3163 | 1/1 | 0.96 | 0.22 | 103,103,103,103 | 0 |
| 56 | MG | 1A | 4620 | 1/1 | 0.96 | 0.20 | 107,107,107,107 | 0 |
| 56 | MG | 2A | 3315 | 1/1 | 0.96 | 0.20 | 90,90,90,90 | 0 |
| 56 | MG | 2A | 3485 | 1/1 | 0.96 | 0.35 | 60,60,60,60 | 0 |
| 56 | MG | 2A | 3316 | 1/1 | 0.96 | 0.26 | 85,85,85,85 | 0 |
| 56 | MG | 1A | 4258 | 1/1 | 0.96 | 0.19 | 68,68,68,68 | 0 |
| 56 | MG | 2A | 3318 | 1/1 | 0.96 | 0.48 | 83,83,83,83 | 0 |
| 56 | MG | 1A | 4089 | 1/1 | 0.96 | 0.31 | 67,67,67,67 | 0 |
| 56 | MG | 2A | 3320 | 1/1 | 0.96 | 0.62 | 88,88,88,88 | 0 |
| 56 | MG | 1a | 1773 | 1/1 | 0.96 | 0.32 | 143,143,143,143 | 0 |
| 56 | MG | 1A | 4934 | 1/1 | 0.96 | 0.33 | 77,77,77,77 | 0 |
| 56 | MG | 1a | 1663 | 1/1 | 0.96 | 0.27 | 115,115,115,115 | 0 |
| 56 | MG | 2A | 3682 | 1/1 | 0.96 | 0.39 | 123,123,123,123 | 0 |
| 56 | MG | 2A | 3495 | 1/1 | 0.96 | 0.26 | 106,106,106,106 | 0 |
| 56 | MG | 1A | 5030 | 1/1 | 0.96 | 0.32 | 72,72,72,72 | 0 |
| 56 | MG | 2A | 3499 | 1/1 | 0.96 | 0.16 | 100,100,100,100 | 0 |
| 56 | MG | 1a | 1665 | 1/1 | 0.96 | 0.12 | 132,132,132,132 | 0 |
| 56 | MG | 1A | 4162 | 1/1 | 0.96 | 0.17 | 56,56,56,56 | 0 |
| 56 | MG | 2A | 3688 | 1/1 | 0.96 | 0.61 | 143,143,143,143 | 0 |
| 56 | MG | 1A | 4438 | 1/1 | 0.96 | 0.09 | 65,65,65,65 | 0 |
| 56 | MG | 2A | 3047 | 1/1 | 0.96 | 0.26 | 99,99,99,99 | 0 |
| 56 | MG | 1A | 4140 | 1/1 | 0.96 | 0.27 | 70,70,70,70 | 0 |
| 56 | MG | 1A | 4164 | 1/1 | 0.96 | 0.27 | 58,58,58,58 | 0 |
| 56 | MG | 2A | 3334 | 1/1 | 0.96 | 0.31 | 105,105,105,105 | 0 |
| 56 | MG | 2A | 3694 | 1/1 | 0.96 | 0.53 | 61,61,61,61 | 0 |
| 56 | MG | 1A | 4070 | 1/1 | 0.96 | 0.21 | 67,67,67,67 | 0 |
| 56 | MG | 1A | 4552 | 1/1 | 0.96 | 0.25 | 71,71,71,71 | 0 |
| 56 | MG | 2A | 3511 | 1/1 | 0.96 | 0.19 | 89,89,89,89 | 0 |
| 56 | MG | 2A | 3182 | 1/1 | 0.96 | 0.50 | 105,105,105,105 | 0 |
| 56 | MG | 2A | 3054 | 1/1 | 0.96 | 0.20 | 100,100,100,100 | 0 |
| 56 | MG | 2A | 3514 | 1/1 | 0.96 | 0.12 | 114,114,114,114 | 0 |
| 56 | MG | 2A | 3702 | 1/1 | 0.96 | 0.25 | 92,92,92,92 | 0 |
| 56 | MG | 2A | 3515 | 1/1 | 0.96 | 0.35 | 115,115,115,115 | 0 |
| 56 | MG | 1U | 202 | 1/1 | 0.96 | 0.21 | 58,58,58,58 | 0 |
| 56 | MG | 1A | 4554 | 1/1 | 0.96 | 0.25 | 79,79,79,79 | 0 |
| 56 | MG | 1A | 4229 | 1/1 | 0.96 | 0.32 | 111,111,111,111 | 0 |
| 56 | MG | 2A | 3187 | 1/1 | 0.96 | 0.18 | 105,105,105,105 | 0 |
| 56 | MG | 2A | 3710 | 1/1 | 0.96 | 0.22 | 95,95,95,95 | 0 |
| 56 | MG | 1A | 4945 | 1/1 | 0.96 | 0.13 | 73,73,73,73 | 0 |
| 56 | MG | 2A | 3189 | 1/1 | 0.96 | 0.27 | 113,113,113,113 | 0 |
| 56 | MG | 2A | 3714 | 1/1 | 0.96 | 0.25 | 101,101,101,101 | 0 |

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| Mol | Type | Chain | Res | Atoms | RSCC | RSR | B-factors(Å$^2$) | Q<0.9 |
|---|---|---|---|---|---|---|---|---|
| 56 | MG | 2A | 3345 | 1/1 | 0.96 | 0.36 | 83,83,83,83 | 0 |
| 56 | MG | 2A | 3716 | 1/1 | 0.96 | 0.24 | 116,116,116,116 | 0 |
| 56 | MG | 2A | 3190 | 1/1 | 0.96 | 0.47 | 98,98,98,98 | 0 |
| 56 | MG | 2s | 103 | 1/1 | 0.96 | 0.10 | 251,251,251,251 | 0 |
| 56 | MG | 2A | 3525 | 1/1 | 0.96 | 0.18 | 106,106,106,106 | 0 |
| 56 | MG | 1a | 1679 | 1/1 | 0.96 | 0.16 | 163,163,163,163 | 0 |
| 56 | MG | 1A | 4391 | 1/1 | 0.96 | 0.23 | 93,93,93,93 | 0 |
| 56 | MG | 1A | 4344 | 1/1 | 0.96 | 0.13 | 70,70,70,70 | 0 |
| 56 | MG | 1A | 4446 | 1/1 | 0.96 | 0.37 | 59,59,59,59 | 0 |
| 56 | MG | 2A | 3195 | 1/1 | 0.96 | 0.49 | 90,90,90,90 | 0 |
| 56 | MG | 2A | 3354 | 1/1 | 0.96 | 0.34 | 79,79,79,79 | 0 |
| 56 | MG | 2w | 201 | 1/1 | 0.96 | 0.13 | 84,84,84,84 | 0 |
| 56 | MG | 1A | 4025 | 1/1 | 0.96 | 0.32 | 67,67,67,67 | 0 |
| 56 | MG | 2x | 101 | 1/1 | 0.96 | 0.87 | 62,62,62,62 | 0 |
| 56 | MG | 2A | 3356 | 1/1 | 0.96 | 0.30 | 80,80,80,80 | 0 |
| 56 | MG | 1A | 4196 | 1/1 | 0.96 | 0.32 | 73,73,73,73 | 0 |
| 56 | MG | 1A | 4269 | 1/1 | 0.96 | 0.15 | 69,69,69,69 | 0 |
| 56 | MG | 2A | 3730 | 1/1 | 0.96 | 0.36 | 99,99,99,99 | 0 |
| 56 | MG | 1A | 4353 | 1/1 | 0.96 | 0.28 | 59,59,59,59 | 0 |
| 56 | MG | 1A | 4572 | 1/1 | 0.96 | 0.18 | 83,83,83,83 | 0 |
| 56 | MG | 1A | 4573 | 1/1 | 0.96 | 0.18 | 70,70,70,70 | 0 |
| 56 | MG | 1A | 4399 | 1/1 | 0.96 | 0.14 | 77,77,77,77 | 0 |
| 56 | MG | 1A | 4871 | 1/1 | 0.96 | 0.24 | 55,55,55,55 | 0 |
| 56 | MG | 1A | 4270 | 1/1 | 0.96 | 0.34 | 68,68,68,68 | 0 |
| 56 | MG | 1A | 4577 | 1/1 | 0.96 | 0.08 | 58,58,58,58 | 0 |
| 56 | MG | 2A | 3074 | 1/1 | 0.96 | 0.15 | 138,138,138,138 | 0 |
| 56 | MG | 1A | 4272 | 1/1 | 0.96 | 0.31 | 68,68,68,68 | 0 |
| 56 | MG | 2A | 3370 | 1/1 | 0.96 | 0.20 | 99,99,99,99 | 0 |
| 56 | MG | 1a | 1806 | 1/1 | 0.96 | 0.19 | 135,135,135,135 | 0 |
| 56 | MG | 2A | 3209 | 1/1 | 0.96 | 0.24 | 93,93,93,93 | 0 |
| 56 | MG | 1a | 1695 | 1/1 | 0.96 | 0.07 | 159,159,159,159 | 0 |
| 56 | MG | 1a | 1808 | 1/1 | 0.96 | 0.40 | 122,122,122,122 | 0 |
| 56 | MG | 2A | 3079 | 1/1 | 0.96 | 0.15 | 125,125,125,125 | 0 |
| 56 | MG | 2a | 1601 | 1/1 | 0.96 | 0.18 | 122,122,122,122 | 0 |
| 56 | MG | 2A | 3748 | 1/1 | 0.96 | 0.33 | 104,104,104,104 | 0 |
| 56 | MG | 2A | 3749 | 1/1 | 0.96 | 0.24 | 93,93,93,93 | 0 |
| 56 | MG | 1a | 1696 | 1/1 | 0.96 | 0.13 | 159,159,159,159 | 0 |
| 56 | MG | 1A | 4029 | 1/1 | 0.96 | 0.27 | 51,51,51,51 | 0 |
| 56 | MG | 2a | 1802 | 1/1 | 0.96 | 0.27 | 166,166,166,166 | 0 |
| 56 | MG | 1A | 5063 | 1/1 | 0.96 | 0.16 | 58,58,58,58 | 0 |
| 56 | MG | 1A | 4128 | 1/1 | 0.96 | 0.20 | 60,60,60,60 | 0 |
| 56 | MG | 1A | 4145 | 1/1 | 0.96 | 0.47 | 51,51,51,51 | 0 |

