



Full wwPDB EM Validation Report ⓘ

Dec 12, 2022 – 10:47 pm GMT

PDB ID : 6QZ0
EMDB ID : EMD-4681
Title : The cryo-EM structure of the head of the genome emptied bacteriophage phi29
Authors : Xu, J.; Wang, D.; Gui, M.; Xiang, Y.
Deposited on : 2019-03-10
Resolution : 3.20 Å (reported)

This is a Full wwPDB EM Validation Report for a publicly released PDB entry.

We welcome your comments at validation@mail.wwpdb.org

A user guide is available at

<https://www.wwpdb.org/validation/2017/EMValidationReportHelp>

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

<http://www.wwpdb.org/validation/2017/FAQs#types>.

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

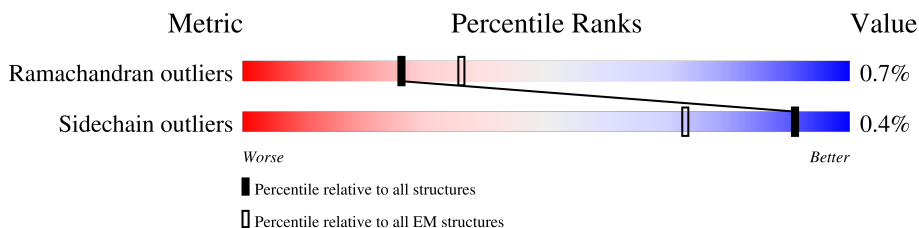
EMDB validation analysis : 0.0.1.dev43
MolProbity : 4.02b-467
Percentile statistics : 20191225.v01 (using entries in the PDB archive December 25th 2019)
MapQ : 1.9.9
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.31.3

1 Overall quality at a glance i

The following experimental techniques were used to determine the structure:
ELECTRON MICROSCOPY

The reported resolution of this entry is 3.20 Å.

Percentile scores (ranging between 0-100) for global validation metrics of the entry are shown in the following graphic. The table shows the number of entries on which the scores are based.



| Metric | Whole archive (#Entries) | EM structures (#Entries) |
|-----------------------|--------------------------|--------------------------|
| Ramachandran outliers | 154571 | 4023 |
| Sidechain outliers | 154315 | 3826 |

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

| Mol | Chain | Length | Quality of chain |
|-----|-------|--------|------------------|
| 1 | 1A | 448 | 38% 96% .. |
| 1 | 1B | 448 | 19% 98% .. |
| 1 | 1C | 448 | 11% 99% . |
| 1 | 1D | 448 | 12% 98% .. |
| 1 | 1E | 448 | 25% 97% . |
| 1 | 1F | 448 | 37% 97% .. |
| 1 | 1G | 448 | 38% 96% .. |
| 1 | 1H | 448 | 19% 98% .. |
| 1 | 1I | 448 | 11% 99% . |

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| Mol | Chain | Length | Quality of chain |
|-----|-------|--------|------------------|
| 1 | 1J | 448 | 11% 98% |
| 1 | 1K | 448 | 26% 97% |
| 1 | 1L | 448 | 37% 97% |
| 1 | 1M | 448 | 37% 96% |
| 1 | 1N | 448 | 19% 98% |
| 1 | 1O | 448 | 11% 99% |
| 1 | 1P | 448 | 12% 98% |
| 1 | 1Q | 448 | 26% 97% |
| 1 | 1R | 448 | 37% 97% |
| 1 | 1S | 448 | 37% 96% |
| 1 | 1T | 448 | 19% 98% |
| 1 | 1U | 448 | 10% 99% |
| 1 | 1V | 448 | 12% 98% |
| 1 | 1W | 448 | 26% 97% |
| 1 | 1X | 448 | 36% 97% |
| 1 | 1Y | 448 | 36% 96% |
| 1 | 1Z | 448 | 18% 98% |
| 1 | 1a | 448 | 10% 99% |
| 1 | 1b | 448 | 12% 98% |
| 1 | 1c | 448 | 25% 97% |
| 1 | 1d | 448 | 37% 97% |
| 1 | 2A | 448 | 12% 96% |
| 1 | 2B | 448 | 14% 98% |
| 1 | 2C | 448 | 13% 99% |
| 1 | 2D | 448 | 19% 99% |

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| Mol | Chain | Length | Quality of chain |
|-----|-------|--------|------------------|
| 1 | 2E | 448 | 17% 98% |
| 1 | 2F | 448 | 12% 96% |
| 1 | 2G | 448 | 14% 98% |
| 1 | 2H | 448 | 12% 99% |
| 1 | 2I | 448 | 19% 99% |
| 1 | 2J | 448 | 17% 98% |
| 1 | 2K | 448 | 12% 96% |
| 1 | 2L | 448 | 14% 98% |
| 1 | 2M | 448 | 13% 99% |
| 1 | 2N | 448 | 20% 99% |
| 1 | 2O | 448 | 17% 98% |
| 1 | 2P | 448 | 12% 96% |
| 1 | 2Q | 448 | 14% 98% |
| 1 | 2R | 448 | 13% 99% |
| 1 | 2S | 448 | 19% 99% |
| 1 | 2T | 448 | 17% 98% |
| 1 | 2U | 448 | 11% 96% |
| 1 | 2V | 448 | 14% 98% |
| 1 | 2W | 448 | 13% 99% |
| 1 | 2X | 448 | 18% 99% |
| 1 | 2Y | 448 | 17% 98% |
| 1 | 3A | 448 | 7% 96% |
| 1 | 3B | 448 | 10% 96% |
| 1 | 3C | 448 | 7% 98% |
| 1 | 3D | 448 | 7% 97% |

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| Mol | Chain | Length | Quality of chain |
|-----|-------|--------|------------------|
| 1 | 3E | 448 | 6% 99% |
| 1 | 3F | 448 | 6% 99% |
| 1 | 3G | 448 | 6% 96% |
| 1 | 3H | 448 | 10% 96% |
| 1 | 3I | 448 | 7% 98% |
| 1 | 3J | 448 | 7% 97% |
| 1 | 3K | 448 | 6% 99% |
| 1 | 3L | 448 | 6% 99% |
| 1 | 3M | 448 | 6% 96% |
| 1 | 3N | 448 | 9% 96% |
| 1 | 3O | 448 | 7% 98% |
| 1 | 3P | 448 | 6% 97% |
| 1 | 3Q | 448 | 7% 99% |
| 1 | 3R | 448 | 6% 99% |
| 1 | 3S | 448 | 6% 96% |
| 1 | 3T | 448 | 9% 96% |
| 1 | 3U | 448 | 7% 98% |
| 1 | 3V | 448 | 7% 97% |
| 1 | 3W | 448 | 6% 99% |
| 1 | 3X | 448 | 7% 99% |
| 1 | 3Y | 448 | 6% 96% |
| 1 | 3Z | 448 | 9% 96% |
| 1 | 3a | 448 | 8% 98% |
| 1 | 3b | 448 | 6% 97% |
| 1 | 3c | 448 | 6% 99% |

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| Mol | Chain | Length | Quality of chain |
|-----|-------|--------|------------------|
| 1 | 3d | 448 | 6% 99% |
| 1 | 4A | 448 | 7% 97% |
| 1 | 4B | 448 | 13% 95% |
| 1 | 4C | 448 | 13% 96% |
| 1 | 4D | 448 | 10% 97% |
| 1 | 4E | 448 | 11% 99% |
| 1 | 4F | 448 | 9% 99% |
| 1 | 4G | 448 | 7% 97% |
| 1 | 4H | 448 | 14% 95% |
| 1 | 4I | 448 | 13% 96% |
| 1 | 4J | 448 | 10% 97% |
| 1 | 4K | 448 | 10% 99% |
| 1 | 4L | 448 | 8% 99% |
| 1 | 4M | 448 | 7% 97% |
| 1 | 4N | 448 | 12% 95% |
| 1 | 4O | 448 | 13% 96% |
| 1 | 4P | 448 | 9% 97% |
| 1 | 4Q | 448 | 12% 99% |
| 1 | 4R | 448 | 8% 99% |
| 1 | 4S | 448 | 7% 97% |
| 1 | 4T | 448 | 13% 95% |
| 1 | 4U | 448 | 13% 96% |
| 1 | 4V | 448 | 9% 97% |
| 1 | 4W | 448 | 10% 99% |
| 1 | 4X | 448 | 9% 99% |

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| Mol | Chain | Length | Quality of chain |
|-----|-------|--------|------------------|
| 1 | 4Y | 448 | 7% 97% |
| 1 | 4Z | 448 | 13% 95% |
| 1 | 4a | 448 | 13% 96% |
| 1 | 4b | 448 | 10% 97% |
| 1 | 4c | 448 | 10% 99% |
| 1 | 4d | 448 | 9% 99% |
| 1 | 5A | 448 | 8% 96% |
| 1 | 5B | 448 | 15% 95% |
| 1 | 5C | 448 | 14% 95% |
| 1 | 5D | 448 | 11% 97% |
| 1 | 5E | 448 | 9% 98% |
| 1 | 5F | 448 | 8% 97% |
| 1 | 5G | 448 | 7% 96% |
| 1 | 5H | 448 | 15% 95% |
| 1 | 5I | 448 | 13% 95% |
| 1 | 5J | 448 | 11% 97% |
| 1 | 5K | 448 | 9% 98% |
| 1 | 5L | 448 | 9% 97% |
| 1 | 5M | 448 | 8% 96% |
| 1 | 5N | 448 | 15% 95% |
| 1 | 5O | 448 | 12% 95% |
| 1 | 5P | 448 | 11% 97% |
| 1 | 5Q | 448 | 10% 98% |
| 1 | 5R | 448 | 8% 97% |
| 1 | 5S | 448 | 8% 96% |

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| Mol | Chain | Length | Quality of chain |
|-----|-------|--------|------------------|
| 1 | 5T | 448 | 14% 95% |
| 1 | 5U | 448 | 14% 94% |
| 1 | 5V | 448 | 10% 97% |
| 1 | 5W | 448 | 10% 98% |
| 1 | 5X | 448 | 8% 97% |
| 1 | 5Y | 448 | 8% 96% |
| 1 | 5Z | 448 | 15% 95% |
| 1 | 5a | 448 | 14% 95% |
| 1 | 5b | 448 | 11% 97% |
| 1 | 5c | 448 | 9% 98% |
| 1 | 5d | 448 | 8% 97% |
| 1 | 6A | 448 | 7% 97% |
| 1 | 6B | 448 | 6% 98% |
| 1 | 6C | 448 | 7% 96% |
| 1 | 6D | 448 | 10% 96% |
| 1 | 6E | 448 | 7% 99% |
| 1 | 6F | 448 | 5% 98% |
| 1 | 6G | 448 | 8% 97% |
| 1 | 6H | 448 | 6% 98% |
| 1 | 6I | 448 | 6% 96% |
| 1 | 6J | 448 | 10% 96% |
| 1 | 6K | 448 | 7% 99% |
| 1 | 6L | 448 | 5% 98% |
| 1 | 6M | 448 | 7% 97% |
| 1 | 6N | 448 | 6% 98% |

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| Mol | Chain | Length | Quality of chain |
|-----|-------|--------|------------------|
| 1 | 6O | 448 | 7% 96% |
| 1 | 6P | 448 | 10% 96% |
| 1 | 6Q | 448 | 7% 99% |
| 1 | 6R | 448 | 6% 98% |
| 1 | 6S | 448 | 8% 97% |
| 1 | 6T | 448 | 7% 98% |
| 1 | 6U | 448 | 8% 96% |
| 1 | 6V | 448 | 9% 96% |
| 1 | 6W | 448 | 7% 99% |
| 1 | 6X | 448 | 6% 98% |
| 1 | 6Y | 448 | 7% 97% |
| 1 | 6Z | 448 | 6% 98% |
| 1 | 6a | 448 | 6% 96% |
| 1 | 6b | 448 | 9% 96% |
| 1 | 6c | 448 | 6% 99% |
| 1 | 6d | 448 | 6% 98% |
| 1 | 7A | 448 | 19% 98% |
| 1 | 7B | 448 | 17% 99% |
| 1 | 7C | 448 | 15% 98% |
| 1 | 7D | 448 | 16% 99% |
| 1 | 7E | 448 | 19% 98% |
| 1 | 7F | 448 | 20% 98% |
| 1 | 7G | 448 | 17% 99% |
| 1 | 7H | 448 | 16% 98% |
| 1 | 7I | 448 | 15% 99% |

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| Mol | Chain | Length | Quality of chain |
|-----|-------|--------|------------------|
| 1 | 7J | 448 | 18% 98% |
| 1 | 7K | 448 | 19% 98% |
| 1 | 7L | 448 | 18% 99% |
| 1 | 7M | 448 | 16% 98% |
| 1 | 7N | 448 | 15% 99% |
| 1 | 7O | 448 | 18% 98% |
| 1 | 7P | 448 | 21% 98% |
| 1 | 7Q | 448 | 18% 99% |
| 1 | 7R | 448 | 15% 98% |
| 1 | 7S | 448 | 15% 99% |
| 1 | 7T | 448 | 19% 98% |
| 1 | 7U | 448 | 19% 98% |
| 1 | 7V | 448 | 18% 99% |
| 1 | 7W | 448 | 16% 98% |
| 1 | 7X | 448 | 15% 99% |
| 1 | 7Y | 448 | 18% 98% |
| 1 | 8A | 448 | 15% 97% |
| 1 | 8B | 448 | 13% 99% |
| 1 | 8C | 448 | 10% 99% |
| 1 | 8D | 448 | 9% 99% |
| 1 | 8E | 448 | 10% 98% |
| 1 | 8F | 448 | 14% 99% |
| 1 | 8G | 448 | 15% 97% |
| 1 | 8H | 448 | 12% 99% |
| 1 | 8I | 448 | 11% 99% |

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| Mol | Chain | Length | Quality of chain |
|-----|-------|--------|------------------|
| 1 | 8J | 448 | 9% 99% |
| 1 | 8K | 448 | 10% 98% |
| 1 | 8L | 448 | 14% 99% |
| 1 | 8M | 448 | 15% 97% |
| 1 | 8N | 448 | 13% 99% |
| 1 | 8O | 448 | 10% 99% |
| 1 | 8P | 448 | 10% 99% |
| 1 | 8Q | 448 | 10% 98% |
| 1 | 8R | 448 | 14% 99% |
| 1 | 8S | 448 | 14% 97% |
| 1 | 8T | 448 | 12% 99% |
| 1 | 8U | 448 | 11% 99% |
| 1 | 8V | 448 | 10% 99% |
| 1 | 8W | 448 | 10% 98% |
| 1 | 8X | 448 | 14% 99% |
| 1 | 8Y | 448 | 14% 97% |
| 1 | 8Z | 448 | 13% 99% |
| 1 | 8a | 448 | 10% 99% |
| 1 | 8b | 448 | 10% 99% |
| 1 | 8c | 448 | 9% 98% |
| 1 | 8d | 448 | 14% 99% |
| 1 | 9A | 448 | 30% 99% |
| 1 | 9B | 448 | 31% 99% |
| 1 | 9C | 448 | 31% 99% |
| 1 | 9D | 448 | 31% 99% |

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| Mol | Chain | Length | Quality of chain |
|-----|-------|--------|------------------|
| 1 | 9E | 448 | 32% 99% |
| 2 | 1e | 281 | 82% 97% |
| 2 | 1f | 281 | 74% 96% |
| 2 | 1g | 281 | 71% 97% |
| 2 | 1h | 281 | 75% 96% |
| 2 | 1i | 281 | 81% 97% |
| 2 | 1j | 281 | 74% 96% |
| 2 | 1k | 281 | 70% 97% |
| 2 | 1l | 281 | 76% 96% |
| 2 | 1m | 281 | 81% 97% |
| 2 | 1n | 281 | 73% 96% |
| 2 | 1o | 281 | 71% 97% |
| 2 | 1p | 281 | 75% 96% |
| 2 | 1q | 281 | 81% 97% |
| 2 | 1r | 281 | 72% 96% |
| 2 | 1s | 281 | 72% 97% |
| 2 | 1t | 281 | 75% 96% |
| 2 | 1u | 281 | 84% 97% |
| 2 | 1v | 281 | 74% 96% |
| 2 | 1w | 281 | 71% 97% |
| 2 | 1x | 281 | 74% 96% |
| 2 | 2Z | 281 | 81% 98% |
| 2 | 2a | 281 | 69% 98% |
| 2 | 2b | 281 | 66% 98% |
| 2 | 2c | 281 | 68% 98% |

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| Mol | Chain | Length | Quality of chain |
|-----|-------|--------|------------------|
| 2 | 2d | 281 | 75% 98% |
| 2 | 2e | 281 | 80% 98% |
| 2 | 2f | 281 | 69% 98% |
| 2 | 2g | 281 | 67% 98% |
| 2 | 2h | 281 | 68% 98% |
| 2 | 2i | 281 | 75% 98% |
| 2 | 2j | 281 | 80% 98% |
| 2 | 2k | 281 | 69% 98% |
| 2 | 2l | 281 | 66% 98% |
| 2 | 2m | 281 | 69% 98% |
| 2 | 2n | 281 | 74% 98% |
| 2 | 2o | 281 | 79% 98% |
| 2 | 2p | 281 | 68% 98% |
| 2 | 2q | 281 | 65% 98% |
| 2 | 2r | 281 | 68% 98% |
| 2 | 2s | 281 | 75% 98% |
| 2 | 2t | 281 | 80% 98% |
| 2 | 2u | 281 | 69% 98% |
| 2 | 2v | 281 | 65% 98% |
| 2 | 2w | 281 | 68% 98% |
| 2 | 2x | 281 | 75% 98% |
| 2 | 3e | 281 | 65% 96% |
| 2 | 3f | 281 | 72% 97% |
| 2 | 3g | 281 | 81% 96% |
| 2 | 3h | 281 | 68% 97% |

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| Mol | Chain | Length | Quality of chain |
|-----|-------|--------|------------------|
| 2 | 3i | 281 | 66% 96% |
| 2 | 3j | 281 | 72% 97% |
| 2 | 3k | 281 | 80% 96% |
| 2 | 3l | 281 | 68% 97% |
| 2 | 3m | 281 | 66% 96% |
| 2 | 3n | 281 | 71% 97% |
| 2 | 3o | 281 | 80% 96% |
| 2 | 3p | 281 | 67% 97% |
| 2 | 3q | 281 | 66% 96% |
| 2 | 3r | 281 | 72% 97% |
| 2 | 3s | 281 | 80% 96% |
| 2 | 3t | 281 | 68% 97% |
| 2 | 3u | 281 | 65% 96% |
| 2 | 3v | 281 | 71% 97% |
| 2 | 3w | 281 | 80% 96% |
| 2 | 3x | 281 | 68% 97% |
| 2 | 4e | 281 | 66% 97% |
| 2 | 4f | 281 | 69% 96% |
| 2 | 4g | 281 | 66% 97% |
| 2 | 4h | 281 | 69% 96% |
| 2 | 4i | 281 | 67% 97% |
| 2 | 4j | 281 | 68% 96% |
| 2 | 4k | 281 | 66% 97% |
| 2 | 4l | 281 | 68% 96% |
| 2 | 4m | 281 | 66% 97% |

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| Mol | Chain | Length | Quality of chain |
|-----|-------|--------|------------------|
| 2 | 4n | 281 | 69% 96% |
| 2 | 5e | 281 | 67% 97% |
| 2 | 5f | 281 | 70% 96% |
| 2 | 5g | 281 | 67% 97% |
| 2 | 5h | 281 | 69% 96% |
| 2 | 5i | 281 | 67% 97% |
| 2 | 5j | 281 | 69% 96% |
| 2 | 5k | 281 | 67% 97% |
| 2 | 5l | 281 | 70% 96% |
| 2 | 5m | 281 | 67% 97% |
| 2 | 5n | 281 | 69% 96% |
| 2 | 6e | 281 | 80% 96% |
| 2 | 6f | 281 | 69% 97% |
| 2 | 6g | 281 | 73% 96% |
| 2 | 6h | 281 | 73% 97% |
| 2 | 6i | 281 | 81% 96% |
| 2 | 6j | 281 | 69% 97% |
| 2 | 6k | 281 | 73% 96% |
| 2 | 6l | 281 | 73% 97% |
| 2 | 6m | 281 | 81% 96% |
| 2 | 6n | 281 | 69% 97% |
| 2 | 6o | 281 | 72% 96% |
| 2 | 6p | 281 | 73% 97% |
| 2 | 6q | 281 | 81% 96% |
| 2 | 6r | 281 | 69% 97% |

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| Mol | Chain | Length | Quality of chain |
|-----|-------|--------|------------------|
| 2 | 6s | 281 | 73% 96% |
| 2 | 6t | 281 | 74% 97% |
| 2 | 6u | 281 | 82% 96% |
| 2 | 6v | 281 | 68% 97% |
| 2 | 6w | 281 | 72% 96% |
| 2 | 6x | 281 | 74% 97% |
| 2 | 7Z | 281 | 65% 98% |
| 2 | 7a | 281 | 68% 98% |
| 2 | 7b | 281 | 73% 98% |
| 2 | 7c | 281 | 81% 98% |
| 2 | 7d | 281 | 77% 98% |
| 2 | 7e | 281 | 65% 98% |
| 2 | 7f | 281 | 68% 98% |
| 2 | 7g | 281 | 74% 98% |
| 2 | 7h | 281 | 81% 98% |
| 2 | 7i | 281 | 78% 98% |
| 2 | 7j | 281 | 65% 98% |
| 2 | 7k | 281 | 68% 98% |
| 2 | 7l | 281 | 74% 98% |
| 2 | 7m | 281 | 80% 98% |
| 2 | 7n | 281 | 78% 98% |
| 2 | 7o | 281 | 66% 98% |
| 2 | 7p | 281 | 68% 98% |
| 2 | 7q | 281 | 74% 98% |
| 2 | 7r | 281 | 81% 98% |

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| Mol | Chain | Length | Quality of chain |
|-----|-------|--------|------------------|
| 2 | 7s | 281 | 79% 98% |
| 2 | 7t | 281 | 66% 98% |
| 2 | 7u | 281 | 68% 98% |
| 2 | 7v | 281 | 74% 98% |
| 2 | 7w | 281 | 82% 98% |
| 2 | 7x | 281 | 78% 98% |
| 2 | 8e | 281 | 86% 96% |
| 2 | 8f | 281 | 77% 97% |
| 2 | 8g | 281 | 79% 97% |
| 2 | 8h | 281 | 84% 96% |
| 2 | 8i | 281 | 75% 97% |
| 2 | 8j | 281 | 80% 96% |
| 2 | 8k | 281 | 85% 96% |
| 2 | 8l | 281 | 75% 97% |
| 2 | 8m | 281 | 79% 97% |
| 2 | 8n | 281 | 82% 96% |
| 2 | 8o | 281 | 74% 97% |
| 2 | 8p | 281 | 80% 96% |
| 2 | 8q | 281 | 84% 96% |
| 2 | 8r | 281 | 75% 97% |
| 2 | 8s | 281 | 80% 97% |
| 2 | 8t | 281 | 83% 96% |
| 2 | 8u | 281 | 75% 97% |
| 2 | 8v | 281 | 79% 96% |
| 2 | 8w | 281 | 87% 96% |

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| Mol | Chain | Length | Quality of chain |
|-----|-------|--------|------------------|
| 2 | 8x | 281 | 77% 97% |
| 2 | 8y | 281 | 81% 97% |
| 2 | 8z | 281 | 83% 96% |
| 2 | 9F | 281 | 75% 98% |
| 2 | 9G | 281 | 75% 98% |
| 2 | 9H | 281 | 77% 98% |
| 2 | 9I | 281 | 77% 98% |
| 2 | 9J | 281 | 75% 98% |
| 2 | 9K | 281 | 75% 97% |
| 2 | 9L | 281 | 79% 96% |
| 2 | 9M | 281 | 87% 96% |
| 2 | 9N | 281 | 76% 97% |
| 2 | 9O | 281 | 80% 97% |
| 2 | 9P | 281 | 83% 96% |
| 2 | 9Q | 281 | 76% 97% |
| 2 | 9R | 281 | 79% 96% |

2 Entry composition [i](#)

There are 2 unique types of molecules in this entry. The entry contains 1161565 atoms, of which 0 are hydrogens and 0 are deuteriums.

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

- Molecule 1 is a protein called Major capsid protein.

| Mol | Chain | Residues | Atoms | | | | | AltConf | Trace |
|-----|-------|----------|---------------|-----------|----------|----------|--------|---------|-------|
| | | | Total | C | N | O | S | | |
| 1 | 1A | 433 | Total 3397 | C 2146 | N 578 | O 665 | S 8 | 0 | 0 |
| 1 | 1B | 445 | Total 3487 | C 2203 | N 592 | O 684 | S 8 | 0 | 0 |
| 1 | 1C | 445 | Total 3487 | C 2203 | N 592 | O 684 | S 8 | 0 | 0 |
| 1 | 1D | 445 | Total 3487 | C 2203 | N 592 | O 684 | S 8 | 0 | 0 |
| 1 | 1E | 435 | Total 3426 | C 2169 | N 579 | O 670 | S 8 | 0 | 0 |
| 1 | 1F | 438 | Total 3449 | C 2182 | N 584 | O 675 | S 8 | 0 | 0 |
| 1 | 2A | 438 | Total 3430 | C 2167 | N 583 | O 672 | S 8 | 0 | 0 |
| 1 | 2B | 445 | Total 3487 | C 2203 | N 592 | O 684 | S 8 | 0 | 0 |
| 1 | 2C | 445 | Total 3487 | C 2203 | N 592 | O 684 | S 8 | 0 | 0 |
| 1 | 2D | 445 | Total 3487 | C 2203 | N 592 | O 684 | S 8 | 0 | 0 |
| 1 | 2E | 445 | Total 3487 | C 2203 | N 592 | O 684 | S 8 | 0 | 0 |
| 1 | 3A | 435 | Total 3422 | C 2167 | N 579 | O 668 | S 8 | 0 | 0 |
| 1 | 3B | 435 | Total 3426 | C 2169 | N 579 | O 670 | S 8 | 0 | 0 |
| 1 | 3C | 445 | Total 3483 | C 2201 | N 592 | O 682 | S 8 | 0 | 0 |
| 1 | 3D | 445 | Total 3487 | C 2203 | N 592 | O 684 | S 8 | 0 | 0 |
| 1 | 3E | 445 | Total 3487 | C 2203 | N 592 | O 684 | S 8 | 0 | 0 |
| 1 | 3F | 445 | Total 3487 | C 2203 | N 592 | O 684 | S 8 | 0 | 0 |

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| Mol | Chain | Residues | Atoms | | | | | AltConf | Trace |
|-----|-------|----------|-------|------|-----|-----|---|---------|-------|
| 1 | 4A | 435 | Total | C | N | O | S | 0 | 0 |
| | | | 3426 | 2169 | 579 | 670 | 8 | | |
| 1 | 4B | 435 | Total | C | N | O | S | 0 | 0 |
| | | | 3426 | 2169 | 579 | 670 | 8 | | |
| 1 | 4C | 435 | Total | C | N | O | S | 0 | 0 |
| | | | 3426 | 2169 | 579 | 670 | 8 | | |
| 1 | 4D | 435 | Total | C | N | O | S | 0 | 0 |
| | | | 3426 | 2169 | 579 | 670 | 8 | | |
| 1 | 4E | 445 | Total | C | N | O | S | 0 | 0 |
| | | | 3487 | 2203 | 592 | 684 | 8 | | |
| 1 | 4F | 445 | Total | C | N | O | S | 0 | 0 |
| | | | 3487 | 2203 | 592 | 684 | 8 | | |
| 1 | 5A | 435 | Total | C | N | O | S | 0 | 0 |
| | | | 3426 | 2169 | 579 | 670 | 8 | | |
| 1 | 5B | 435 | Total | C | N | O | S | 0 | 0 |
| | | | 3426 | 2169 | 579 | 670 | 8 | | |
| 1 | 5C | 435 | Total | C | N | O | S | 0 | 0 |
| | | | 3426 | 2169 | 579 | 670 | 8 | | |
| 1 | 5D | 435 | Total | C | N | O | S | 0 | 0 |
| | | | 3426 | 2169 | 579 | 670 | 8 | | |
| 1 | 5E | 445 | Total | C | N | O | S | 0 | 0 |
| | | | 3487 | 2203 | 592 | 684 | 8 | | |
| 1 | 5F | 445 | Total | C | N | O | S | 0 | 0 |
| | | | 3487 | 2203 | 592 | 684 | 8 | | |
| 1 | 6A | 445 | Total | C | N | O | S | 0 | 0 |
| | | | 3487 | 2203 | 592 | 684 | 8 | | |
| 1 | 6B | 445 | Total | C | N | O | S | 0 | 0 |
| | | | 3487 | 2203 | 592 | 684 | 8 | | |
| 1 | 6C | 435 | Total | C | N | O | S | 0 | 0 |
| | | | 3426 | 2169 | 579 | 670 | 8 | | |
| 1 | 6D | 435 | Total | C | N | O | S | 0 | 0 |
| | | | 3426 | 2169 | 579 | 670 | 8 | | |
| 1 | 6E | 445 | Total | C | N | O | S | 0 | 0 |
| | | | 3487 | 2203 | 592 | 684 | 8 | | |
| 1 | 6F | 445 | Total | C | N | O | S | 0 | 0 |
| | | | 3487 | 2203 | 592 | 684 | 8 | | |
| 1 | 7A | 445 | Total | C | N | O | S | 0 | 0 |
| | | | 3487 | 2203 | 592 | 684 | 8 | | |
| 1 | 7B | 445 | Total | C | N | O | S | 0 | 0 |
| | | | 3487 | 2203 | 592 | 684 | 8 | | |
| 1 | 7C | 445 | Total | C | N | O | S | 0 | 0 |
| | | | 3487 | 2203 | 592 | 684 | 8 | | |

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| Mol | Chain | Residues | Atoms | | | | | AltConf | Trace |
|-----|-------|----------|---------------|-----------|----------|----------|--------|---------|-------|
| 1 | 7D | 445 | Total 3487 | C 2203 | N 592 | O 684 | S 8 | 0 | 0 |
| 1 | 7E | 445 | Total 3487 | C 2203 | N 592 | O 684 | S 8 | 0 | 0 |
| 1 | 8A | 445 | Total 3487 | C 2203 | N 592 | O 684 | S 8 | 0 | 0 |
| 1 | 8B | 445 | Total 3487 | C 2203 | N 592 | O 684 | S 8 | 0 | 0 |
| 1 | 8C | 445 | Total 3487 | C 2203 | N 592 | O 684 | S 8 | 0 | 0 |
| 1 | 8D | 445 | Total 3487 | C 2203 | N 592 | O 684 | S 8 | 0 | 0 |
| 1 | 8E | 445 | Total 3487 | C 2203 | N 592 | O 684 | S 8 | 0 | 0 |
| 1 | 8F | 445 | Total 3487 | C 2203 | N 592 | O 684 | S 8 | 0 | 0 |
| 1 | 9A | 445 | Total 3487 | C 2203 | N 592 | O 684 | S 8 | 0 | 0 |
| 1 | 1G | 433 | Total 3397 | C 2146 | N 578 | O 665 | S 8 | 0 | 0 |
| 1 | 1H | 445 | Total 3487 | C 2203 | N 592 | O 684 | S 8 | 0 | 0 |
| 1 | 1I | 445 | Total 3487 | C 2203 | N 592 | O 684 | S 8 | 0 | 0 |
| 1 | 1J | 445 | Total 3487 | C 2203 | N 592 | O 684 | S 8 | 0 | 0 |
| 1 | 1K | 435 | Total 3426 | C 2169 | N 579 | O 670 | S 8 | 0 | 0 |
| 1 | 1L | 438 | Total 3449 | C 2182 | N 584 | O 675 | S 8 | 0 | 0 |
| 1 | 2F | 438 | Total 3430 | C 2167 | N 583 | O 672 | S 8 | 0 | 0 |
| 1 | 2G | 445 | Total 3487 | C 2203 | N 592 | O 684 | S 8 | 0 | 0 |
| 1 | 2H | 445 | Total 3487 | C 2203 | N 592 | O 684 | S 8 | 0 | 0 |
| 1 | 2I | 445 | Total 3487 | C 2203 | N 592 | O 684 | S 8 | 0 | 0 |
| 1 | 2J | 445 | Total 3487 | C 2203 | N 592 | O 684 | S 8 | 0 | 0 |
| 1 | 3G | 435 | Total 3422 | C 2167 | N 579 | O 668 | S 8 | 0 | 0 |

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| Mol | Chain | Residues | Atoms | | | | | AltConf | Trace |
|-----|-------|----------|-------|------|-----|-----|---|---------|-------|
| 1 | 3H | 435 | Total | C | N | O | S | 0 | 0 |
| | | | 3426 | 2169 | 579 | 670 | 8 | | |
| 1 | 3I | 445 | Total | C | N | O | S | 0 | 0 |
| | | | 3483 | 2201 | 592 | 682 | 8 | | |
| 1 | 3J | 445 | Total | C | N | O | S | 0 | 0 |
| | | | 3487 | 2203 | 592 | 684 | 8 | | |
| 1 | 3K | 445 | Total | C | N | O | S | 0 | 0 |
| | | | 3487 | 2203 | 592 | 684 | 8 | | |
| 1 | 3L | 445 | Total | C | N | O | S | 0 | 0 |
| | | | 3487 | 2203 | 592 | 684 | 8 | | |
| 1 | 4G | 435 | Total | C | N | O | S | 0 | 0 |
| | | | 3426 | 2169 | 579 | 670 | 8 | | |
| 1 | 4H | 435 | Total | C | N | O | S | 0 | 0 |
| | | | 3426 | 2169 | 579 | 670 | 8 | | |
| 1 | 4I | 435 | Total | C | N | O | S | 0 | 0 |
| | | | 3426 | 2169 | 579 | 670 | 8 | | |
| 1 | 4J | 435 | Total | C | N | O | S | 0 | 0 |
| | | | 3426 | 2169 | 579 | 670 | 8 | | |
| 1 | 4K | 445 | Total | C | N | O | S | 0 | 0 |
| | | | 3487 | 2203 | 592 | 684 | 8 | | |
| 1 | 4L | 445 | Total | C | N | O | S | 0 | 0 |
| | | | 3487 | 2203 | 592 | 684 | 8 | | |
| 1 | 5G | 435 | Total | C | N | O | S | 0 | 0 |
| | | | 3426 | 2169 | 579 | 670 | 8 | | |
| 1 | 5H | 435 | Total | C | N | O | S | 0 | 0 |
| | | | 3426 | 2169 | 579 | 670 | 8 | | |
| 1 | 5I | 435 | Total | C | N | O | S | 0 | 0 |
| | | | 3426 | 2169 | 579 | 670 | 8 | | |
| 1 | 5J | 435 | Total | C | N | O | S | 0 | 0 |
| | | | 3426 | 2169 | 579 | 670 | 8 | | |
| 1 | 5K | 445 | Total | C | N | O | S | 0 | 0 |
| | | | 3487 | 2203 | 592 | 684 | 8 | | |
| 1 | 5L | 445 | Total | C | N | O | S | 0 | 0 |
| | | | 3487 | 2203 | 592 | 684 | 8 | | |
| 1 | 6G | 445 | Total | C | N | O | S | 0 | 0 |
| | | | 3487 | 2203 | 592 | 684 | 8 | | |
| 1 | 6H | 445 | Total | C | N | O | S | 0 | 0 |
| | | | 3487 | 2203 | 592 | 684 | 8 | | |
| 1 | 6I | 435 | Total | C | N | O | S | 0 | 0 |
| | | | 3426 | 2169 | 579 | 670 | 8 | | |
| 1 | 6J | 435 | Total | C | N | O | S | 0 | 0 |
| | | | 3426 | 2169 | 579 | 670 | 8 | | |

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| Mol | Chain | Residues | Atoms | | | | | AltConf | Trace |
|-----|-------|----------|---------------|-----------|----------|----------|--------|---------|-------|
| 1 | 6K | 445 | Total 3487 | C 2203 | N 592 | O 684 | S 8 | 0 | 0 |
| 1 | 6L | 445 | Total 3487 | C 2203 | N 592 | O 684 | S 8 | 0 | 0 |
| 1 | 7F | 445 | Total 3487 | C 2203 | N 592 | O 684 | S 8 | 0 | 0 |
| 1 | 7G | 445 | Total 3487 | C 2203 | N 592 | O 684 | S 8 | 0 | 0 |
| 1 | 7H | 445 | Total 3487 | C 2203 | N 592 | O 684 | S 8 | 0 | 0 |
| 1 | 7I | 445 | Total 3487 | C 2203 | N 592 | O 684 | S 8 | 0 | 0 |
| 1 | 7J | 445 | Total 3487 | C 2203 | N 592 | O 684 | S 8 | 0 | 0 |
| 1 | 8G | 445 | Total 3487 | C 2203 | N 592 | O 684 | S 8 | 0 | 0 |
| 1 | 8H | 445 | Total 3487 | C 2203 | N 592 | O 684 | S 8 | 0 | 0 |
| 1 | 8I | 445 | Total 3487 | C 2203 | N 592 | O 684 | S 8 | 0 | 0 |
| 1 | 8J | 445 | Total 3487 | C 2203 | N 592 | O 684 | S 8 | 0 | 0 |
| 1 | 8K | 445 | Total 3487 | C 2203 | N 592 | O 684 | S 8 | 0 | 0 |
| 1 | 8L | 445 | Total 3487 | C 2203 | N 592 | O 684 | S 8 | 0 | 0 |
| 1 | 9B | 445 | Total 3487 | C 2203 | N 592 | O 684 | S 8 | 0 | 0 |
| 1 | 1M | 433 | Total 3397 | C 2146 | N 578 | O 665 | S 8 | 0 | 0 |
| 1 | 1N | 445 | Total 3487 | C 2203 | N 592 | O 684 | S 8 | 0 | 0 |
| 1 | 1O | 445 | Total 3487 | C 2203 | N 592 | O 684 | S 8 | 0 | 0 |
| 1 | 1P | 445 | Total 3487 | C 2203 | N 592 | O 684 | S 8 | 0 | 0 |
| 1 | 1Q | 435 | Total 3426 | C 2169 | N 579 | O 670 | S 8 | 0 | 0 |
| 1 | 1R | 438 | Total 3449 | C 2182 | N 584 | O 675 | S 8 | 0 | 0 |
| 1 | 2K | 438 | Total 3430 | C 2167 | N 583 | O 672 | S 8 | 0 | 0 |

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| Mol | Chain | Residues | Atoms | | | | | AltConf | Trace |
|-----|-------|----------|---------------|-----------|----------|----------|--------|---------|-------|
| 1 | 2L | 445 | Total 3487 | C 2203 | N 592 | O 684 | S 8 | 0 | 0 |
| 1 | 2M | 445 | Total 3487 | C 2203 | N 592 | O 684 | S 8 | 0 | 0 |
| 1 | 2N | 445 | Total 3487 | C 2203 | N 592 | O 684 | S 8 | 0 | 0 |
| 1 | 2O | 445 | Total 3487 | C 2203 | N 592 | O 684 | S 8 | 0 | 0 |
| 1 | 3M | 435 | Total 3422 | C 2167 | N 579 | O 668 | S 8 | 0 | 0 |
| 1 | 3N | 435 | Total 3426 | C 2169 | N 579 | O 670 | S 8 | 0 | 0 |
| 1 | 3O | 445 | Total 3483 | C 2201 | N 592 | O 682 | S 8 | 0 | 0 |
| 1 | 3P | 445 | Total 3487 | C 2203 | N 592 | O 684 | S 8 | 0 | 0 |
| 1 | 3Q | 445 | Total 3487 | C 2203 | N 592 | O 684 | S 8 | 0 | 0 |
| 1 | 3R | 445 | Total 3487 | C 2203 | N 592 | O 684 | S 8 | 0 | 0 |
| 1 | 4M | 435 | Total 3426 | C 2169 | N 579 | O 670 | S 8 | 0 | 0 |
| 1 | 4N | 435 | Total 3426 | C 2169 | N 579 | O 670 | S 8 | 0 | 0 |
| 1 | 4O | 435 | Total 3426 | C 2169 | N 579 | O 670 | S 8 | 0 | 0 |
| 1 | 4P | 435 | Total 3426 | C 2169 | N 579 | O 670 | S 8 | 0 | 0 |
| 1 | 4Q | 445 | Total 3487 | C 2203 | N 592 | O 684 | S 8 | 0 | 0 |
| 1 | 4R | 445 | Total 3487 | C 2203 | N 592 | O 684 | S 8 | 0 | 0 |
| 1 | 5M | 435 | Total 3426 | C 2169 | N 579 | O 670 | S 8 | 0 | 0 |
| 1 | 5N | 435 | Total 3426 | C 2169 | N 579 | O 670 | S 8 | 0 | 0 |
| 1 | 5O | 435 | Total 3426 | C 2169 | N 579 | O 670 | S 8 | 0 | 0 |
| 1 | 5P | 435 | Total 3426 | C 2169 | N 579 | O 670 | S 8 | 0 | 0 |
| 1 | 5Q | 445 | Total 3487 | C 2203 | N 592 | O 684 | S 8 | 0 | 0 |

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| Mol | Chain | Residues | Atoms | | | | | AltConf | Trace |
|-----|-------|----------|-------|------|-----|-----|---|---------|-------|
| 1 | 5R | 445 | Total | C | N | O | S | 0 | 0 |
| | | | 3487 | 2203 | 592 | 684 | 8 | | |
| 1 | 6M | 445 | Total | C | N | O | S | 0 | 0 |
| | | | 3487 | 2203 | 592 | 684 | 8 | | |
| 1 | 6N | 445 | Total | C | N | O | S | 0 | 0 |
| | | | 3487 | 2203 | 592 | 684 | 8 | | |
| 1 | 6O | 435 | Total | C | N | O | S | 0 | 0 |
| | | | 3426 | 2169 | 579 | 670 | 8 | | |
| 1 | 6P | 435 | Total | C | N | O | S | 0 | 0 |
| | | | 3426 | 2169 | 579 | 670 | 8 | | |
| 1 | 6Q | 445 | Total | C | N | O | S | 0 | 0 |
| | | | 3487 | 2203 | 592 | 684 | 8 | | |
| 1 | 6R | 445 | Total | C | N | O | S | 0 | 0 |
| | | | 3487 | 2203 | 592 | 684 | 8 | | |
| 1 | 7K | 445 | Total | C | N | O | S | 0 | 0 |
| | | | 3487 | 2203 | 592 | 684 | 8 | | |
| 1 | 7L | 445 | Total | C | N | O | S | 0 | 0 |
| | | | 3487 | 2203 | 592 | 684 | 8 | | |
| 1 | 7M | 445 | Total | C | N | O | S | 0 | 0 |
| | | | 3487 | 2203 | 592 | 684 | 8 | | |
| 1 | 7N | 445 | Total | C | N | O | S | 0 | 0 |
| | | | 3487 | 2203 | 592 | 684 | 8 | | |
| 1 | 7O | 445 | Total | C | N | O | S | 0 | 0 |
| | | | 3487 | 2203 | 592 | 684 | 8 | | |
| 1 | 8M | 445 | Total | C | N | O | S | 0 | 0 |
| | | | 3487 | 2203 | 592 | 684 | 8 | | |
| 1 | 8N | 445 | Total | C | N | O | S | 0 | 0 |
| | | | 3487 | 2203 | 592 | 684 | 8 | | |
| 1 | 8O | 445 | Total | C | N | O | S | 0 | 0 |
| | | | 3487 | 2203 | 592 | 684 | 8 | | |
| 1 | 8P | 445 | Total | C | N | O | S | 0 | 0 |
| | | | 3487 | 2203 | 592 | 684 | 8 | | |
| 1 | 8Q | 445 | Total | C | N | O | S | 0 | 0 |
| | | | 3487 | 2203 | 592 | 684 | 8 | | |
| 1 | 8R | 445 | Total | C | N | O | S | 0 | 0 |
| | | | 3487 | 2203 | 592 | 684 | 8 | | |
| 1 | 9C | 445 | Total | C | N | O | S | 0 | 0 |
| | | | 3487 | 2203 | 592 | 684 | 8 | | |
| 1 | 1S | 433 | Total | C | N | O | S | 0 | 0 |
| | | | 3397 | 2146 | 578 | 665 | 8 | | |
| 1 | 1T | 445 | Total | C | N | O | S | 0 | 0 |
| | | | 3487 | 2203 | 592 | 684 | 8 | | |

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| Mol | Chain | Residues | Atoms | | | | | AltConf | Trace |
|-----|-------|----------|-------|------|-----|-----|---|---------|-------|
| 1 | 1U | 445 | Total | C | N | O | S | 0 | 0 |
| | | | 3487 | 2203 | 592 | 684 | 8 | | |
| 1 | 1V | 445 | Total | C | N | O | S | 0 | 0 |
| | | | 3487 | 2203 | 592 | 684 | 8 | | |
| 1 | 1W | 435 | Total | C | N | O | S | 0 | 0 |
| | | | 3426 | 2169 | 579 | 670 | 8 | | |
| 1 | 1X | 438 | Total | C | N | O | S | 0 | 0 |
| | | | 3449 | 2182 | 584 | 675 | 8 | | |
| 1 | 2P | 438 | Total | C | N | O | S | 0 | 0 |
| | | | 3430 | 2167 | 583 | 672 | 8 | | |
| 1 | 2Q | 445 | Total | C | N | O | S | 0 | 0 |
| | | | 3487 | 2203 | 592 | 684 | 8 | | |
| 1 | 2R | 445 | Total | C | N | O | S | 0 | 0 |
| | | | 3487 | 2203 | 592 | 684 | 8 | | |
| 1 | 2S | 445 | Total | C | N | O | S | 0 | 0 |
| | | | 3487 | 2203 | 592 | 684 | 8 | | |
| 1 | 2T | 445 | Total | C | N | O | S | 0 | 0 |
| | | | 3487 | 2203 | 592 | 684 | 8 | | |
| 1 | 3S | 435 | Total | C | N | O | S | 0 | 0 |
| | | | 3422 | 2167 | 579 | 668 | 8 | | |
| 1 | 3T | 435 | Total | C | N | O | S | 0 | 0 |
| | | | 3426 | 2169 | 579 | 670 | 8 | | |
| 1 | 3U | 445 | Total | C | N | O | S | 0 | 0 |
| | | | 3483 | 2201 | 592 | 682 | 8 | | |
| 1 | 3V | 445 | Total | C | N | O | S | 0 | 0 |
| | | | 3487 | 2203 | 592 | 684 | 8 | | |
| 1 | 3W | 445 | Total | C | N | O | S | 0 | 0 |
| | | | 3487 | 2203 | 592 | 684 | 8 | | |
| 1 | 3X | 445 | Total | C | N | O | S | 0 | 0 |
| | | | 3487 | 2203 | 592 | 684 | 8 | | |
| 1 | 4S | 435 | Total | C | N | O | S | 0 | 0 |
| | | | 3426 | 2169 | 579 | 670 | 8 | | |
| 1 | 4T | 435 | Total | C | N | O | S | 0 | 0 |
| | | | 3426 | 2169 | 579 | 670 | 8 | | |
| 1 | 4U | 435 | Total | C | N | O | S | 0 | 0 |
| | | | 3426 | 2169 | 579 | 670 | 8 | | |
| 1 | 4V | 435 | Total | C | N | O | S | 0 | 0 |
| | | | 3426 | 2169 | 579 | 670 | 8 | | |
| 1 | 4W | 445 | Total | C | N | O | S | 0 | 0 |
| | | | 3487 | 2203 | 592 | 684 | 8 | | |
| 1 | 4X | 445 | Total | C | N | O | S | 0 | 0 |
| | | | 3487 | 2203 | 592 | 684 | 8 | | |

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| Mol | Chain | Residues | Atoms | | | | | AltConf | Trace |
|-----|-------|----------|-------|------|-----|-----|---|---------|-------|
| 1 | 5S | 435 | Total | C | N | O | S | 0 | 0 |
| | | | 3426 | 2169 | 579 | 670 | 8 | | |
| 1 | 5T | 435 | Total | C | N | O | S | 0 | 0 |
| | | | 3426 | 2169 | 579 | 670 | 8 | | |
| 1 | 5U | 435 | Total | C | N | O | S | 0 | 0 |
| | | | 3426 | 2169 | 579 | 670 | 8 | | |
| 1 | 5V | 435 | Total | C | N | O | S | 0 | 0 |
| | | | 3426 | 2169 | 579 | 670 | 8 | | |
| 1 | 5W | 445 | Total | C | N | O | S | 0 | 0 |
| | | | 3487 | 2203 | 592 | 684 | 8 | | |
| 1 | 5X | 445 | Total | C | N | O | S | 0 | 0 |
| | | | 3487 | 2203 | 592 | 684 | 8 | | |
| 1 | 6S | 445 | Total | C | N | O | S | 0 | 0 |
| | | | 3487 | 2203 | 592 | 684 | 8 | | |
| 1 | 6T | 445 | Total | C | N | O | S | 0 | 0 |
| | | | 3487 | 2203 | 592 | 684 | 8 | | |
| 1 | 6U | 435 | Total | C | N | O | S | 0 | 0 |
| | | | 3426 | 2169 | 579 | 670 | 8 | | |
| 1 | 6V | 435 | Total | C | N | O | S | 0 | 0 |
| | | | 3426 | 2169 | 579 | 670 | 8 | | |
| 1 | 6W | 445 | Total | C | N | O | S | 0 | 0 |
| | | | 3487 | 2203 | 592 | 684 | 8 | | |
| 1 | 6X | 445 | Total | C | N | O | S | 0 | 0 |
| | | | 3487 | 2203 | 592 | 684 | 8 | | |
| 1 | 7P | 445 | Total | C | N | O | S | 0 | 0 |
| | | | 3487 | 2203 | 592 | 684 | 8 | | |
| 1 | 7Q | 445 | Total | C | N | O | S | 0 | 0 |
| | | | 3487 | 2203 | 592 | 684 | 8 | | |
| 1 | 7R | 445 | Total | C | N | O | S | 0 | 0 |
| | | | 3487 | 2203 | 592 | 684 | 8 | | |
| 1 | 7S | 445 | Total | C | N | O | S | 0 | 0 |
| | | | 3487 | 2203 | 592 | 684 | 8 | | |
| 1 | 7T | 445 | Total | C | N | O | S | 0 | 0 |
| | | | 3487 | 2203 | 592 | 684 | 8 | | |
| 1 | 8S | 445 | Total | C | N | O | S | 0 | 0 |
| | | | 3487 | 2203 | 592 | 684 | 8 | | |
| 1 | 8T | 445 | Total | C | N | O | S | 0 | 0 |
| | | | 3487 | 2203 | 592 | 684 | 8 | | |
| 1 | 8U | 445 | Total | C | N | O | S | 0 | 0 |
| | | | 3487 | 2203 | 592 | 684 | 8 | | |
| 1 | 8V | 445 | Total | C | N | O | S | 0 | 0 |
| | | | 3487 | 2203 | 592 | 684 | 8 | | |

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| Mol | Chain | Residues | Atoms | | | | | AltConf | Trace |
|-----|-------|----------|---------------|-----------|----------|----------|--------|---------|-------|
| 1 | 8W | 445 | Total 3487 | C 2203 | N 592 | O 684 | S 8 | 0 | 0 |
| 1 | 8X | 445 | Total 3487 | C 2203 | N 592 | O 684 | S 8 | 0 | 0 |
| 1 | 9D | 445 | Total 3487 | C 2203 | N 592 | O 684 | S 8 | 0 | 0 |
| 1 | 1Y | 433 | Total 3397 | C 2146 | N 578 | O 665 | S 8 | 0 | 0 |
| 1 | 1Z | 445 | Total 3487 | C 2203 | N 592 | O 684 | S 8 | 0 | 0 |
| 1 | 1a | 445 | Total 3487 | C 2203 | N 592 | O 684 | S 8 | 0 | 0 |
| 1 | 1b | 445 | Total 3487 | C 2203 | N 592 | O 684 | S 8 | 0 | 0 |
| 1 | 1c | 435 | Total 3426 | C 2169 | N 579 | O 670 | S 8 | 0 | 0 |
| 1 | 1d | 438 | Total 3449 | C 2182 | N 584 | O 675 | S 8 | 0 | 0 |
| 1 | 2U | 438 | Total 3430 | C 2167 | N 583 | O 672 | S 8 | 0 | 0 |
| 1 | 2V | 445 | Total 3487 | C 2203 | N 592 | O 684 | S 8 | 0 | 0 |
| 1 | 2W | 445 | Total 3487 | C 2203 | N 592 | O 684 | S 8 | 0 | 0 |
| 1 | 2X | 445 | Total 3487 | C 2203 | N 592 | O 684 | S 8 | 0 | 0 |
| 1 | 2Y | 445 | Total 3487 | C 2203 | N 592 | O 684 | S 8 | 0 | 0 |
| 1 | 3Y | 435 | Total 3422 | C 2167 | N 579 | O 668 | S 8 | 0 | 0 |
| 1 | 3Z | 435 | Total 3426 | C 2169 | N 579 | O 670 | S 8 | 0 | 0 |
| 1 | 3a | 445 | Total 3483 | C 2201 | N 592 | O 682 | S 8 | 0 | 0 |
| 1 | 3b | 445 | Total 3487 | C 2203 | N 592 | O 684 | S 8 | 0 | 0 |
| 1 | 3c | 445 | Total 3487 | C 2203 | N 592 | O 684 | S 8 | 0 | 0 |
| 1 | 3d | 445 | Total 3487 | C 2203 | N 592 | O 684 | S 8 | 0 | 0 |
| 1 | 4Y | 435 | Total 3426 | C 2169 | N 579 | O 670 | S 8 | 0 | 0 |

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| Mol | Chain | Residues | Atoms | | | | | AltConf | Trace |
|-----|-------|----------|-------|------|-----|-----|---|---------|-------|
| 1 | 4Z | 435 | Total | C | N | O | S | 0 | 0 |
| | | | 3426 | 2169 | 579 | 670 | 8 | | |
| 1 | 4a | 435 | Total | C | N | O | S | 0 | 0 |
| | | | 3426 | 2169 | 579 | 670 | 8 | | |
| 1 | 4b | 435 | Total | C | N | O | S | 0 | 0 |
| | | | 3426 | 2169 | 579 | 670 | 8 | | |
| 1 | 4c | 445 | Total | C | N | O | S | 0 | 0 |
| | | | 3487 | 2203 | 592 | 684 | 8 | | |
| 1 | 4d | 445 | Total | C | N | O | S | 0 | 0 |
| | | | 3487 | 2203 | 592 | 684 | 8 | | |
| 1 | 5Y | 435 | Total | C | N | O | S | 0 | 0 |
| | | | 3426 | 2169 | 579 | 670 | 8 | | |
| 1 | 5Z | 435 | Total | C | N | O | S | 0 | 0 |
| | | | 3426 | 2169 | 579 | 670 | 8 | | |
| 1 | 5a | 435 | Total | C | N | O | S | 0 | 0 |
| | | | 3426 | 2169 | 579 | 670 | 8 | | |
| 1 | 5b | 435 | Total | C | N | O | S | 0 | 0 |
| | | | 3426 | 2169 | 579 | 670 | 8 | | |
| 1 | 5c | 445 | Total | C | N | O | S | 0 | 0 |
| | | | 3487 | 2203 | 592 | 684 | 8 | | |
| 1 | 5d | 445 | Total | C | N | O | S | 0 | 0 |
| | | | 3487 | 2203 | 592 | 684 | 8 | | |
| 1 | 6Y | 445 | Total | C | N | O | S | 0 | 0 |
| | | | 3487 | 2203 | 592 | 684 | 8 | | |
| 1 | 6Z | 445 | Total | C | N | O | S | 0 | 0 |
| | | | 3487 | 2203 | 592 | 684 | 8 | | |
| 1 | 6a | 435 | Total | C | N | O | S | 0 | 0 |
| | | | 3426 | 2169 | 579 | 670 | 8 | | |
| 1 | 6b | 435 | Total | C | N | O | S | 0 | 0 |
| | | | 3426 | 2169 | 579 | 670 | 8 | | |
| 1 | 6c | 445 | Total | C | N | O | S | 0 | 0 |
| | | | 3487 | 2203 | 592 | 684 | 8 | | |
| 1 | 6d | 445 | Total | C | N | O | S | 0 | 0 |
| | | | 3487 | 2203 | 592 | 684 | 8 | | |
| 1 | 7U | 445 | Total | C | N | O | S | 0 | 0 |
| | | | 3487 | 2203 | 592 | 684 | 8 | | |
| 1 | 7V | 445 | Total | C | N | O | S | 0 | 0 |
| | | | 3487 | 2203 | 592 | 684 | 8 | | |
| 1 | 7W | 445 | Total | C | N | O | S | 0 | 0 |
| | | | 3487 | 2203 | 592 | 684 | 8 | | |
| 1 | 7X | 445 | Total | C | N | O | S | 0 | 0 |
| | | | 3487 | 2203 | 592 | 684 | 8 | | |

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| Mol | Chain | Residues | Atoms | | | | | AltConf | Trace |
|-----|-------|----------|-------|------|-----|-----|---|---------|-------|
| 1 | 7Y | 445 | Total | C | N | O | S | 0 | 0 |
| | | | 3487 | 2203 | 592 | 684 | 8 | | |
| 1 | 8Y | 445 | Total | C | N | O | S | 0 | 0 |
| | | | 3487 | 2203 | 592 | 684 | 8 | | |
| 1 | 8Z | 445 | Total | C | N | O | S | 0 | 0 |
| | | | 3487 | 2203 | 592 | 684 | 8 | | |
| 1 | 8a | 445 | Total | C | N | O | S | 0 | 0 |
| | | | 3487 | 2203 | 592 | 684 | 8 | | |
| 1 | 8b | 445 | Total | C | N | O | S | 0 | 0 |
| | | | 3487 | 2203 | 592 | 684 | 8 | | |
| 1 | 8c | 445 | Total | C | N | O | S | 0 | 0 |
| | | | 3487 | 2203 | 592 | 684 | 8 | | |
| 1 | 8d | 445 | Total | C | N | O | S | 0 | 0 |
| | | | 3487 | 2203 | 592 | 684 | 8 | | |
| 1 | 9E | 445 | Total | C | N | O | S | 0 | 0 |
| | | | 3487 | 2203 | 592 | 684 | 8 | | |

- Molecule 2 is a protein called Capsid fiber protein.

| Mol | Chain | Residues | Atoms | | | | | AltConf | Trace |
|-----|-------|----------|-------|------|-----|-----|---|---------|-------|
| 2 | 1e | 280 | Total | C | N | O | S | 8 | 0 |
| | | | 2106 | 1317 | 349 | 436 | 4 | | |
| 2 | 1f | 279 | Total | C | N | O | S | 8 | 0 |
| | | | 2098 | 1312 | 348 | 435 | 3 | | |
| 2 | 1g | 280 | Total | C | N | O | S | 8 | 0 |
| | | | 2106 | 1317 | 349 | 436 | 4 | | |
| 2 | 1h | 279 | Total | C | N | O | S | 8 | 0 |
| | | | 2098 | 1312 | 348 | 435 | 3 | | |
| 2 | 2Z | 280 | Total | C | N | O | S | 8 | 0 |
| | | | 2106 | 1317 | 349 | 436 | 4 | | |
| 2 | 2a | 280 | Total | C | N | O | S | 8 | 0 |
| | | | 2106 | 1317 | 349 | 436 | 4 | | |
| 2 | 2b | 280 | Total | C | N | O | S | 8 | 0 |
| | | | 2106 | 1317 | 349 | 436 | 4 | | |
| 2 | 2c | 280 | Total | C | N | O | S | 8 | 0 |
| | | | 2106 | 1317 | 349 | 436 | 4 | | |
| 2 | 2d | 280 | Total | C | N | O | S | 8 | 0 |
| | | | 2106 | 1317 | 349 | 436 | 4 | | |
| 2 | 3e | 279 | Total | C | N | O | S | 8 | 0 |
| | | | 2098 | 1312 | 348 | 435 | 3 | | |
| 2 | 3f | 280 | Total | C | N | O | S | 8 | 0 |
| | | | 2106 | 1317 | 349 | 436 | 4 | | |

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| Mol | Chain | Residues | Atoms | | | | | AltConf | Trace |
|-----|-------|----------|---------------|-----------|----------|----------|--------|---------|-------|
| | | | Total | C | N | O | S | | |
| 2 | 3g | 279 | Total 2098 | C 1312 | N 348 | O 435 | S 3 | 8 | 0 |
| 2 | 3h | 280 | Total 2106 | C 1317 | N 349 | O 436 | S 4 | 8 | 0 |
| 2 | 4e | 280 | Total 2106 | C 1317 | N 349 | O 436 | S 4 | 8 | 0 |
| 2 | 4f | 279 | Total 2098 | C 1312 | N 348 | O 435 | S 3 | 8 | 0 |
| 2 | 5e | 280 | Total 2106 | C 1317 | N 349 | O 436 | S 4 | 8 | 0 |
| 2 | 5f | 279 | Total 2098 | C 1312 | N 348 | O 435 | S 3 | 8 | 0 |
| 2 | 6e | 279 | Total 2098 | C 1312 | N 348 | O 435 | S 3 | 8 | 0 |
| 2 | 6f | 280 | Total 2106 | C 1317 | N 349 | O 436 | S 4 | 8 | 0 |
| 2 | 6g | 279 | Total 2098 | C 1312 | N 348 | O 435 | S 3 | 8 | 0 |
| 2 | 6h | 280 | Total 2106 | C 1317 | N 349 | O 436 | S 4 | 8 | 0 |
| 2 | 7Z | 280 | Total 2106 | C 1317 | N 349 | O 436 | S 4 | 8 | 0 |
| 2 | 7a | 280 | Total 2106 | C 1317 | N 349 | O 436 | S 4 | 8 | 0 |
| 2 | 7b | 280 | Total 2106 | C 1317 | N 349 | O 436 | S 4 | 8 | 0 |
| 2 | 7c | 280 | Total 2106 | C 1317 | N 349 | O 436 | S 4 | 8 | 0 |
| 2 | 7d | 280 | Total 2106 | C 1317 | N 349 | O 436 | S 4 | 8 | 0 |
| 2 | 8e | 279 | Total 2098 | C 1312 | N 348 | O 435 | S 3 | 8 | 0 |
| 2 | 8f | 280 | Total 2106 | C 1317 | N 349 | O 436 | S 4 | 8 | 0 |
| 2 | 8g | 280 | Total 2106 | C 1317 | N 349 | O 436 | S 4 | 8 | 0 |
| 2 | 8h | 279 | Total 2098 | C 1312 | N 348 | O 435 | S 3 | 8 | 0 |
| 2 | 8i | 280 | Total 2106 | C 1317 | N 349 | O 436 | S 4 | 8 | 0 |
| 2 | 8j | 279 | Total 2098 | C 1312 | N 348 | O 435 | S 3 | 8 | 0 |

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| Mol | Chain | Residues | Atoms | | | | | AltConf | Trace |
|-----|-------|----------|---------------|-----------|----------|----------|--------|---------|-------|
| | | | Total | C | N | O | S | | |
| 2 | 9F | 280 | Total 2106 | C 1317 | N 349 | O 436 | S 4 | 8 | 0 |
| 2 | 1i | 280 | Total 2106 | C 1317 | N 349 | O 436 | S 4 | 8 | 0 |
| 2 | 1j | 279 | Total 2098 | C 1312 | N 348 | O 435 | S 3 | 8 | 0 |
| 2 | 1k | 280 | Total 2106 | C 1317 | N 349 | O 436 | S 4 | 8 | 0 |
| 2 | 1l | 279 | Total 2098 | C 1312 | N 348 | O 435 | S 3 | 8 | 0 |
| 2 | 2e | 280 | Total 2106 | C 1317 | N 349 | O 436 | S 4 | 8 | 0 |
| 2 | 2f | 280 | Total 2106 | C 1317 | N 349 | O 436 | S 4 | 8 | 0 |
| 2 | 2g | 280 | Total 2106 | C 1317 | N 349 | O 436 | S 4 | 8 | 0 |
| 2 | 2h | 280 | Total 2106 | C 1317 | N 349 | O 436 | S 4 | 8 | 0 |
| 2 | 2i | 280 | Total 2106 | C 1317 | N 349 | O 436 | S 4 | 8 | 0 |
| 2 | 3i | 279 | Total 2098 | C 1312 | N 348 | O 435 | S 3 | 8 | 0 |
| 2 | 3j | 280 | Total 2106 | C 1317 | N 349 | O 436 | S 4 | 8 | 0 |
| 2 | 3k | 279 | Total 2098 | C 1312 | N 348 | O 435 | S 3 | 8 | 0 |
| 2 | 3l | 280 | Total 2106 | C 1317 | N 349 | O 436 | S 4 | 8 | 0 |
| 2 | 4g | 280 | Total 2106 | C 1317 | N 349 | O 436 | S 4 | 8 | 0 |
| 2 | 4h | 279 | Total 2098 | C 1312 | N 348 | O 435 | S 3 | 8 | 0 |
| 2 | 5g | 280 | Total 2106 | C 1317 | N 349 | O 436 | S 4 | 8 | 0 |
| 2 | 5h | 279 | Total 2098 | C 1312 | N 348 | O 435 | S 3 | 8 | 0 |
| 2 | 6i | 279 | Total 2098 | C 1312 | N 348 | O 435 | S 3 | 8 | 0 |
| 2 | 6j | 280 | Total 2106 | C 1317 | N 349 | O 436 | S 4 | 8 | 0 |
| 2 | 6k | 279 | Total 2098 | C 1312 | N 348 | O 435 | S 3 | 8 | 0 |

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| Mol | Chain | Residues | Atoms | | | | | AltConf | Trace |
|-----|-------|----------|---------------|-----------|----------|----------|--------|---------|-------|
| | | | Total | C | N | O | S | | |
| 2 | 6l | 280 | Total 2106 | C 1317 | N 349 | O 436 | S 4 | 8 | 0 |
| 2 | 7e | 280 | Total 2106 | C 1317 | N 349 | O 436 | S 4 | 8 | 0 |
| 2 | 7f | 280 | Total 2106 | C 1317 | N 349 | O 436 | S 4 | 8 | 0 |
| 2 | 7g | 280 | Total 2106 | C 1317 | N 349 | O 436 | S 4 | 8 | 0 |
| 2 | 7h | 280 | Total 2106 | C 1317 | N 349 | O 436 | S 4 | 8 | 0 |
| 2 | 7i | 280 | Total 2106 | C 1317 | N 349 | O 436 | S 4 | 8 | 0 |
| 2 | 8k | 279 | Total 2098 | C 1312 | N 348 | O 435 | S 3 | 8 | 0 |
| 2 | 8l | 280 | Total 2106 | C 1317 | N 349 | O 436 | S 4 | 8 | 0 |
| 2 | 8m | 280 | Total 2106 | C 1317 | N 349 | O 436 | S 4 | 8 | 0 |
| 2 | 8n | 279 | Total 2098 | C 1312 | N 348 | O 435 | S 3 | 8 | 0 |
| 2 | 8o | 280 | Total 2106 | C 1317 | N 349 | O 436 | S 4 | 8 | 0 |
| 2 | 8p | 279 | Total 2098 | C 1312 | N 348 | O 435 | S 3 | 8 | 0 |
| 2 | 9G | 280 | Total 2106 | C 1317 | N 349 | O 436 | S 4 | 8 | 0 |
| 2 | 1m | 280 | Total 2106 | C 1317 | N 349 | O 436 | S 4 | 8 | 0 |
| 2 | 1n | 279 | Total 2098 | C 1312 | N 348 | O 435 | S 3 | 8 | 0 |
| 2 | 1o | 280 | Total 2106 | C 1317 | N 349 | O 436 | S 4 | 8 | 0 |
| 2 | 1p | 279 | Total 2098 | C 1312 | N 348 | O 435 | S 3 | 8 | 0 |
| 2 | 2j | 280 | Total 2106 | C 1317 | N 349 | O 436 | S 4 | 8 | 0 |
| 2 | 2k | 280 | Total 2106 | C 1317 | N 349 | O 436 | S 4 | 8 | 0 |
| 2 | 2l | 280 | Total 2106 | C 1317 | N 349 | O 436 | S 4 | 8 | 0 |
| 2 | 2m | 280 | Total 2106 | C 1317 | N 349 | O 436 | S 4 | 8 | 0 |

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| Mol | Chain | Residues | Atoms | | | | | AltConf | Trace |
|-----|-------|----------|---------------|-----------|----------|----------|--------|---------|-------|
| | | | Total | C | N | O | S | | |
| 2 | 2n | 280 | Total 2106 | C 1317 | N 349 | O 436 | S 4 | 8 | 0 |
| 2 | 3m | 279 | Total 2098 | C 1312 | N 348 | O 435 | S 3 | 8 | 0 |
| 2 | 3n | 280 | Total 2106 | C 1317 | N 349 | O 436 | S 4 | 8 | 0 |
| 2 | 3o | 279 | Total 2098 | C 1312 | N 348 | O 435 | S 3 | 8 | 0 |
| 2 | 3p | 280 | Total 2106 | C 1317 | N 349 | O 436 | S 4 | 8 | 0 |
| 2 | 4i | 280 | Total 2106 | C 1317 | N 349 | O 436 | S 4 | 8 | 0 |
| 2 | 4j | 279 | Total 2098 | C 1312 | N 348 | O 435 | S 3 | 8 | 0 |
| 2 | 5i | 280 | Total 2106 | C 1317 | N 349 | O 436 | S 4 | 8 | 0 |
| 2 | 5j | 279 | Total 2098 | C 1312 | N 348 | O 435 | S 3 | 8 | 0 |
| 2 | 6m | 279 | Total 2098 | C 1312 | N 348 | O 435 | S 3 | 8 | 0 |
| 2 | 6n | 280 | Total 2106 | C 1317 | N 349 | O 436 | S 4 | 8 | 0 |
| 2 | 6o | 279 | Total 2098 | C 1312 | N 348 | O 435 | S 3 | 8 | 0 |
| 2 | 6p | 280 | Total 2106 | C 1317 | N 349 | O 436 | S 4 | 8 | 0 |
| 2 | 7j | 280 | Total 2106 | C 1317 | N 349 | O 436 | S 4 | 8 | 0 |
| 2 | 7k | 280 | Total 2106 | C 1317 | N 349 | O 436 | S 4 | 8 | 0 |
| 2 | 7l | 280 | Total 2106 | C 1317 | N 349 | O 436 | S 4 | 8 | 0 |
| 2 | 7m | 280 | Total 2106 | C 1317 | N 349 | O 436 | S 4 | 8 | 0 |
| 2 | 7n | 280 | Total 2106 | C 1317 | N 349 | O 436 | S 4 | 8 | 0 |
| 2 | 8q | 279 | Total 2098 | C 1312 | N 348 | O 435 | S 3 | 8 | 0 |
| 2 | 8r | 280 | Total 2106 | C 1317 | N 349 | O 436 | S 4 | 8 | 0 |
| 2 | 8s | 280 | Total 2106 | C 1317 | N 349 | O 436 | S 4 | 8 | 0 |

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| Mol | Chain | Residues | Atoms | | | | | AltConf | Trace |
|-----|-------|----------|---------------|-----------|----------|----------|--------|---------|-------|
| | | | Total | C | N | O | S | | |
| 2 | 8t | 279 | Total 2098 | C 1312 | N 348 | O 435 | S 3 | 8 | 0 |
| 2 | 8u | 280 | Total 2106 | C 1317 | N 349 | O 436 | S 4 | 8 | 0 |
| 2 | 8v | 279 | Total 2098 | C 1312 | N 348 | O 435 | S 3 | 8 | 0 |
| 2 | 9H | 280 | Total 2106 | C 1317 | N 349 | O 436 | S 4 | 8 | 0 |
| 2 | 1q | 280 | Total 2106 | C 1317 | N 349 | O 436 | S 4 | 8 | 0 |
| 2 | 1r | 279 | Total 2098 | C 1312 | N 348 | O 435 | S 3 | 8 | 0 |
| 2 | 1s | 280 | Total 2106 | C 1317 | N 349 | O 436 | S 4 | 8 | 0 |
| 2 | 1t | 279 | Total 2098 | C 1312 | N 348 | O 435 | S 3 | 8 | 0 |
| 2 | 2o | 280 | Total 2106 | C 1317 | N 349 | O 436 | S 4 | 8 | 0 |
| 2 | 2p | 280 | Total 2106 | C 1317 | N 349 | O 436 | S 4 | 8 | 0 |
| 2 | 2q | 280 | Total 2106 | C 1317 | N 349 | O 436 | S 4 | 8 | 0 |
| 2 | 2r | 280 | Total 2106 | C 1317 | N 349 | O 436 | S 4 | 8 | 0 |
| 2 | 2s | 280 | Total 2106 | C 1317 | N 349 | O 436 | S 4 | 8 | 0 |
| 2 | 3q | 279 | Total 2098 | C 1312 | N 348 | O 435 | S 3 | 8 | 0 |
| 2 | 3r | 280 | Total 2106 | C 1317 | N 349 | O 436 | S 4 | 8 | 0 |
| 2 | 3s | 279 | Total 2098 | C 1312 | N 348 | O 435 | S 3 | 8 | 0 |
| 2 | 3t | 280 | Total 2106 | C 1317 | N 349 | O 436 | S 4 | 8 | 0 |
| 2 | 4k | 280 | Total 2106 | C 1317 | N 349 | O 436 | S 4 | 8 | 0 |
| 2 | 4l | 279 | Total 2098 | C 1312 | N 348 | O 435 | S 3 | 8 | 0 |
| 2 | 5k | 280 | Total 2106 | C 1317 | N 349 | O 436 | S 4 | 8 | 0 |
| 2 | 5l | 279 | Total 2098 | C 1312 | N 348 | O 435 | S 3 | 8 | 0 |

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| Mol | Chain | Residues | Atoms | | | | | AltConf | Trace |
|-----|-------|----------|---------------|-----------|----------|----------|--------|---------|-------|
| | | | Total | C | N | O | S | | |
| 2 | 6q | 279 | Total 2098 | C 1312 | N 348 | O 435 | S 3 | 8 | 0 |
| 2 | 6r | 280 | Total 2106 | C 1317 | N 349 | O 436 | S 4 | 8 | 0 |
| 2 | 6s | 279 | Total 2098 | C 1312 | N 348 | O 435 | S 3 | 8 | 0 |
| 2 | 6t | 280 | Total 2106 | C 1317 | N 349 | O 436 | S 4 | 8 | 0 |
| 2 | 7o | 280 | Total 2106 | C 1317 | N 349 | O 436 | S 4 | 8 | 0 |
| 2 | 7p | 280 | Total 2106 | C 1317 | N 349 | O 436 | S 4 | 8 | 0 |
| 2 | 7q | 280 | Total 2106 | C 1317 | N 349 | O 436 | S 4 | 8 | 0 |
| 2 | 7r | 280 | Total 2106 | C 1317 | N 349 | O 436 | S 4 | 8 | 0 |
| 2 | 7s | 280 | Total 2106 | C 1317 | N 349 | O 436 | S 4 | 8 | 0 |
| 2 | 8w | 279 | Total 2098 | C 1312 | N 348 | O 435 | S 3 | 8 | 0 |
| 2 | 8x | 280 | Total 2106 | C 1317 | N 349 | O 436 | S 4 | 8 | 0 |
| 2 | 8y | 280 | Total 2106 | C 1317 | N 349 | O 436 | S 4 | 8 | 0 |
| 2 | 8z | 279 | Total 2098 | C 1312 | N 348 | O 435 | S 3 | 8 | 0 |
| 2 | 9K | 280 | Total 2106 | C 1317 | N 349 | O 436 | S 4 | 8 | 0 |
| 2 | 9L | 279 | Total 2098 | C 1312 | N 348 | O 435 | S 3 | 8 | 0 |
| 2 | 9I | 280 | Total 2106 | C 1317 | N 349 | O 436 | S 4 | 8 | 0 |
| 2 | 1u | 280 | Total 2106 | C 1317 | N 349 | O 436 | S 4 | 8 | 0 |
| 2 | 1v | 279 | Total 2098 | C 1312 | N 348 | O 435 | S 3 | 8 | 0 |
| 2 | 1w | 280 | Total 2106 | C 1317 | N 349 | O 436 | S 4 | 8 | 0 |
| 2 | 1x | 279 | Total 2098 | C 1312 | N 348 | O 435 | S 3 | 8 | 0 |
| 2 | 2t | 280 | Total 2106 | C 1317 | N 349 | O 436 | S 4 | 8 | 0 |

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| Mol | Chain | Residues | Atoms | | | | | AltConf | Trace |
|-----|-------|----------|---------------|-----------|----------|----------|--------|---------|-------|
| | | | Total | C | N | O | S | | |
| 2 | 2u | 280 | Total 2106 | C 1317 | N 349 | O 436 | S 4 | 8 | 0 |
| 2 | 2v | 280 | Total 2106 | C 1317 | N 349 | O 436 | S 4 | 8 | 0 |
| 2 | 2w | 280 | Total 2106 | C 1317 | N 349 | O 436 | S 4 | 8 | 0 |
| 2 | 2x | 280 | Total 2106 | C 1317 | N 349 | O 436 | S 4 | 8 | 0 |
| 2 | 3u | 279 | Total 2098 | C 1312 | N 348 | O 435 | S 3 | 8 | 0 |
| 2 | 3v | 280 | Total 2106 | C 1317 | N 349 | O 436 | S 4 | 8 | 0 |
| 2 | 3w | 279 | Total 2098 | C 1312 | N 348 | O 435 | S 3 | 8 | 0 |
| 2 | 3x | 280 | Total 2106 | C 1317 | N 349 | O 436 | S 4 | 8 | 0 |
| 2 | 4m | 280 | Total 2106 | C 1317 | N 349 | O 436 | S 4 | 8 | 0 |
| 2 | 4n | 279 | Total 2098 | C 1312 | N 348 | O 435 | S 3 | 8 | 0 |
| 2 | 5m | 280 | Total 2106 | C 1317 | N 349 | O 436 | S 4 | 8 | 0 |
| 2 | 5n | 279 | Total 2098 | C 1312 | N 348 | O 435 | S 3 | 8 | 0 |
| 2 | 6u | 279 | Total 2098 | C 1312 | N 348 | O 435 | S 3 | 8 | 0 |
| 2 | 6v | 280 | Total 2106 | C 1317 | N 349 | O 436 | S 4 | 8 | 0 |
| 2 | 6w | 279 | Total 2098 | C 1312 | N 348 | O 435 | S 3 | 8 | 0 |
| 2 | 6x | 280 | Total 2106 | C 1317 | N 349 | O 436 | S 4 | 8 | 0 |
| 2 | 7t | 280 | Total 2106 | C 1317 | N 349 | O 436 | S 4 | 8 | 0 |
| 2 | 7u | 280 | Total 2106 | C 1317 | N 349 | O 436 | S 4 | 8 | 0 |
| 2 | 7v | 280 | Total 2106 | C 1317 | N 349 | O 436 | S 4 | 8 | 0 |
| 2 | 7w | 280 | Total 2106 | C 1317 | N 349 | O 436 | S 4 | 8 | 0 |
| 2 | 7x | 280 | Total 2106 | C 1317 | N 349 | O 436 | S 4 | 8 | 0 |

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| Mol | Chain | Residues | Atoms | | | | | AltConf | Trace |
|-----|-------|----------|-------|------|-----|-----|---|---------|-------|
| | | | Total | C | N | O | S | | |
| 2 | 9M | 279 | 2098 | 1312 | 348 | 435 | 3 | 8 | 0 |
| 2 | 9N | 280 | 2106 | 1317 | 349 | 436 | 4 | 8 | 0 |
| 2 | 9O | 280 | 2106 | 1317 | 349 | 436 | 4 | 8 | 0 |
| 2 | 9P | 279 | 2098 | 1312 | 348 | 435 | 3 | 8 | 0 |
| 2 | 9Q | 280 | 2106 | 1317 | 349 | 436 | 4 | 8 | 0 |
| 2 | 9R | 279 | 2098 | 1312 | 348 | 435 | 3 | 8 | 0 |
| 2 | 9J | 280 | 2106 | 1317 | 349 | 436 | 4 | 8 | 0 |

There are 330 discrepancies between the modelled and reference sequences:

| Chain | Residue | Modelled | Actual | Comment | Reference |
|-------|---------|----------|--------|-----------|------------|
| 1e | 123 | GLU | ASP | conflict | UNP B3VMP4 |
| 1e | 281 | LEU | - | insertion | UNP B3VMP4 |
| 1f | 123 | GLU | ASP | conflict | UNP B3VMP4 |
| 1f | 281 | LEU | - | insertion | UNP B3VMP4 |
| 1g | 123 | GLU | ASP | conflict | UNP B3VMP4 |
| 1g | 281 | LEU | - | insertion | UNP B3VMP4 |
| 1h | 123 | GLU | ASP | conflict | UNP B3VMP4 |
| 1h | 281 | LEU | - | insertion | UNP B3VMP4 |
| 2Z | 123 | GLU | ASP | conflict | UNP B3VMP4 |
| 2Z | 281 | LEU | - | insertion | UNP B3VMP4 |
| 2a | 123 | GLU | ASP | conflict | UNP B3VMP4 |
| 2a | 281 | LEU | - | insertion | UNP B3VMP4 |
| 2b | 123 | GLU | ASP | conflict | UNP B3VMP4 |
| 2b | 281 | LEU | - | insertion | UNP B3VMP4 |
| 2c | 123 | GLU | ASP | conflict | UNP B3VMP4 |
| 2c | 281 | LEU | - | insertion | UNP B3VMP4 |
| 2d | 123 | GLU | ASP | conflict | UNP B3VMP4 |
| 2d | 281 | LEU | - | insertion | UNP B3VMP4 |
| 3e | 123 | GLU | ASP | conflict | UNP B3VMP4 |
| 3e | 281 | LEU | - | insertion | UNP B3VMP4 |
| 3f | 123 | GLU | ASP | conflict | UNP B3VMP4 |
| 3f | 281 | LEU | - | insertion | UNP B3VMP4 |
| 3g | 123 | GLU | ASP | conflict | UNP B3VMP4 |
| 3g | 281 | LEU | - | insertion | UNP B3VMP4 |
| 3h | 123 | GLU | ASP | conflict | UNP B3VMP4 |

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| Chain | Residue | Modelled | Actual | Comment | Reference |
|-------|---------|----------|--------|-----------|------------|
| 3h | 281 | LEU | - | insertion | UNP B3VMP4 |
| 4e | 123 | GLU | ASP | conflict | UNP B3VMP4 |
| 4e | 281 | LEU | - | insertion | UNP B3VMP4 |
| 4f | 123 | GLU | ASP | conflict | UNP B3VMP4 |
| 4f | 281 | LEU | - | insertion | UNP B3VMP4 |
| 5e | 123 | GLU | ASP | conflict | UNP B3VMP4 |
| 5e | 281 | LEU | - | insertion | UNP B3VMP4 |
| 5f | 123 | GLU | ASP | conflict | UNP B3VMP4 |
| 5f | 281 | LEU | - | insertion | UNP B3VMP4 |
| 6e | 123 | GLU | ASP | conflict | UNP B3VMP4 |
| 6e | 281 | LEU | - | insertion | UNP B3VMP4 |
| 6f | 123 | GLU | ASP | conflict | UNP B3VMP4 |
| 6f | 281 | LEU | - | insertion | UNP B3VMP4 |
| 6g | 123 | GLU | ASP | conflict | UNP B3VMP4 |
| 6g | 281 | LEU | - | insertion | UNP B3VMP4 |
| 6h | 123 | GLU | ASP | conflict | UNP B3VMP4 |
| 6h | 281 | LEU | - | insertion | UNP B3VMP4 |
| 7Z | 123 | GLU | ASP | conflict | UNP B3VMP4 |
| 7Z | 281 | LEU | - | insertion | UNP B3VMP4 |
| 7a | 123 | GLU | ASP | conflict | UNP B3VMP4 |
| 7a | 281 | LEU | - | insertion | UNP B3VMP4 |
| 7b | 123 | GLU | ASP | conflict | UNP B3VMP4 |
| 7b | 281 | LEU | - | insertion | UNP B3VMP4 |
| 7c | 123 | GLU | ASP | conflict | UNP B3VMP4 |
| 7c | 281 | LEU | - | insertion | UNP B3VMP4 |
| 7d | 123 | GLU | ASP | conflict | UNP B3VMP4 |
| 7d | 281 | LEU | - | insertion | UNP B3VMP4 |
| 8e | 123 | GLU | ASP | conflict | UNP B3VMP4 |
| 8e | 281 | LEU | - | insertion | UNP B3VMP4 |
| 8f | 123 | GLU | ASP | conflict | UNP B3VMP4 |
| 8f | 281 | LEU | - | insertion | UNP B3VMP4 |
| 8g | 123 | GLU | ASP | conflict | UNP B3VMP4 |
| 8g | 281 | LEU | - | insertion | UNP B3VMP4 |
| 8h | 123 | GLU | ASP | conflict | UNP B3VMP4 |
| 8h | 281 | LEU | - | insertion | UNP B3VMP4 |
| 8i | 123 | GLU | ASP | conflict | UNP B3VMP4 |
| 8i | 281 | LEU | - | insertion | UNP B3VMP4 |
| 8j | 123 | GLU | ASP | conflict | UNP B3VMP4 |
| 8j | 281 | LEU | - | insertion | UNP B3VMP4 |
| 9F | 123 | GLU | ASP | conflict | UNP B3VMP4 |
| 9F | 281 | LEU | - | insertion | UNP B3VMP4 |
| 1i | 123 | GLU | ASP | conflict | UNP B3VMP4 |

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| Chain | Residue | Modelled | Actual | Comment | Reference |
|-------|---------|----------|--------|-----------|------------|
| 1i | 281 | LEU | - | insertion | UNP B3VMP4 |
| 1j | 123 | GLU | ASP | conflict | UNP B3VMP4 |
| 1j | 281 | LEU | - | insertion | UNP B3VMP4 |
| 1k | 123 | GLU | ASP | conflict | UNP B3VMP4 |
| 1k | 281 | LEU | - | insertion | UNP B3VMP4 |
| 1l | 123 | GLU | ASP | conflict | UNP B3VMP4 |
| 1l | 281 | LEU | - | insertion | UNP B3VMP4 |
| 2e | 123 | GLU | ASP | conflict | UNP B3VMP4 |
| 2e | 281 | LEU | - | insertion | UNP B3VMP4 |
| 2f | 123 | GLU | ASP | conflict | UNP B3VMP4 |
| 2f | 281 | LEU | - | insertion | UNP B3VMP4 |
| 2g | 123 | GLU | ASP | conflict | UNP B3VMP4 |
| 2g | 281 | LEU | - | insertion | UNP B3VMP4 |
| 2h | 123 | GLU | ASP | conflict | UNP B3VMP4 |
| 2h | 281 | LEU | - | insertion | UNP B3VMP4 |
| 2i | 123 | GLU | ASP | conflict | UNP B3VMP4 |
| 2i | 281 | LEU | - | insertion | UNP B3VMP4 |
| 3i | 123 | GLU | ASP | conflict | UNP B3VMP4 |
| 3i | 281 | LEU | - | insertion | UNP B3VMP4 |
| 3j | 123 | GLU | ASP | conflict | UNP B3VMP4 |
| 3j | 281 | LEU | - | insertion | UNP B3VMP4 |
| 3k | 123 | GLU | ASP | conflict | UNP B3VMP4 |
| 3k | 281 | LEU | - | insertion | UNP B3VMP4 |
| 3l | 123 | GLU | ASP | conflict | UNP B3VMP4 |
| 3l | 281 | LEU | - | insertion | UNP B3VMP4 |
| 4g | 123 | GLU | ASP | conflict | UNP B3VMP4 |
| 4g | 281 | LEU | - | insertion | UNP B3VMP4 |
| 4h | 123 | GLU | ASP | conflict | UNP B3VMP4 |
| 4h | 281 | LEU | - | insertion | UNP B3VMP4 |
| 5g | 123 | GLU | ASP | conflict | UNP B3VMP4 |
| 5g | 281 | LEU | - | insertion | UNP B3VMP4 |
| 5h | 123 | GLU | ASP | conflict | UNP B3VMP4 |
| 5h | 281 | LEU | - | insertion | UNP B3VMP4 |
| 6i | 123 | GLU | ASP | conflict | UNP B3VMP4 |
| 6i | 281 | LEU | - | insertion | UNP B3VMP4 |
| 6j | 123 | GLU | ASP | conflict | UNP B3VMP4 |
| 6j | 281 | LEU | - | insertion | UNP B3VMP4 |
| 6k | 123 | GLU | ASP | conflict | UNP B3VMP4 |
| 6k | 281 | LEU | - | insertion | UNP B3VMP4 |
| 6l | 123 | GLU | ASP | conflict | UNP B3VMP4 |
| 6l | 281 | LEU | - | insertion | UNP B3VMP4 |
| 7e | 123 | GLU | ASP | conflict | UNP B3VMP4 |

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| Chain | Residue | Modelled | Actual | Comment | Reference |
|-------|---------|----------|--------|-----------|------------|
| 7e | 281 | LEU | - | insertion | UNP B3VMP4 |
| 7f | 123 | GLU | ASP | conflict | UNP B3VMP4 |
| 7f | 281 | LEU | - | insertion | UNP B3VMP4 |
| 7g | 123 | GLU | ASP | conflict | UNP B3VMP4 |
| 7g | 281 | LEU | - | insertion | UNP B3VMP4 |
| 7h | 123 | GLU | ASP | conflict | UNP B3VMP4 |
| 7h | 281 | LEU | - | insertion | UNP B3VMP4 |
| 7i | 123 | GLU | ASP | conflict | UNP B3VMP4 |
| 7i | 281 | LEU | - | insertion | UNP B3VMP4 |
| 8k | 123 | GLU | ASP | conflict | UNP B3VMP4 |
| 8k | 281 | LEU | - | insertion | UNP B3VMP4 |
| 8l | 123 | GLU | ASP | conflict | UNP B3VMP4 |
| 8l | 281 | LEU | - | insertion | UNP B3VMP4 |
| 8m | 123 | GLU | ASP | conflict | UNP B3VMP4 |
| 8m | 281 | LEU | - | insertion | UNP B3VMP4 |
| 8n | 123 | GLU | ASP | conflict | UNP B3VMP4 |
| 8n | 281 | LEU | - | insertion | UNP B3VMP4 |
| 8o | 123 | GLU | ASP | conflict | UNP B3VMP4 |
| 8o | 281 | LEU | - | insertion | UNP B3VMP4 |
| 8p | 123 | GLU | ASP | conflict | UNP B3VMP4 |
| 8p | 281 | LEU | - | insertion | UNP B3VMP4 |
| 9G | 123 | GLU | ASP | conflict | UNP B3VMP4 |
| 9G | 281 | LEU | - | insertion | UNP B3VMP4 |
| 1m | 123 | GLU | ASP | conflict | UNP B3VMP4 |
| 1m | 281 | LEU | - | insertion | UNP B3VMP4 |
| 1n | 123 | GLU | ASP | conflict | UNP B3VMP4 |
| 1n | 281 | LEU | - | insertion | UNP B3VMP4 |
| 1o | 123 | GLU | ASP | conflict | UNP B3VMP4 |
| 1o | 281 | LEU | - | insertion | UNP B3VMP4 |
| 1p | 123 | GLU | ASP | conflict | UNP B3VMP4 |
| 1p | 281 | LEU | - | insertion | UNP B3VMP4 |
| 2j | 123 | GLU | ASP | conflict | UNP B3VMP4 |
| 2j | 281 | LEU | - | insertion | UNP B3VMP4 |
| 2k | 123 | GLU | ASP | conflict | UNP B3VMP4 |
| 2k | 281 | LEU | - | insertion | UNP B3VMP4 |
| 2l | 123 | GLU | ASP | conflict | UNP B3VMP4 |
| 2l | 281 | LEU | - | insertion | UNP B3VMP4 |
| 2m | 123 | GLU | ASP | conflict | UNP B3VMP4 |
| 2m | 281 | LEU | - | insertion | UNP B3VMP4 |
| 2n | 123 | GLU | ASP | conflict | UNP B3VMP4 |
| 2n | 281 | LEU | - | insertion | UNP B3VMP4 |
| 3m | 123 | GLU | ASP | conflict | UNP B3VMP4 |

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| Chain | Residue | Modelled | Actual | Comment | Reference |
|-------|---------|----------|--------|-----------|------------|
| 3m | 281 | LEU | - | insertion | UNP B3VMP4 |
| 3n | 123 | GLU | ASP | conflict | UNP B3VMP4 |
| 3n | 281 | LEU | - | insertion | UNP B3VMP4 |
| 3o | 123 | GLU | ASP | conflict | UNP B3VMP4 |
| 3o | 281 | LEU | - | insertion | UNP B3VMP4 |
| 3p | 123 | GLU | ASP | conflict | UNP B3VMP4 |
| 3p | 281 | LEU | - | insertion | UNP B3VMP4 |
| 4i | 123 | GLU | ASP | conflict | UNP B3VMP4 |
| 4i | 281 | LEU | - | insertion | UNP B3VMP4 |
| 4j | 123 | GLU | ASP | conflict | UNP B3VMP4 |
| 4j | 281 | LEU | - | insertion | UNP B3VMP4 |
| 5i | 123 | GLU | ASP | conflict | UNP B3VMP4 |
| 5i | 281 | LEU | - | insertion | UNP B3VMP4 |
| 5j | 123 | GLU | ASP | conflict | UNP B3VMP4 |
| 5j | 281 | LEU | - | insertion | UNP B3VMP4 |
| 6m | 123 | GLU | ASP | conflict | UNP B3VMP4 |
| 6m | 281 | LEU | - | insertion | UNP B3VMP4 |
| 6n | 123 | GLU | ASP | conflict | UNP B3VMP4 |
| 6n | 281 | LEU | - | insertion | UNP B3VMP4 |
| 6o | 123 | GLU | ASP | conflict | UNP B3VMP4 |
| 6o | 281 | LEU | - | insertion | UNP B3VMP4 |
| 6p | 123 | GLU | ASP | conflict | UNP B3VMP4 |
| 6p | 281 | LEU | - | insertion | UNP B3VMP4 |
| 7j | 123 | GLU | ASP | conflict | UNP B3VMP4 |
| 7j | 281 | LEU | - | insertion | UNP B3VMP4 |
| 7k | 123 | GLU | ASP | conflict | UNP B3VMP4 |
| 7k | 281 | LEU | - | insertion | UNP B3VMP4 |
| 7l | 123 | GLU | ASP | conflict | UNP B3VMP4 |
| 7l | 281 | LEU | - | insertion | UNP B3VMP4 |
| 7m | 123 | GLU | ASP | conflict | UNP B3VMP4 |
| 7m | 281 | LEU | - | insertion | UNP B3VMP4 |
| 7n | 123 | GLU | ASP | conflict | UNP B3VMP4 |
| 7n | 281 | LEU | - | insertion | UNP B3VMP4 |
| 8q | 123 | GLU | ASP | conflict | UNP B3VMP4 |
| 8q | 281 | LEU | - | insertion | UNP B3VMP4 |
| 8r | 123 | GLU | ASP | conflict | UNP B3VMP4 |
| 8r | 281 | LEU | - | insertion | UNP B3VMP4 |
| 8s | 123 | GLU | ASP | conflict | UNP B3VMP4 |
| 8s | 281 | LEU | - | insertion | UNP B3VMP4 |
| 8t | 123 | GLU | ASP | conflict | UNP B3VMP4 |
| 8t | 281 | LEU | - | insertion | UNP B3VMP4 |
| 8u | 123 | GLU | ASP | conflict | UNP B3VMP4 |

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| Chain | Residue | Modelled | Actual | Comment | Reference |
|-------|---------|----------|--------|-----------|------------|
| 8u | 281 | LEU | - | insertion | UNP B3VMP4 |
| 8v | 123 | GLU | ASP | conflict | UNP B3VMP4 |
| 8v | 281 | LEU | - | insertion | UNP B3VMP4 |
| 9H | 123 | GLU | ASP | conflict | UNP B3VMP4 |
| 9H | 281 | LEU | - | insertion | UNP B3VMP4 |
| 1q | 123 | GLU | ASP | conflict | UNP B3VMP4 |
| 1q | 281 | LEU | - | insertion | UNP B3VMP4 |
| 1r | 123 | GLU | ASP | conflict | UNP B3VMP4 |
| 1r | 281 | LEU | - | insertion | UNP B3VMP4 |
| 1s | 123 | GLU | ASP | conflict | UNP B3VMP4 |
| 1s | 281 | LEU | - | insertion | UNP B3VMP4 |
| 1t | 123 | GLU | ASP | conflict | UNP B3VMP4 |
| 1t | 281 | LEU | - | insertion | UNP B3VMP4 |
| 2o | 123 | GLU | ASP | conflict | UNP B3VMP4 |
| 2o | 281 | LEU | - | insertion | UNP B3VMP4 |
| 2p | 123 | GLU | ASP | conflict | UNP B3VMP4 |
| 2p | 281 | LEU | - | insertion | UNP B3VMP4 |
| 2q | 123 | GLU | ASP | conflict | UNP B3VMP4 |
| 2q | 281 | LEU | - | insertion | UNP B3VMP4 |
| 2r | 123 | GLU | ASP | conflict | UNP B3VMP4 |
| 2r | 281 | LEU | - | insertion | UNP B3VMP4 |
| 2s | 123 | GLU | ASP | conflict | UNP B3VMP4 |
| 2s | 281 | LEU | - | insertion | UNP B3VMP4 |
| 3q | 123 | GLU | ASP | conflict | UNP B3VMP4 |
| 3q | 281 | LEU | - | insertion | UNP B3VMP4 |
| 3r | 123 | GLU | ASP | conflict | UNP B3VMP4 |
| 3r | 281 | LEU | - | insertion | UNP B3VMP4 |
| 3s | 123 | GLU | ASP | conflict | UNP B3VMP4 |
| 3s | 281 | LEU | - | insertion | UNP B3VMP4 |
| 3t | 123 | GLU | ASP | conflict | UNP B3VMP4 |
| 3t | 281 | LEU | - | insertion | UNP B3VMP4 |
| 4k | 123 | GLU | ASP | conflict | UNP B3VMP4 |
| 4k | 281 | LEU | - | insertion | UNP B3VMP4 |
| 4l | 123 | GLU | ASP | conflict | UNP B3VMP4 |
| 4l | 281 | LEU | - | insertion | UNP B3VMP4 |
| 5k | 123 | GLU | ASP | conflict | UNP B3VMP4 |
| 5k | 281 | LEU | - | insertion | UNP B3VMP4 |
| 5l | 123 | GLU | ASP | conflict | UNP B3VMP4 |
| 5l | 281 | LEU | - | insertion | UNP B3VMP4 |
| 6q | 123 | GLU | ASP | conflict | UNP B3VMP4 |
| 6q | 281 | LEU | - | insertion | UNP B3VMP4 |
| 6r | 123 | GLU | ASP | conflict | UNP B3VMP4 |