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| Mol | Type | Chain | Res | Atoms | RSCC | RSR | B-factors(Å$^2$) | Q<0.9 |
|---|---|---|---|---|---|---|---|---|
| 56 | MG | 2A | 3219 | 1/1 | 0.96 | 0.28 | 110,110,110,110 | 0 |
| 56 | MG | 1a | 1815 | 1/1 | 0.96 | 0.24 | 171,171,171,171 | 0 |
| 56 | MG | 2A | 3352 | 1/1 | 0.97 | 0.18 | 89,89,89,89 | 0 |
| 56 | MG | 1A | 4496 | 1/1 | 0.97 | 0.76 | 60,60,60,60 | 0 |
| 56 | MG | 2A | 3656 | 1/1 | 0.97 | 0.51 | 109,109,109,109 | 0 |
| 56 | MG | 1A | 5057 | 1/1 | 0.97 | 0.21 | 170,170,170,170 | 0 |
| 56 | MG | 2A | 3827 | 1/1 | 0.97 | 0.10 | 105,105,105,105 | 0 |
| 56 | MG | 2a | 1655 | 1/1 | 0.97 | 0.06 | 142,142,142,142 | 0 |
| 56 | MG | 1A | 4111 | 1/1 | 0.97 | 0.30 | 49,49,49,49 | 0 |
| 56 | MG | 1A | 4041 | 1/1 | 0.97 | 0.64 | 74,74,74,74 | 0 |
| 56 | MG | 1A | 4556 | 1/1 | 0.97 | 0.17 | 58,58,58,58 | 0 |
| 56 | MG | 2A | 3507 | 1/1 | 0.97 | 0.22 | 128,128,128,128 | 0 |
| 56 | MG | 1A | 4557 | 1/1 | 0.97 | 0.38 | 58,58,58,58 | 0 |
| 56 | MG | 2A | 3665 | 1/1 | 0.97 | 0.22 | 129,129,129,129 | 0 |
| 56 | MG | 1A | 4558 | 1/1 | 0.97 | 0.25 | 66,66,66,66 | 0 |
| 56 | MG | 1A | 4407 | 1/1 | 0.97 | 0.25 | 52,52,52,52 | 0 |
| 56 | MG | 1A | 4127 | 1/1 | 0.97 | 0.45 | 63,63,63,63 | 0 |
| 56 | MG | 1a | 1716 | 1/1 | 0.97 | 0.22 | 120,120,120,120 | 0 |
| 56 | MG | 1a | 1717 | 1/1 | 0.97 | 0.43 | 110,110,110,110 | 0 |
| 56 | MG | 1A | 4167 | 1/1 | 0.97 | 0.37 | 58,58,58,58 | 0 |
| 56 | MG | 2A | 3840 | 1/1 | 0.97 | 0.26 | 117,117,117,117 | 0 |
| 56 | MG | 1a | 1610 | 1/1 | 0.97 | 0.34 | 90,90,90,90 | 0 |
| 56 | MG | 2A | 3368 | 1/1 | 0.97 | 0.25 | 100,100,100,100 | 0 |
| 56 | MG | 2A | 3518 | 1/1 | 0.97 | 0.10 | 96,96,96,96 | 0 |
| 56 | MG | 1a | 1720 | 1/1 | 0.97 | 0.40 | 124,124,124,124 | 0 |
| 56 | MG | 2A | 3679 | 1/1 | 0.97 | 0.49 | 106,106,106,106 | 0 |
| 56 | MG | 1A | 4088 | 1/1 | 0.97 | 0.24 | 66,66,66,66 | 0 |
| 56 | MG | 1A | 4302 | 1/1 | 0.97 | 0.42 | 80,80,80,80 | 0 |
| 56 | MG | 1A | 4564 | 1/1 | 0.97 | 0.34 | 56,56,56,56 | 0 |
| 56 | MG | 1A | 4413 | 1/1 | 0.97 | 0.20 | 63,63,63,63 | 0 |
| 56 | MG | 1a | 1726 | 1/1 | 0.97 | 0.09 | 127,127,127,127 | 0 |
| 56 | MG | 1A | 4782 | 1/1 | 0.97 | 0.23 | 81,81,81,81 | 0 |
| 56 | MG | 1A | 4877 | 1/1 | 0.97 | 0.15 | 81,81,81,81 | 0 |
| 56 | MG | 2A | 3378 | 1/1 | 0.97 | 0.15 | 106,106,106,106 | 0 |
| 56 | MG | 1B | 210 | 1/1 | 0.97 | 0.54 | 89,89,89,89 | 0 |
| 56 | MG | 1A | 4878 | 1/1 | 0.97 | 0.34 | 77,77,77,77 | 0 |
| 56 | MG | 1A | 4332 | 1/1 | 0.97 | 0.34 | 75,75,75,75 | 0 |
| 56 | MG | 1A | 4103 | 1/1 | 0.97 | 0.26 | 50,50,50,50 | 0 |
| 56 | MG | 1A | 4569 | 1/1 | 0.97 | 0.32 | 60,60,60,60 | 0 |
| 56 | MG | 1A | 4974 | 1/1 | 0.97 | 0.11 | 74,74,74,74 | 0 |
| 56 | MG | 2A | 3386 | 1/1 | 0.97 | 0.21 | 125,125,125,125 | 0 |
| 56 | MG | 1a | 1847 | 1/1 | 0.97 | 0.12 | 184,184,184,184 | 0 |

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| Mol | Type | Chain | Res | Atoms | RSCC | RSR | B-factors(Å$^2$) | Q<0.9 |
|---|---|---|---|---|---|---|---|---|
| 56 | MG | 2A | 3696 | 1/1 | 0.97 | 0.27 | 105,105,105,105 | 0 |
| 56 | MG | 1A | 4570 | 1/1 | 0.97 | 0.30 | 60,60,60,60 | 0 |
| 56 | MG | 1A | 4508 | 1/1 | 0.97 | 0.25 | 70,70,70,70 | 0 |
| 56 | MG | 1A | 4641 | 1/1 | 0.97 | 0.16 | 79,79,79,79 | 0 |
| 56 | MG | 2A | 3124 | 1/1 | 0.97 | 0.20 | 125,125,125,125 | 0 |
| 56 | MG | 1a | 1851 | 1/1 | 0.97 | 0.16 | 175,175,175,175 | 0 |
| 56 | MG | 1A | 4109 | 1/1 | 0.97 | 0.21 | 54,54,54,54 | 0 |
| 56 | MG | 2A | 3703 | 1/1 | 0.97 | 0.43 | 94,94,94,94 | 0 |
| 56 | MG | 1A | 4574 | 1/1 | 0.97 | 0.25 | 57,57,57,57 | 0 |
| 56 | MG | 2A | 3705 | 1/1 | 0.97 | 0.26 | 98,98,98,98 | 0 |
| 56 | MG | 1A | 4793 | 1/1 | 0.97 | 0.17 | 108,108,108,108 | 0 |
| 56 | MG | 1A | 4335 | 1/1 | 0.97 | 0.19 | 76,76,76,76 | 0 |
| 56 | MG | 1A | 4983 | 1/1 | 0.97 | 0.21 | 56,56,56,56 | 0 |
| 56 | MG | 1a | 1633 | 1/1 | 0.97 | 0.18 | 109,109,109,109 | 0 |
| 56 | MG | 2A | 3011 | 1/1 | 0.97 | 0.29 | 104,104,104,104 | 0 |
| 56 | MG | 2a | 1891 | 1/1 | 0.97 | 0.11 | 157,157,157,157 | 0 |
| 56 | MG | 2A | 3711 | 1/1 | 0.97 | 0.17 | 95,95,95,95 | 0 |
| 56 | MG | 1A | 4713 | 1/1 | 0.97 | 0.26 | 55,55,55,55 | 0 |
| 56 | MG | 2A | 3013 | 1/1 | 0.97 | 0.38 | 118,118,118,118 | 0 |
| 56 | MG | 1a | 1635 | 1/1 | 0.97 | 0.16 | 121,121,121,121 | 0 |
| 56 | MG | 1A | 4458 | 1/1 | 0.97 | 0.34 | 60,60,60,60 | 0 |
| 56 | MG | 1A | 4418 | 1/1 | 0.97 | 0.20 | 52,52,52,52 | 0 |
| 56 | MG | 2A | 3406 | 1/1 | 0.97 | 0.14 | 140,140,140,140 | 0 |
| 56 | MG | 1a | 1750 | 1/1 | 0.97 | 0.17 | 134,134,134,134 | 0 |
| 56 | MG | 2D | 304 | 1/1 | 0.97 | 0.13 | 107,107,107,107 | 0 |
| 56 | MG | 2D | 305 | 1/1 | 0.97 | 0.12 | 96,96,96,96 | 0 |
| 56 | MG | 1A | 4717 | 1/1 | 0.97 | 0.64 | 81,81,81,81 | 0 |
| 56 | MG | 1A | 4513 | 1/1 | 0.97 | 0.28 | 78,78,78,78 | 0 |
| 56 | MG | 2a | 1720 | 1/1 | 0.97 | 0.10 | 153,153,153,153 | 0 |
| 56 | MG | 1A | 4159 | 1/1 | 0.97 | 0.18 | 50,50,50,50 | 0 |
| 56 | MG | 1A | 4205 | 1/1 | 0.97 | 0.20 | 56,56,56,56 | 0 |
| 56 | MG | 2A | 3723 | 1/1 | 0.97 | 0.20 | 96,96,96,96 | 0 |
| 56 | MG | 1A | 4206 | 1/1 | 0.97 | 0.36 | 55,55,55,55 | 0 |
| 56 | MG | 1A | 4808 | 1/1 | 0.97 | 0.23 | 53,53,53,53 | 0 |
| 56 | MG | 1A | 4517 | 1/1 | 0.97 | 0.78 | 81,81,81,81 | 0 |
| 56 | MG | 1A | 4810 | 1/1 | 0.97 | 0.12 | 63,63,63,63 | 0 |
| 56 | MG | 1a | 1759 | 1/1 | 0.97 | 0.19 | 104,104,104,104 | 0 |
| 56 | MG | 2A | 3274 | 1/1 | 0.97 | 0.21 | 83,83,83,83 | 0 |
| 56 | MG | 2N | 202 | 1/1 | 0.97 | 0.40 | 84,84,84,84 | 0 |
| 56 | MG | 1A | 4276 | 1/1 | 0.97 | 0.30 | 67,67,67,67 | 0 |
| 56 | MG | 2A | 3731 | 1/1 | 0.97 | 0.24 | 86,86,86,86 | 0 |
| 56 | MG | 2A | 3276 | 1/1 | 0.97 | 0.29 | 85,85,85,85 | 0 |

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| Mol | Type | Chain | Res | Atoms | RSCC | RSR | B-factors(Å$^2$) | Q<0.9 |
|---|---|---|---|---|---|---|---|---|
| 56 | MG | 2A | 3568 | 1/1 | 0.97 | 0.22 | 92,92,92,92 | 0 |
| 56 | MG | 1A | 4423 | 1/1 | 0.97 | 0.21 | 53,53,53,53 | 0 |
| 56 | MG | 2A | 3422 | 1/1 | 0.97 | 0.10 | 130,130,130,130 | 0 |
| 56 | MG | 1A | 4813 | 1/1 | 0.97 | 0.14 | 70,70,70,70 | 0 |
| 56 | MG | 1A | 4814 | 1/1 | 0.97 | 0.69 | 59,59,59,59 | 0 |
| 56 | MG | 1A | 4907 | 1/1 | 0.97 | 0.20 | 52,52,52,52 | 0 |
| 56 | MG | 1A | 4465 | 1/1 | 0.97 | 0.19 | 60,60,60,60 | 0 |
| 56 | MG | 1A | 5008 | 1/1 | 0.97 | 0.21 | 76,76,76,76 | 0 |
| 56 | MG | 1A | 4277 | 1/1 | 0.97 | 0.58 | 53,53,53,53 | 0 |
| 56 | MG | 1A | 5010 | 1/1 | 0.97 | 0.28 | 75,75,75,75 | 0 |
| 56 | MG | 1A | 4342 | 1/1 | 0.97 | 0.17 | 65,65,65,65 | 0 |
| 56 | MG | 1A | 4658 | 1/1 | 0.97 | 0.33 | 96,96,96,96 | 0 |
| 56 | MG | 1A | 4468 | 1/1 | 0.97 | 0.21 | 58,58,58,58 | 0 |
| 56 | MG | 2A | 3433 | 1/1 | 0.97 | 0.48 | 92,92,92,92 | 0 |
| 56 | MG | 1A | 4914 | 1/1 | 0.97 | 0.18 | 74,74,74,74 | 0 |
| 56 | MG | 2a | 1750 | 1/1 | 0.97 | 0.91 | 120,120,120,120 | 0 |
| 56 | MG | 2a | 1751 | 1/1 | 0.97 | 0.26 | 116,116,116,116 | 0 |
| 56 | MG | 2A | 3290 | 1/1 | 0.97 | 0.30 | 112,112,112,112 | 0 |
| 56 | MG | 1a | 1886 | 1/1 | 0.97 | 0.22 | 125,125,125,125 | 0 |
| 56 | MG | 1a | 1887 | 1/1 | 0.97 | 0.17 | 130,130,130,130 | 0 |
| 56 | MG | 2A | 3293 | 1/1 | 0.97 | 0.52 | 94,94,94,94 | 0 |
| 56 | MG | 1a | 1888 | 1/1 | 0.97 | 0.16 | 119,119,119,119 | 0 |
| 56 | MG | 2A | 3165 | 1/1 | 0.97 | 0.21 | 98,98,98,98 | 0 |
| 56 | MG | 2A | 3296 | 1/1 | 0.97 | 0.37 | 94,94,94,94 | 0 |
| 56 | MG | 1A | 4469 | 1/1 | 0.97 | 0.19 | 56,56,56,56 | 0 |
| 56 | MG | 2A | 3445 | 1/1 | 0.97 | 0.47 | 86,86,86,86 | 0 |
| 56 | MG | 1A | 4470 | 1/1 | 0.97 | 0.18 | 54,54,54,54 | 0 |
| 56 | MG | 1P | 204 | 1/1 | 0.97 | 0.10 | 88,88,88,88 | 0 |
| 56 | MG | 1A | 4426 | 1/1 | 0.97 | 0.18 | 77,77,77,77 | 0 |
| 56 | MG | 1A | 4919 | 1/1 | 0.97 | 0.29 | 62,62,62,62 | 0 |
| 56 | MG | 2A | 3600 | 1/1 | 0.97 | 0.07 | 118,118,118,118 | 0 |
| 56 | MG | 2A | 3764 | 1/1 | 0.97 | 0.10 | 151,151,151,151 | 0 |
| 56 | MG | 2A | 3049 | 1/1 | 0.97 | 0.34 | 94,94,94,94 | 0 |
| 56 | MG | 2A | 3602 | 1/1 | 0.97 | 0.18 | 97,97,97,97 | 0 |
| 56 | MG | 2A | 3304 | 1/1 | 0.97 | 0.50 | 127,127,127,127 | 0 |
| 56 | MG | 27 | 102 | 1/1 | 0.97 | 0.56 | 89,89,89,89 | 0 |
| 56 | MG | 27 | 103 | 1/1 | 0.97 | 0.12 | 97,97,97,97 | 0 |
| 56 | MG | 1A | 4122 | 1/1 | 0.97 | 0.40 | 66,66,66,66 | 0 |
| 56 | MG | 1A | 4251 | 1/1 | 0.97 | 0.23 | 60,60,60,60 | 0 |
| 56 | MG | 1A | 4826 | 1/1 | 0.97 | 0.39 | 91,91,91,91 | 0 |
| 56 | MG | 1a | 1668 | 1/1 | 0.97 | 0.07 | 139,139,139,139 | 0 |
| 56 | MG | 1A | 4476 | 1/1 | 0.97 | 0.17 | 66,66,66,66 | 0 |