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| Chain | Residue | Modelled | Actual | Comment | Reference |
|-------|---------|----------|--------|-----------|------------|
| 6r | 281 | LEU | - | insertion | UNP B3VMP4 |
| 6s | 123 | GLU | ASP | conflict | UNP B3VMP4 |
| 6s | 281 | LEU | - | insertion | UNP B3VMP4 |
| 6t | 123 | GLU | ASP | conflict | UNP B3VMP4 |
| 6t | 281 | LEU | - | insertion | UNP B3VMP4 |
| 7o | 123 | GLU | ASP | conflict | UNP B3VMP4 |
| 7o | 281 | LEU | - | insertion | UNP B3VMP4 |
| 7p | 123 | GLU | ASP | conflict | UNP B3VMP4 |
| 7p | 281 | LEU | - | insertion | UNP B3VMP4 |
| 7q | 123 | GLU | ASP | conflict | UNP B3VMP4 |
| 7q | 281 | LEU | - | insertion | UNP B3VMP4 |
| 7r | 123 | GLU | ASP | conflict | UNP B3VMP4 |
| 7r | 281 | LEU | - | insertion | UNP B3VMP4 |
| 7s | 123 | GLU | ASP | conflict | UNP B3VMP4 |
| 7s | 281 | LEU | - | insertion | UNP B3VMP4 |
| 8w | 123 | GLU | ASP | conflict | UNP B3VMP4 |
| 8w | 281 | LEU | - | insertion | UNP B3VMP4 |
| 8x | 123 | GLU | ASP | conflict | UNP B3VMP4 |
| 8x | 281 | LEU | - | insertion | UNP B3VMP4 |
| 8y | 123 | GLU | ASP | conflict | UNP B3VMP4 |
| 8y | 281 | LEU | - | insertion | UNP B3VMP4 |
| 8z | 123 | GLU | ASP | conflict | UNP B3VMP4 |
| 8z | 281 | LEU | - | insertion | UNP B3VMP4 |
| 9K | 123 | GLU | ASP | conflict | UNP B3VMP4 |
| 9K | 281 | LEU | - | insertion | UNP B3VMP4 |
| 9L | 123 | GLU | ASP | conflict | UNP B3VMP4 |
| 9L | 281 | LEU | - | insertion | UNP B3VMP4 |
| 9I | 123 | GLU | ASP | conflict | UNP B3VMP4 |
| 9I | 281 | LEU | - | insertion | UNP B3VMP4 |
| 1u | 123 | GLU | ASP | conflict | UNP B3VMP4 |
| 1u | 281 | LEU | - | insertion | UNP B3VMP4 |
| 1v | 123 | GLU | ASP | conflict | UNP B3VMP4 |
| 1v | 281 | LEU | - | insertion | UNP B3VMP4 |
| 1w | 123 | GLU | ASP | conflict | UNP B3VMP4 |
| 1w | 281 | LEU | - | insertion | UNP B3VMP4 |
| 1x | 123 | GLU | ASP | conflict | UNP B3VMP4 |
| 1x | 281 | LEU | - | insertion | UNP B3VMP4 |
| 2t | 123 | GLU | ASP | conflict | UNP B3VMP4 |
| 2t | 281 | LEU | - | insertion | UNP B3VMP4 |
| 2u | 123 | GLU | ASP | conflict | UNP B3VMP4 |
| 2u | 281 | LEU | - | insertion | UNP B3VMP4 |
| 2v | 123 | GLU | ASP | conflict | UNP B3VMP4 |

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| Chain | Residue | Modelled | Actual | Comment | Reference |
|-------|---------|----------|--------|-----------|------------|
| 2v | 281 | LEU | - | insertion | UNP B3VMP4 |
| 2w | 123 | GLU | ASP | conflict | UNP B3VMP4 |
| 2w | 281 | LEU | - | insertion | UNP B3VMP4 |
| 2x | 123 | GLU | ASP | conflict | UNP B3VMP4 |
| 2x | 281 | LEU | - | insertion | UNP B3VMP4 |
| 3u | 123 | GLU | ASP | conflict | UNP B3VMP4 |
| 3u | 281 | LEU | - | insertion | UNP B3VMP4 |
| 3v | 123 | GLU | ASP | conflict | UNP B3VMP4 |
| 3v | 281 | LEU | - | insertion | UNP B3VMP4 |
| 3w | 123 | GLU | ASP | conflict | UNP B3VMP4 |
| 3w | 281 | LEU | - | insertion | UNP B3VMP4 |
| 3x | 123 | GLU | ASP | conflict | UNP B3VMP4 |
| 3x | 281 | LEU | - | insertion | UNP B3VMP4 |
| 4m | 123 | GLU | ASP | conflict | UNP B3VMP4 |
| 4m | 281 | LEU | - | insertion | UNP B3VMP4 |
| 4n | 123 | GLU | ASP | conflict | UNP B3VMP4 |
| 4n | 281 | LEU | - | insertion | UNP B3VMP4 |
| 5m | 123 | GLU | ASP | conflict | UNP B3VMP4 |
| 5m | 281 | LEU | - | insertion | UNP B3VMP4 |
| 5n | 123 | GLU | ASP | conflict | UNP B3VMP4 |
| 5n | 281 | LEU | - | insertion | UNP B3VMP4 |
| 6u | 123 | GLU | ASP | conflict | UNP B3VMP4 |
| 6u | 281 | LEU | - | insertion | UNP B3VMP4 |
| 6v | 123 | GLU | ASP | conflict | UNP B3VMP4 |
| 6v | 281 | LEU | - | insertion | UNP B3VMP4 |
| 6w | 123 | GLU | ASP | conflict | UNP B3VMP4 |
| 6w | 281 | LEU | - | insertion | UNP B3VMP4 |
| 6x | 123 | GLU | ASP | conflict | UNP B3VMP4 |
| 6x | 281 | LEU | - | insertion | UNP B3VMP4 |
| 7t | 123 | GLU | ASP | conflict | UNP B3VMP4 |
| 7t | 281 | LEU | - | insertion | UNP B3VMP4 |
| 7u | 123 | GLU | ASP | conflict | UNP B3VMP4 |
| 7u | 281 | LEU | - | insertion | UNP B3VMP4 |
| 7v | 123 | GLU | ASP | conflict | UNP B3VMP4 |
| 7v | 281 | LEU | - | insertion | UNP B3VMP4 |
| 7w | 123 | GLU | ASP | conflict | UNP B3VMP4 |
| 7w | 281 | LEU | - | insertion | UNP B3VMP4 |
| 7x | 123 | GLU | ASP | conflict | UNP B3VMP4 |
| 7x | 281 | LEU | - | insertion | UNP B3VMP4 |
| 9M | 123 | GLU | ASP | conflict | UNP B3VMP4 |
| 9M | 281 | LEU | - | insertion | UNP B3VMP4 |
| 9N | 123 | GLU | ASP | conflict | UNP B3VMP4 |

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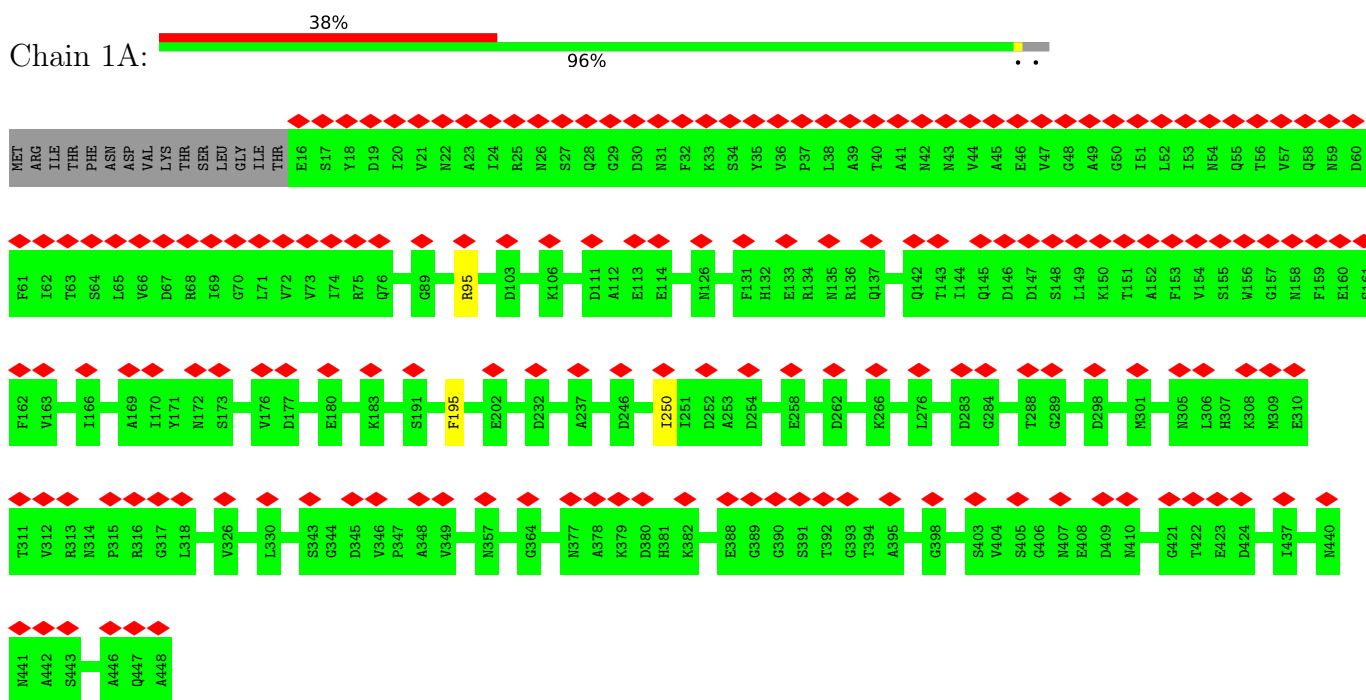
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| Chain | Residue | Modelled | Actual | Comment | Reference |
|--------------|----------------|-----------------|---------------|----------------|------------------|
| 9N | 281 | LEU | - | insertion | UNP B3VMP4 |
| 9O | 123 | GLU | ASP | conflict | UNP B3VMP4 |
| 9O | 281 | LEU | - | insertion | UNP B3VMP4 |
| 9P | 123 | GLU | ASP | conflict | UNP B3VMP4 |
| 9P | 281 | LEU | - | insertion | UNP B3VMP4 |
| 9Q | 123 | GLU | ASP | conflict | UNP B3VMP4 |
| 9Q | 281 | LEU | - | insertion | UNP B3VMP4 |
| 9R | 123 | GLU | ASP | conflict | UNP B3VMP4 |
| 9R | 281 | LEU | - | insertion | UNP B3VMP4 |
| 9J | 123 | GLU | ASP | conflict | UNP B3VMP4 |
| 9J | 281 | LEU | - | insertion | UNP B3VMP4 |

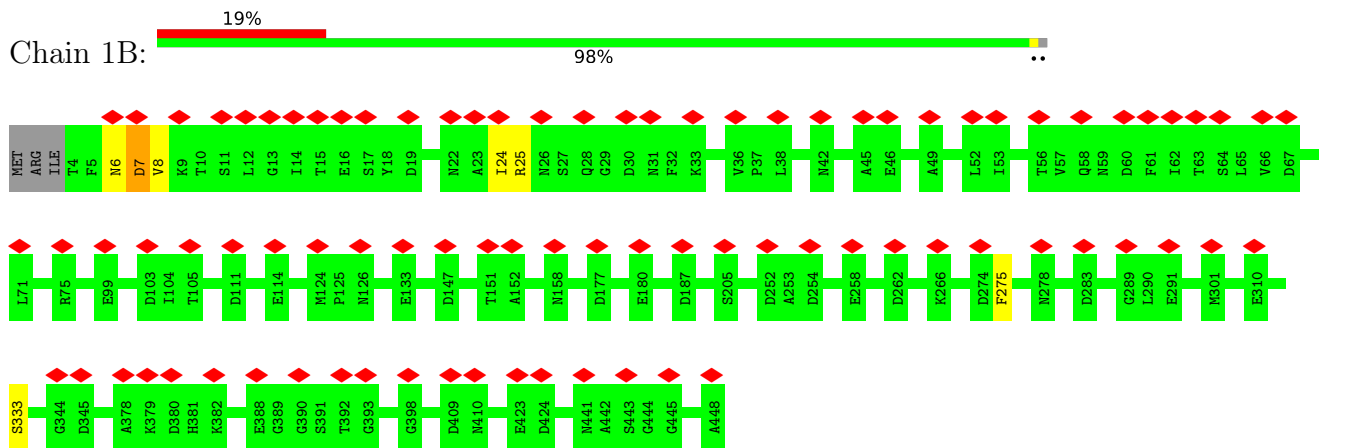
3 Residue-property plots

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

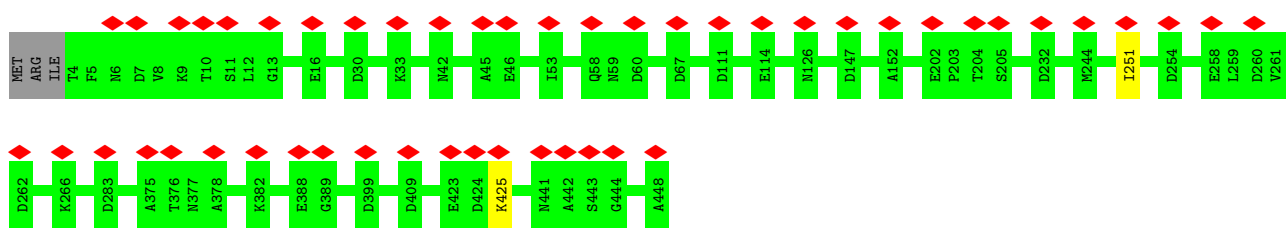
- Molecule 1: Major capsid protein



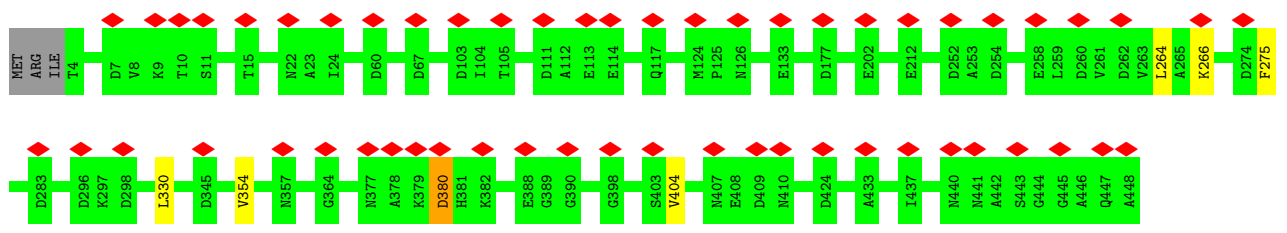
- Molecule 1: Major capsid protein



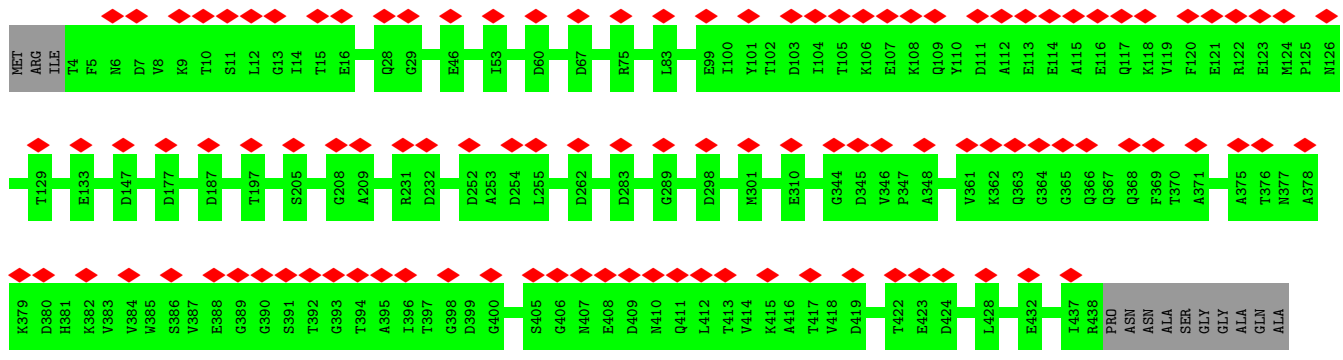
- Molecule 1: Major capsid protein



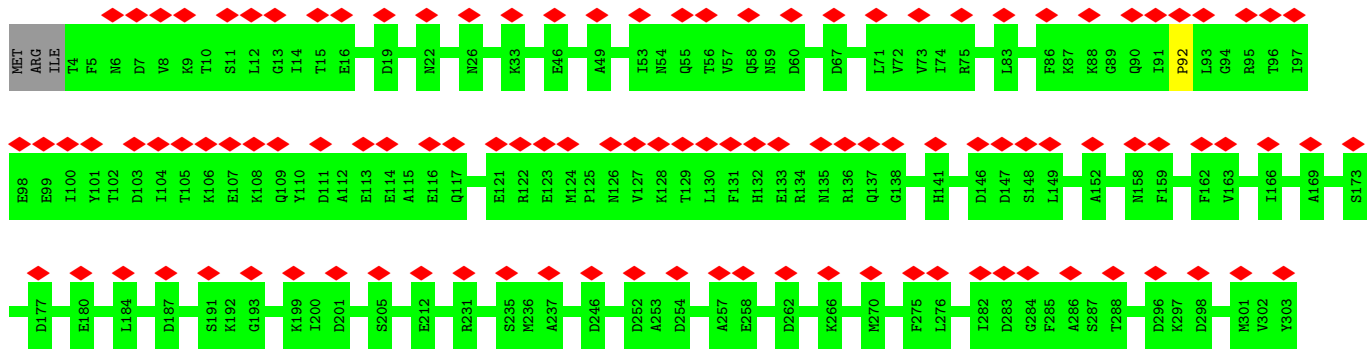
• Molecule 1: Major capsid protein

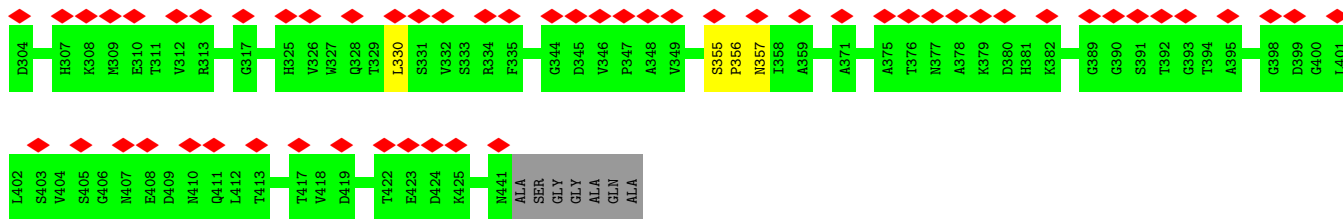


• Molecule 1: Major capsid protein

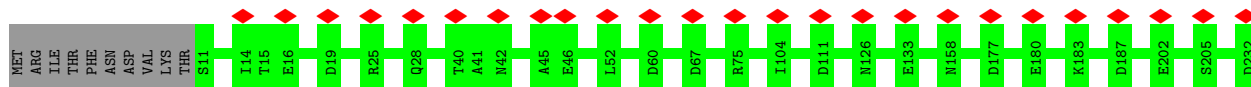


• Molecule 1: Major capsid protein

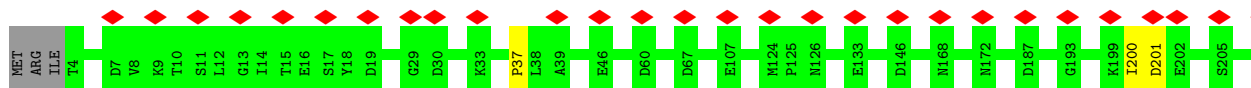




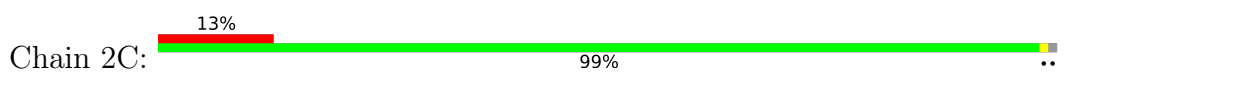
• Molecule 1: Major capsid protein



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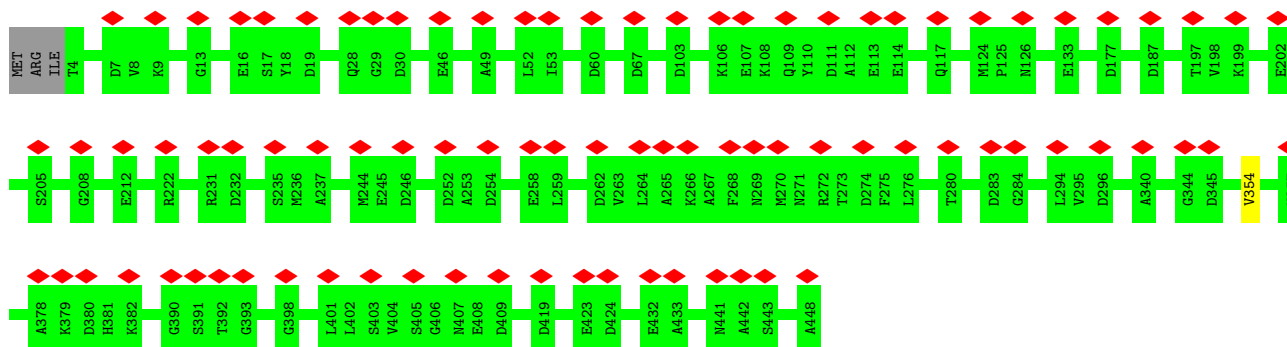


• Molecule 1: Major capsid protein

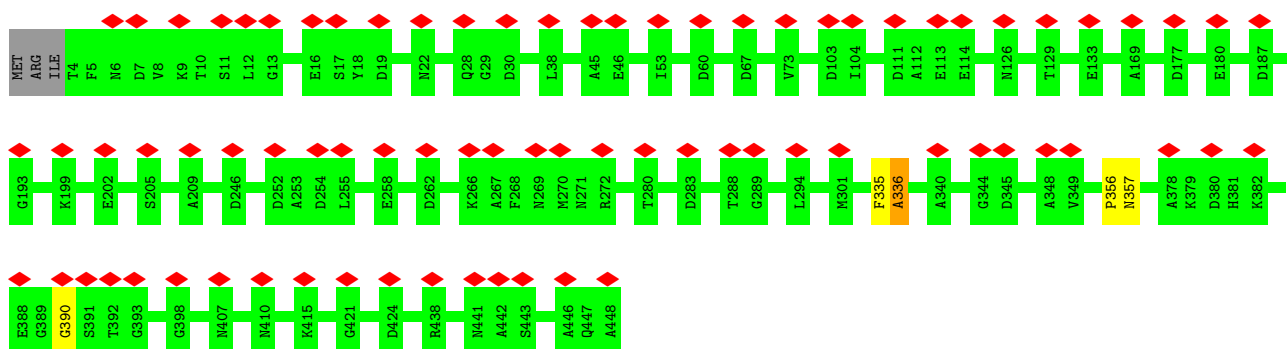


• Molecule 1: Major capsid protein

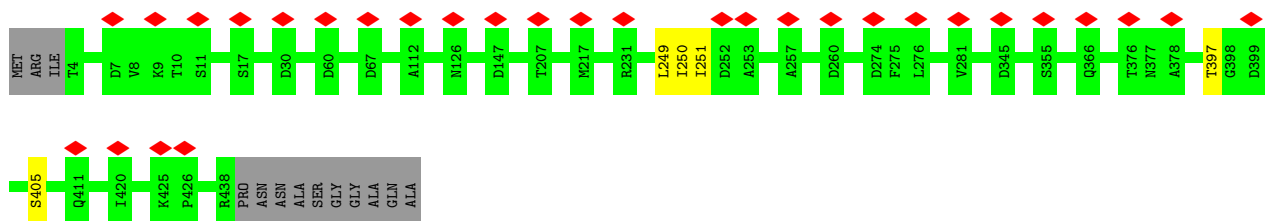




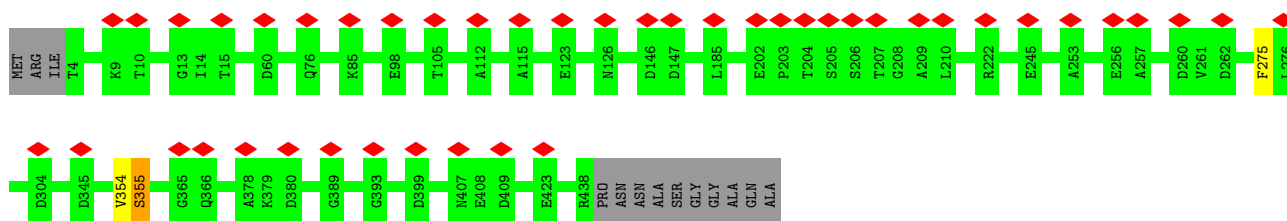
• Molecule 1: Major capsid protein



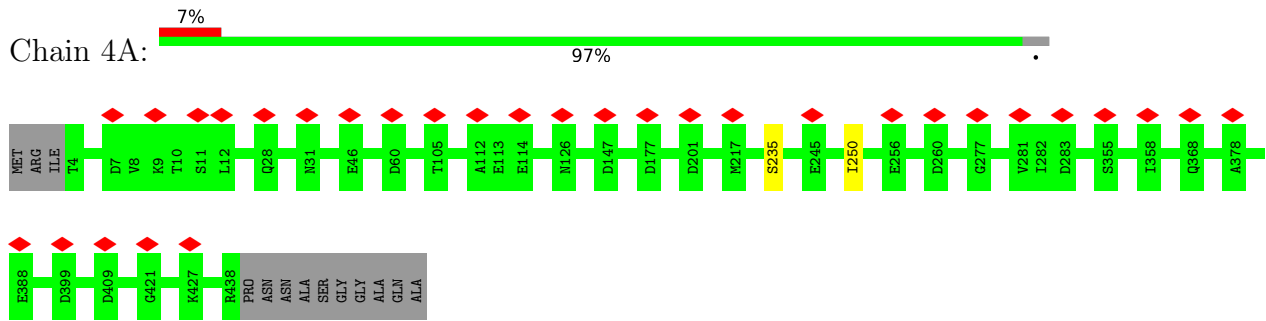
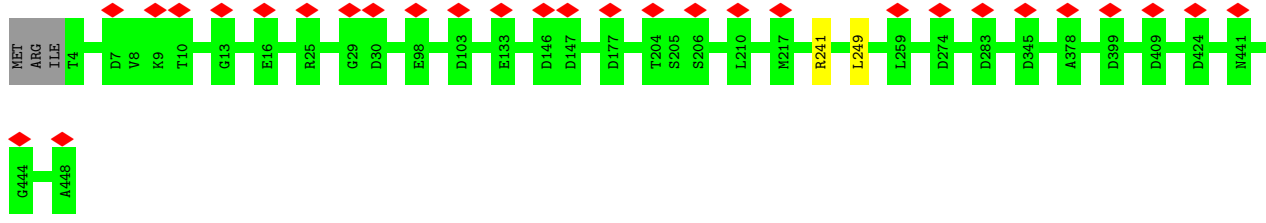
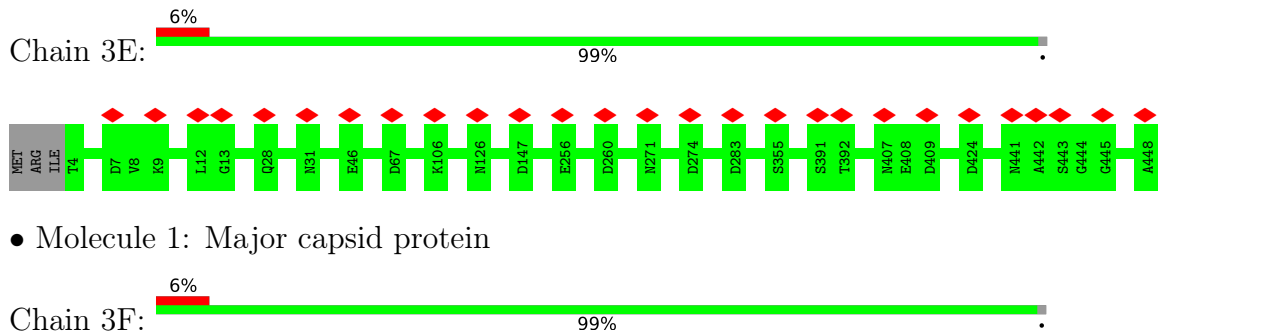
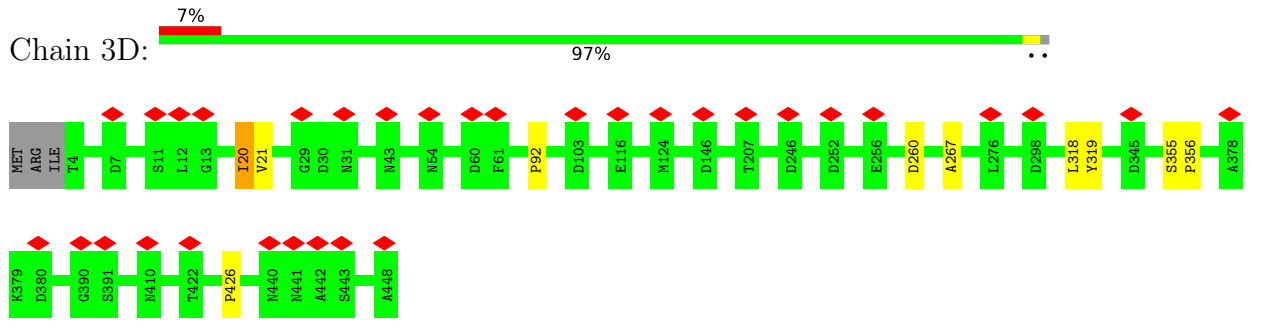
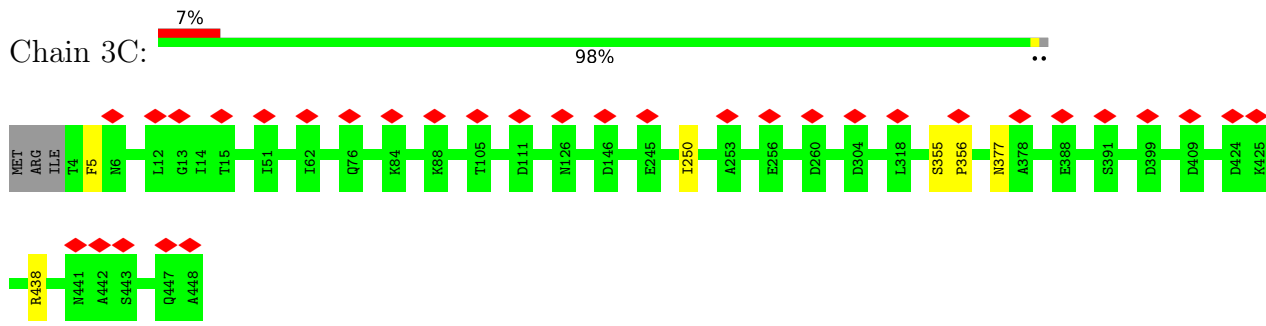
• Molecule 1: Major capsid protein



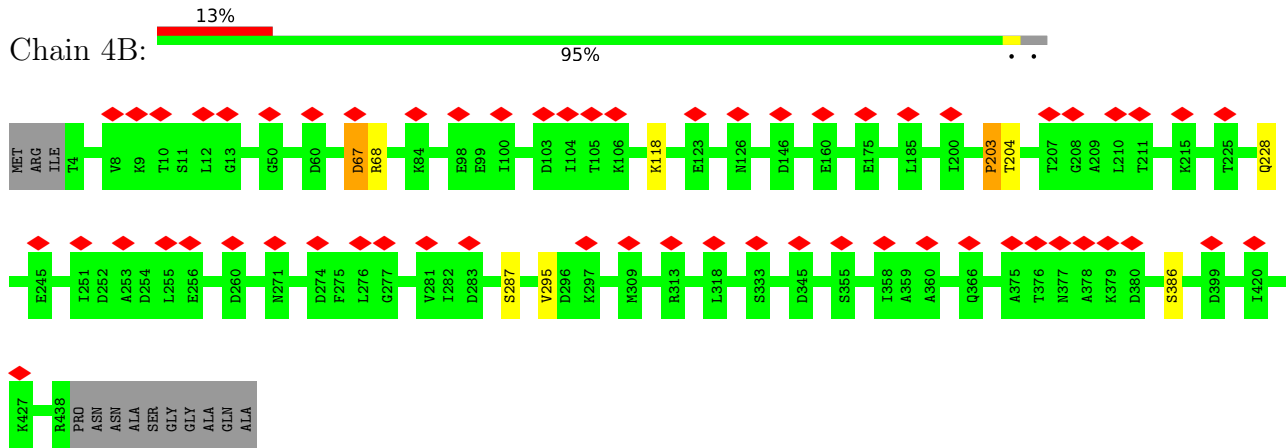
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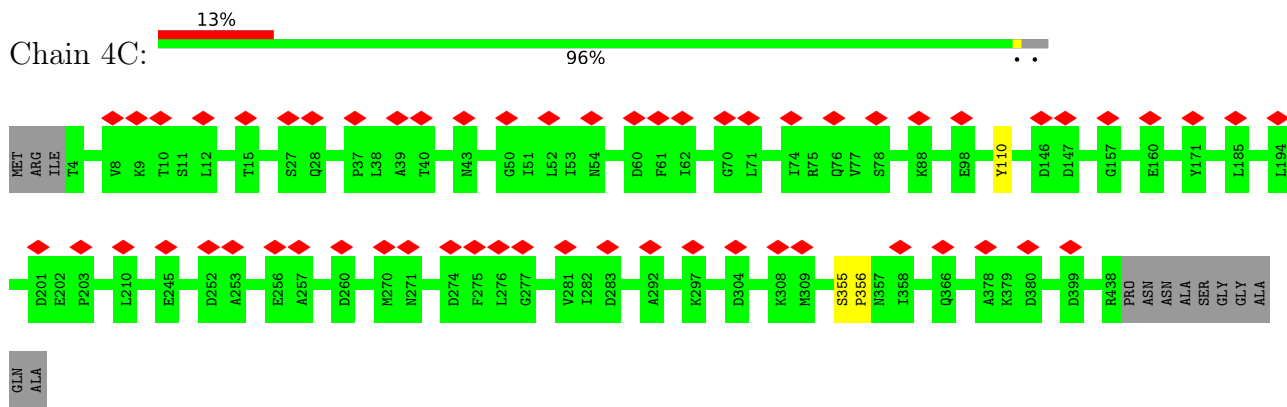
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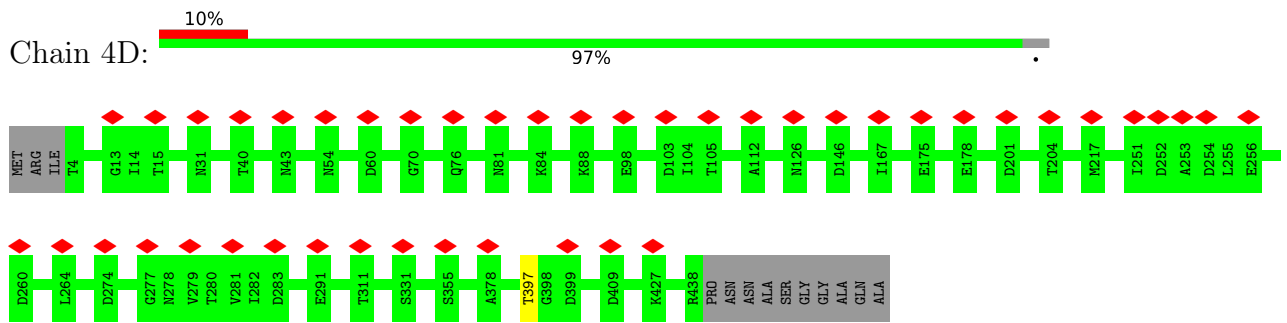
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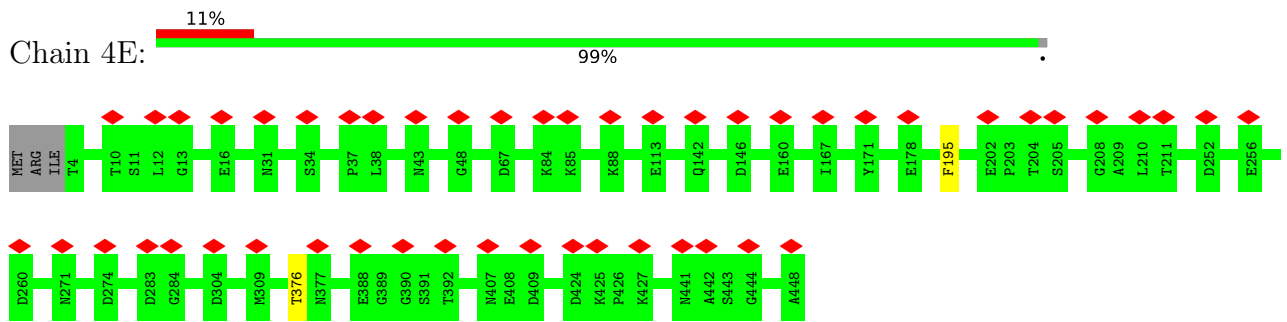
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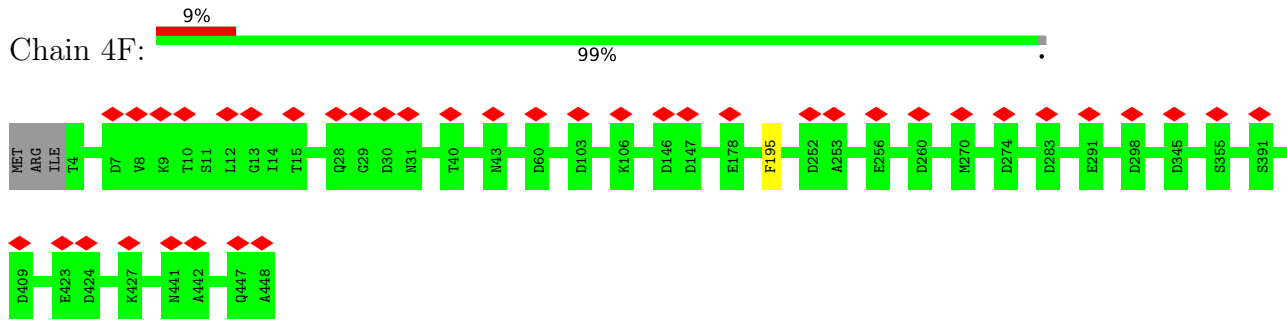
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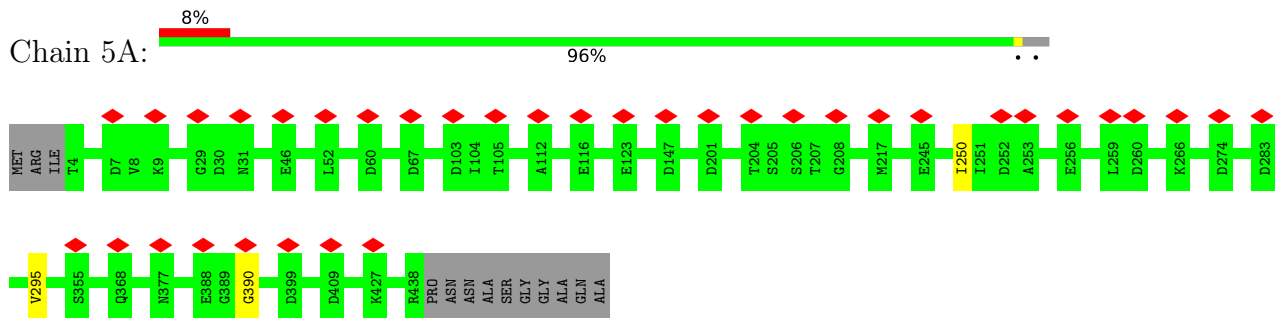
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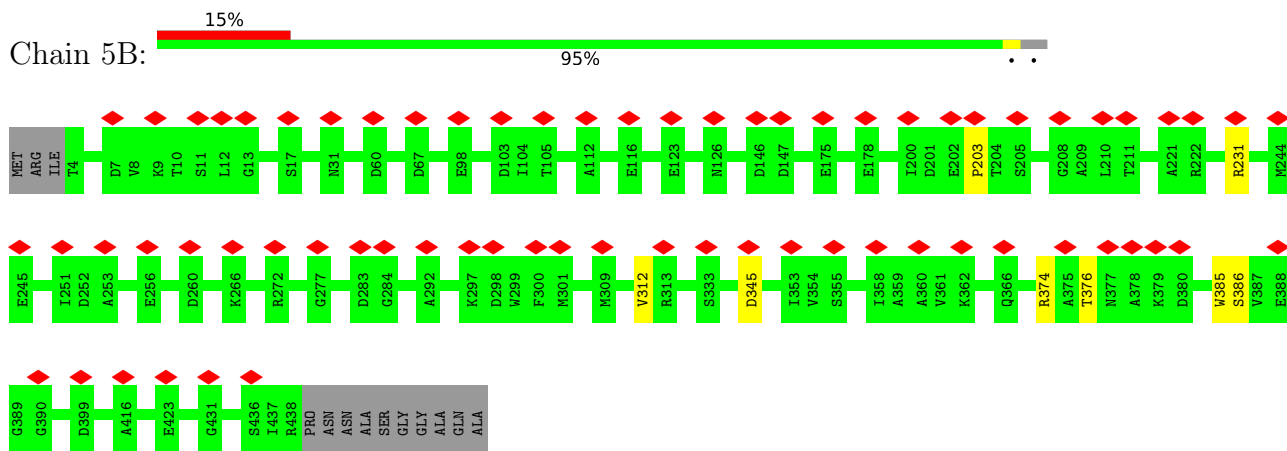
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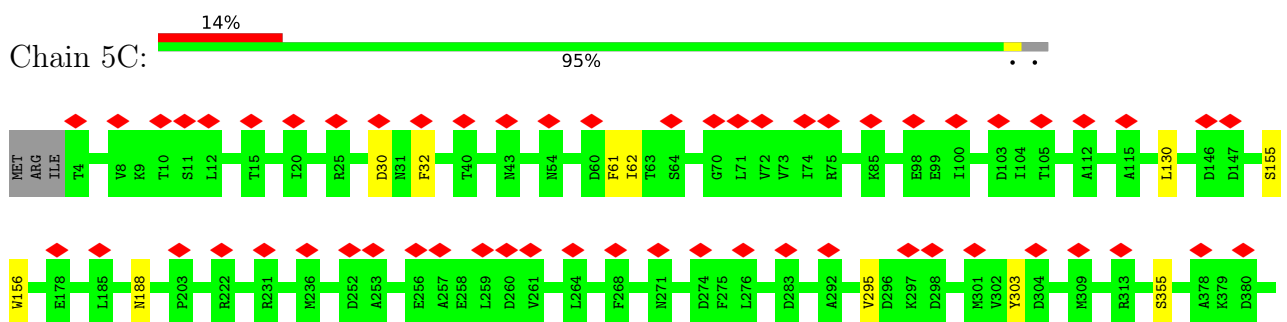
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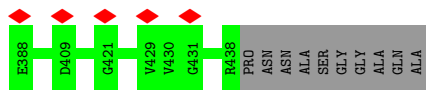


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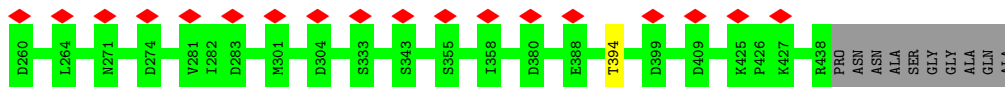
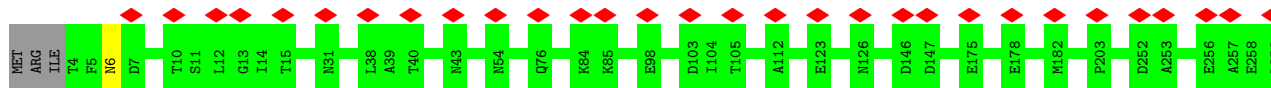


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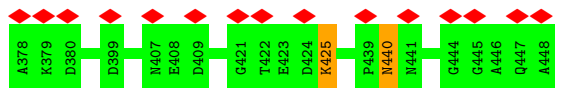
• Molecule 1: Major capsid protein



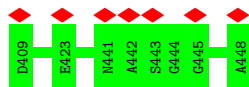
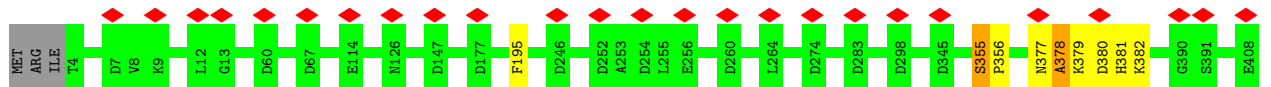
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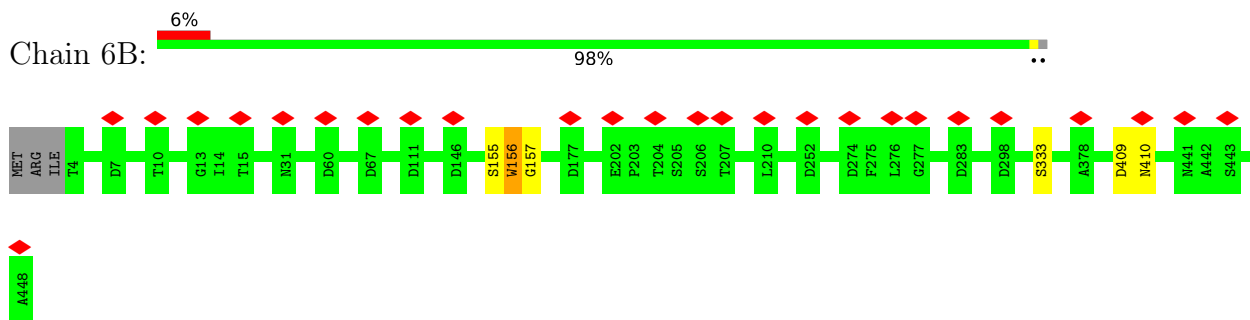
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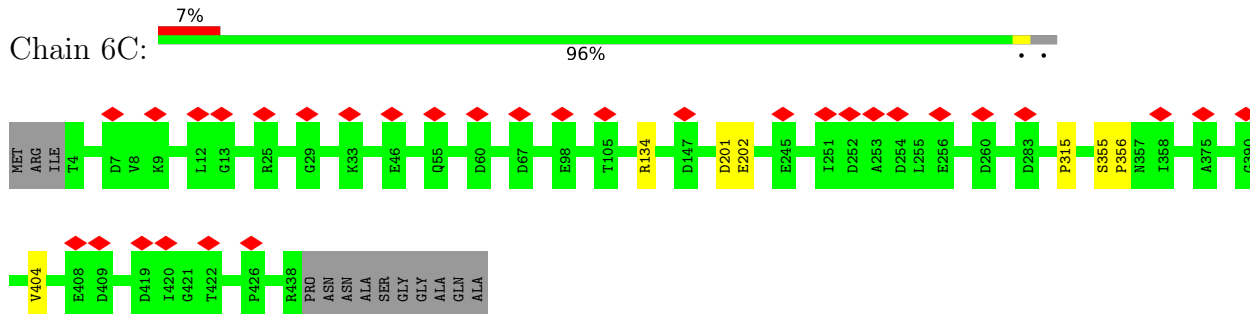
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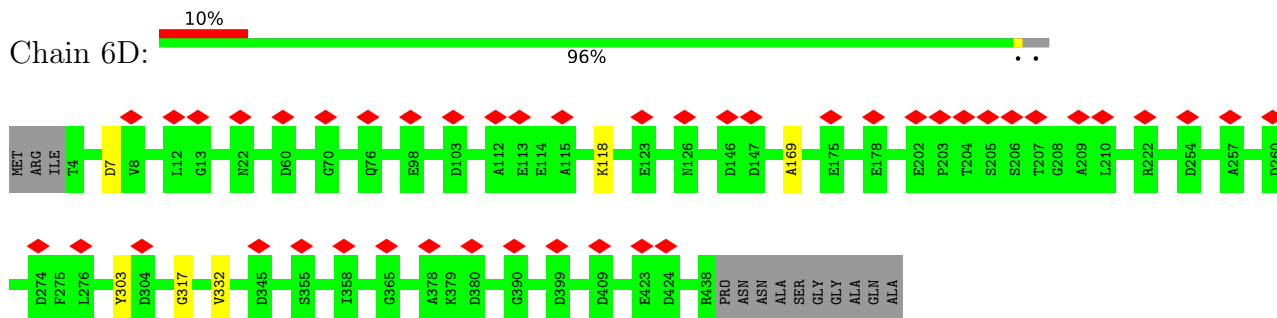
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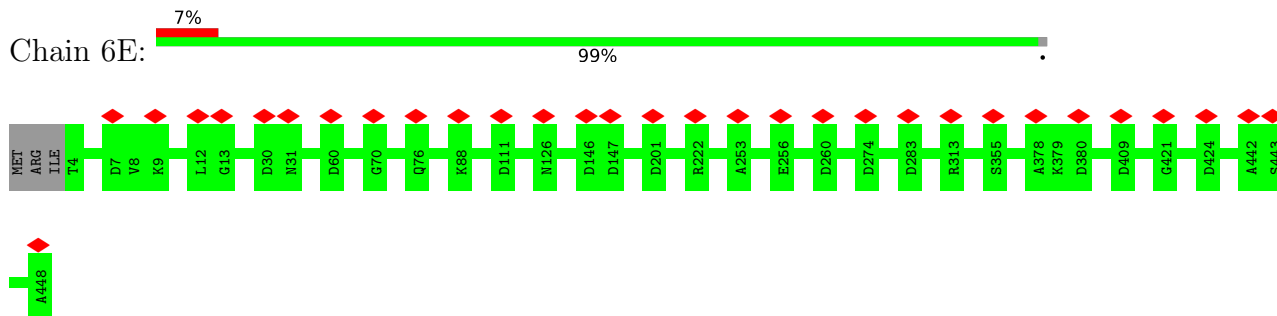
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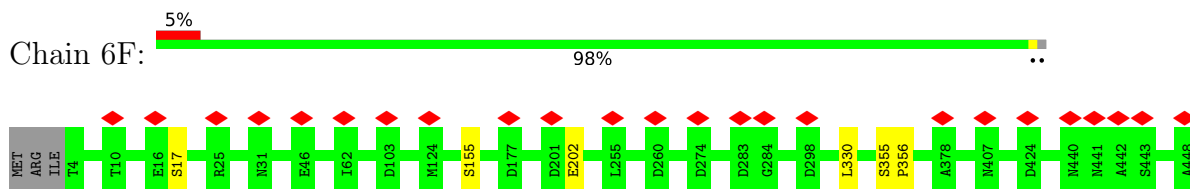
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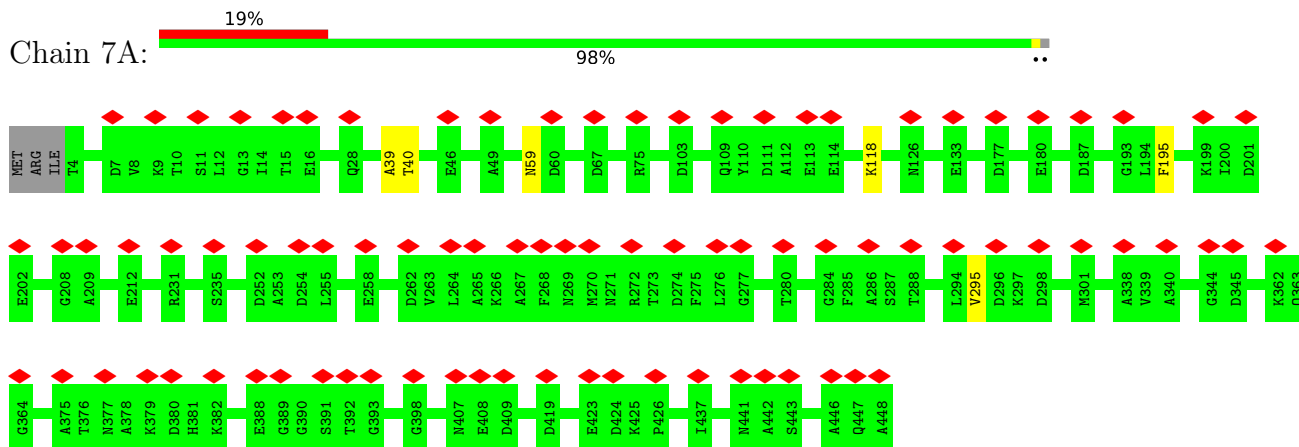
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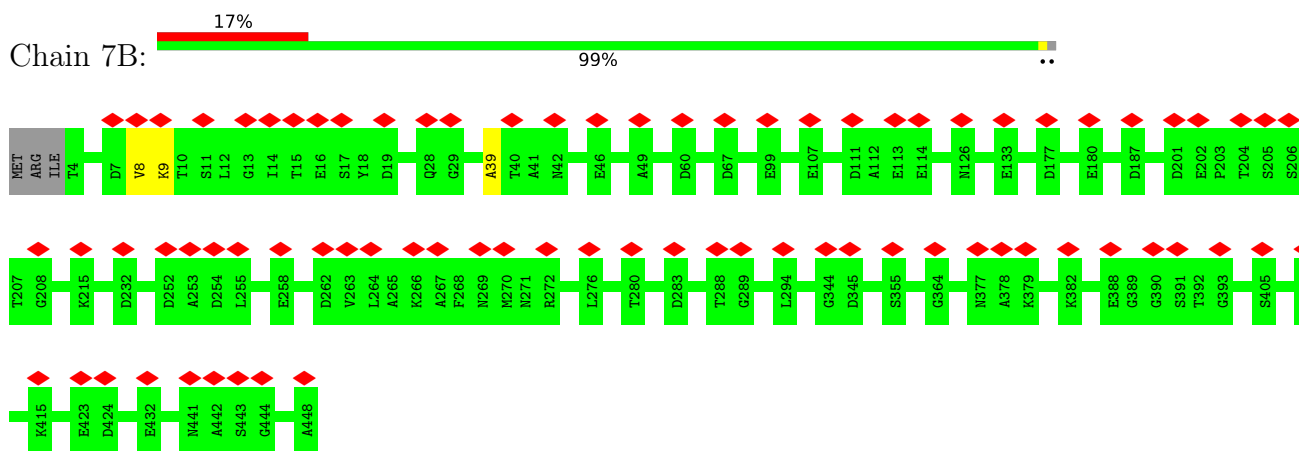
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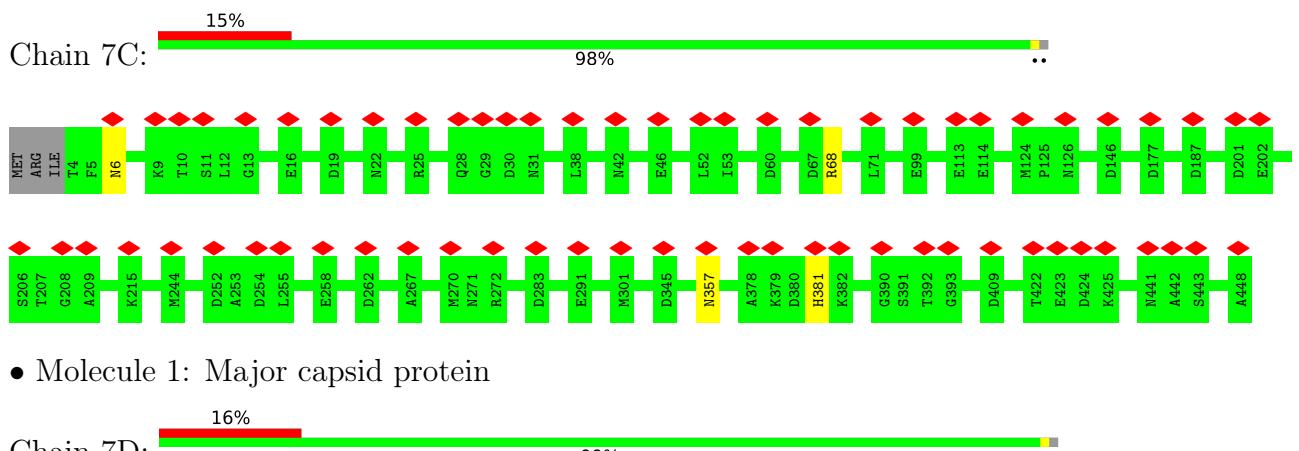
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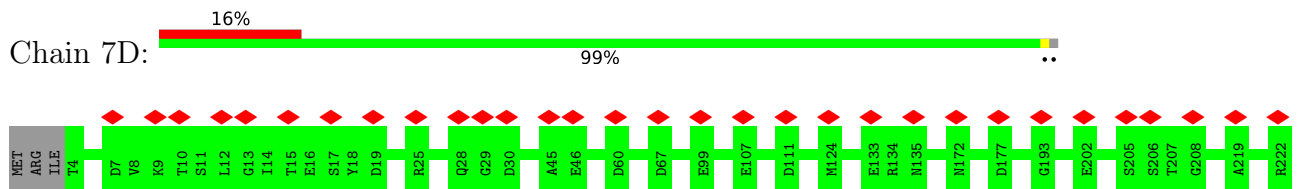
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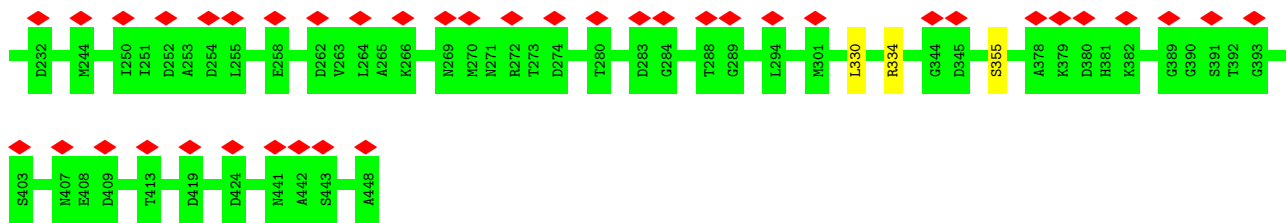


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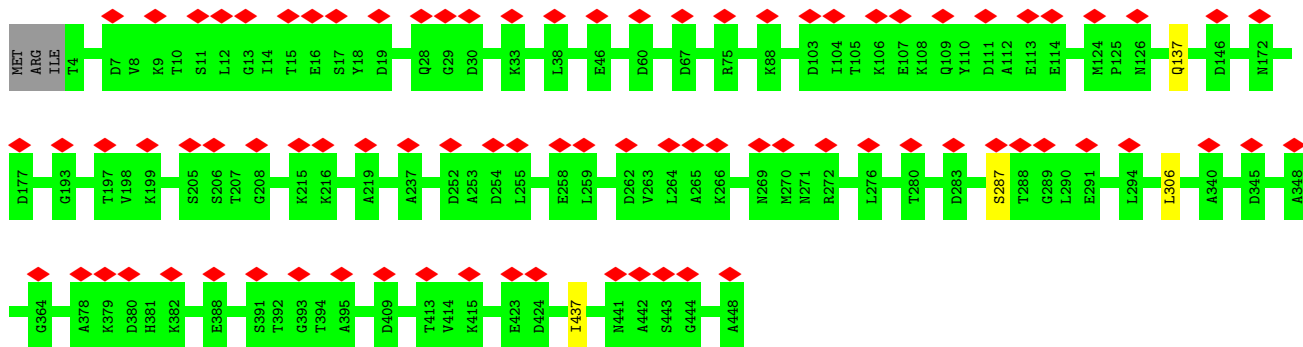


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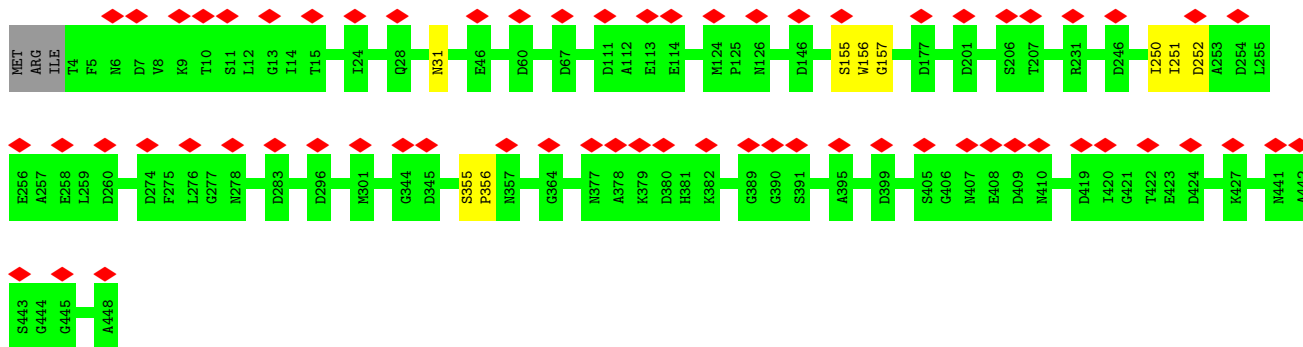




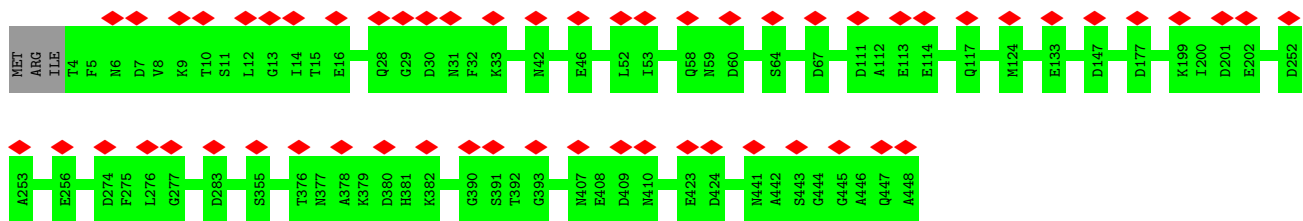
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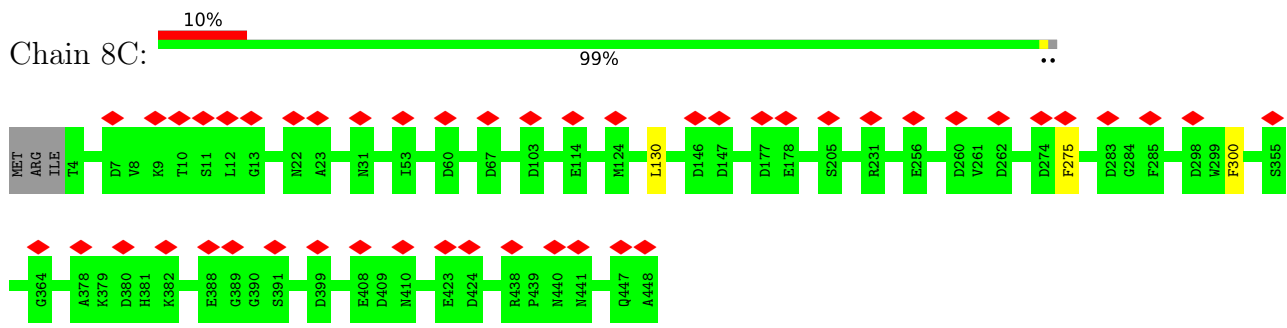
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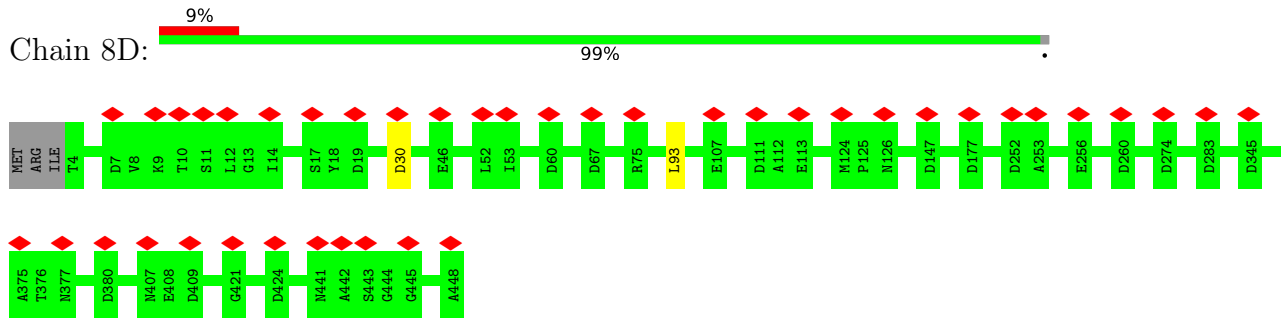
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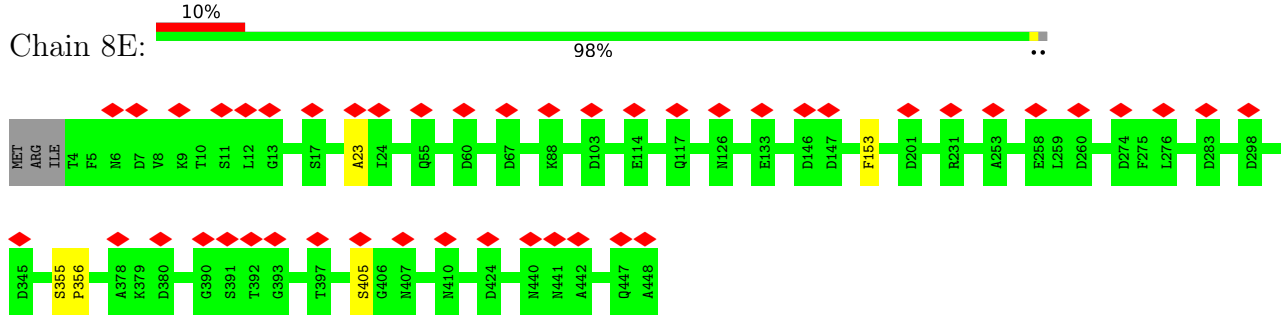
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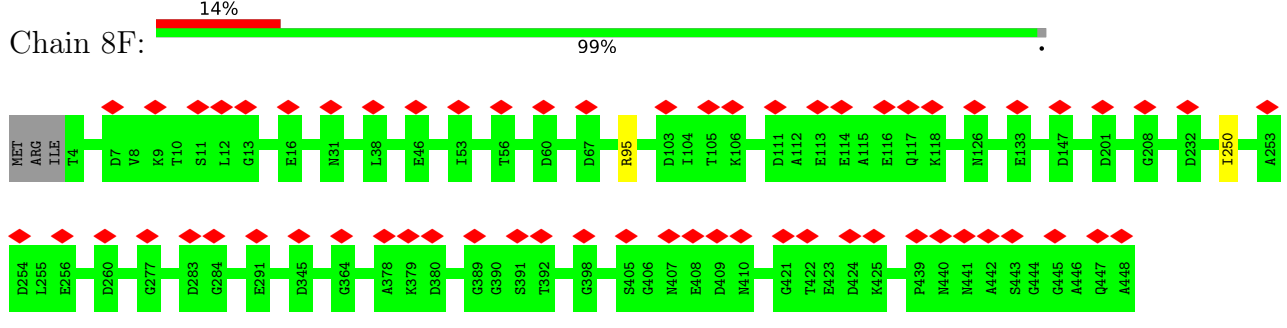
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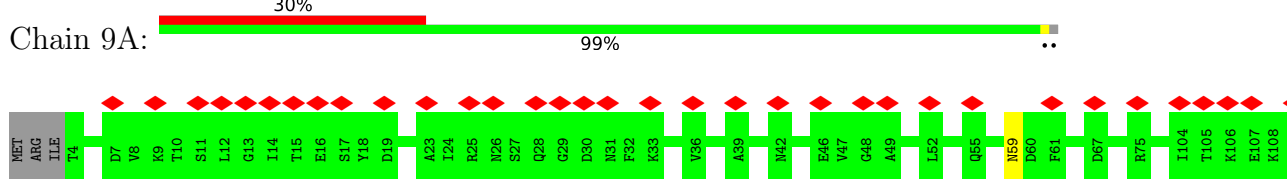
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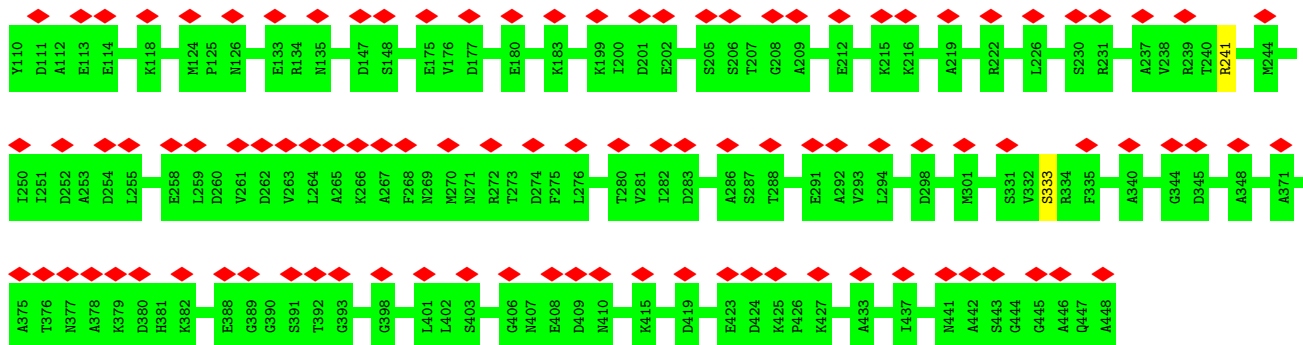


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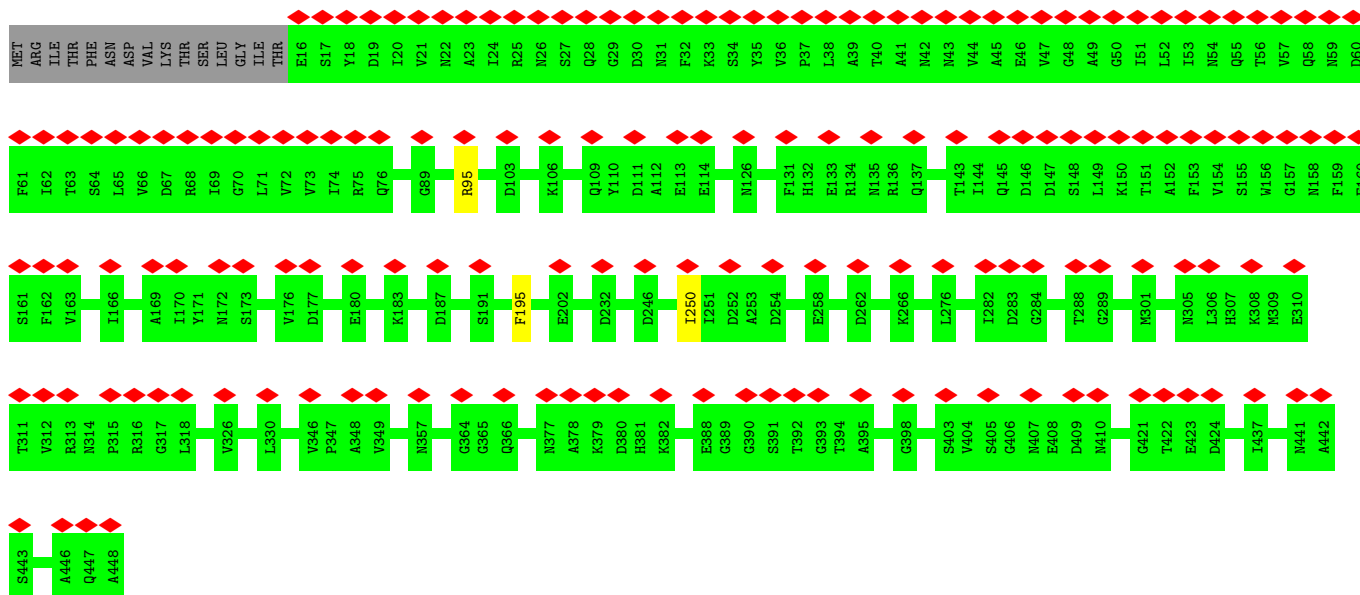
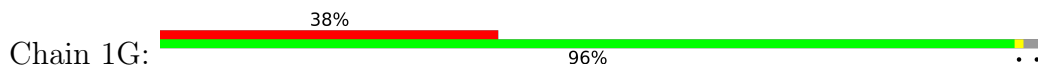


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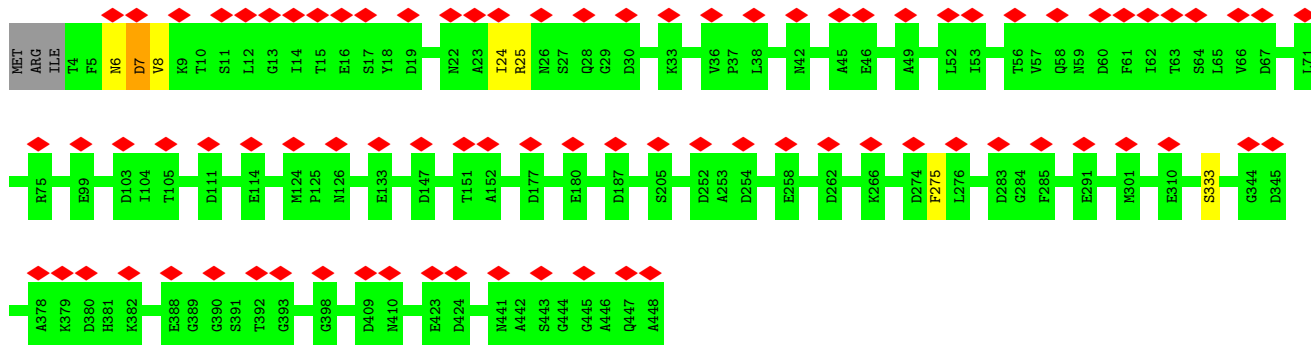




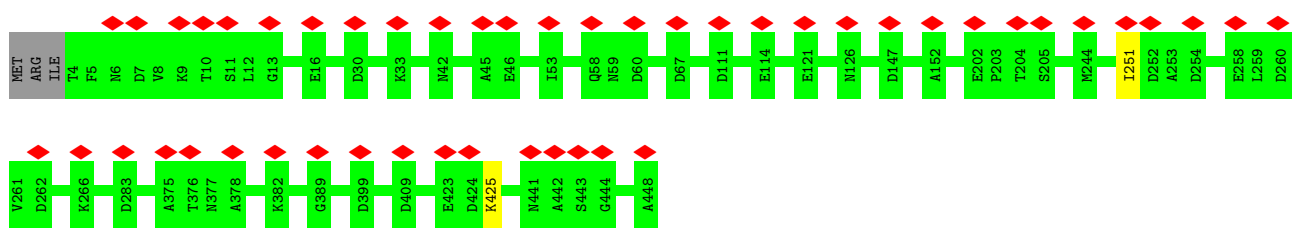
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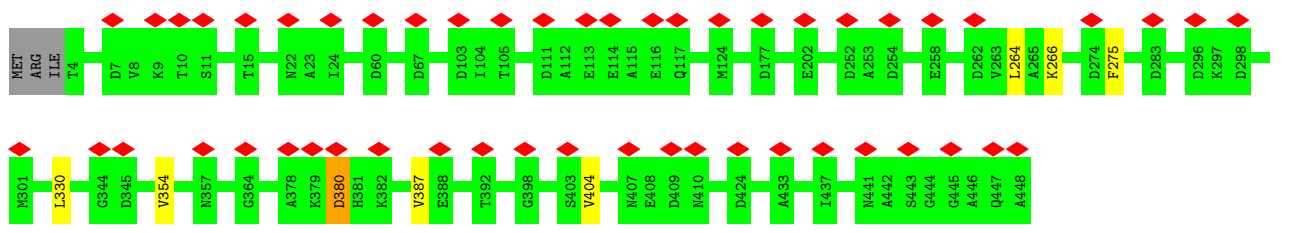
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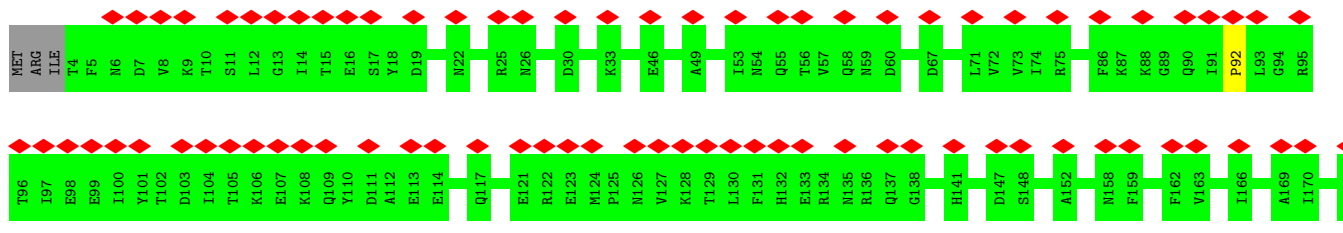
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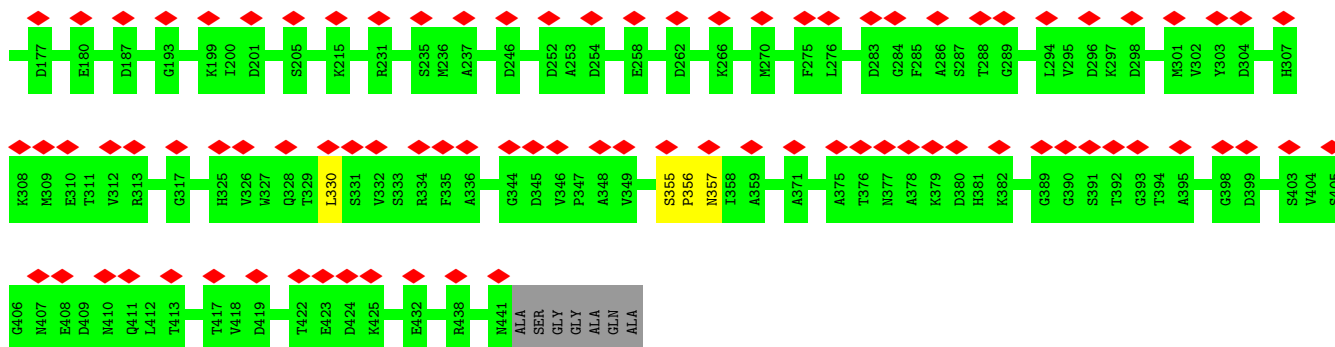


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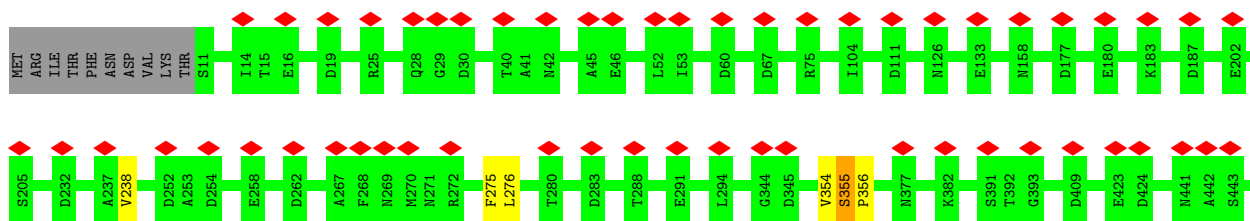
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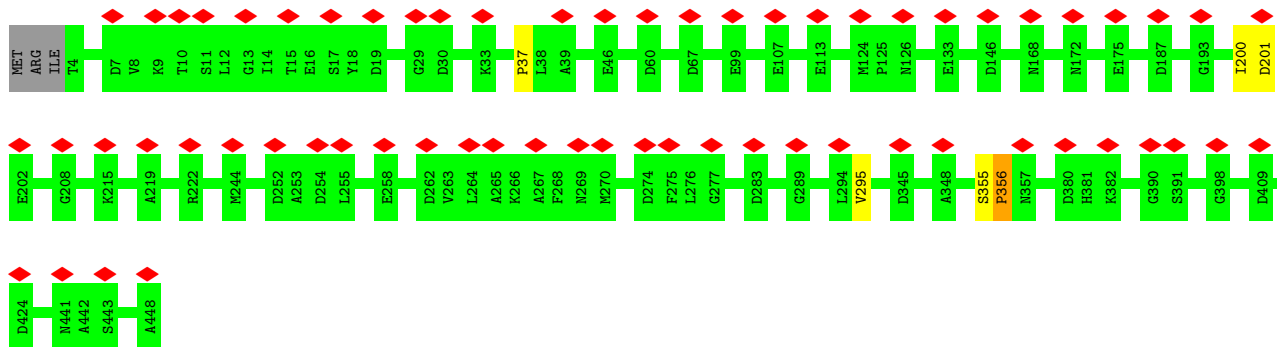
- Molecule 1: Major capsid protein

Chain 2F: 12% 96%



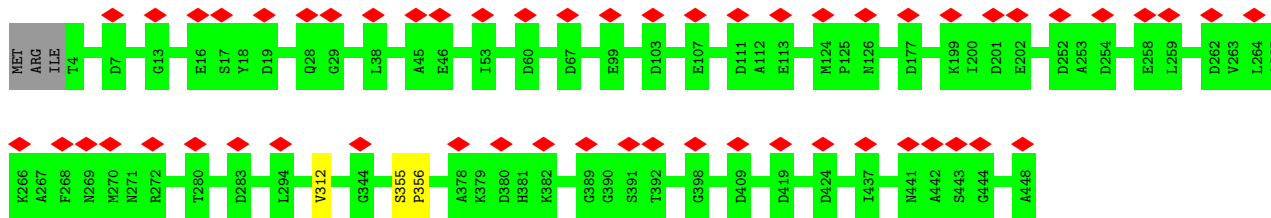
- Molecule 1: Major capsid protein

Chain 2G: 14% 98%

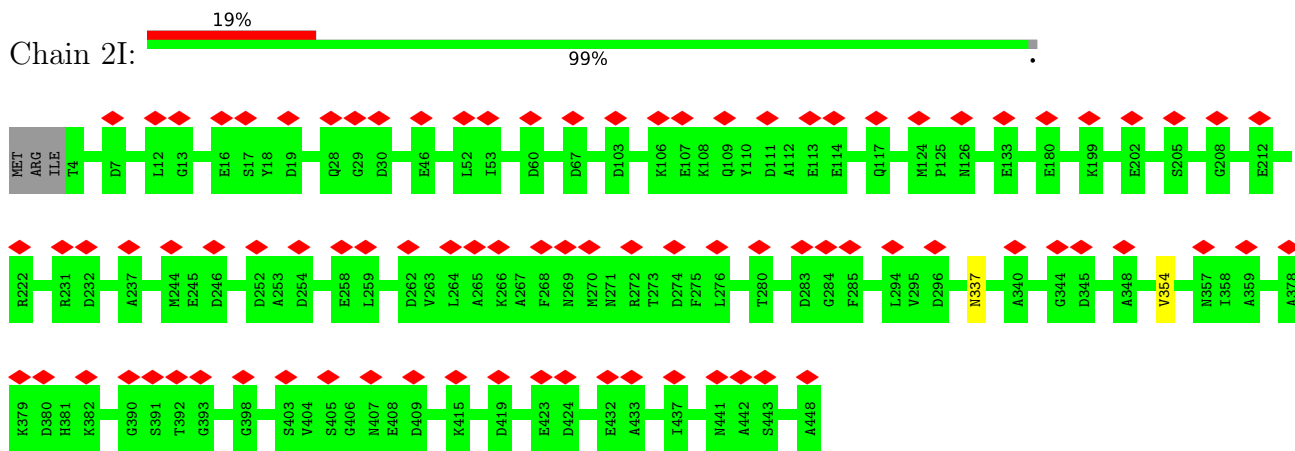


- Molecule 1: Major capsid protein

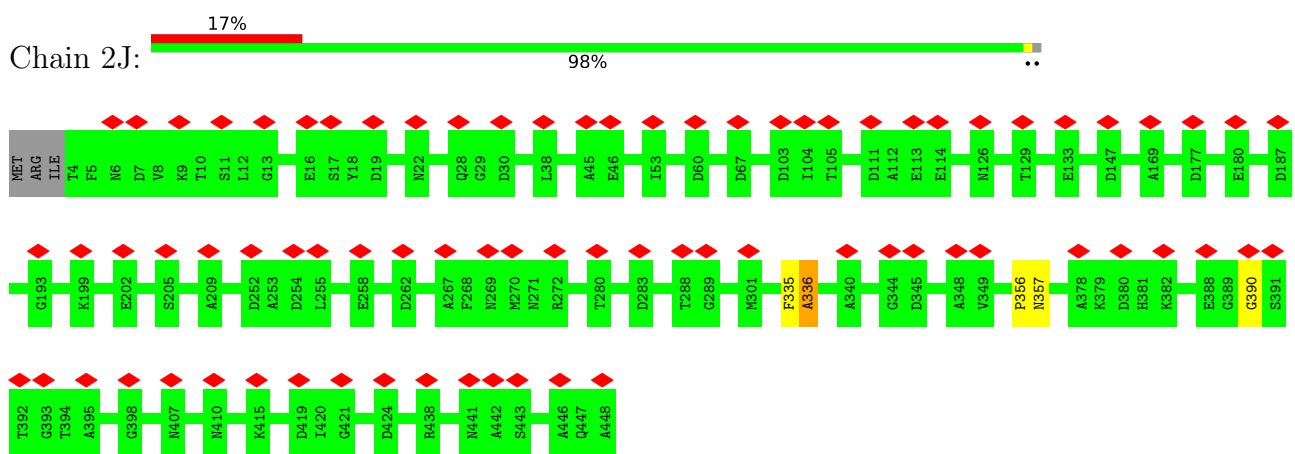
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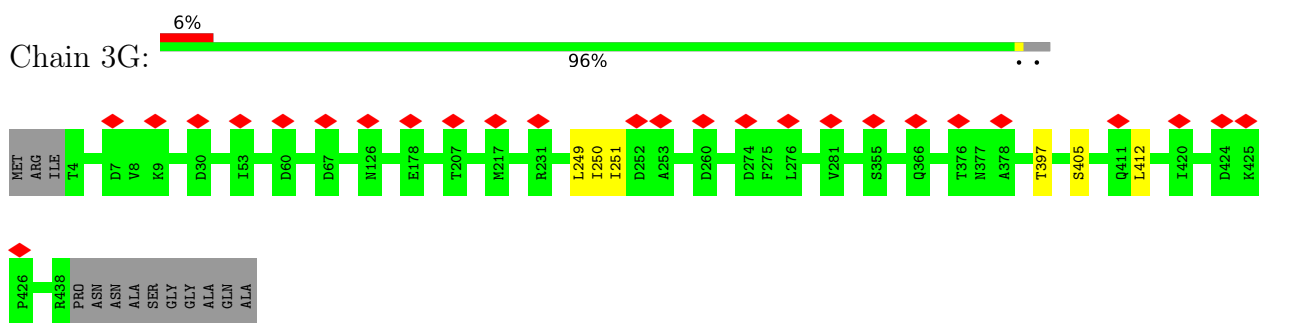
- Molecule 1: Major capsid protein



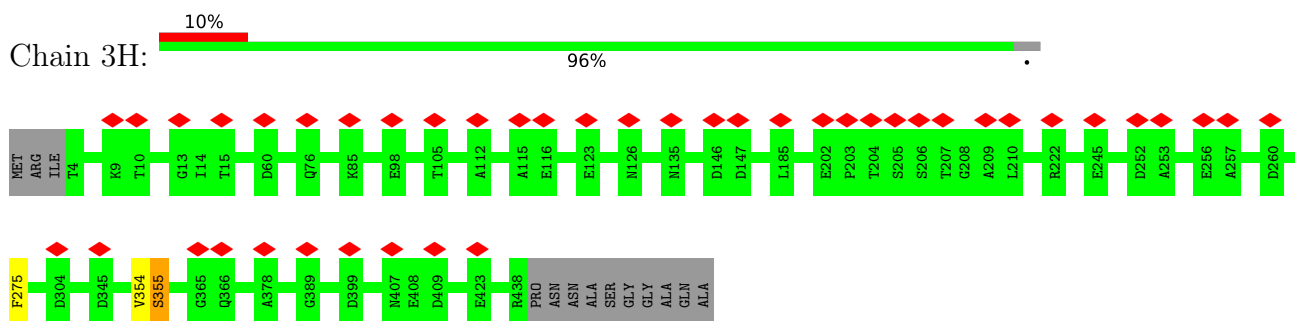
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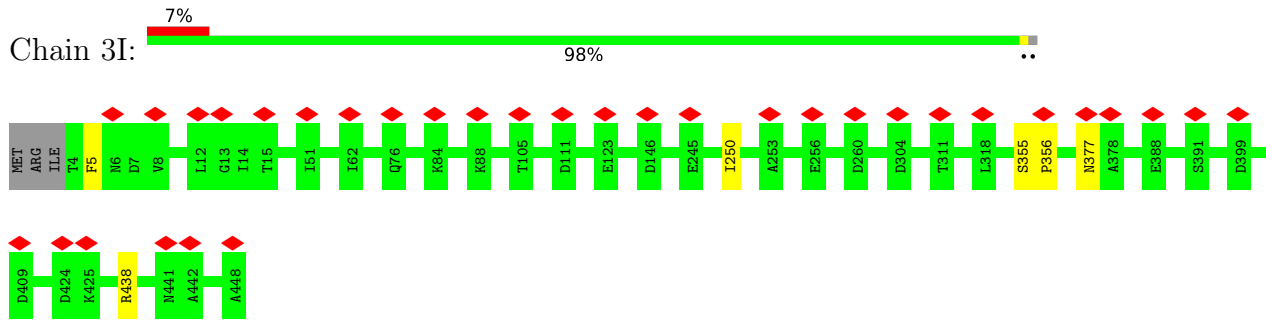
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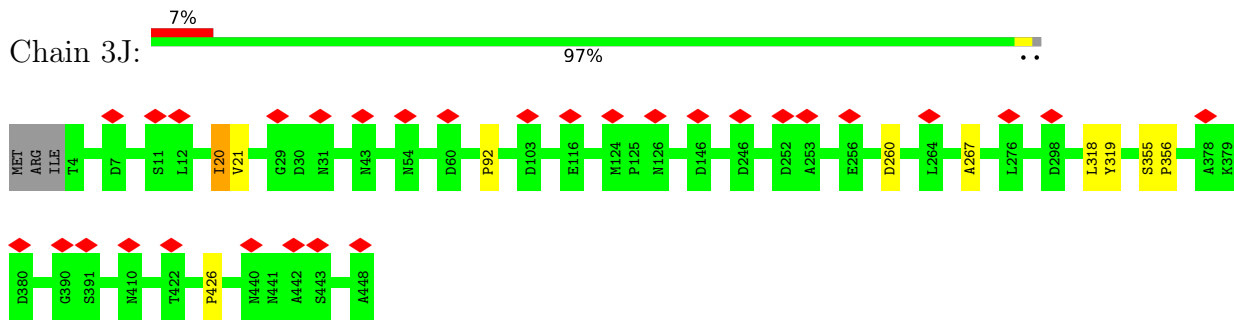
• Molecule 1: Major capsid protein



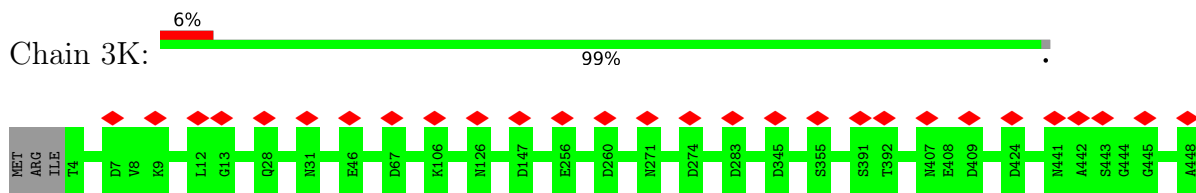
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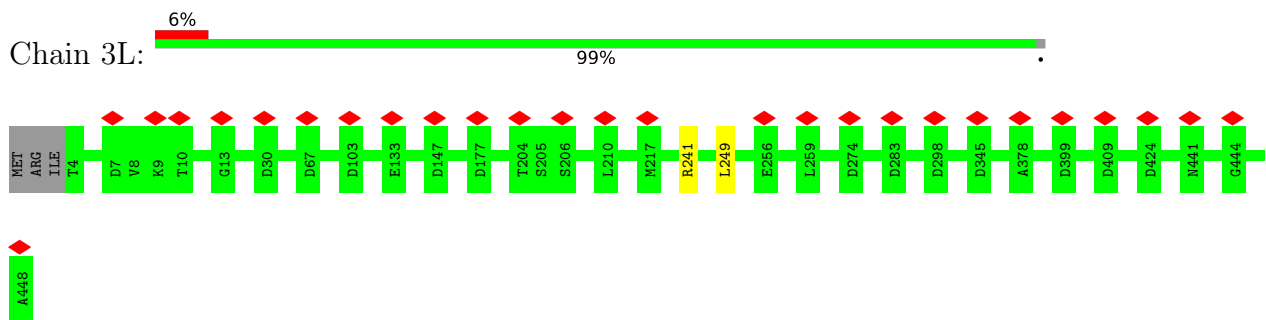
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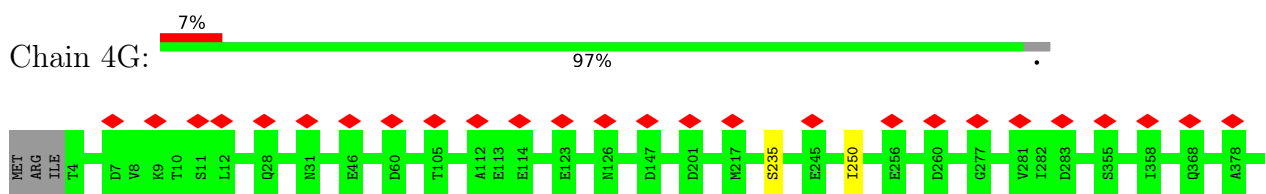
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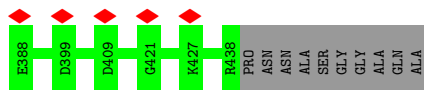


- Molecule 1: Major capsid protein

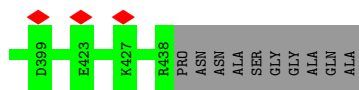
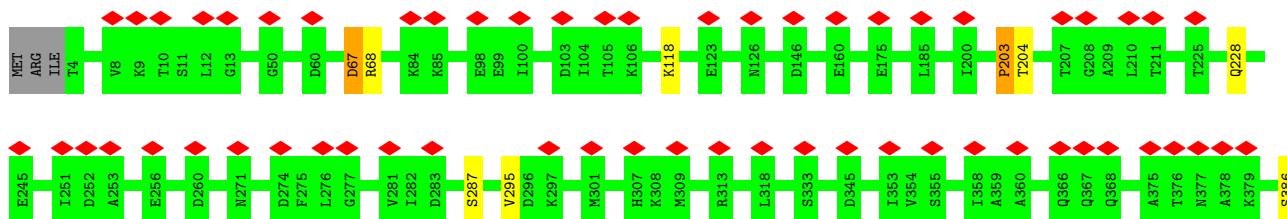


- Molecule 1: Major capsid protein

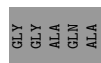
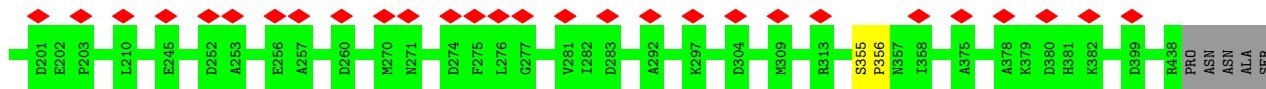
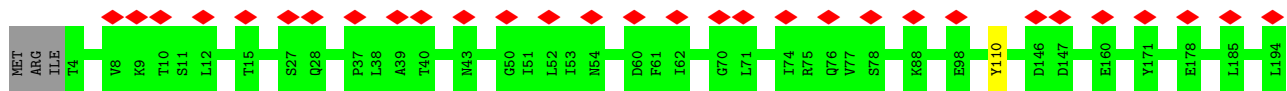




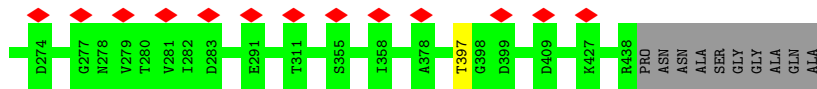
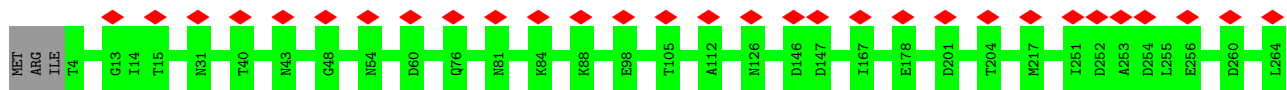
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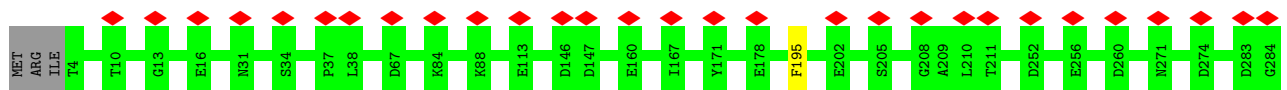
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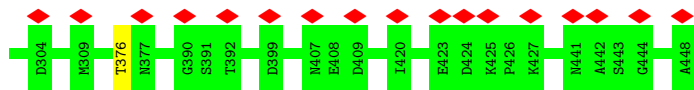


• Molecule 1: Major capsid protein

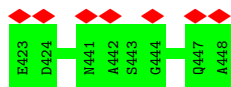
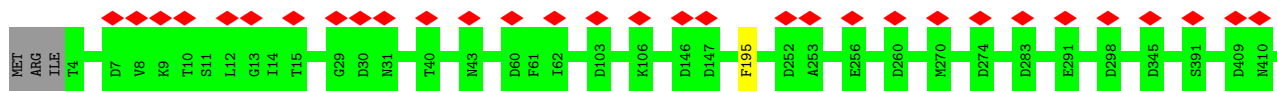


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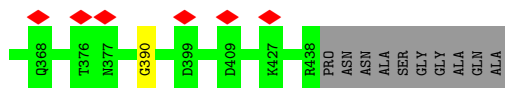
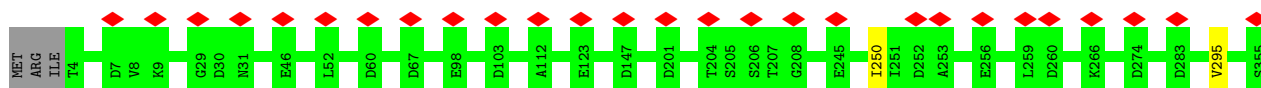