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| Mol | Type | Chain | Res | Atoms | RSCC | RSR | B-factors(Å$^2$) | Q<0.9 |
|---|---|---|---|---|---|---|---|---|
| 56 | MG | 2A | 3177 | 1/1 | 0.97 | 0.47 | 113,113,113,113 | 0 |
| 56 | MG | 1A | 4666 | 1/1 | 0.97 | 0.49 | 78,78,78,78 | 0 |
| 56 | MG | 2A | 3313 | 1/1 | 0.97 | 0.22 | 95,95,95,95 | 0 |
| 56 | MG | 1A | 4741 | 1/1 | 0.97 | 0.28 | 75,75,75,75 | 0 |
| 56 | MG | 1A | 4252 | 1/1 | 0.97 | 0.40 | 54,54,54,54 | 0 |
| 56 | MG | 1A | 4281 | 1/1 | 0.97 | 0.30 | 70,70,70,70 | 0 |
| 56 | MG | 1A | 4096 | 1/1 | 0.97 | 0.36 | 55,55,55,55 | 0 |
| 56 | MG | 2q | 203 | 1/1 | 0.97 | 0.28 | 151,151,151,151 | 0 |
| 56 | MG | 2a | 1605 | 1/1 | 0.97 | 0.27 | 127,127,127,127 | 0 |
| 56 | MG | 1A | 4534 | 1/1 | 0.97 | 0.20 | 78,78,78,78 | 0 |
| 56 | MG | 1A | 5032 | 1/1 | 0.97 | 0.20 | 83,83,83,83 | 0 |
| 56 | MG | 1A | 4351 | 1/1 | 0.97 | 0.09 | 67,67,67,67 | 0 |
| 56 | MG | 2A | 3620 | 1/1 | 0.97 | 0.43 | 122,122,122,122 | 0 |
| 56 | MG | 1A | 4254 | 1/1 | 0.97 | 0.30 | 66,66,66,66 | 0 |
| 56 | MG | 1A | 4255 | 1/1 | 0.97 | 0.29 | 65,65,65,65 | 0 |
| 56 | MG | 2A | 3623 | 1/1 | 0.97 | 0.31 | 147,147,147,147 | 0 |
| 56 | MG | 2A | 3326 | 1/1 | 0.97 | 0.40 | 85,85,85,85 | 0 |
| 56 | MG | 1A | 4256 | 1/1 | 0.97 | 0.34 | 65,65,65,65 | 0 |
| 56 | MG | 1A | 4539 | 1/1 | 0.97 | 0.19 | 69,69,69,69 | 0 |
| 56 | MG | 2A | 3790 | 1/1 | 0.97 | 0.33 | 96,96,96,96 | 0 |
| 56 | MG | 2A | 3068 | 1/1 | 0.97 | 0.23 | 148,148,148,148 | 0 |
| 56 | MG | 1A | 4176 | 1/1 | 0.97 | 0.22 | 59,59,59,59 | 0 |
| 56 | MG | 1A | 5039 | 1/1 | 0.97 | 0.11 | 68,68,68,68 | 0 |
| 56 | MG | 1A | 4213 | 1/1 | 0.97 | 0.40 | 57,57,57,57 | 0 |
| 56 | MG | 1A | 4177 | 1/1 | 0.97 | 0.20 | 58,58,58,58 | 0 |
| 56 | MG | 2A | 3796 | 1/1 | 0.97 | 0.18 | 96,96,96,96 | 0 |
| 56 | MG | 1A | 4440 | 1/1 | 0.97 | 0.22 | 73,73,73,73 | 0 |
| 56 | MG | 1A | 5043 | 1/1 | 0.97 | 0.62 | 71,71,71,71 | 0 |
| 56 | MG | 1A | 4400 | 1/1 | 0.97 | 0.17 | 75,75,75,75 | 0 |
| 56 | MG | 1A | 5046 | 1/1 | 0.97 | 0.10 | 78,78,78,78 | 0 |
| 56 | MG | 1A | 4260 | 1/1 | 0.97 | 0.37 | 58,58,58,58 | 0 |
| 56 | MG | 1A | 5048 | 1/1 | 0.97 | 0.09 | 65,65,65,65 | 0 |
| 56 | MG | 2A | 3804 | 1/1 | 0.97 | 0.29 | 114,114,114,114 | 0 |
| 56 | MG | 1A | 4760 | 1/1 | 0.97 | 0.25 | 67,67,67,67 | 0 |
| 56 | MG | 2a | 1631 | 1/1 | 0.97 | 0.09 | 151,151,151,151 | 0 |
| 56 | MG | 1A | 4152 | 1/1 | 0.97 | 0.31 | 56,56,56,56 | 0 |
| 56 | MG | 2A | 3081 | 1/1 | 0.97 | 0.18 | 125,125,125,125 | 0 |
| 56 | MG | 2a | 1813 | 1/1 | 0.97 | 0.10 | 143,143,143,143 | 0 |
| 56 | MG | 1A | 4852 | 1/1 | 0.97 | 0.44 | 71,71,71,71 | 0 |
| 56 | MG | 1a | 1811 | 1/1 | 0.97 | 0.17 | 99,99,99,99 | 0 |
| 56 | MG | 15 | 102 | 1/1 | 0.97 | 0.21 | 60,60,60,60 | 0 |
| 56 | MG | 2A | 3812 | 1/1 | 0.97 | 0.45 | 144,144,144,144 | 0 |

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| Mol | Type | Chain | Res | Atoms | RSCC | RSR | B-factors(Å$^2$) | Q<0.9 |
|---|---|---|---|---|---|---|---|---|
| 56 | MG | 2a | 1818 | 1/1 | 0.97 | 0.16 | 156,156,156,156 | 0 |
| 56 | MG | 1A | 4237 | 1/1 | 0.97 | 0.37 | 73,73,73,73 | 0 |
| 57 | ZN | 1Y | 302 | 1/1 | 0.97 | 0.12 | 96,96,96,96 | 0 |
| 56 | MG | 2a | 1820 | 1/1 | 0.97 | 0.22 | 155,155,155,155 | 0 |
| 57 | ZN | 15 | 103 | 1/1 | 0.97 | 0.16 | 74,74,74,74 | 0 |
| 56 | MG | 1A | 4493 | 1/1 | 0.97 | 0.34 | 68,68,68,68 | 0 |
| 56 | MG | 2A | 3494 | 1/1 | 0.97 | 0.33 | 134,134,134,134 | 0 |
| 56 | MG | 17 | 102 | 1/1 | 0.97 | 0.80 | 61,61,61,61 | 0 |
| 57 | ZN | 25 | 102 | 1/1 | 0.97 | 0.20 | 119,119,119,119 | 0 |
| 56 | MG | 1A | 4494 | 1/1 | 0.97 | 0.18 | 78,78,78,78 | 0 |
| 56 | MG | 2A | 3498 | 1/1 | 0.97 | 0.12 | 102,102,102,102 | 0 |
| 56 | MG | 2A | 3819 | 1/1 | 0.97 | 0.12 | 42,42,42,42 | 0 |
| 58 | SF4 | 1d | 304 | 8/8 | 0.97 | 0.20 | 150,150,150,150 | 0 |
| 56 | MG | 18 | 101 | 1/1 | 0.97 | 0.30 | 56,56,56,56 | 0 |
| 56 | MG | 1A | 4194 | 1/1 | 0.97 | 0.22 | 68,68,68,68 | 0 |
| 56 | MG | 2a | 1833 | 1/1 | 0.97 | 0.26 | 161,161,161,161 | 0 |
| 56 | MG | 1A | 4271 | 1/1 | 0.98 | 0.58 | 62,62,62,62 | 0 |
| 56 | MG | 1A | 5045 | 1/1 | 0.98 | 0.61 | 67,67,67,67 | 0 |
| 56 | MG | 1A | 4225 | 1/1 | 0.98 | 0.25 | 73,73,73,73 | 0 |
| 56 | MG | 1a | 1741 | 1/1 | 0.98 | 0.08 | 139,139,139,139 | 0 |
| 56 | MG | 1T | 202 | 1/1 | 0.98 | 0.21 | 83,83,83,83 | 0 |
| 56 | MG | 1A | 4201 | 1/1 | 0.98 | 0.53 | 70,70,70,70 | 0 |
| 56 | MG | 1A | 4362 | 1/1 | 0.98 | 0.19 | 67,67,67,67 | 0 |
| 56 | MG | 2A | 3261 | 1/1 | 0.98 | 0.39 | 80,80,80,80 | 0 |
| 56 | MG | 2A | 3596 | 1/1 | 0.98 | 0.10 | 100,100,100,100 | 0 |
| 56 | MG | 1A | 4607 | 1/1 | 0.98 | 0.24 | 67,67,67,67 | 0 |
| 56 | MG | 1A | 4967 | 1/1 | 0.98 | 0.10 | 83,83,83,83 | 0 |
| 56 | MG | 1A | 4002 | 1/1 | 0.98 | 0.13 | 65,65,65,65 | 0 |
| 56 | MG | 2A | 3265 | 1/1 | 0.98 | 0.13 | 90,90,90,90 | 0 |
| 56 | MG | 1A | 4827 | 1/1 | 0.98 | 0.23 | 69,69,69,69 | 0 |
| 56 | MG | 2A | 3846 | 1/1 | 0.98 | 0.25 | 108,108,108,108 | 0 |
| 56 | MG | 1A | 4171 | 1/1 | 0.98 | 0.47 | 49,49,49,49 | 0 |
| 56 | MG | 2A | 3848 | 1/1 | 0.98 | 0.12 | 61,61,61,61 | 0 |
| 56 | MG | 2A | 3375 | 1/1 | 0.98 | 0.25 | 103,103,103,103 | 0 |
| 56 | MG | 1A | 4147 | 1/1 | 0.98 | 0.28 | 57,57,57,57 | 0 |
| 56 | MG | 2A | 3851 | 1/1 | 0.98 | 0.20 | 110,110,110,110 | 0 |
| 56 | MG | 2A | 3852 | 1/1 | 0.98 | 0.14 | 96,96,96,96 | 0 |
| 56 | MG | 1A | 4709 | 1/1 | 0.98 | 0.14 | 68,68,68,68 | 0 |
| 56 | MG | 1A | 4366 | 1/1 | 0.98 | 0.30 | 60,60,60,60 | 0 |
| 56 | MG | 1A | 4187 | 1/1 | 0.98 | 0.31 | 67,67,67,67 | 0 |
| 56 | MG | 1A | 4769 | 1/1 | 0.98 | 0.13 | 72,72,72,72 | 0 |
| 56 | MG | 1A | 4904 | 1/1 | 0.98 | 0.19 | 63,63,63,63 | 0 |

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| Mol | Type | Chain | Res | Atoms | RSCC | RSR | B-factors(Å$^2$) | Q<0.9 |
|---|---|---|---|---|---|---|---|---|
| 56 | MG | 1A | 4770 | 1/1 | 0.98 | 0.30 | 65,65,65,65 | 0 |
| 56 | MG | 1A | 4771 | 1/1 | 0.98 | 0.25 | 70,70,70,70 | 0 |
| 56 | MG | 2a | 1638 | 1/1 | 0.98 | 0.25 | 148,148,148,148 | 0 |
| 56 | MG | 2A | 3496 | 1/1 | 0.98 | 0.17 | 99,99,99,99 | 0 |
| 56 | MG | 1A | 4614 | 1/1 | 0.98 | 0.18 | 71,71,71,71 | 0 |
| 56 | MG | 1A | 4188 | 1/1 | 0.98 | 0.30 | 68,68,68,68 | 0 |
| 56 | MG | 2a | 1642 | 1/1 | 0.98 | 0.08 | 143,143,143,143 | 0 |
| 56 | MG | 1A | 4617 | 1/1 | 0.98 | 0.21 | 98,98,98,98 | 0 |
| 56 | MG | 2a | 1644 | 1/1 | 0.98 | 0.41 | 125,125,125,125 | 0 |
| 56 | MG | 2A | 3616 | 1/1 | 0.98 | 0.16 | 93,93,93,93 | 0 |
| 56 | MG | 1A | 4102 | 1/1 | 0.98 | 0.14 | 53,53,53,53 | 0 |
| 56 | MG | 1A | 4174 | 1/1 | 0.98 | 0.19 | 59,59,59,59 | 0 |
| 56 | MG | 1A | 4913 | 1/1 | 0.98 | 0.14 | 72,72,72,72 | 0 |
| 56 | MG | 1A | 4718 | 1/1 | 0.98 | 0.11 | 99,99,99,99 | 0 |
| 56 | MG | 2A | 3741 | 1/1 | 0.98 | 0.20 | 85,85,85,85 | 0 |
| 56 | MG | 1a | 1675 | 1/1 | 0.98 | 0.29 | 124,124,124,124 | 0 |
| 56 | MG | 1a | 1676 | 1/1 | 0.98 | 0.08 | 151,151,151,151 | 0 |
| 56 | MG | 15 | 101 | 1/1 | 0.98 | 0.23 | 61,61,61,61 | 0 |
| 56 | MG | 1A | 4161 | 1/1 | 0.98 | 0.21 | 58,58,58,58 | 0 |
| 56 | MG | 2A | 3396 | 1/1 | 0.98 | 0.16 | 126,126,126,126 | 0 |
| 56 | MG | 1A | 4668 | 1/1 | 0.98 | 0.28 | 93,93,93,93 | 0 |
| 56 | MG | 1A | 4044 | 1/1 | 0.98 | 0.15 | 62,62,62,62 | 0 |
| 56 | MG | 1A | 4991 | 1/1 | 0.98 | 0.15 | 66,66,66,66 | 0 |
| 56 | MG | 1A | 4338 | 1/1 | 0.98 | 0.14 | 67,67,67,67 | 0 |
| 56 | MG | 2a | 1660 | 1/1 | 0.98 | 0.44 | 142,142,142,142 | 0 |
| 56 | MG | 1A | 4283 | 1/1 | 0.98 | 0.35 | 65,65,65,65 | 0 |
| 56 | MG | 1A | 4995 | 1/1 | 0.98 | 0.18 | 77,77,77,77 | 0 |
| 56 | MG | 18 | 103 | 1/1 | 0.98 | 0.19 | 75,75,75,75 | 0 |
| 56 | MG | 1A | 4139 | 1/1 | 0.98 | 0.27 | 68,68,68,68 | 0 |
| 56 | MG | 1A | 4998 | 1/1 | 0.98 | 0.16 | 80,80,80,80 | 0 |
| 56 | MG | 1A | 4851 | 1/1 | 0.98 | 0.24 | 72,72,72,72 | 0 |
| 56 | MG | 1A | 4533 | 1/1 | 0.98 | 0.32 | 68,68,68,68 | 0 |
| 56 | MG | 1A | 4674 | 1/1 | 0.98 | 0.24 | 91,91,91,91 | 0 |
| 56 | MG | 2A | 3638 | 1/1 | 0.98 | 0.10 | 114,114,114,114 | 0 |
| 56 | MG | 2A | 3409 | 1/1 | 0.98 | 0.09 | 116,116,116,116 | 0 |
| 56 | MG | 1A | 4215 | 1/1 | 0.98 | 0.42 | 54,54,54,54 | 0 |
| 56 | MG | 1A | 4216 | 1/1 | 0.98 | 0.21 | 62,62,62,62 | 0 |
| 56 | MG | 1a | 1693 | 1/1 | 0.98 | 0.14 | 136,136,136,136 | 0 |
| 56 | MG | 2A | 3303 | 1/1 | 0.98 | 0.19 | 113,113,113,113 | 0 |
| 56 | MG | 1a | 1785 | 1/1 | 0.98 | 0.33 | 136,136,136,136 | 0 |
| 56 | MG | 1A | 4729 | 1/1 | 0.98 | 0.36 | 64,64,64,64 | 0 |
| 56 | MG | 1A | 4928 | 1/1 | 0.98 | 0.15 | 77,77,77,77 | 0 |