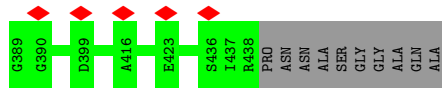
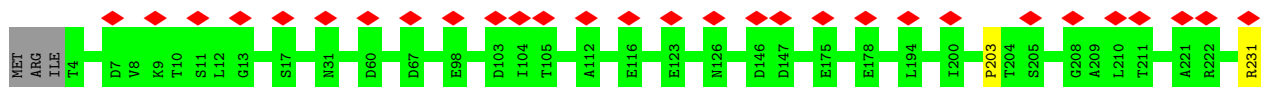
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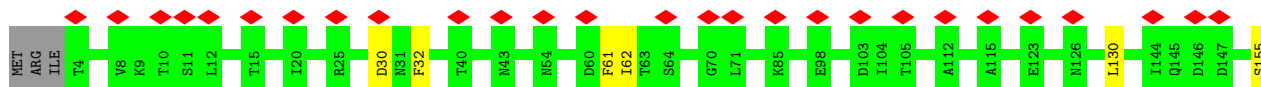
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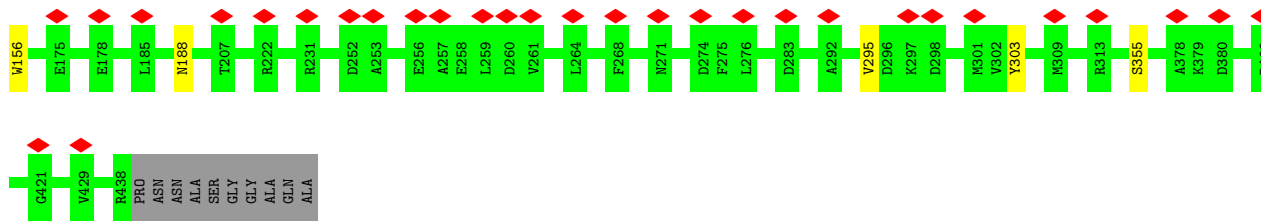


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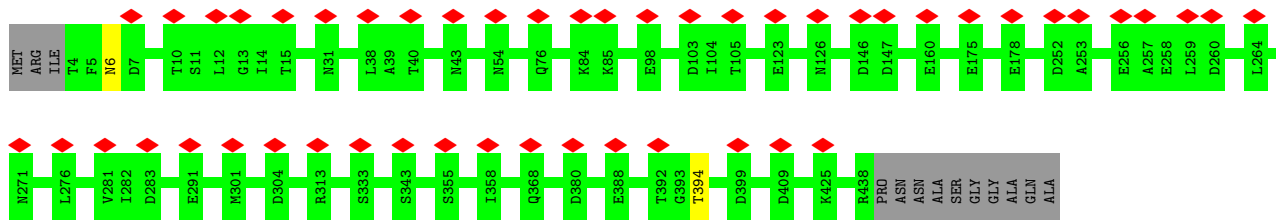


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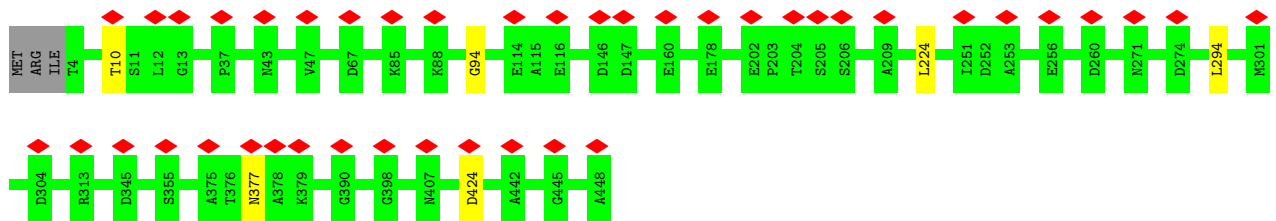




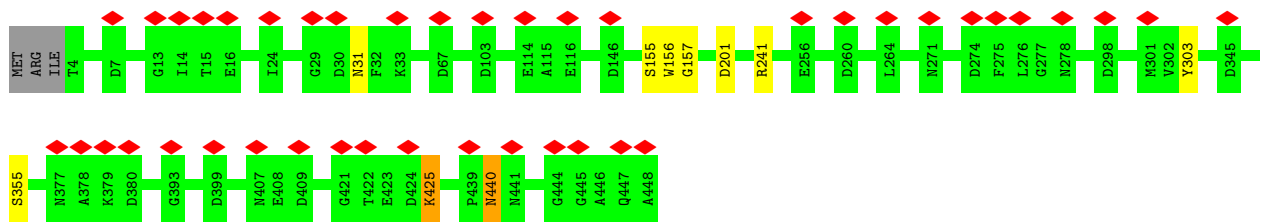
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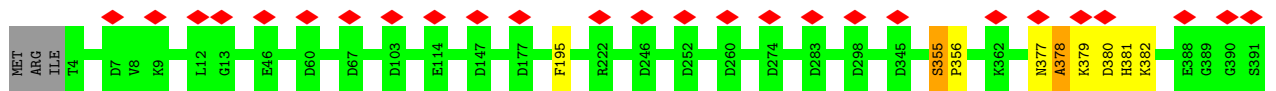
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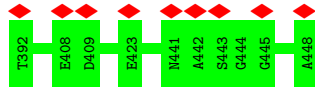


• Molecule 1: Major capsid protein

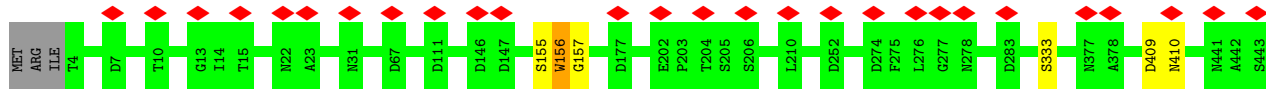


• Molecule 1: Major capsid protein

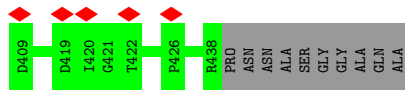
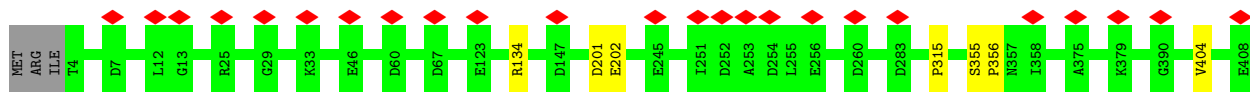




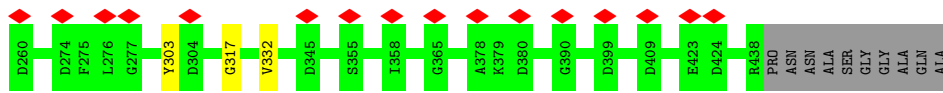
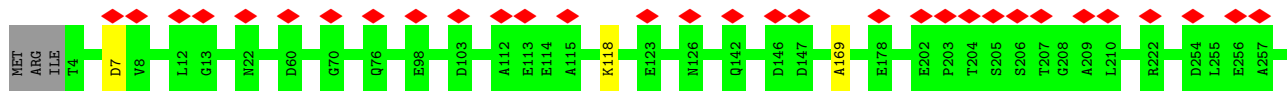
• Molecule 1: Major capsid protein



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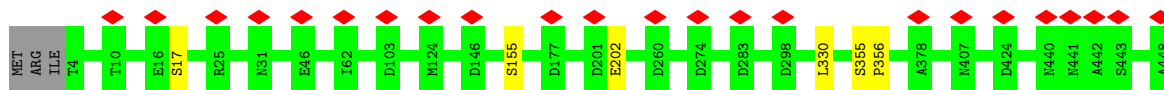
• Molecule 1: Major capsid protein



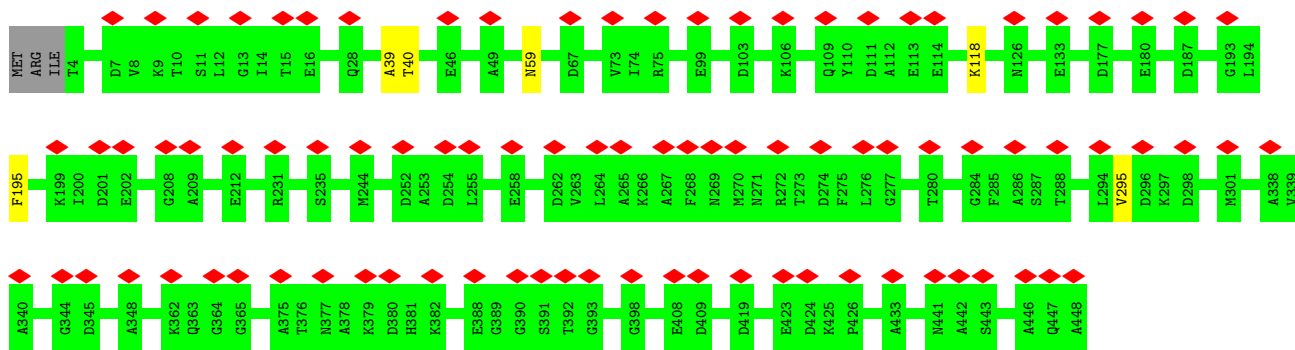
• Molecule 1: Major capsid protein



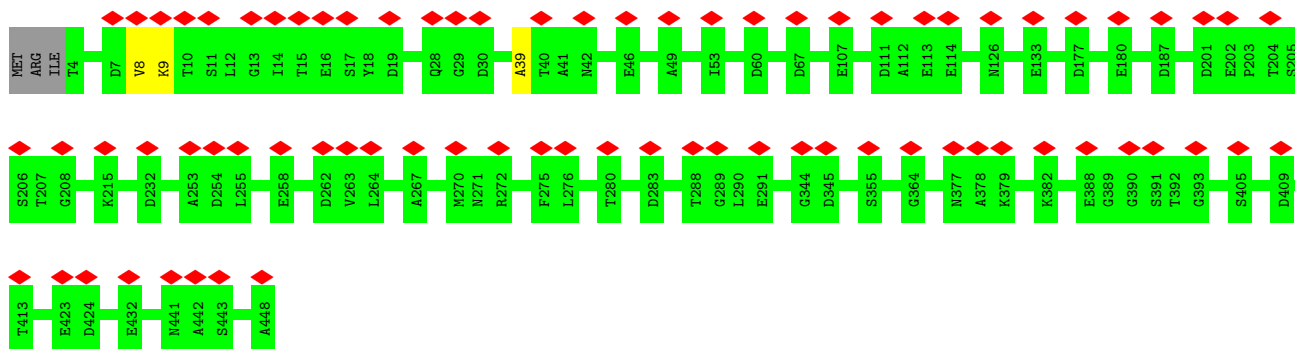
• Molecule 1: Major capsid protein



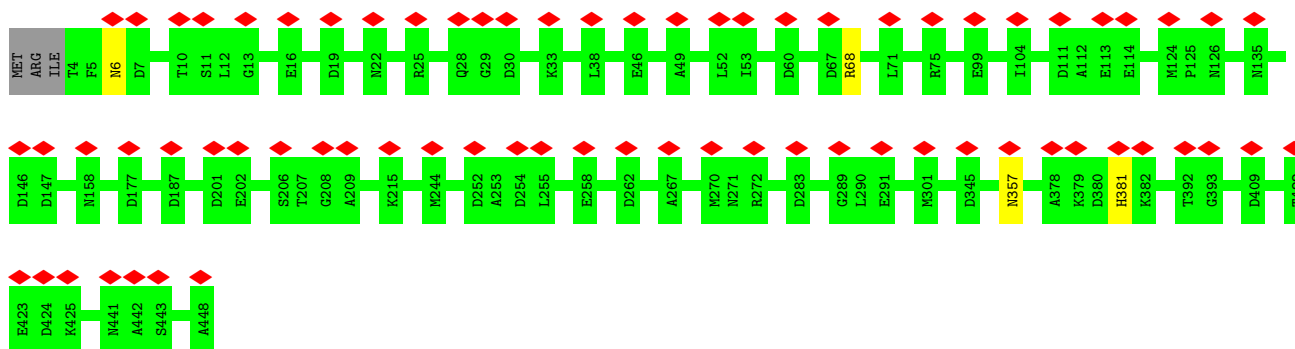
• Molecule 1: Major capsid protein



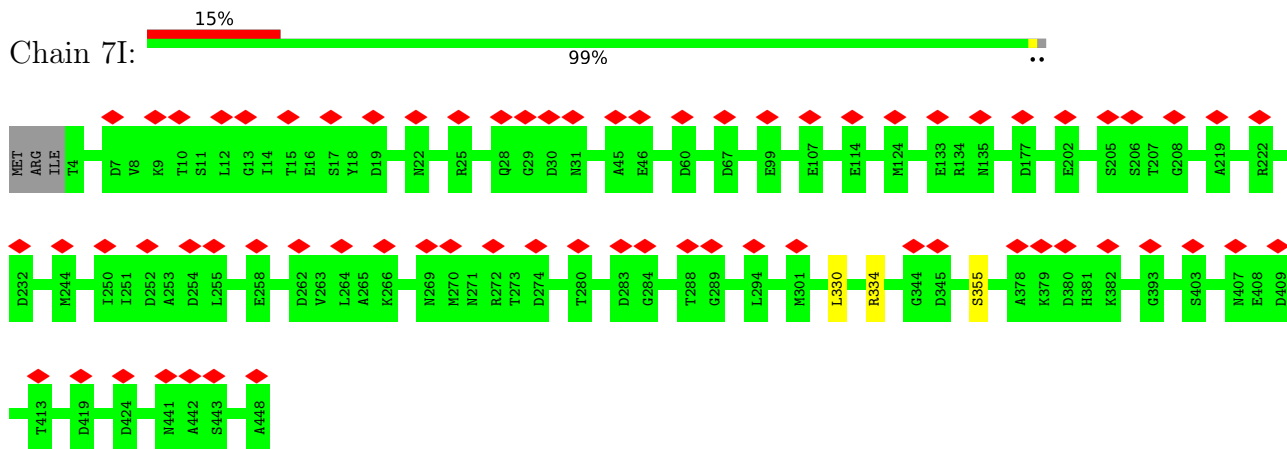
• Molecule 1: Major capsid protein



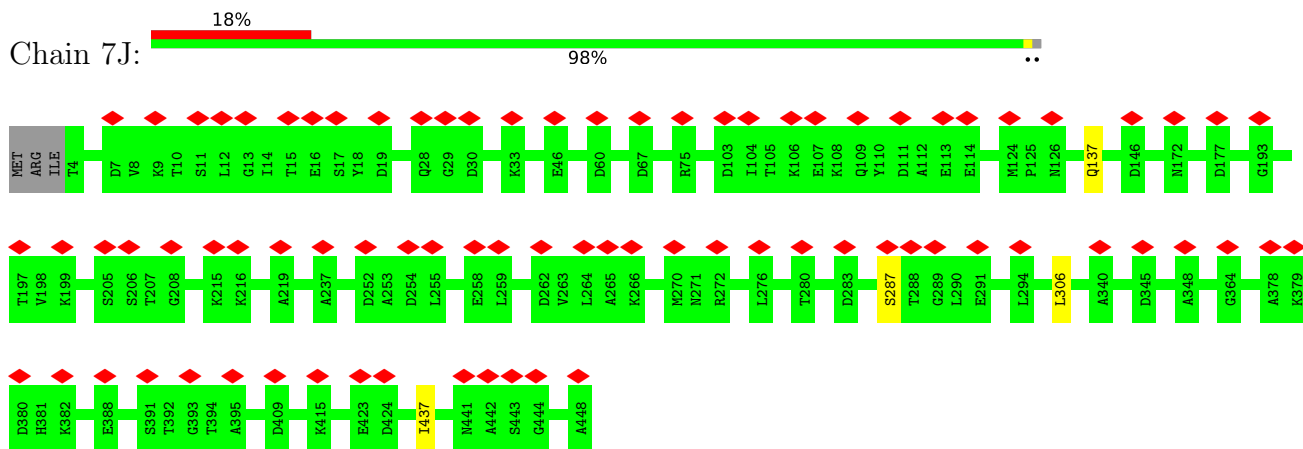
• Molecule 1: Major capsid protein



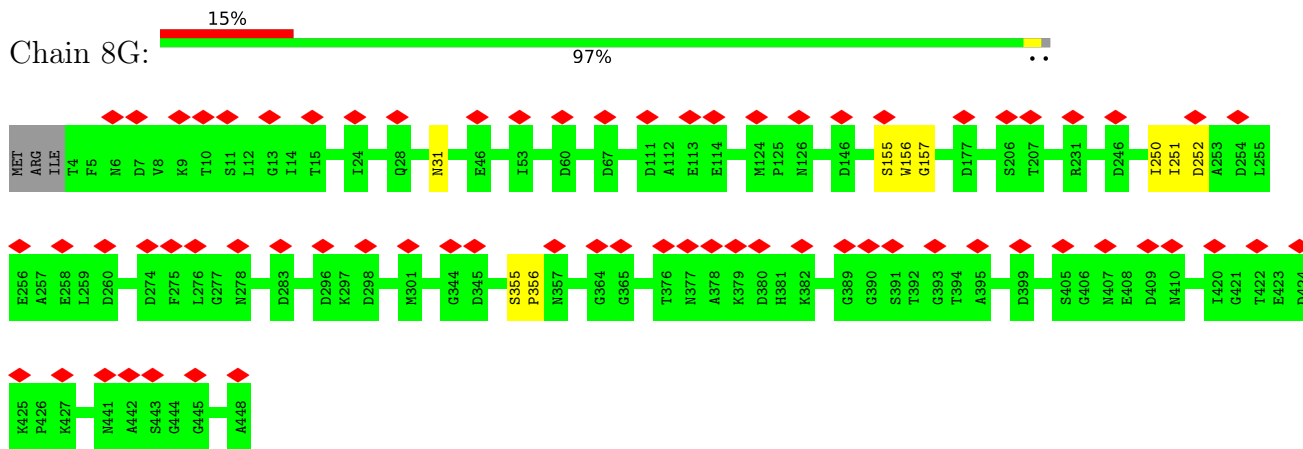
• Molecule 1: Major capsid protein



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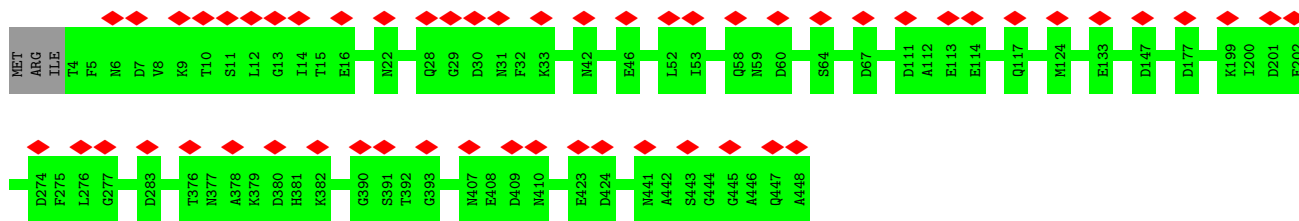


• Molecule 1: Major capsid protein

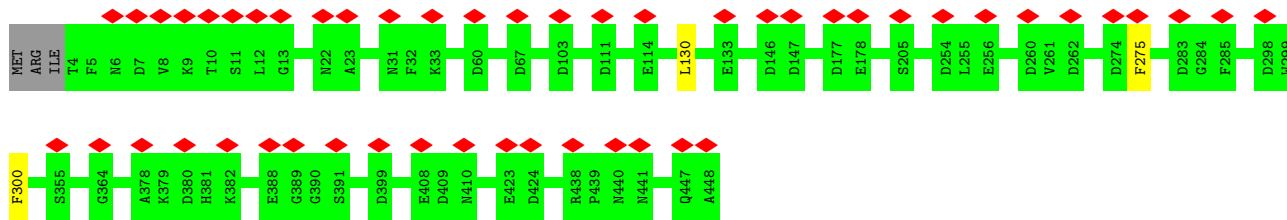


• Molecule 1: Major capsid protein

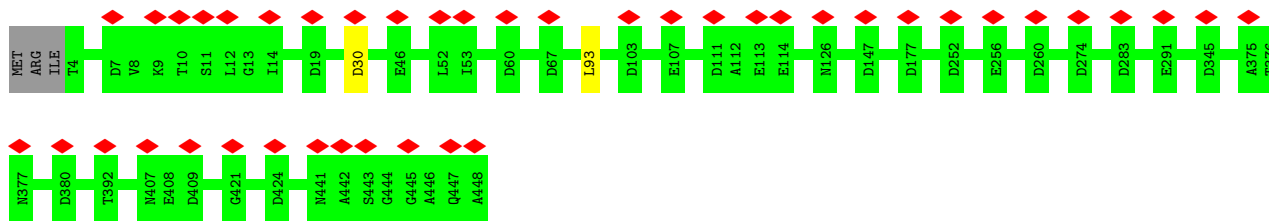




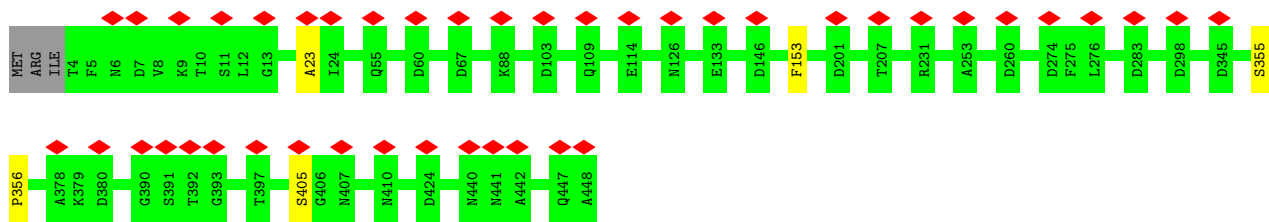
• Molecule 1: Major capsid protein



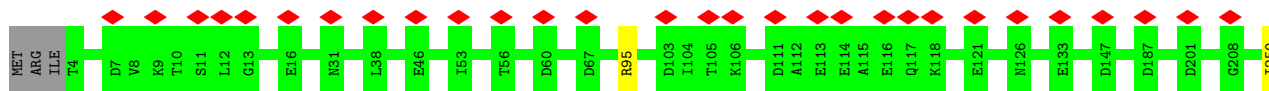
• Molecule 1: Major capsid protein

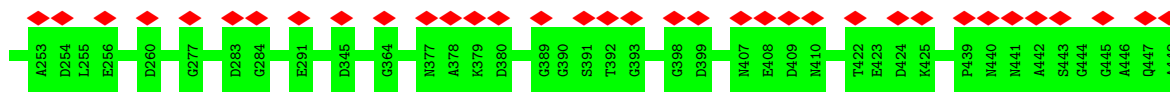


• Molecule 1: Major capsid protein



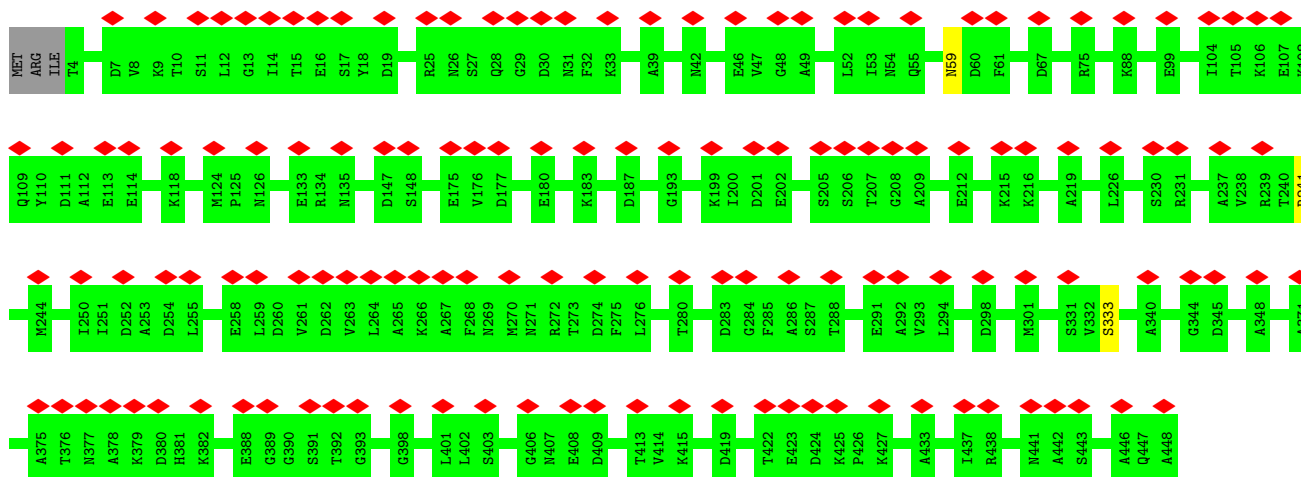
• Molecule 1: Major capsid protein





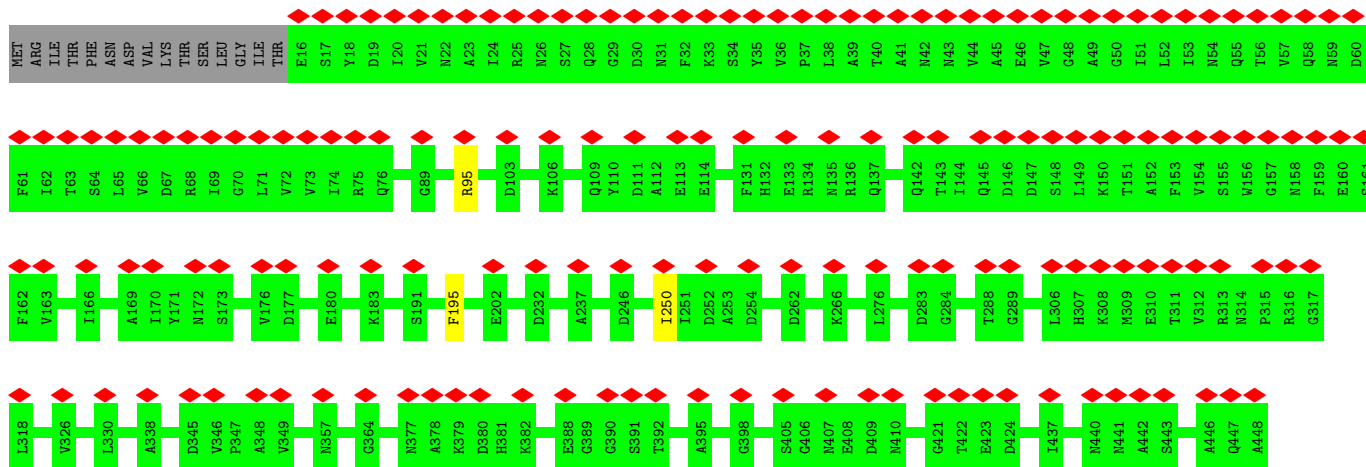
- Molecule 1: Major capsid protein

Chain 9B: 31% 99%



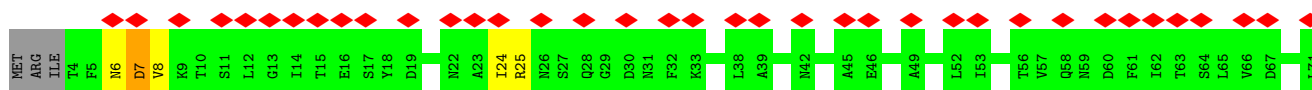
- Molecule 1: Major capsid protein

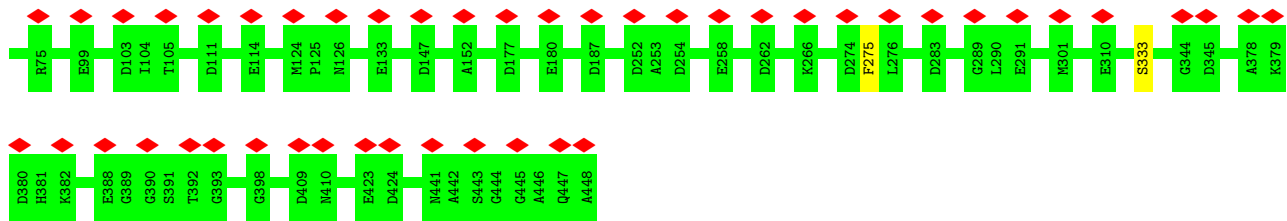
Chain 1M: 37% 96%



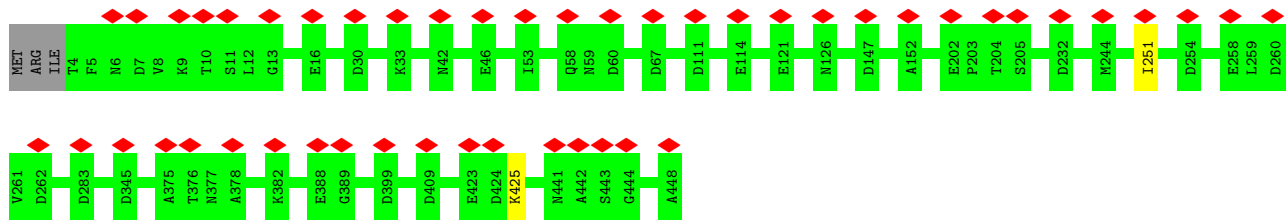
- Molecule 1: Major capsid protein

Chain 1N: 19% 98%

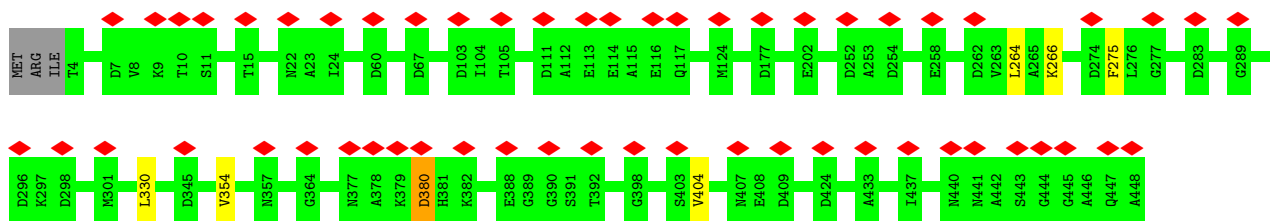




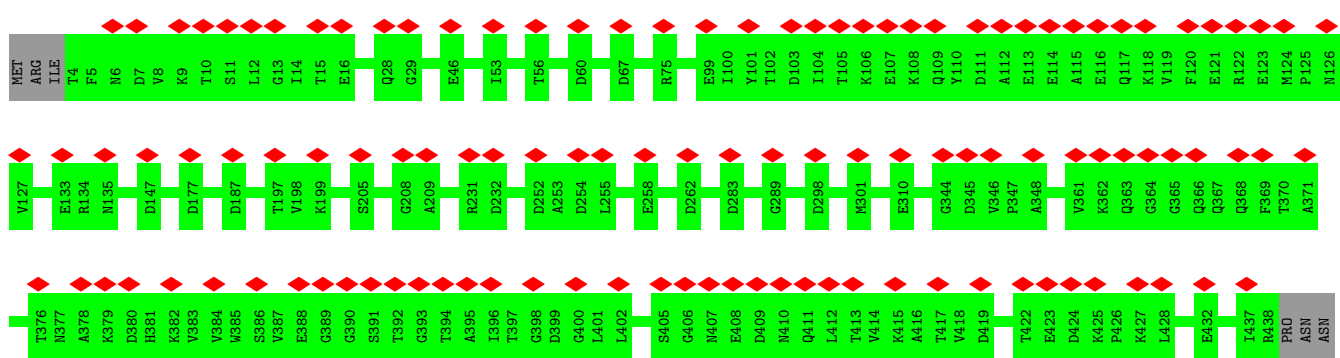
• Molecule 1: Major capsid protein



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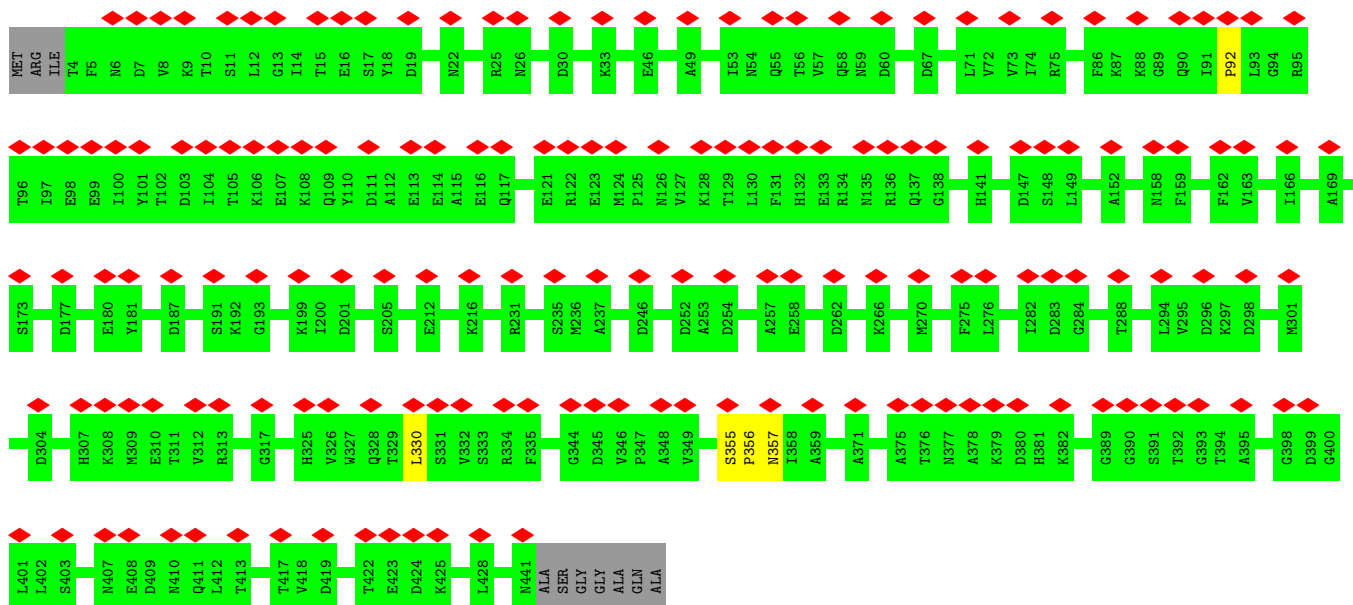


• Molecule 1: Major capsid protein

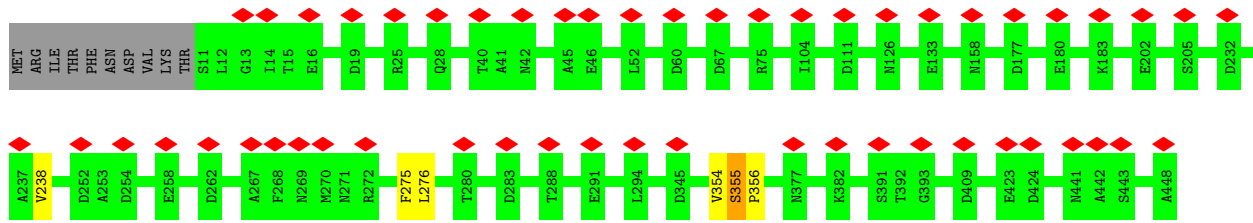


• Molecule 1: Major capsid protein

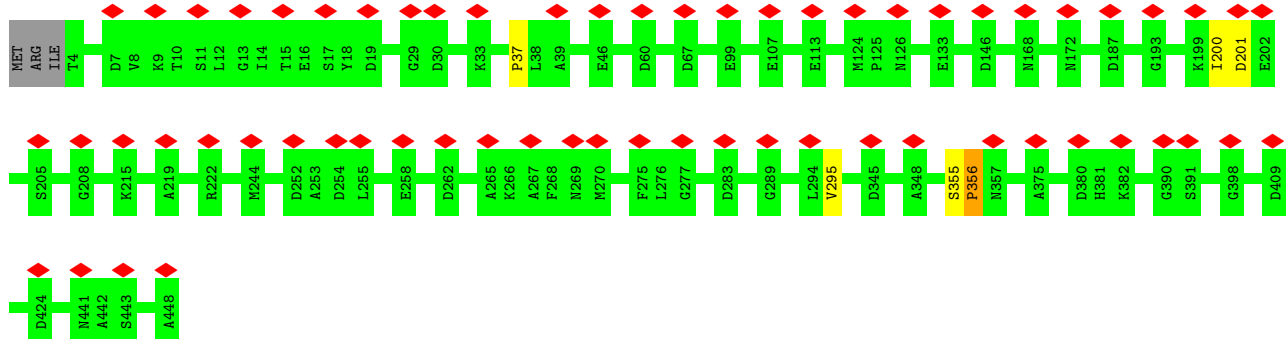




• Molecule 1: Major capsid protein

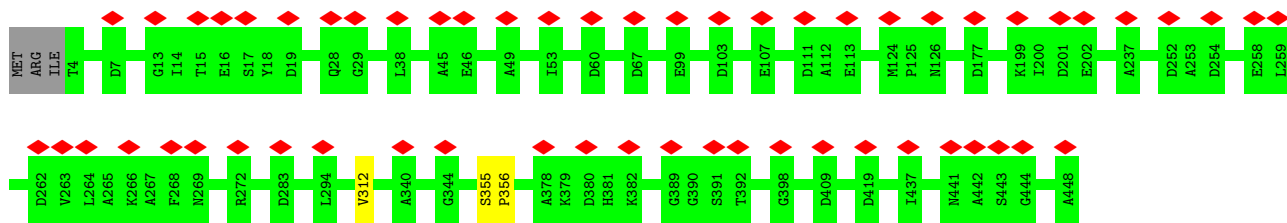


• Molecule 1: Major capsid protein

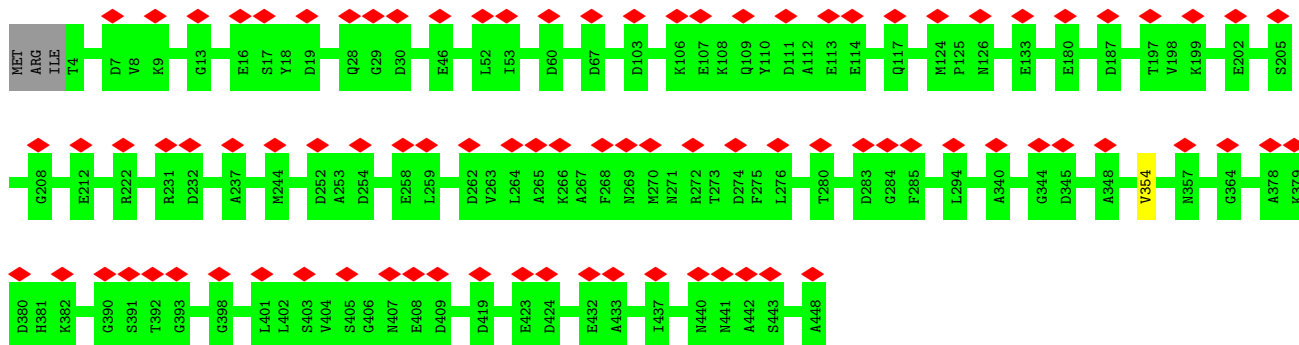


• Molecule 1: Major capsid protein

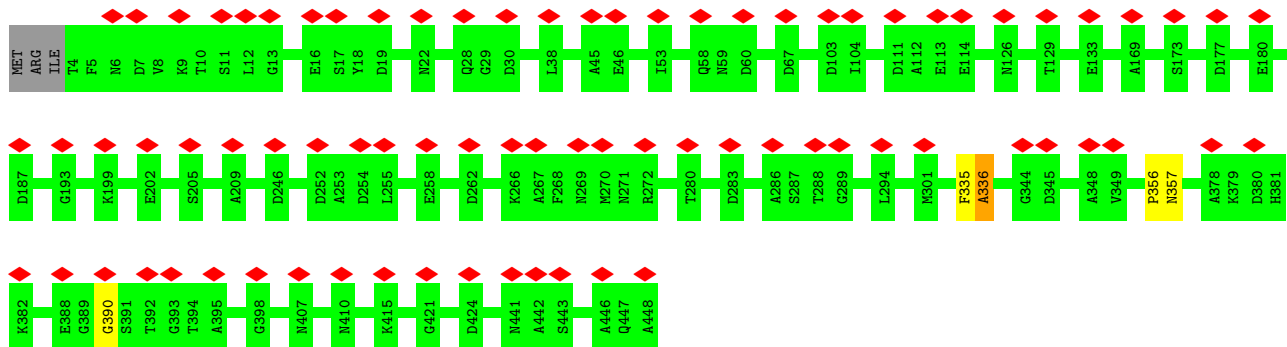




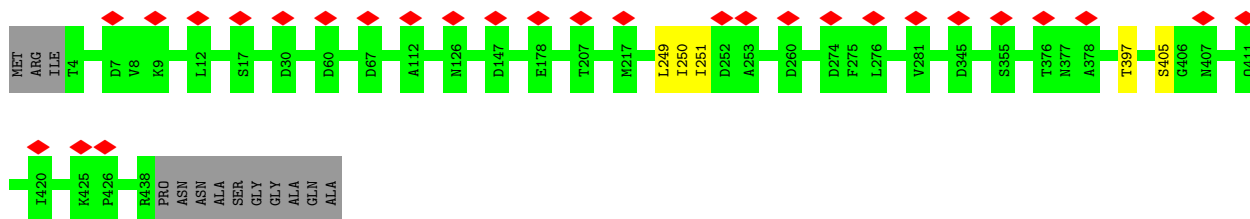
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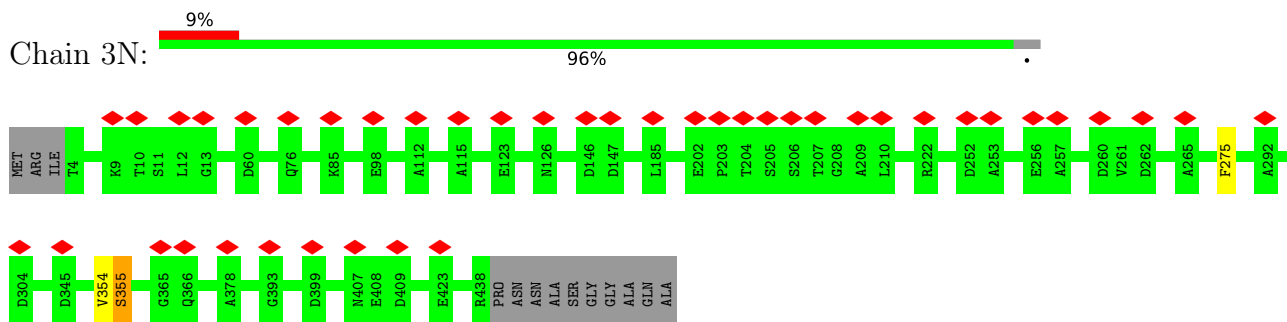
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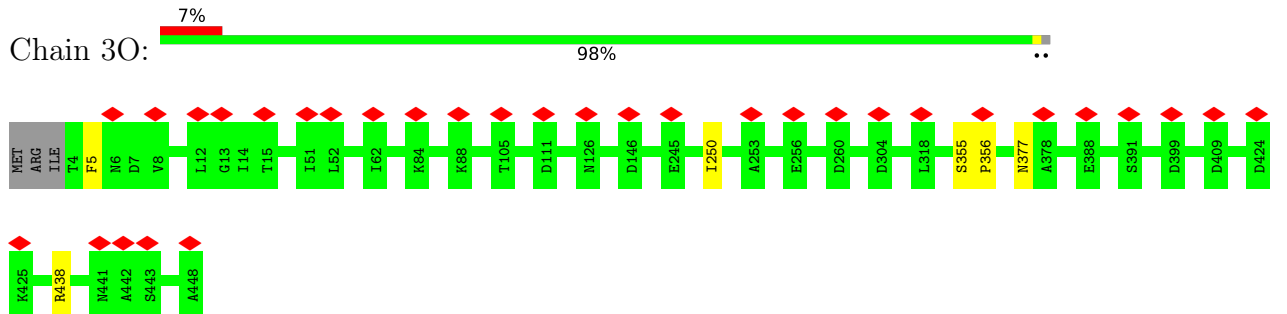
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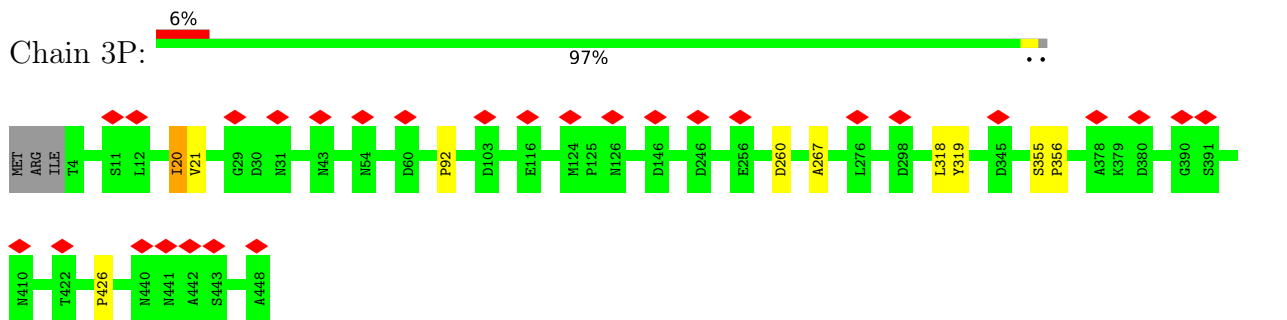
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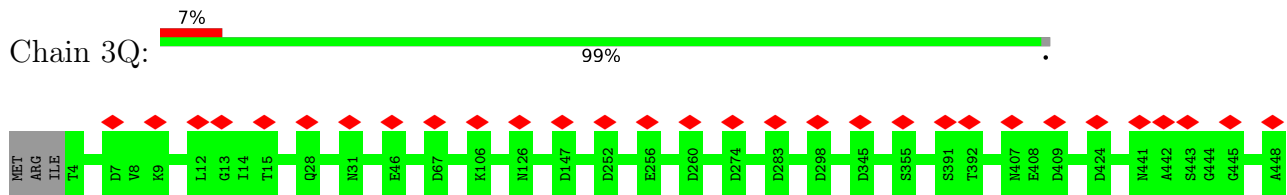
• Molecule 1: Major capsid protein



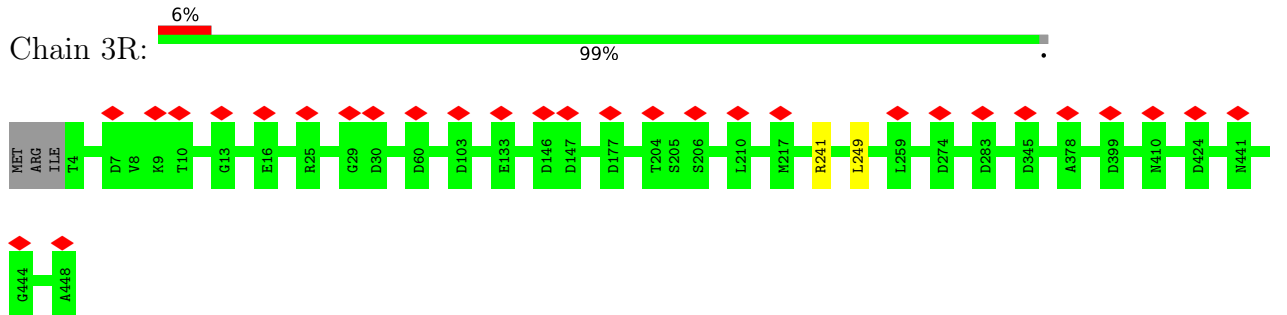
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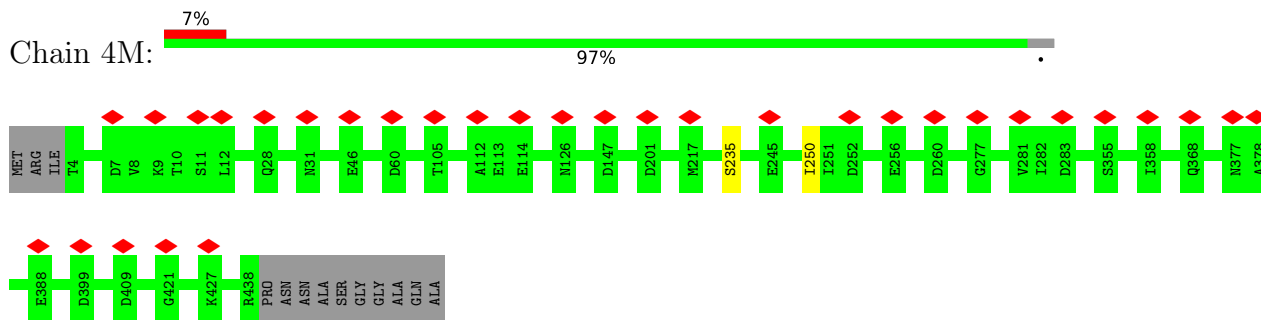
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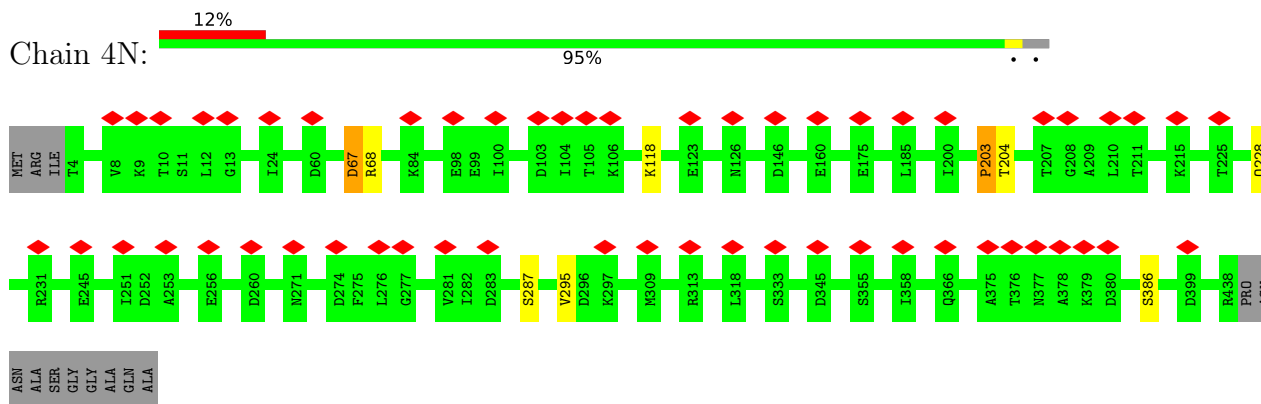
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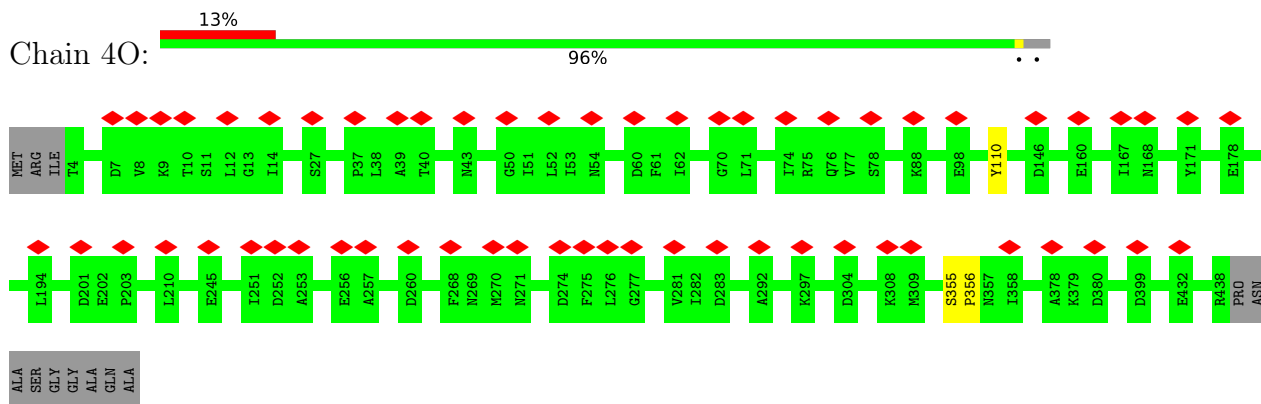
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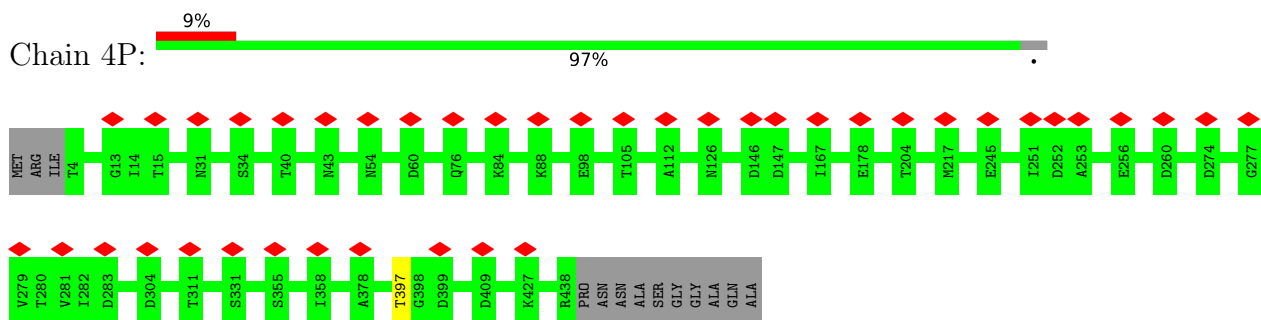
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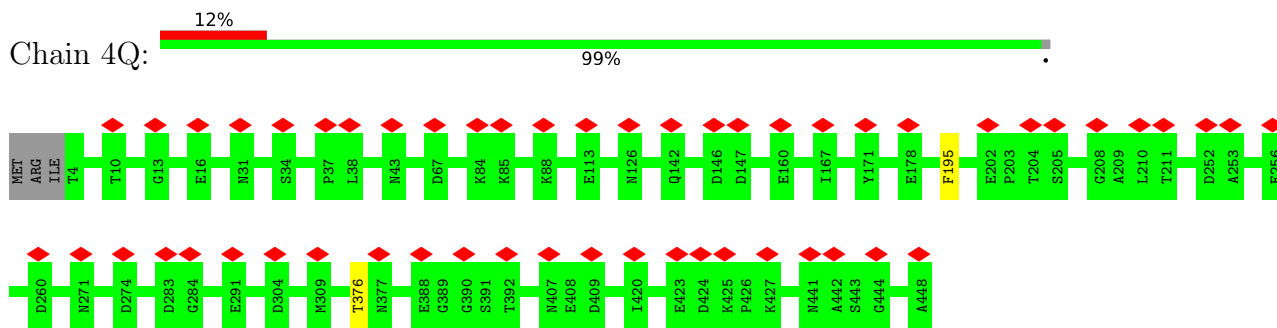
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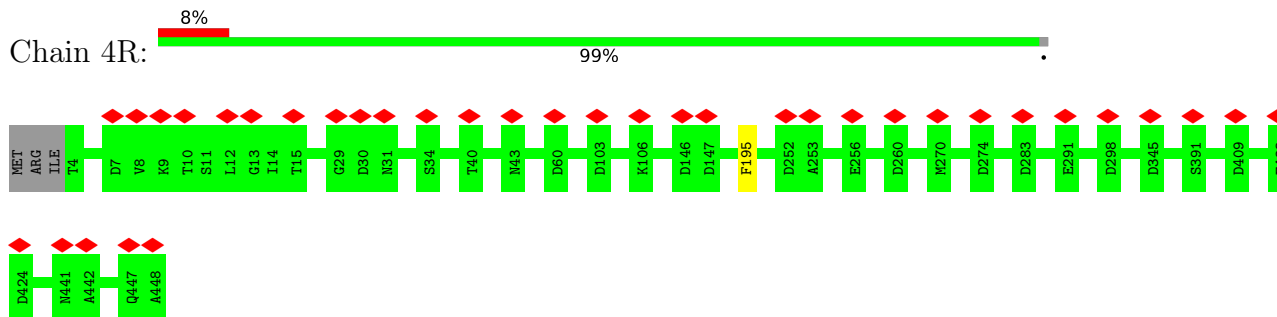
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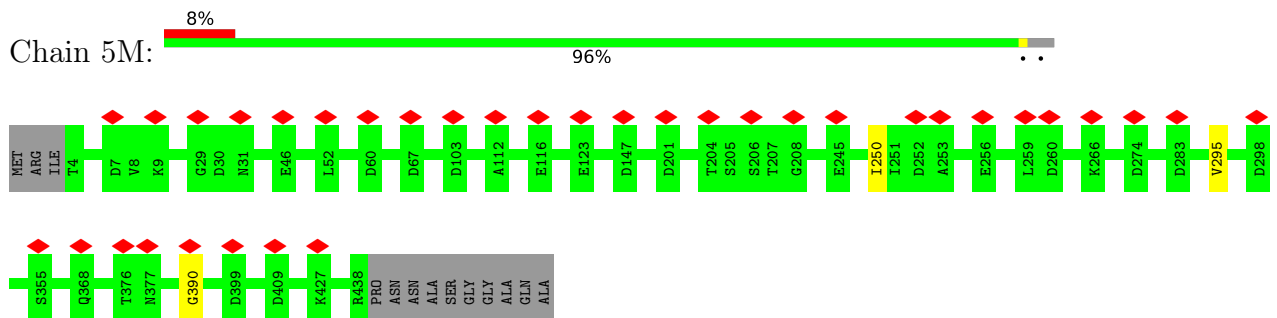
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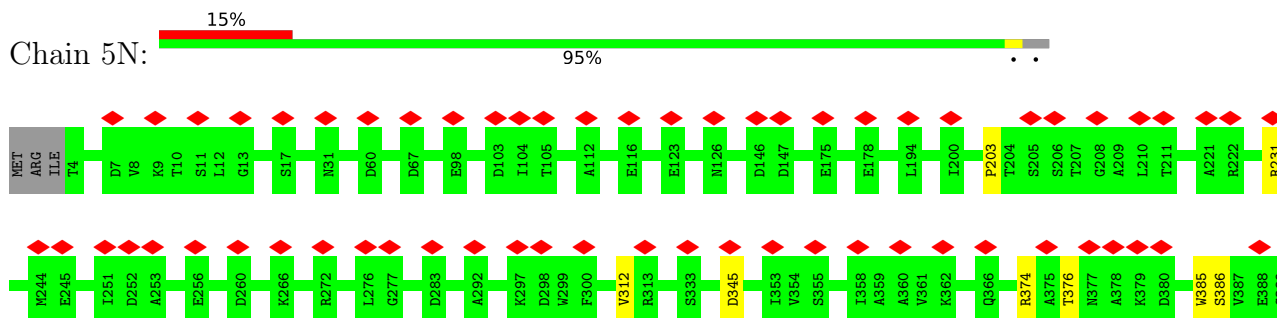
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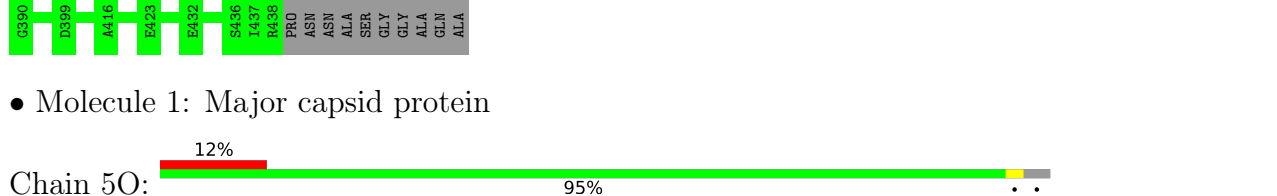
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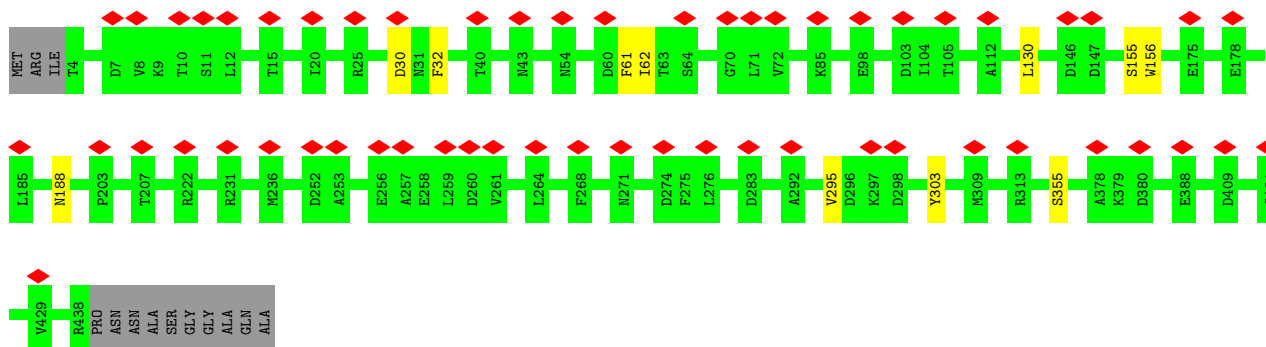
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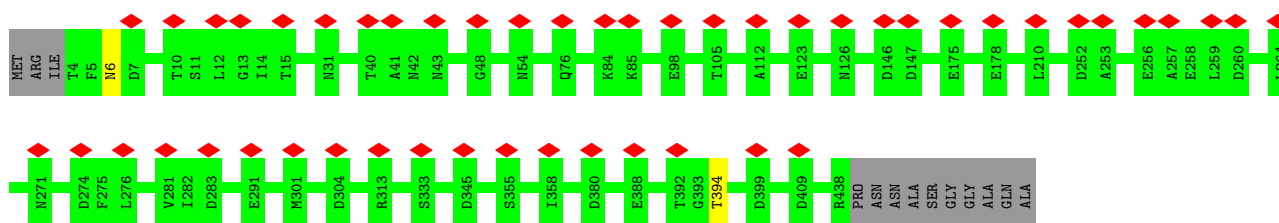
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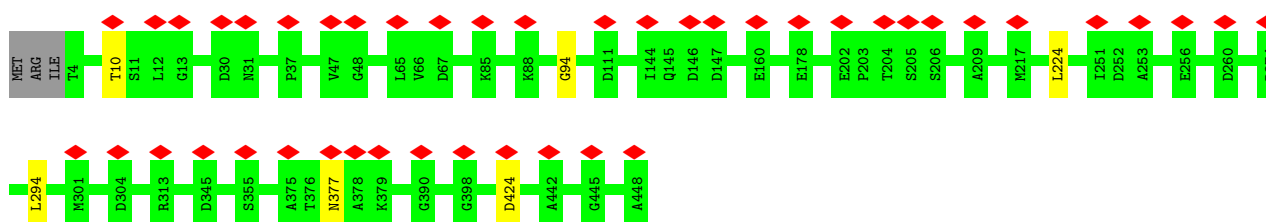
• Molecule 1: Major capsid protein



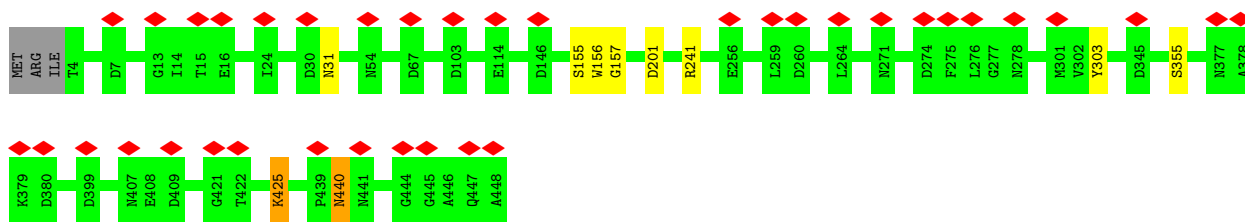
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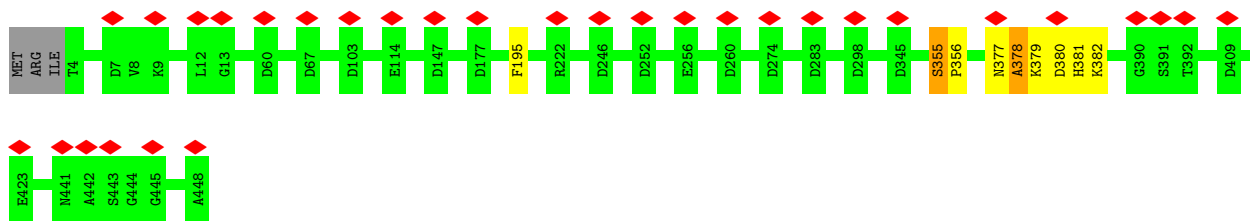


• Molecule 1: Major capsid protein

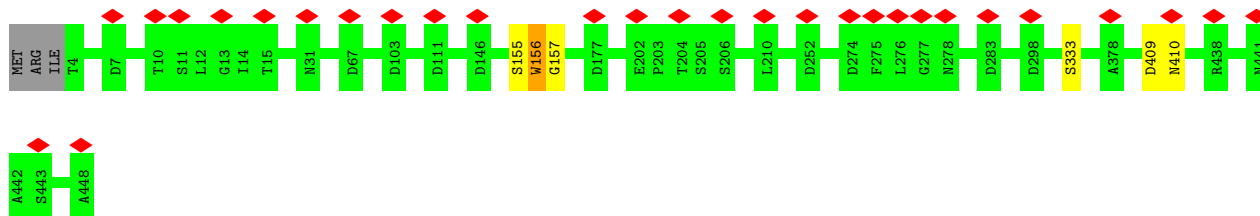


• Molecule 1: Major capsid protein

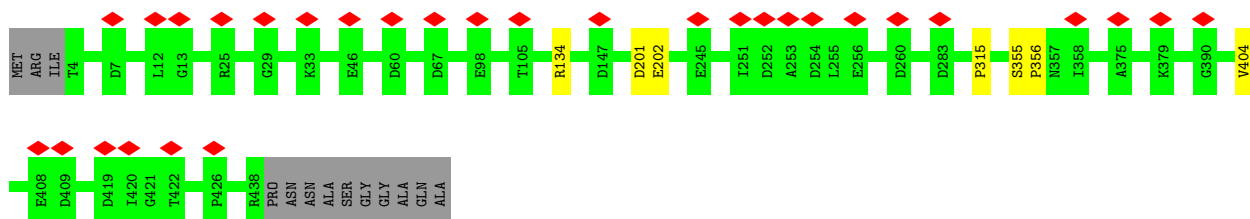




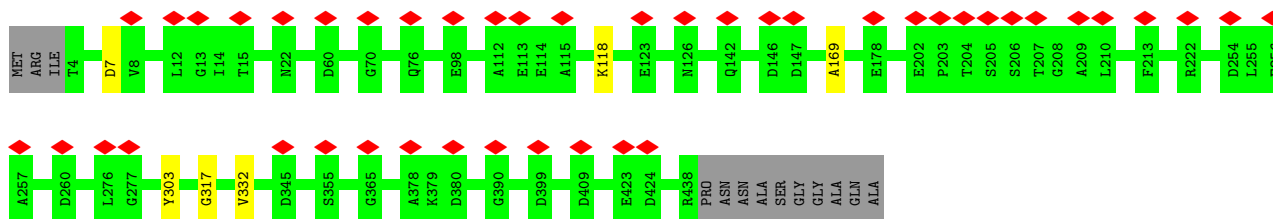
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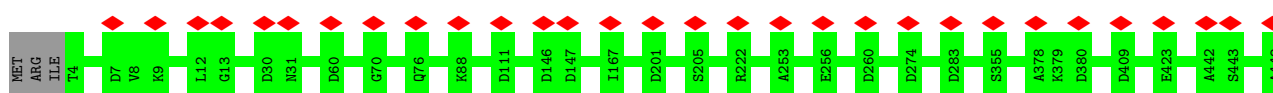
• Molecule 1: Major capsid protein



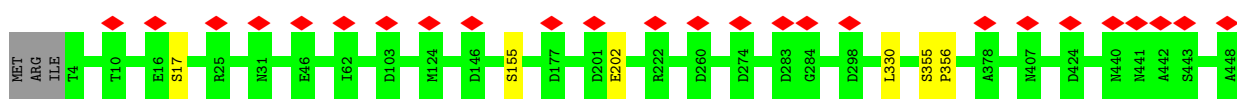
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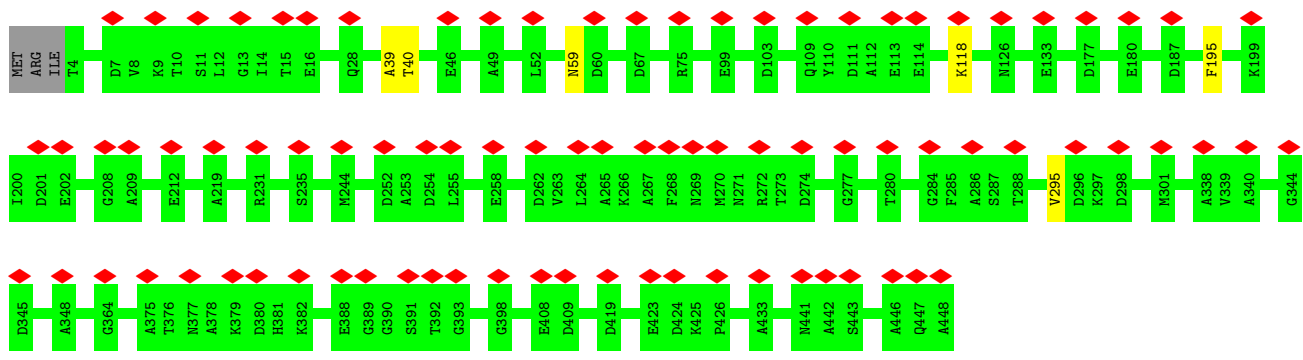
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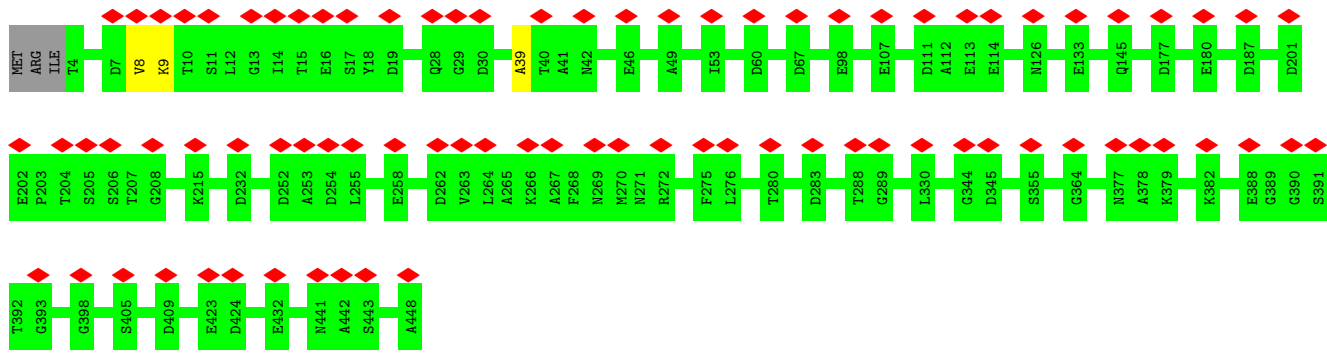
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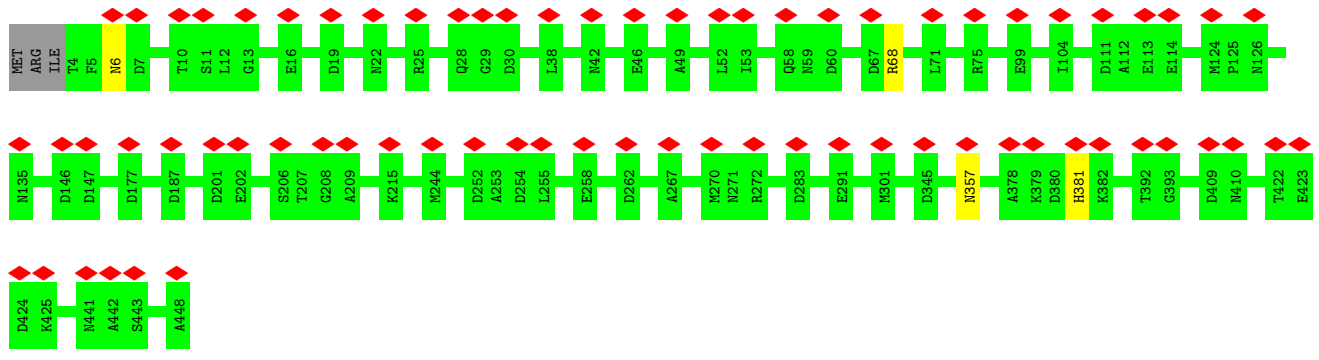
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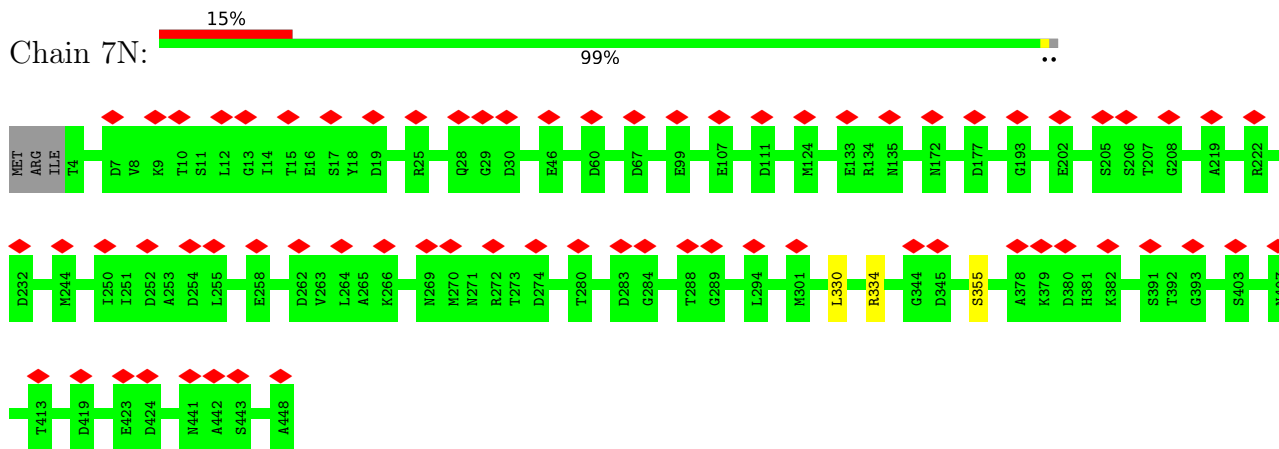
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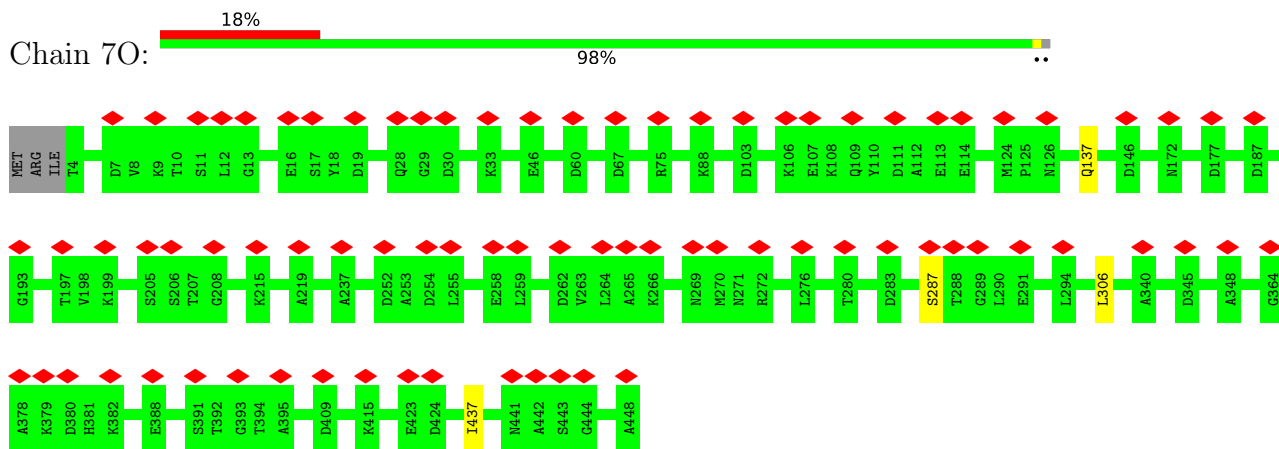
• Molecule 1: Major capsid protein



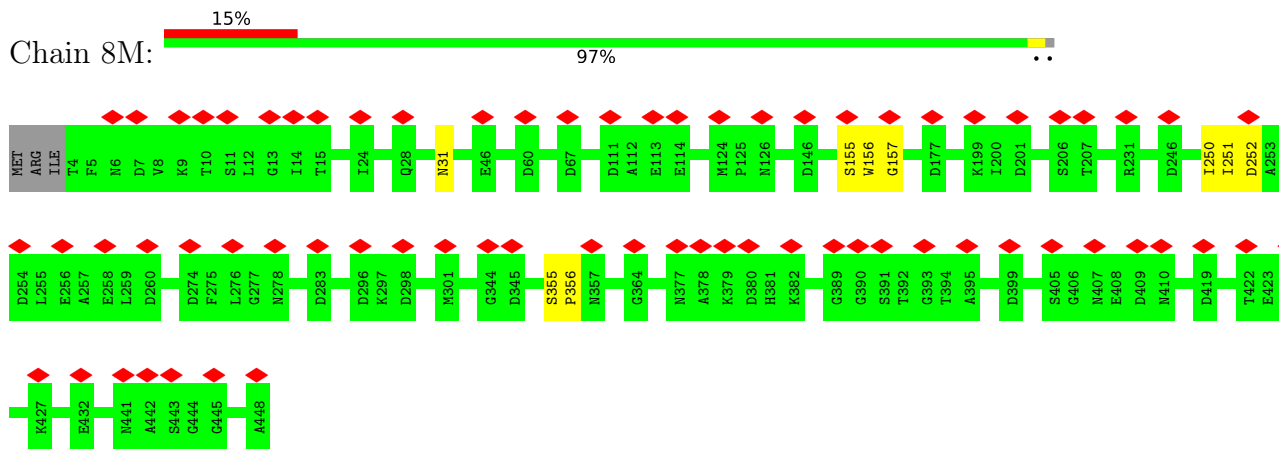
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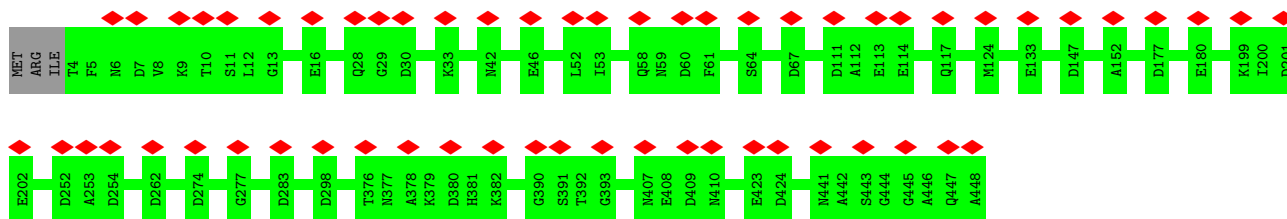


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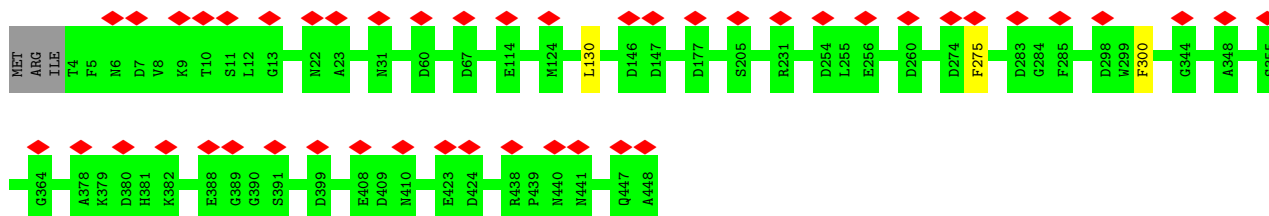


• Molecule 1: Major capsid protein

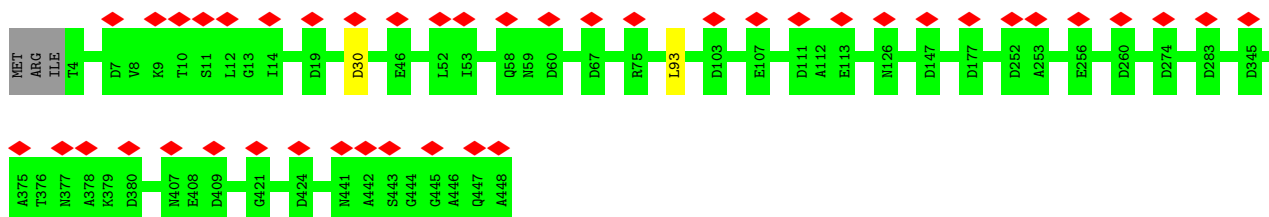




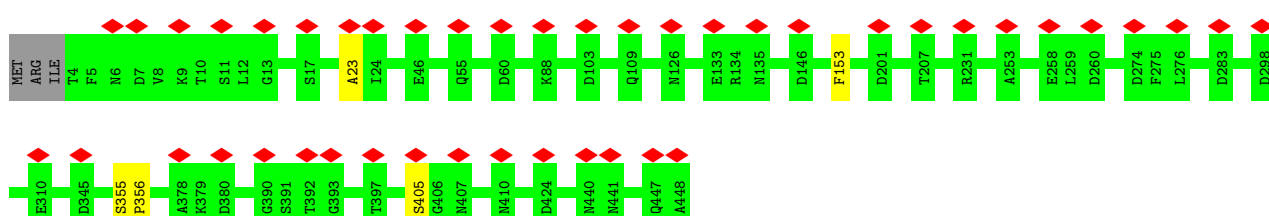
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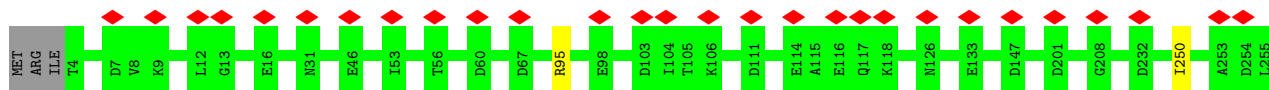
• Molecule 1: Major capsid protein

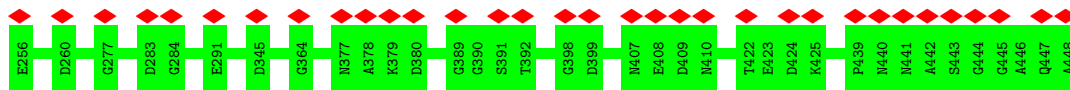


• Molecule 1: Major capsid protein

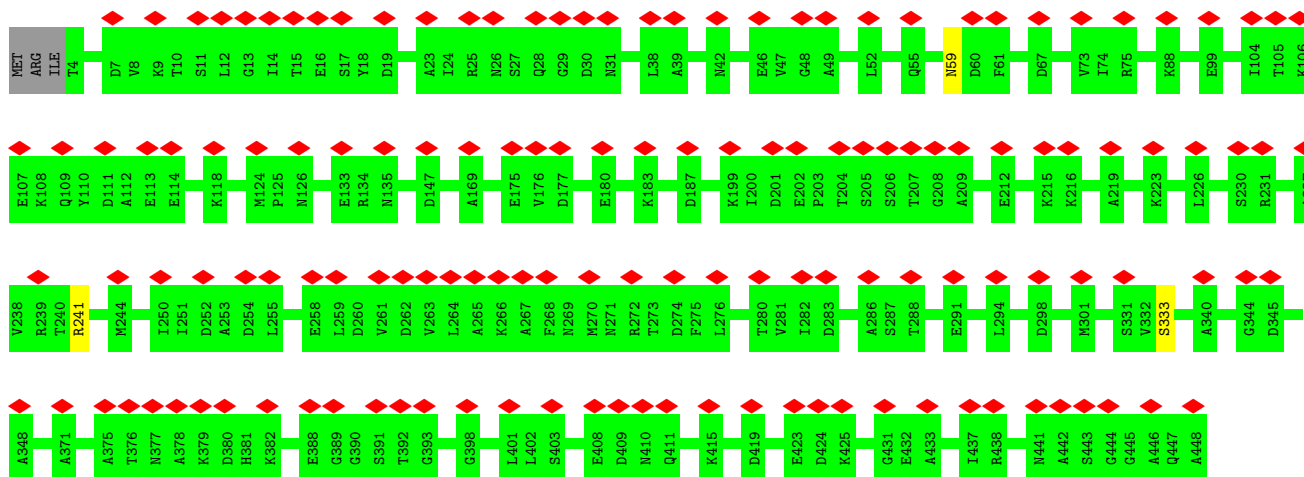


• Molecule 1: Major capsid protein

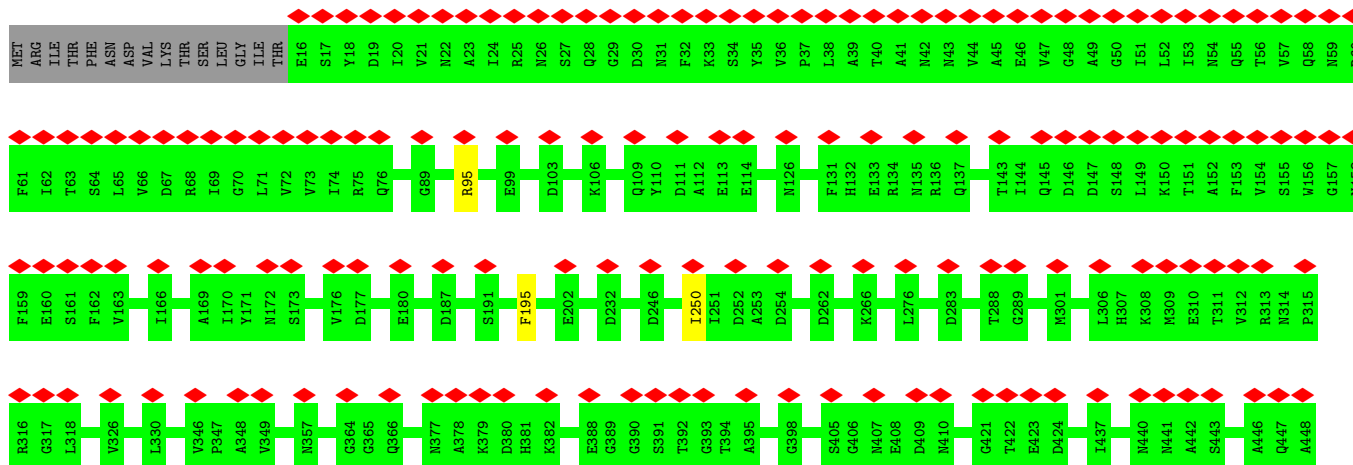




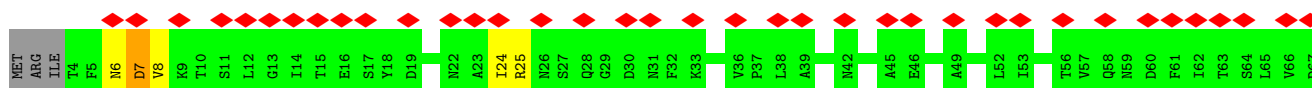
• Molecule 1: Major capsid protein

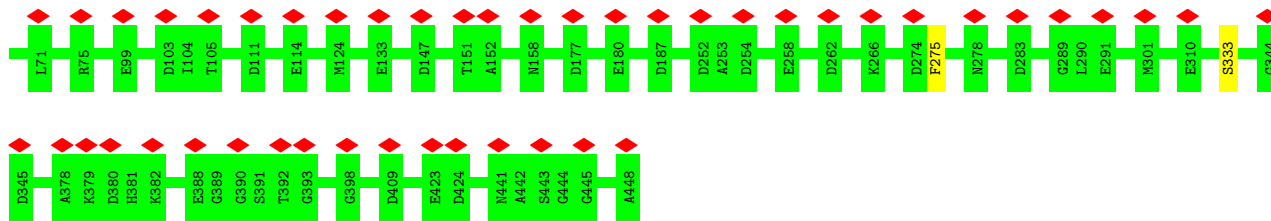


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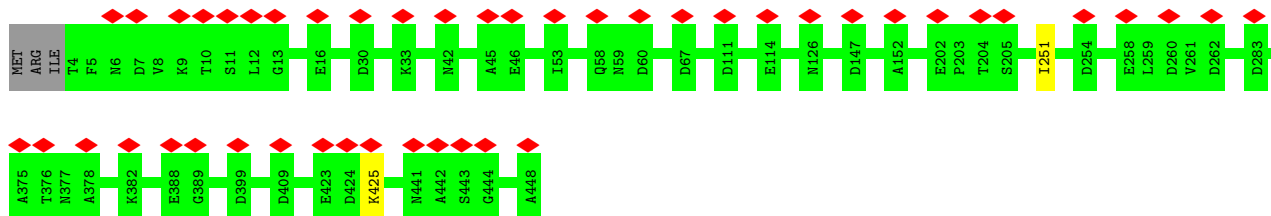


• Molecule 1: Major capsid protein

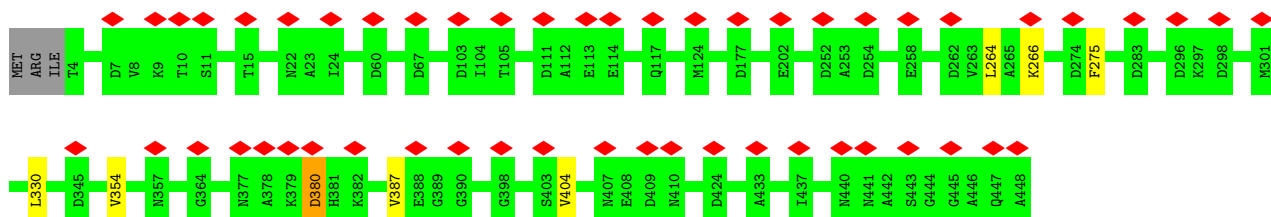




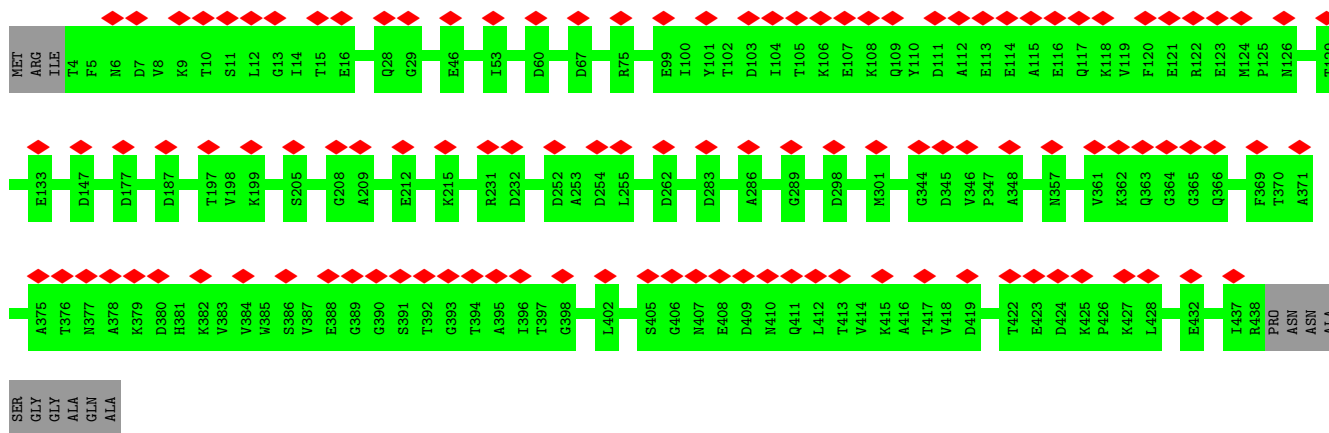
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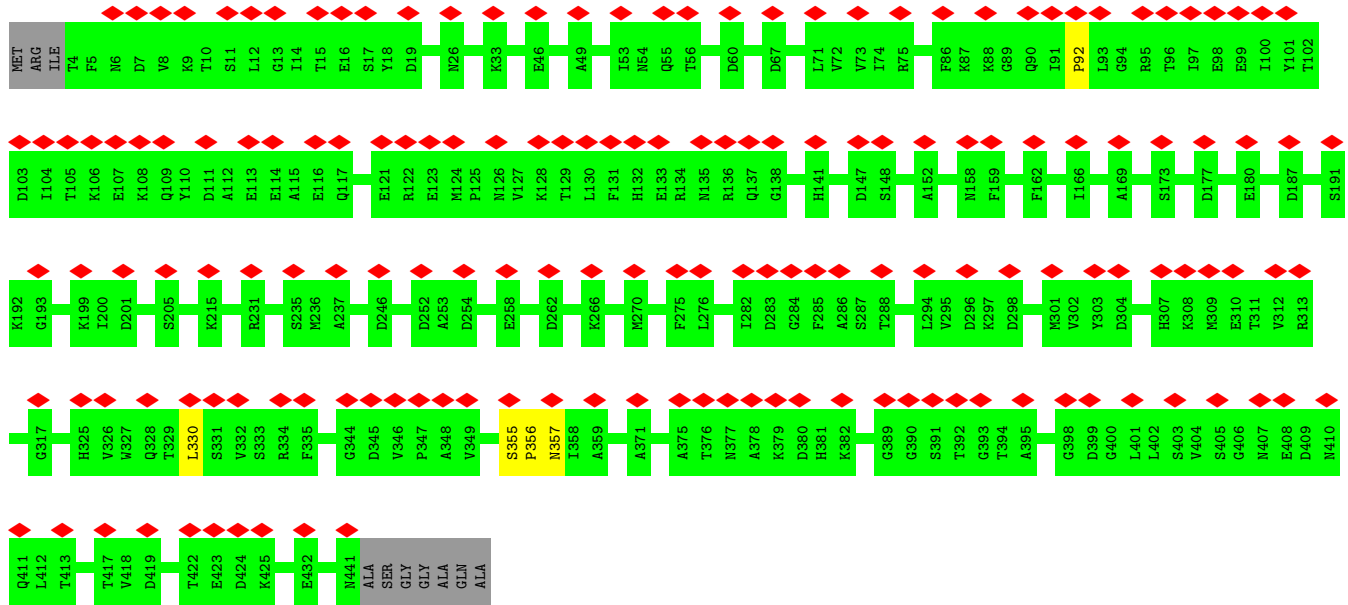


• Molecule 1: Major capsid protein

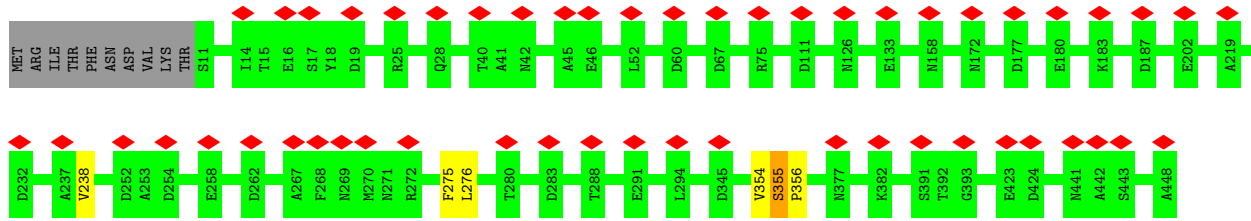


• Molecule 1: Major capsid protein

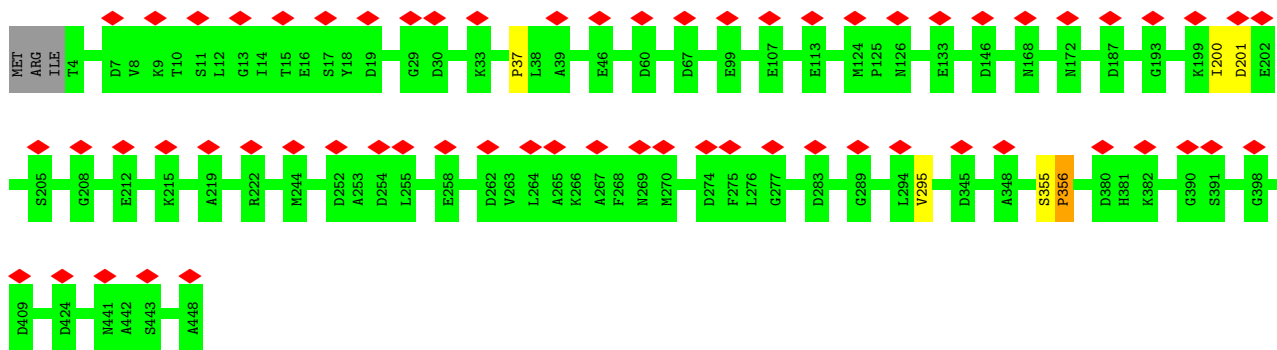




• Molecule 1: Major capsid protein

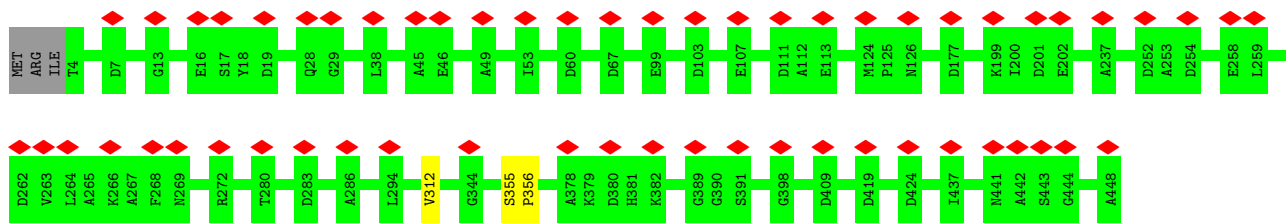


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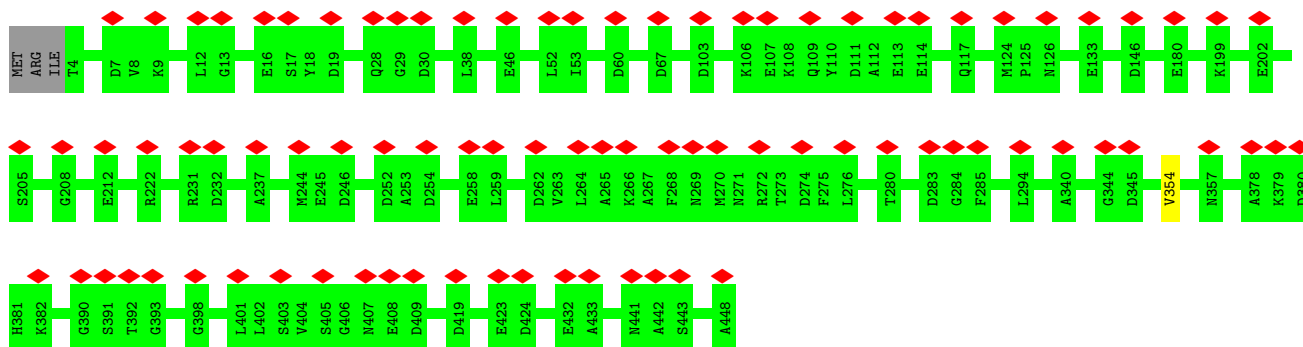


• Molecule 1: Major capsid protein

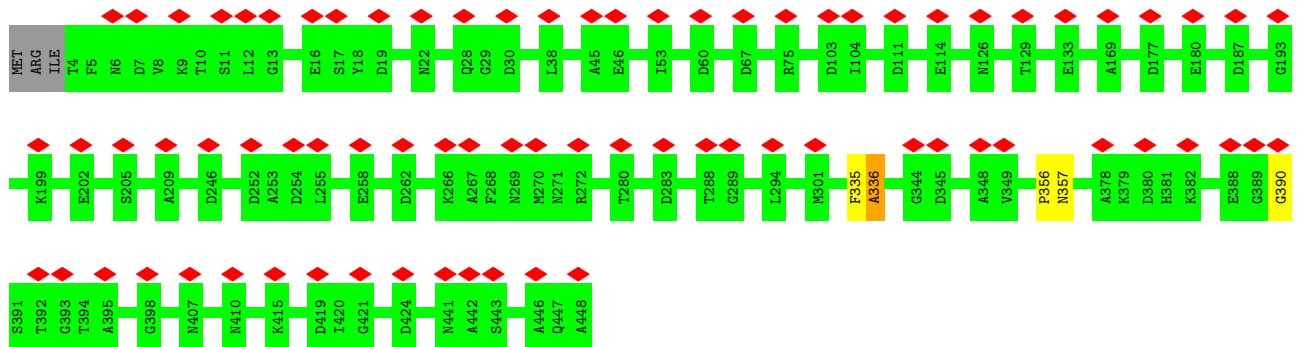




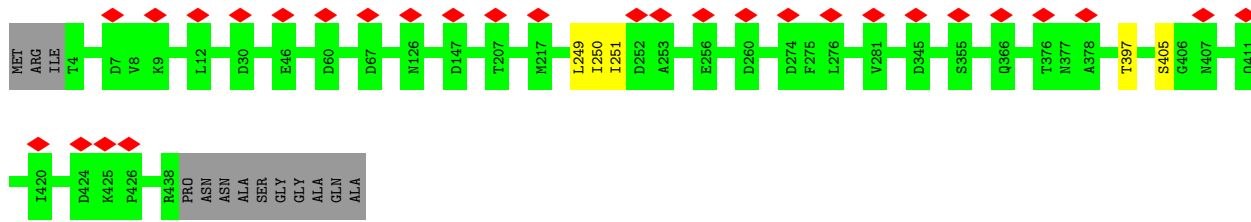
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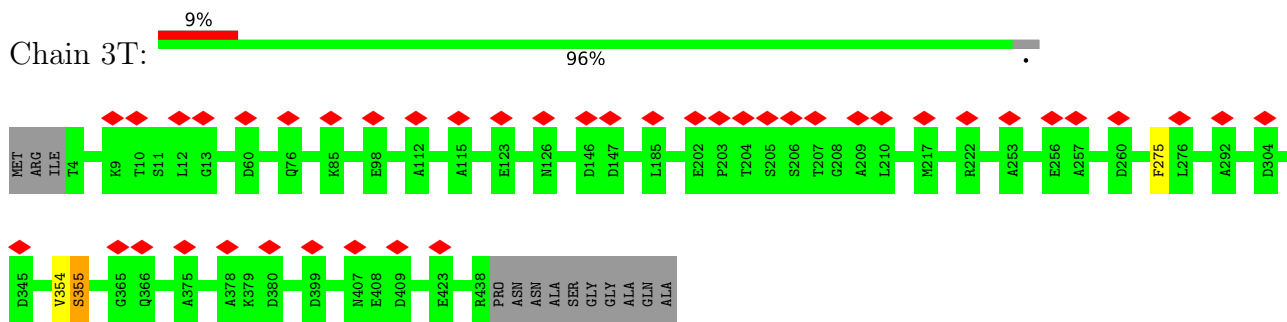
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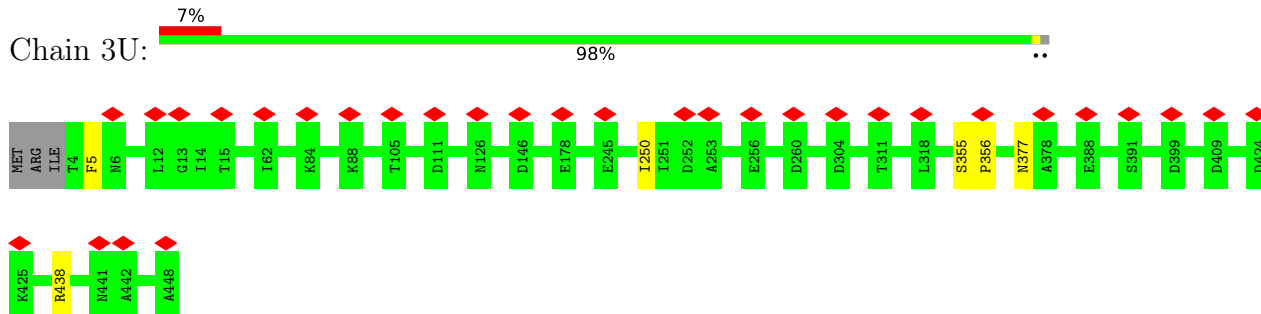
• Molecule 1: Major capsid protein



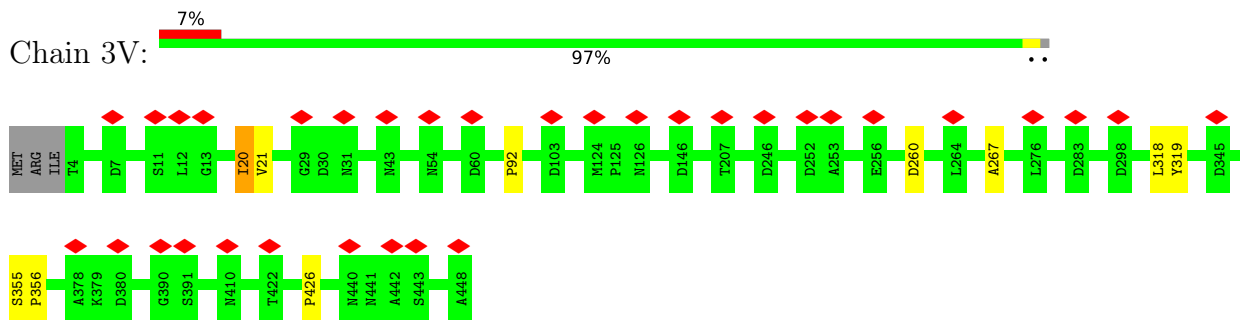
• Molecule 1: Major capsid protein



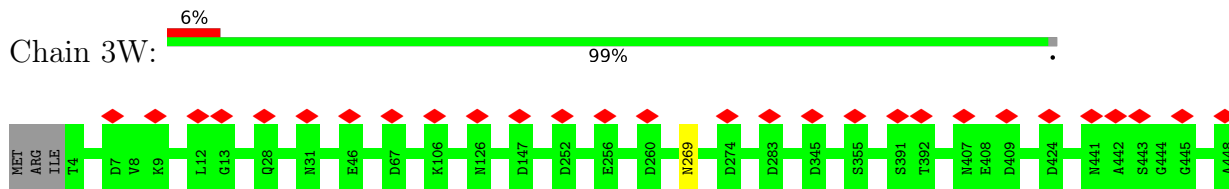
• Molecule 1: Major capsid protein



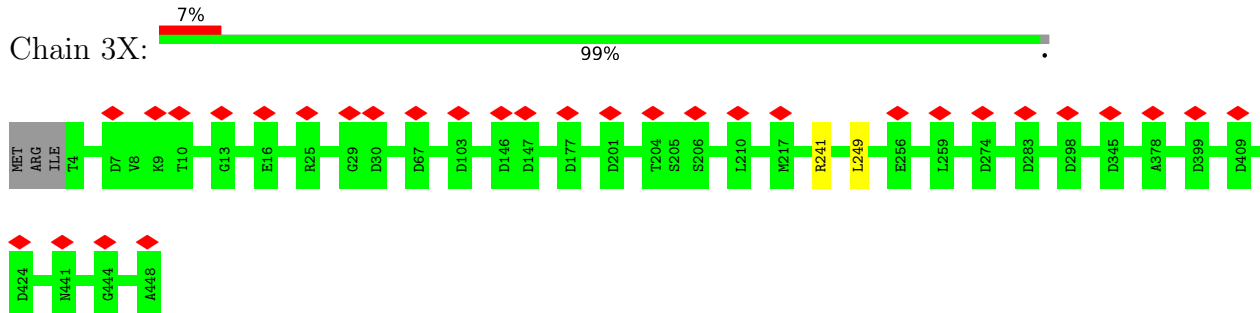
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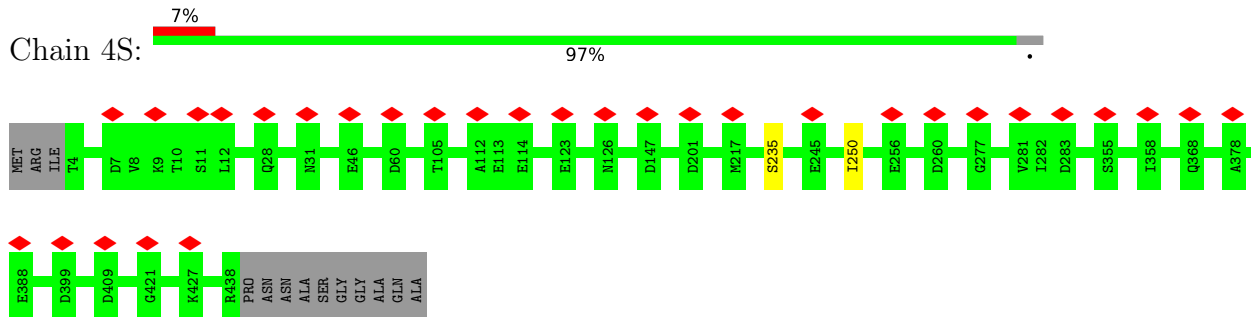
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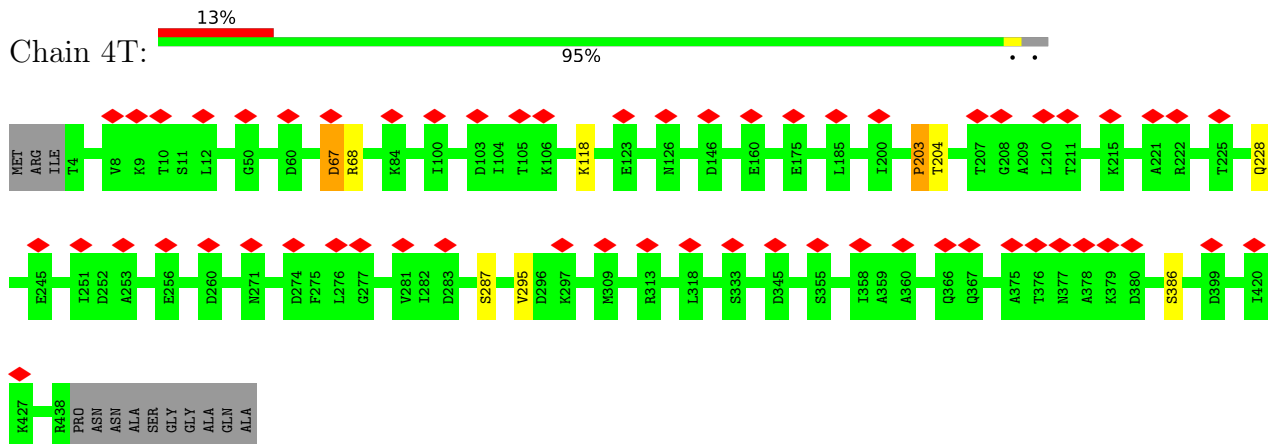
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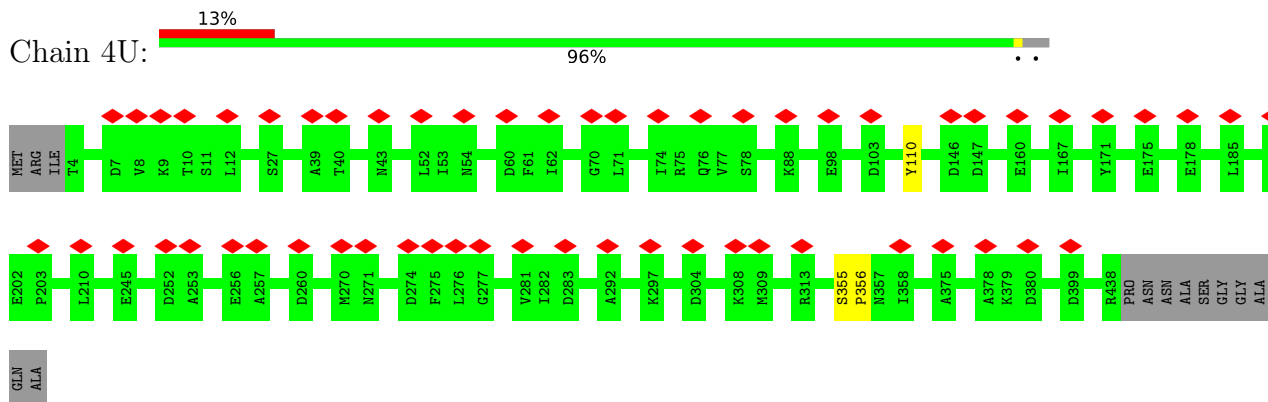
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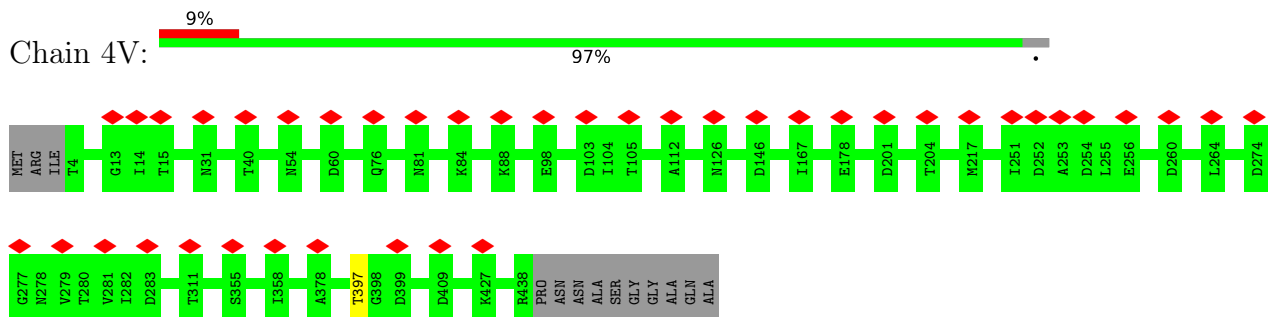
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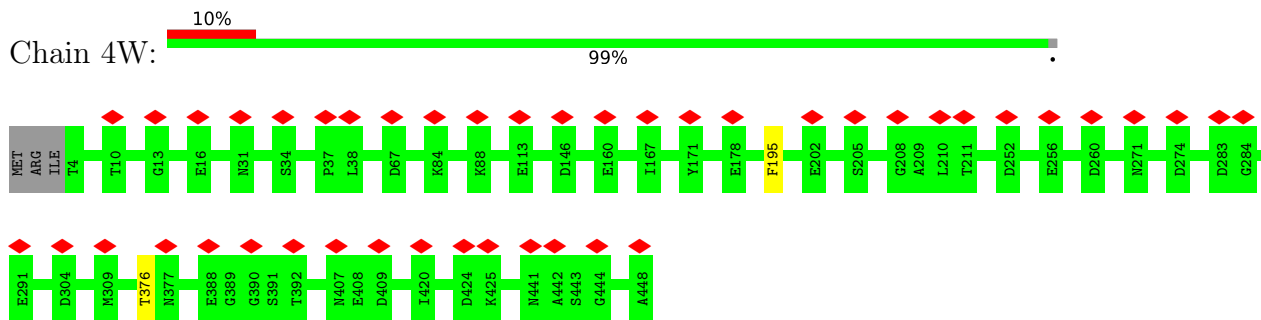
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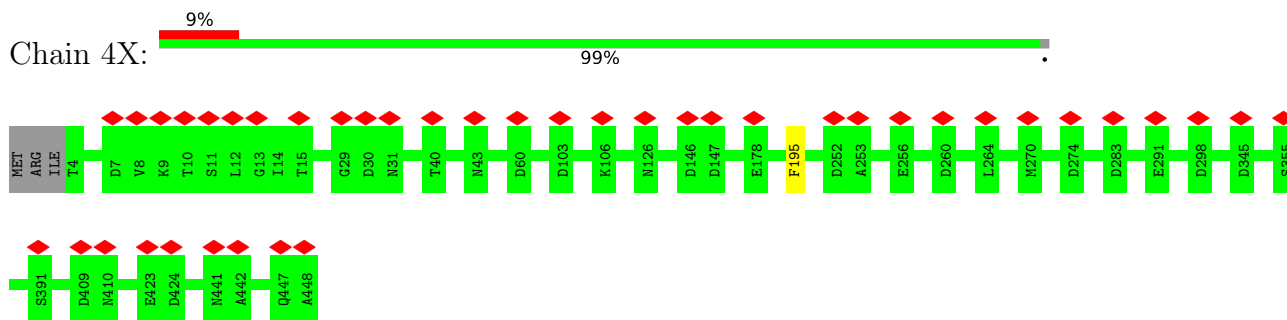
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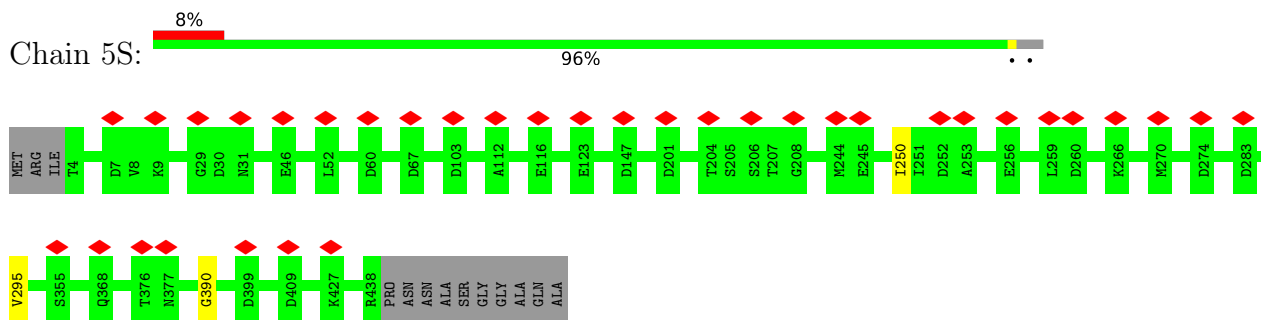
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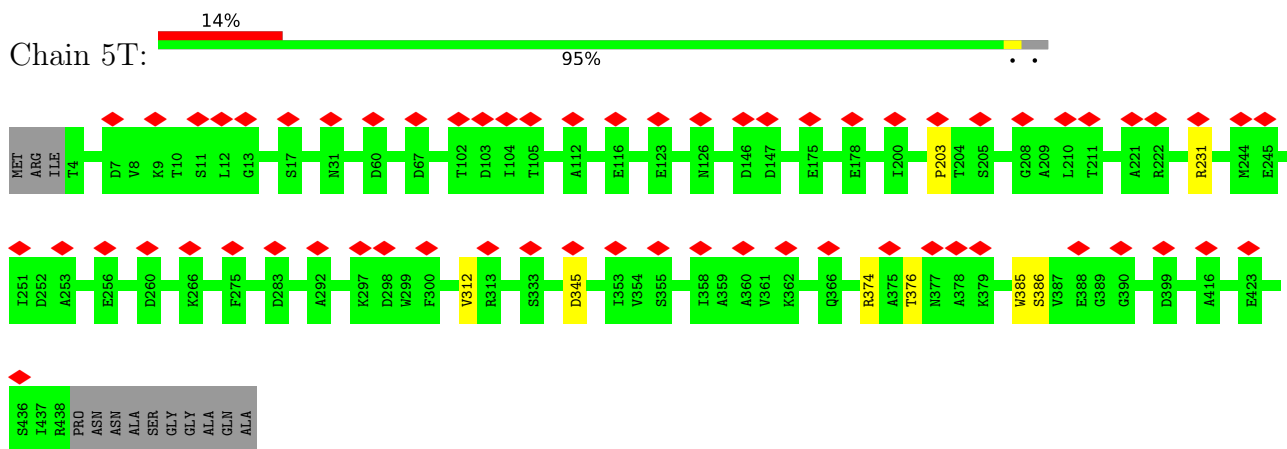
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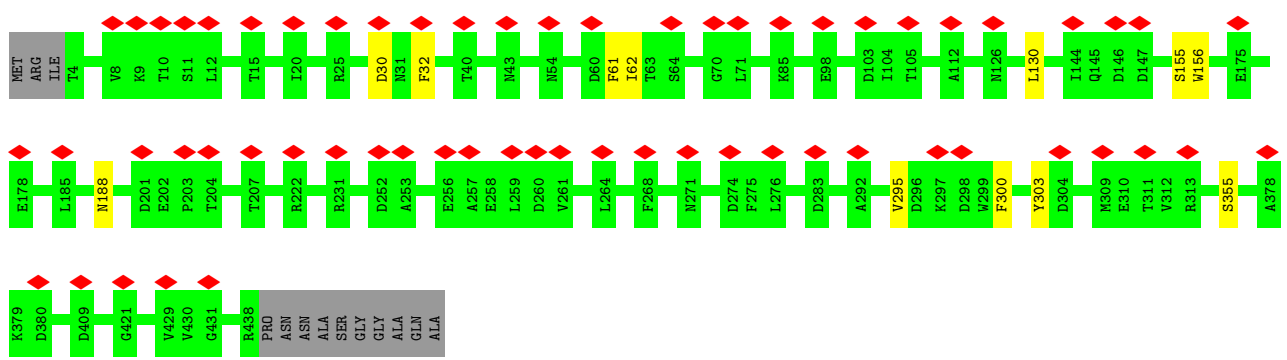
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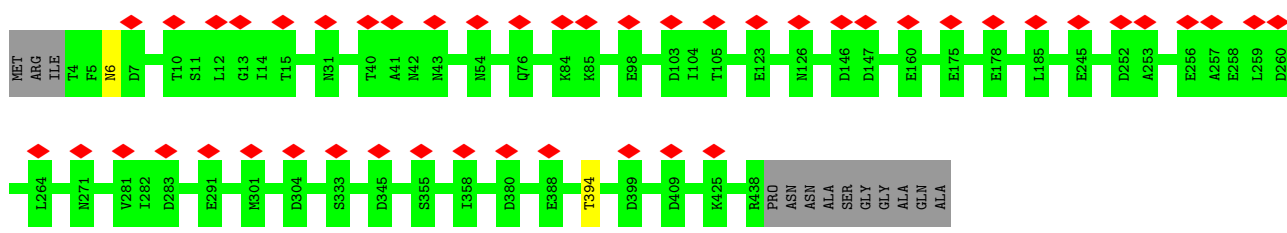
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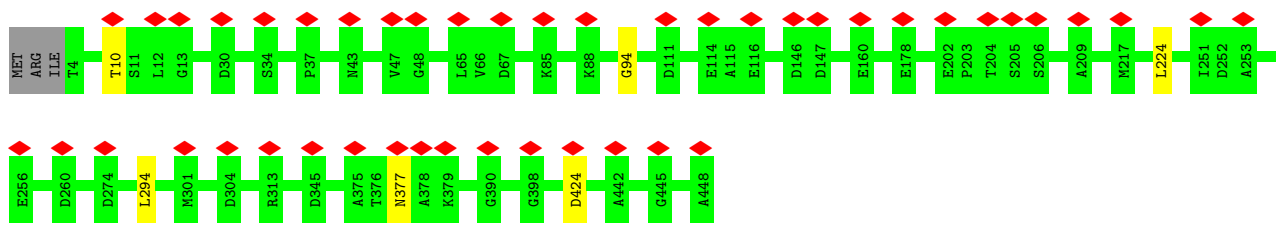
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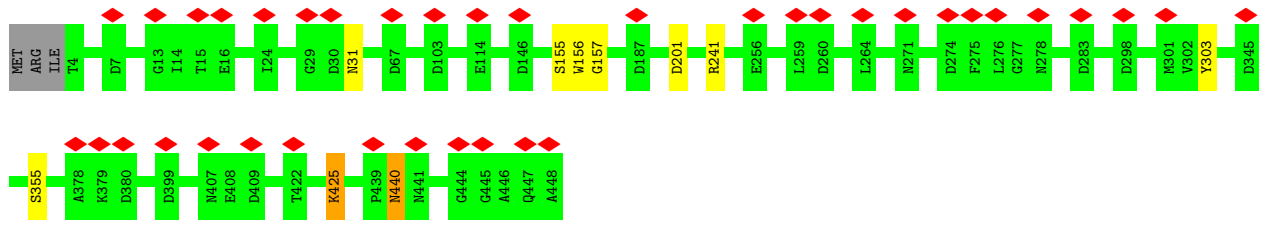
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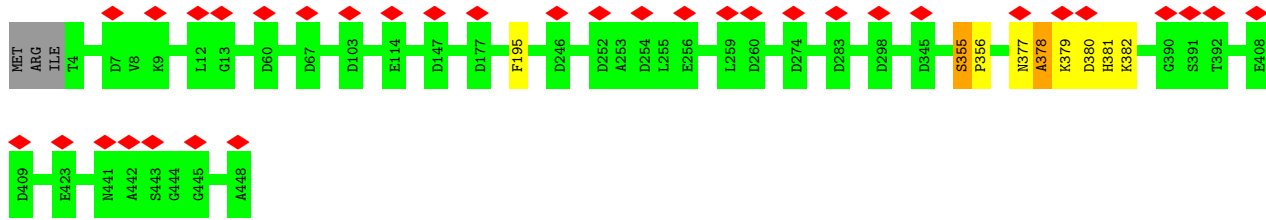


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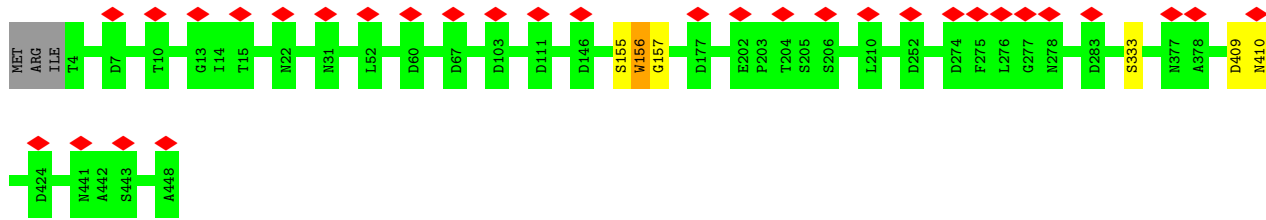


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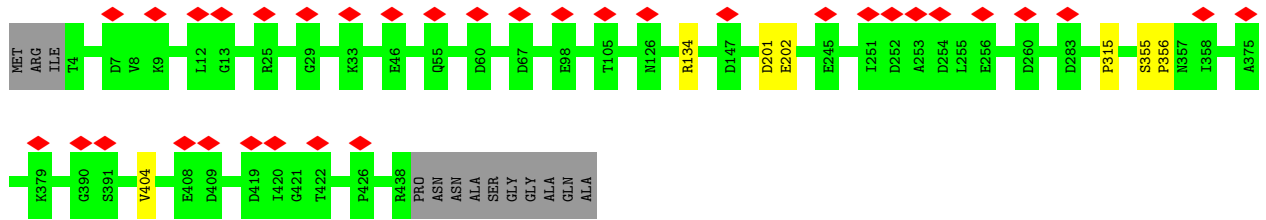




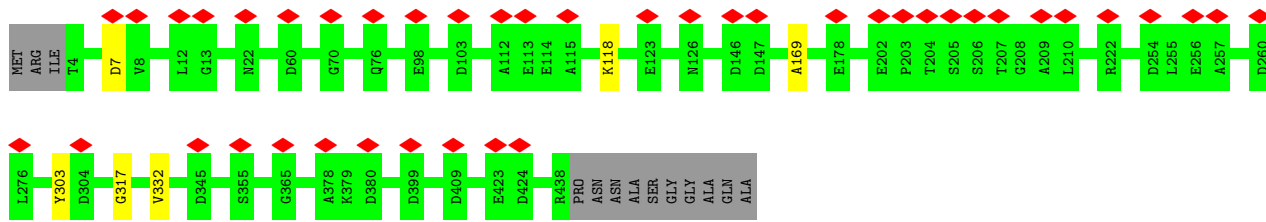
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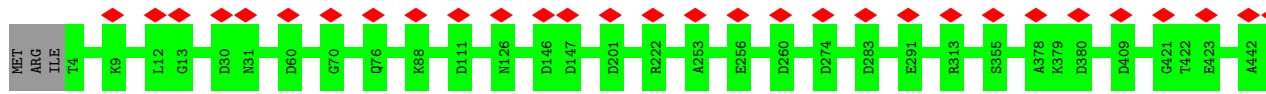
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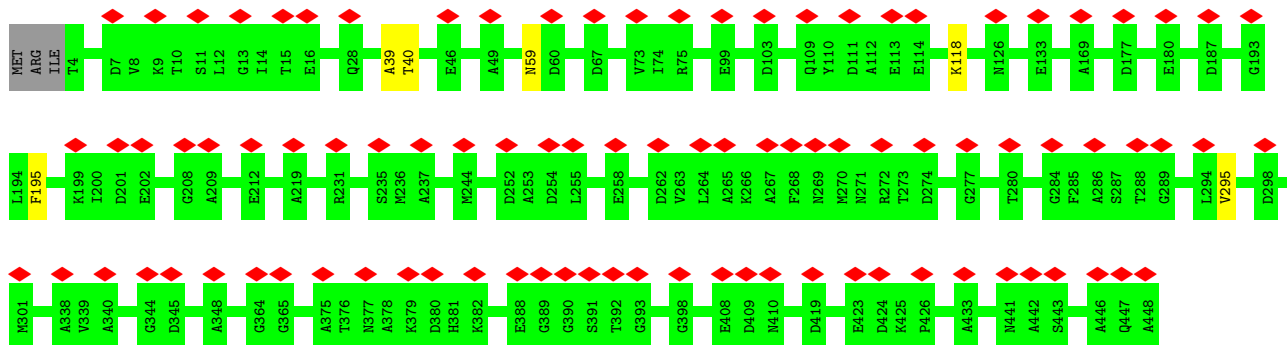




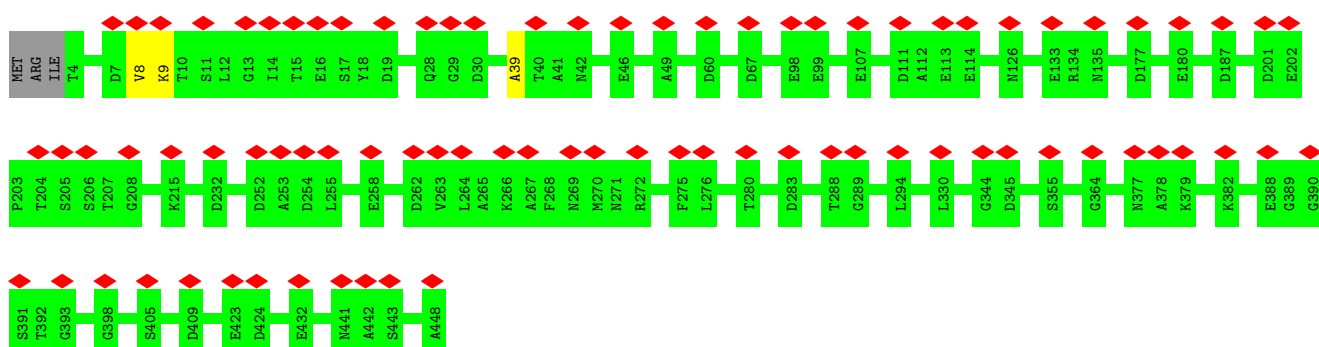
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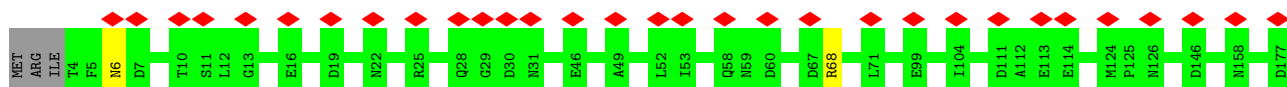
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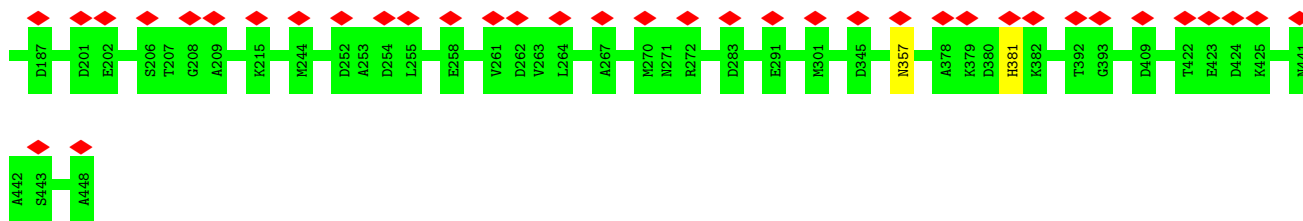


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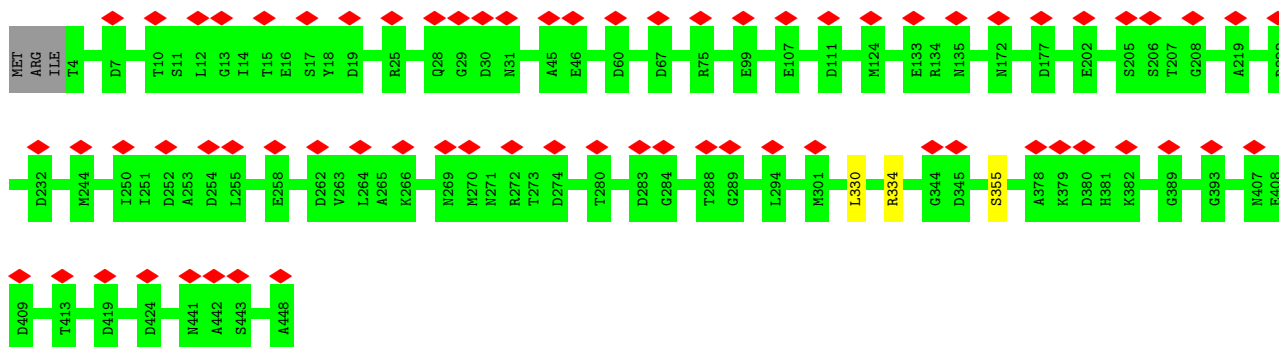


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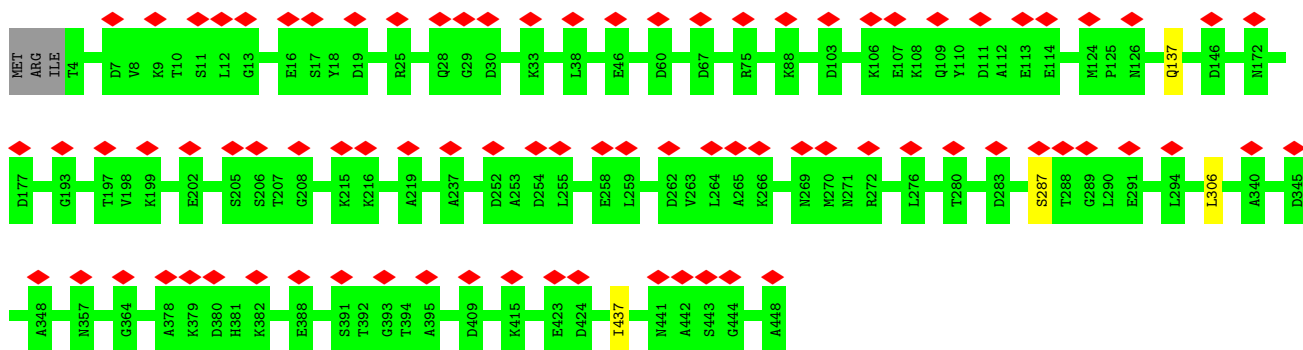




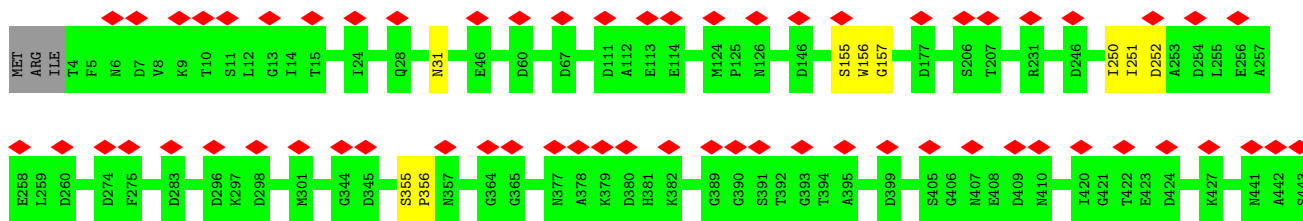
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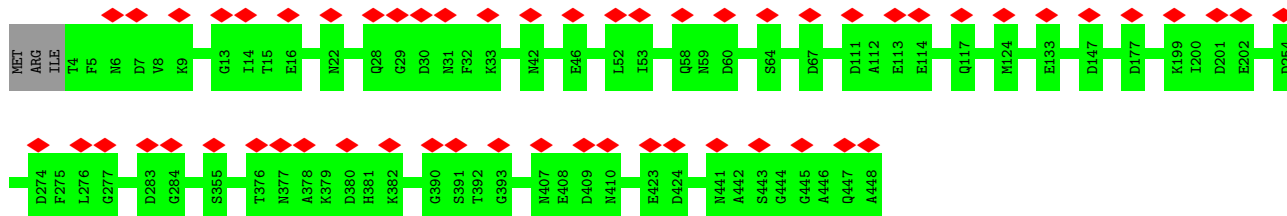


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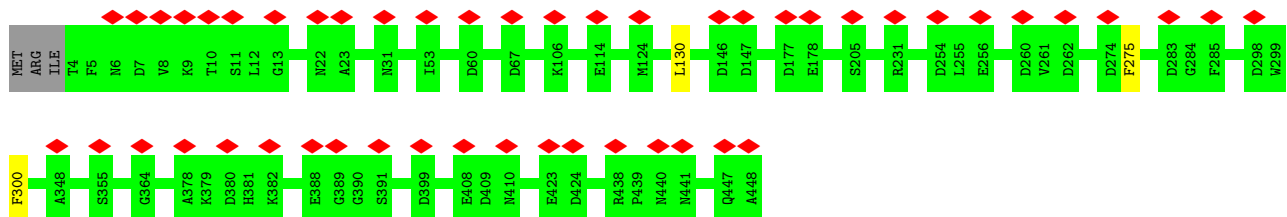




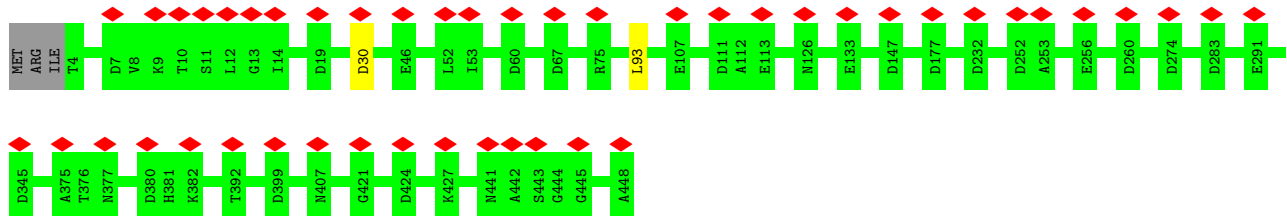
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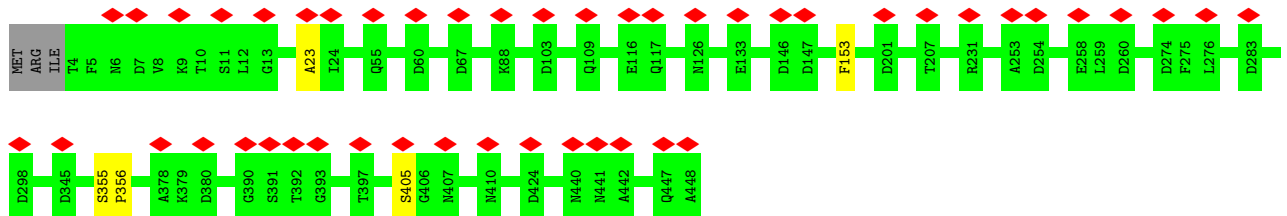
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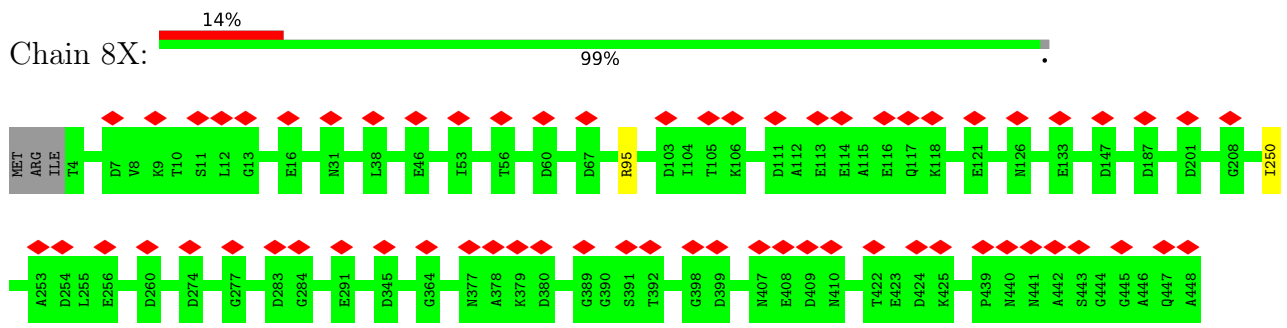
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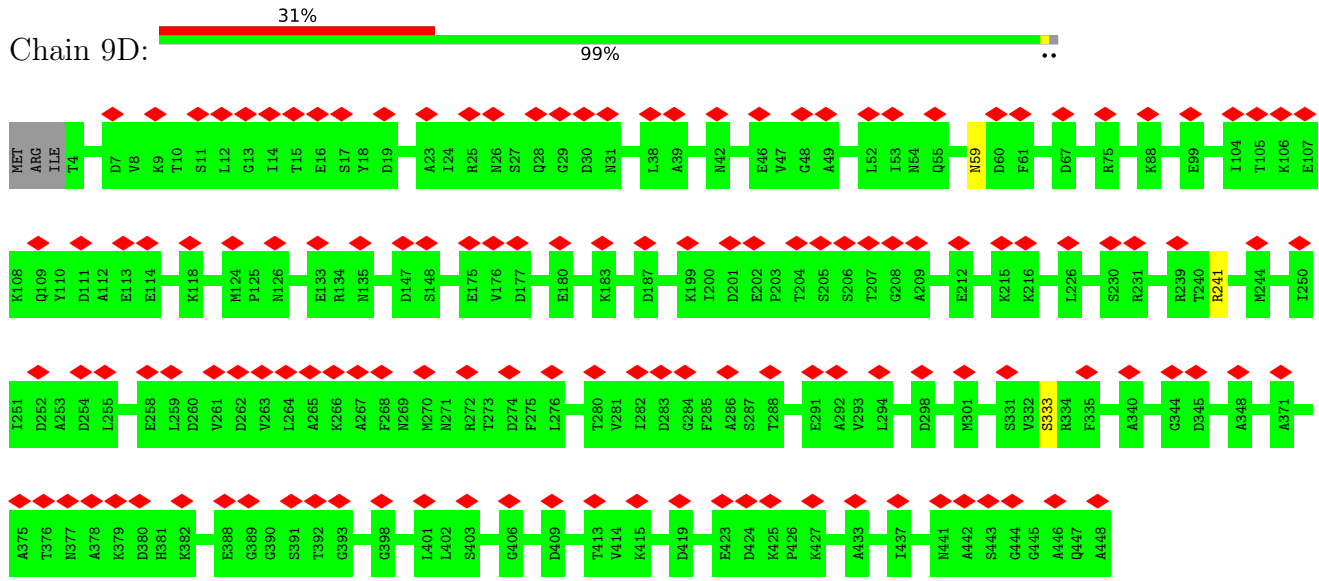
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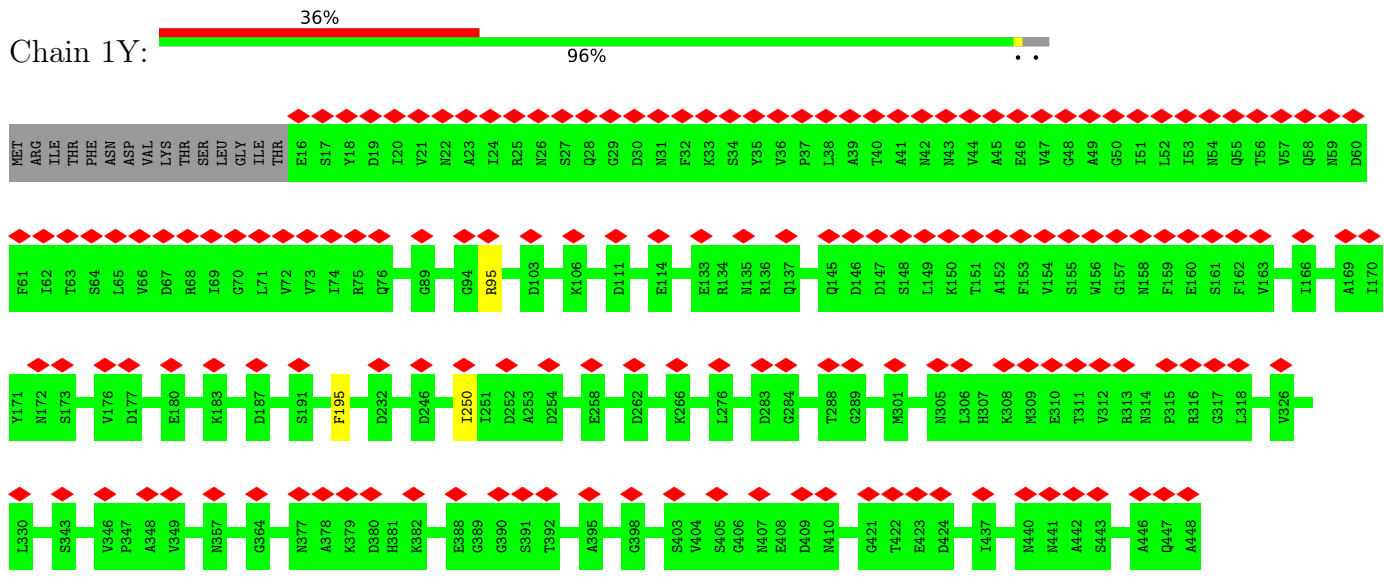
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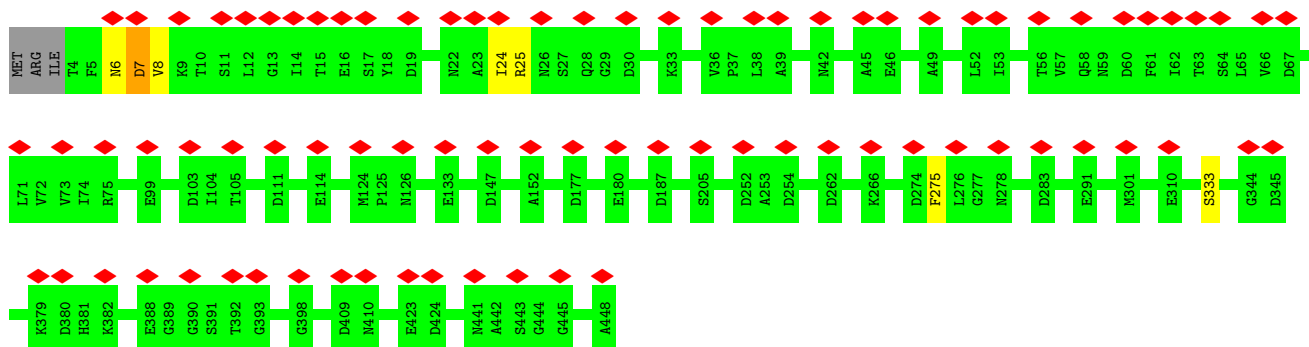


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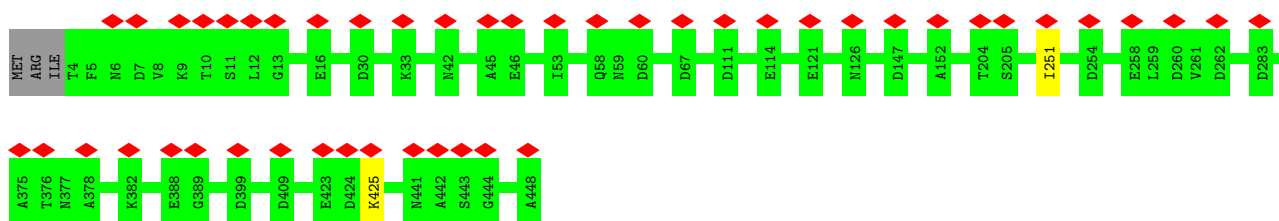


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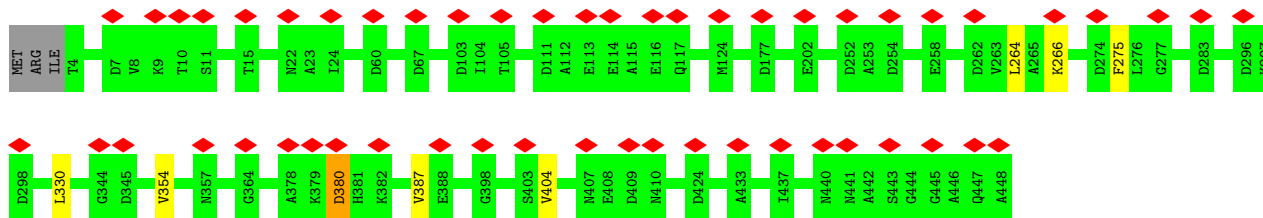




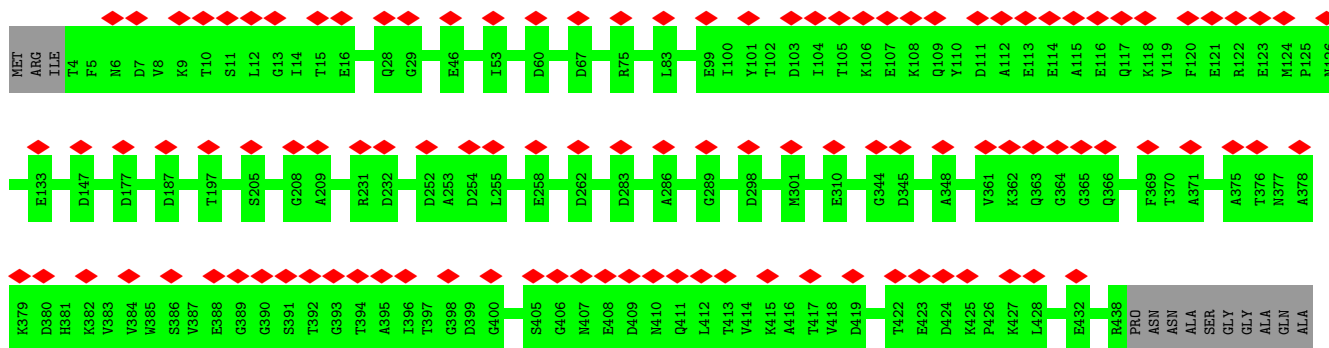
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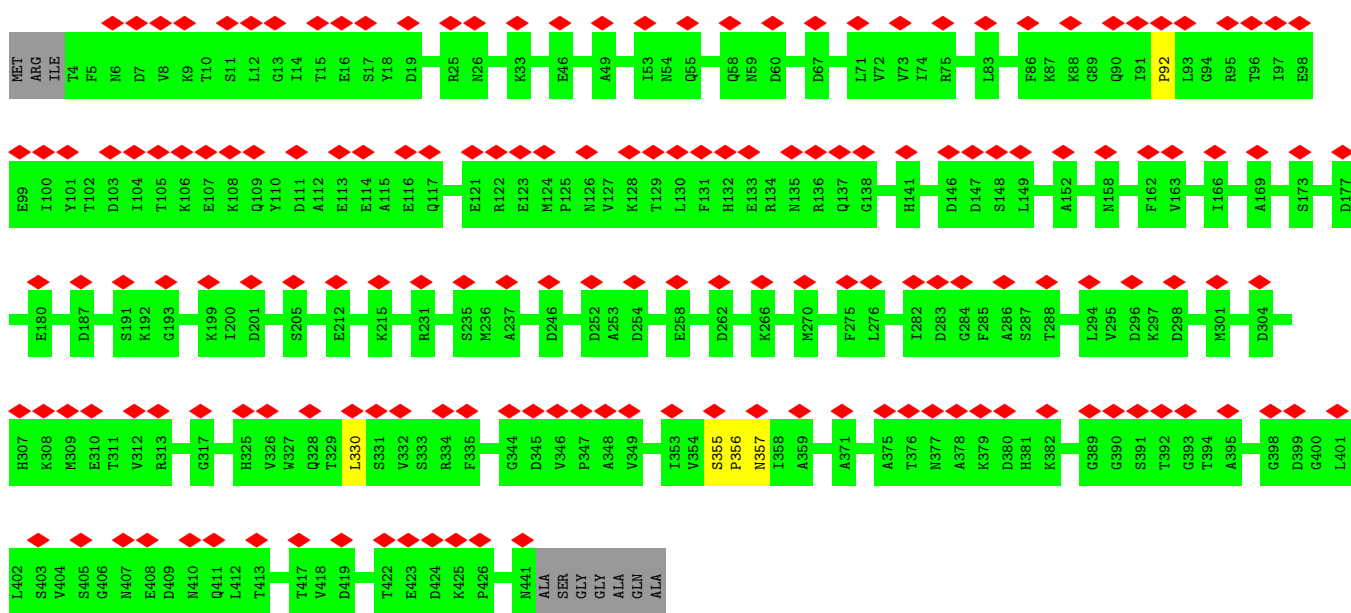
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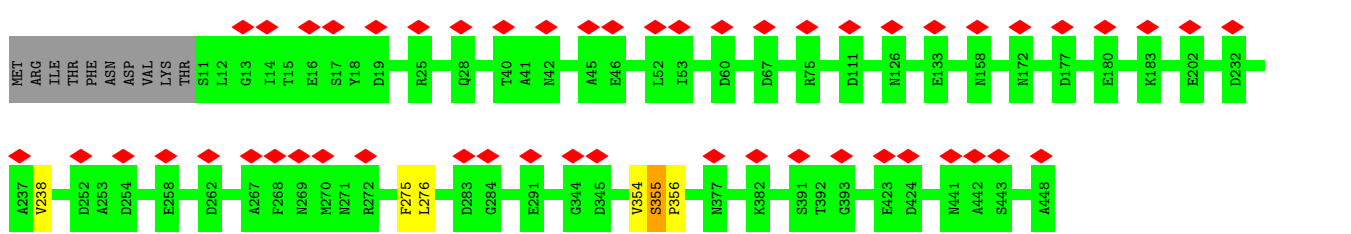
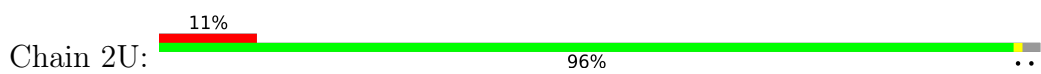
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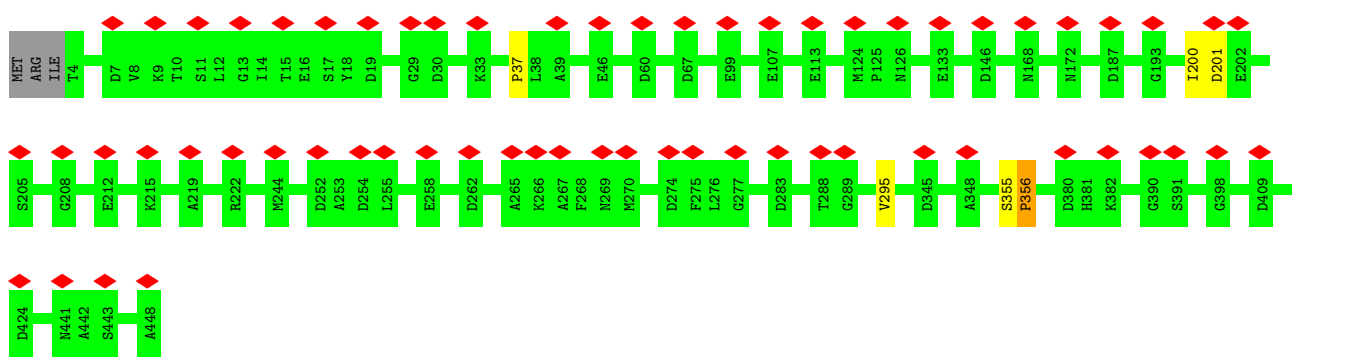
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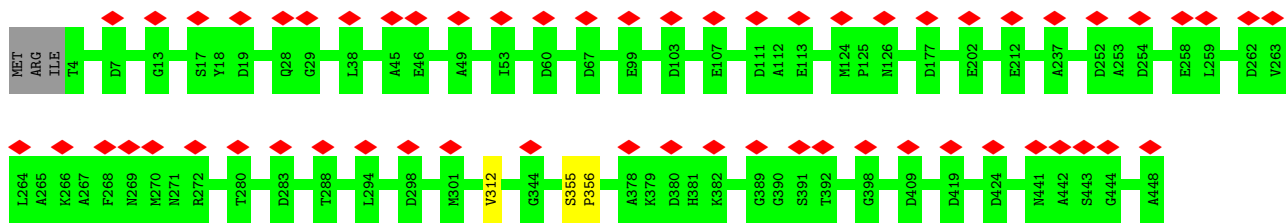


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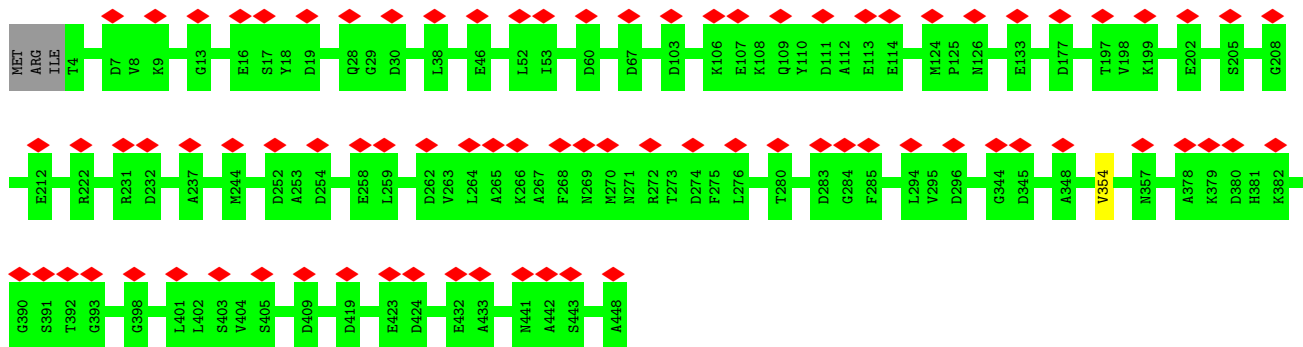


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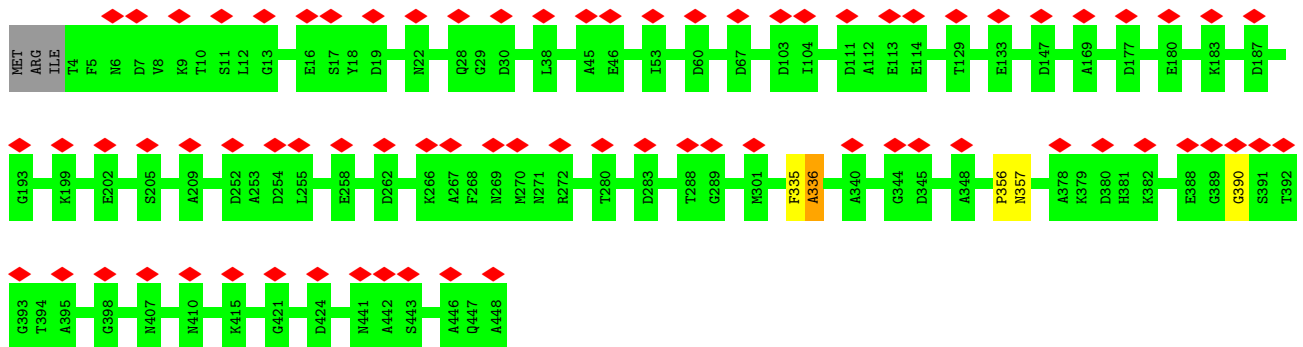




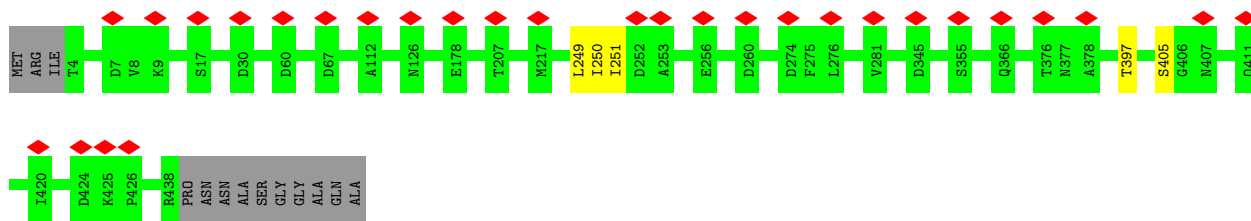
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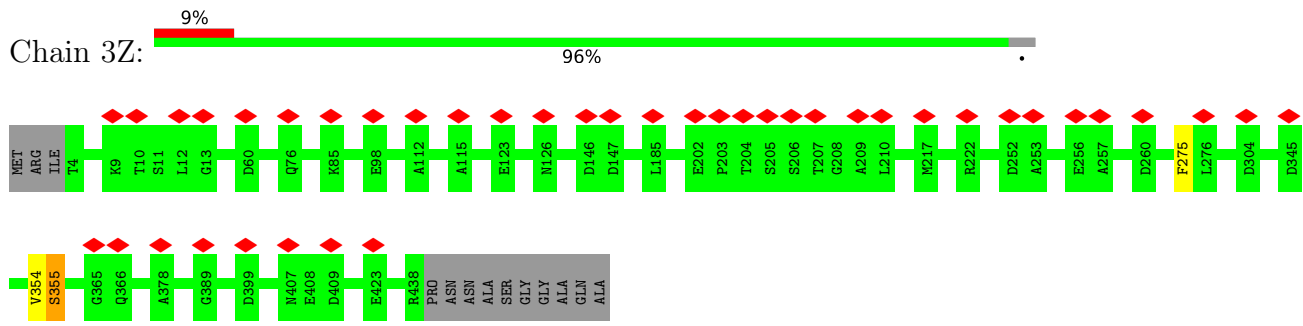
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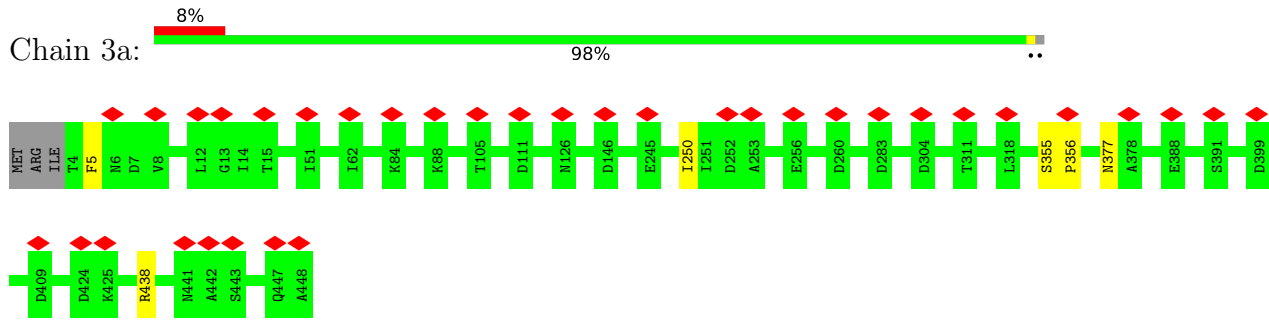
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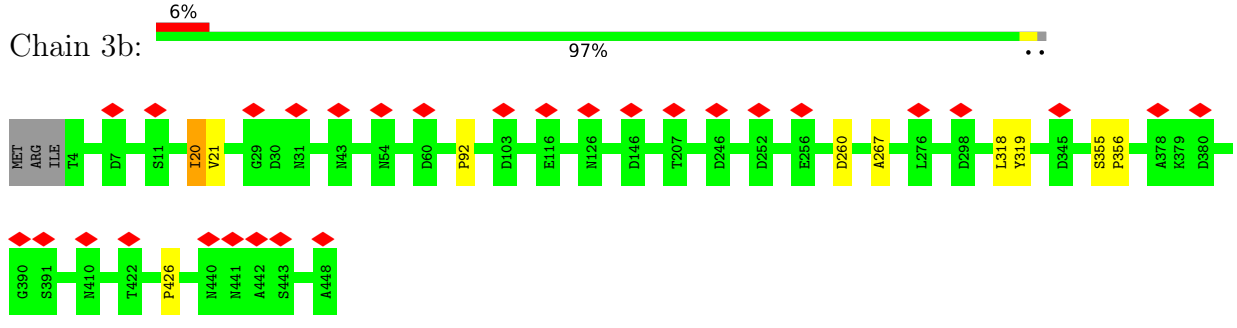
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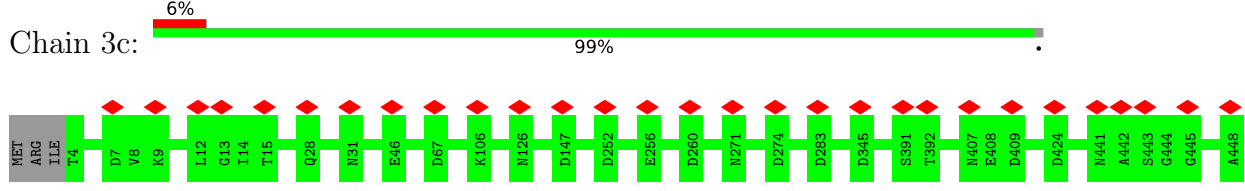
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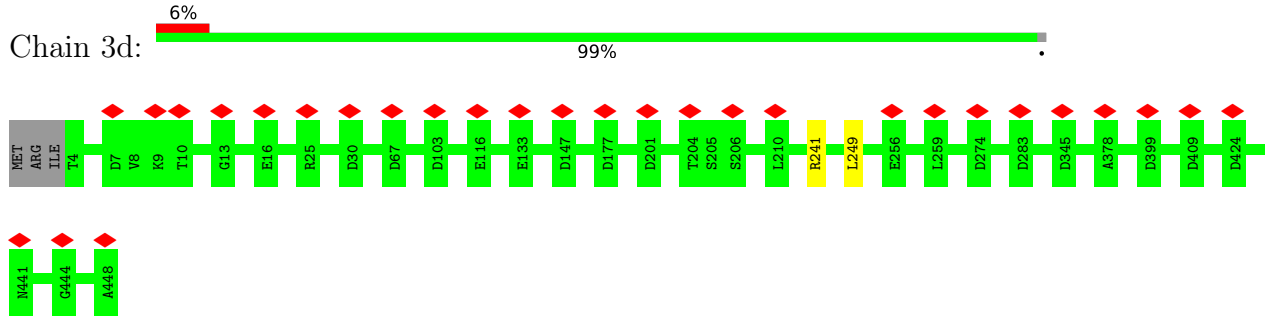
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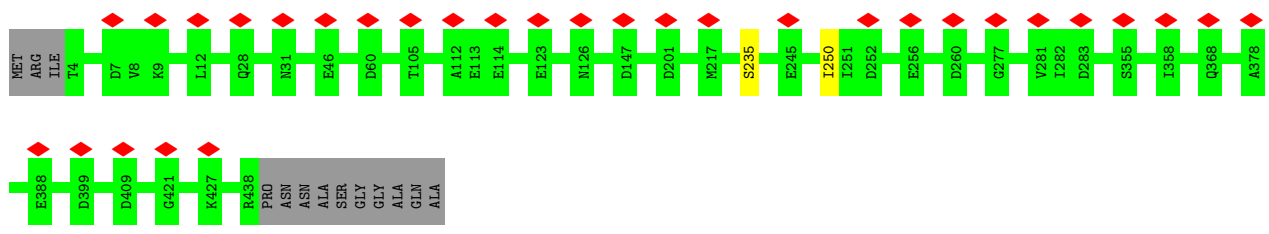
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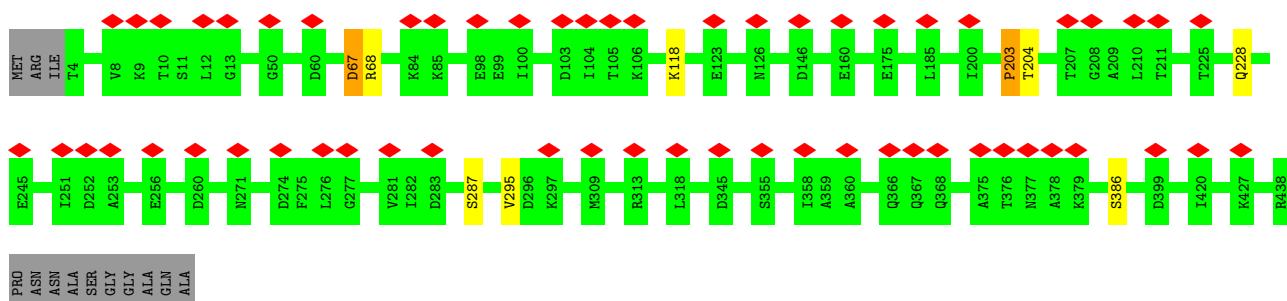
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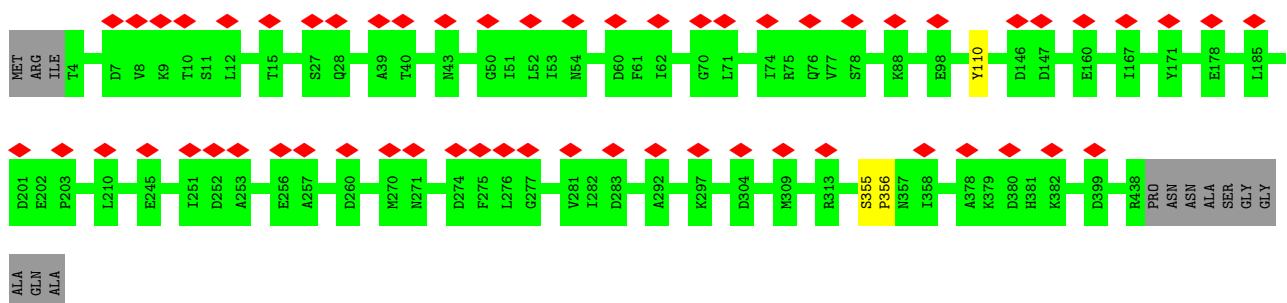
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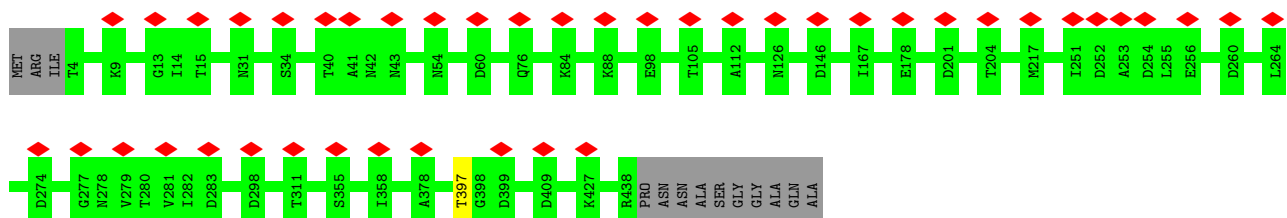
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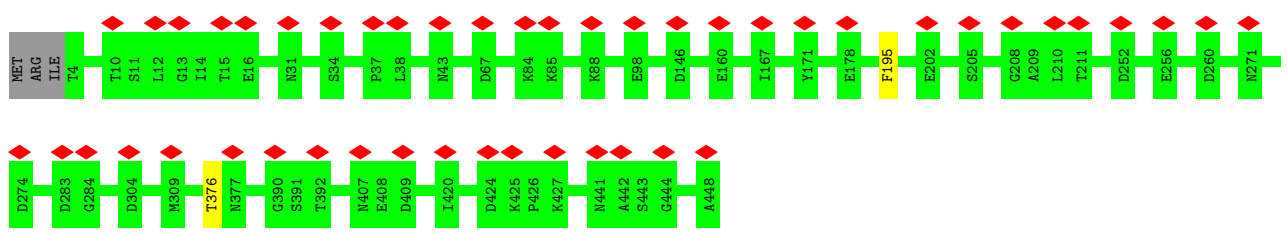
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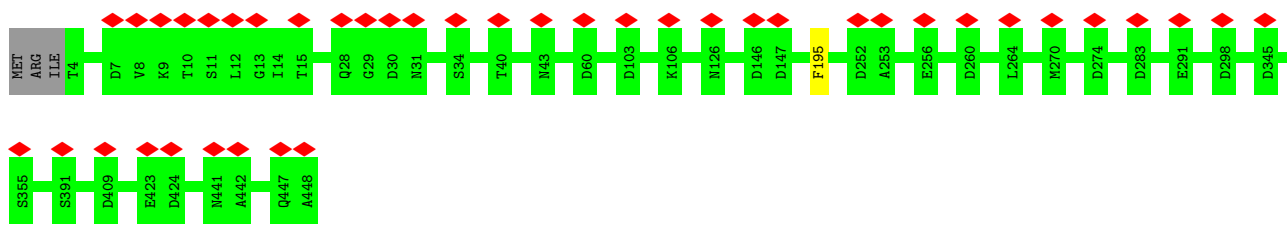
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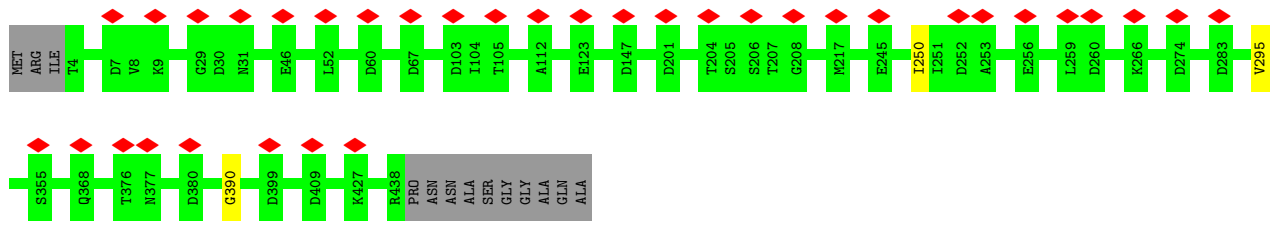
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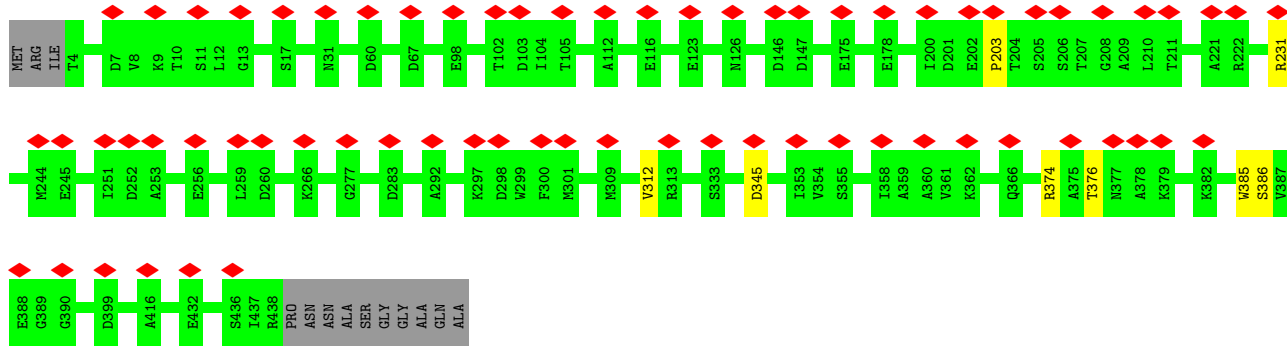
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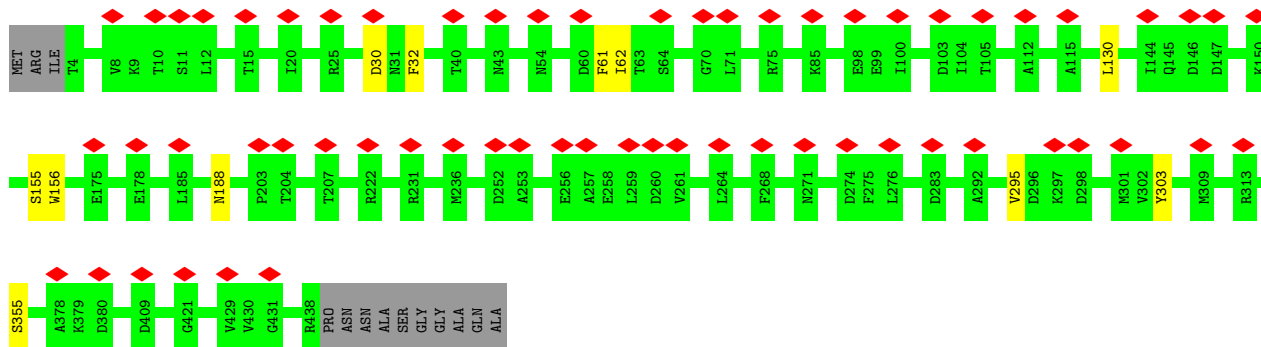


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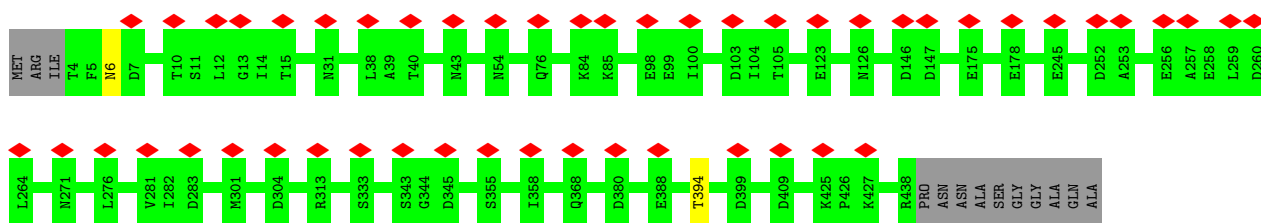


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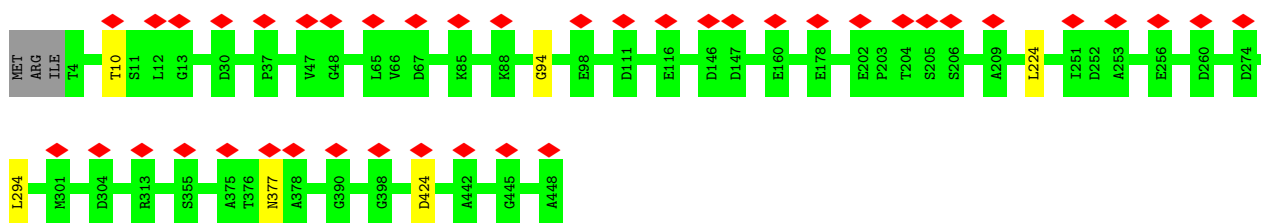




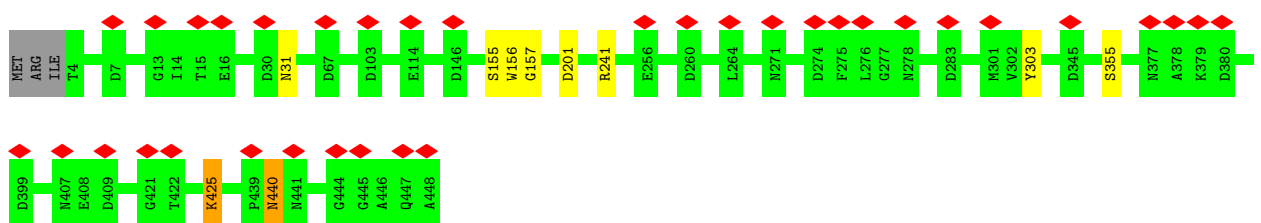
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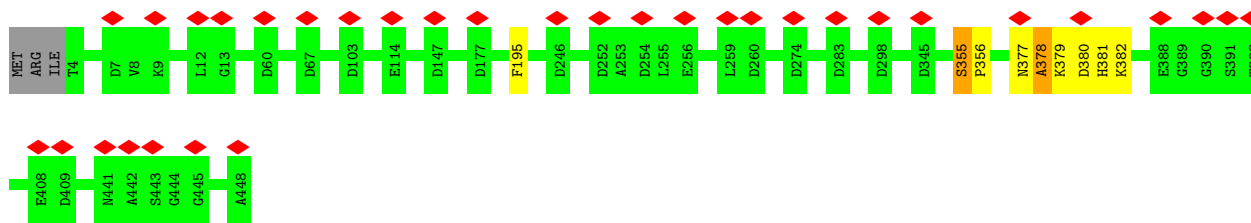


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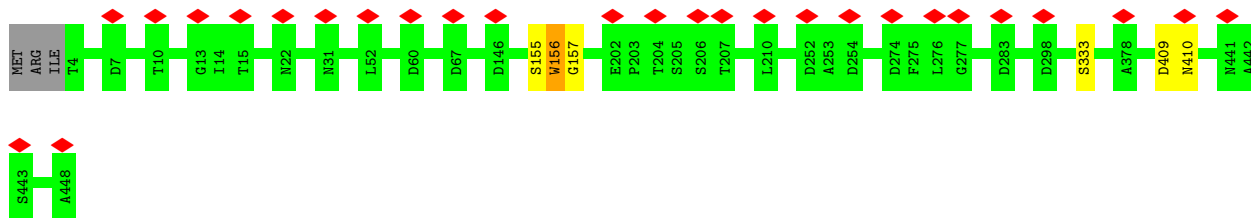


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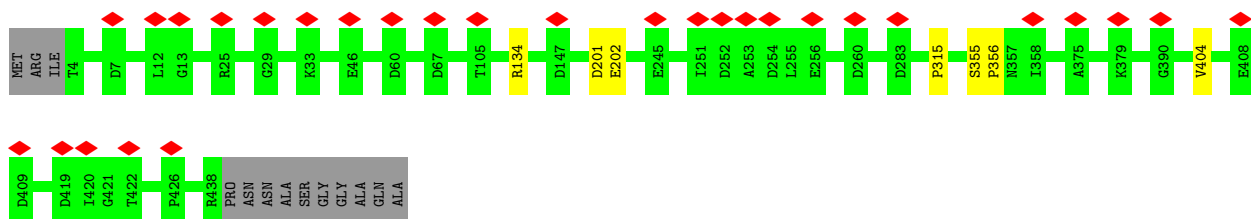




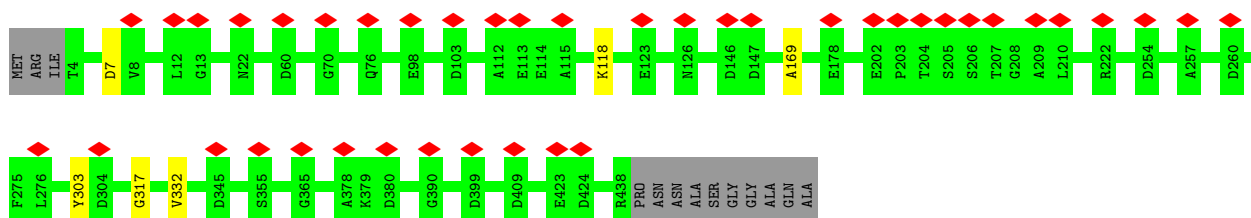
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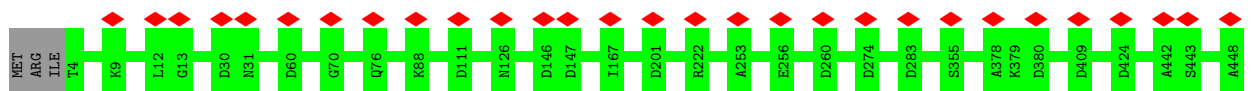
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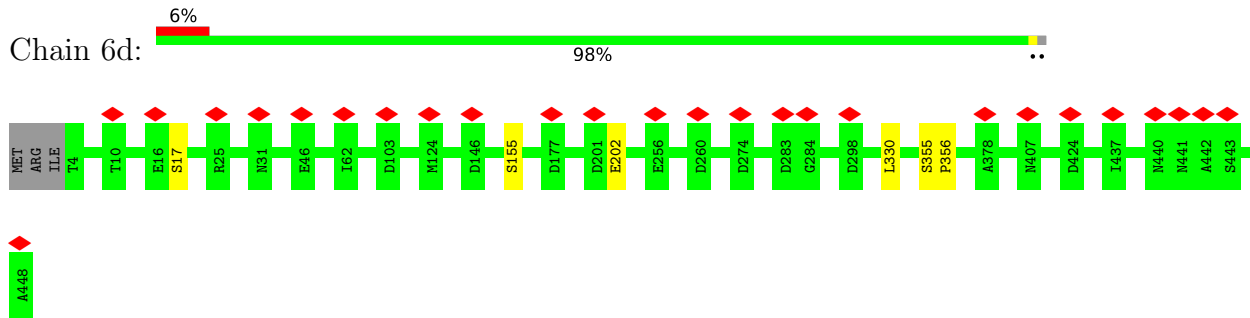
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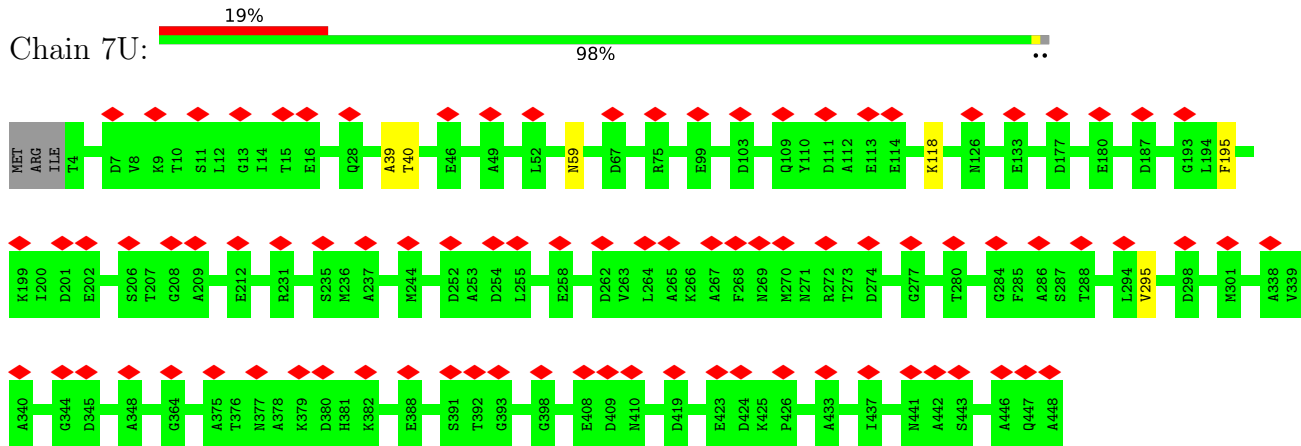
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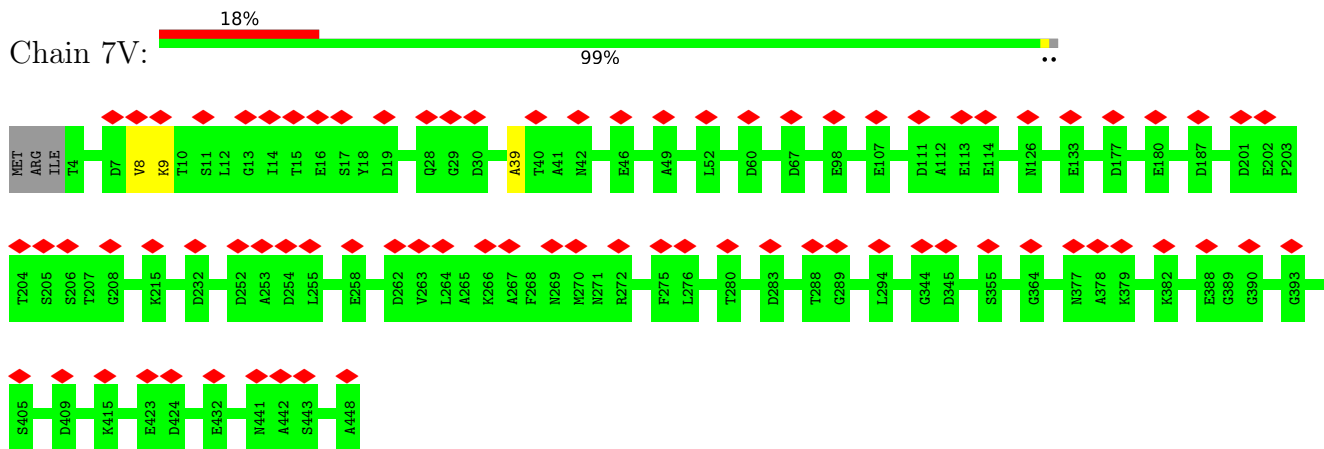
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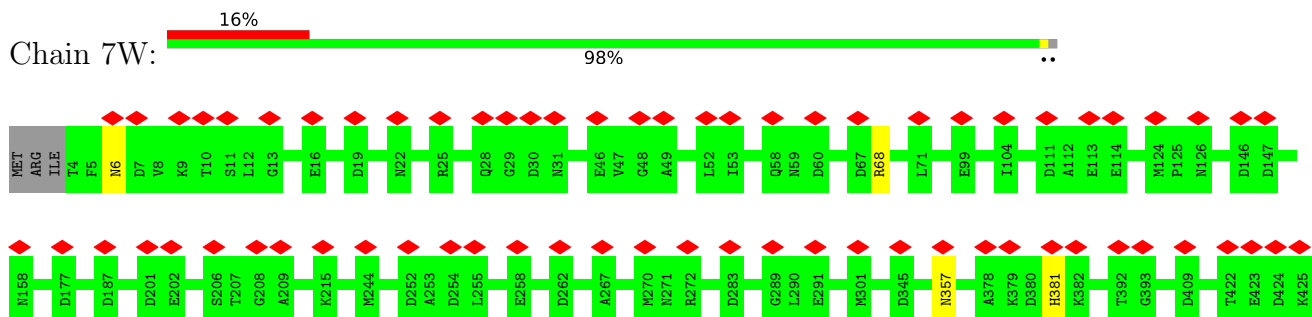
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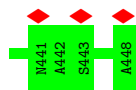


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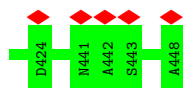
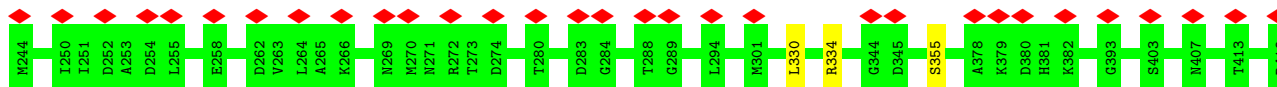
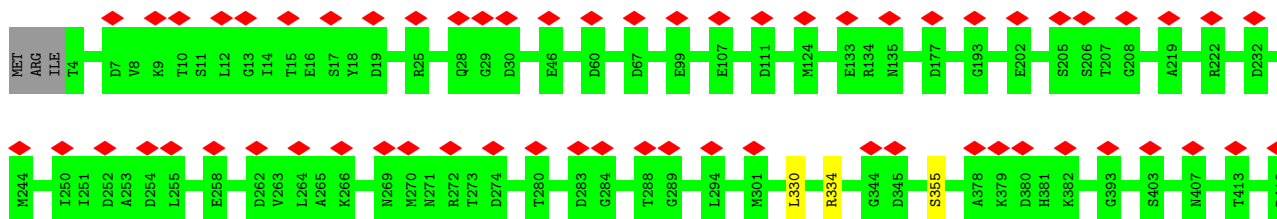


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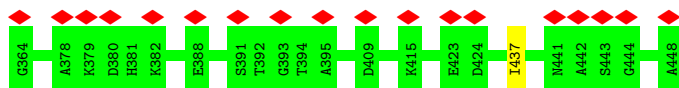
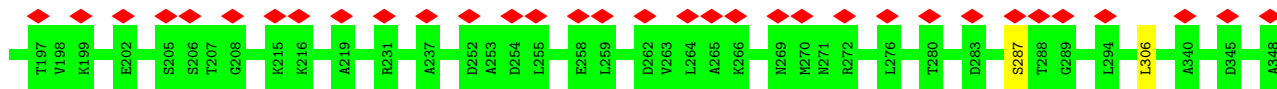
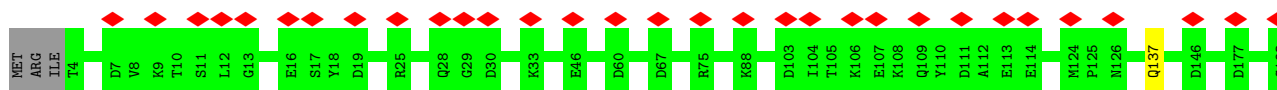




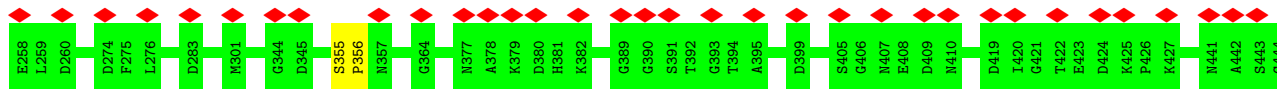
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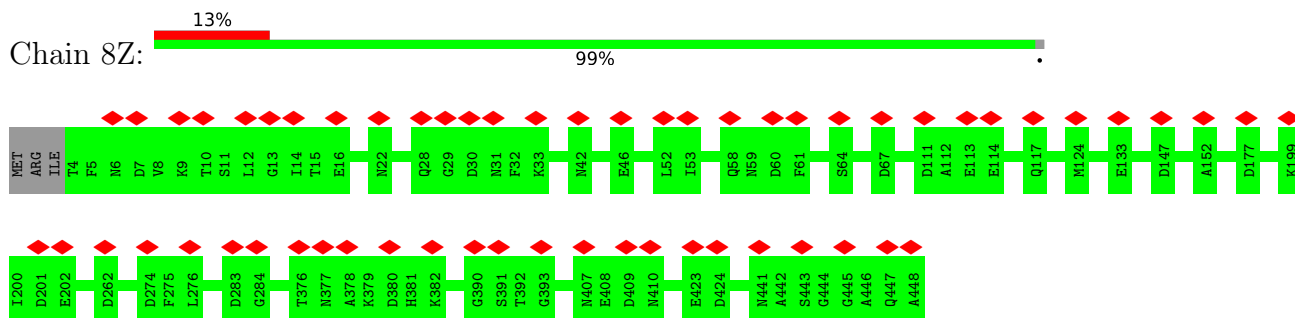
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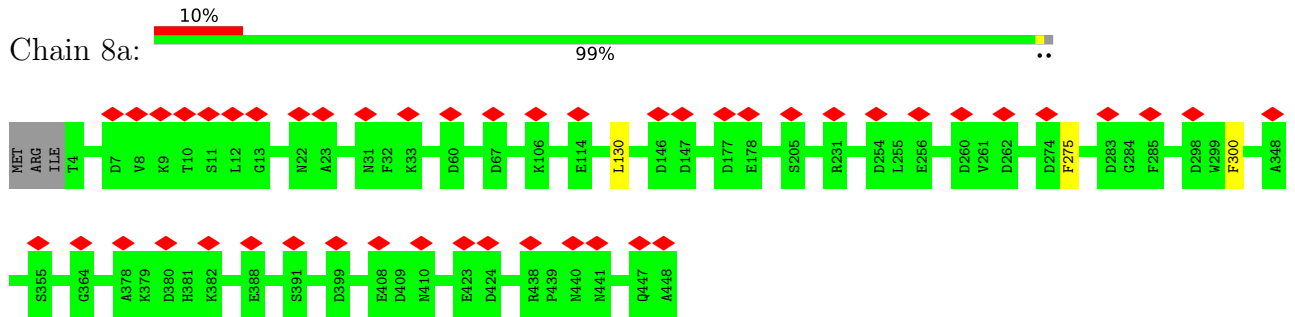
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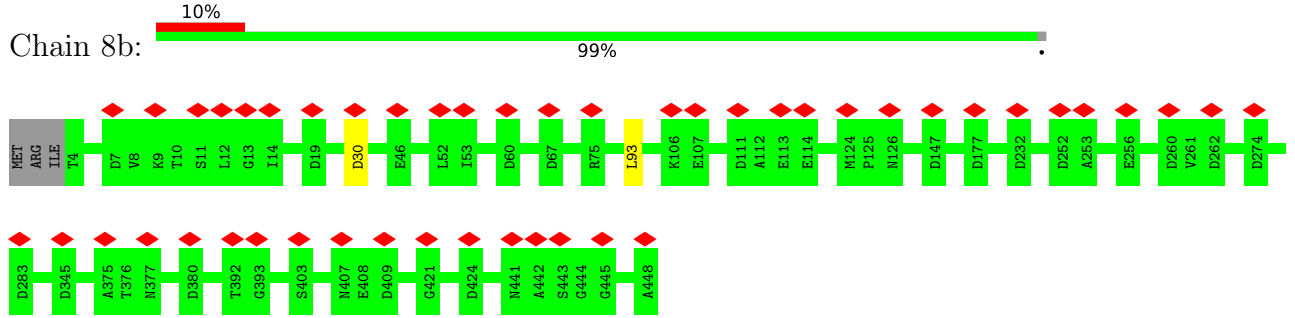
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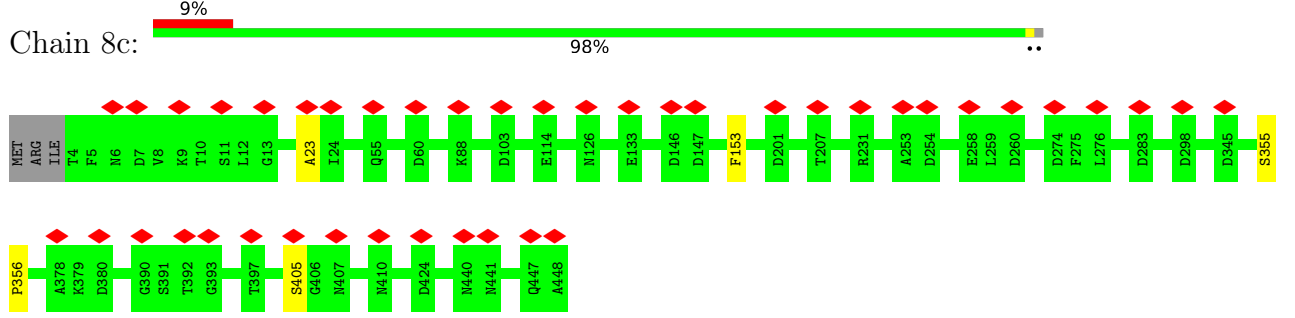
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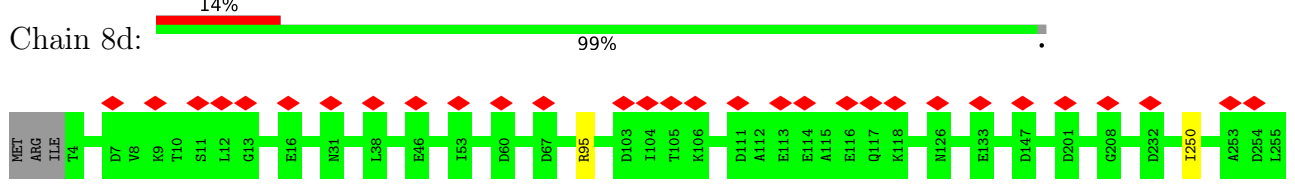
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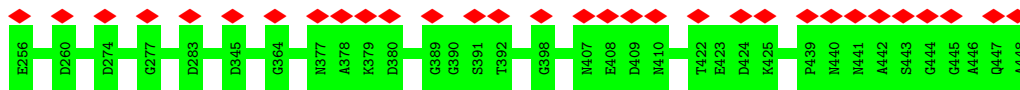