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| Mol | Type | Chain | Res | Atoms | RSCC | RSR | B-factors(Å$^2$) | Q<0.9 |
|---|---|---|---|---|---|---|---|---|
| 56 | MG | 1A | 4262 | 1/1 | 0.98 | 0.22 | 66,66,66,66 | 0 |
| 56 | MG | 1A | 4731 | 1/1 | 0.98 | 0.15 | 54,54,54,54 | 0 |
| 56 | MG | 1A | 4073 | 1/1 | 0.98 | 0.20 | 71,71,71,71 | 0 |
| 56 | MG | 1A | 4345 | 1/1 | 0.98 | 0.25 | 65,65,65,65 | 0 |
| 56 | MG | 2A | 3311 | 1/1 | 0.98 | 0.36 | 102,102,102,102 | 0 |
| 56 | MG | 1A | 4796 | 1/1 | 0.98 | 0.15 | 100,100,100,100 | 0 |
| 56 | MG | 2a | 1685 | 1/1 | 0.98 | 0.37 | 167,167,167,167 | 0 |
| 56 | MG | 2A | 3653 | 1/1 | 0.98 | 0.13 | 117,117,117,117 | 0 |
| 56 | MG | 2A | 3114 | 1/1 | 0.98 | 0.17 | 153,153,153,153 | 0 |
| 56 | MG | 1A | 4346 | 1/1 | 0.98 | 0.14 | 72,72,72,72 | 0 |
| 56 | MG | 1A | 4347 | 1/1 | 0.98 | 0.18 | 66,66,66,66 | 0 |
| 56 | MG | 1A | 4384 | 1/1 | 0.98 | 0.21 | 66,66,66,66 | 0 |
| 56 | MG | 2a | 1823 | 1/1 | 0.98 | 0.10 | 153,153,153,153 | 0 |
| 56 | MG | 2A | 3118 | 1/1 | 0.98 | 0.17 | 135,135,135,135 | 0 |
| 56 | MG | 2a | 1825 | 1/1 | 0.98 | 0.19 | 169,169,169,169 | 0 |
| 56 | MG | 2A | 3659 | 1/1 | 0.98 | 0.53 | 149,149,149,149 | 0 |
| 56 | MG | 1A | 4801 | 1/1 | 0.98 | 0.19 | 76,76,76,76 | 0 |
| 56 | MG | 1A | 5017 | 1/1 | 0.98 | 0.29 | 68,68,68,68 | 0 |
| 56 | MG | 1A | 4289 | 1/1 | 0.98 | 0.27 | 68,68,68,68 | 0 |
| 56 | MG | 2a | 1830 | 1/1 | 0.98 | 0.06 | 147,147,147,147 | 0 |
| 56 | MG | 2A | 3322 | 1/1 | 0.98 | 0.27 | 88,88,88,88 | 0 |
| 56 | MG | 1A | 4939 | 1/1 | 0.98 | 0.17 | 71,71,71,71 | 0 |
| 56 | MG | 1A | 4870 | 1/1 | 0.98 | 0.16 | 54,54,54,54 | 0 |
| 56 | MG | 2A | 3325 | 1/1 | 0.98 | 0.36 | 88,88,88,88 | 0 |
| 56 | MG | 2a | 1836 | 1/1 | 0.98 | 0.39 | 124,124,124,124 | 0 |
| 56 | MG | 1A | 4803 | 1/1 | 0.98 | 0.11 | 101,101,101,101 | 0 |
| 56 | MG | 2A | 3669 | 1/1 | 0.98 | 0.20 | 92,92,92,92 | 0 |
| 56 | MG | 2A | 3670 | 1/1 | 0.98 | 0.10 | 92,92,92,92 | 0 |
| 56 | MG | 2A | 3436 | 1/1 | 0.98 | 0.24 | 104,104,104,104 | 0 |
| 56 | MG | 1A | 4195 | 1/1 | 0.98 | 0.23 | 68,68,68,68 | 0 |
| 56 | MG | 2A | 3438 | 1/1 | 0.98 | 0.54 | 79,79,79,79 | 0 |
| 56 | MG | 2A | 3674 | 1/1 | 0.98 | 0.52 | 145,145,145,145 | 0 |
| 56 | MG | 1a | 1711 | 1/1 | 0.98 | 0.11 | 125,125,125,125 | 0 |
| 56 | MG | 1A | 4001 | 1/1 | 0.98 | 0.31 | 65,65,65,65 | 0 |
| 56 | MG | 1a | 1713 | 1/1 | 0.98 | 0.26 | 109,109,109,109 | 0 |
| 56 | MG | 2A | 3799 | 1/1 | 0.98 | 0.13 | 116,116,116,116 | 0 |
| 56 | MG | 2a | 1848 | 1/1 | 0.98 | 0.13 | 157,157,157,157 | 0 |
| 56 | MG | 1E | 307 | 1/1 | 0.98 | 0.38 | 62,62,62,62 | 0 |
| 56 | MG | 1A | 4944 | 1/1 | 0.98 | 0.17 | 88,88,88,88 | 0 |
| 56 | MG | 2A | 3557 | 1/1 | 0.98 | 0.22 | 90,90,90,90 | 0 |
| 56 | MG | 2A | 3228 | 1/1 | 0.98 | 0.14 | 98,98,98,98 | 0 |
| 56 | MG | 1A | 4220 | 1/1 | 0.98 | 0.29 | 60,60,60,60 | 0 |