• Molecule 1: Major capsid protein

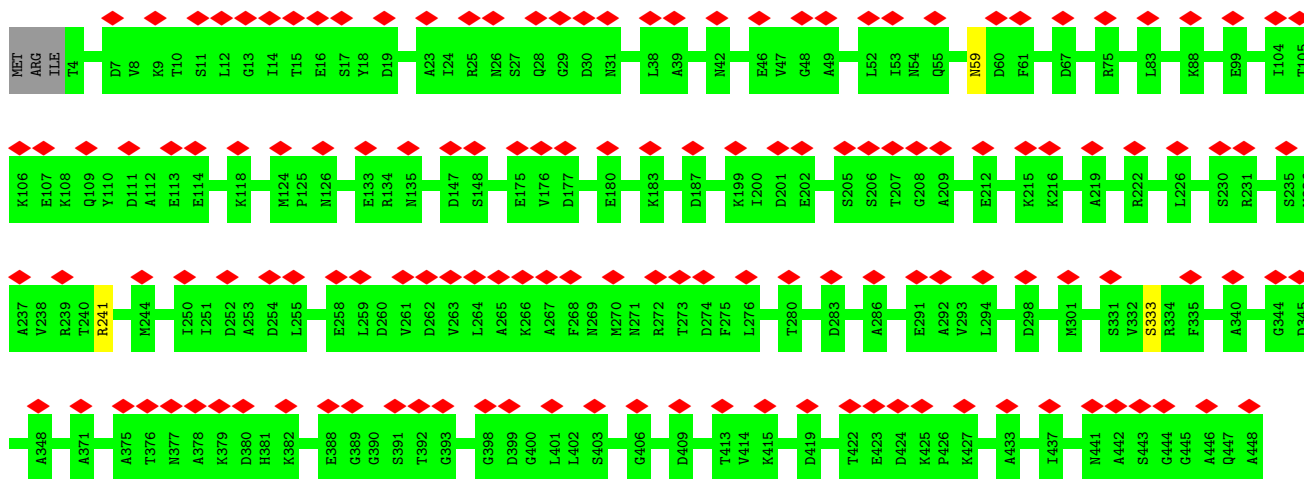


• Molecule 1: Major capsid protein

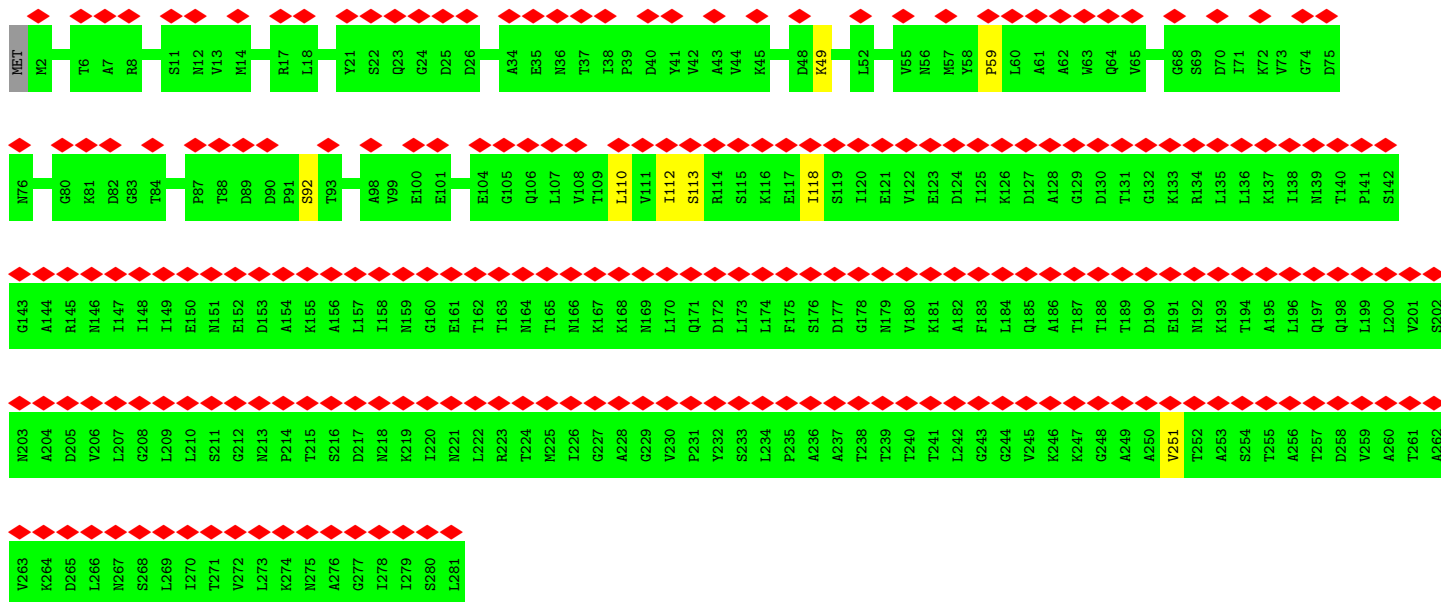
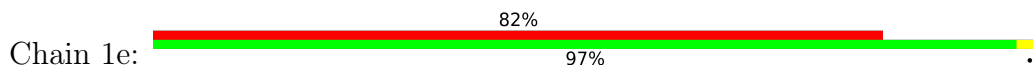




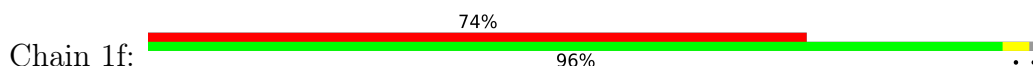
• Molecule 1: Major capsid protein

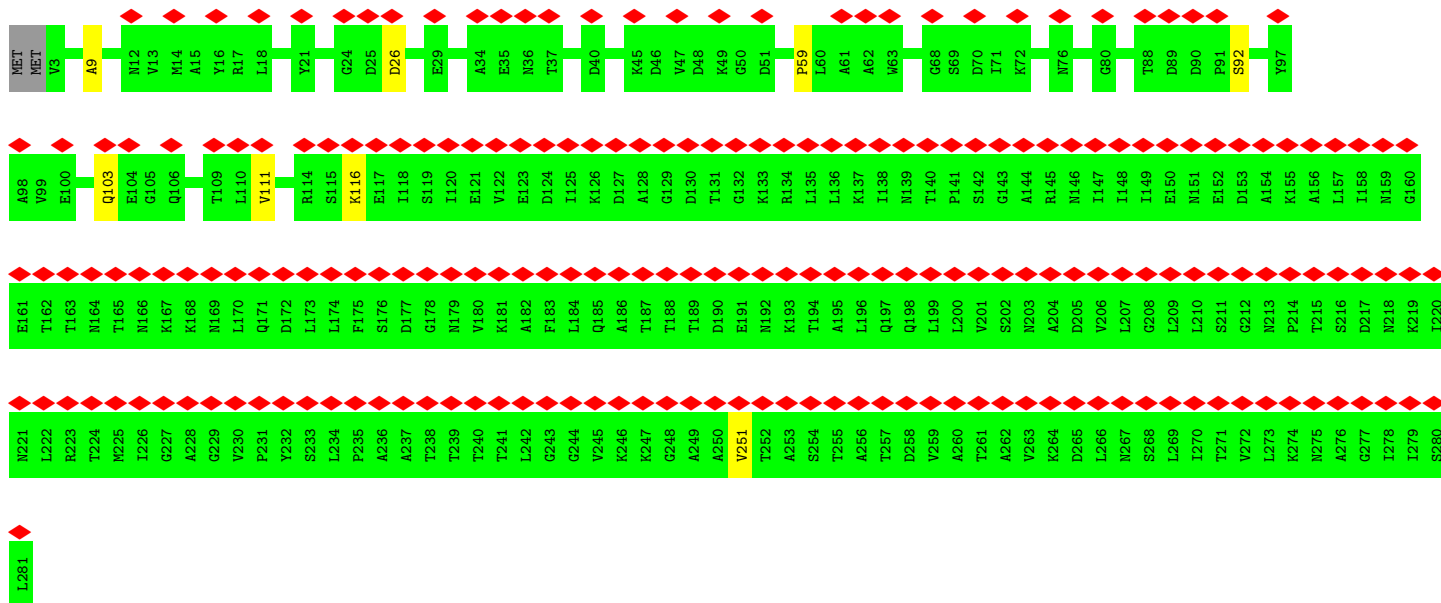


• Molecule 2: Capsid fiber protein

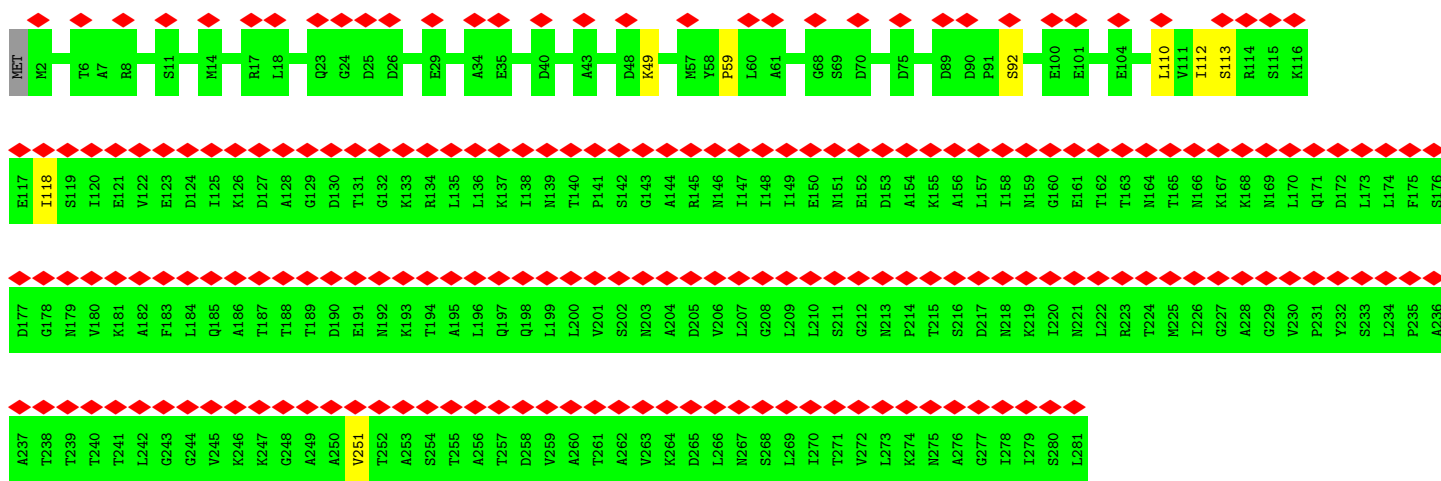


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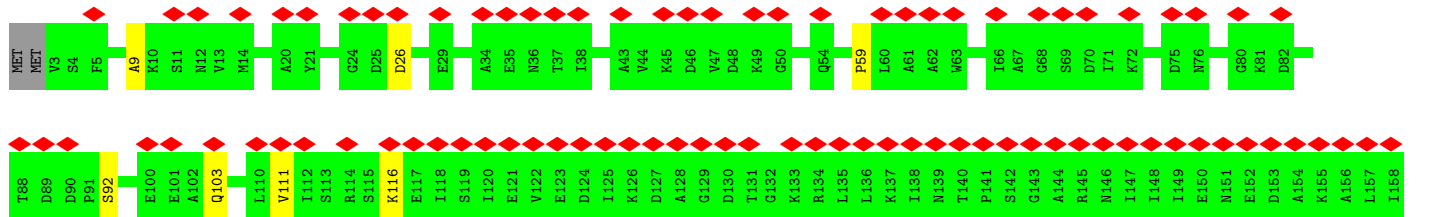
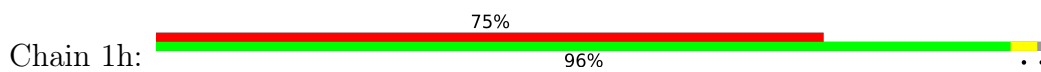


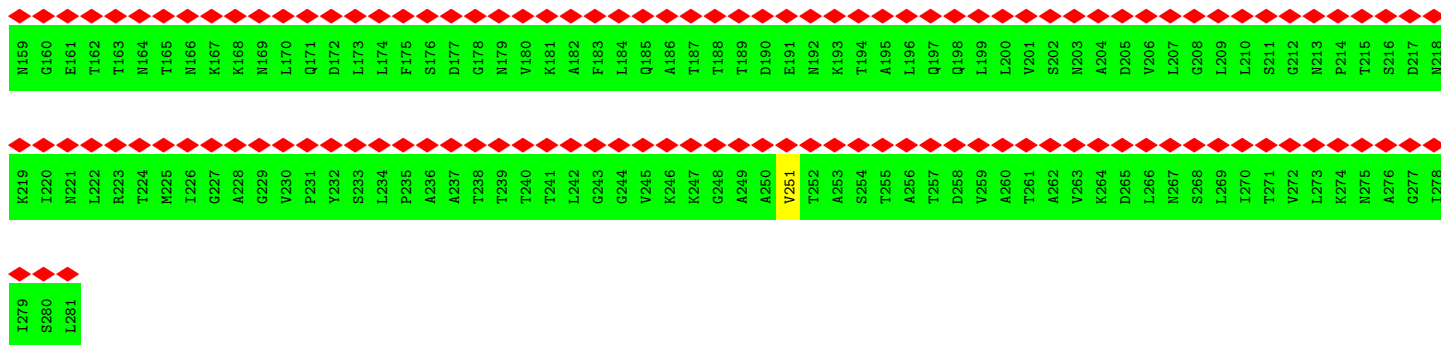


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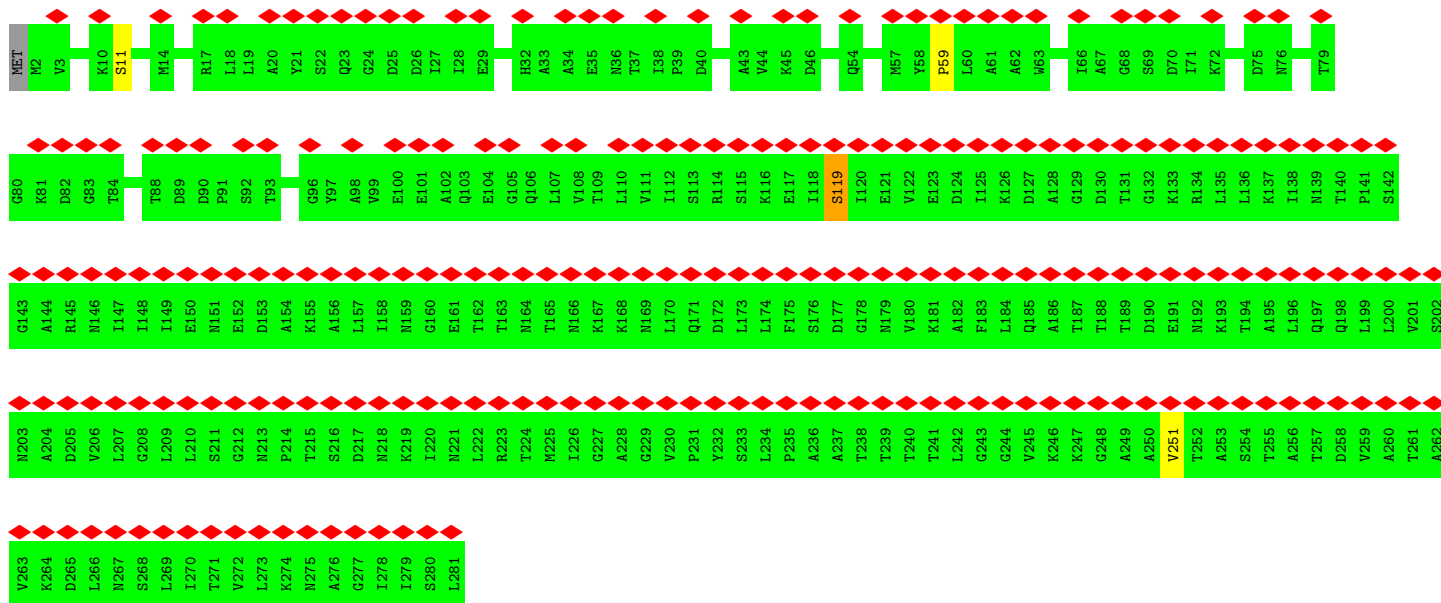
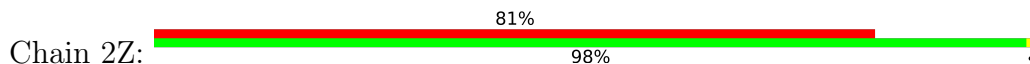


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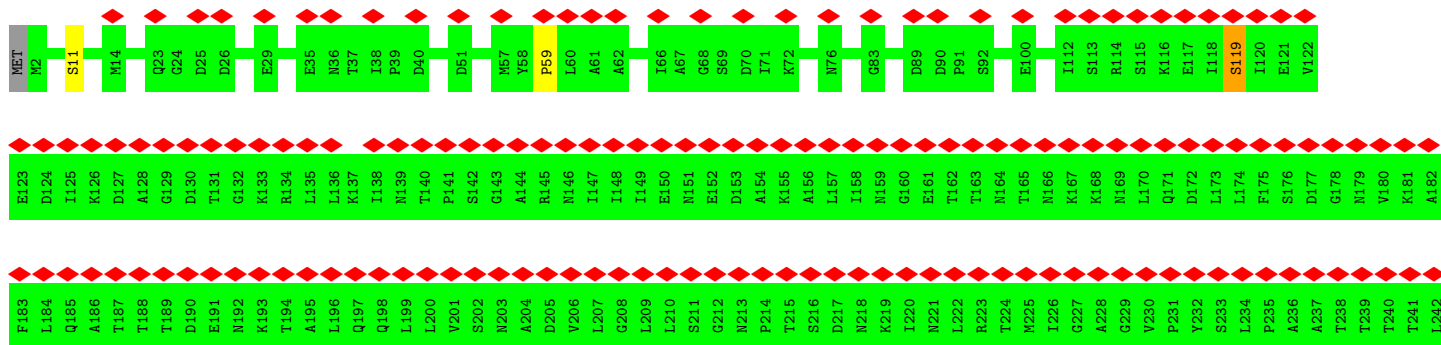


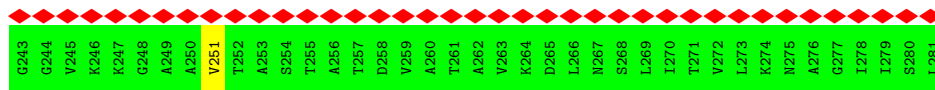


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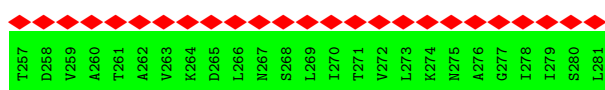
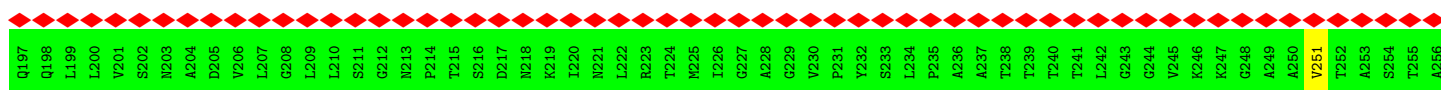
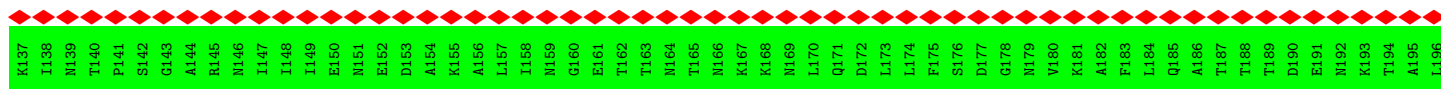
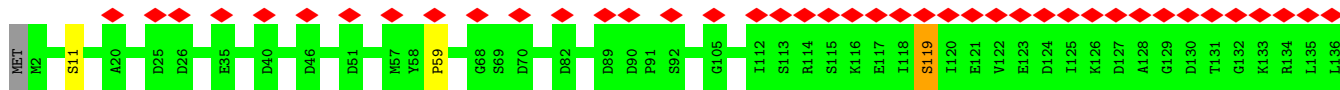


• Molecule 2: Capsid fiber protein

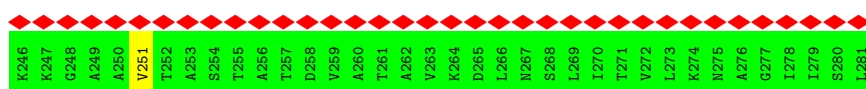
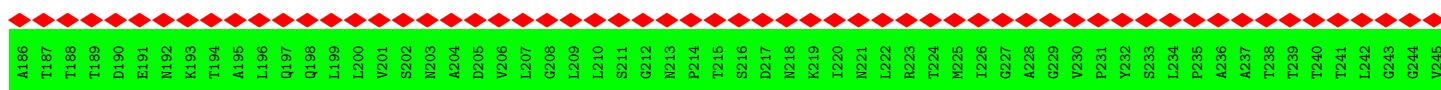
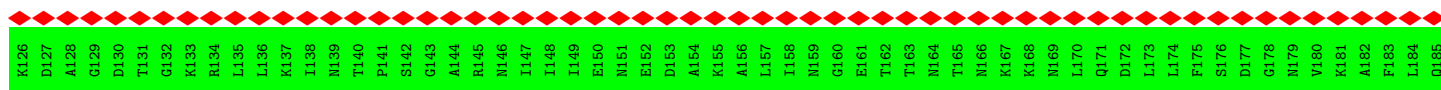
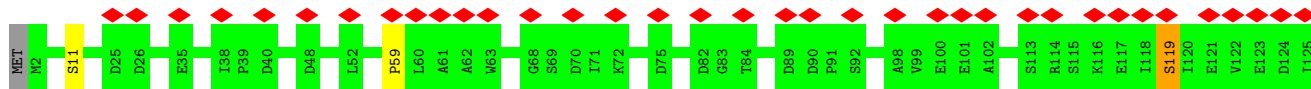




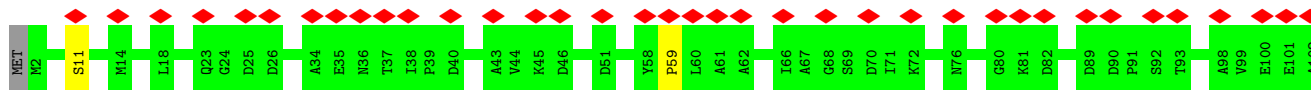
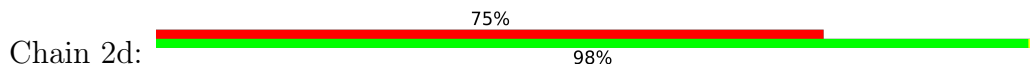
• Molecule 2: Capsid fiber protein

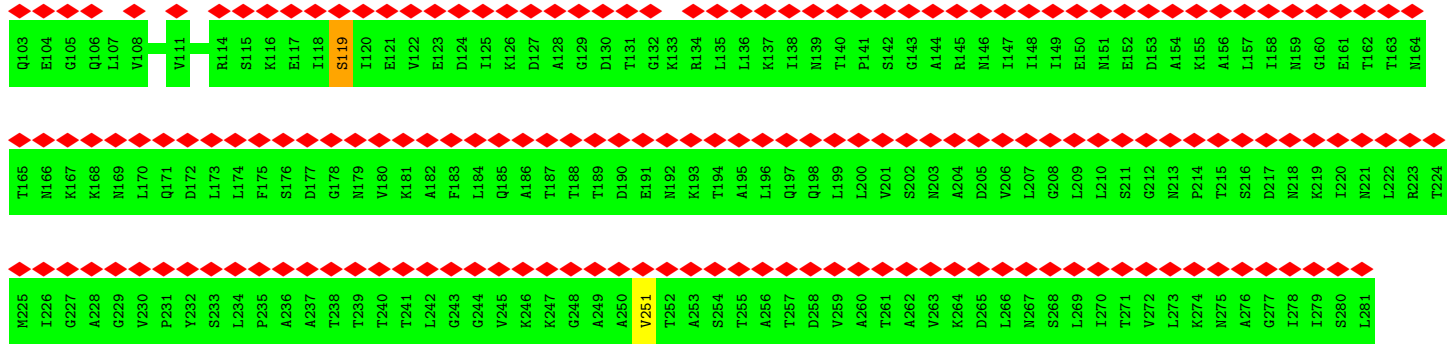


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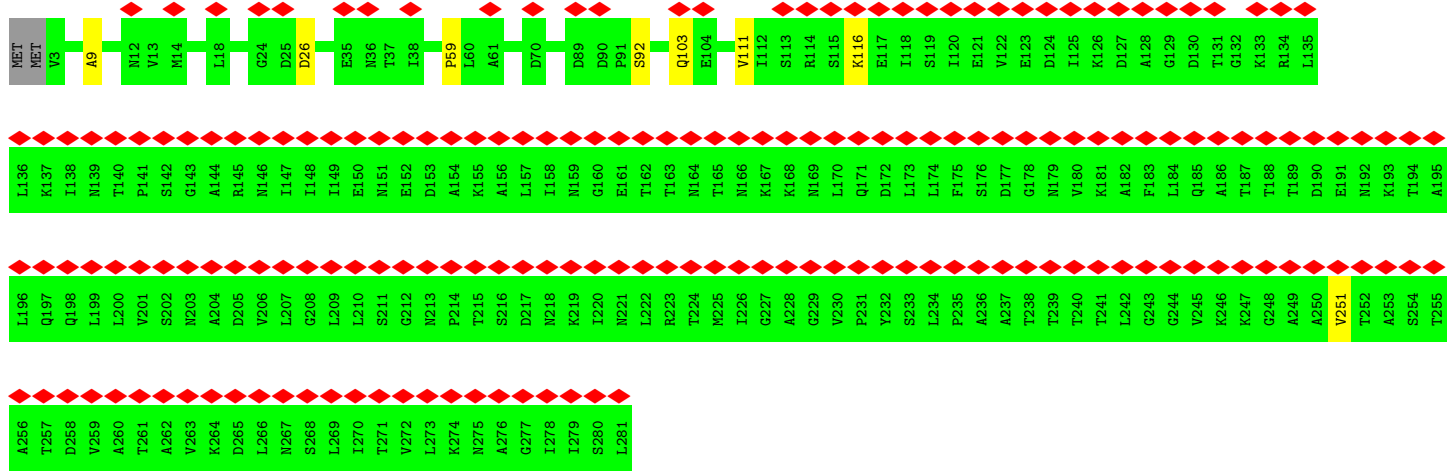


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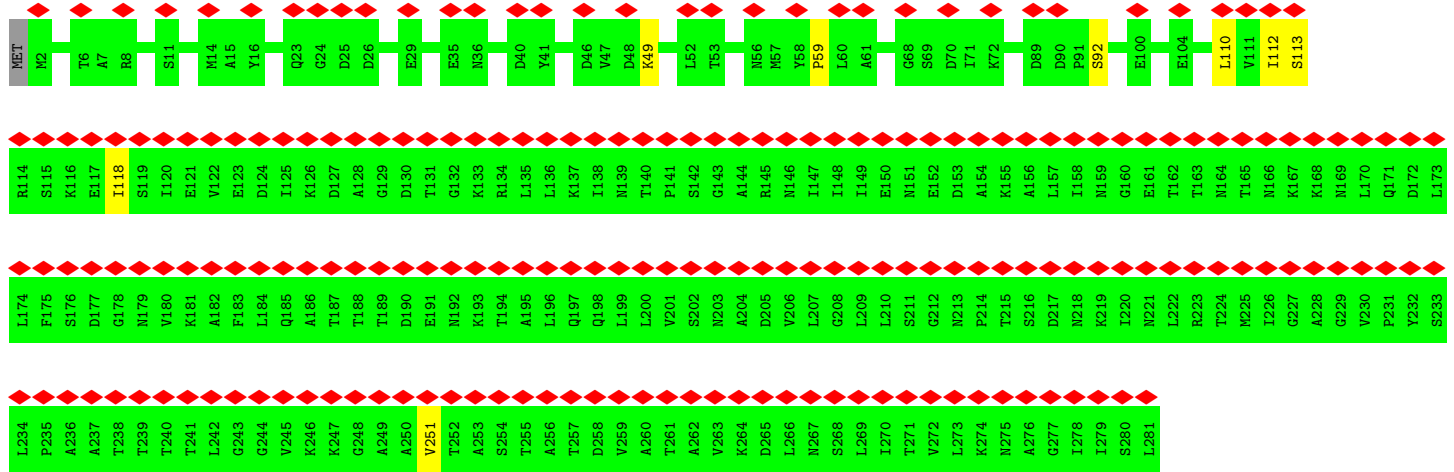




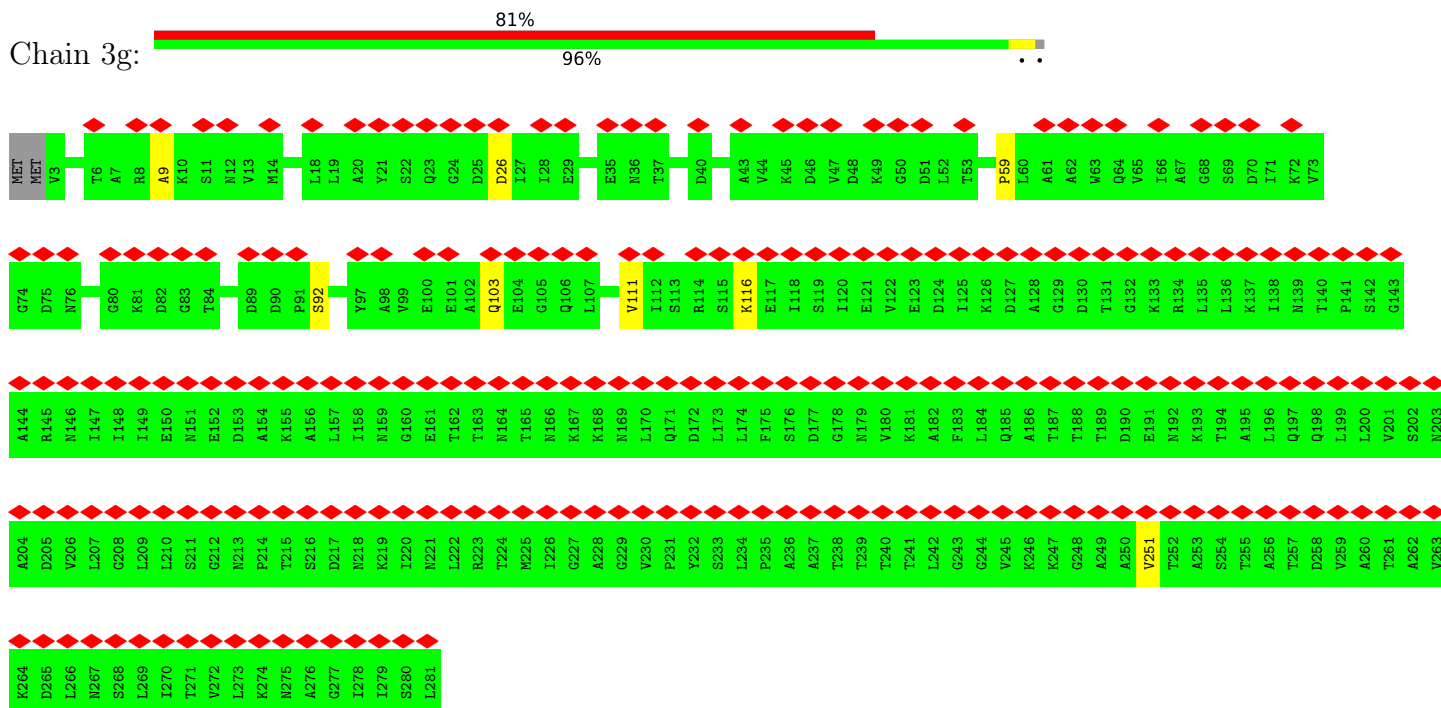
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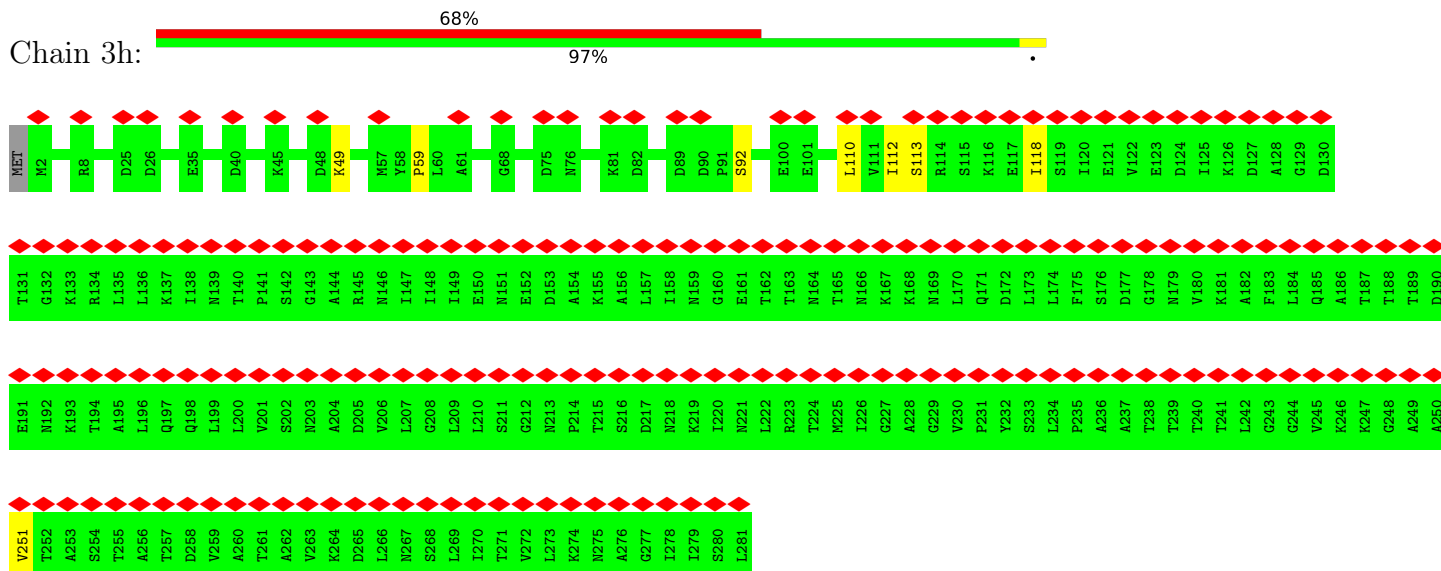
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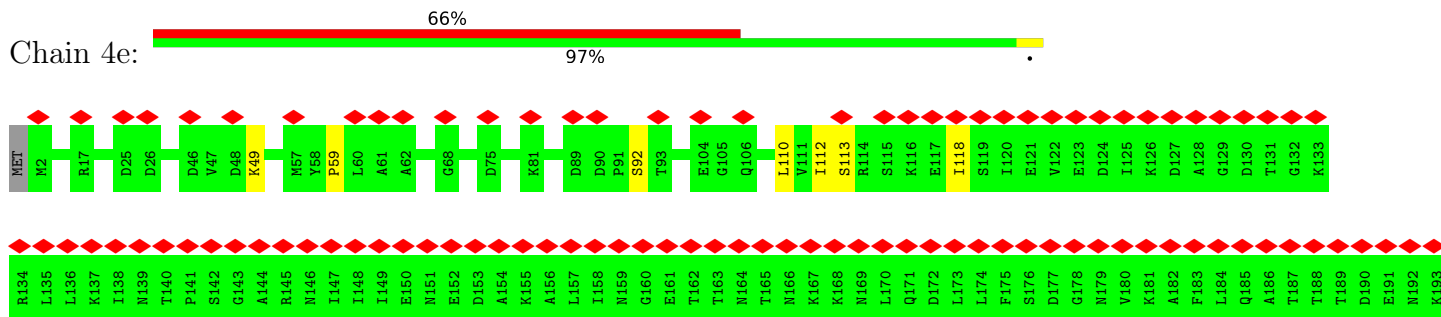
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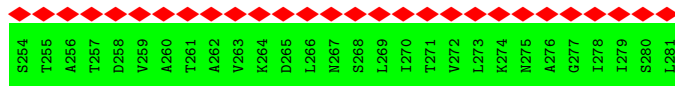
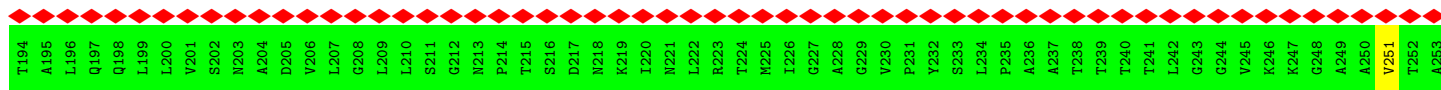


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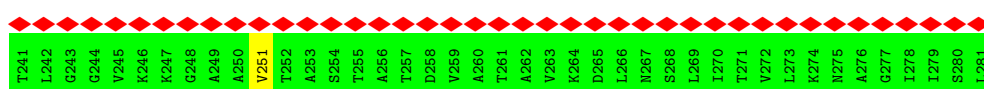
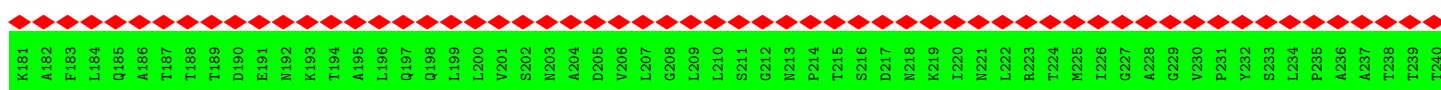
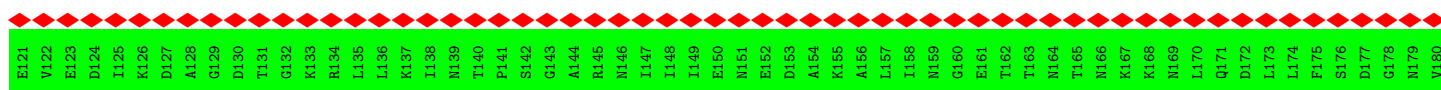
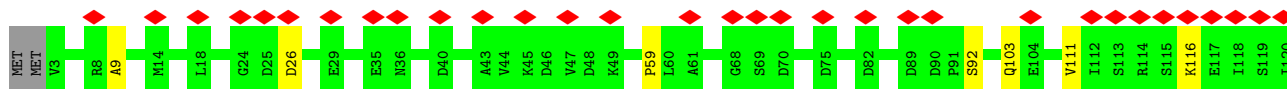


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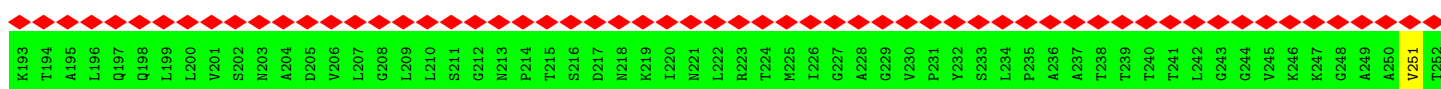
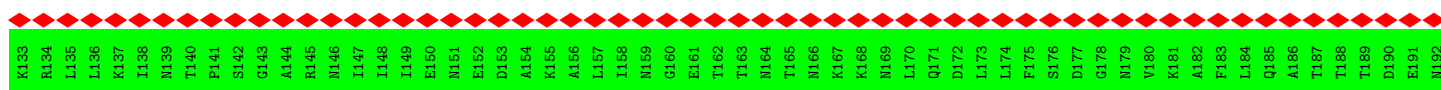
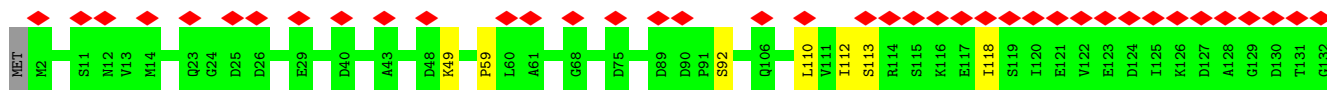




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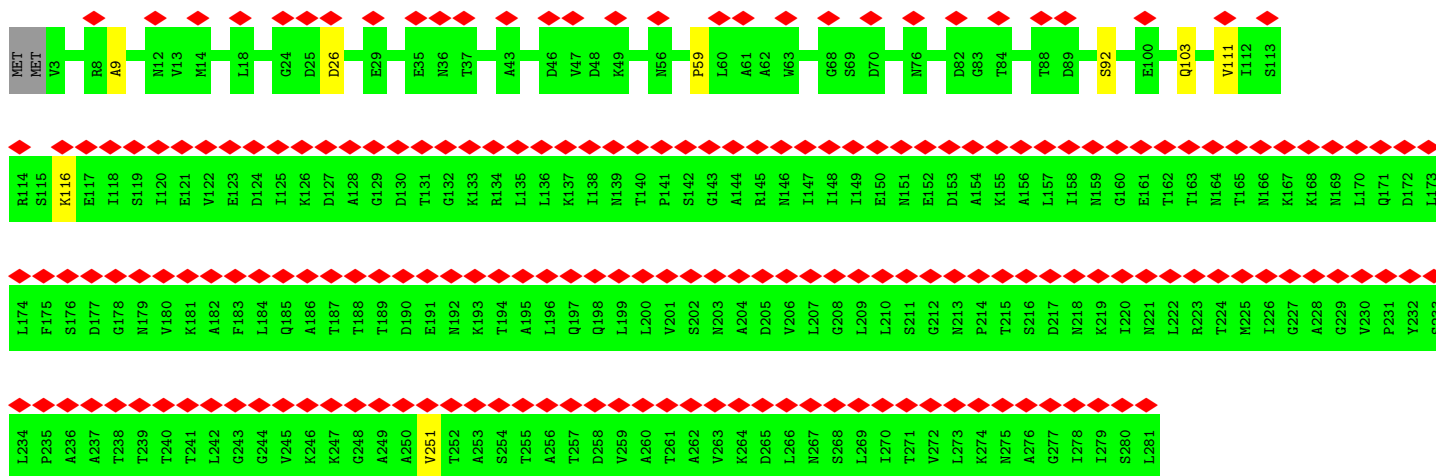


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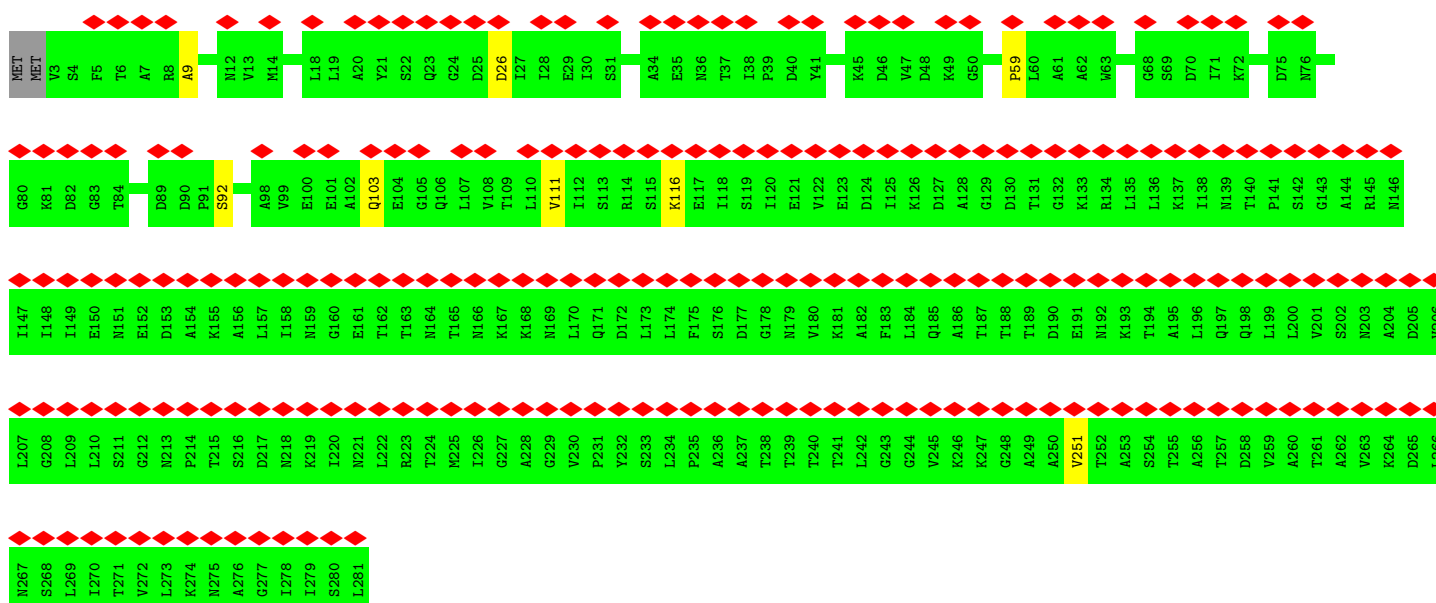
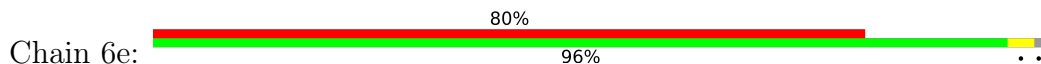


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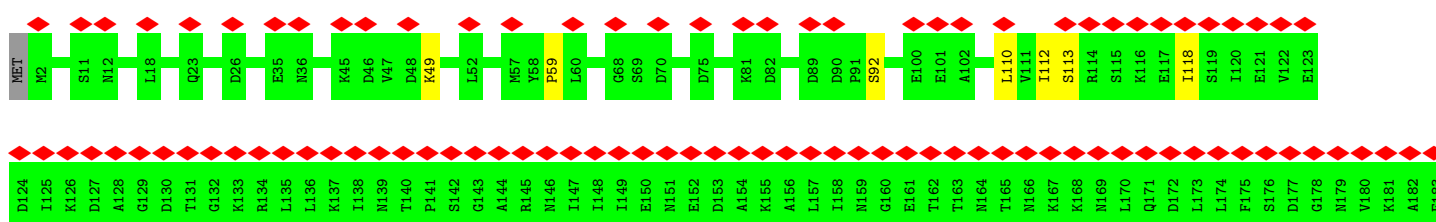


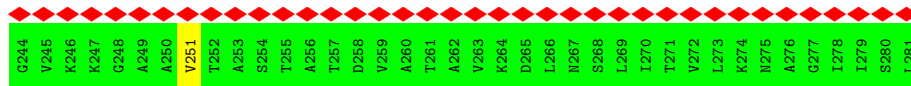
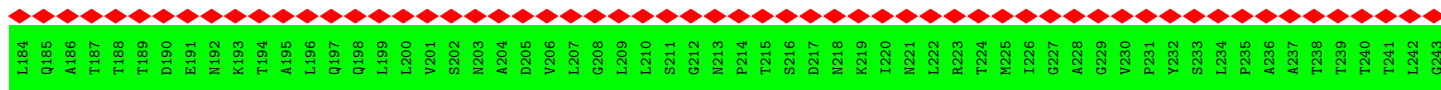


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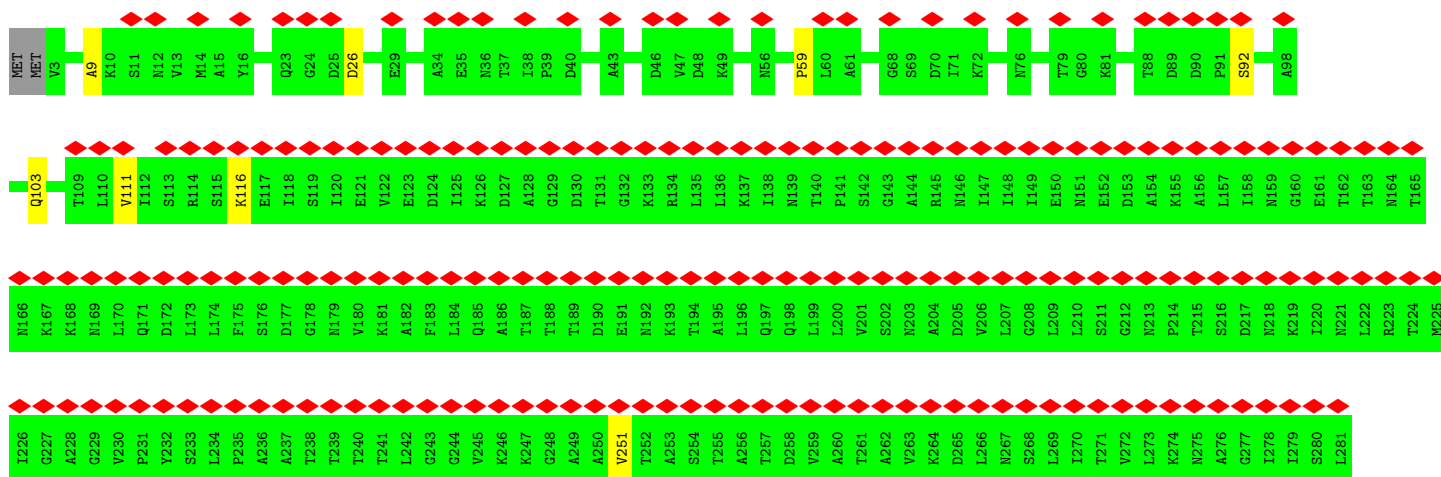
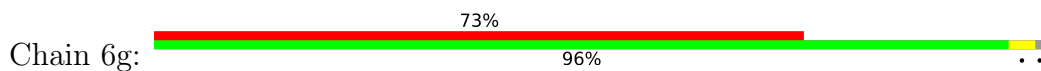


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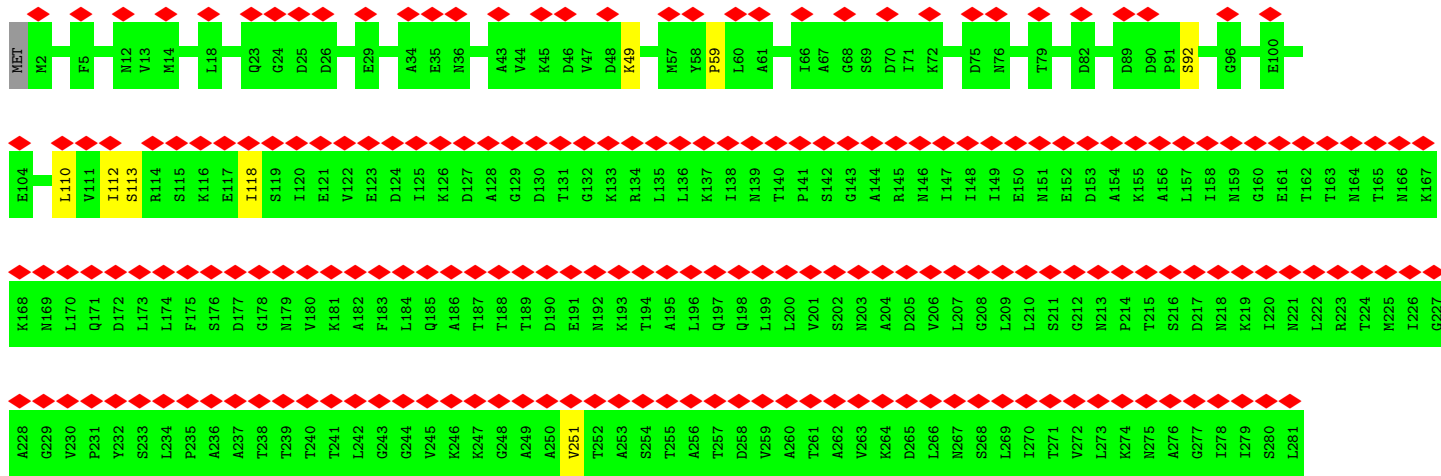
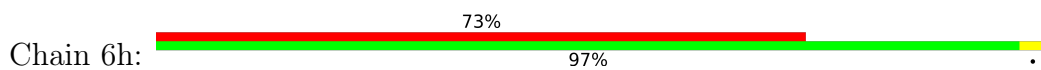




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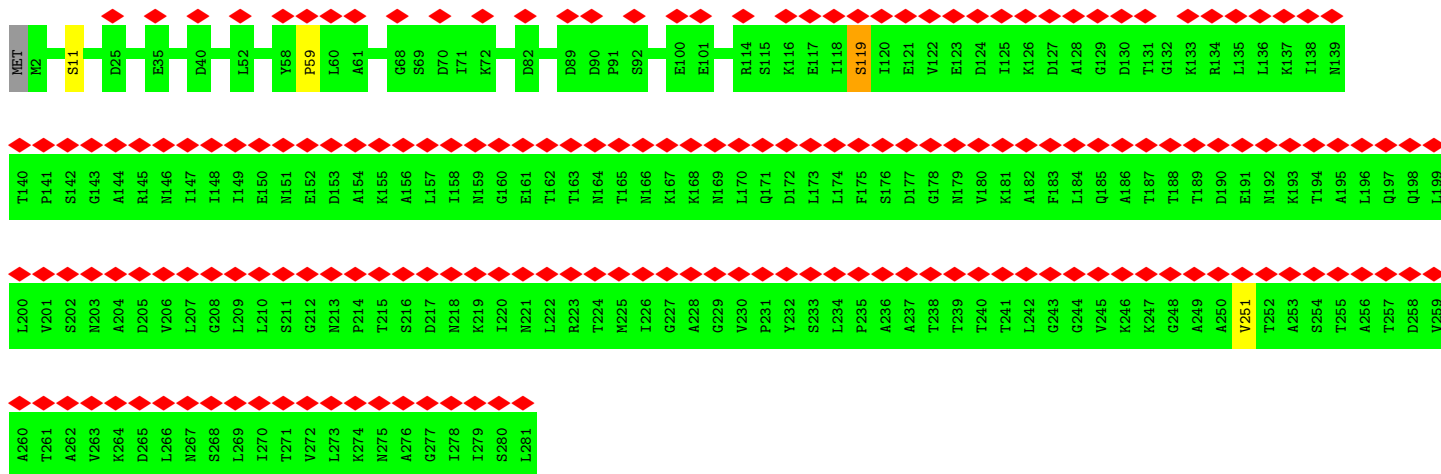


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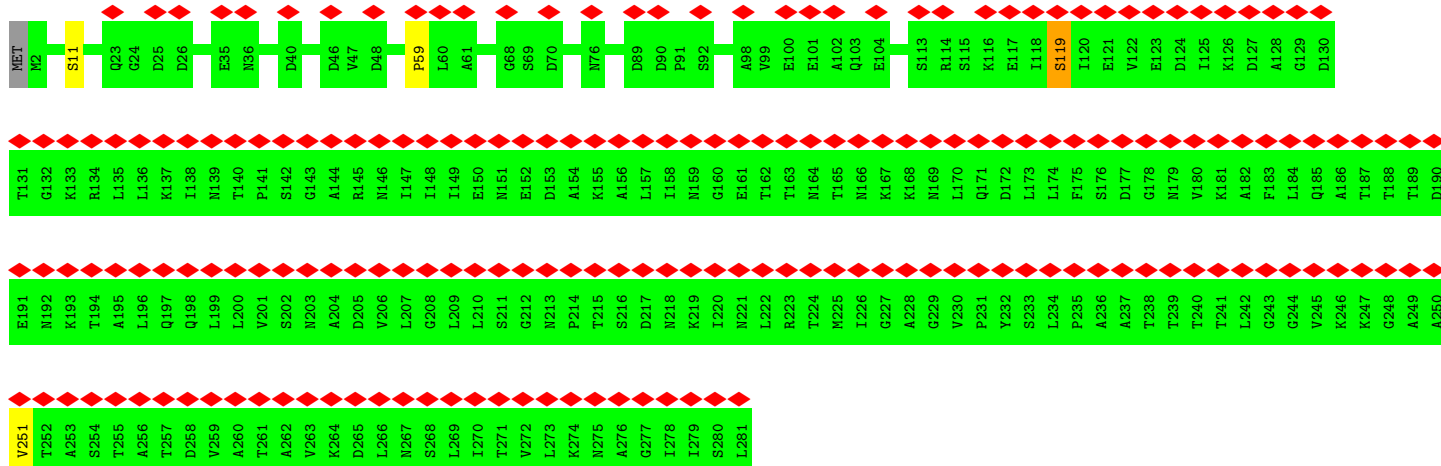


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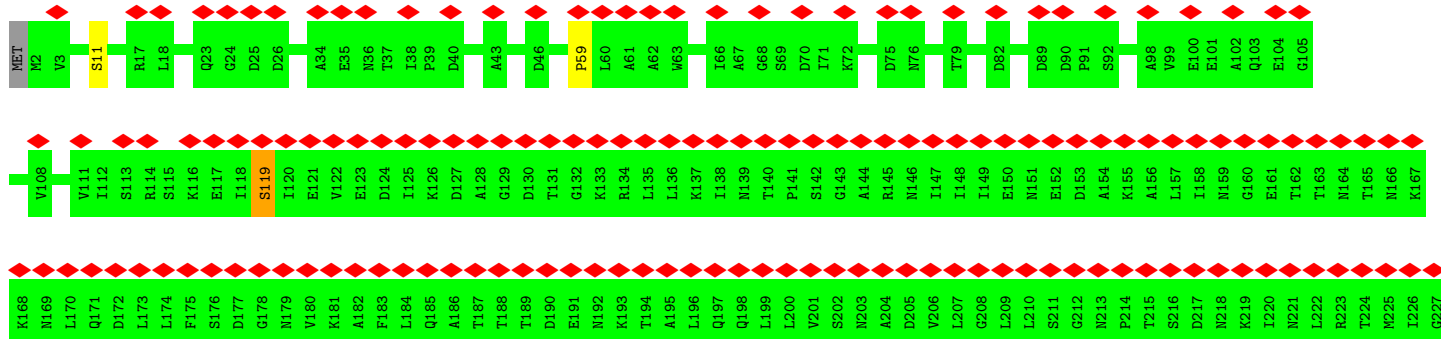
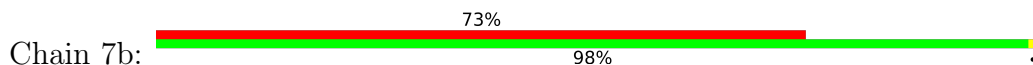


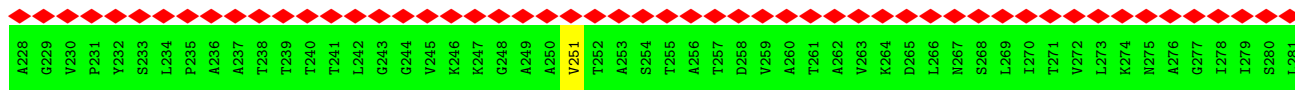


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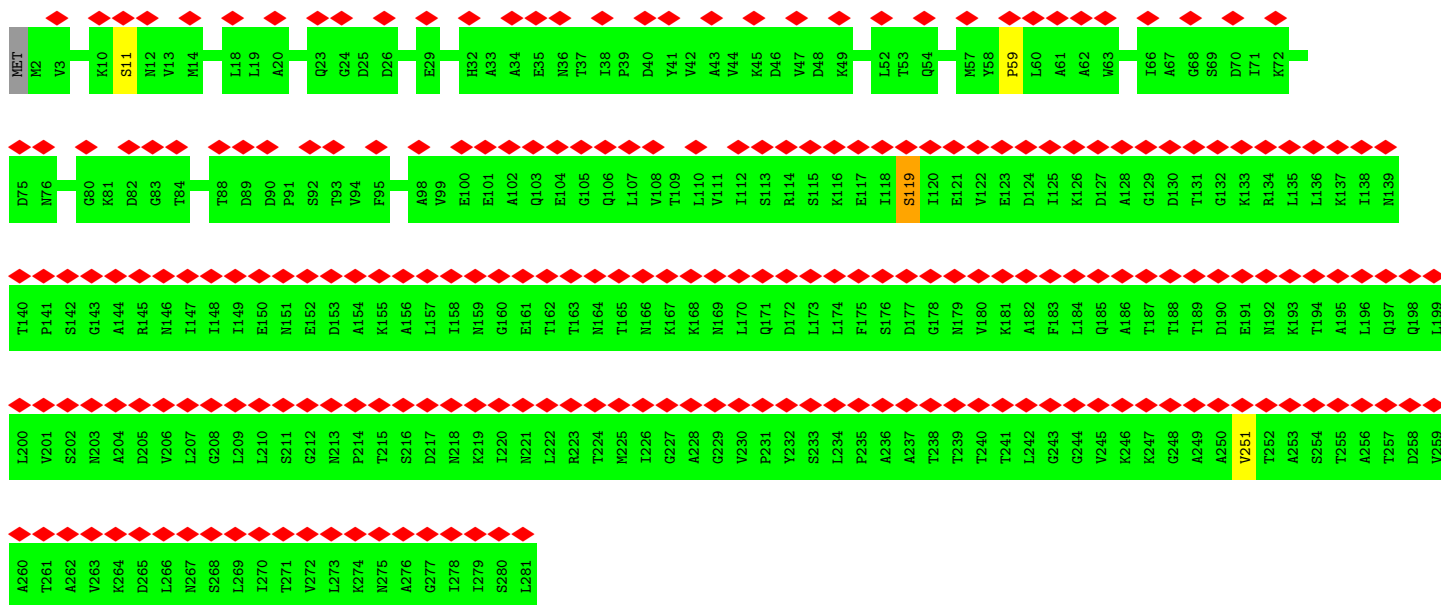
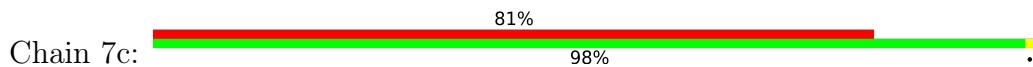


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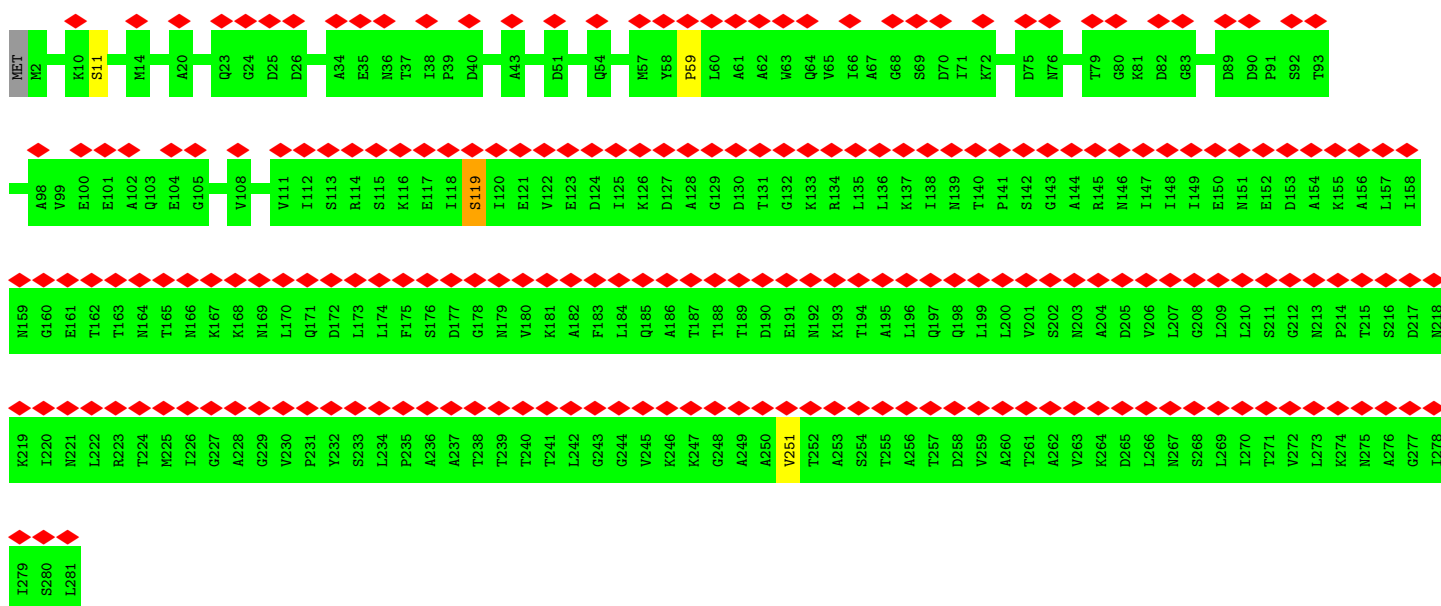
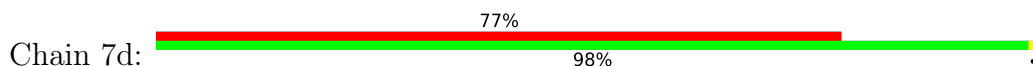




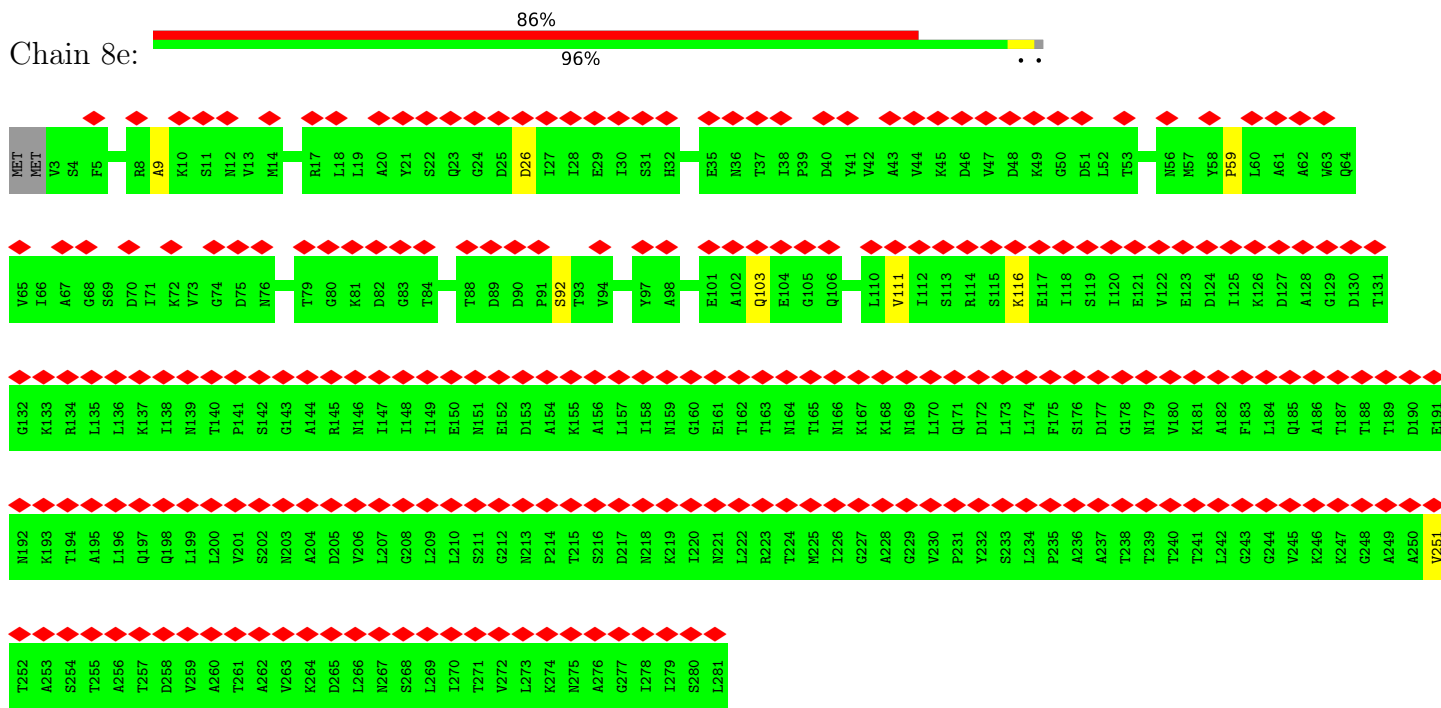
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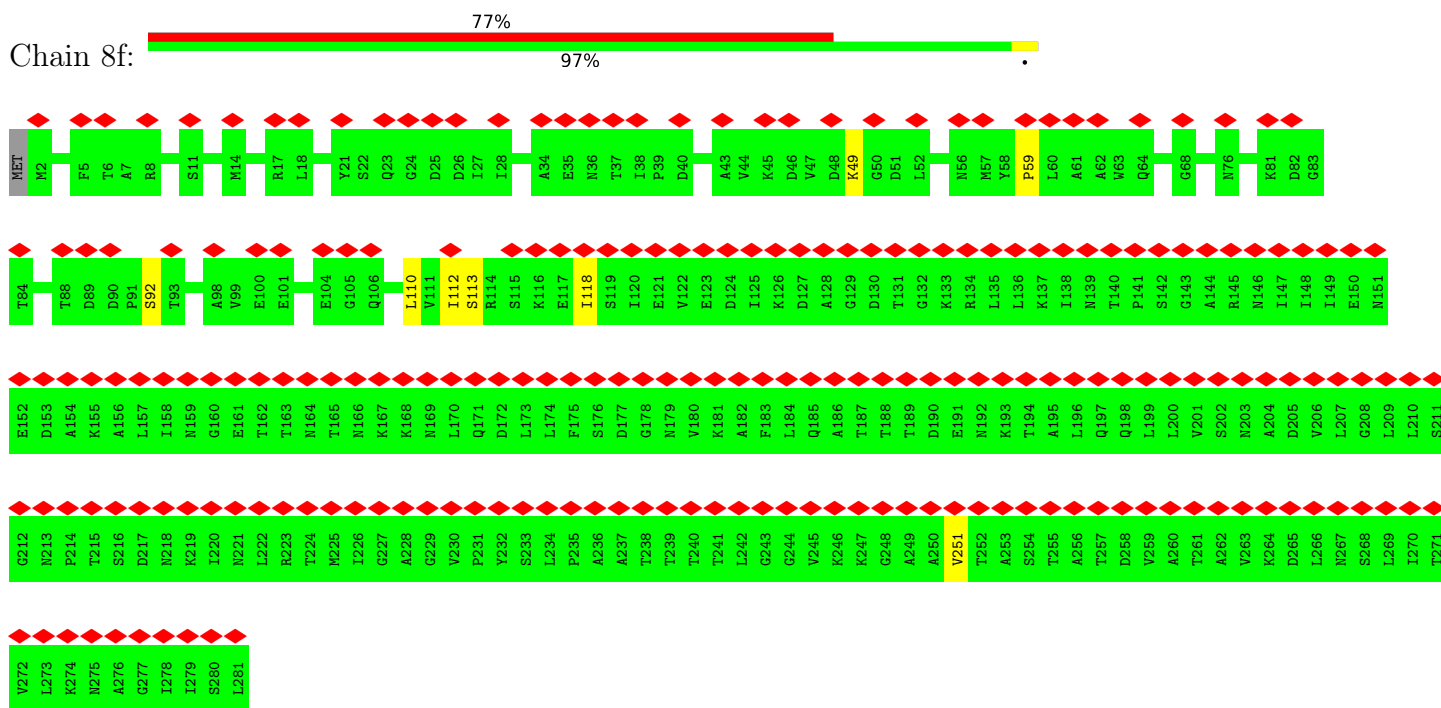
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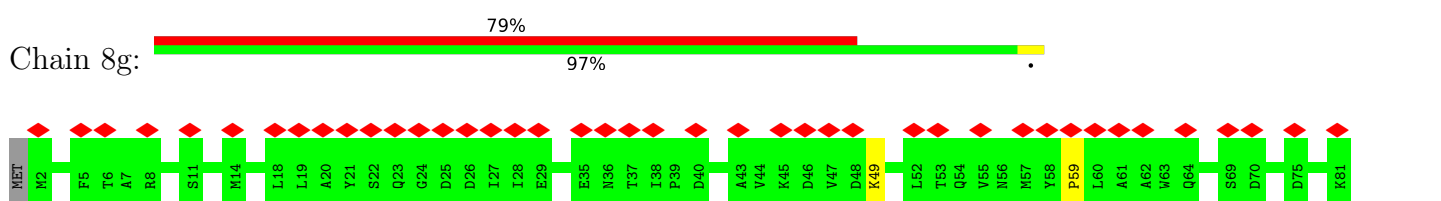
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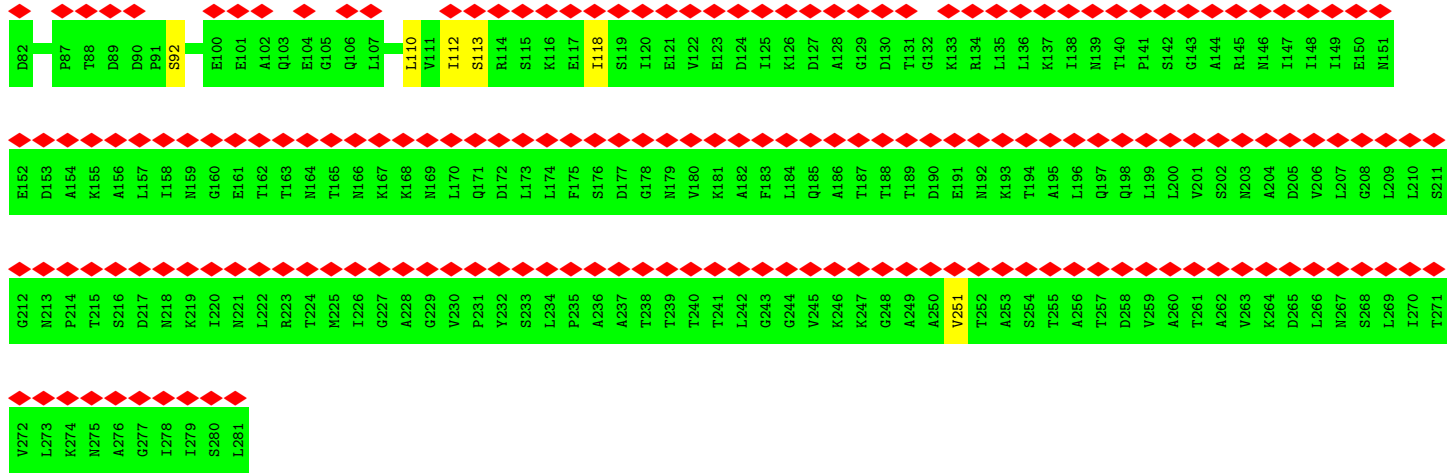


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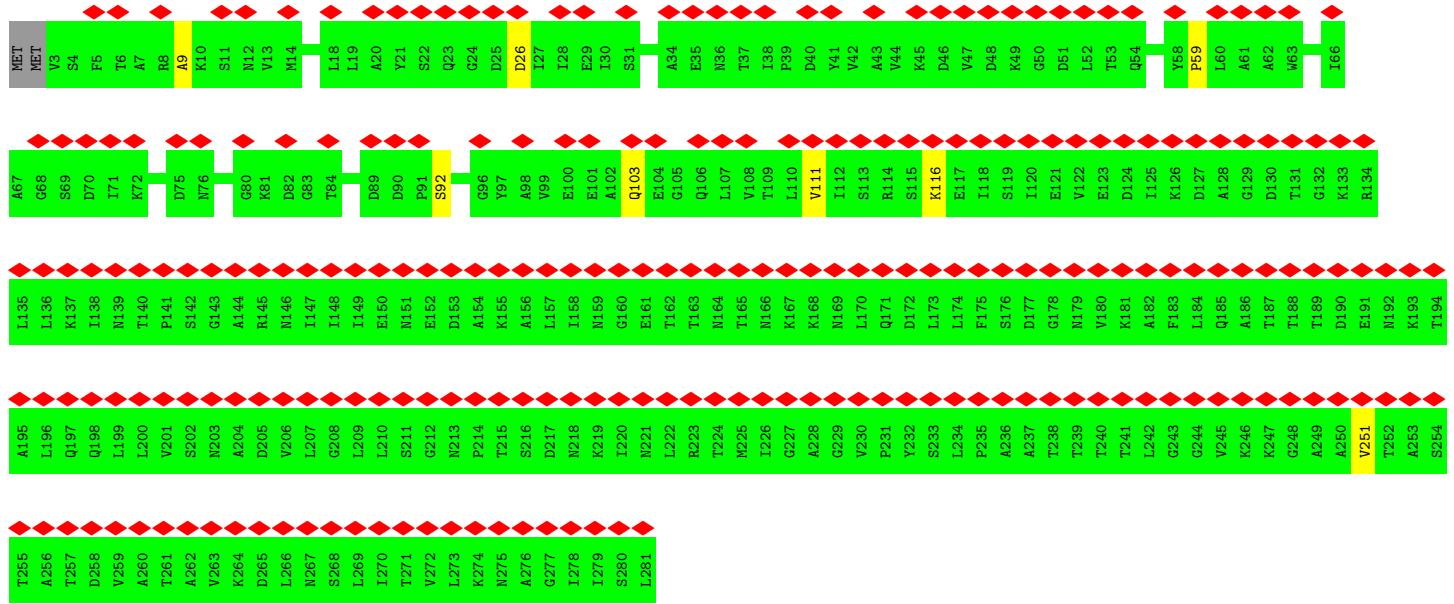
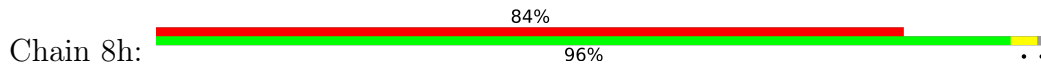


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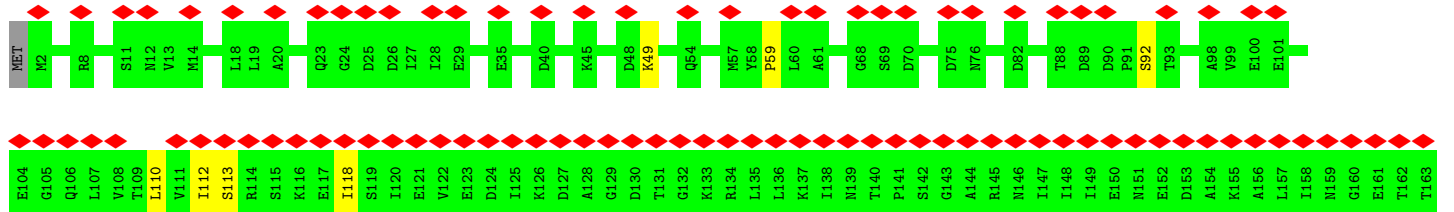
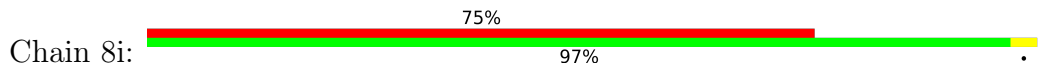


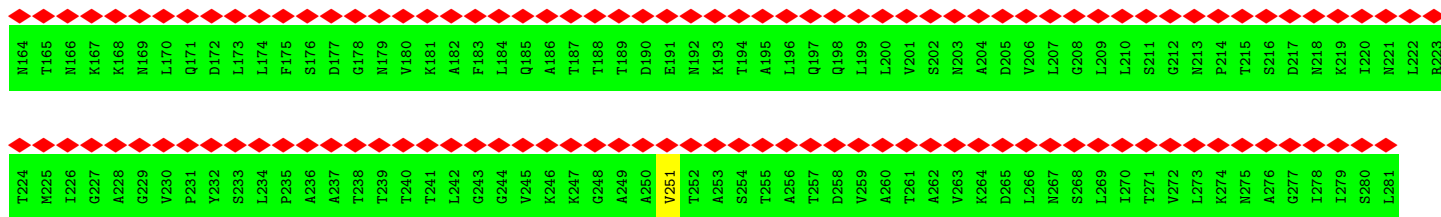


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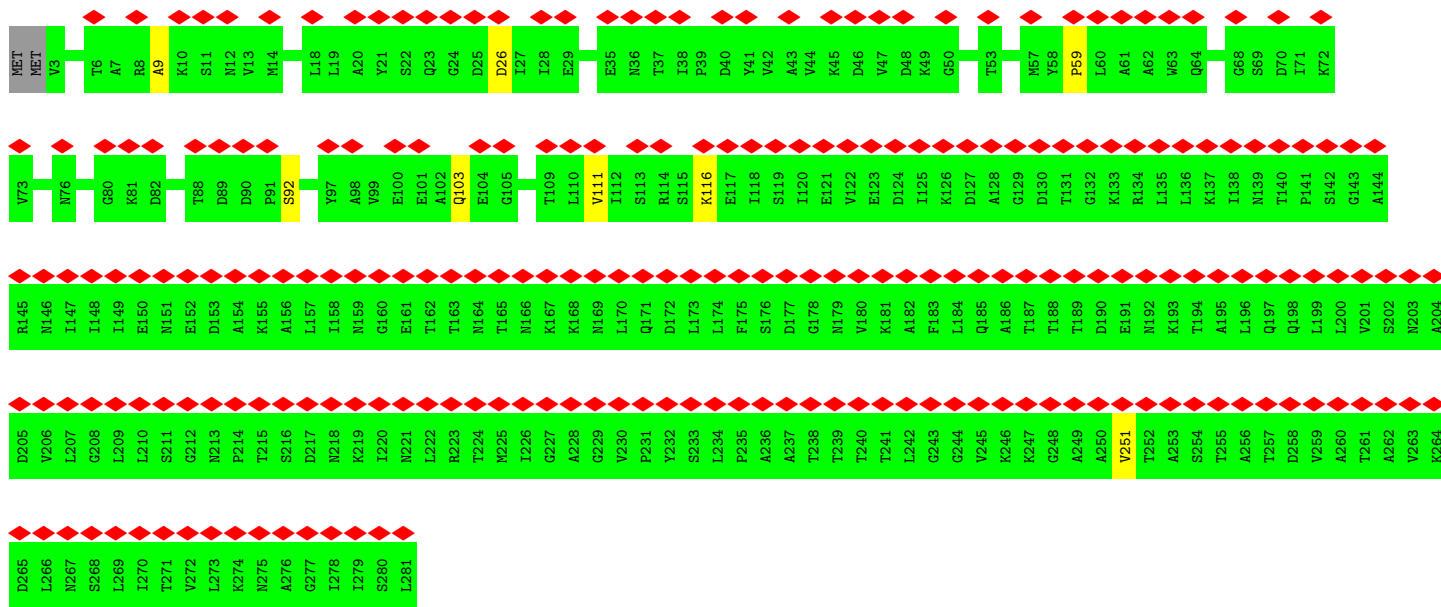
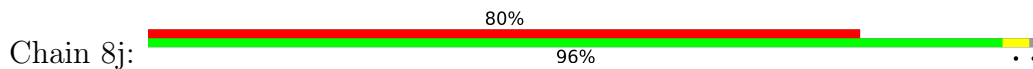


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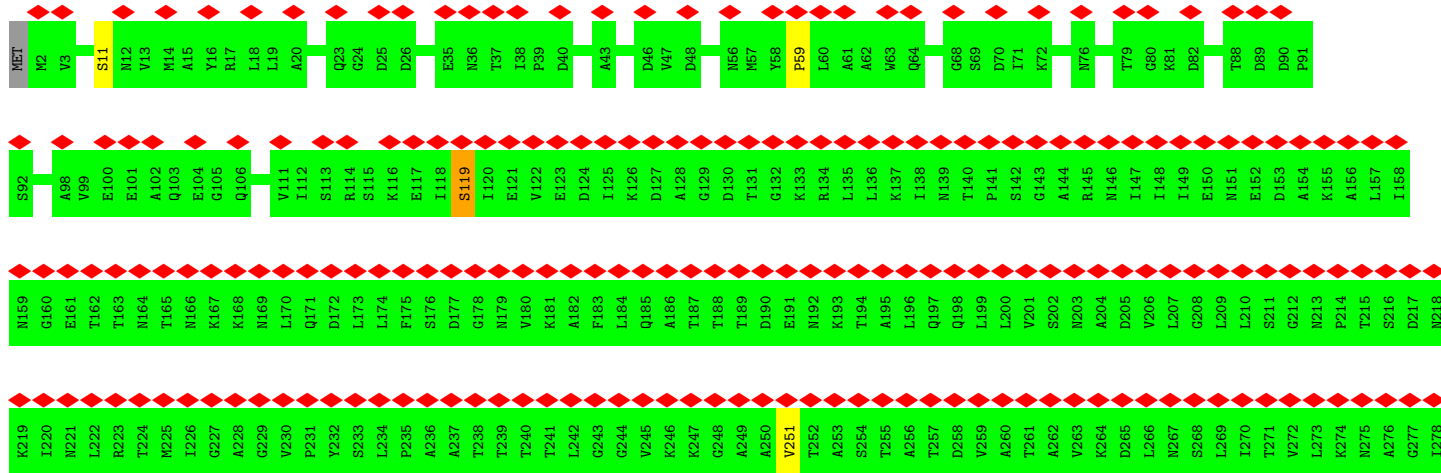
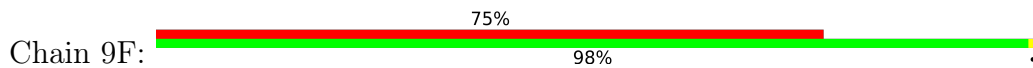




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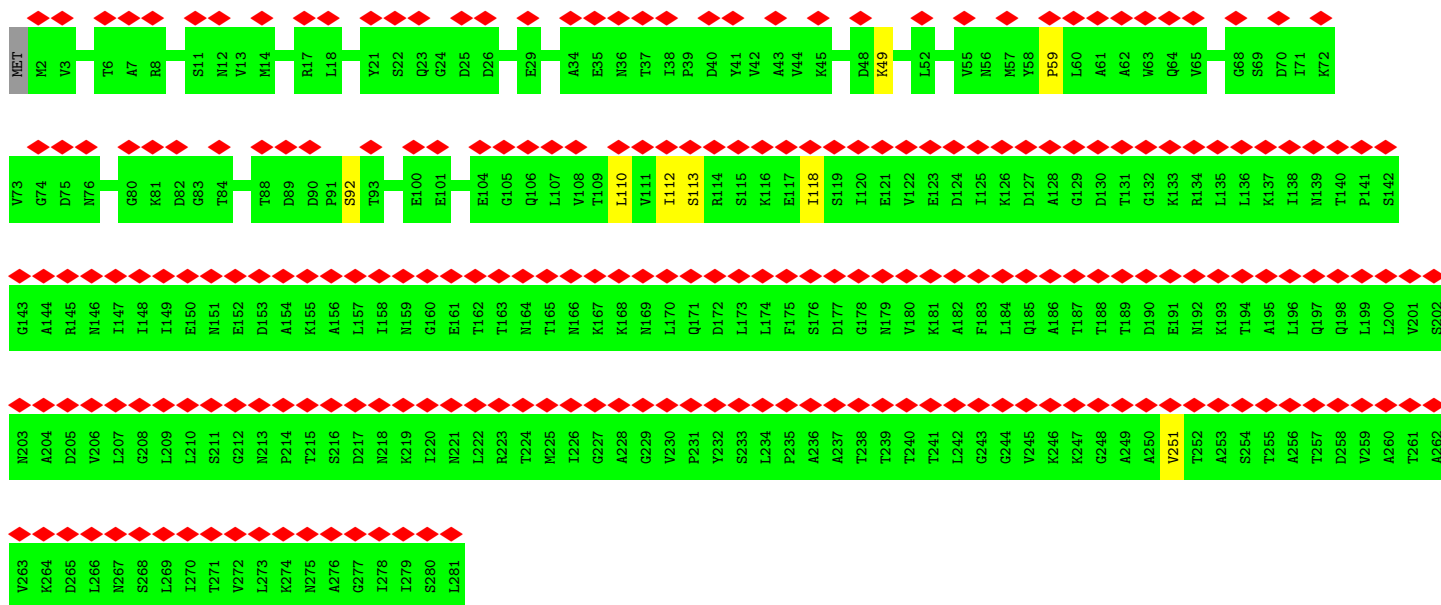
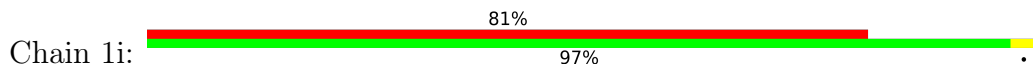


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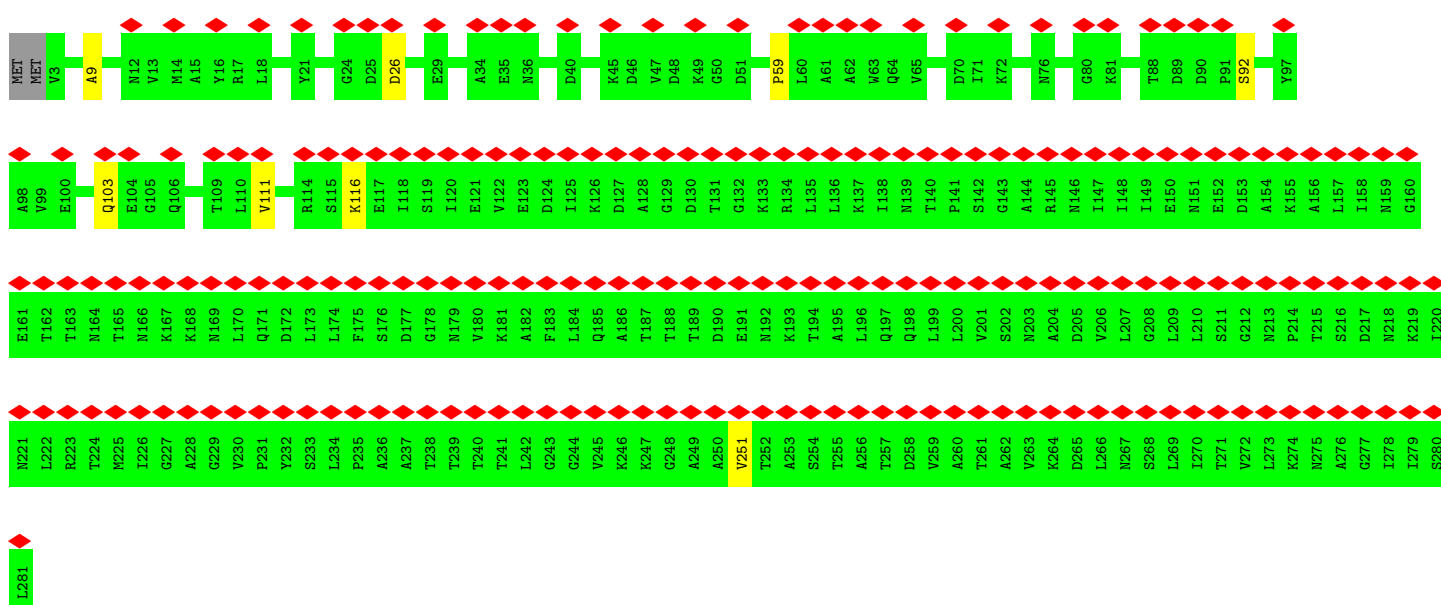
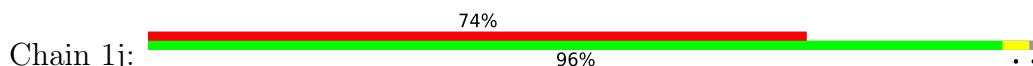




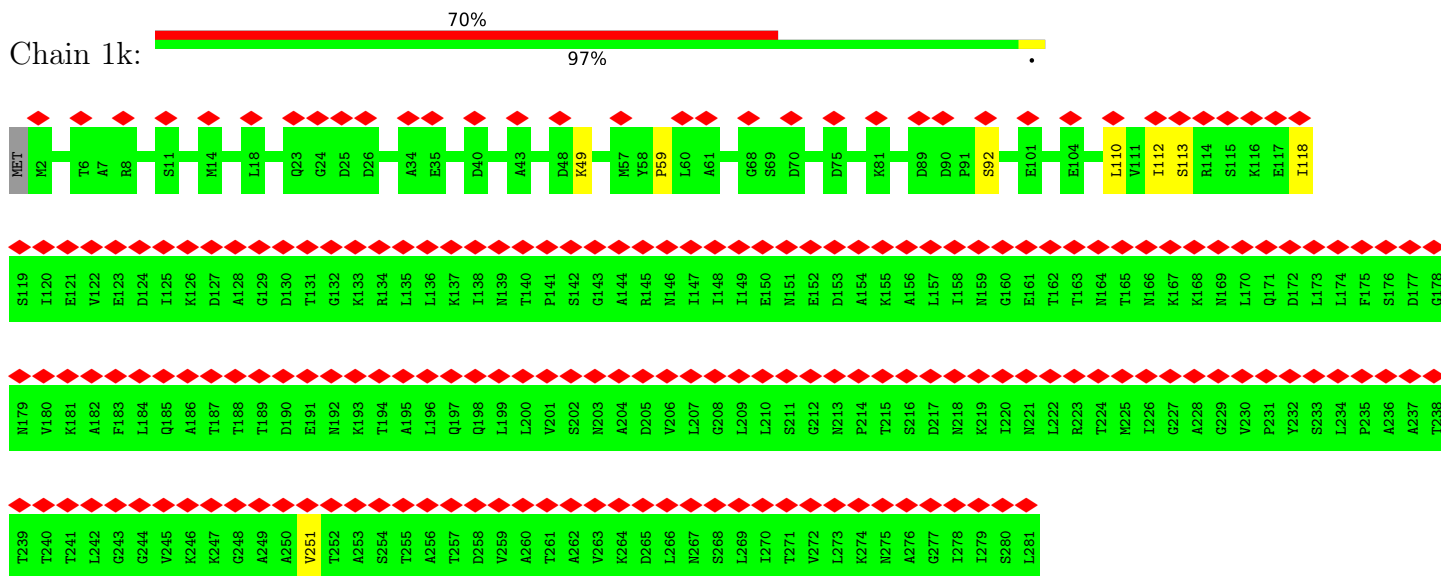
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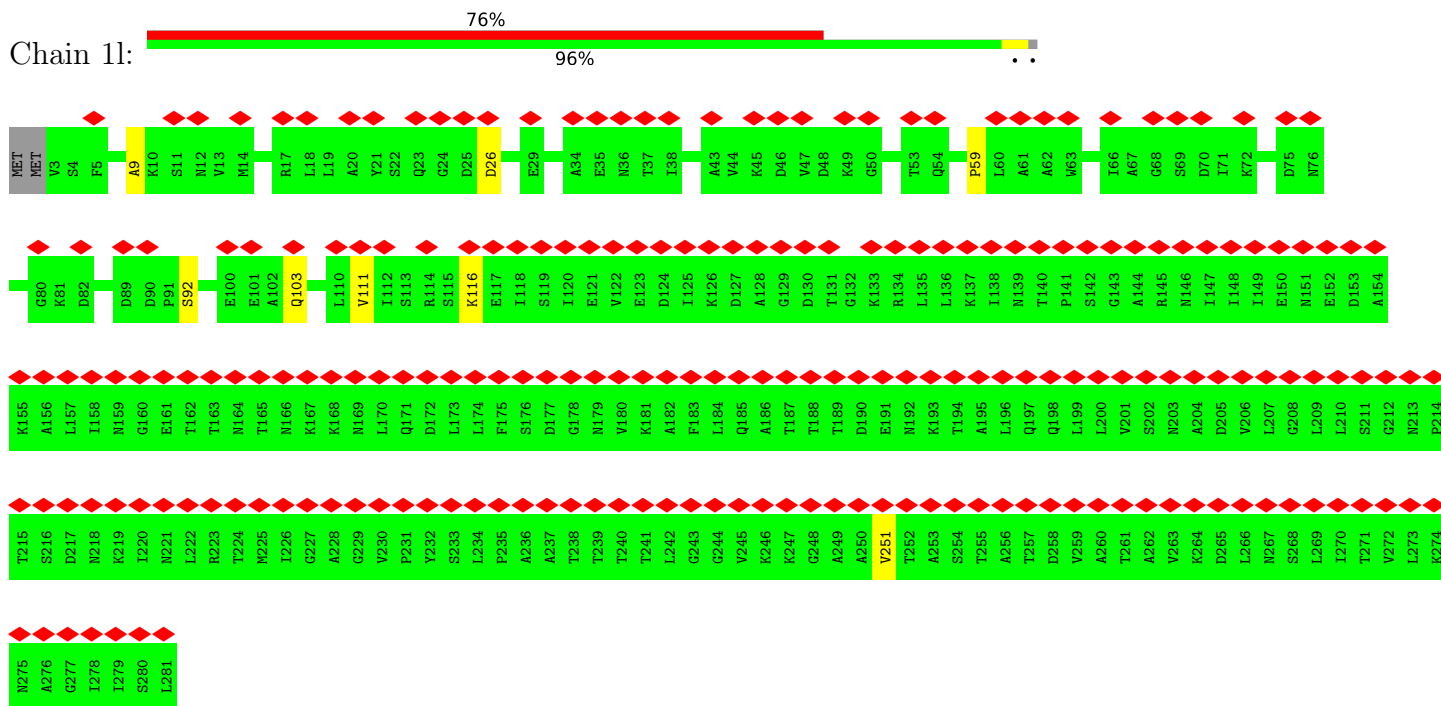
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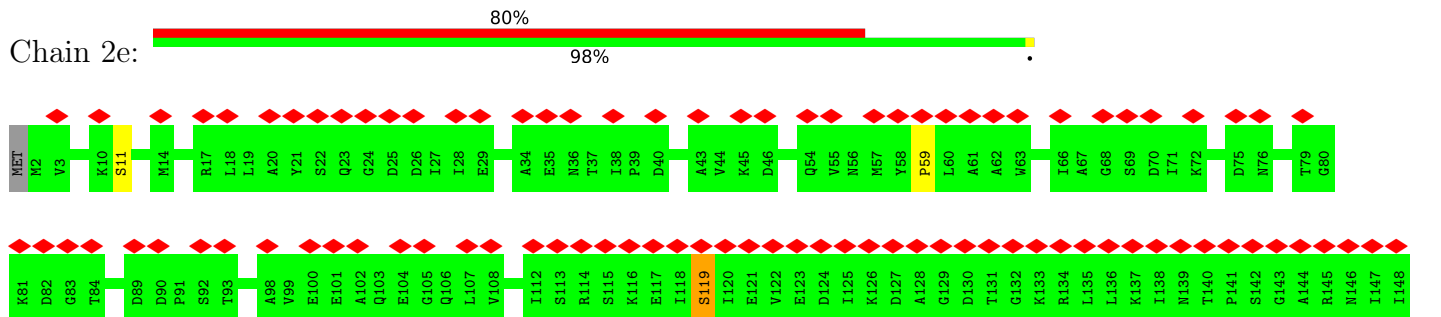
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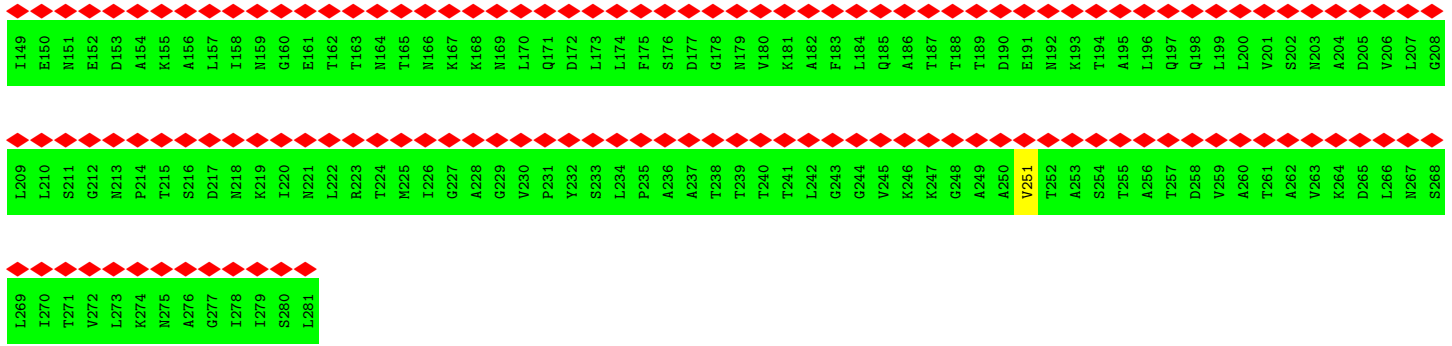


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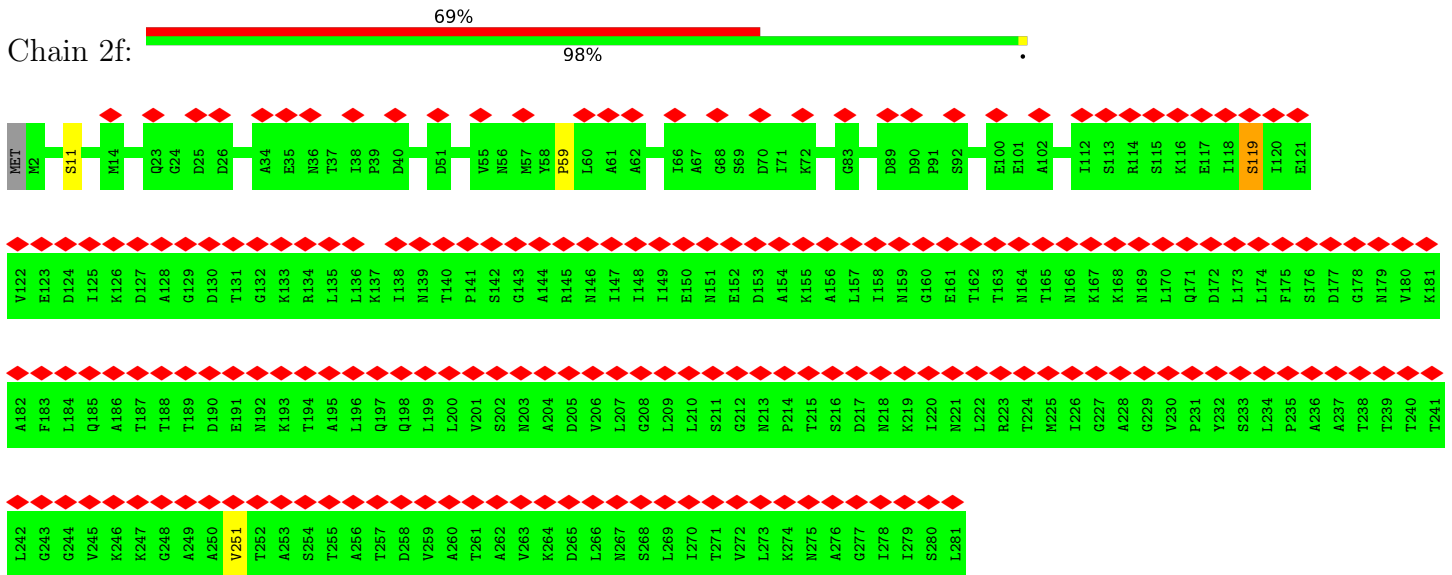


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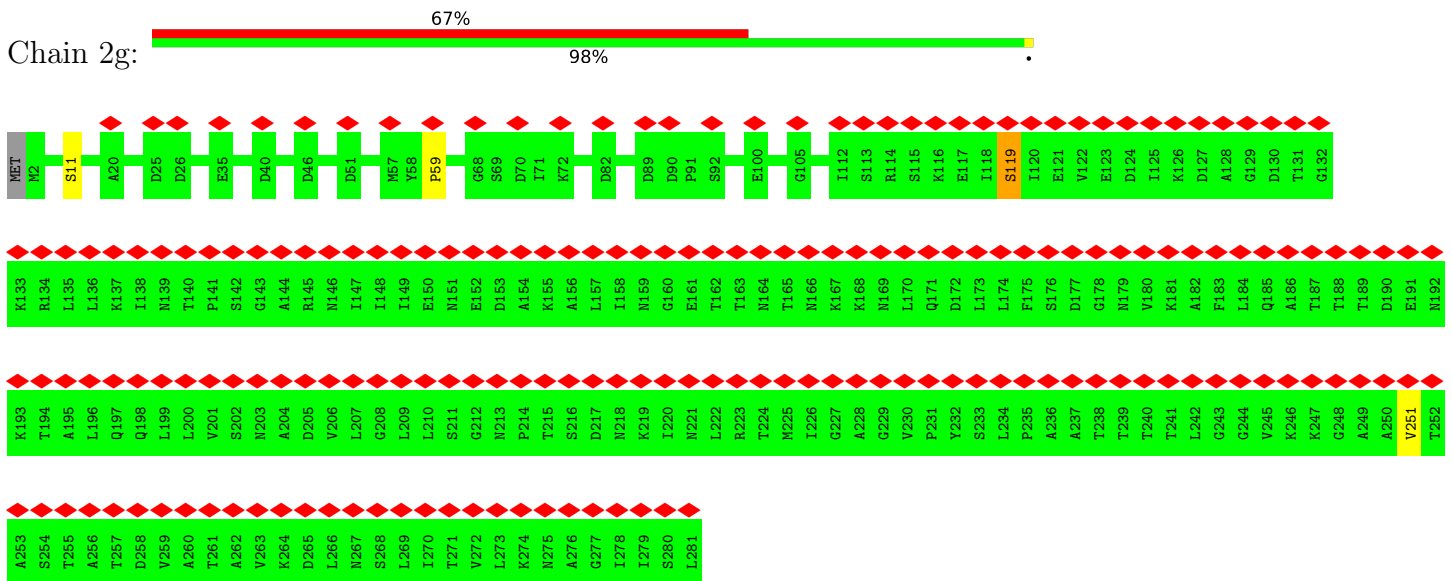




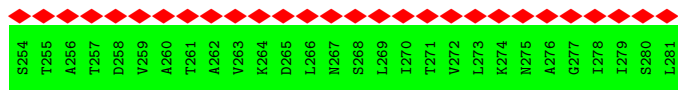
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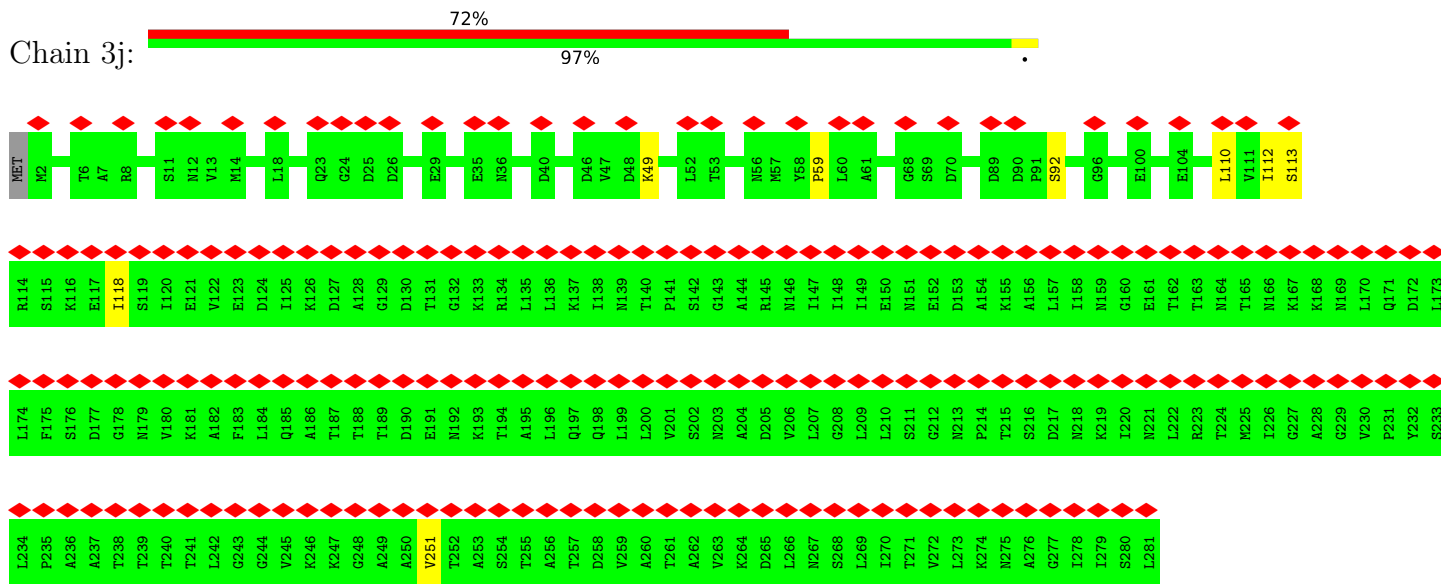
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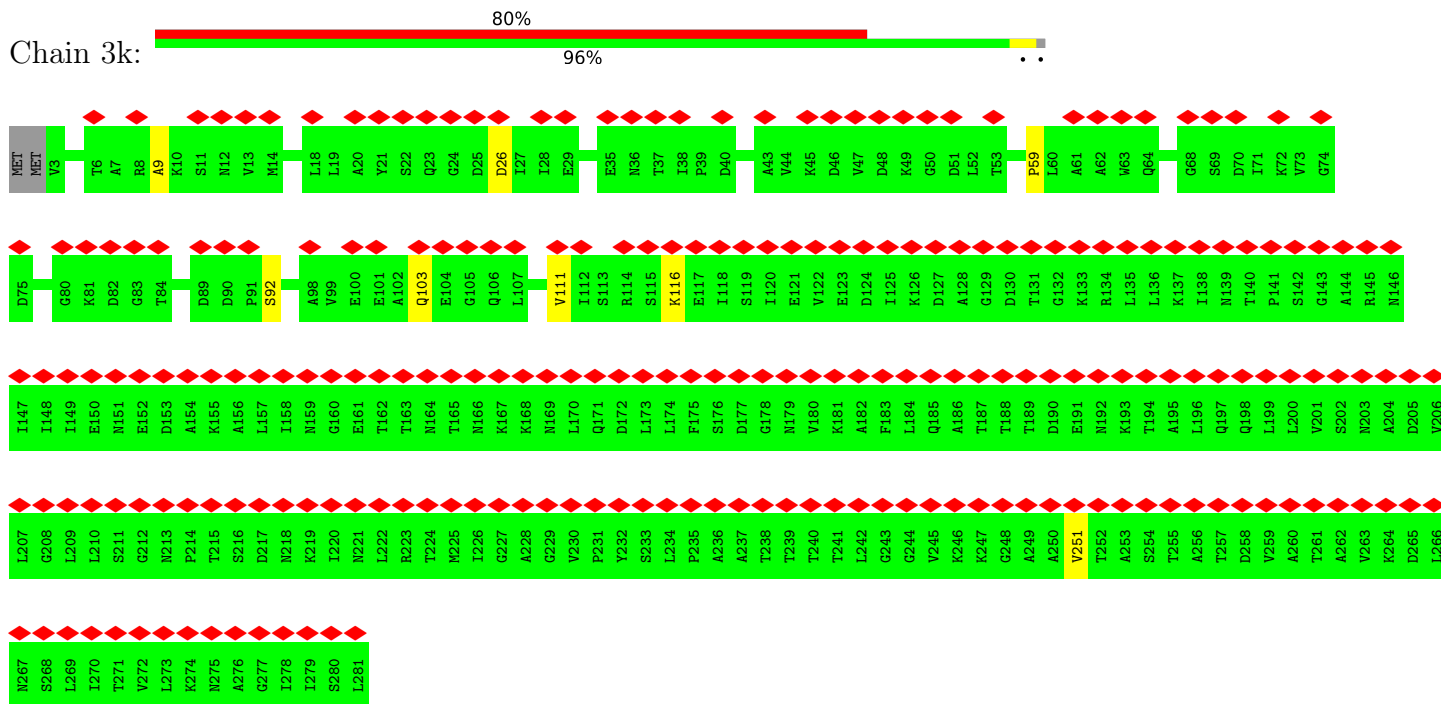
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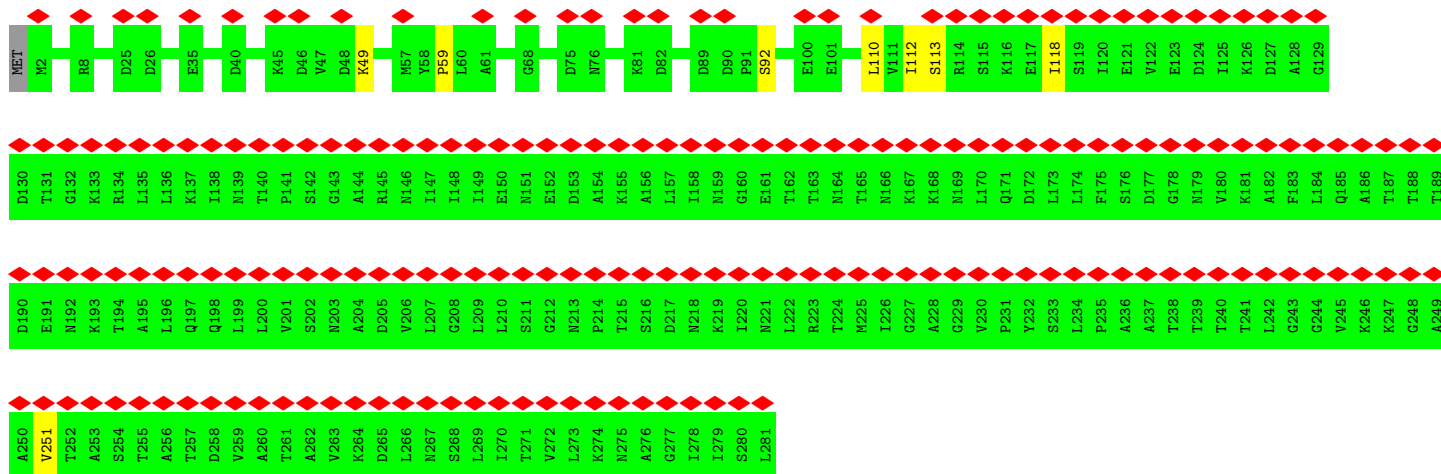


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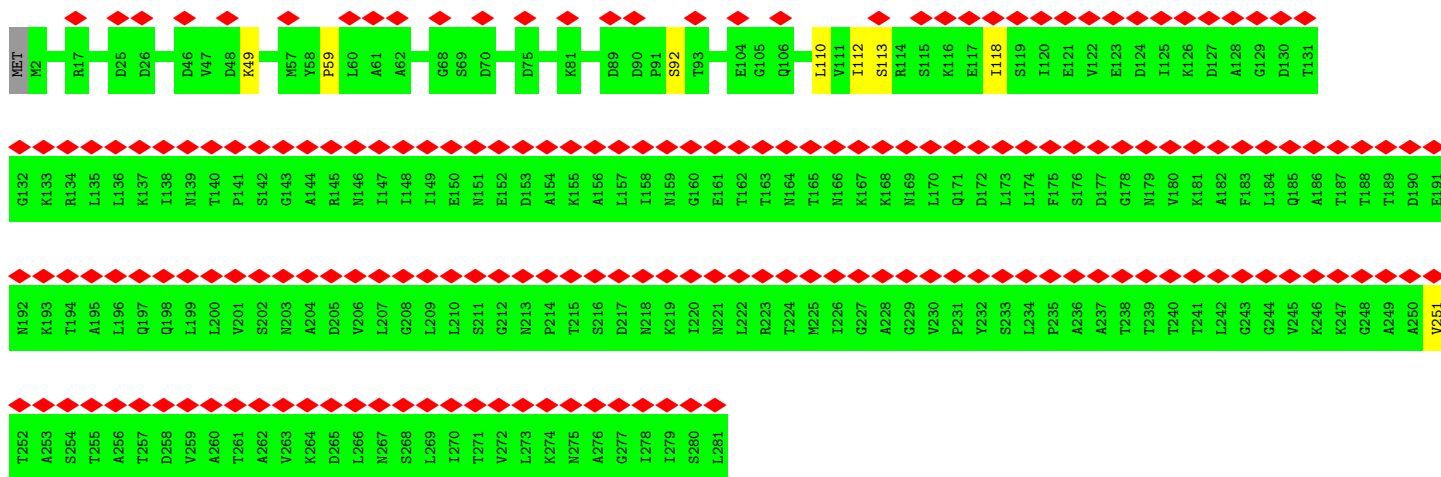


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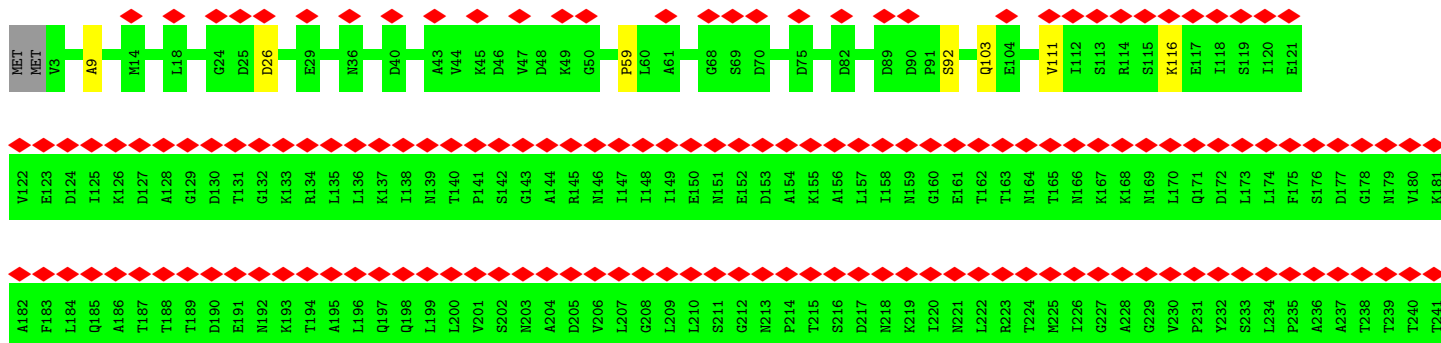


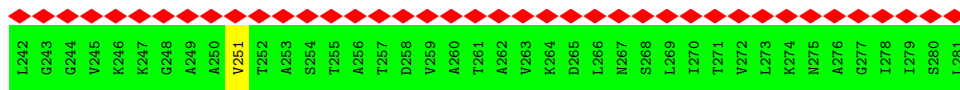


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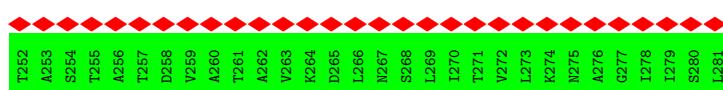
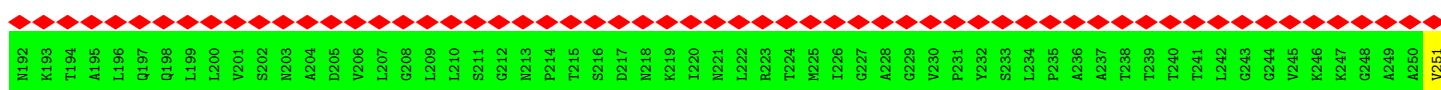
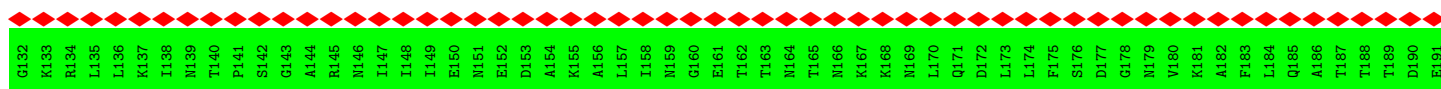
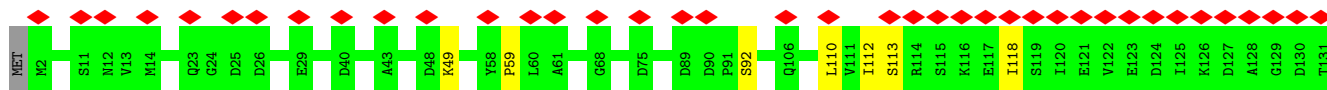


• Molecule 2: Capsid fiber protein

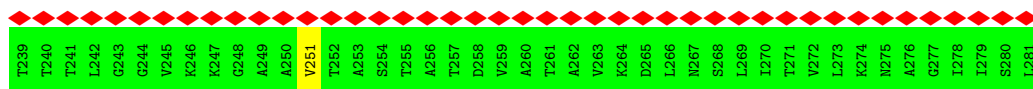
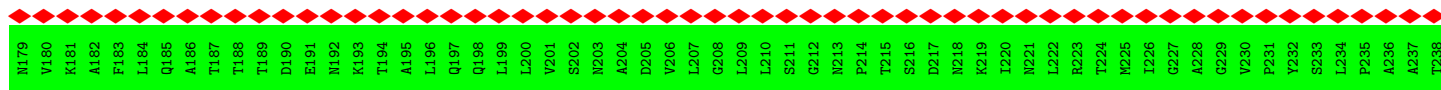
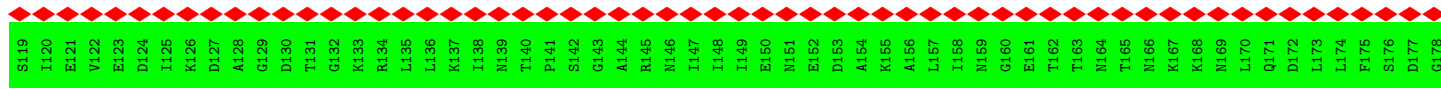
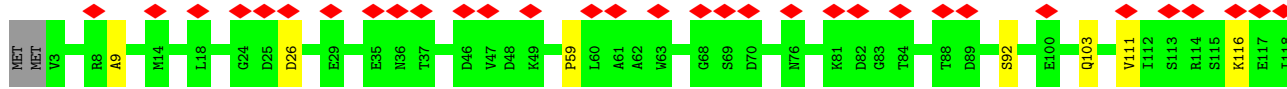




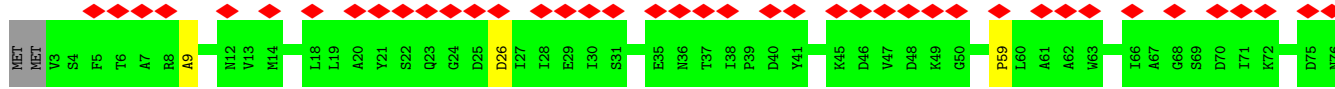
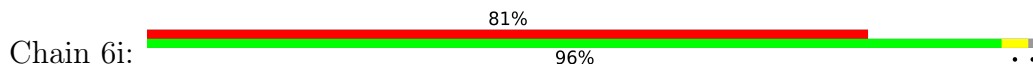
• Molecule 2: Capsid fiber protein



• Molecule 2: Capsid fiber protein

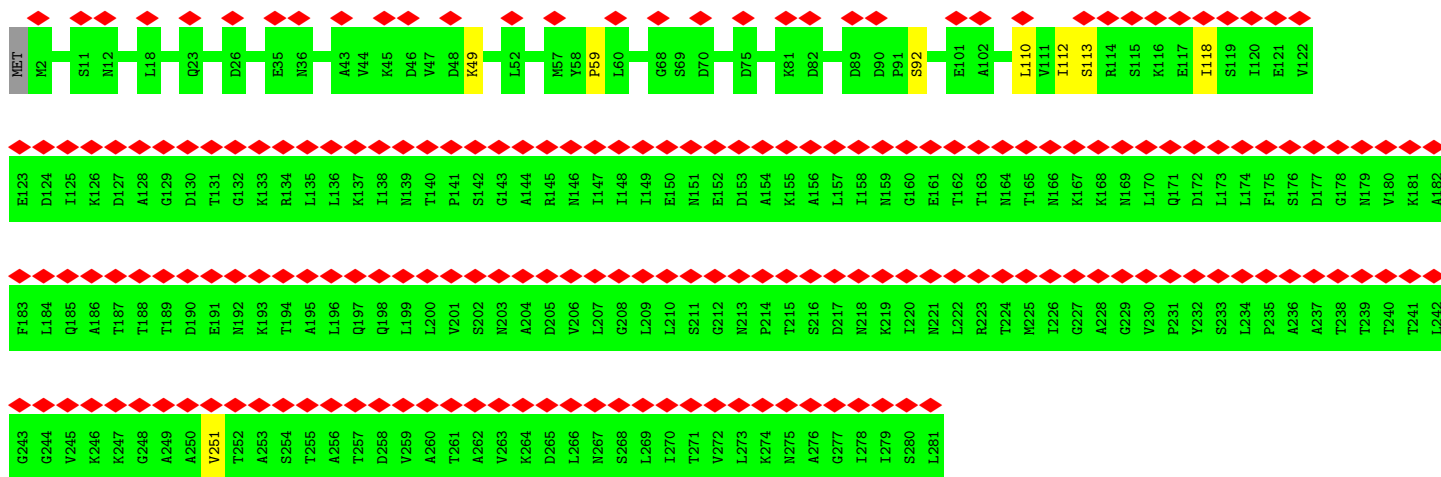


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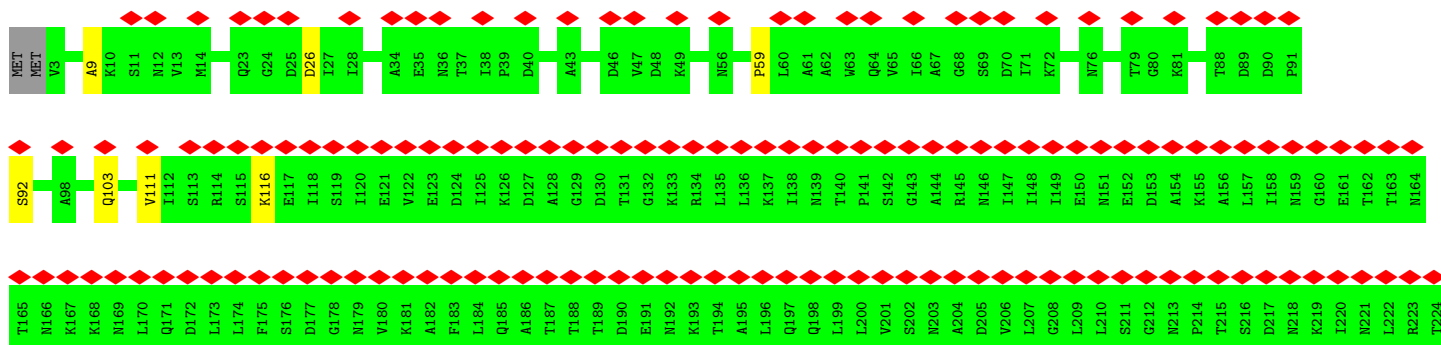
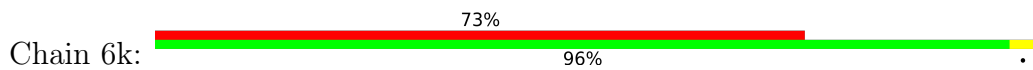


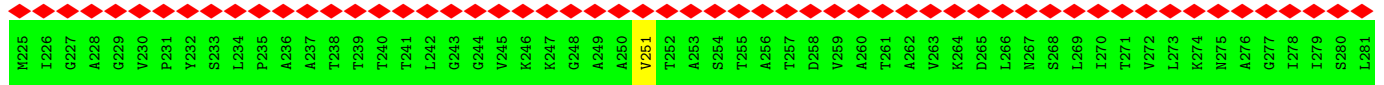


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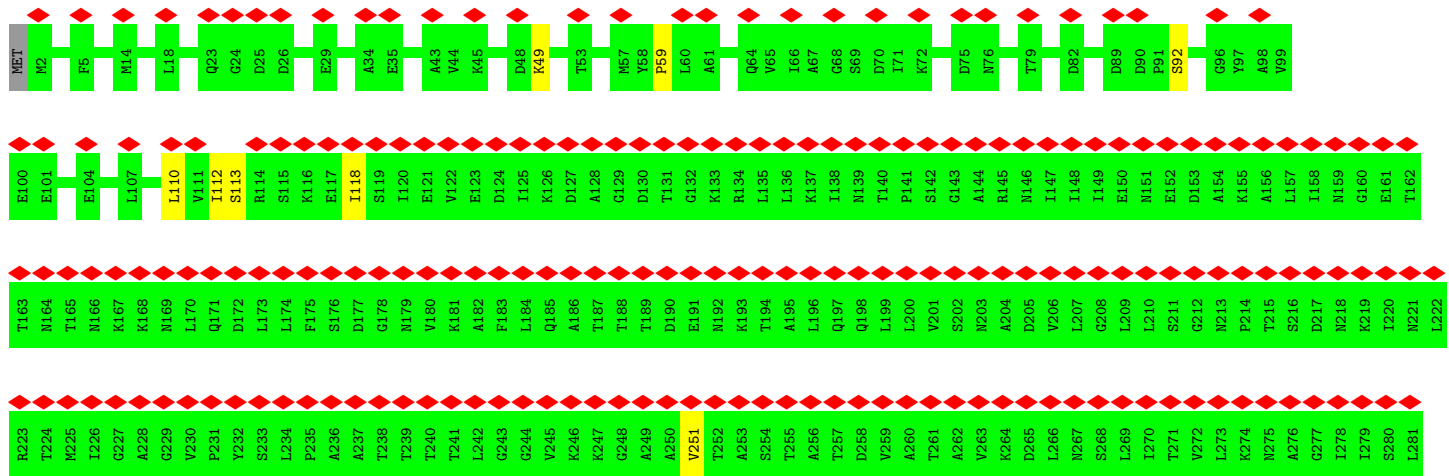
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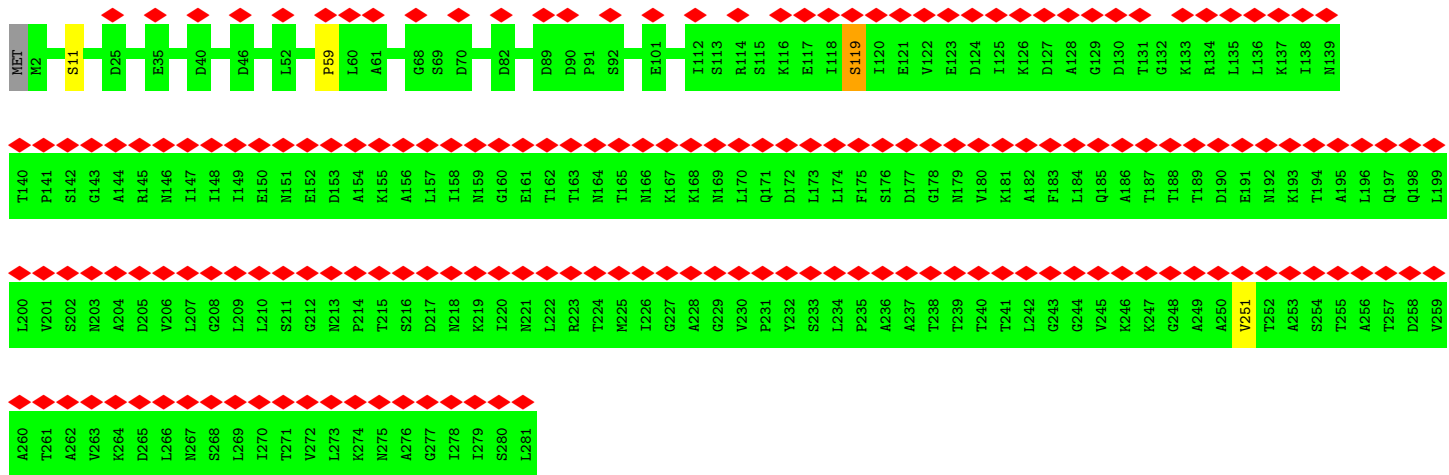
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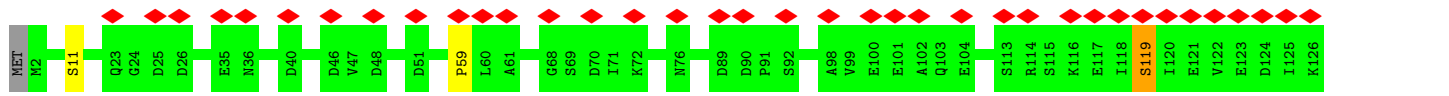
• Molecule 2: Capsid fiber protein

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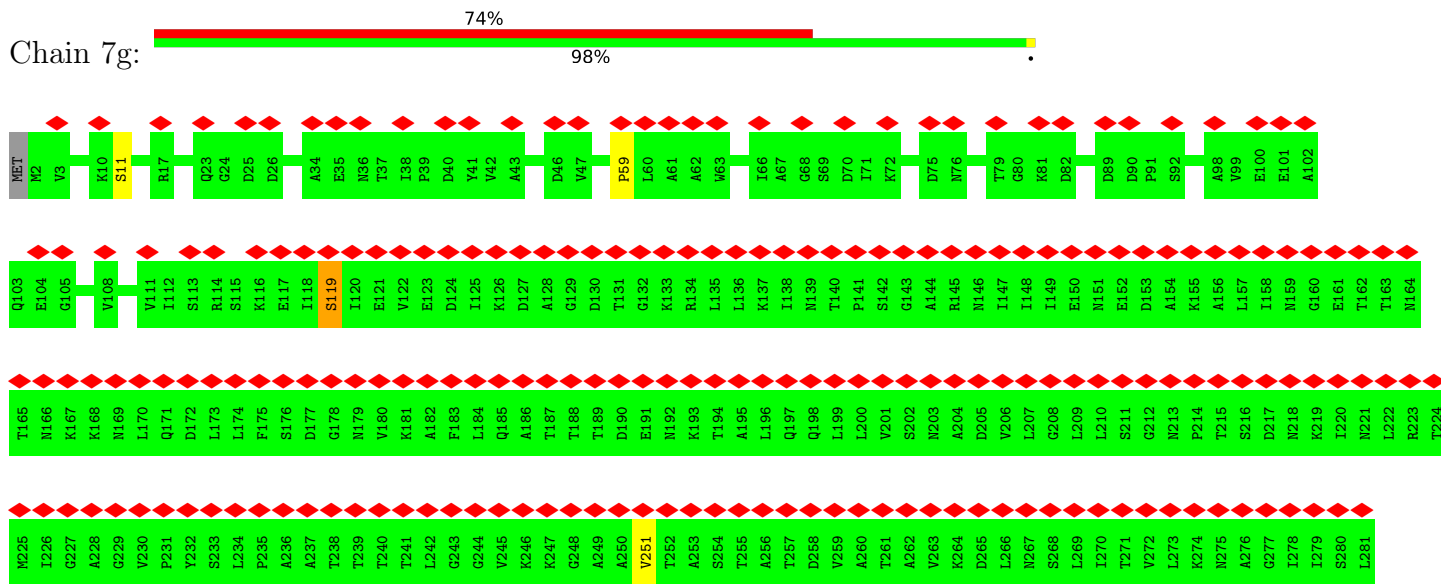
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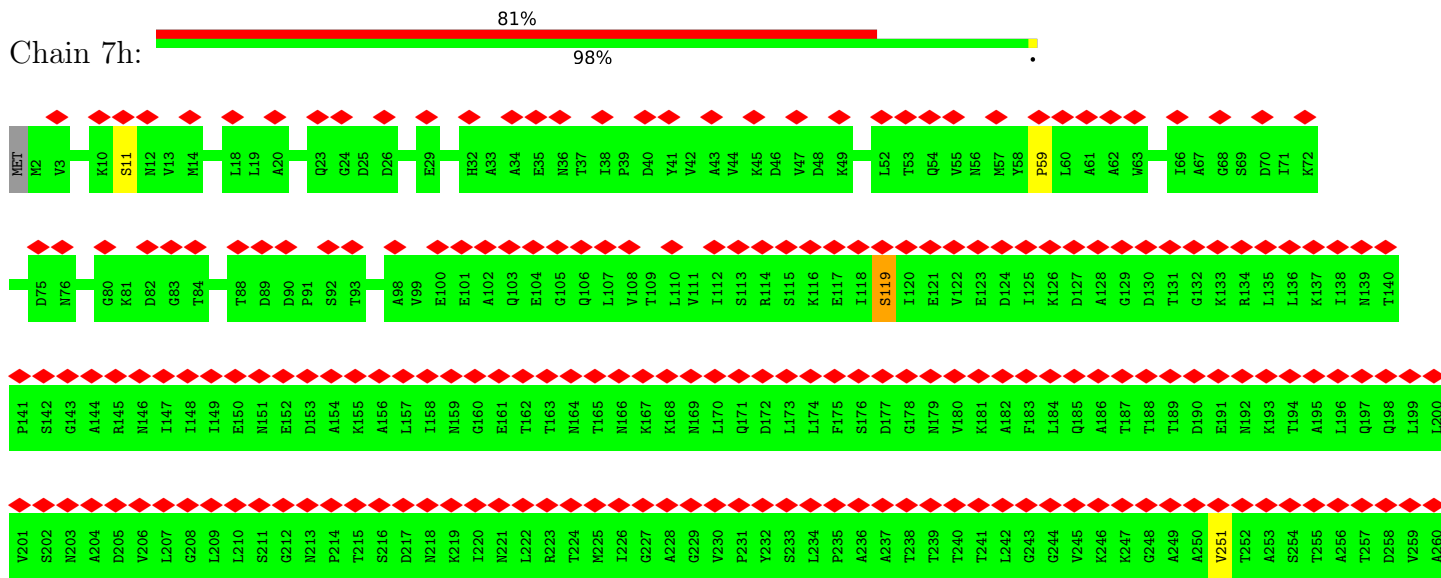


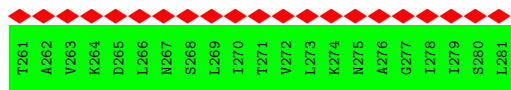


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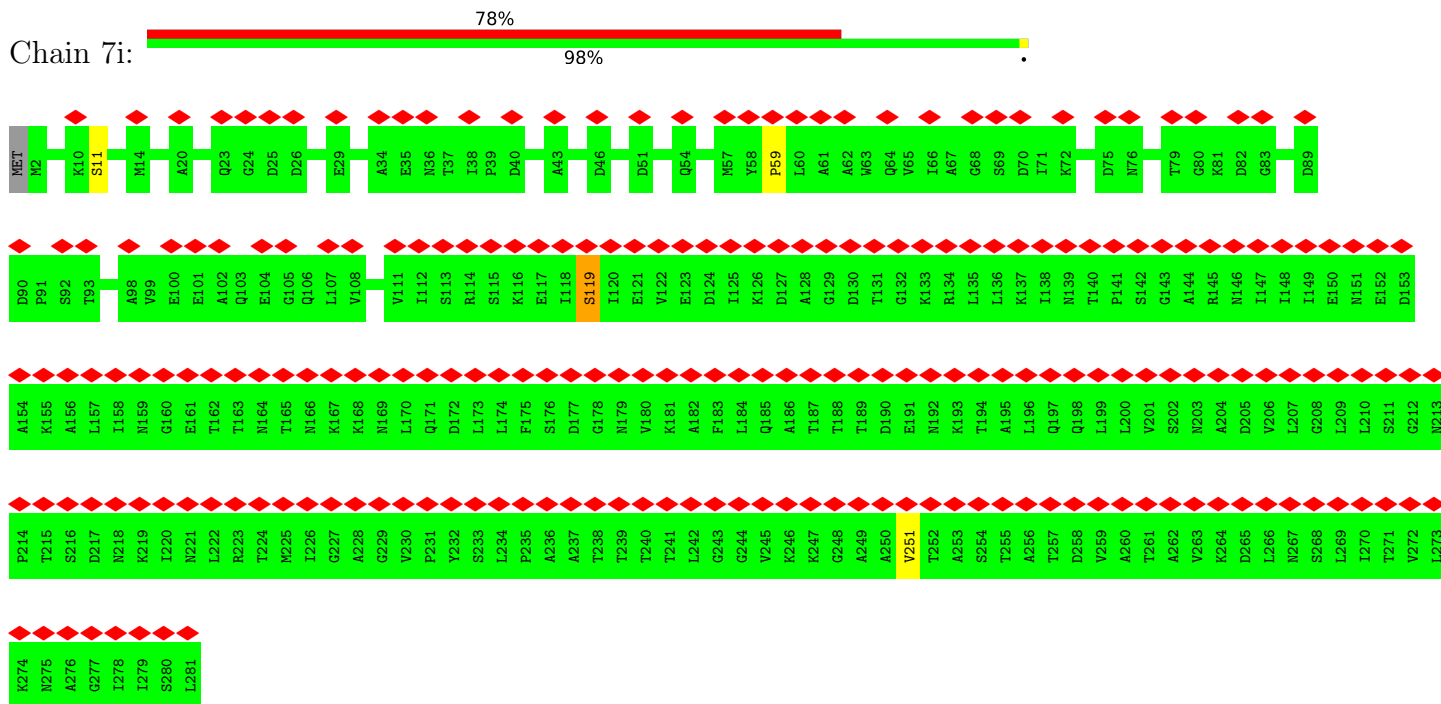


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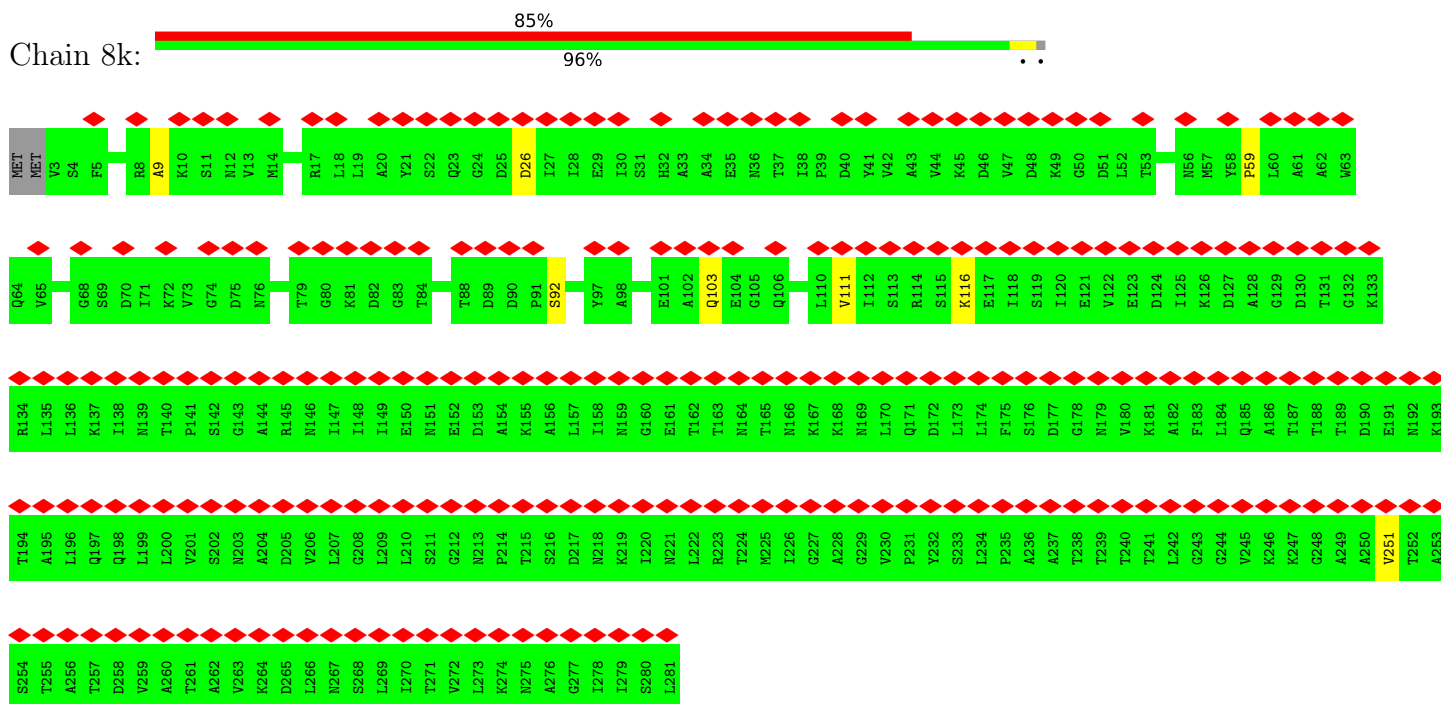




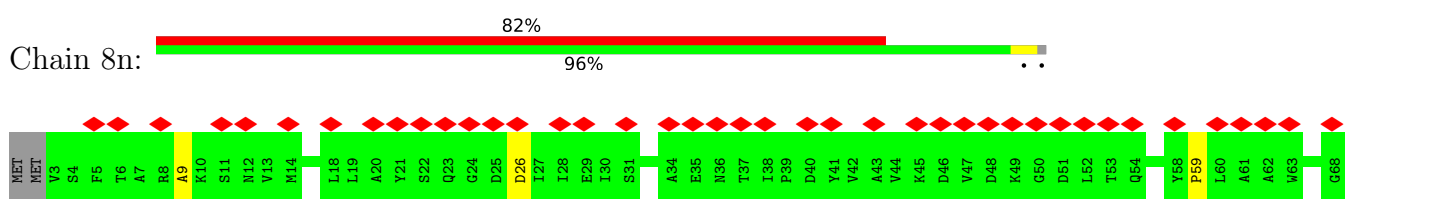
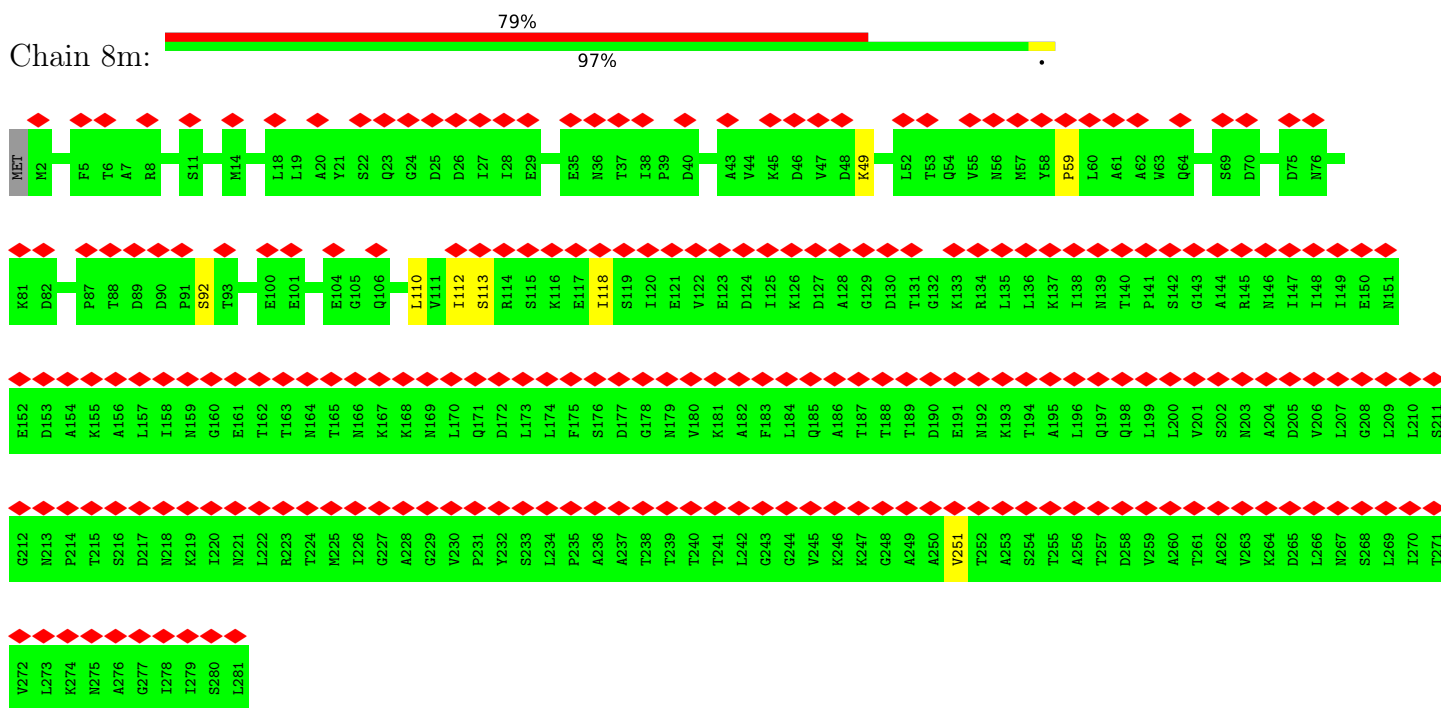
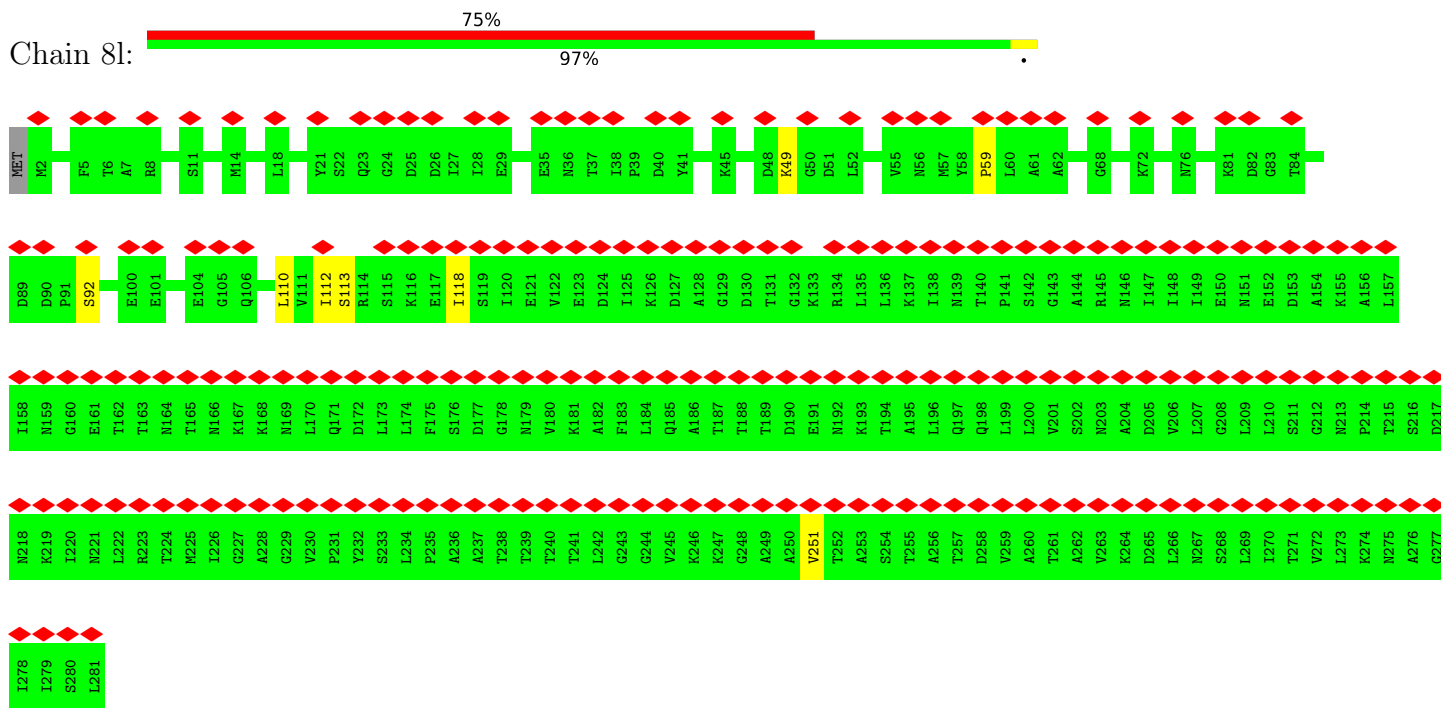
• Molecule 2: Capsid fiber protein

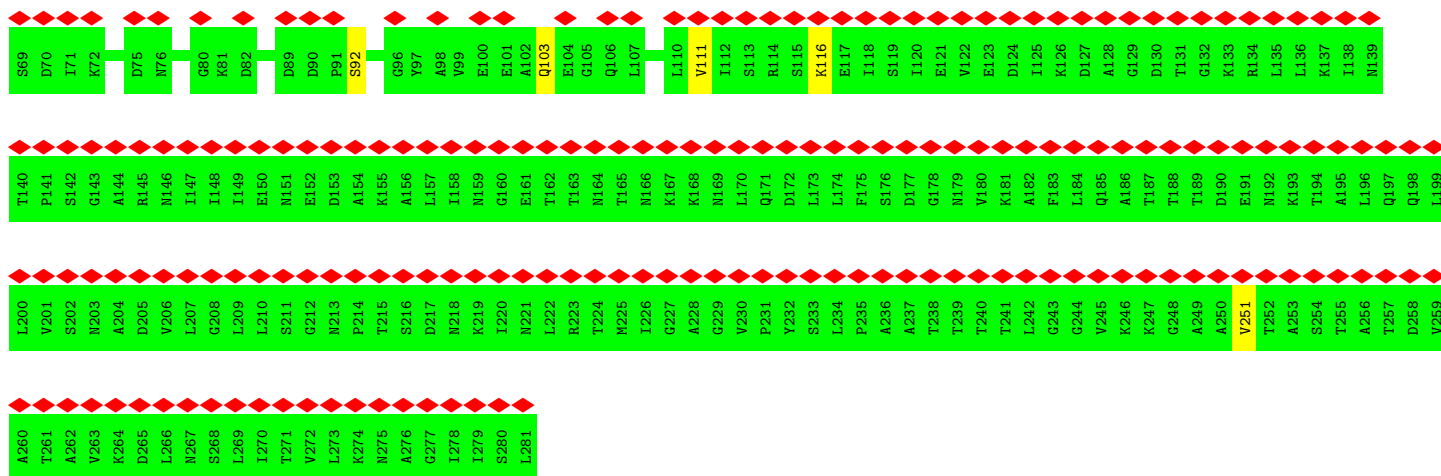


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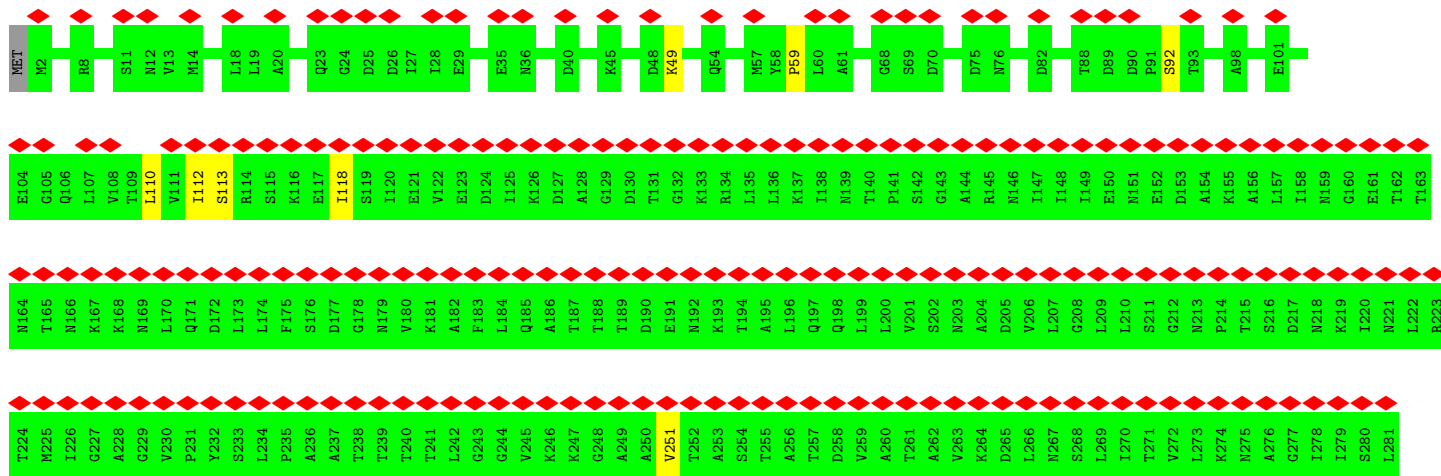
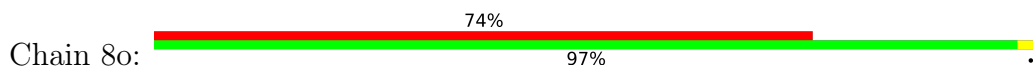


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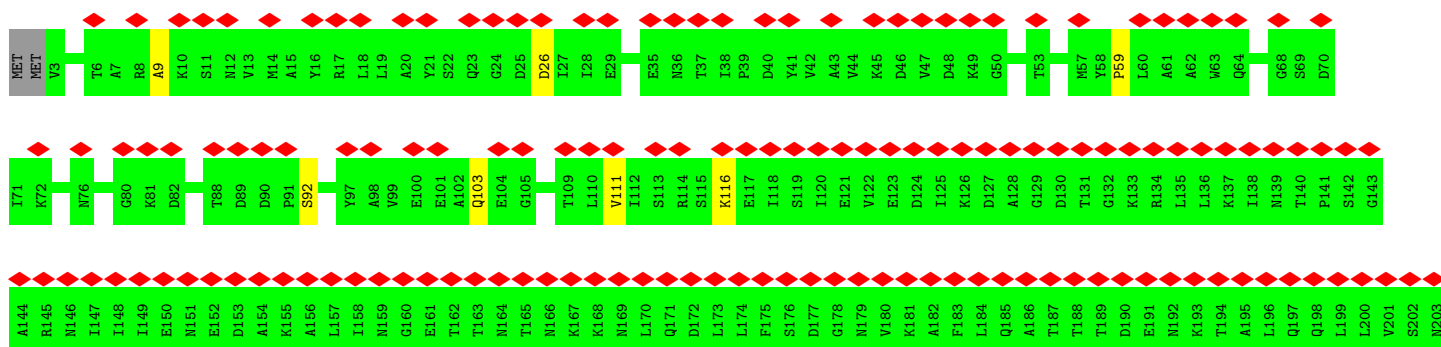
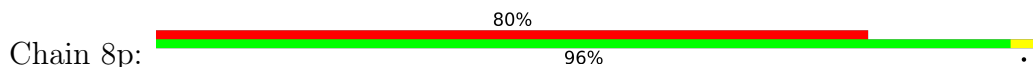




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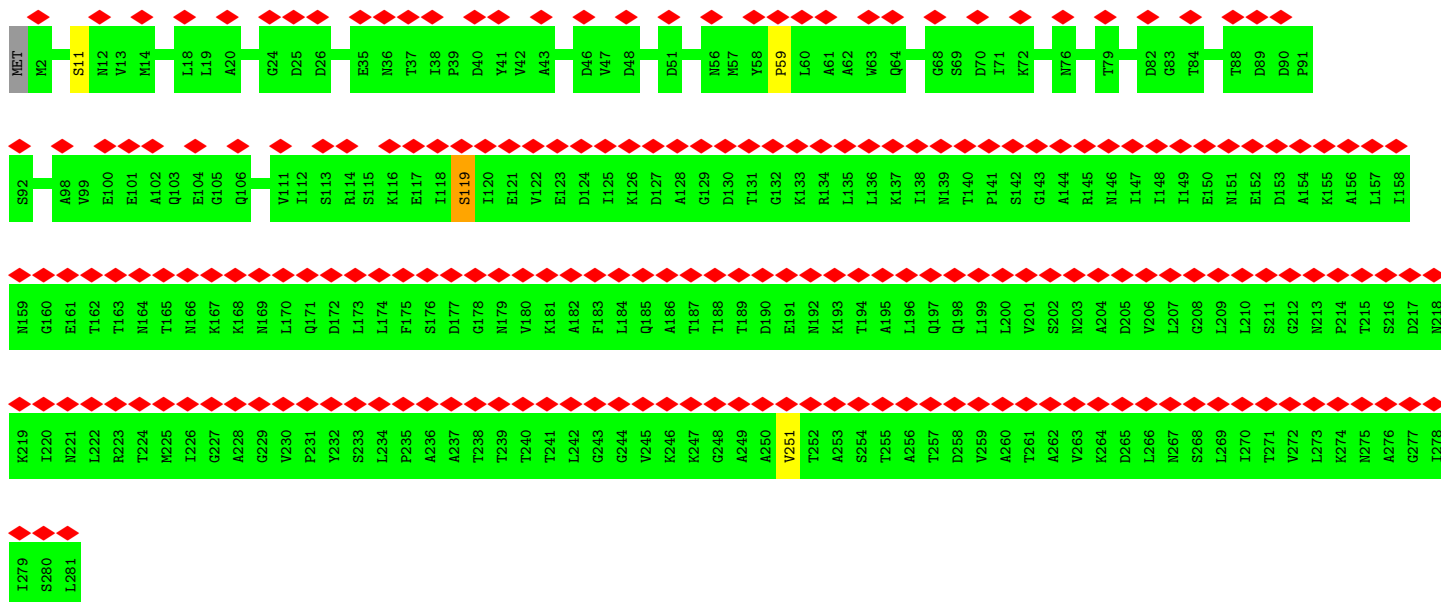
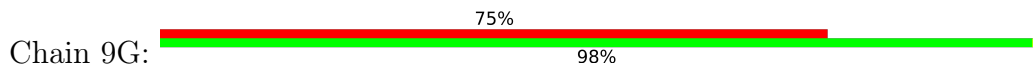


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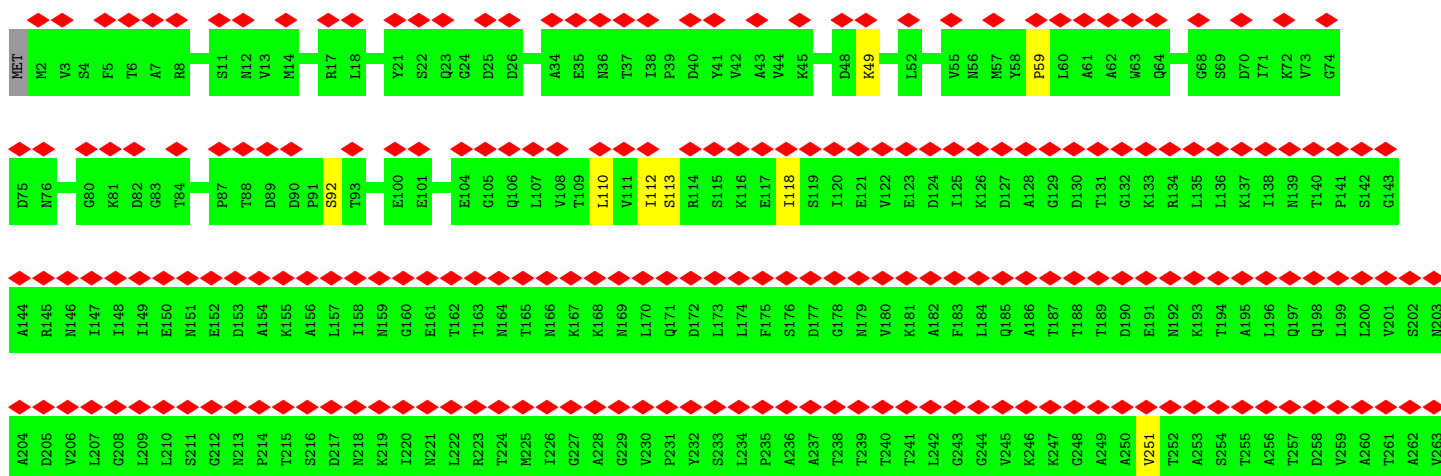
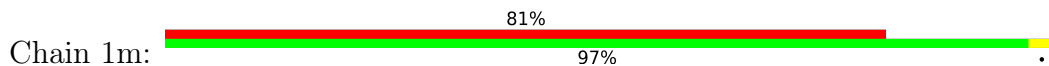


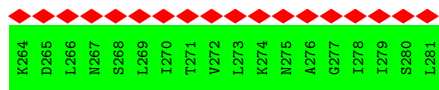


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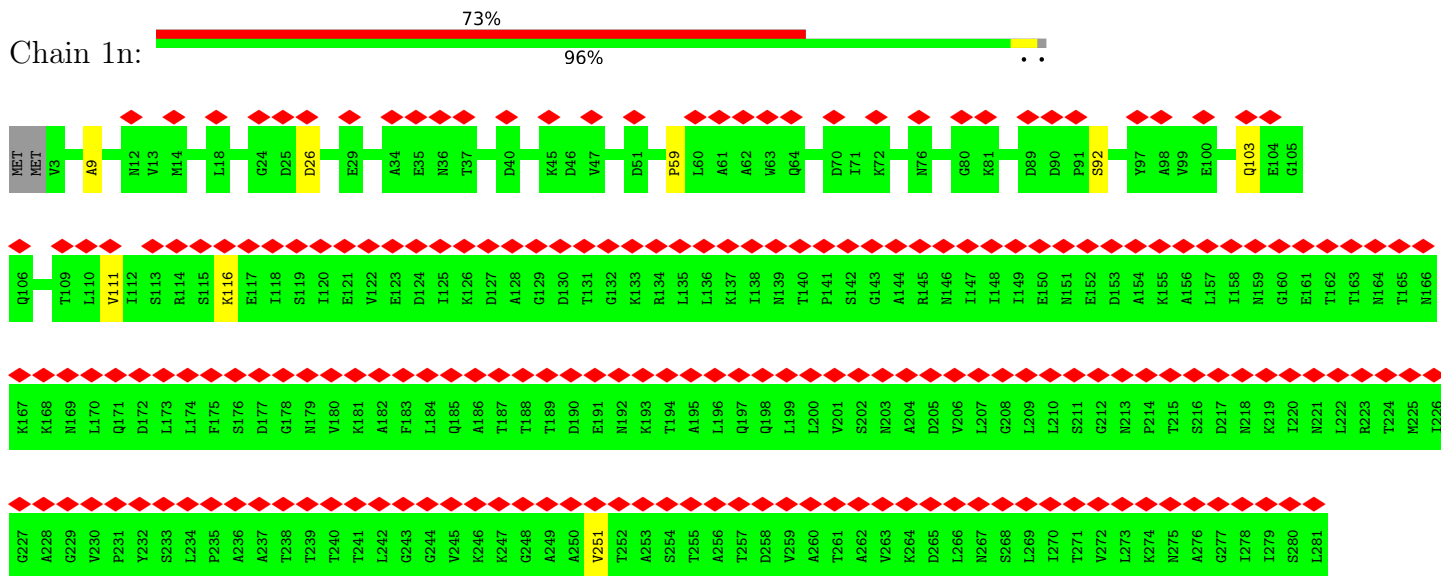


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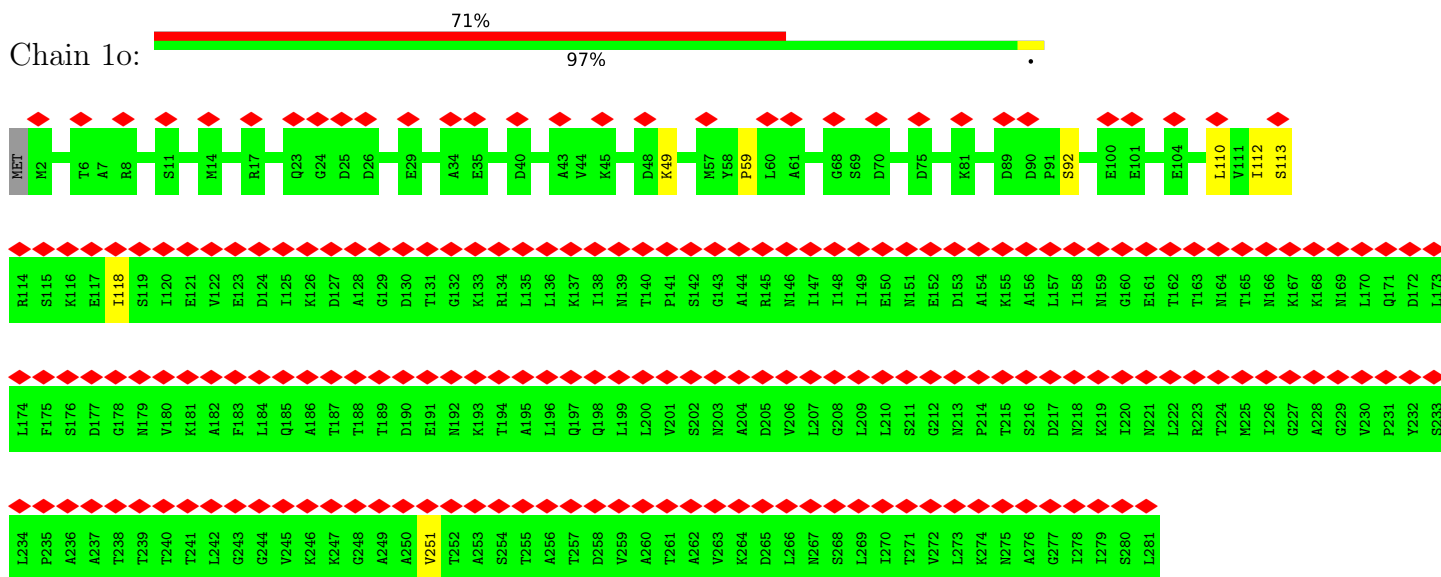




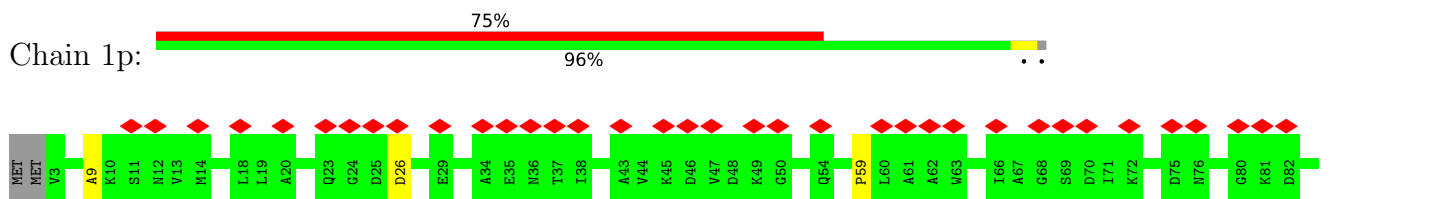
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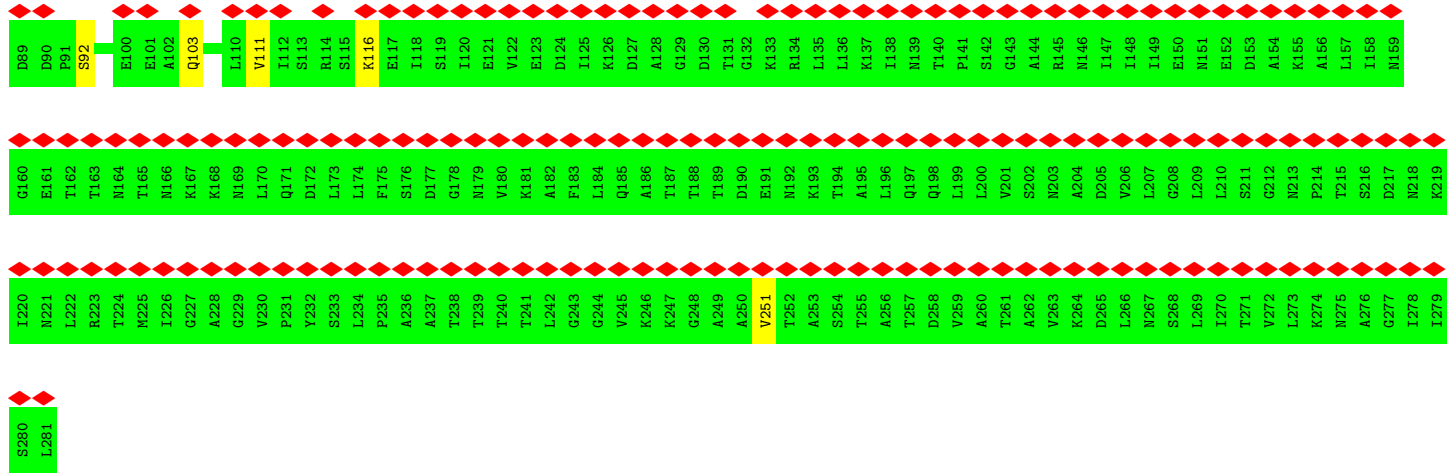


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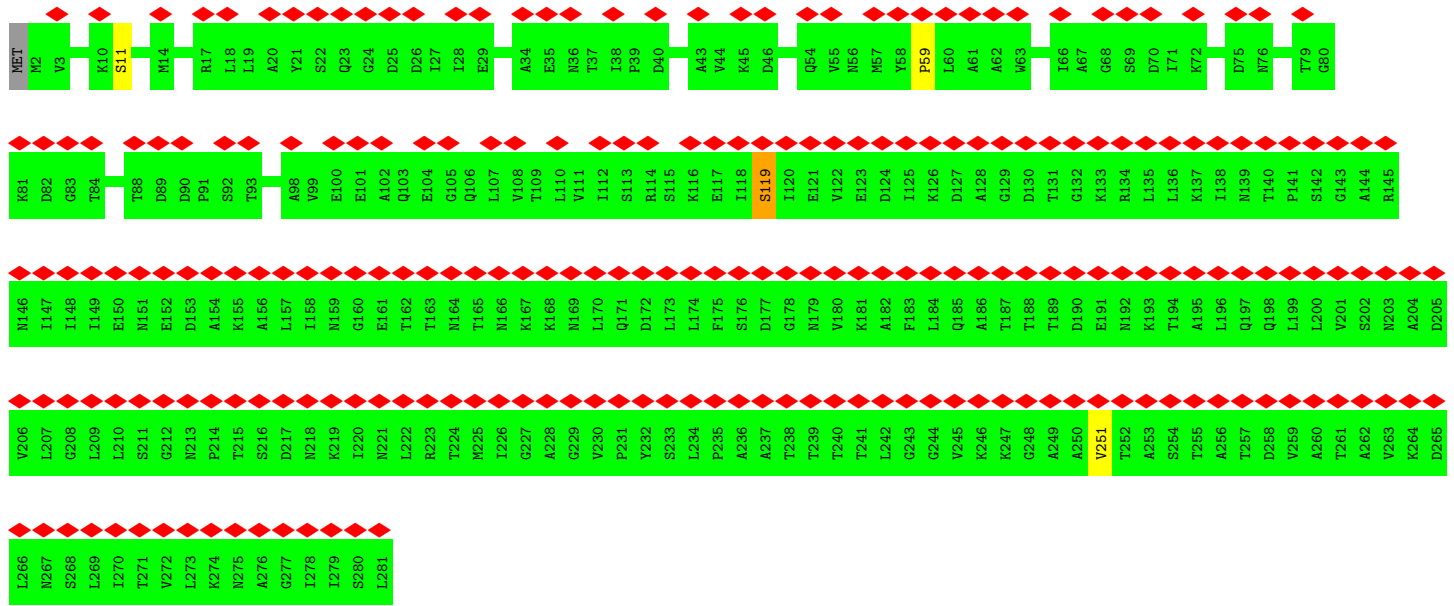
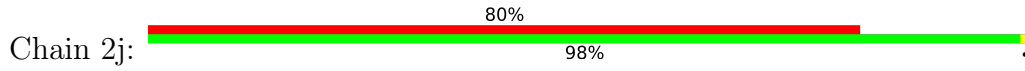


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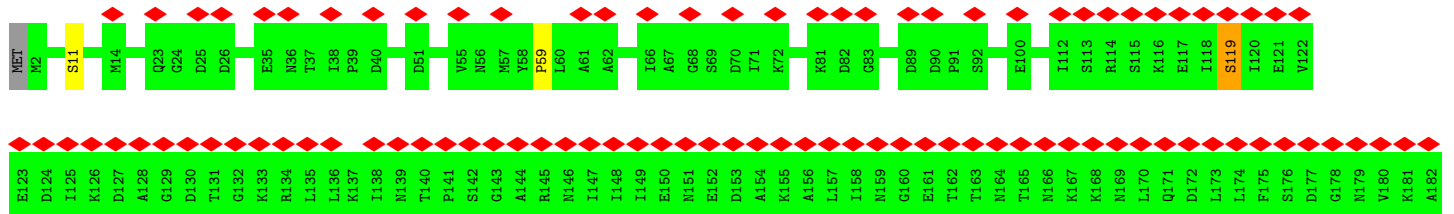


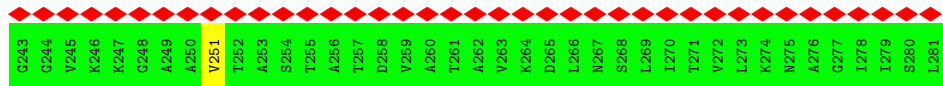
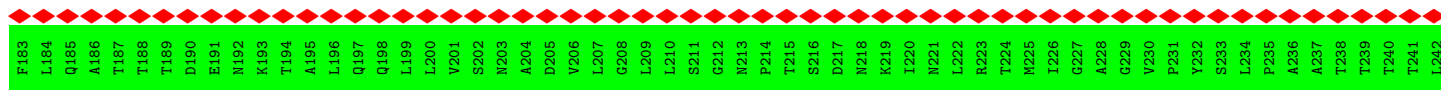


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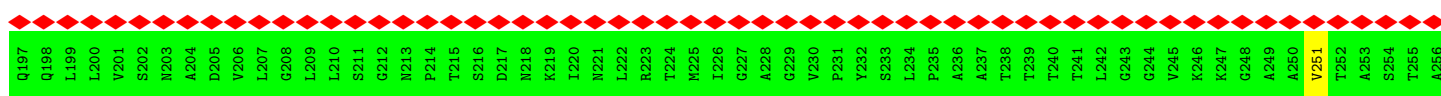
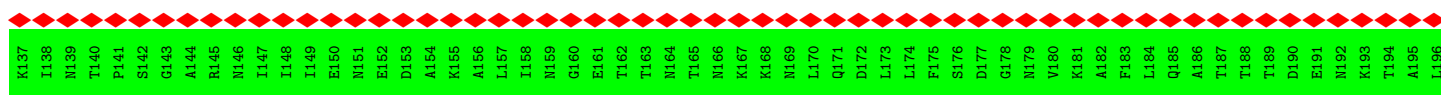
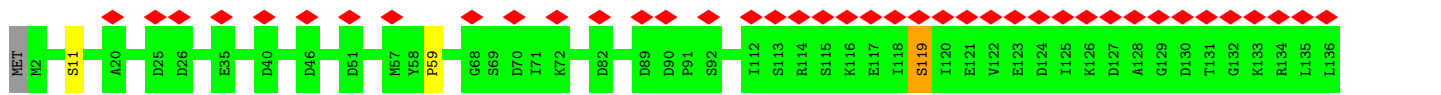


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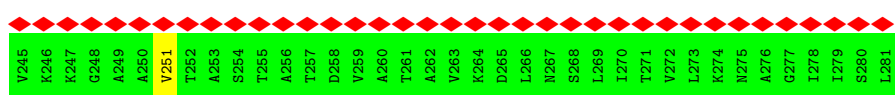
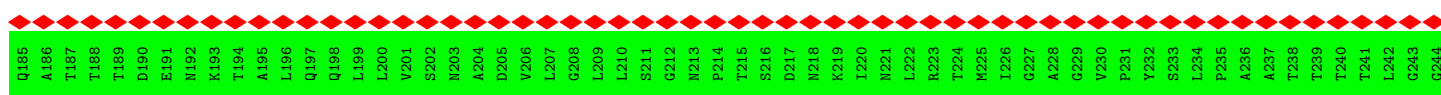
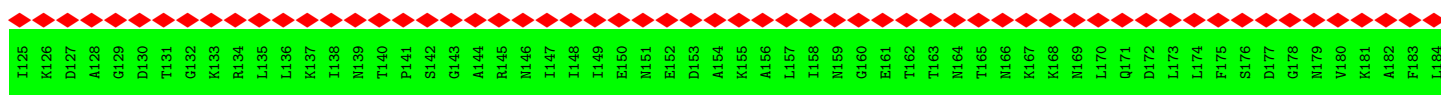
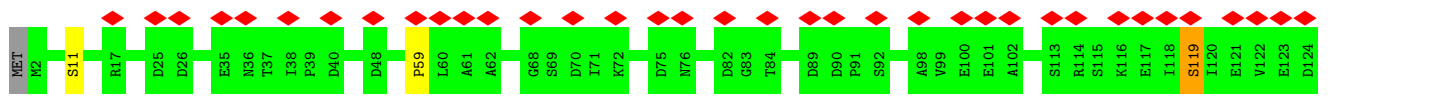
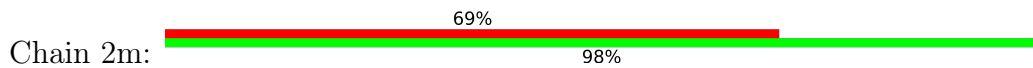




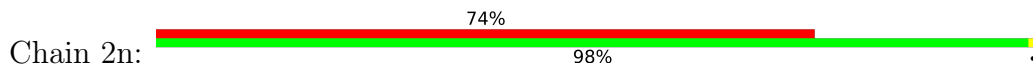
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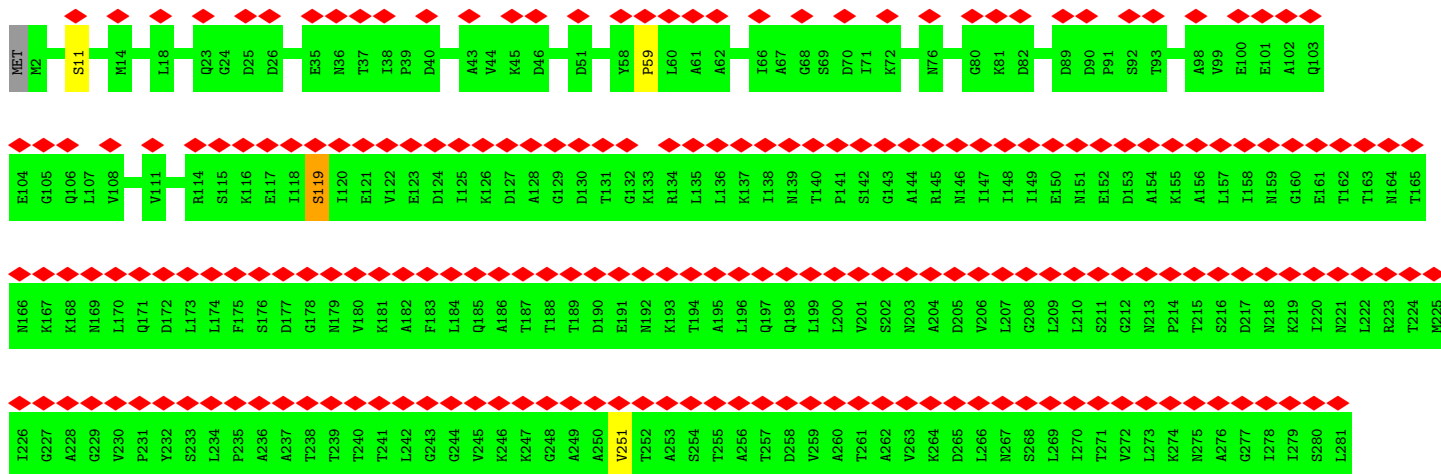


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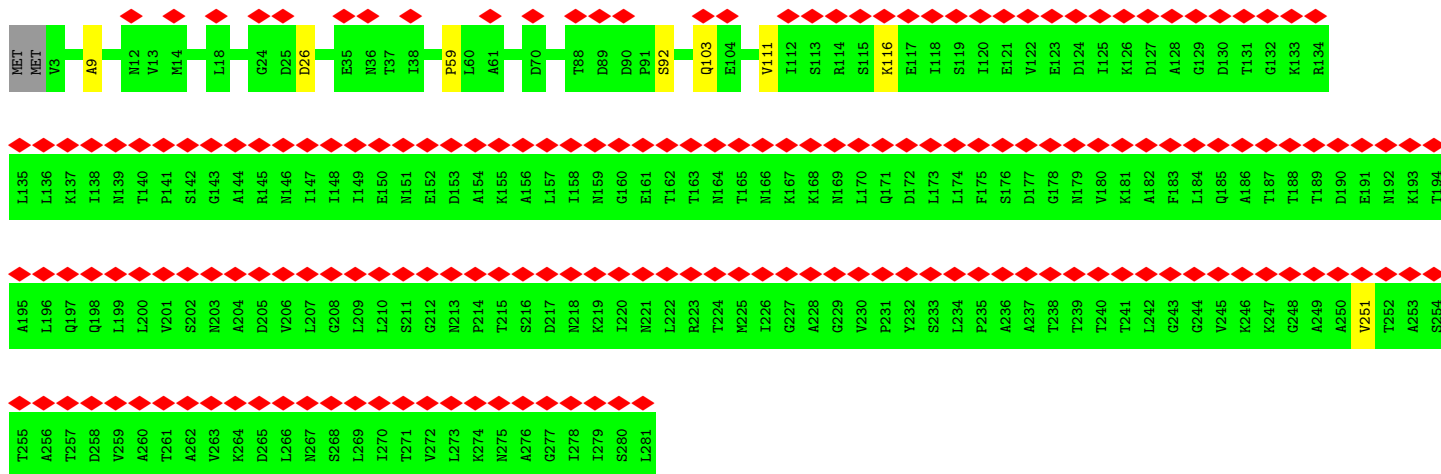


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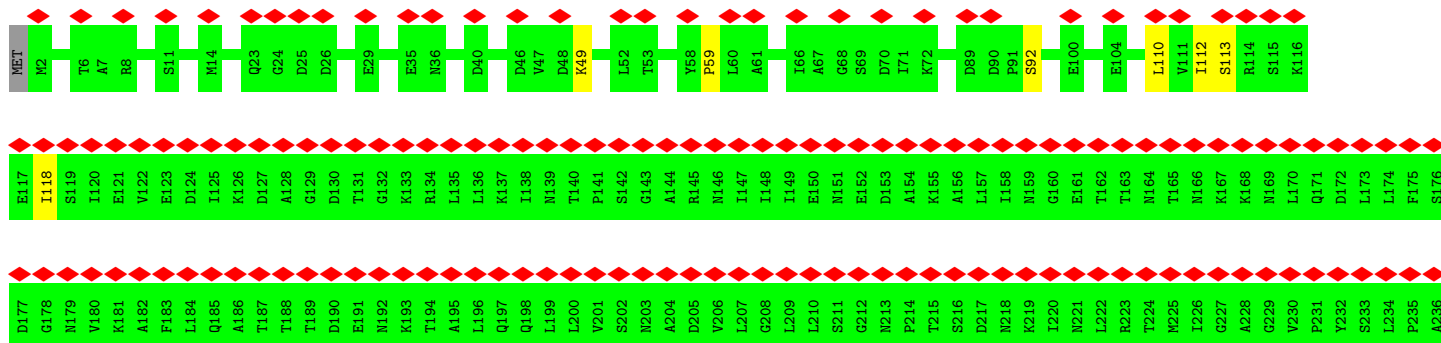


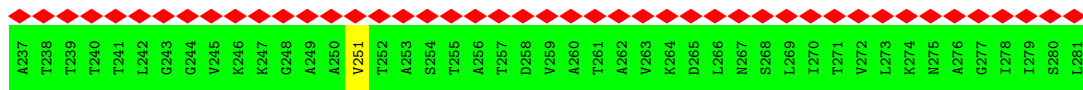


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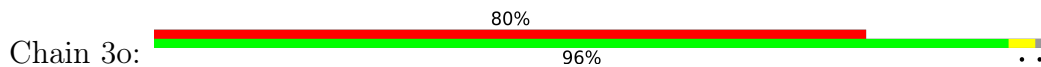


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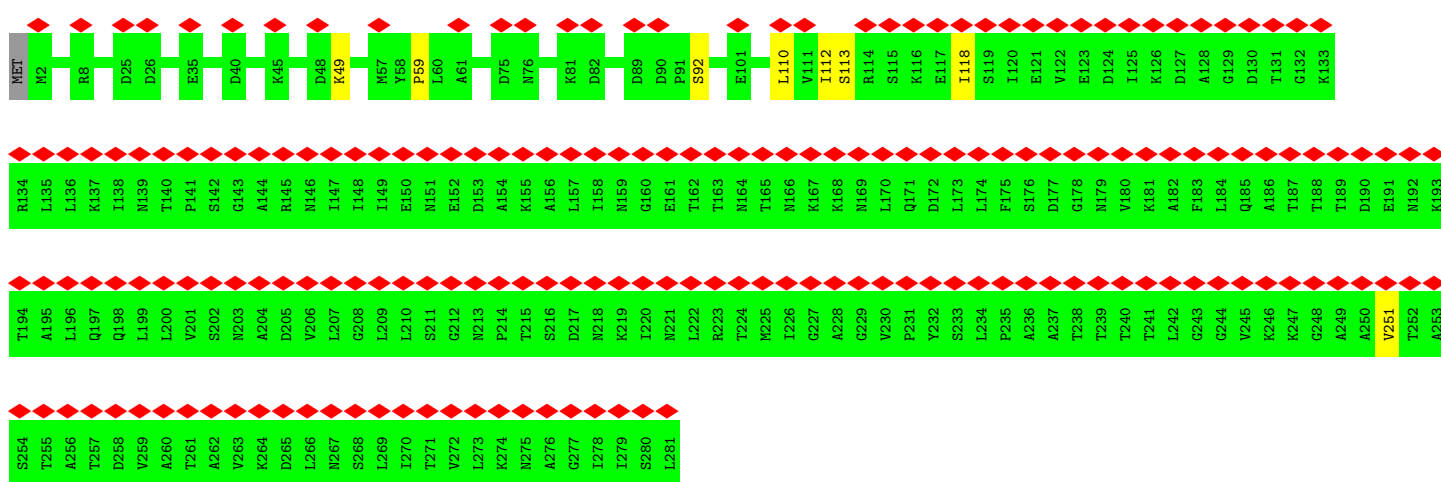




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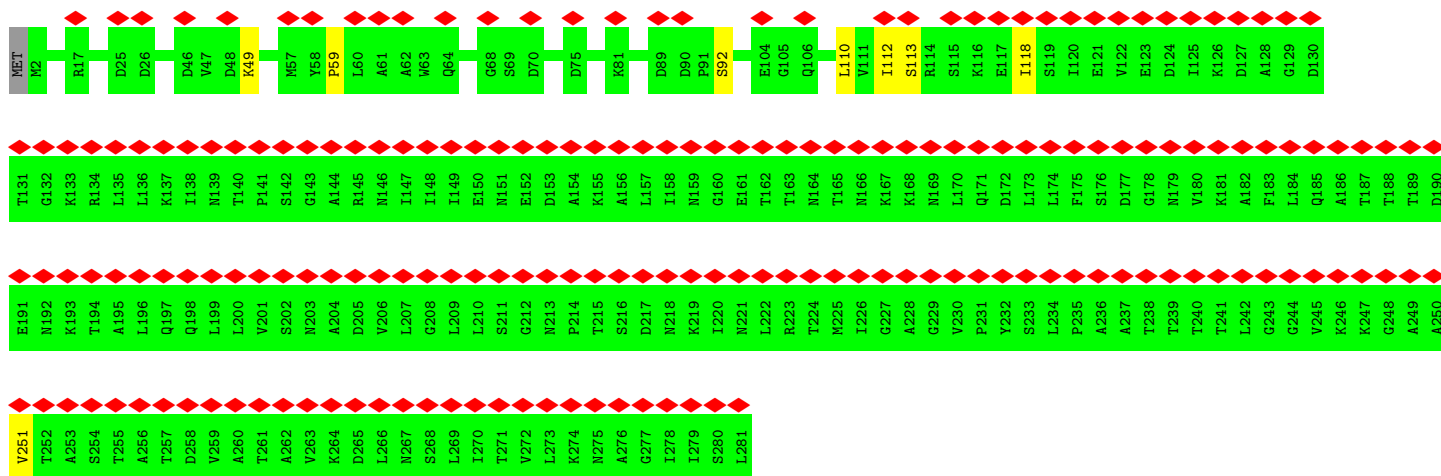


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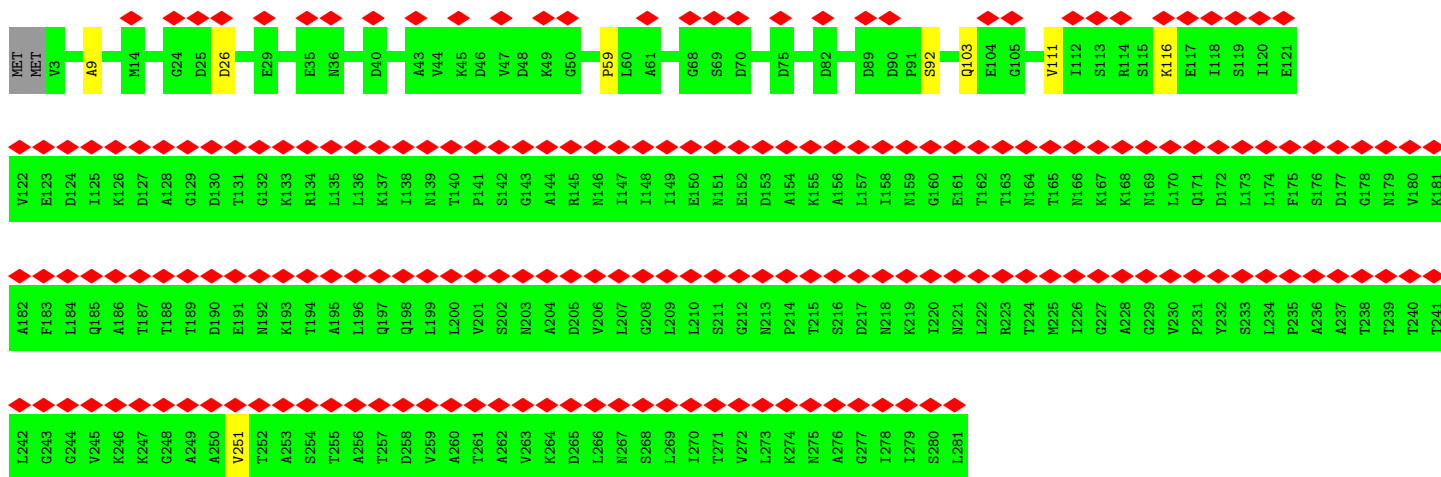


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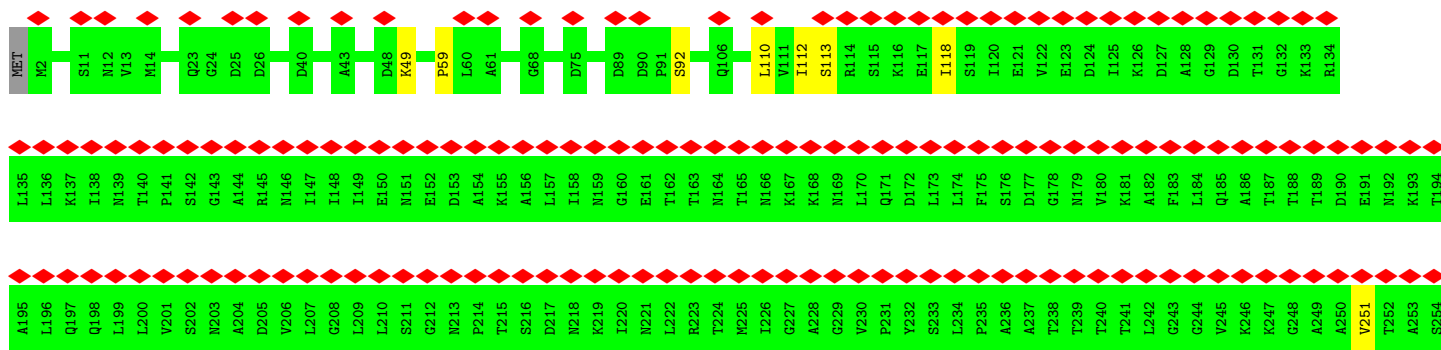
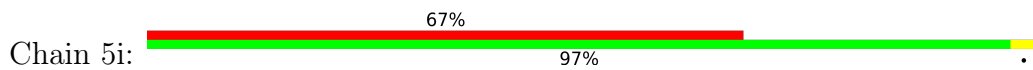


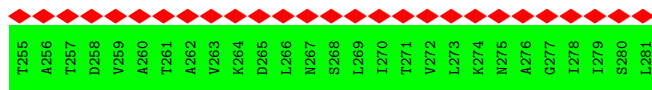


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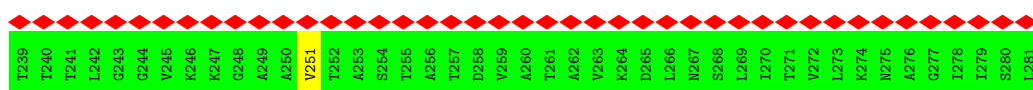
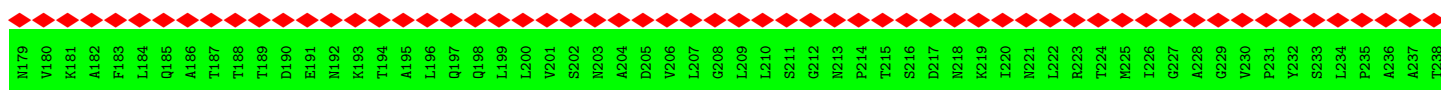
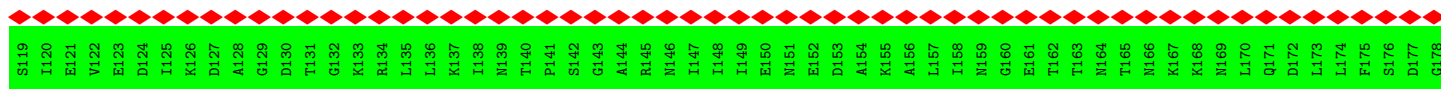