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| Mol | Type | Chain | Res | Atoms | RSCC | RSR | B-factors(Å$^2$) | Q<0.9 |
|---|---|---|---|---|---|---|---|---|
| 56 | MG | 1A | 4352 | 1/1 | 0.98 | 0.24 | 61,61,61,61 | 0 |
| 56 | MG | 1A | 4056 | 1/1 | 0.98 | 0.49 | 66,66,66,66 | 0 |
| 56 | MG | 2A | 3807 | 1/1 | 0.98 | 0.23 | 132,132,132,132 | 0 |
| 56 | MG | 1N | 201 | 1/1 | 0.98 | 0.35 | 72,72,72,72 | 0 |
| 56 | MG | 1A | 4591 | 1/1 | 0.98 | 0.13 | 85,85,85,85 | 0 |
| 56 | MG | 1A | 4880 | 1/1 | 0.98 | 0.20 | 83,83,83,83 | 0 |
| 56 | MG | 1a | 1722 | 1/1 | 0.98 | 0.53 | 113,113,113,113 | 0 |
| 56 | MG | 2A | 3452 | 1/1 | 0.98 | 0.53 | 90,90,90,90 | 0 |
| 56 | MG | 1a | 1816 | 1/1 | 0.98 | 0.33 | 183,183,183,183 | 0 |
| 56 | MG | 2a | 1725 | 1/1 | 0.98 | 0.12 | 142,142,142,142 | 0 |
| 56 | MG | 2A | 3237 | 1/1 | 0.98 | 0.15 | 112,112,112,112 | 0 |
| 56 | MG | 1A | 4392 | 1/1 | 0.98 | 0.08 | 103,103,103,103 | 0 |
| 56 | MG | 1A | 4951 | 1/1 | 0.98 | 0.20 | 68,68,68,68 | 0 |
| 56 | MG | 1A | 4952 | 1/1 | 0.98 | 0.16 | 65,65,65,65 | 0 |
| 56 | MG | 1A | 4004 | 1/1 | 0.98 | 0.52 | 45,45,45,45 | 0 |
| 56 | MG | 1A | 4125 | 1/1 | 0.98 | 0.35 | 79,79,79,79 | 0 |
| 57 | ZN | 16 | 102 | 1/1 | 0.98 | 0.16 | 82,82,82,82 | 0 |
| 56 | MG | 1A | 4471 | 1/1 | 0.98 | 0.38 | 60,60,60,60 | 0 |
| 56 | MG | 1P | 205 | 1/1 | 0.98 | 0.10 | 95,95,95,95 | 0 |
| 56 | MG | 1A | 4017 | 1/1 | 0.98 | 0.26 | 69,69,69,69 | 0 |
| 56 | MG | 1a | 1643 | 1/1 | 0.98 | 0.23 | 130,130,130,130 | 0 |
| 56 | MG | 1A | 4553 | 1/1 | 0.98 | 0.22 | 91,91,91,91 | 0 |
| 56 | MG | 2A | 3149 | 1/1 | 0.98 | 0.48 | 110,110,110,110 | 0 |
| 56 | MG | 1A | 4599 | 1/1 | 0.98 | 0.13 | 60,60,60,60 | 0 |
| 56 | MG | 1A | 4358 | 1/1 | 0.98 | 0.14 | 72,72,72,72 | 0 |
| 58 | SF4 | 2d | 303 | 8/8 | 0.98 | 0.13 | 166,166,166,166 | 0 |
| 56 | MG | 1A | 4555 | 1/1 | 0.98 | 0.35 | 57,57,57,57 | 0 |
| 56 | MG | 1a | 1736 | 1/1 | 0.98 | 0.63 | 145,145,145,145 | 0 |
| 56 | MG | 1A | 4397 | 1/1 | 0.98 | 0.12 | 72,72,72,72 | 0 |
| 56 | MG | 1A | 4043 | 1/1 | 0.99 | 0.23 | 56,56,56,56 | 0 |
| 56 | MG | 2A | 3471 | 1/1 | 0.99 | 0.17 | 113,113,113,113 | 0 |
| 56 | MG | 2A | 3053 | 1/1 | 0.99 | 0.16 | 96,96,96,96 | 0 |
| 56 | MG | 1A | 4744 | 1/1 | 0.99 | 0.20 | 69,69,69,69 | 0 |
| 56 | MG | 1A | 4210 | 1/1 | 0.99 | 0.29 | 58,58,58,58 | 0 |
| 56 | MG | 1D | 304 | 1/1 | 0.99 | 0.44 | 75,75,75,75 | 0 |
| 56 | MG | 1A | 4716 | 1/1 | 0.99 | 0.20 | 72,72,72,72 | 0 |
| 56 | MG | 1v | 703 | 1/1 | 0.99 | 0.18 | 116,116,116,116 | 0 |
| 56 | MG | 1A | 4611 | 1/1 | 0.99 | 0.16 | 54,54,54,54 | 0 |
| 56 | MG | 1A | 4853 | 1/1 | 0.99 | 0.18 | 78,78,78,78 | 0 |
| 56 | MG | 1A | 4104 | 1/1 | 0.99 | 0.18 | 56,56,56,56 | 0 |
| 56 | MG | 1A | 4567 | 1/1 | 0.99 | 0.24 | 56,56,56,56 | 0 |
| 56 | MG | 1y | 103 | 1/1 | 0.99 | 0.72 | 89,89,89,89 | 0 |

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| Mol | Type | Chain | Res | Atoms | RSCC | RSR | B-factors(Å$^2$) | Q<0.9 |
|---|---|---|---|---|---|---|---|---|
| 56 | MG | 1A | 4856 | 1/1 | 0.99 | 0.14 | 60,60,60,60 | 0 |
| 56 | MG | 1A | 4817 | 1/1 | 0.99 | 0.17 | 65,65,65,65 | 0 |
| 56 | MG | 1A | 4092 | 1/1 | 0.99 | 0.11 | 60,60,60,60 | 0 |
| 56 | MG | 1A | 4994 | 1/1 | 0.99 | 0.16 | 79,79,79,79 | 0 |
| 56 | MG | 1E | 306 | 1/1 | 0.99 | 0.11 | 83,83,83,83 | 0 |
| 56 | MG | 1A | 4615 | 1/1 | 0.99 | 0.14 | 67,67,67,67 | 0 |
| 56 | MG | 1a | 1778 | 1/1 | 0.99 | 0.53 | 126,126,126,126 | 0 |
| 56 | MG | 1A | 4996 | 1/1 | 0.99 | 0.19 | 71,71,71,71 | 0 |
| 56 | MG | 1A | 4150 | 1/1 | 0.99 | 0.16 | 59,59,59,59 | 0 |
| 56 | MG | 1A | 4388 | 1/1 | 0.99 | 0.21 | 79,79,79,79 | 0 |
| 56 | MG | 1A | 4571 | 1/1 | 0.99 | 0.15 | 79,79,79,79 | 0 |
| 56 | MG | 1A | 5000 | 1/1 | 0.99 | 0.12 | 63,63,63,63 | 0 |
| 56 | MG | 1A | 5001 | 1/1 | 0.99 | 0.09 | 65,65,65,65 | 0 |
| 56 | MG | 2A | 3210 | 1/1 | 0.99 | 0.26 | 93,93,93,93 | 0 |
| 56 | MG | 1O | 202 | 1/1 | 0.99 | 0.47 | 82,82,82,82 | 0 |
| 56 | MG | 1A | 4906 | 1/1 | 0.99 | 0.15 | 57,57,57,57 | 0 |
| 56 | MG | 1A | 4076 | 1/1 | 0.99 | 0.18 | 77,77,77,77 | 0 |
| 56 | MG | 1A | 4325 | 1/1 | 0.99 | 0.22 | 63,63,63,63 | 0 |
| 56 | MG | 2A | 3353 | 1/1 | 0.99 | 0.20 | 83,83,83,83 | 0 |
| 56 | MG | 1A | 4789 | 1/1 | 0.99 | 0.26 | 96,96,96,96 | 0 |
| 56 | MG | 1A | 4758 | 1/1 | 0.99 | 0.23 | 75,75,75,75 | 0 |
| 56 | MG | 2A | 3820 | 1/1 | 0.99 | 0.15 | 106,106,106,106 | 0 |
| 56 | MG | 2A | 3580 | 1/1 | 0.99 | 0.27 | 118,118,118,118 | 0 |
| 56 | MG | 1A | 4207 | 1/1 | 0.99 | 0.32 | 52,52,52,52 | 0 |
| 56 | MG | 2A | 3357 | 1/1 | 0.99 | 0.08 | 87,87,87,87 | 0 |
| 56 | MG | 2A | 3662 | 1/1 | 0.99 | 0.15 | 96,96,96,96 | 0 |
| 56 | MG | 2A | 3286 | 1/1 | 0.99 | 0.20 | 101,101,101,101 | 0 |
| 56 | MG | 1a | 1614 | 1/1 | 0.99 | 0.10 | 93,93,93,93 | 0 |
| 56 | MG | 1a | 1793 | 1/1 | 0.99 | 0.12 | 128,128,128,128 | 0 |
| 56 | MG | 1A | 5061 | 1/1 | 0.99 | 0.12 | 91,91,91,91 | 0 |
| 56 | MG | 2A | 3510 | 1/1 | 0.99 | 0.07 | 94,94,94,94 | 0 |
| 56 | MG | 1a | 1616 | 1/1 | 0.99 | 0.11 | 99,99,99,99 | 0 |
| 56 | MG | 2A | 3589 | 1/1 | 0.99 | 0.13 | 127,127,127,127 | 0 |
| 56 | MG | 1A | 4792 | 1/1 | 0.99 | 0.14 | 66,66,66,66 | 0 |
| 56 | MG | 1A | 4869 | 1/1 | 0.99 | 0.23 | 54,54,54,54 | 0 |
| 56 | MG | 2A | 3592 | 1/1 | 0.99 | 0.23 | 129,129,129,129 | 0 |
| 56 | MG | 1A | 4597 | 1/1 | 0.99 | 0.09 | 65,65,65,65 | 0 |
| 56 | MG | 1A | 4474 | 1/1 | 0.99 | 0.26 | 56,56,56,56 | 0 |
| 56 | MG | 1A | 4872 | 1/1 | 0.99 | 0.17 | 54,54,54,54 | 0 |
| 56 | MG | 1A | 4873 | 1/1 | 0.99 | 0.16 | 55,55,55,55 | 0 |
| 56 | MG | 2A | 3757 | 1/1 | 0.99 | 0.20 | 127,127,127,127 | 0 |
| 56 | MG | 1A | 4918 | 1/1 | 0.99 | 0.19 | 61,61,61,61 | 0 |