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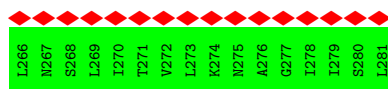
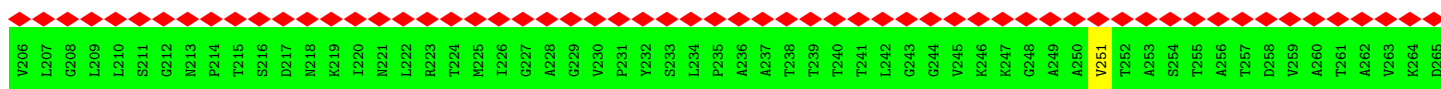
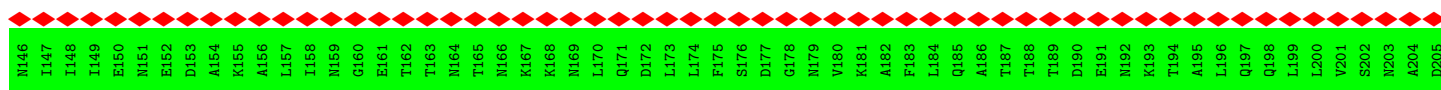
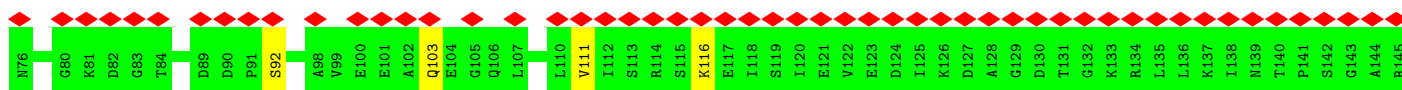
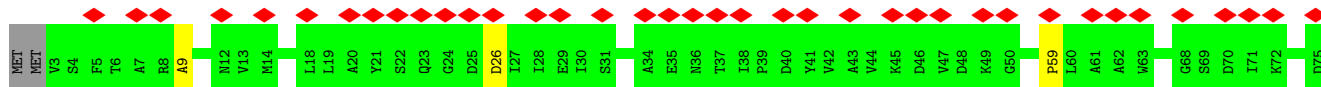
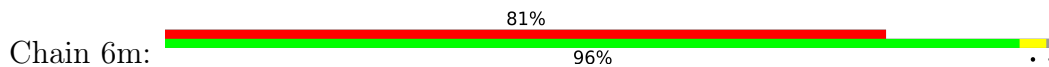




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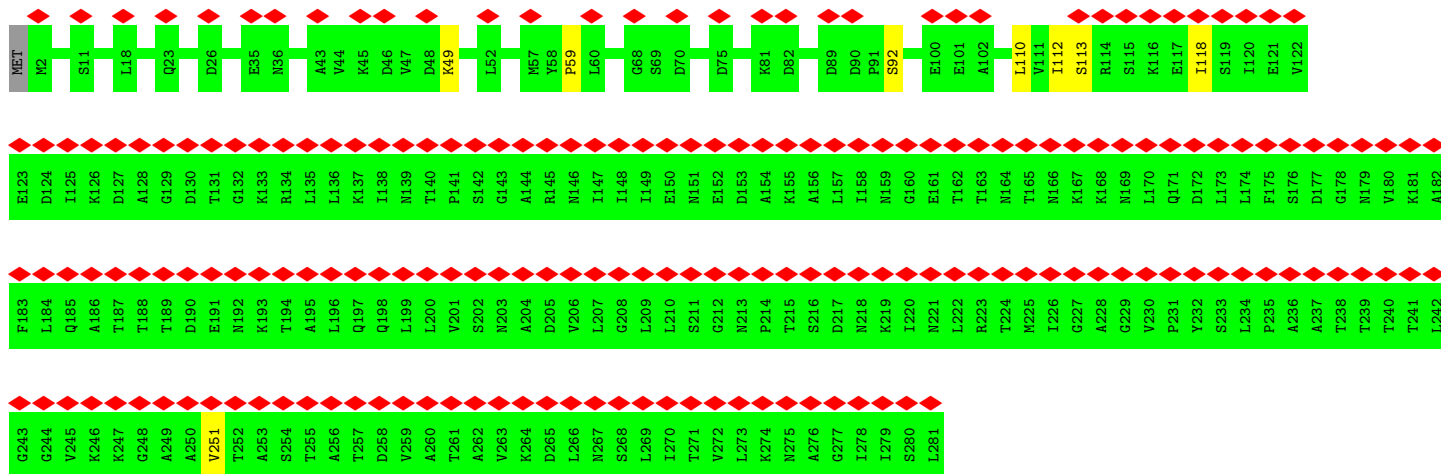


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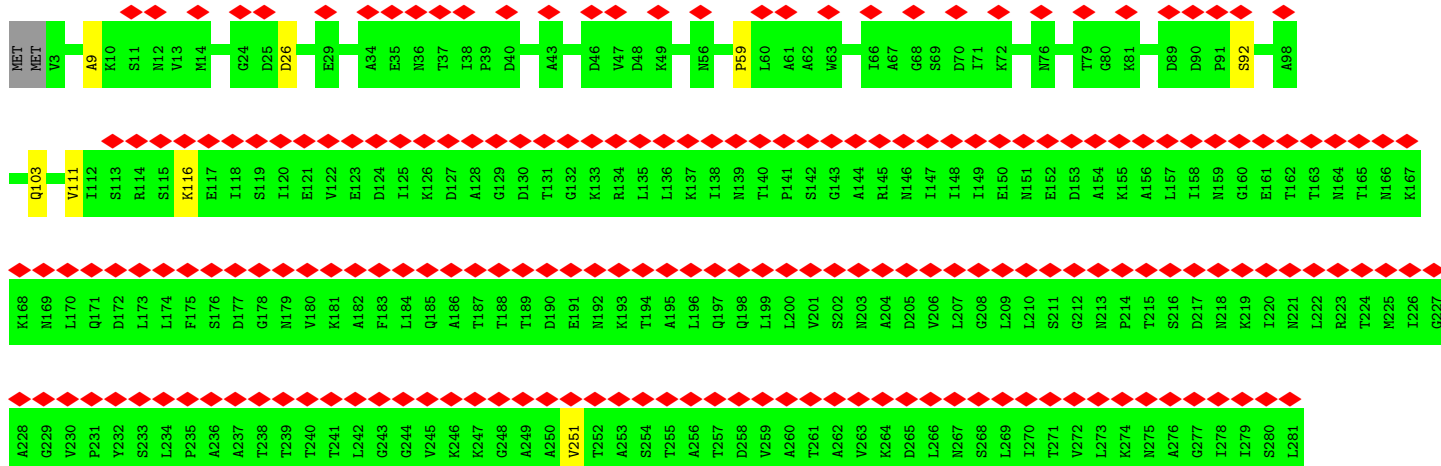


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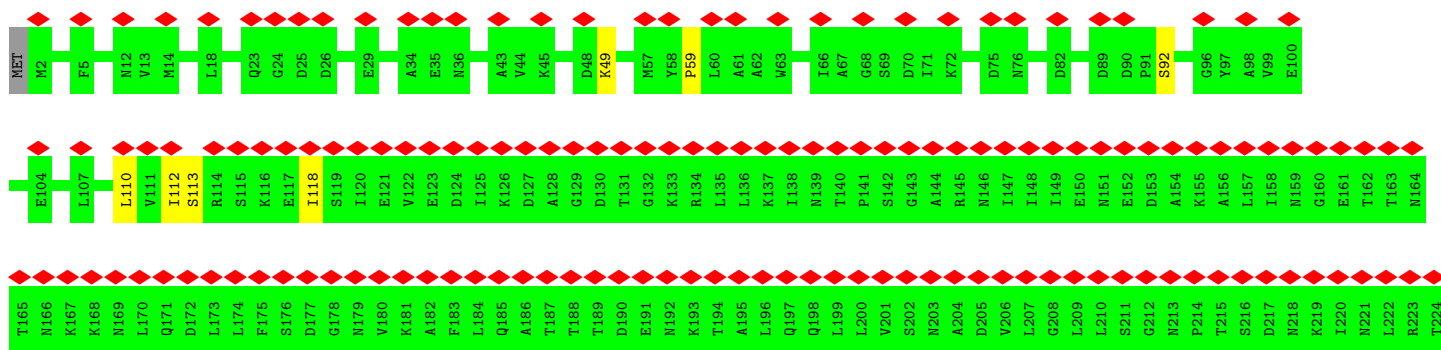
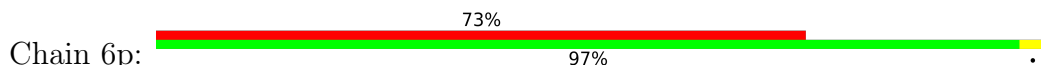


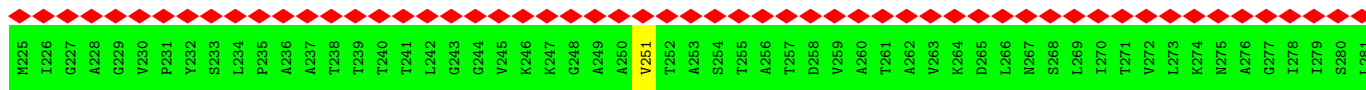


• Molecule 2: Capsid fiber protein



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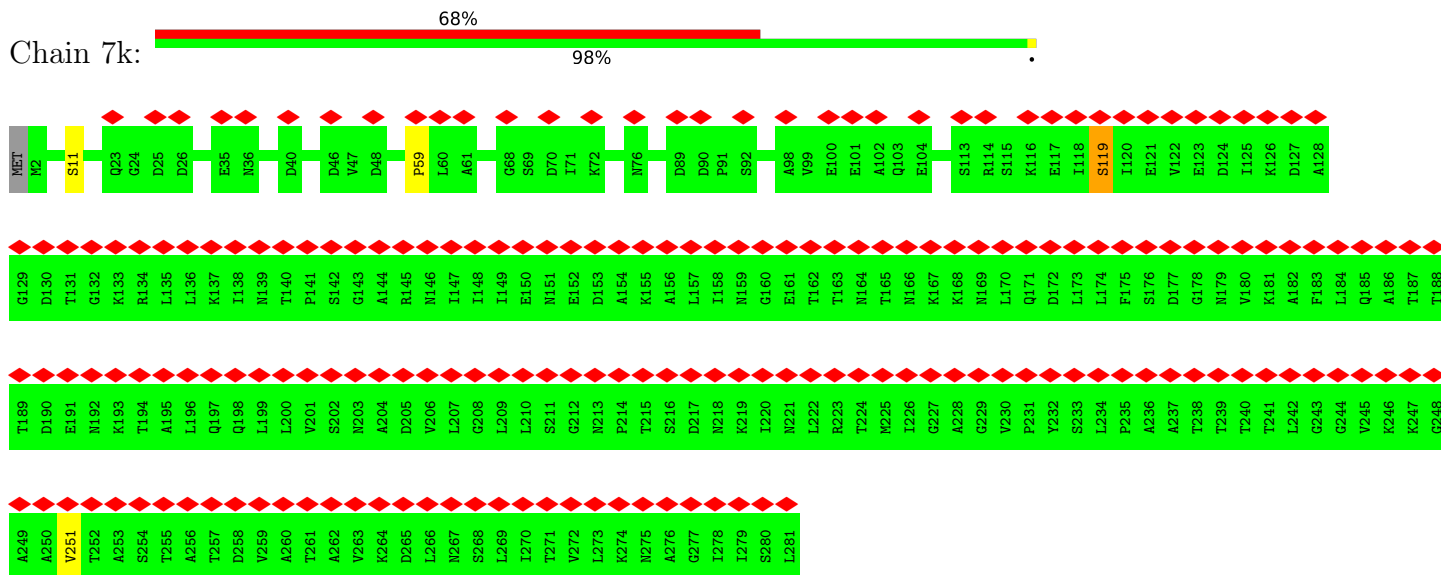




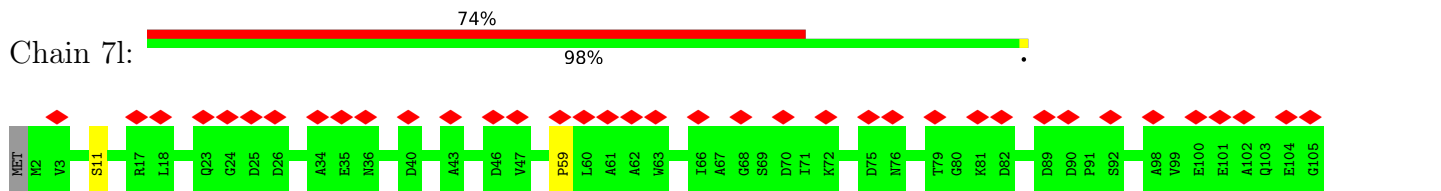
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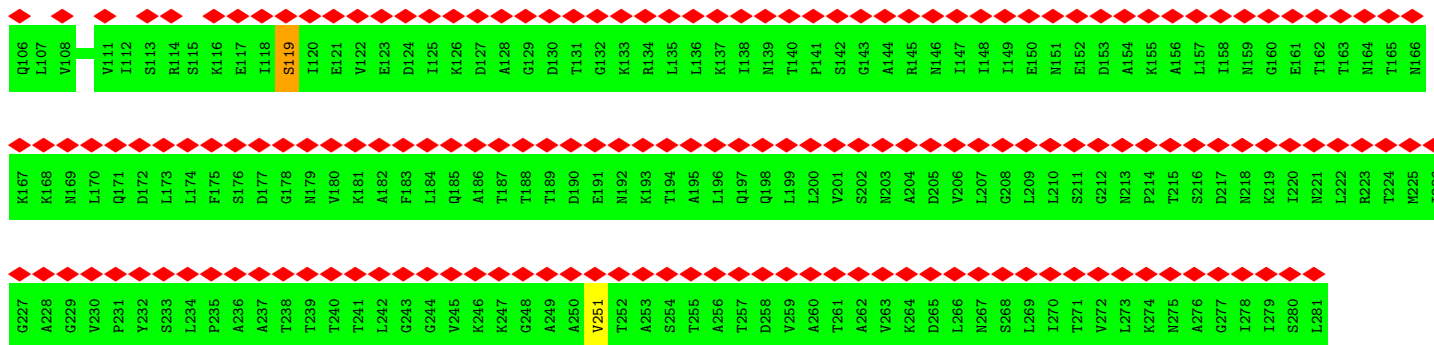


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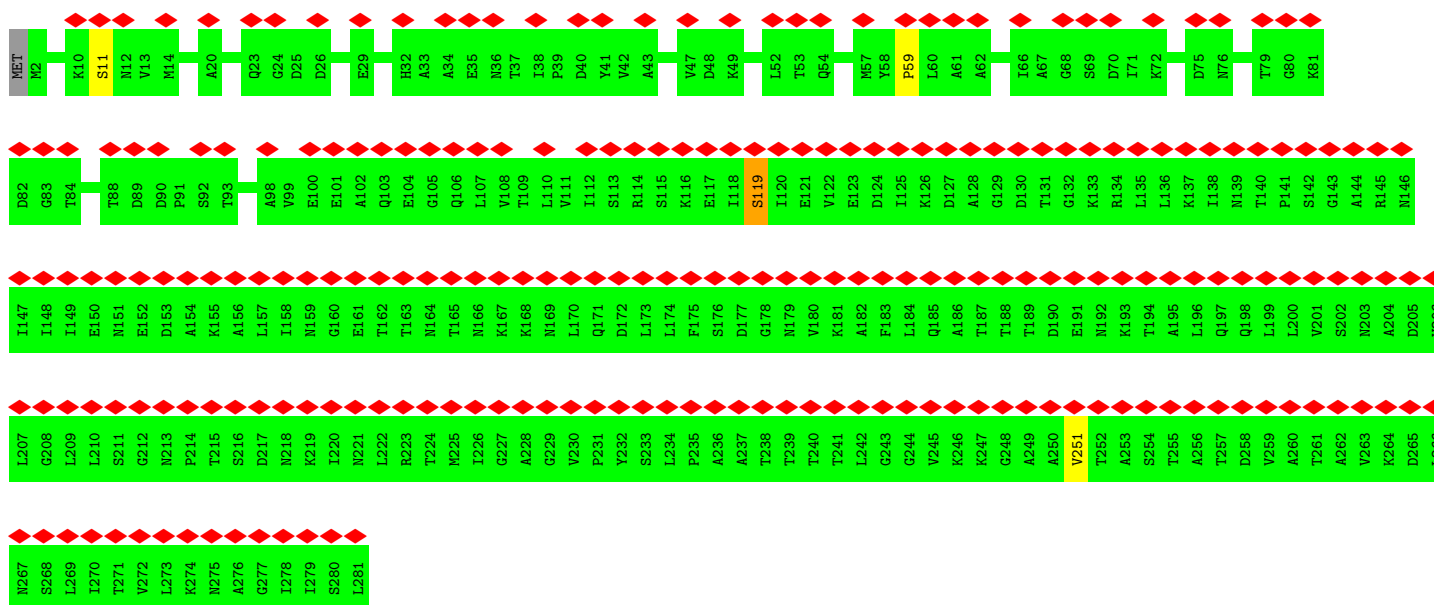
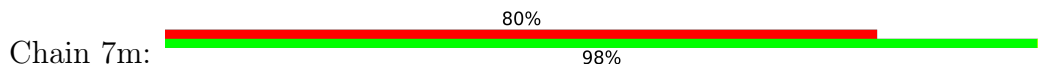


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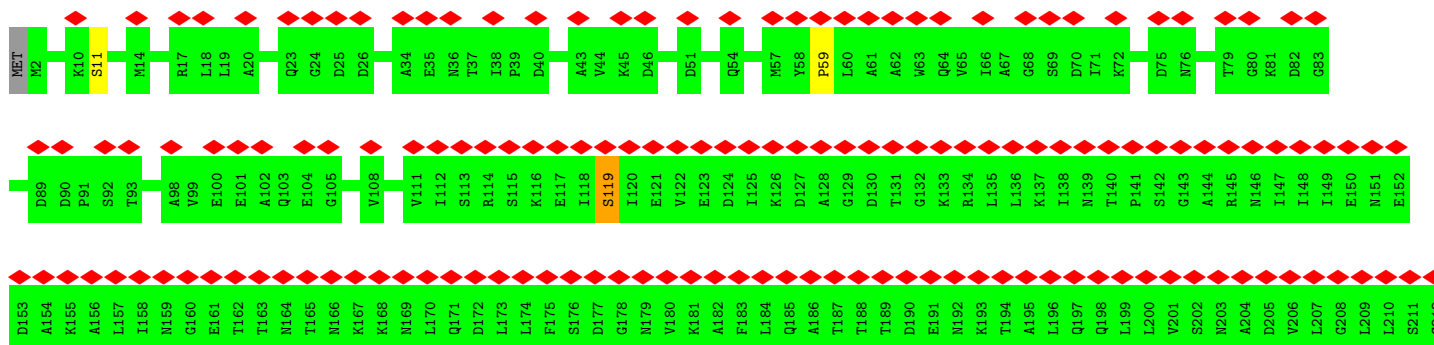
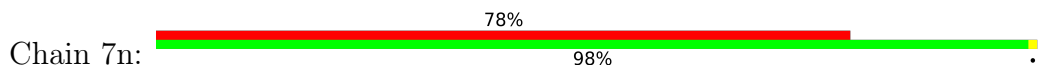




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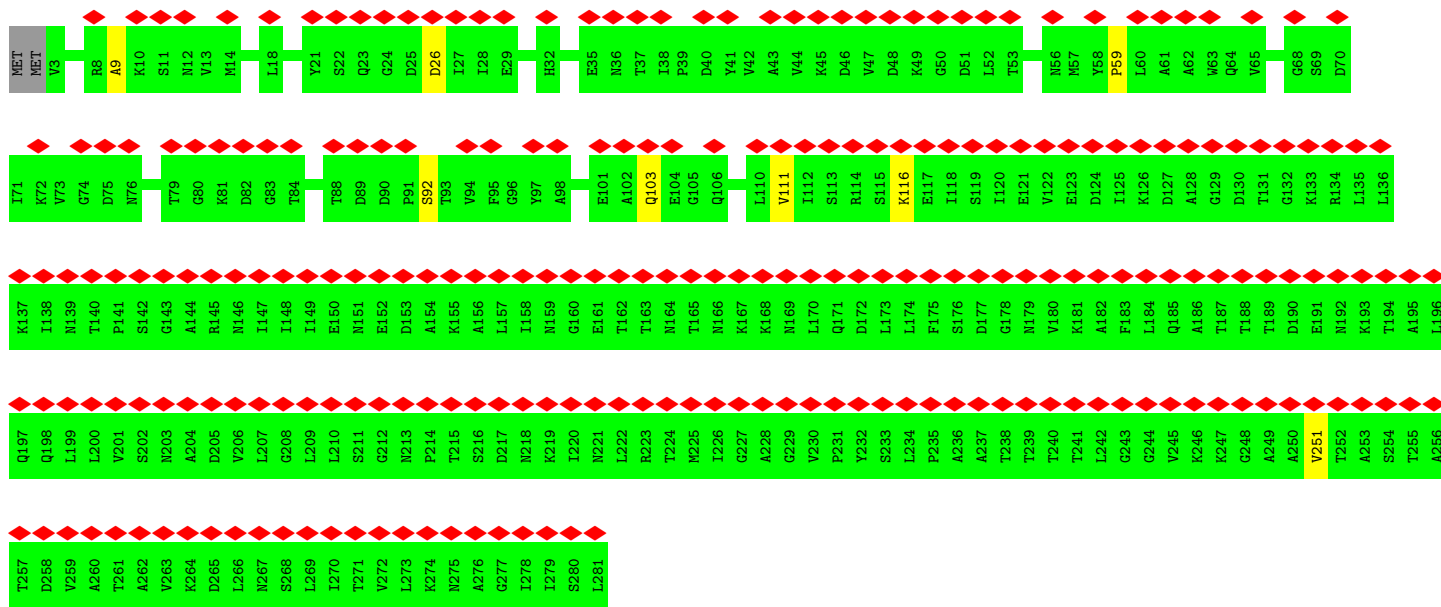
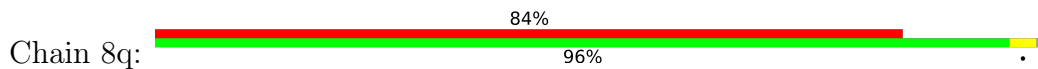


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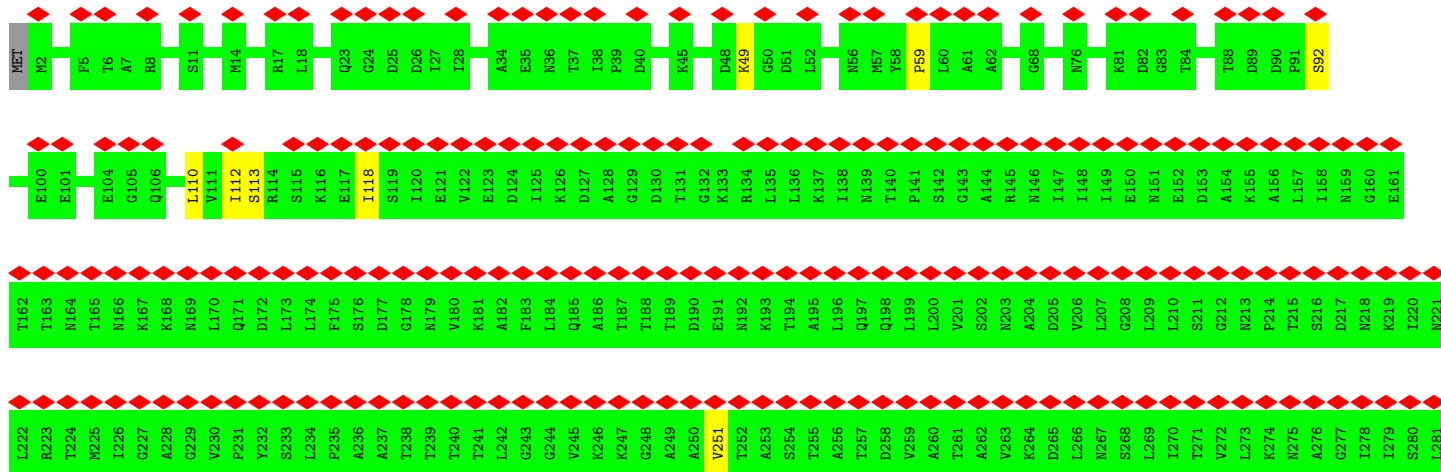
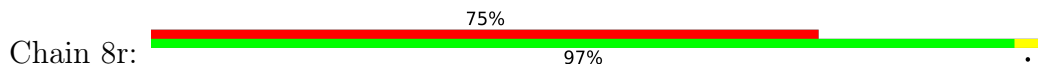




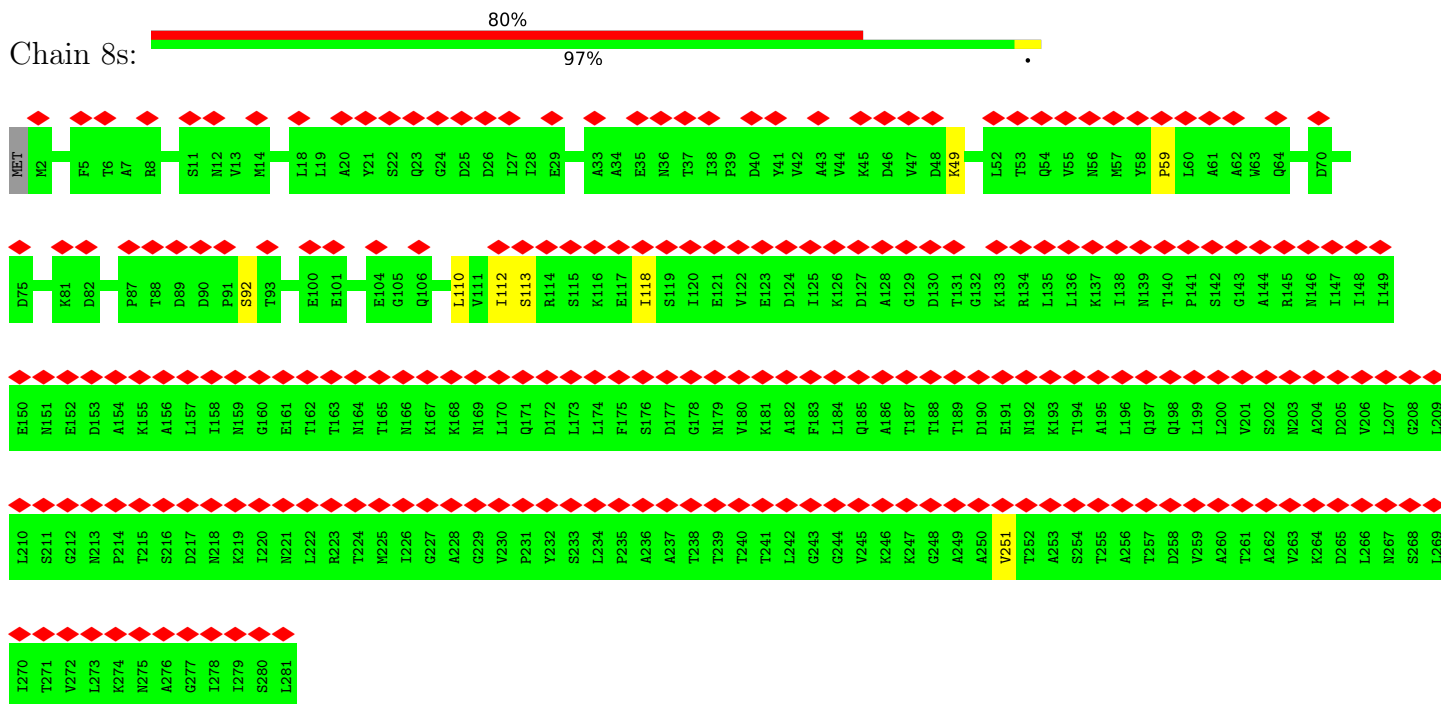
• Molecule 2: Capsid fiber protein



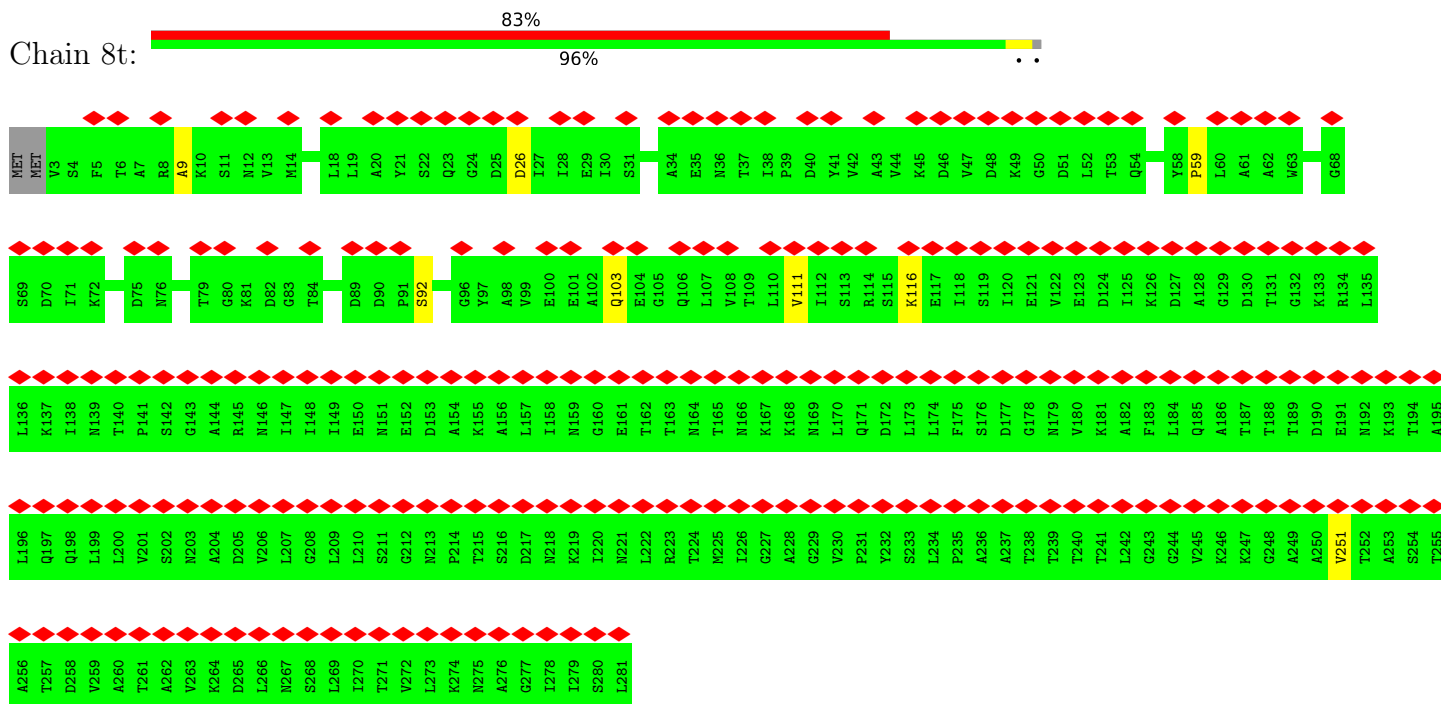
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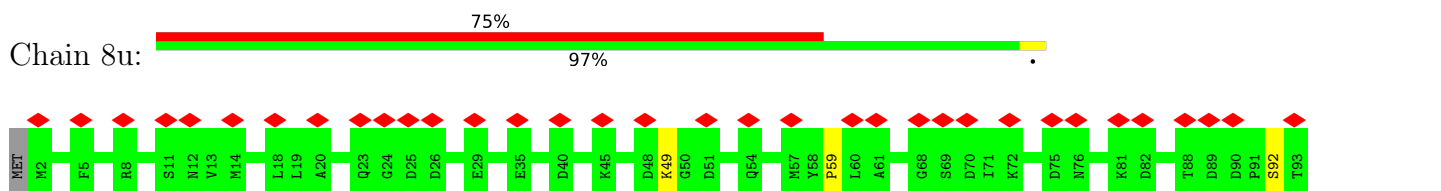
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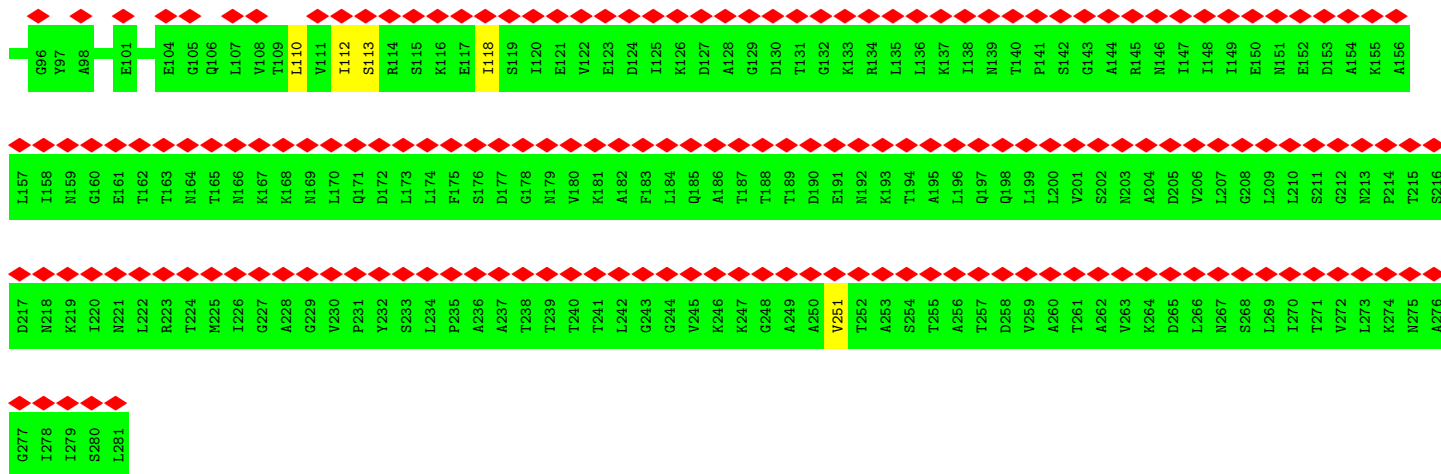


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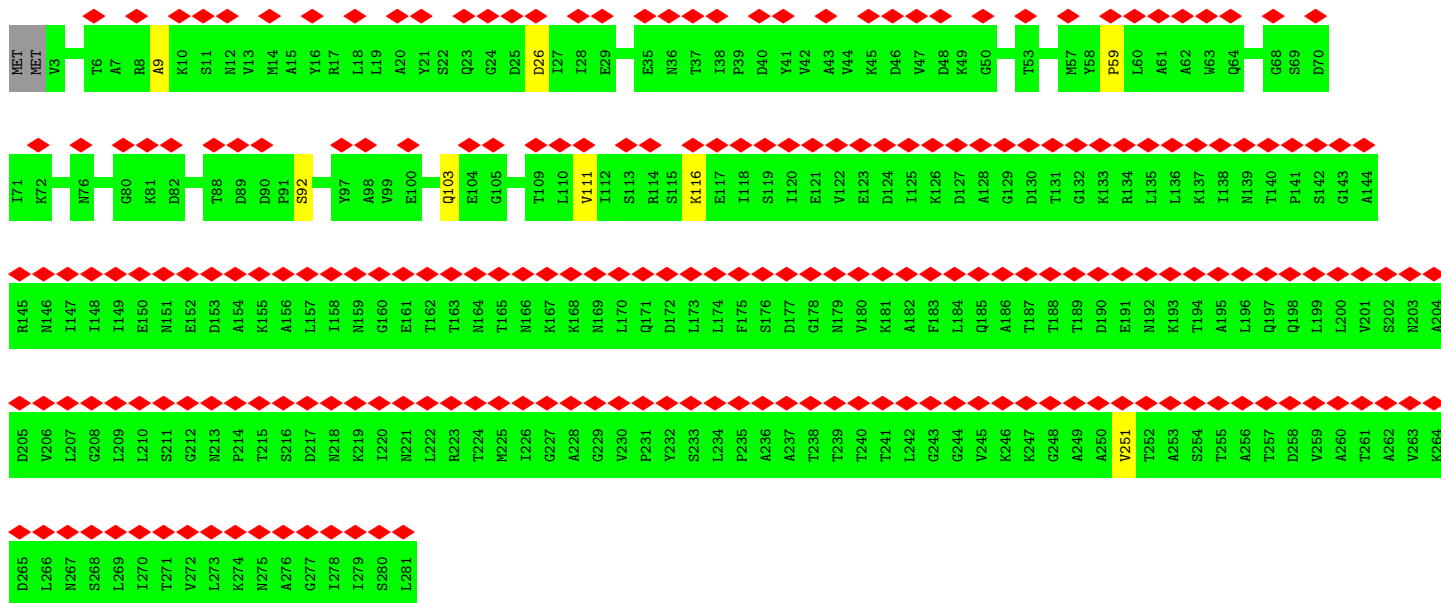
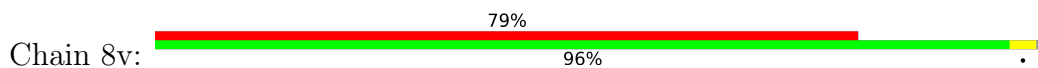


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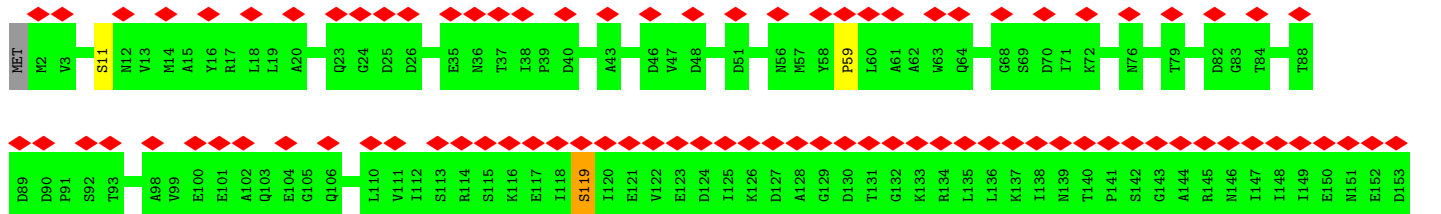
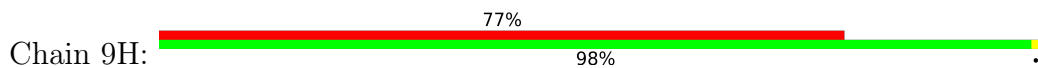


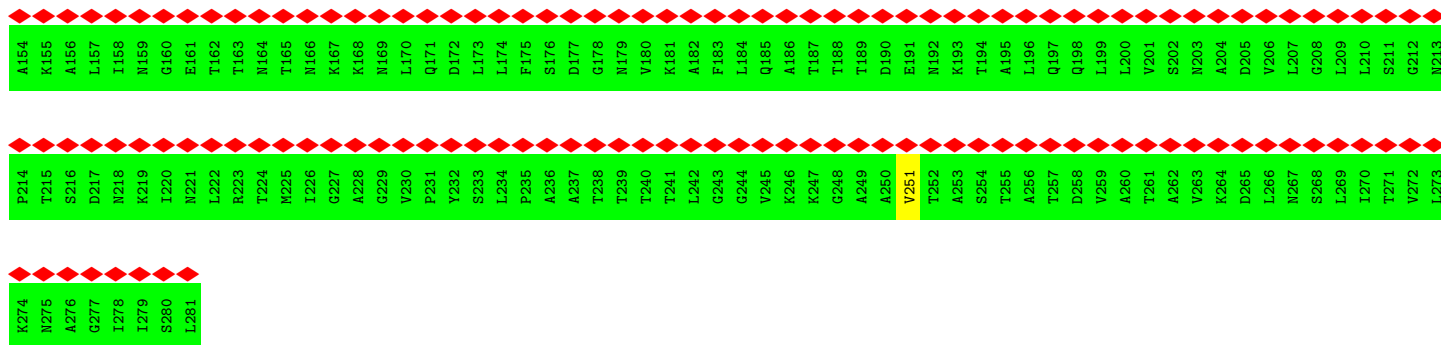


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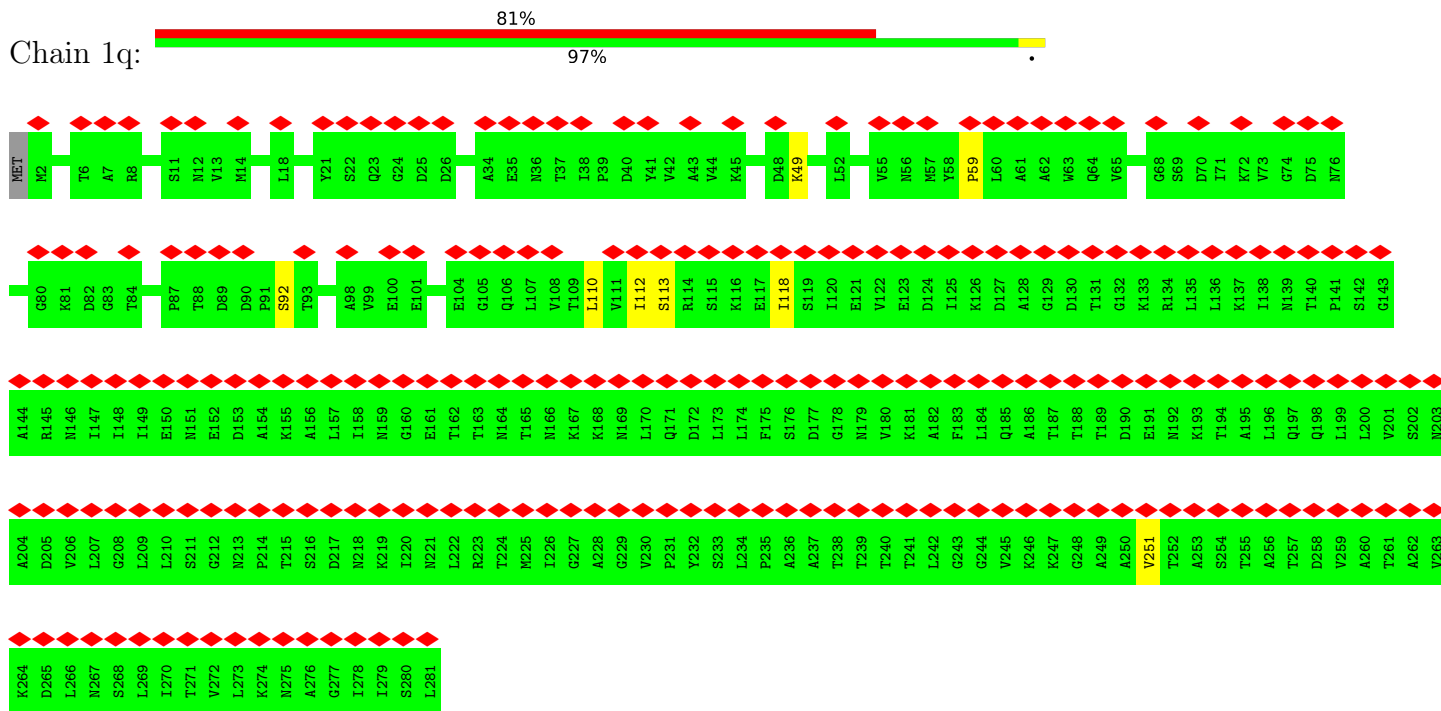


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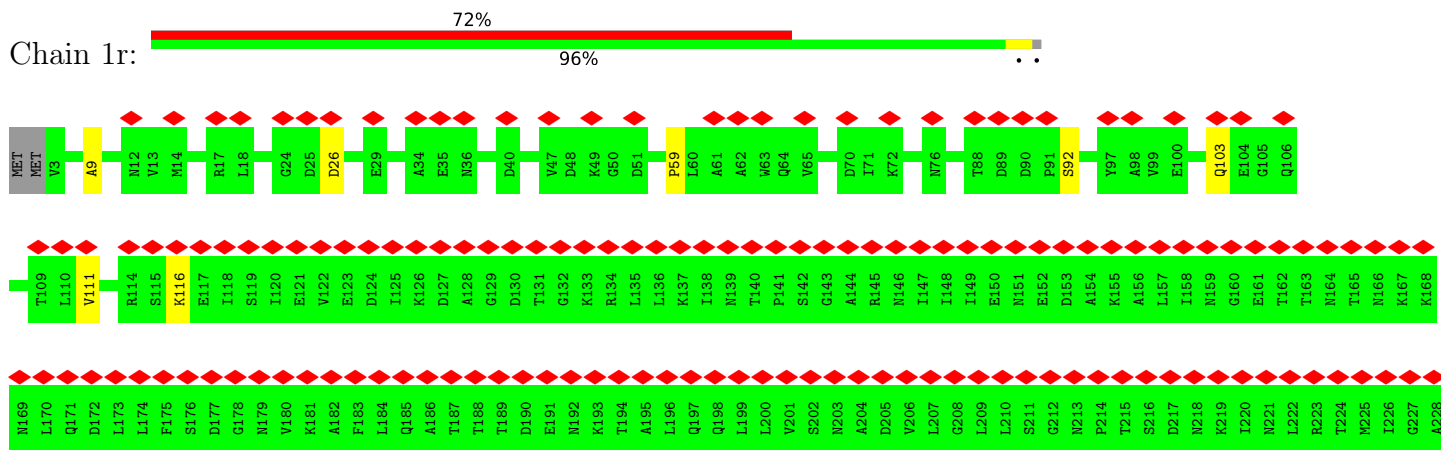


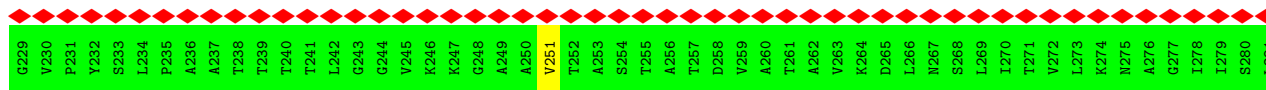


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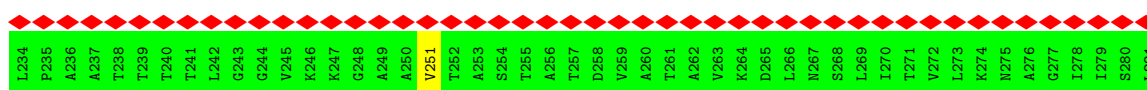
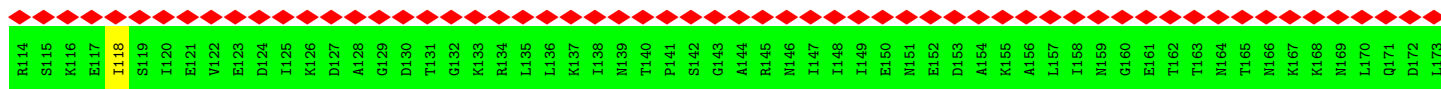
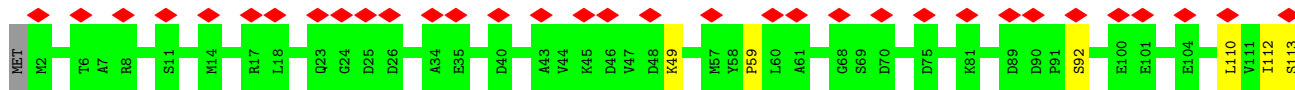
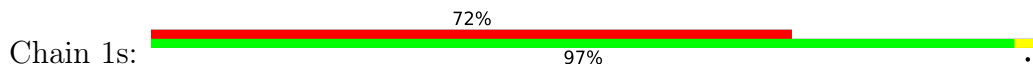


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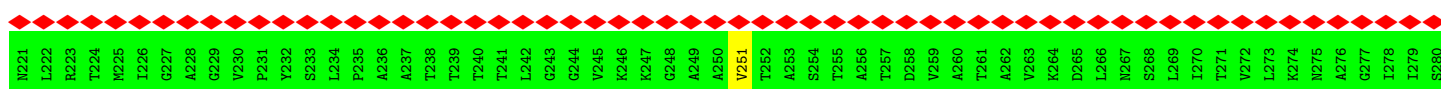
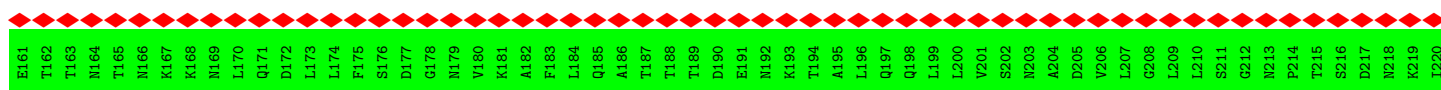
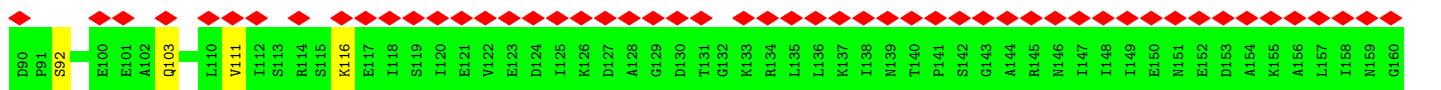
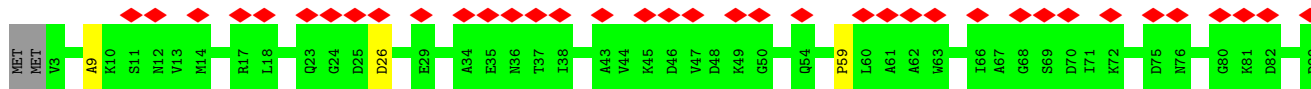
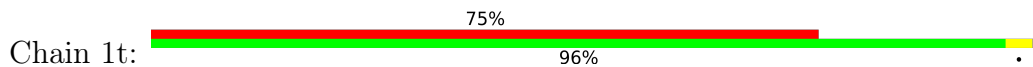




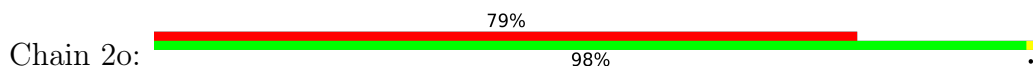
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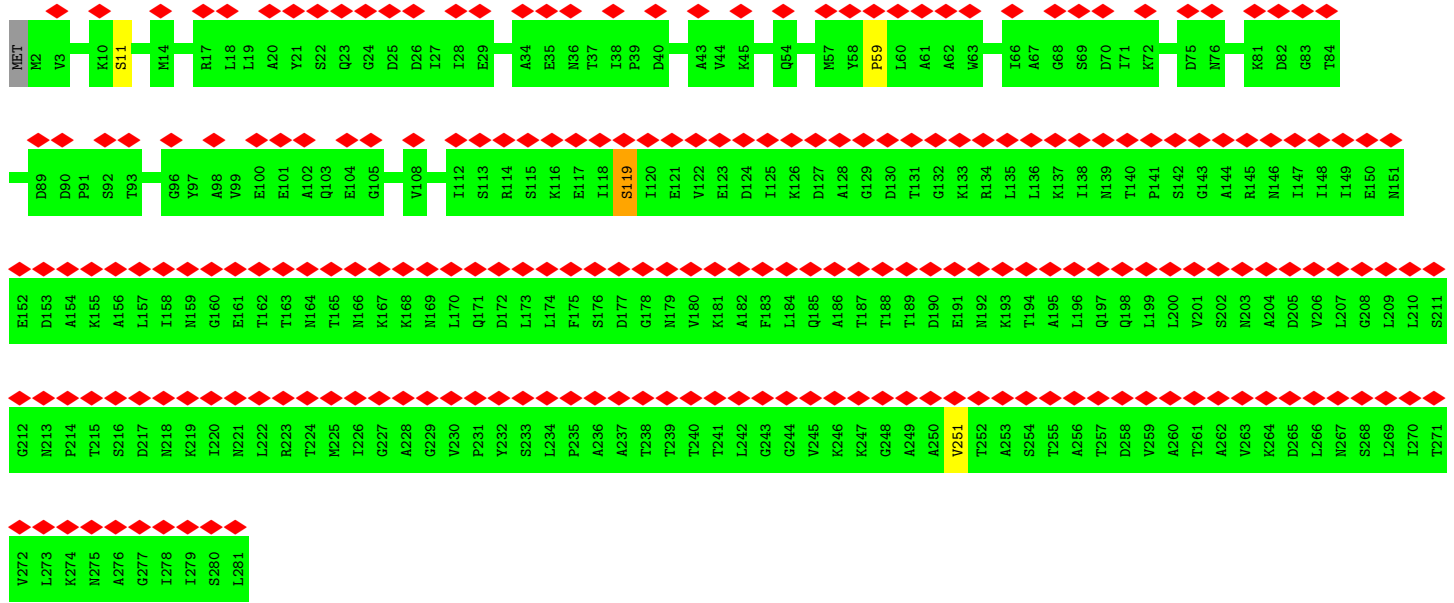


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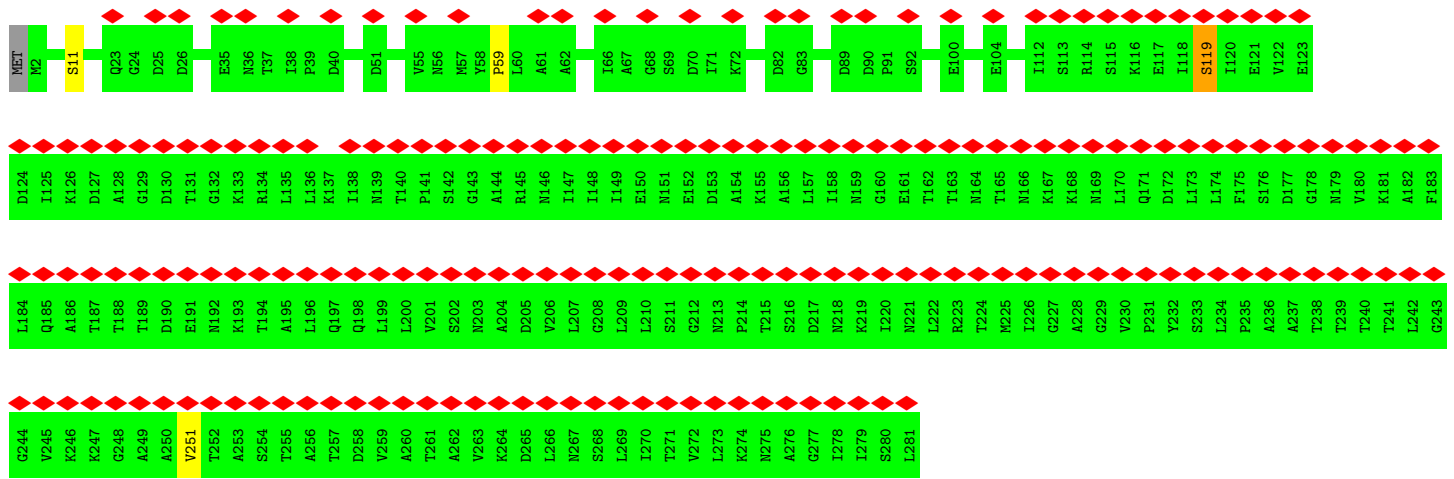


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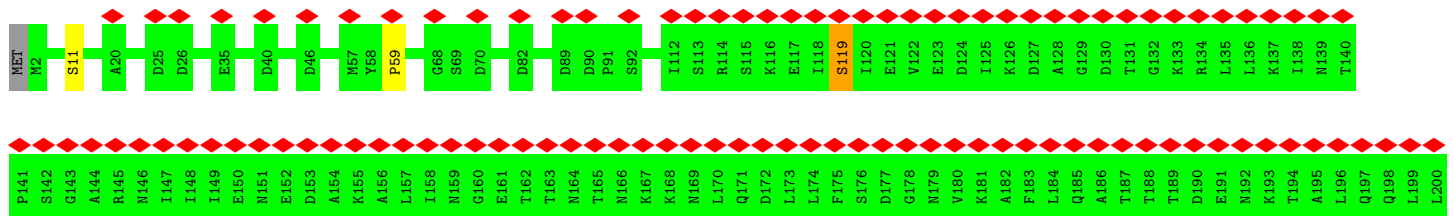


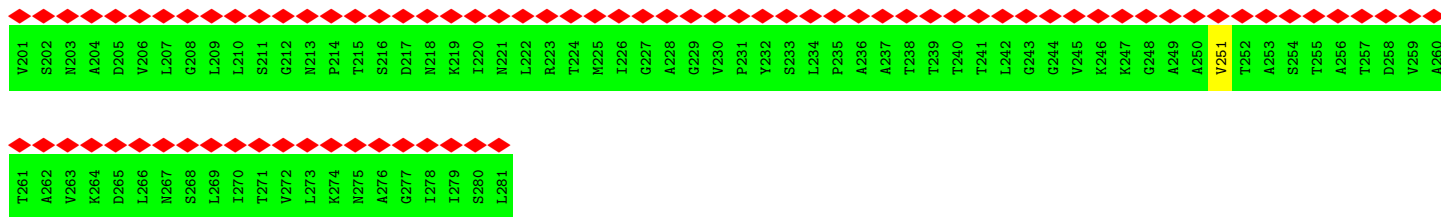


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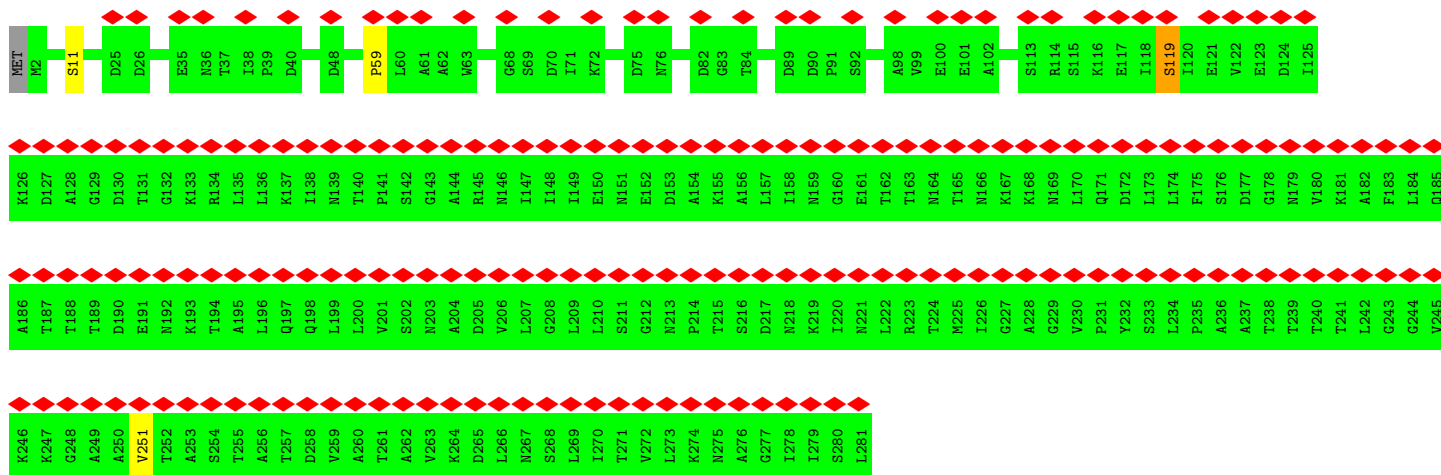


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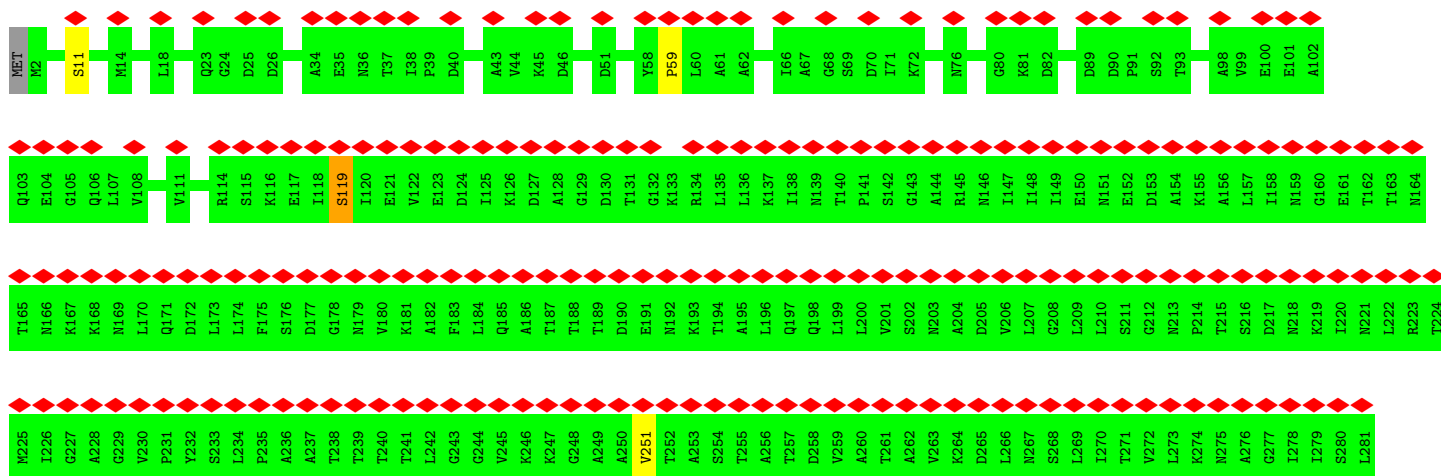
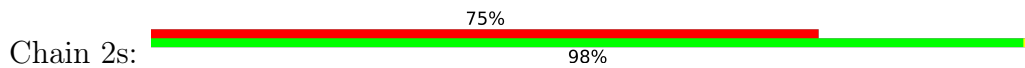




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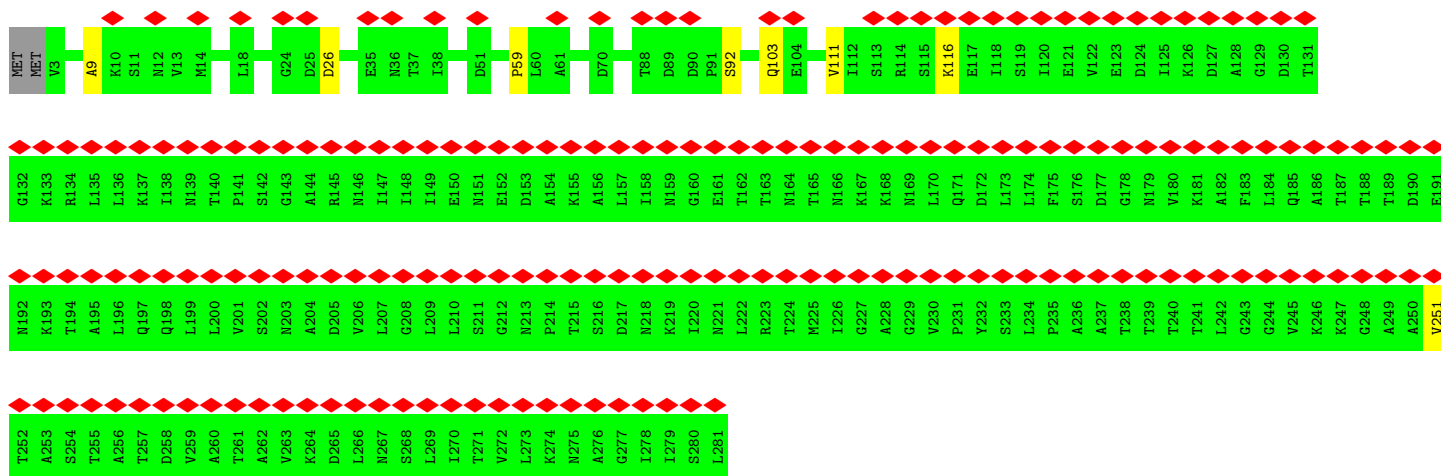


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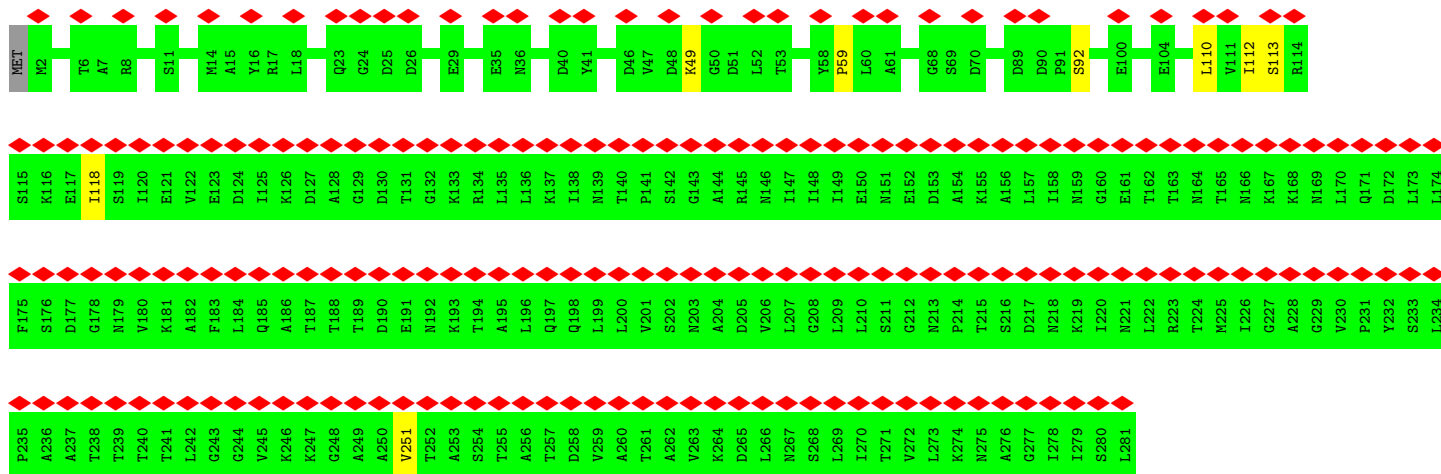
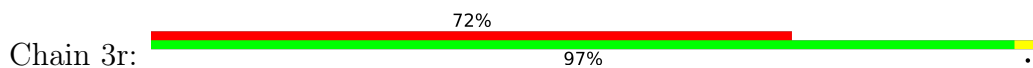


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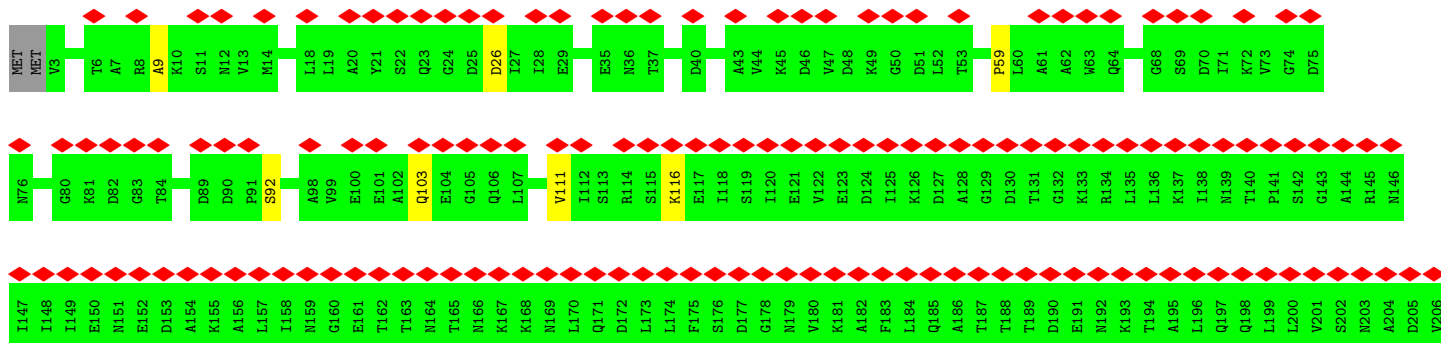
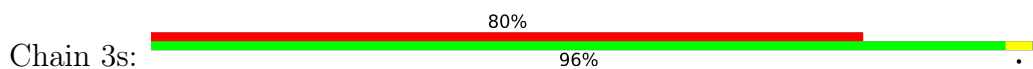




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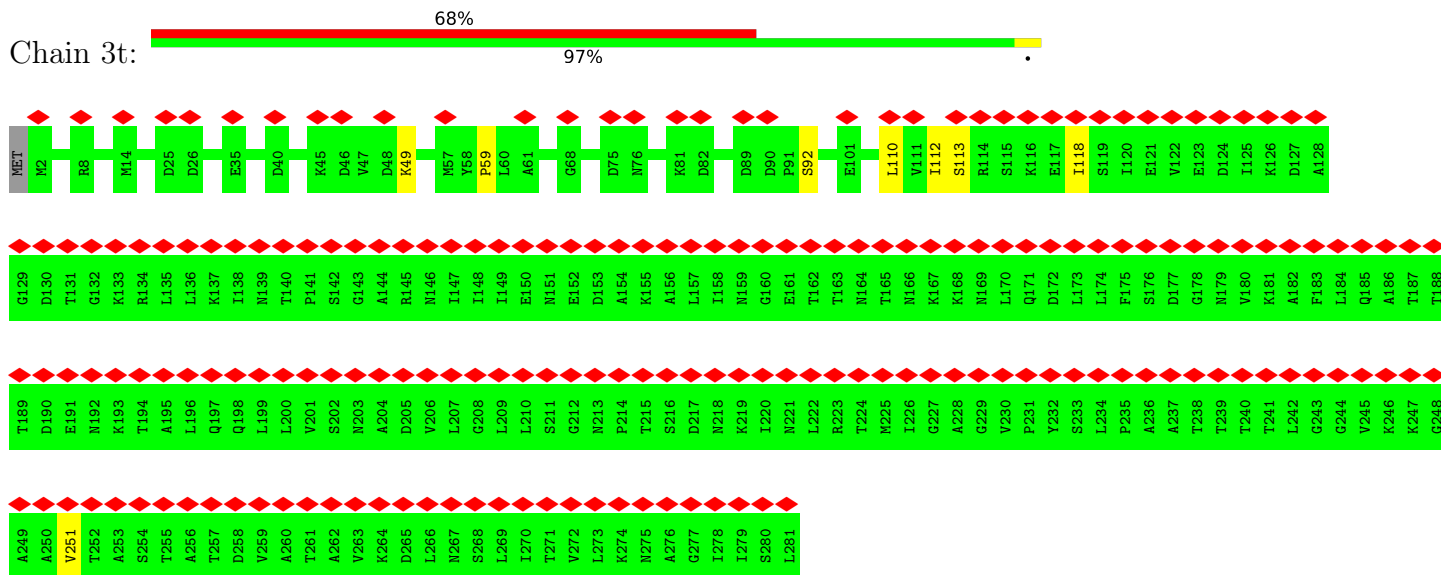


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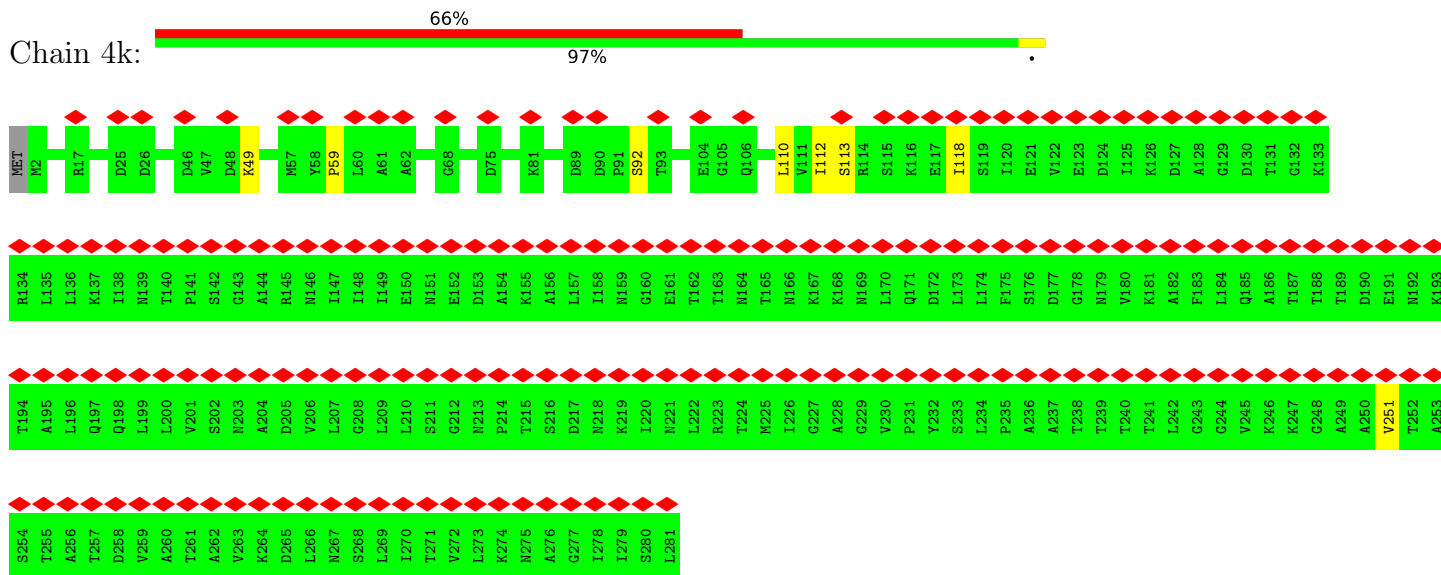




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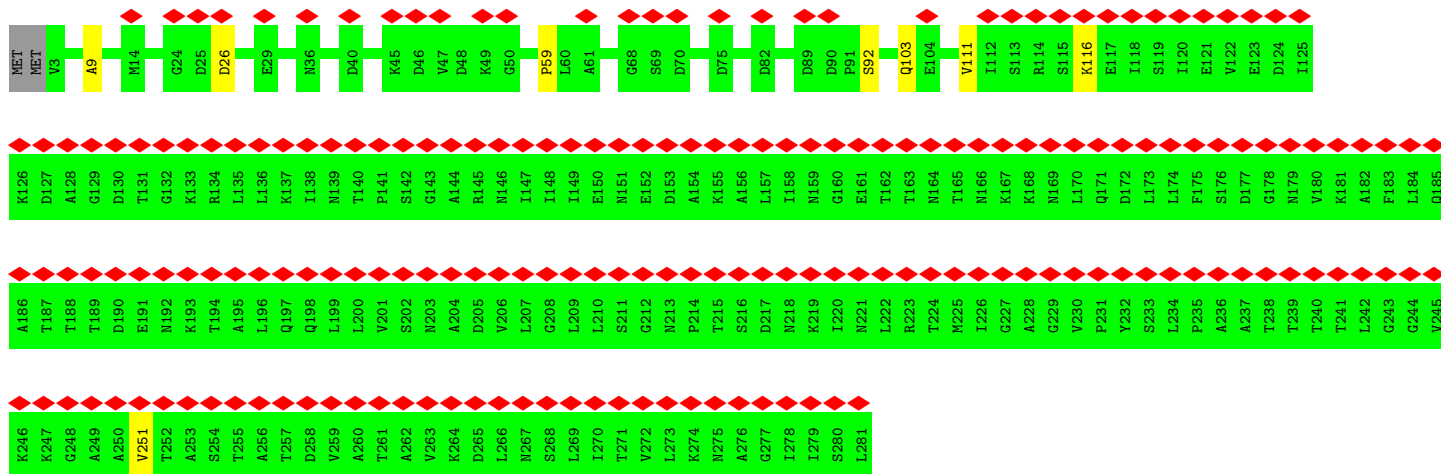


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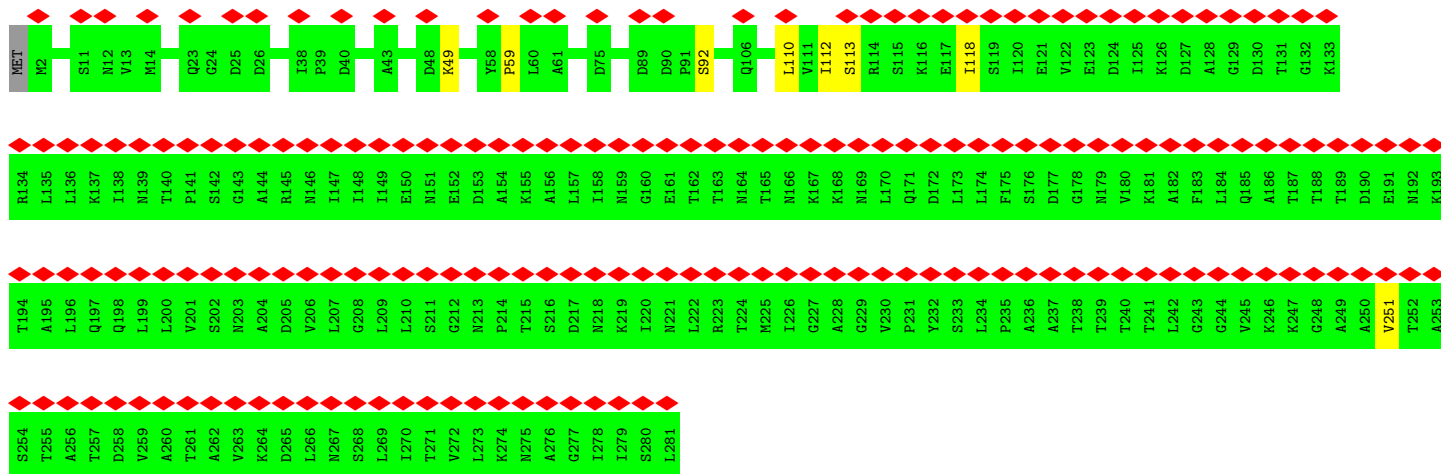


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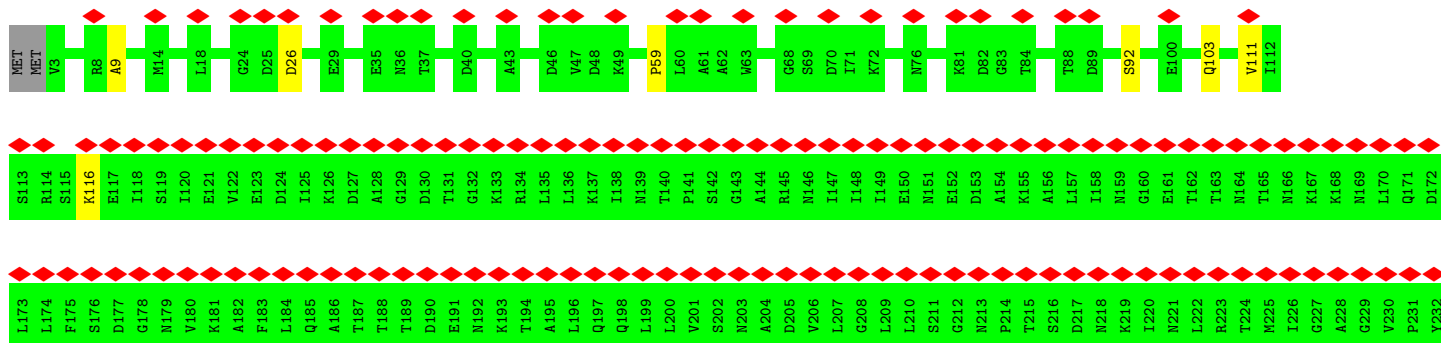


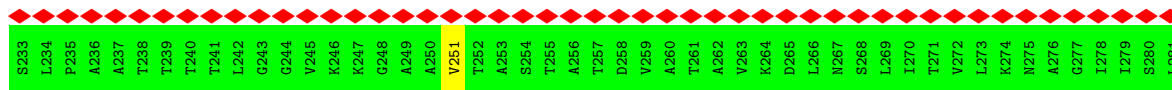


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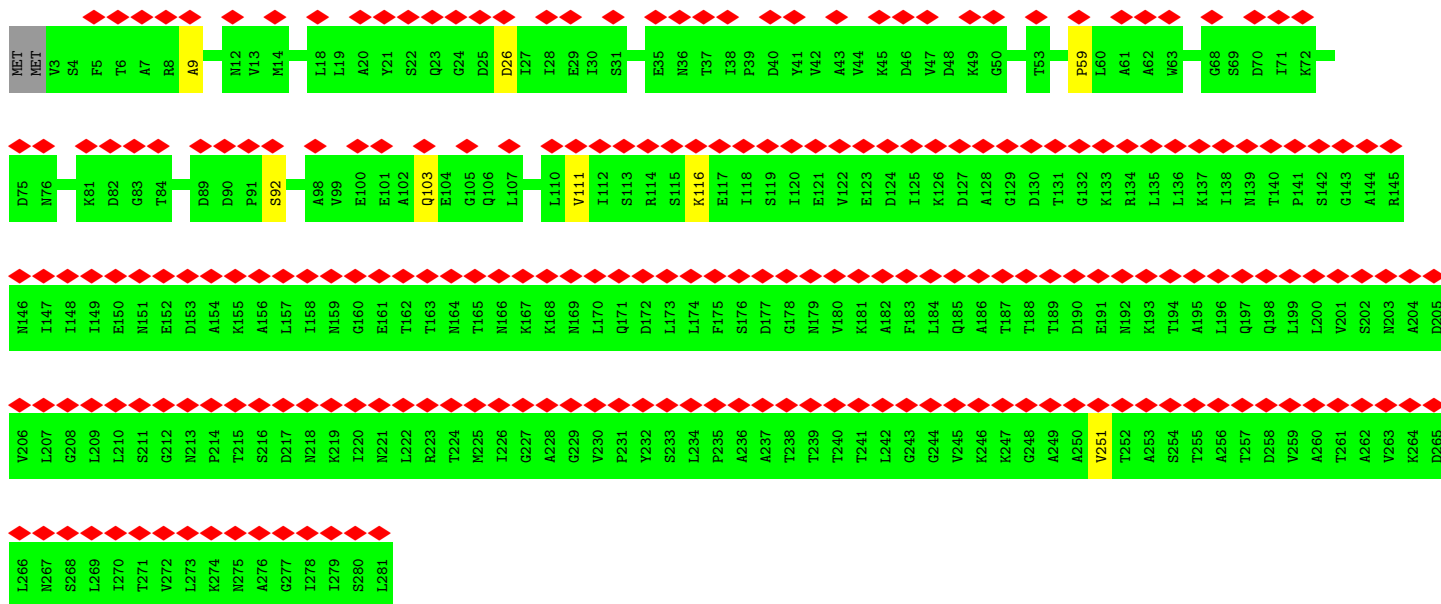
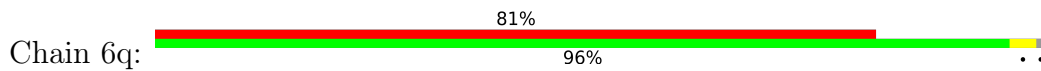


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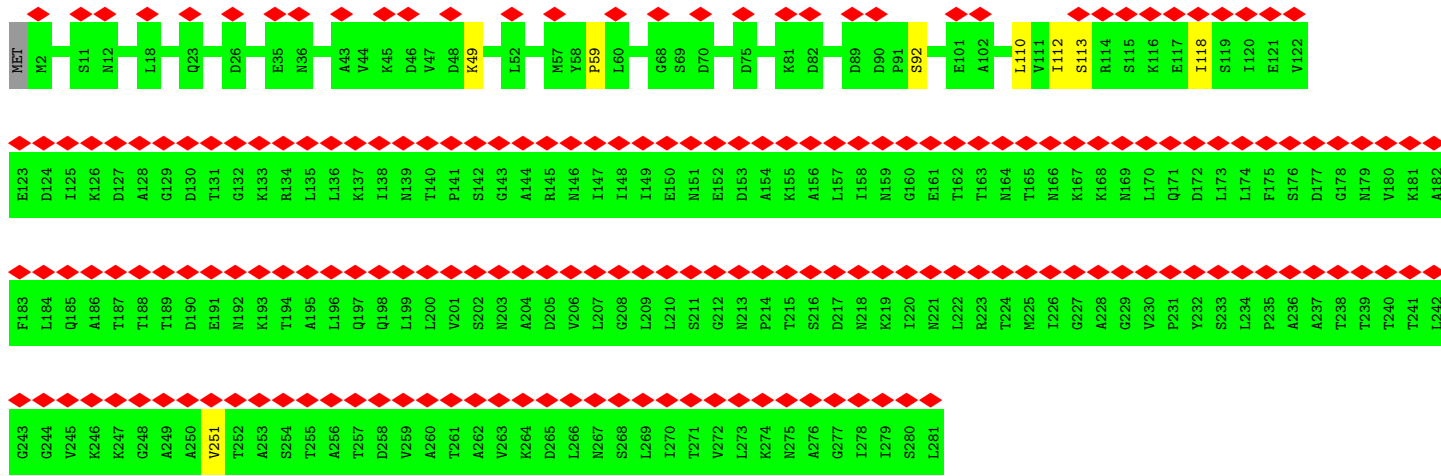




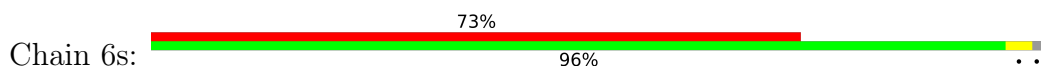
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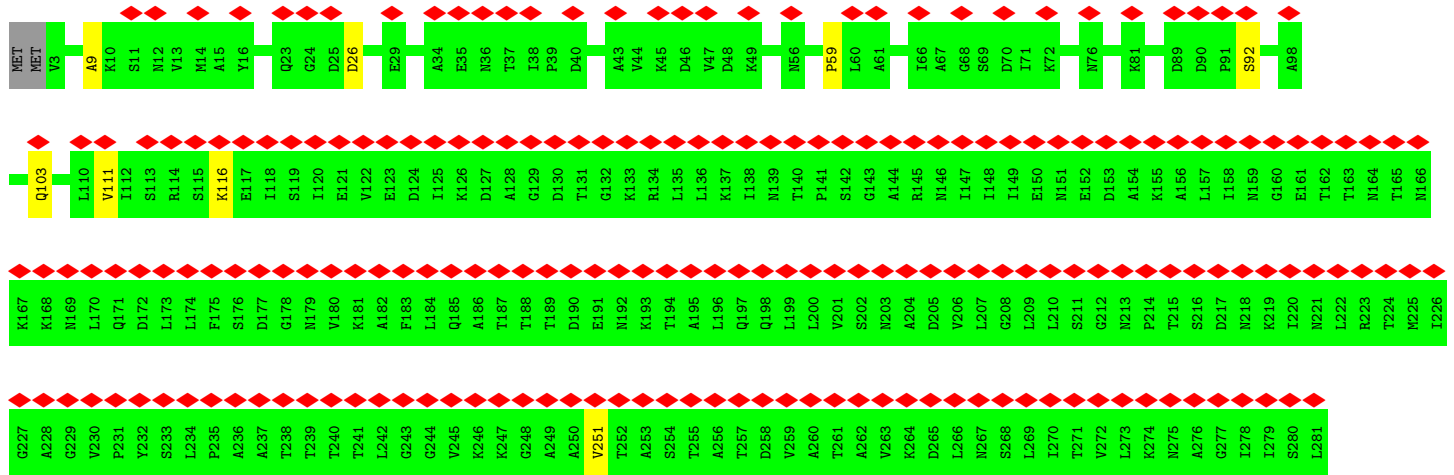


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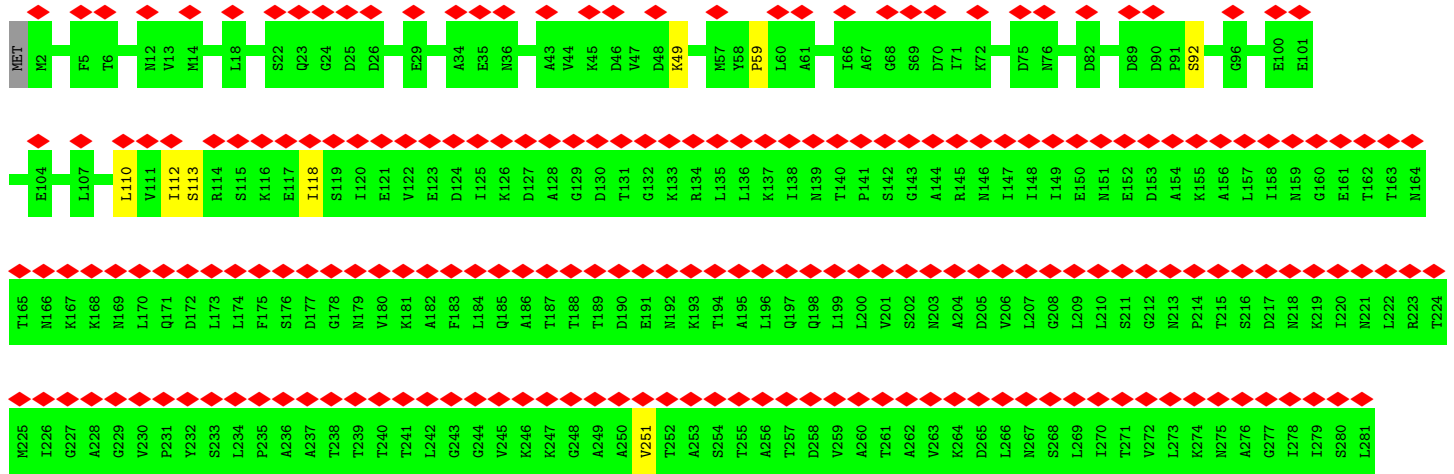
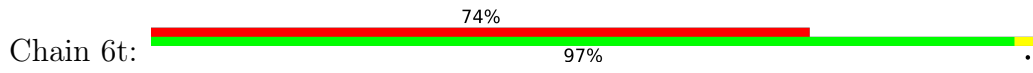


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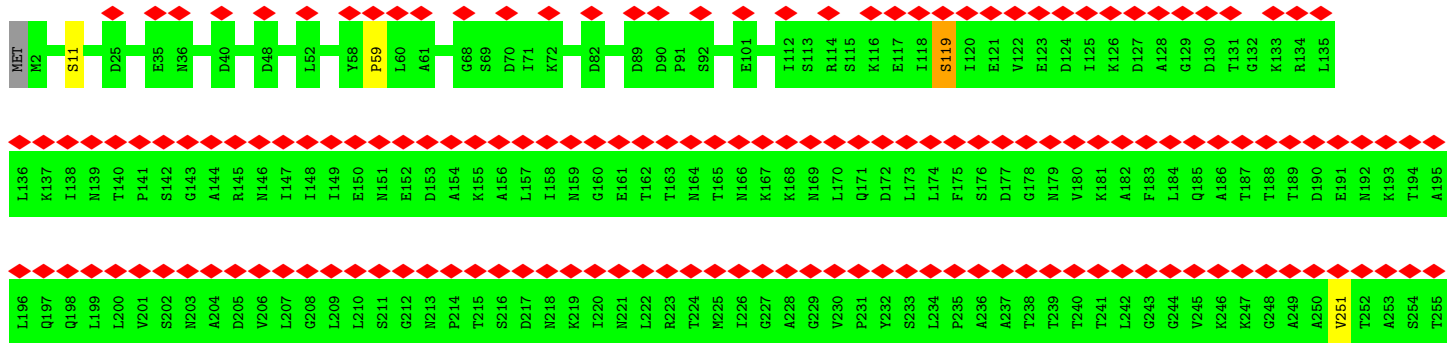


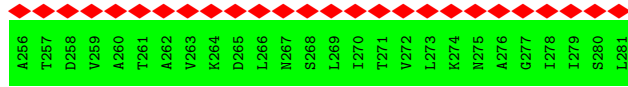


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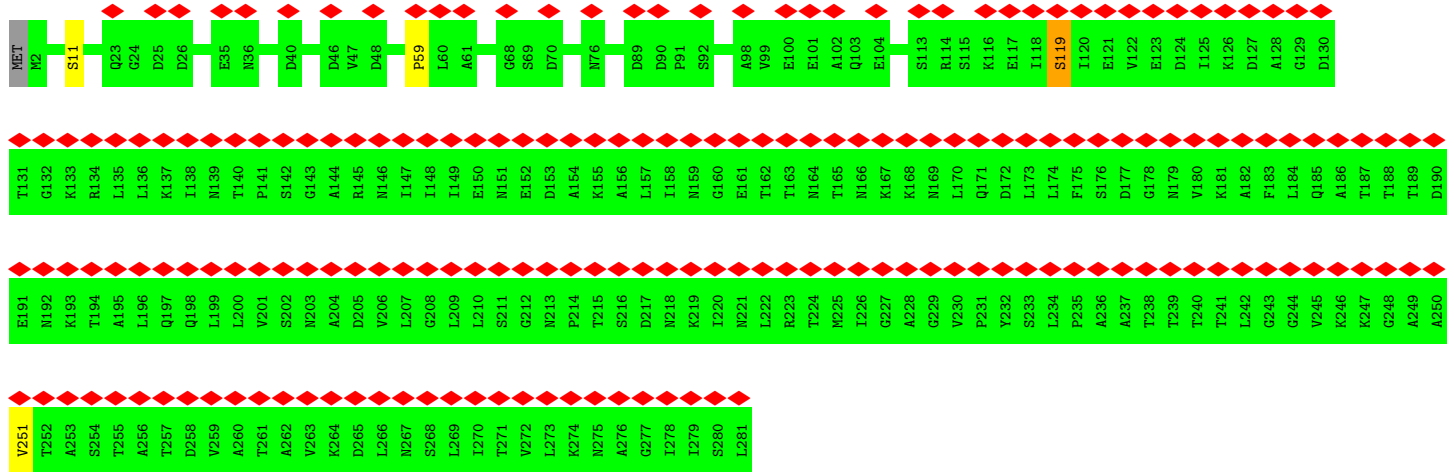


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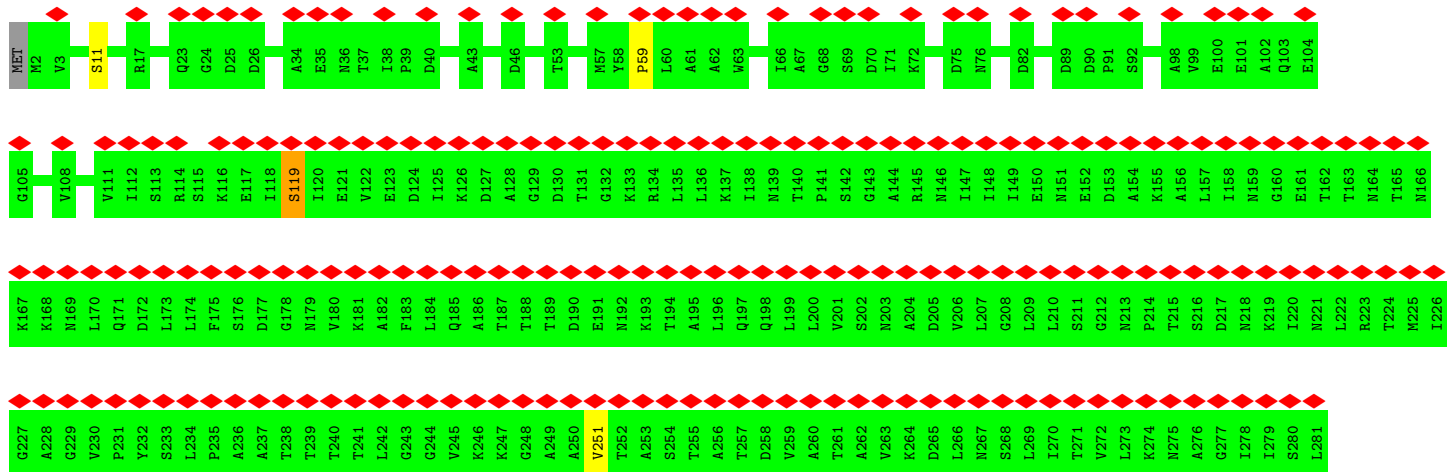
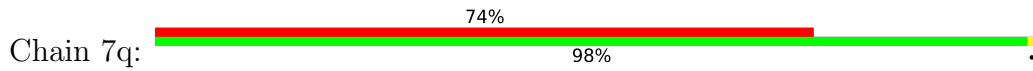




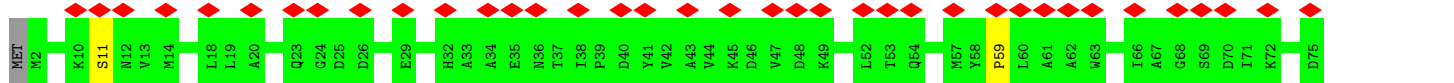
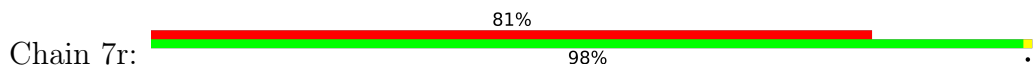
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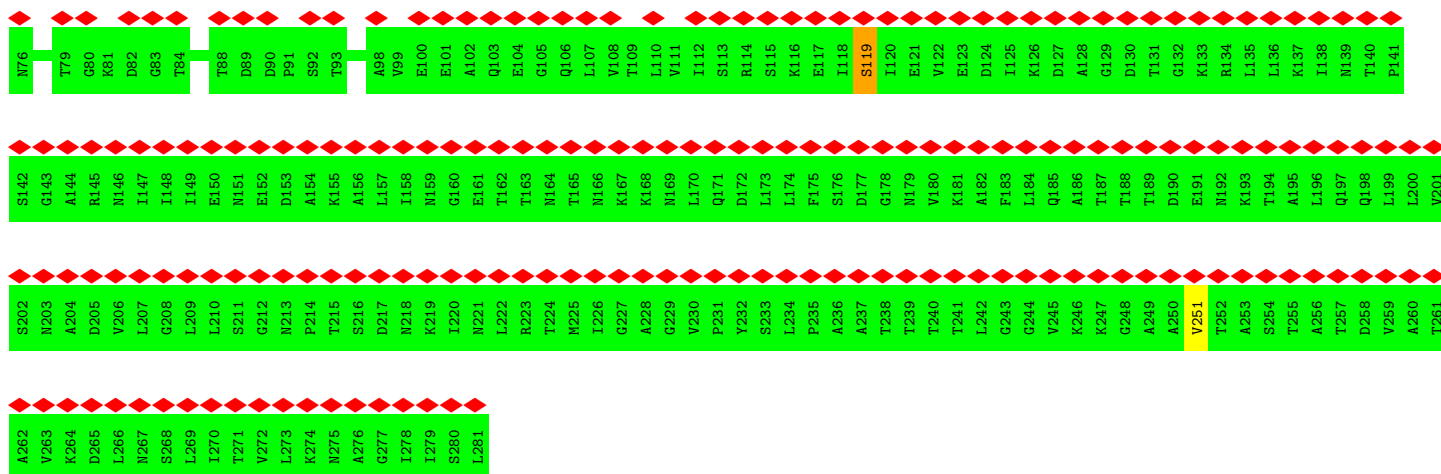