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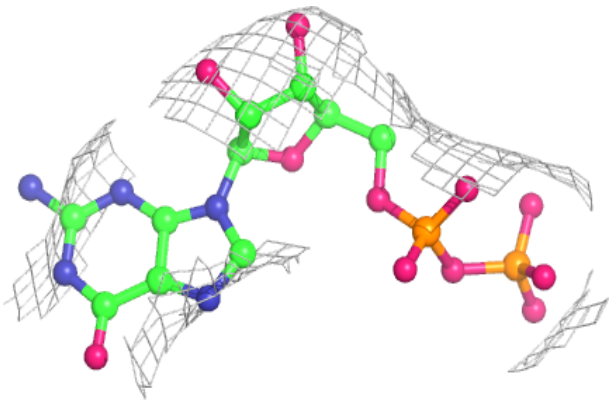
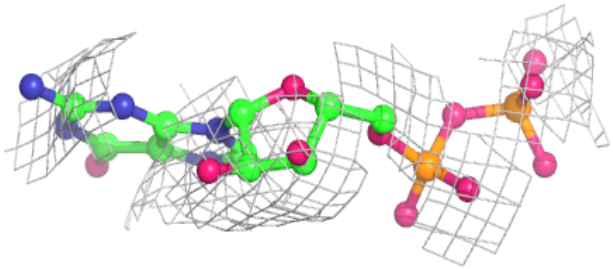
| Mol | Type | Chain | Res | Atoms | RSCC | RSR | B-factors(Å$^2$) | Q<0.9 |
|---|---|---|---|---|---|---|---|---|
| 56 | MG | 1A | 4293 | 1/1 | 0.99 | 0.25 | 78,78,78,78 | 0 |
| 56 | MG | 1A | 4248 | 1/1 | 0.99 | 0.20 | 56,56,56,56 | 0 |
| 56 | MG | 1A | 4295 | 1/1 | 0.99 | 0.34 | 83,83,83,83 | 0 |
| 56 | MG | 1A | 5018 | 1/1 | 0.99 | 0.21 | 71,71,71,71 | 0 |
| 56 | MG | 1A | 4410 | 1/1 | 0.99 | 0.43 | 47,47,47,47 | 0 |
| 56 | MG | 1A | 4800 | 1/1 | 0.99 | 0.22 | 69,69,69,69 | 0 |
| 56 | MG | 1A | 4498 | 1/1 | 0.99 | 0.30 | 63,63,63,63 | 0 |
| 56 | MG | 1A | 4735 | 1/1 | 0.99 | 0.13 | 65,65,65,65 | 0 |
| 56 | MG | 2a | 1831 | 1/1 | 0.99 | 0.06 | 145,145,145,145 | 0 |
| 56 | MG | 1A | 4971 | 1/1 | 0.99 | 0.14 | 63,63,63,63 | 0 |
| 56 | MG | 1A | 4680 | 1/1 | 0.99 | 0.15 | 82,82,82,82 | 0 |
| 56 | MG | 1A | 4839 | 1/1 | 0.99 | 0.19 | 63,63,63,63 | 0 |
| 56 | MG | 1A | 4654 | 1/1 | 0.99 | 0.10 | 84,84,84,84 | 0 |
| 56 | MG | 2A | 3455 | 1/1 | 0.99 | 0.15 | 90,90,90,90 | 0 |
| 56 | MG | 1a | 1876 | 1/1 | 0.99 | 0.08 | 102,102,102,102 | 0 |
| 56 | MG | 1A | 4427 | 1/1 | 0.99 | 0.25 | 53,53,53,53 | 0 |
| 56 | MG | 2A | 3384 | 1/1 | 0.99 | 0.34 | 105,105,105,105 | 0 |
| 57 | ZN | 19 | 102 | 1/1 | 0.99 | 0.20 | 80,80,80,80 | 0 |
| 56 | MG | 1A | 4842 | 1/1 | 0.99 | 0.34 | 78,78,78,78 | 0 |
| 56 | MG | 1A | 5029 | 1/1 | 0.99 | 0.10 | 69,69,69,69 | 0 |
| 56 | MG | 2A | 3314 | 1/1 | 0.99 | 0.21 | 93,93,93,93 | 0 |
| 56 | MG | 2A | 3045 | 1/1 | 0.99 | 0.33 | 93,93,93,93 | 0 |
| 56 | MG | 1A | 4843 | 1/1 | 0.99 | 0.26 | 76,76,76,76 | 0 |
| 56 | MG | 1A | 4480 | 1/1 | 0.99 | 0.19 | 80,80,80,80 | 0 |
| 56 | MG | 2a | 1679 | 1/1 | 0.99 | 0.12 | 166,166,166,166 | 0 |
| 56 | MG | 2A | 3180 | 1/1 | 0.99 | 0.16 | 116,116,116,116 | 0 |
| 56 | MG | 1A | 4979 | 1/1 | 0.99 | 0.13 | 58,58,58,58 | 0 |
| 56 | MG | 1A | 4208 | 1/1 | 0.99 | 0.17 | 56,56,56,56 | 0 |
| 56 | MG | 1A | 4355 | 1/1 | 0.99 | 0.16 | 67,67,67,67 | 0 |
| 56 | MG | 1A | 4382 | 1/1 | 0.99 | 0.27 | 68,68,68,68 | 0 |
| 56 | MG | 1A | 4755 | 1/1 | 1.00 | 0.36 | 60,60,60,60 | 0 |
| 56 | MG | 1A | 4794 | 1/1 | 1.00 | 0.07 | 67,67,67,67 | 0 |

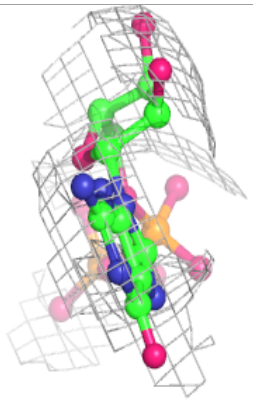
The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation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

**Electron density around GDP 2v 704:**

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

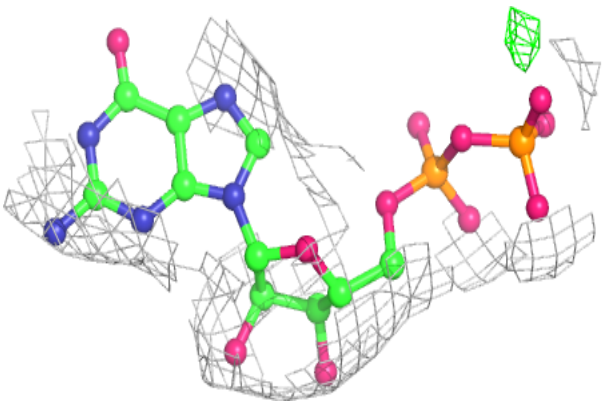


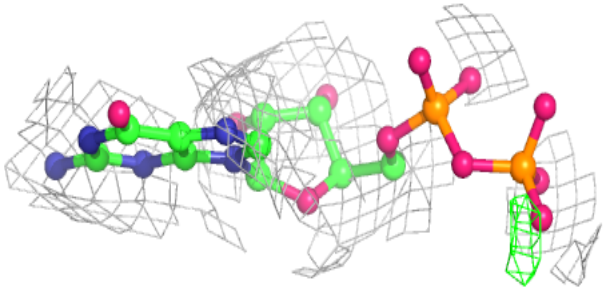


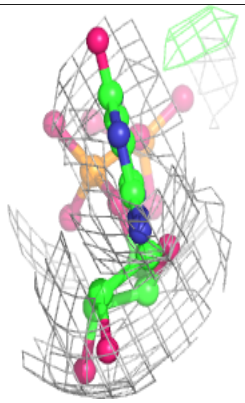


**Electron density around GDP 1v 704:**

$2mF_o$-$DF_c$ (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.