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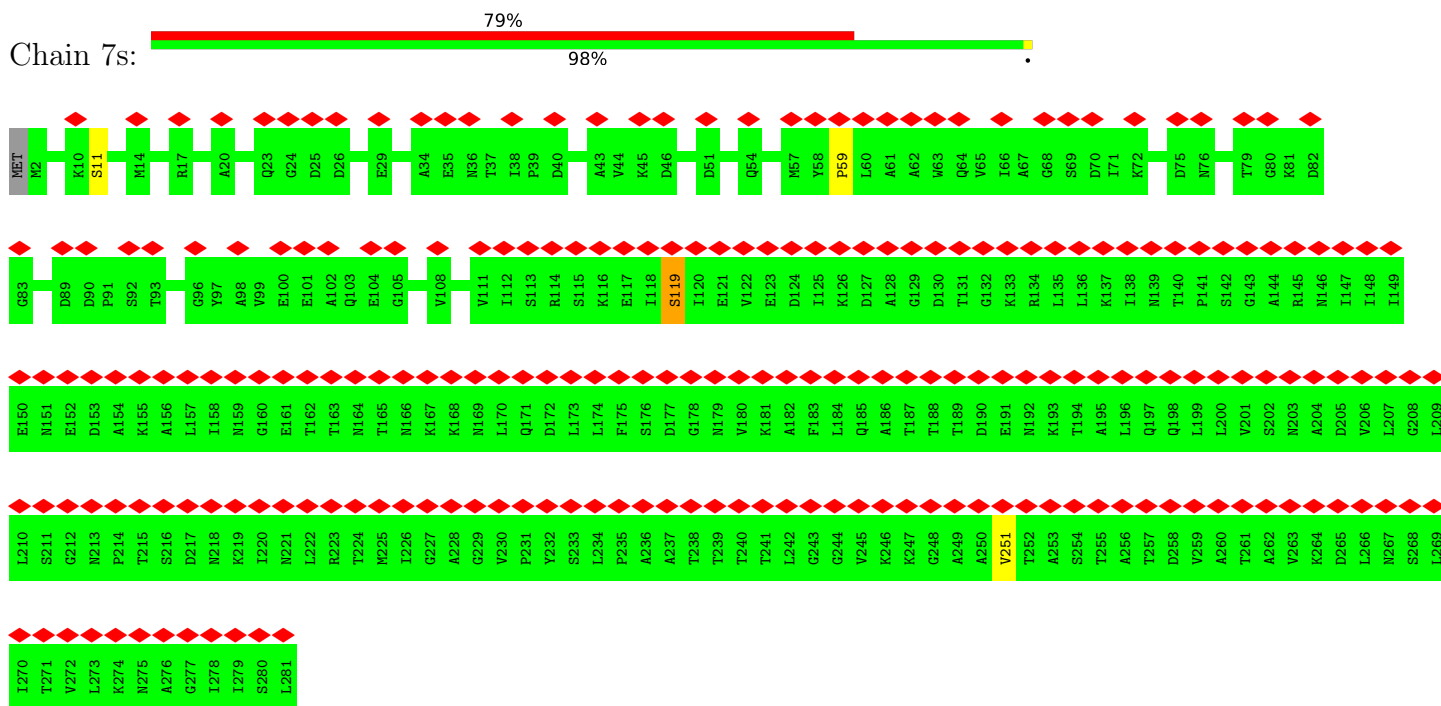


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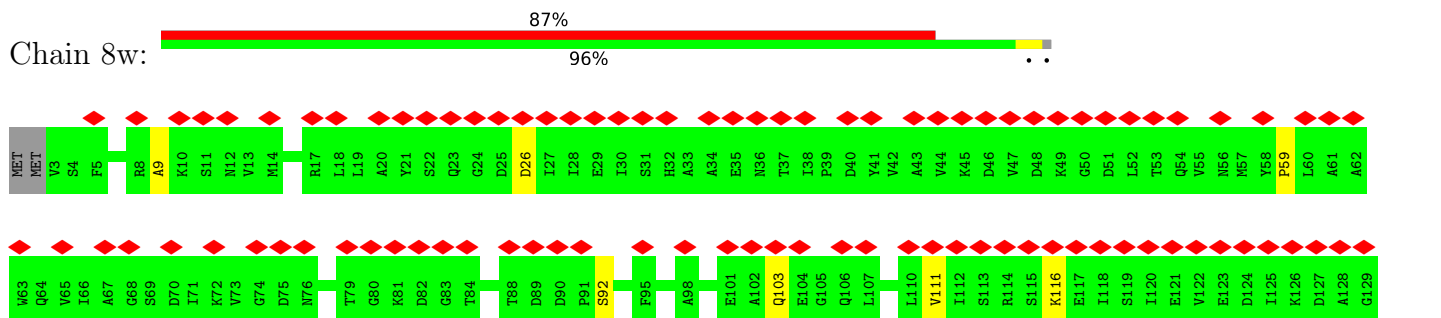


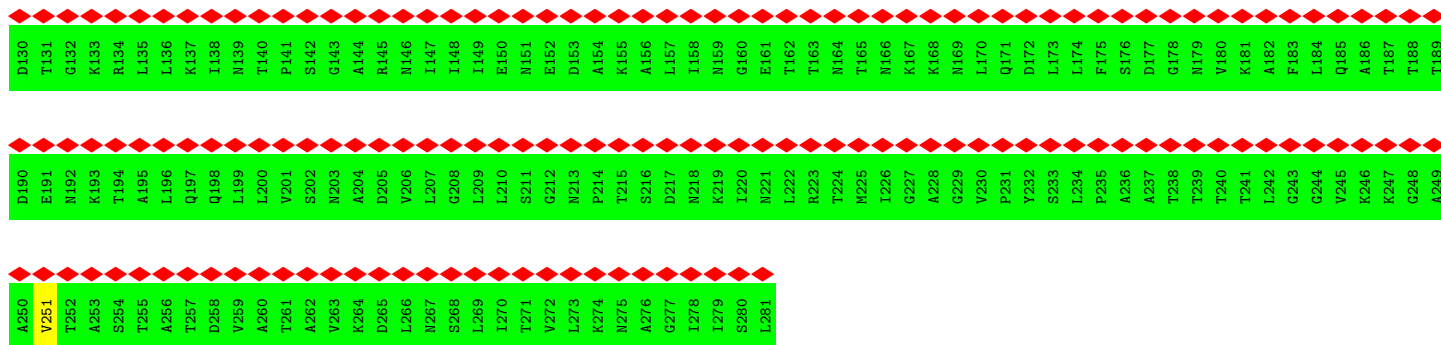


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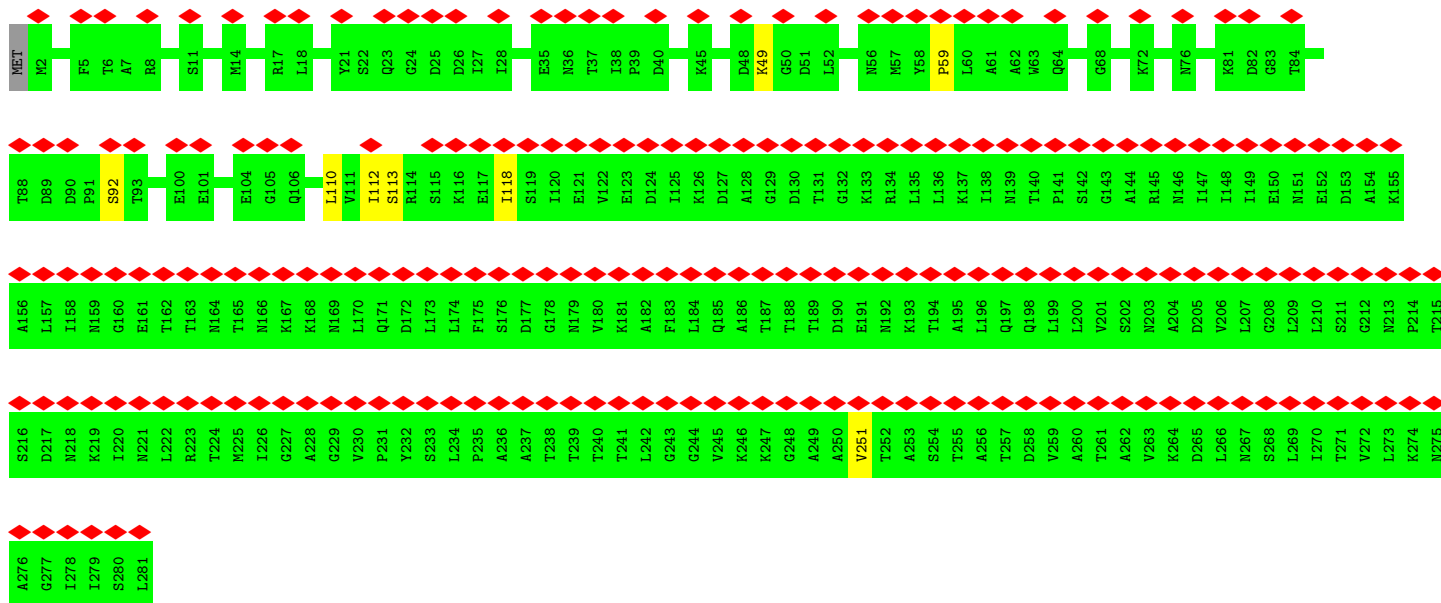
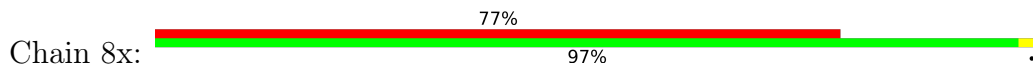


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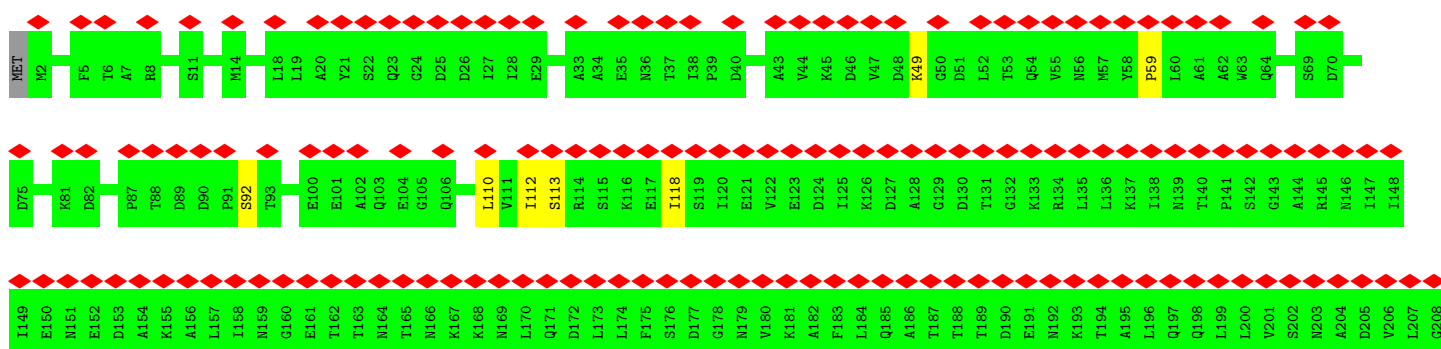
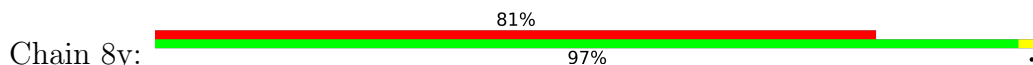


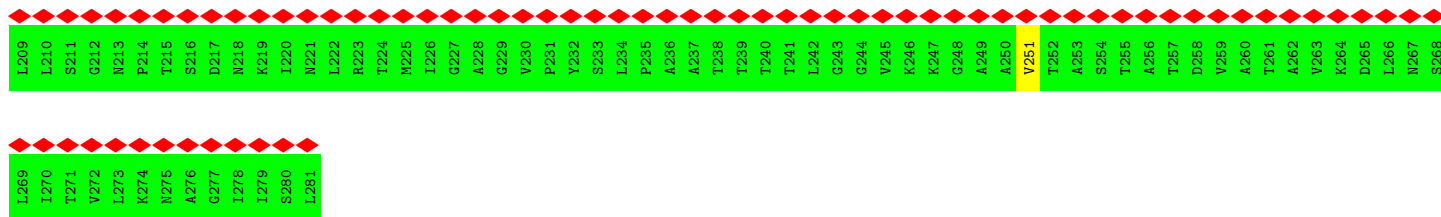


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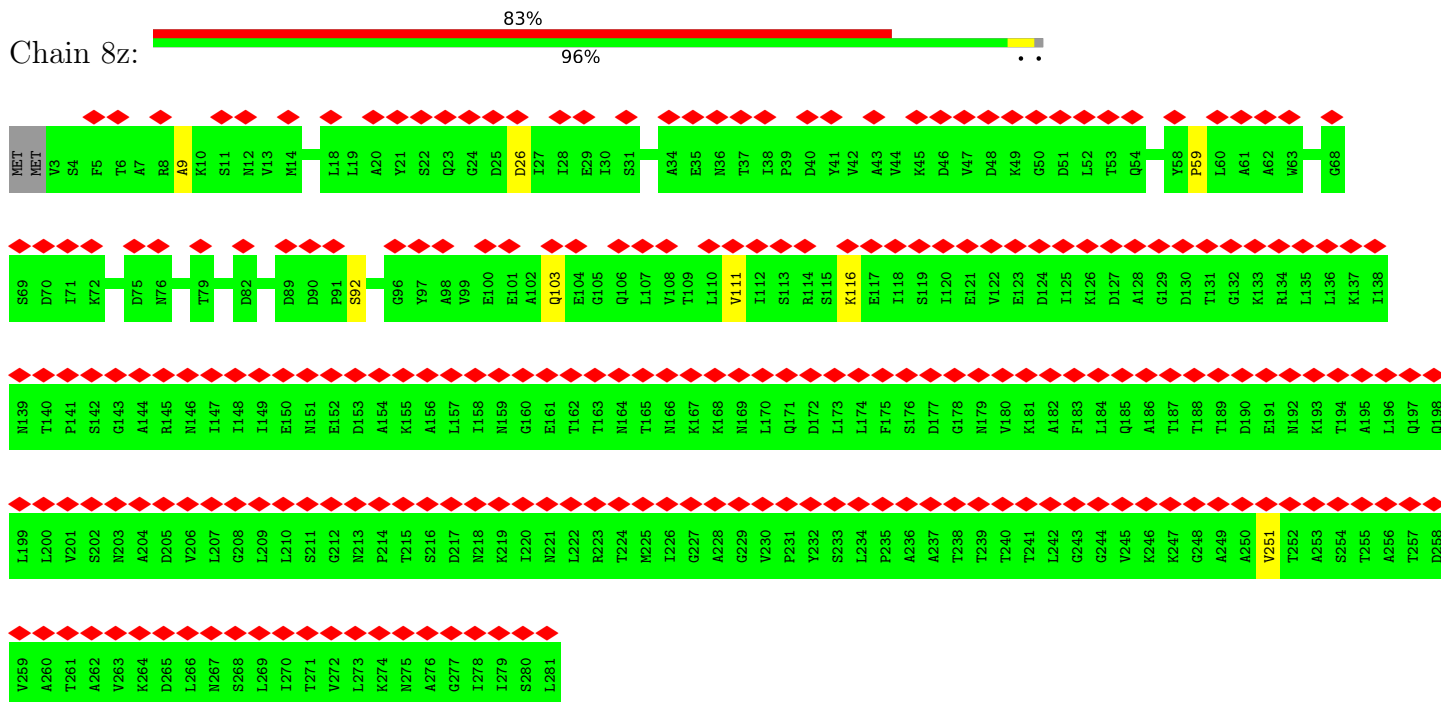


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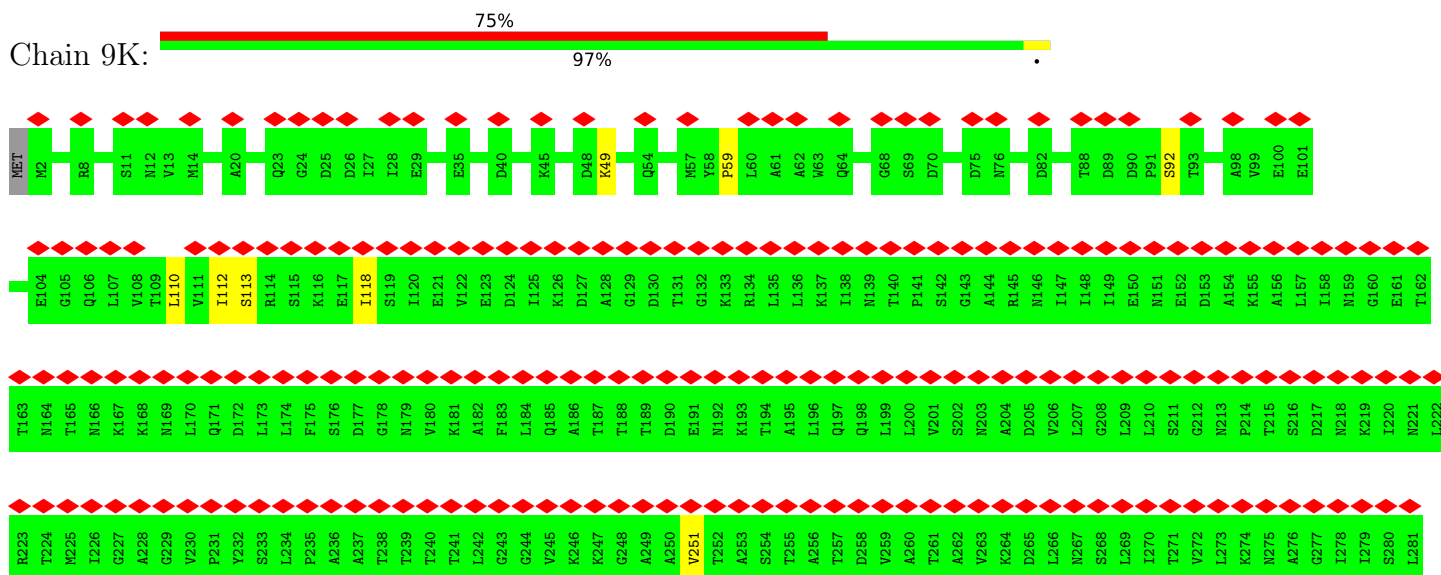




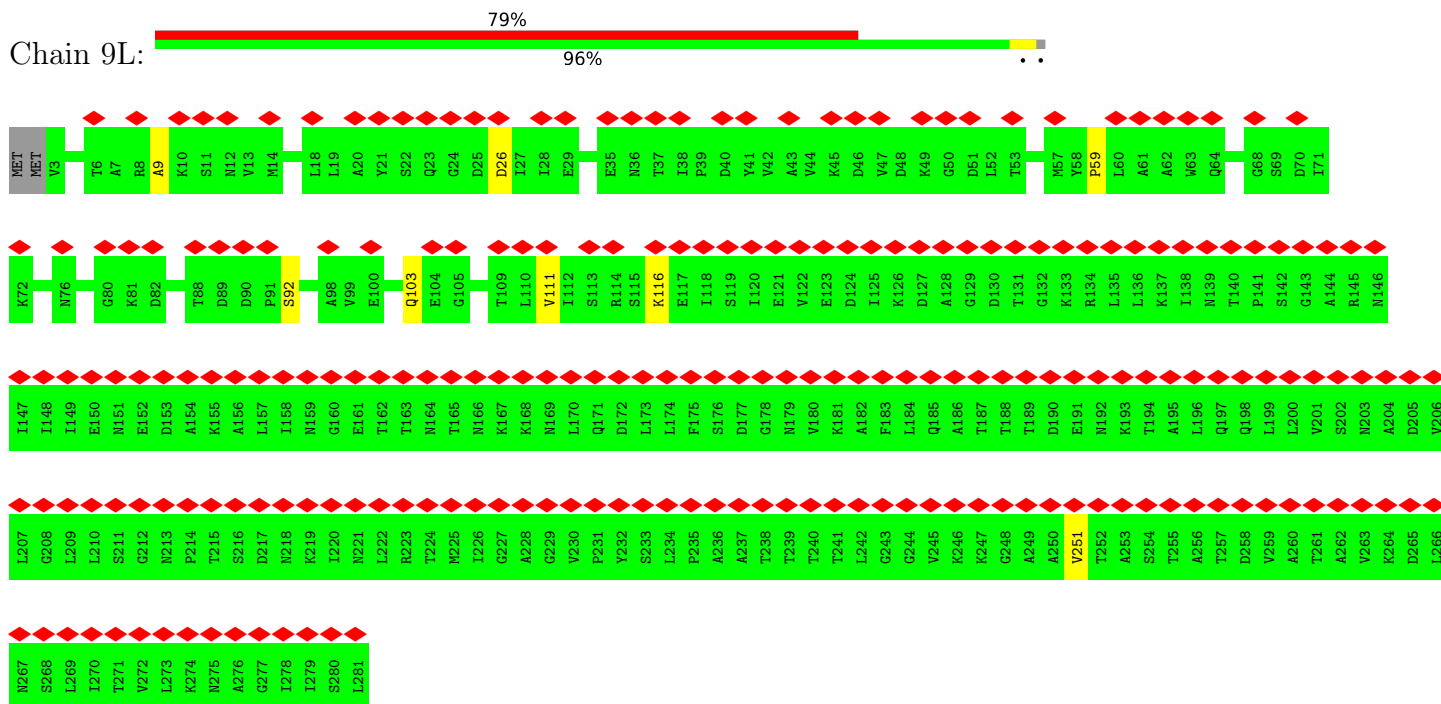
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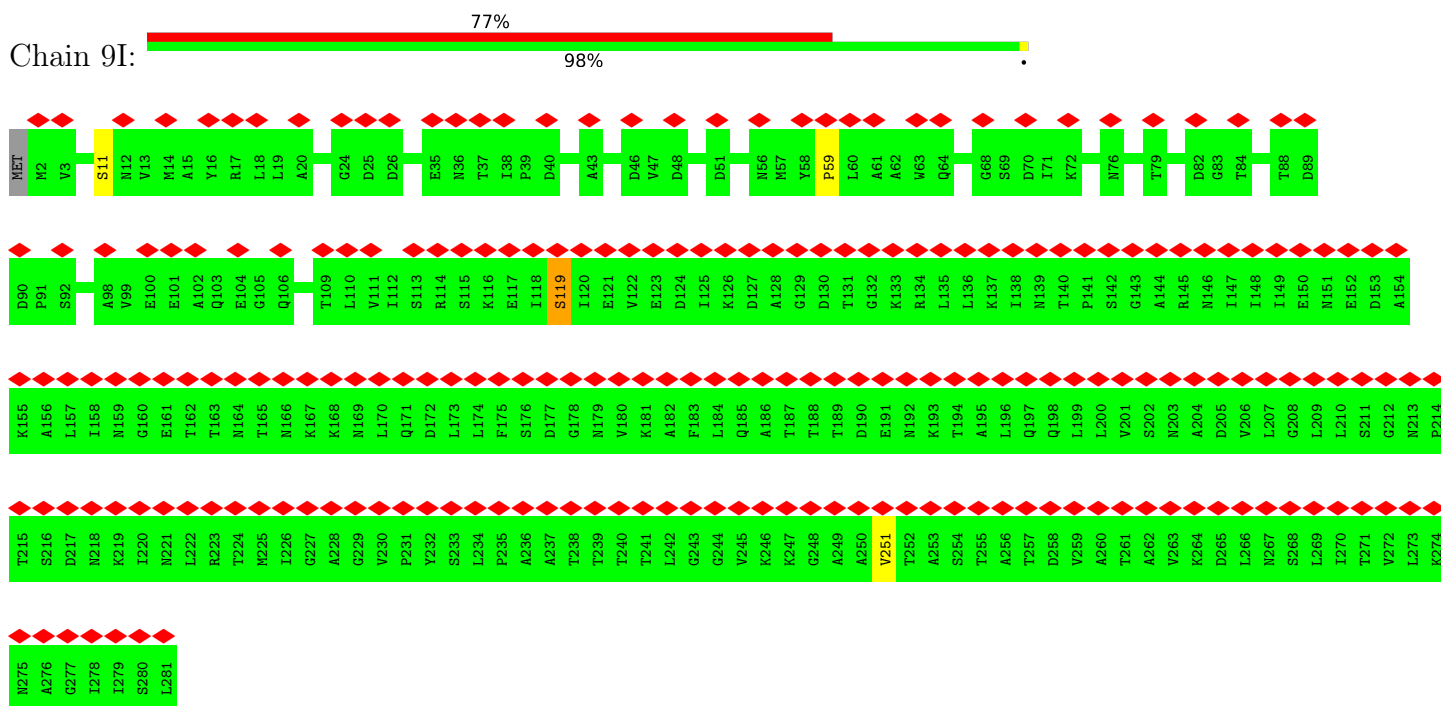
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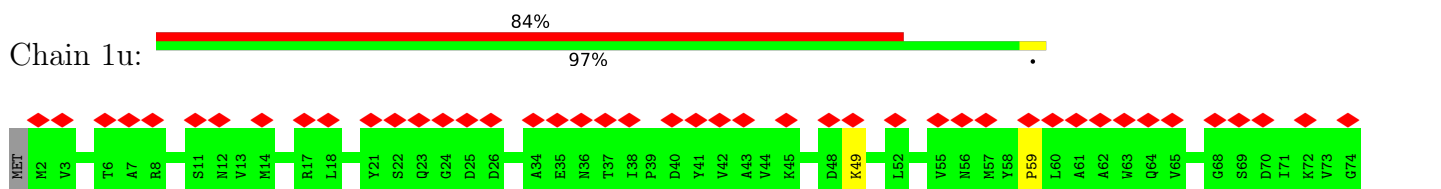
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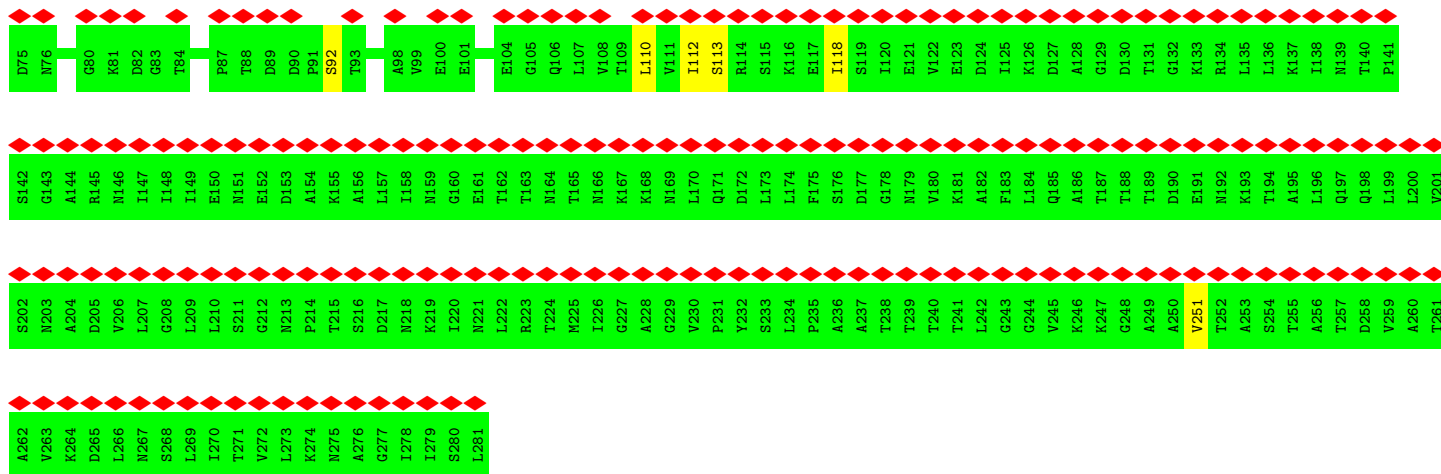


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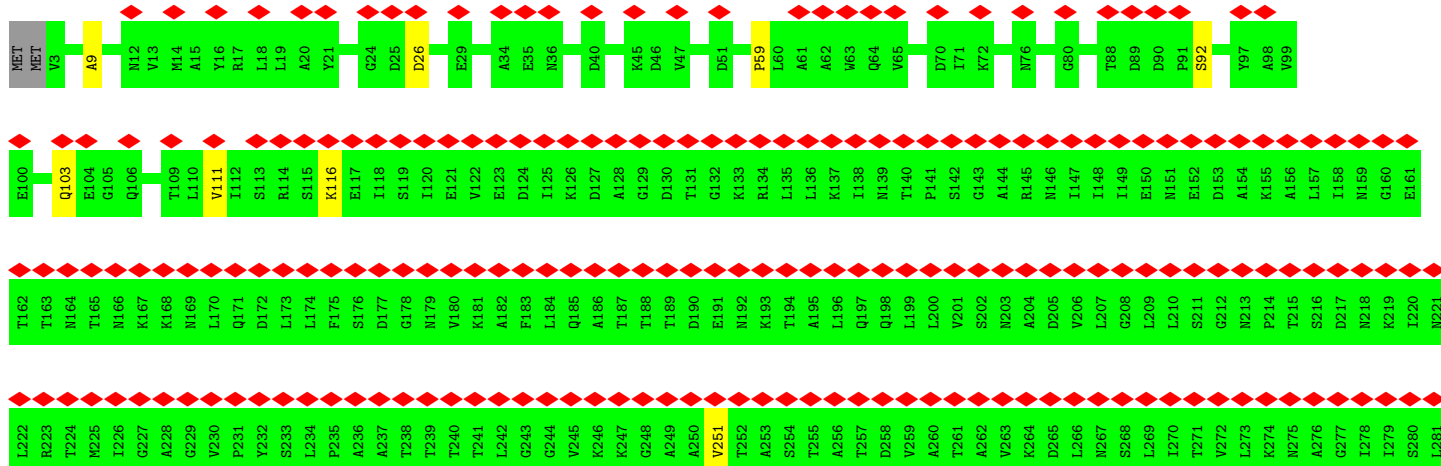
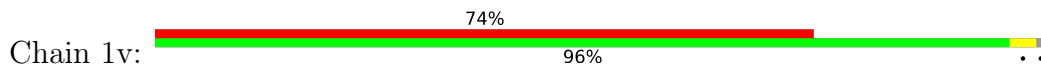


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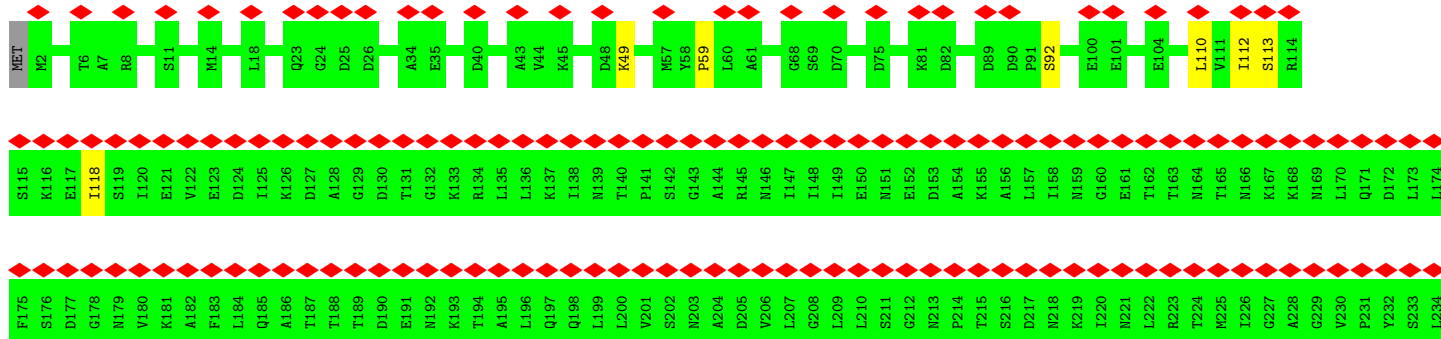
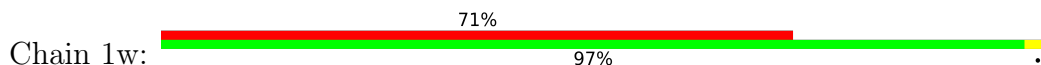


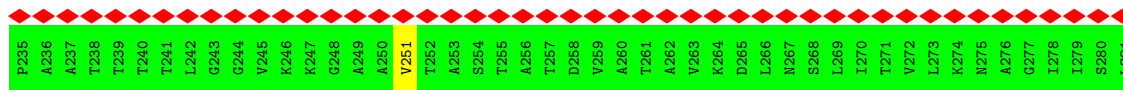


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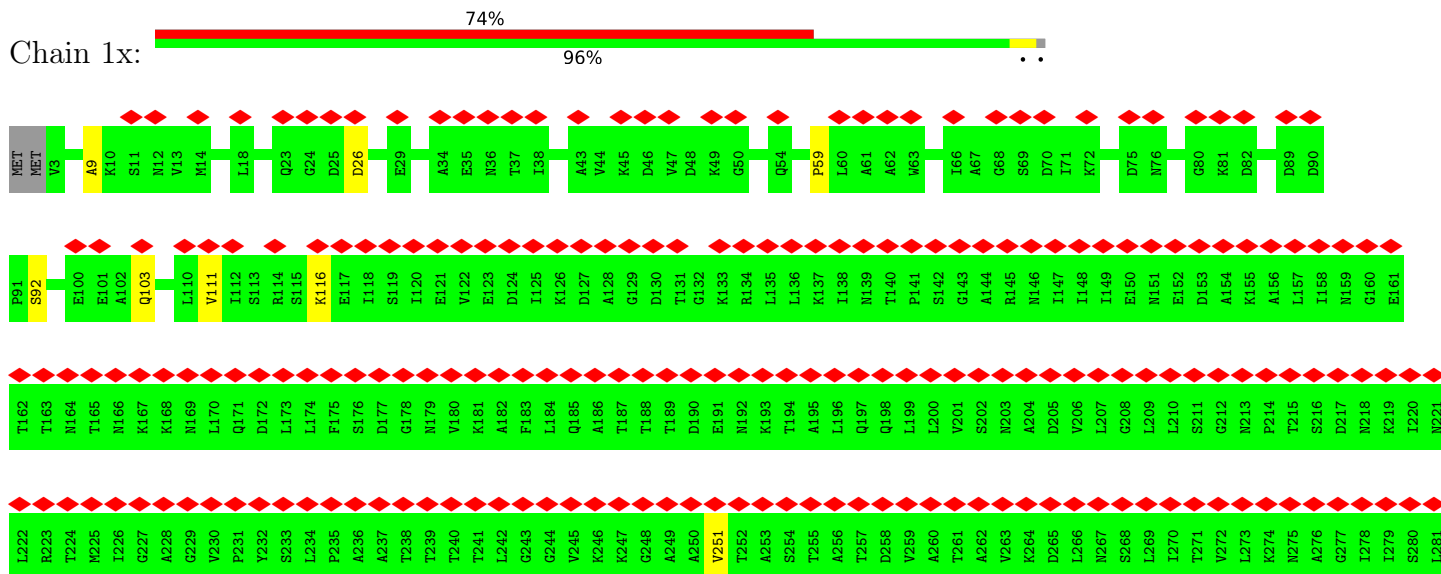


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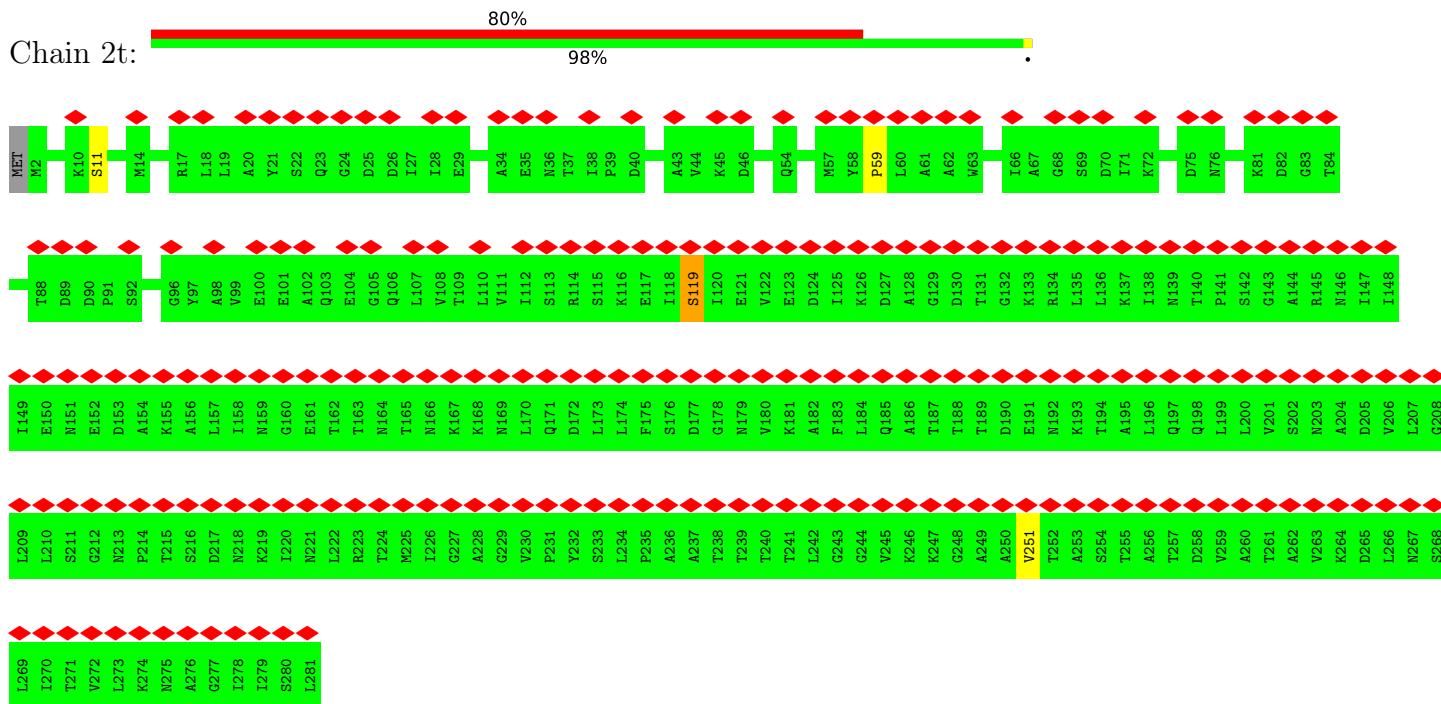




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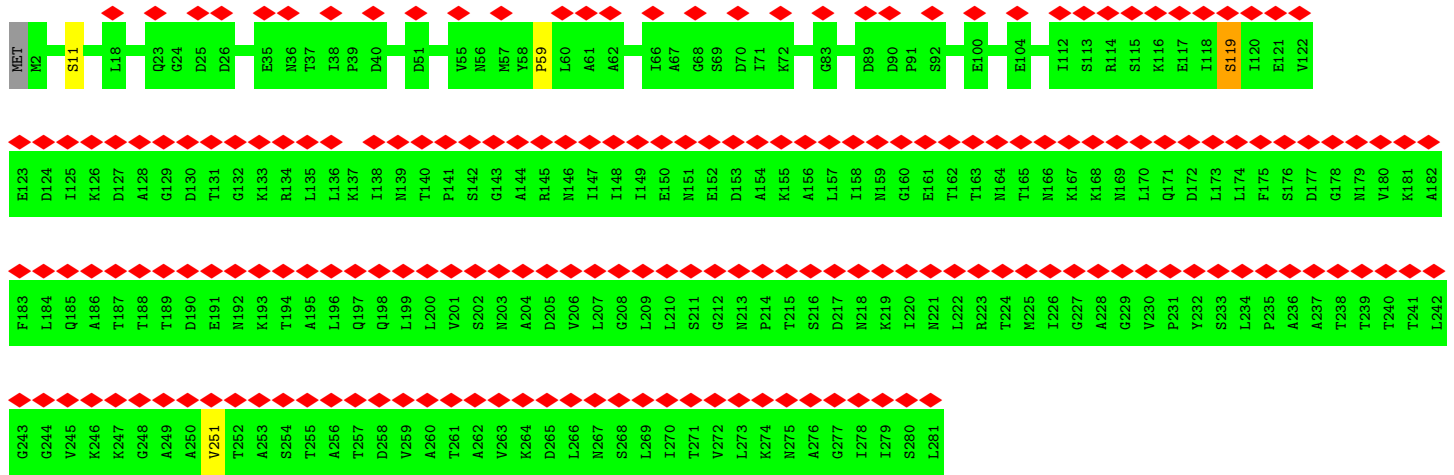


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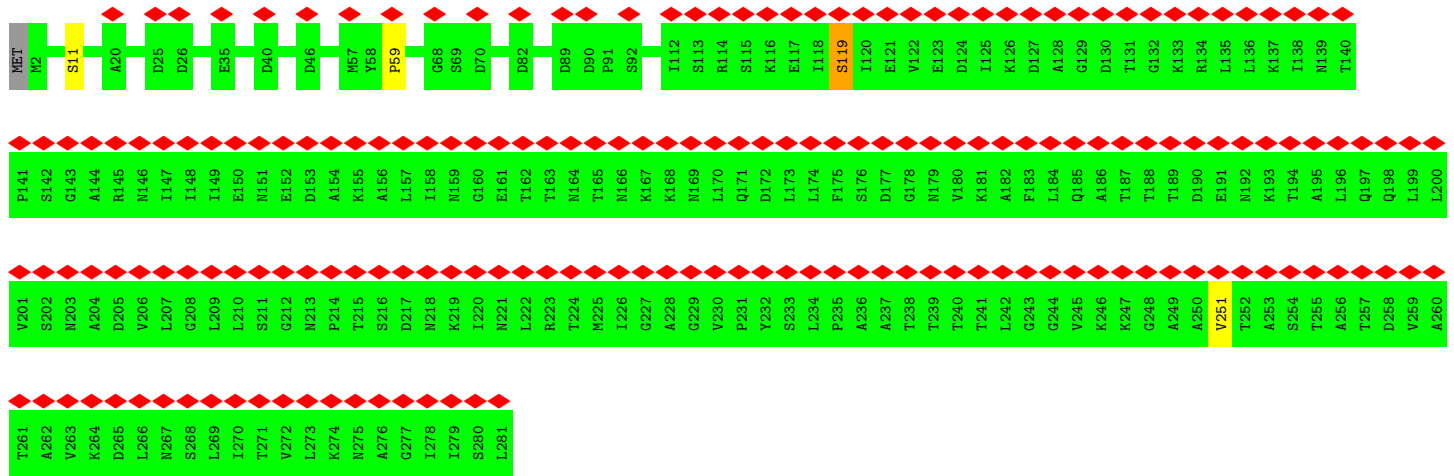


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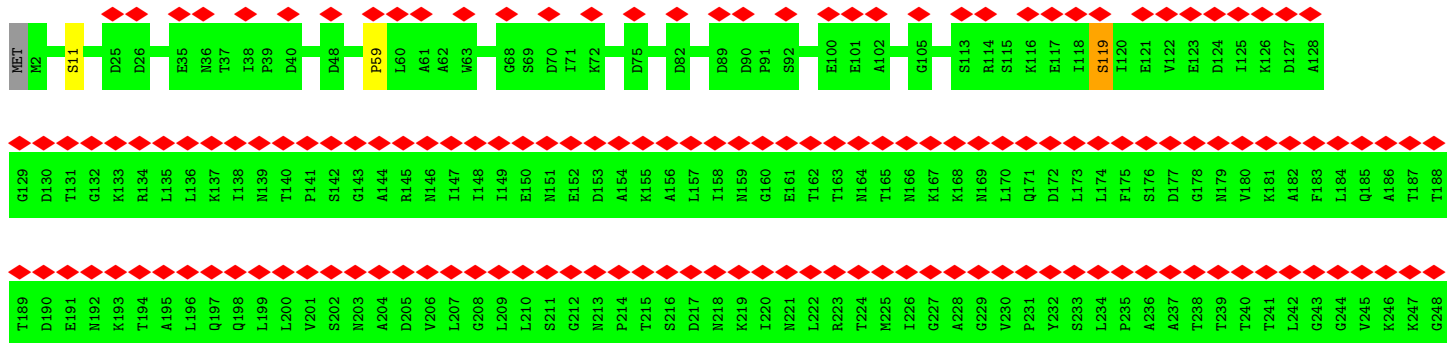


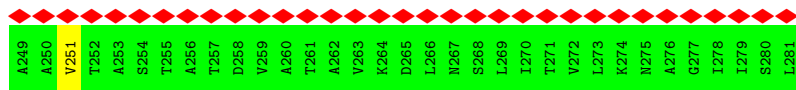


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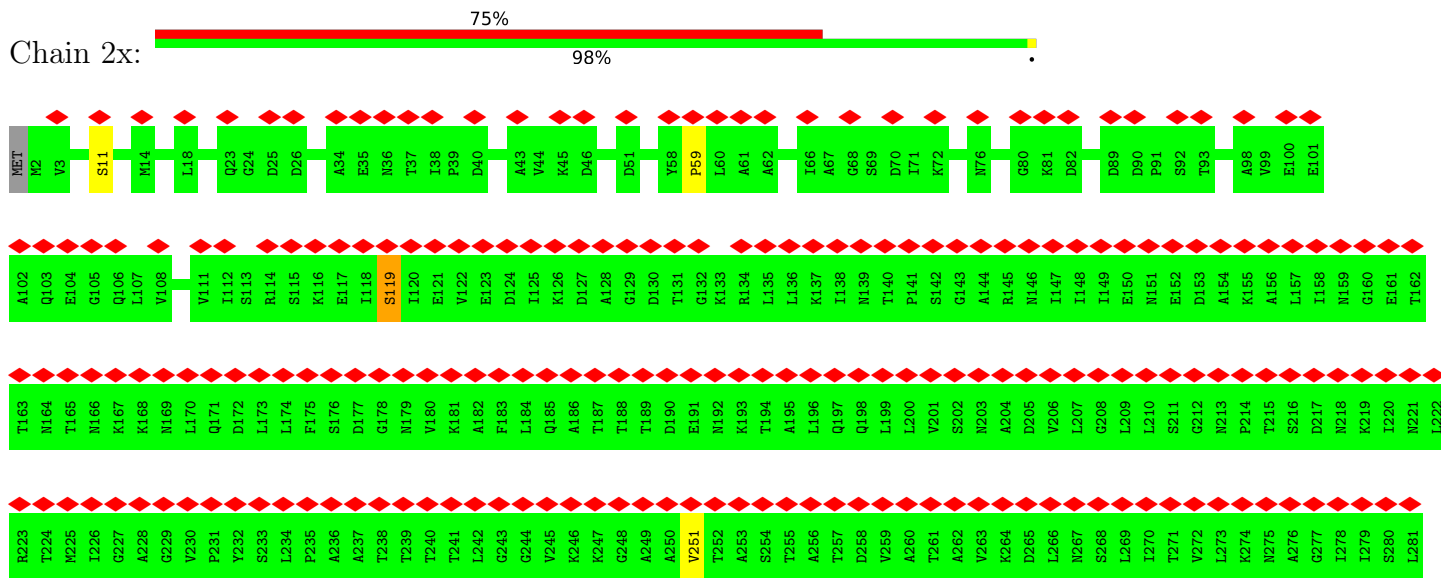


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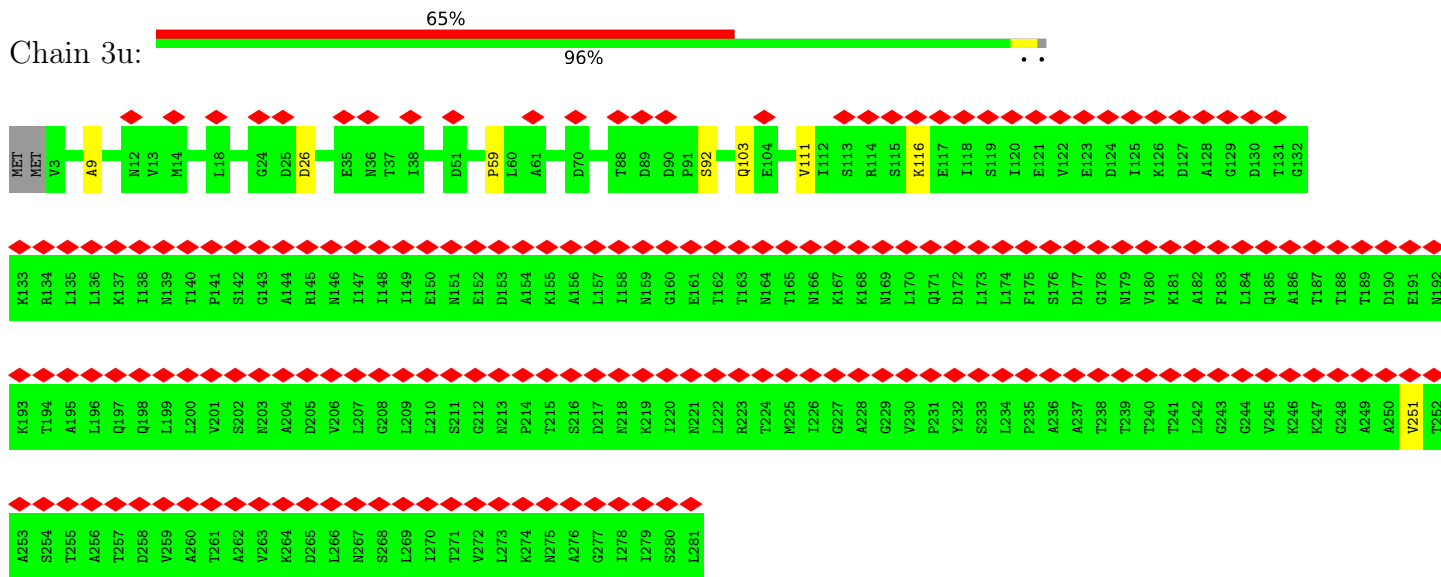




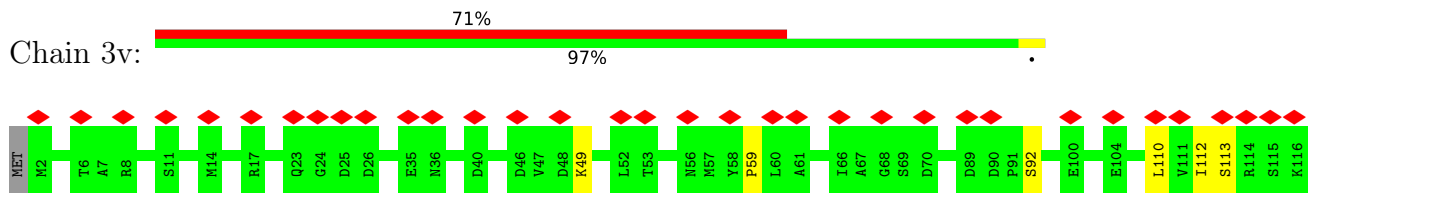
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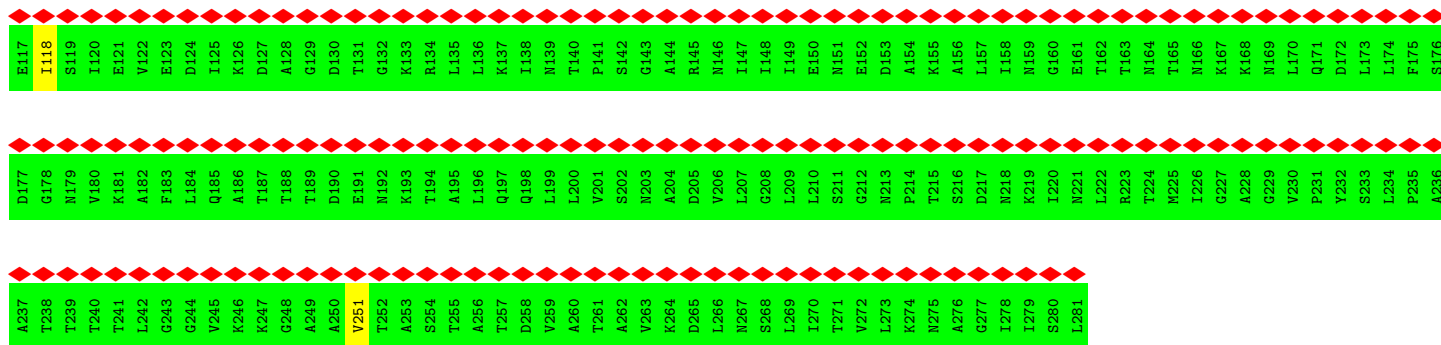


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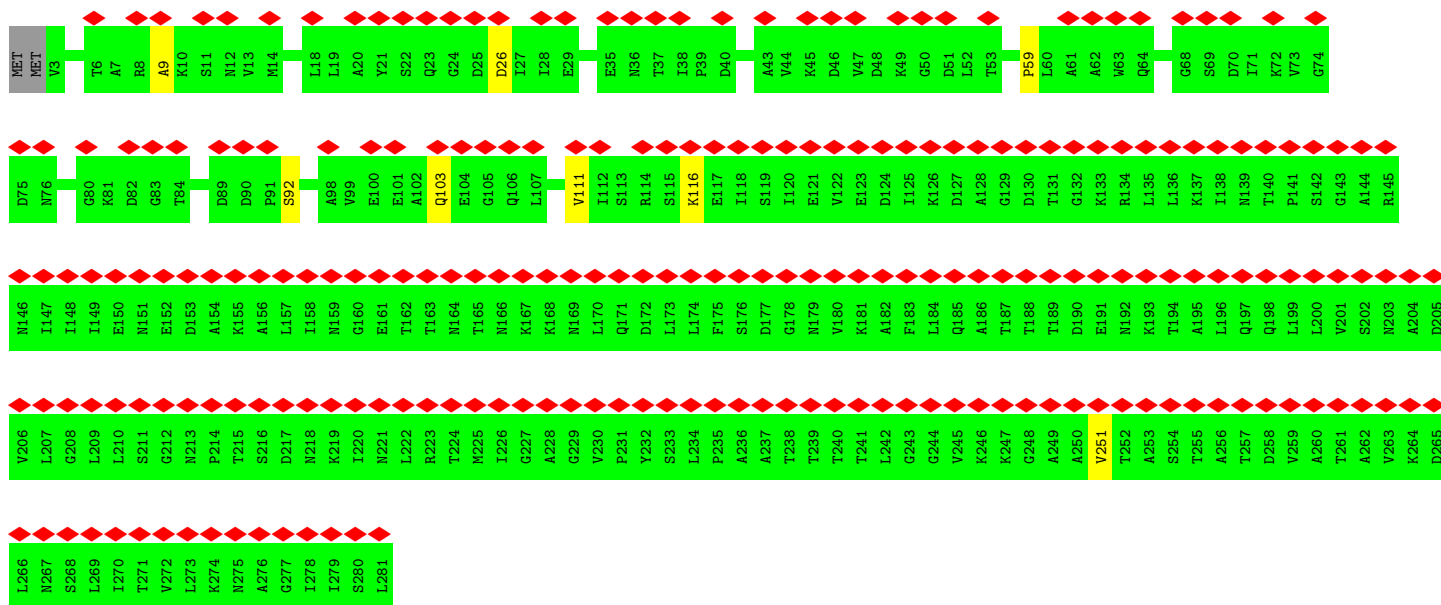
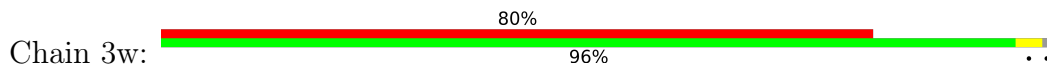


• Molecule 2: Capsid fiber protein

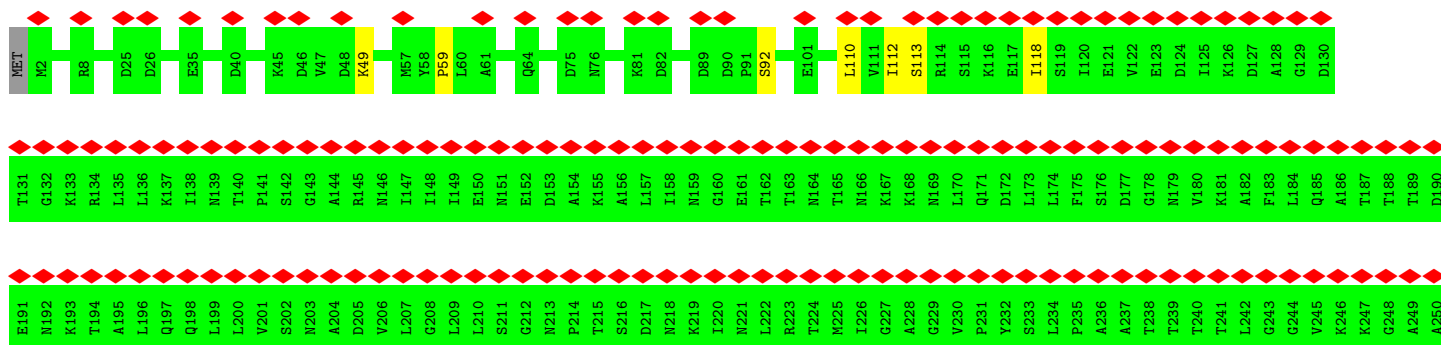


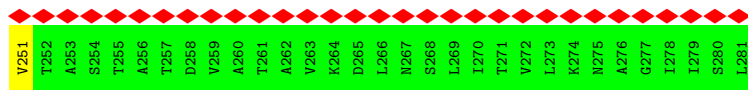


• Molecule 2: Capsid fiber protein

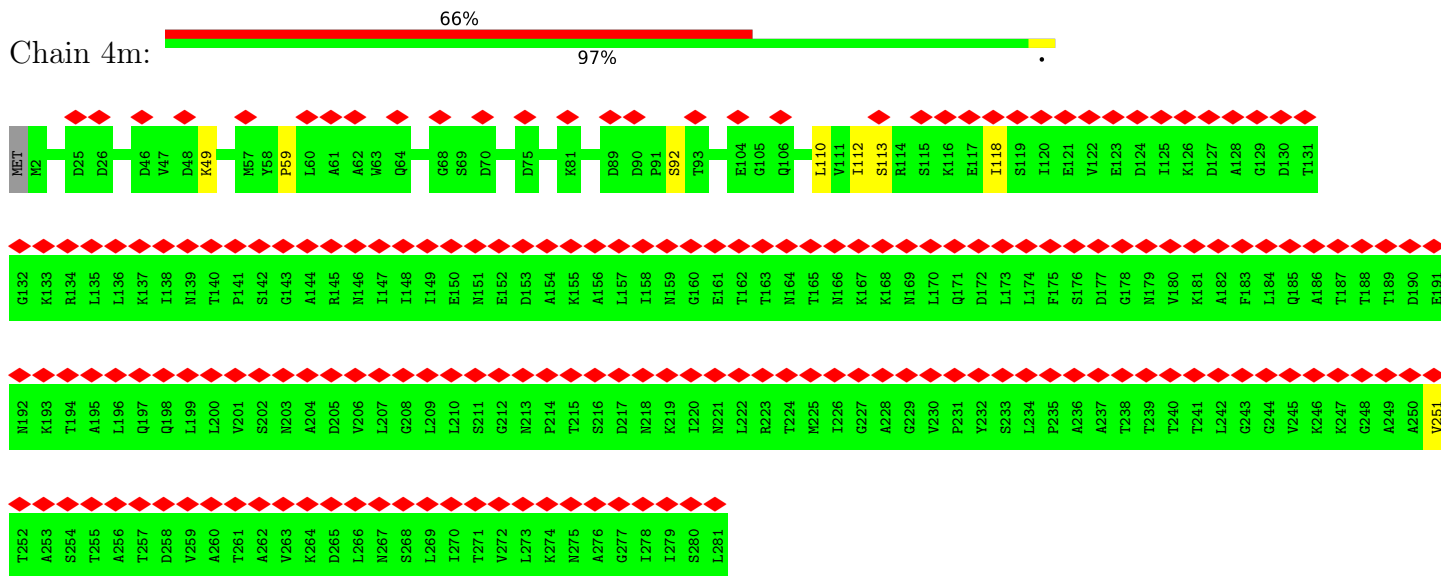


• Molecule 2: Capsid fiber protein

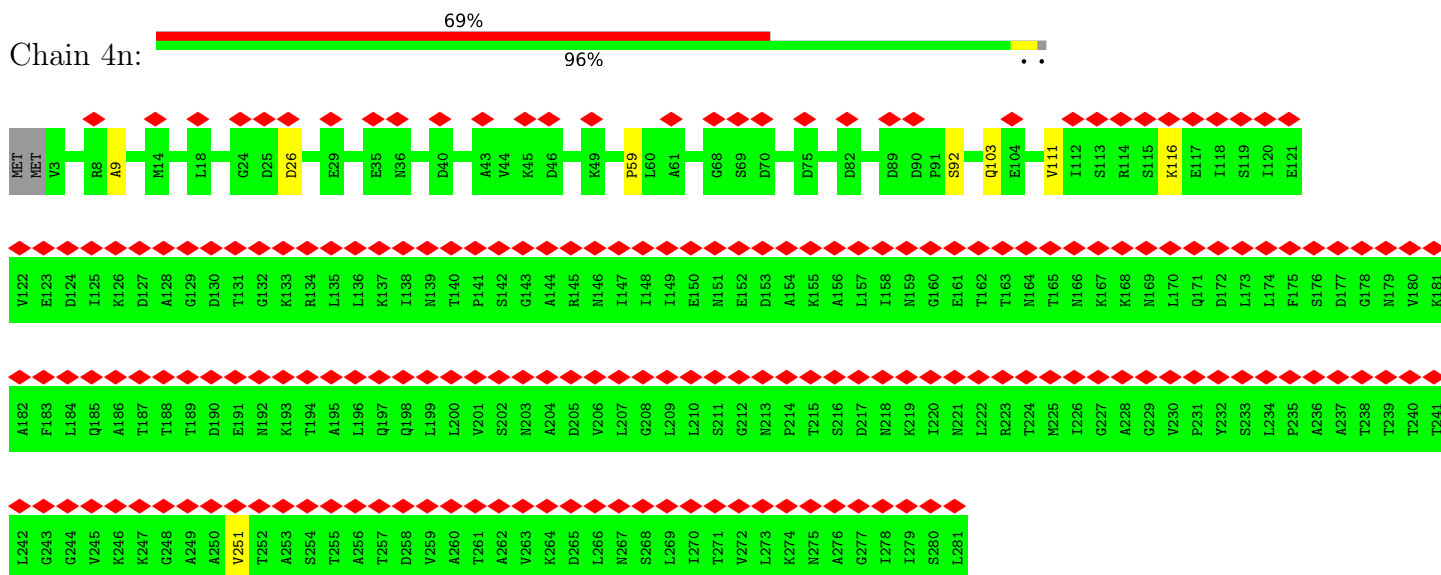




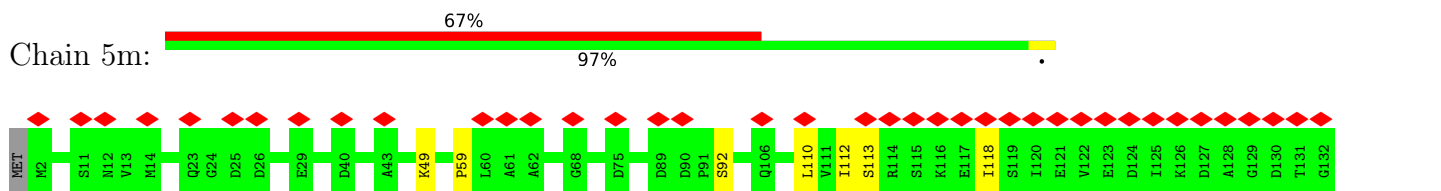
• Molecule 2: Capsid fiber protein

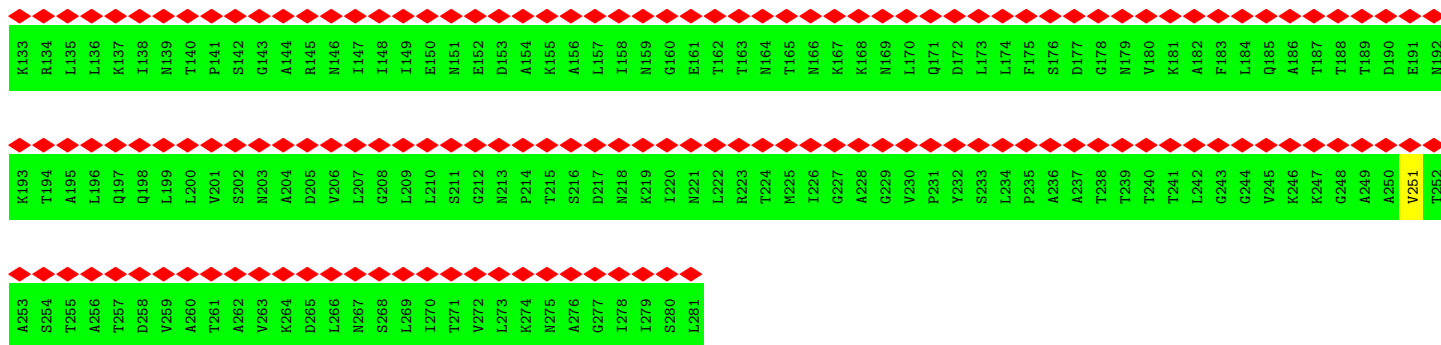


• Molecule 2: Capsid fiber protein

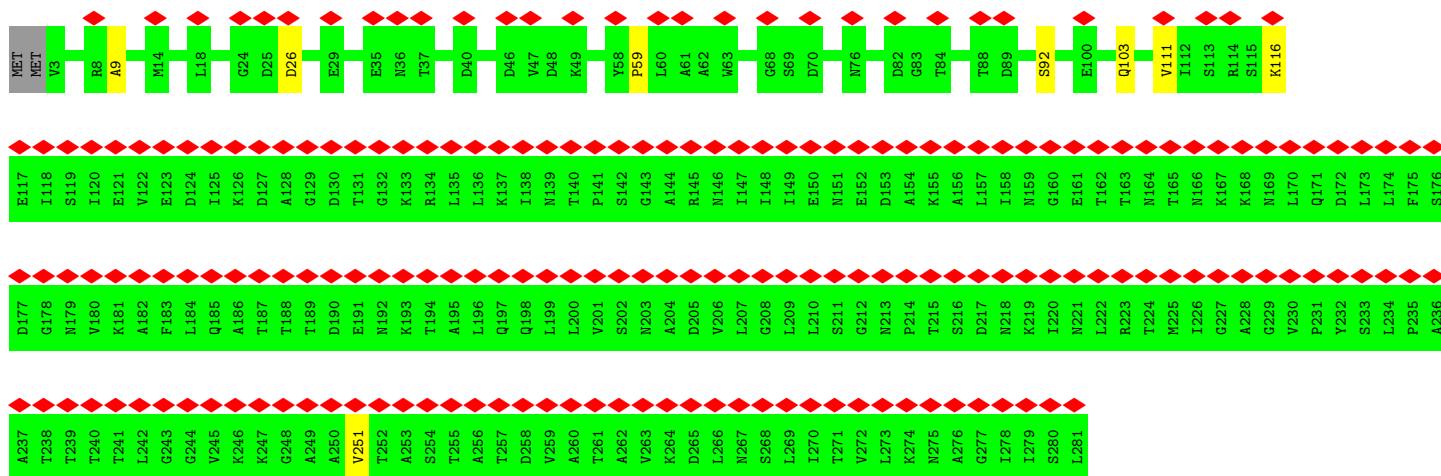


• Molecule 2: Capsid fiber protein

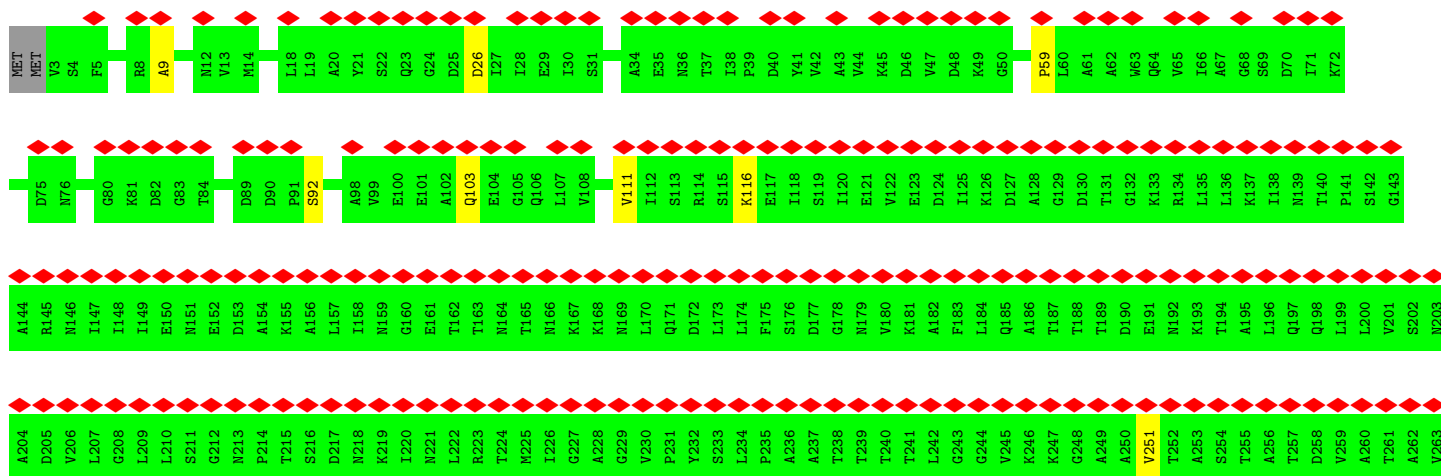
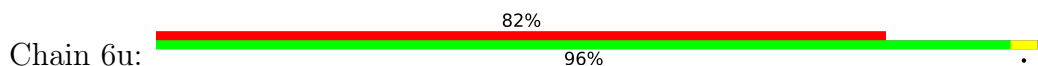


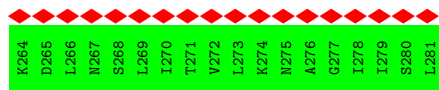


• Molecule 2: Capsid fiber protein

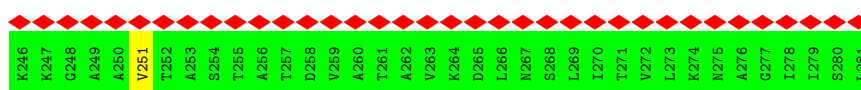
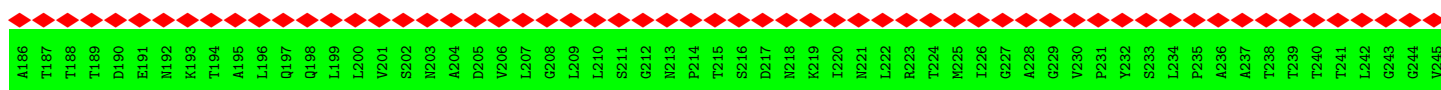
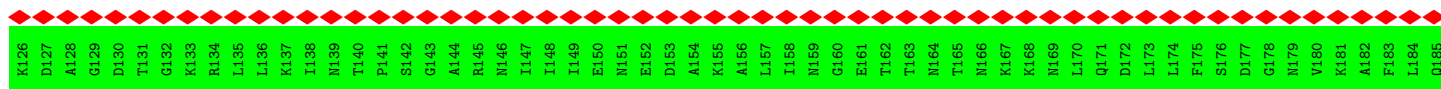
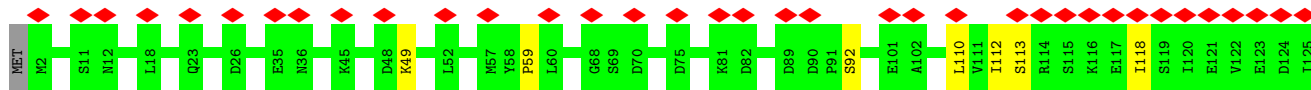


• Molecule 2: Capsid fiber protein

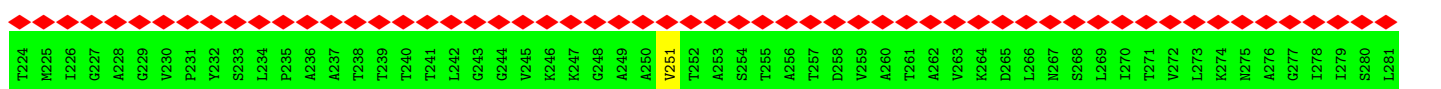
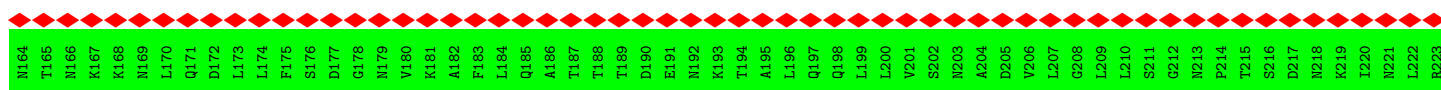
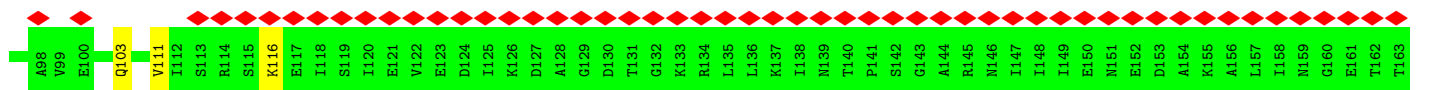
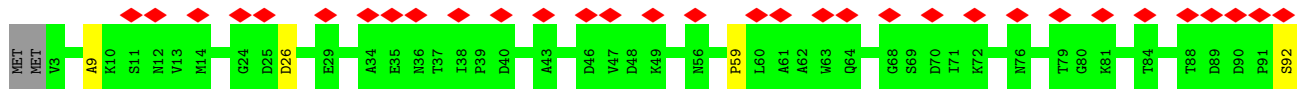
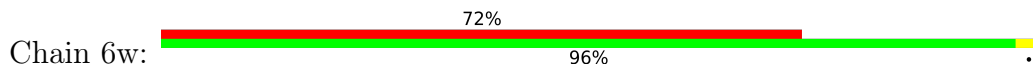




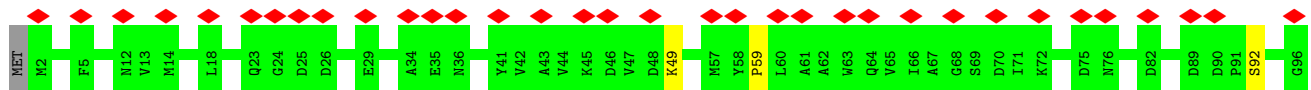
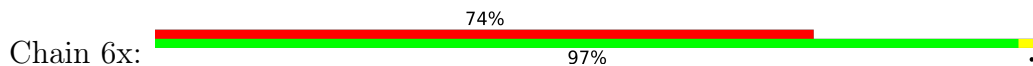
• Molecule 2: Capsid fiber protein

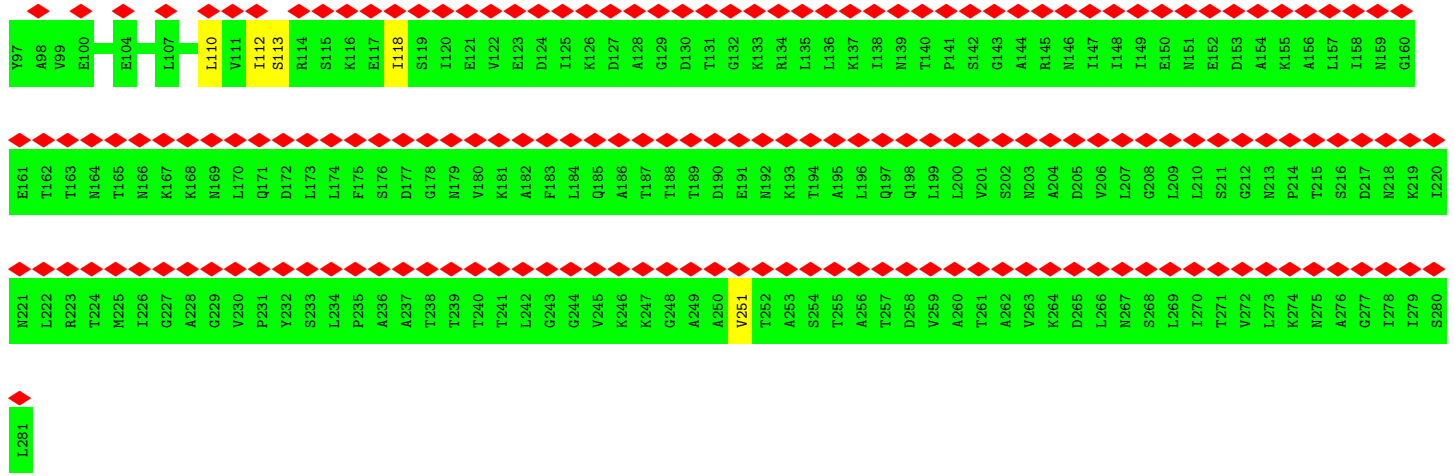


• Molecule 2: Capsid fiber protein

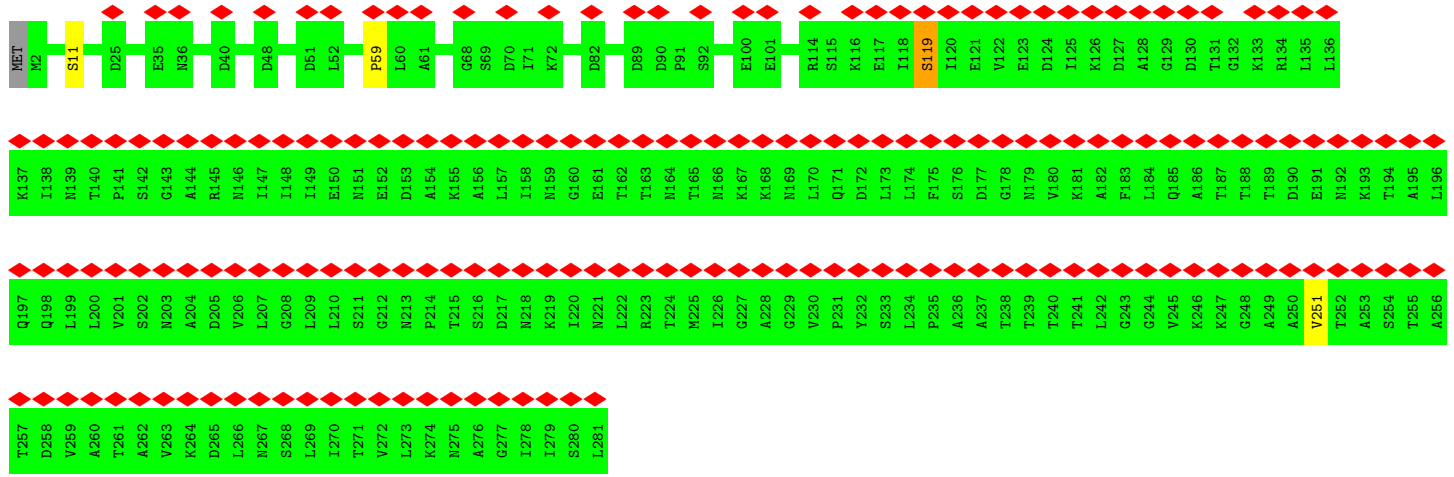


• Molecule 2: Capsid fiber protein

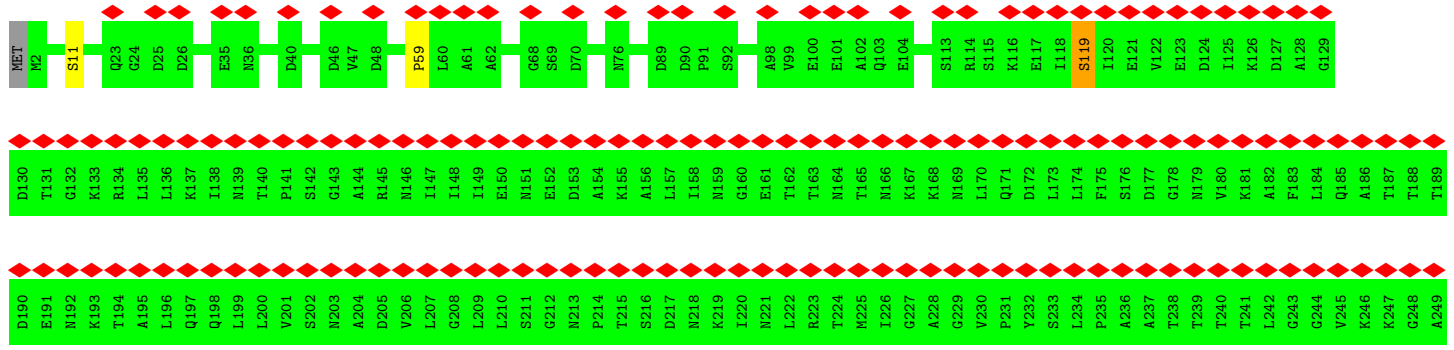


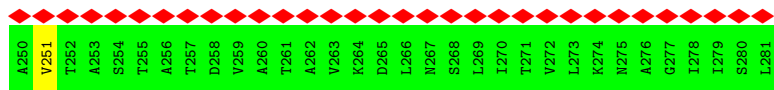


• Molecule 2: Capsid fiber protein

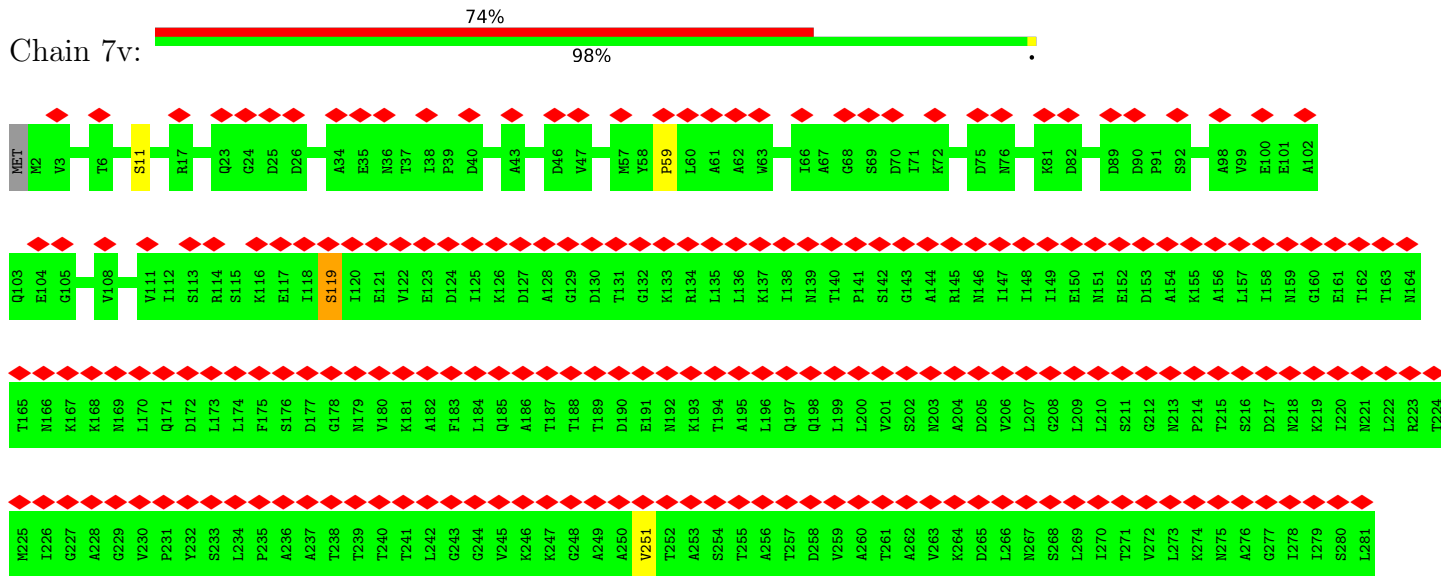


• Molecule 2: Capsid fiber protein

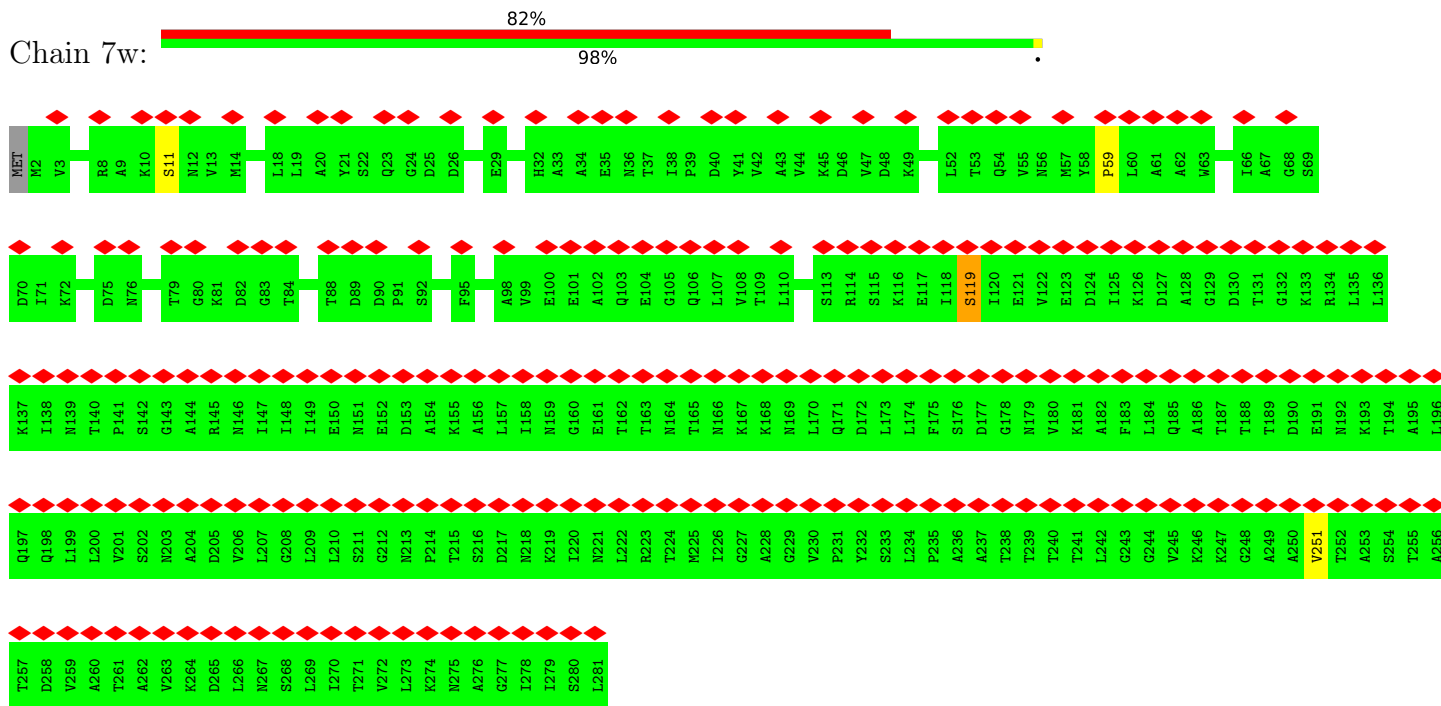




• Molecule 2: Capsid fiber protein

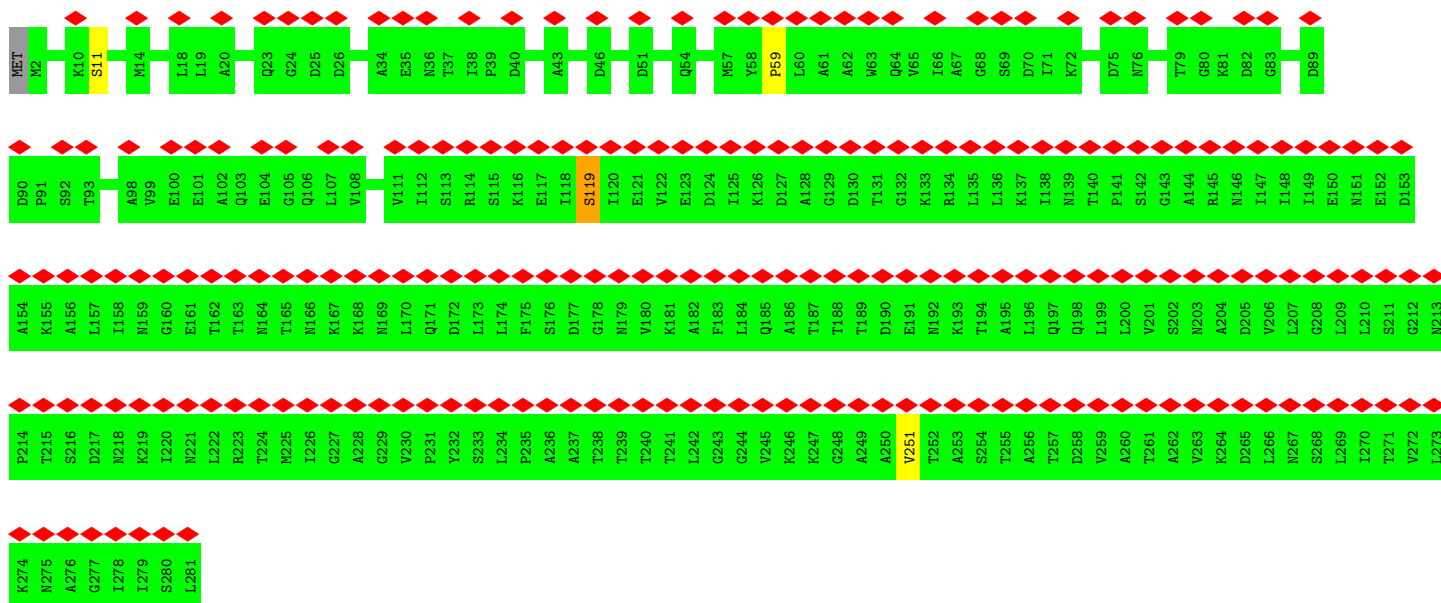


• Molecule 2: Capsid fiber protein

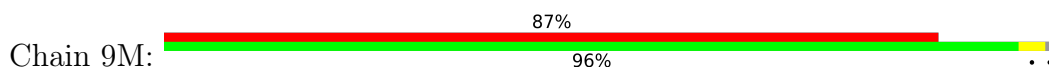


• Molecule 2: Capsid fiber protein

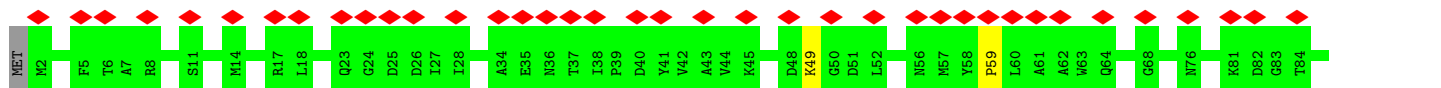
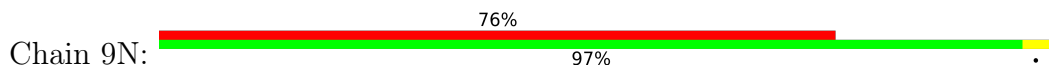


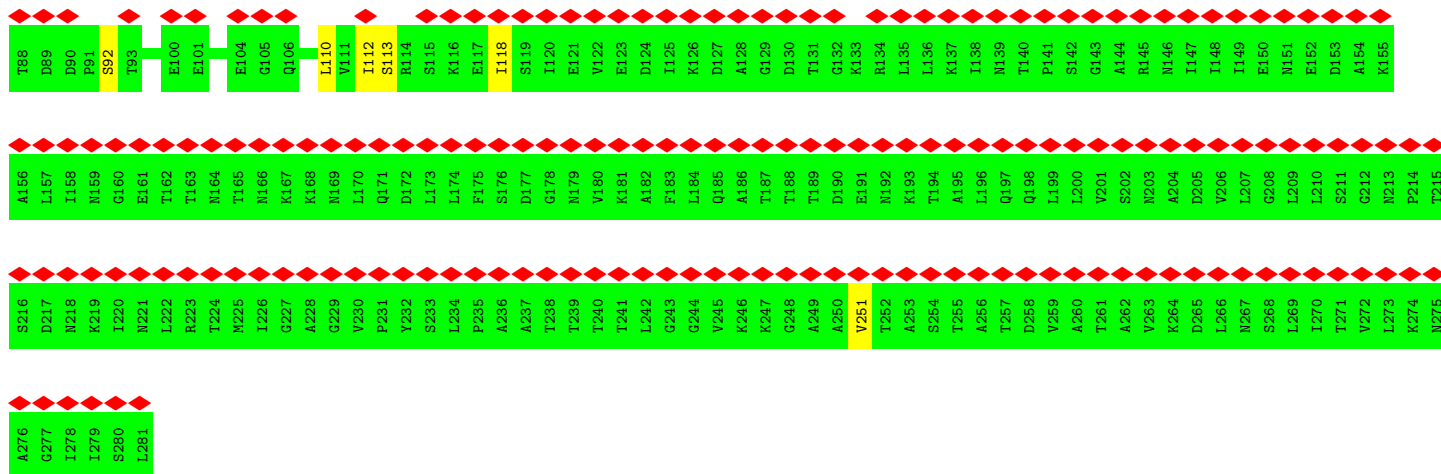


• Molecule 2: Capsid fiber protein

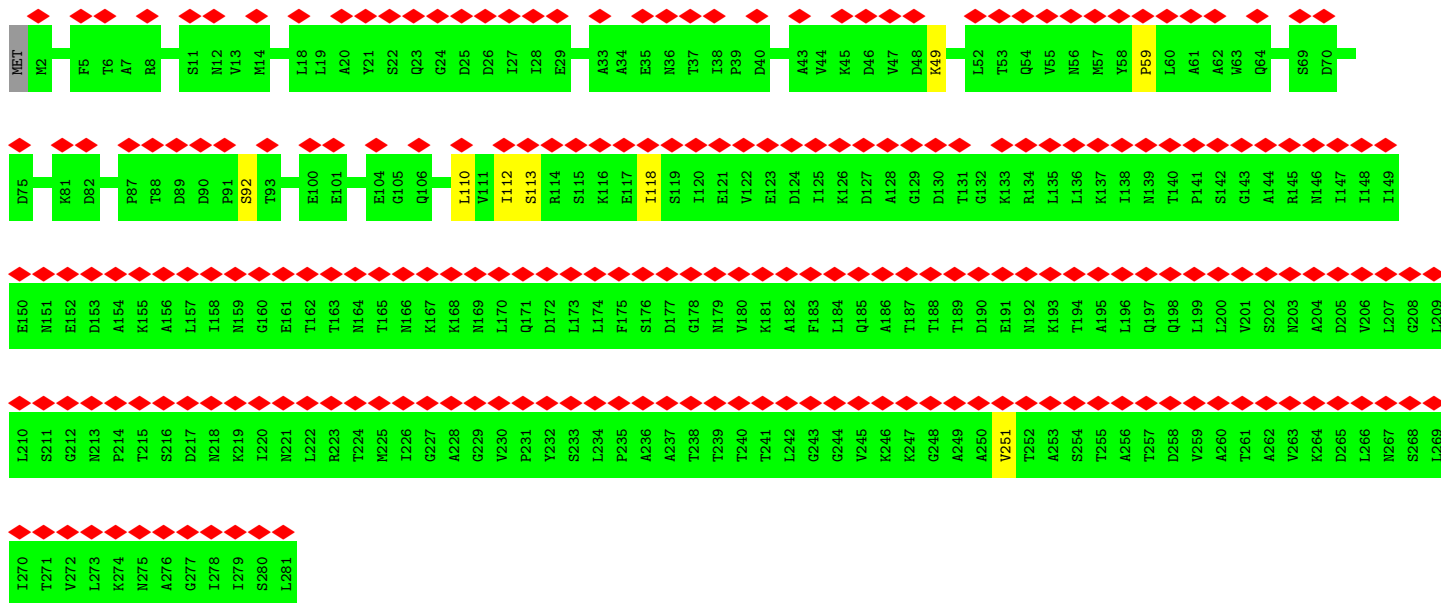
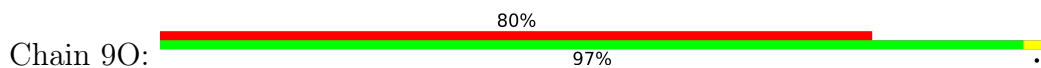


• Molecule 2: Capsid fiber protein

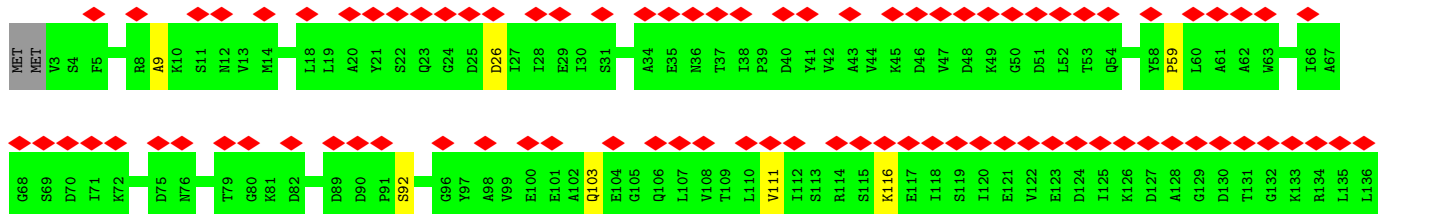
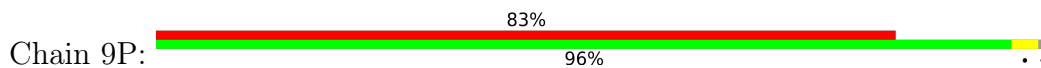


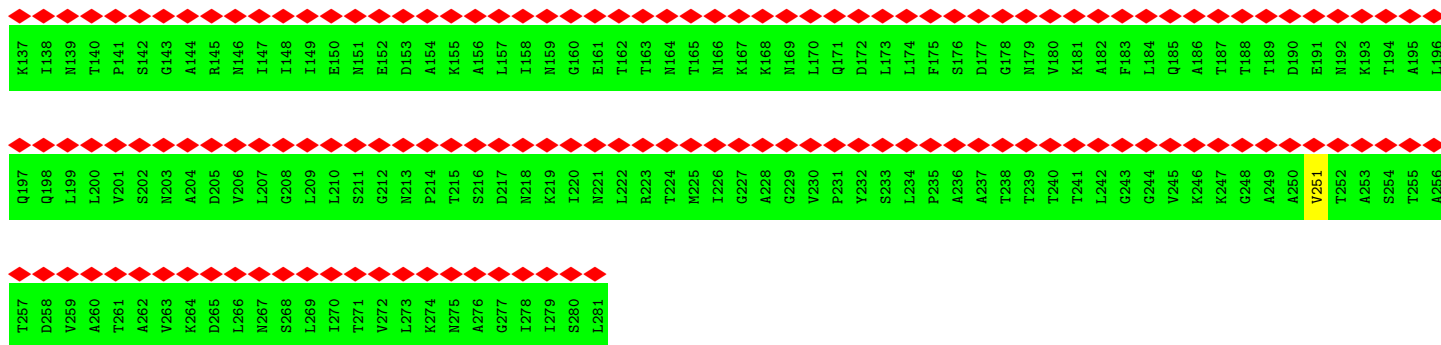


• Molecule 2: Capsid fiber protein

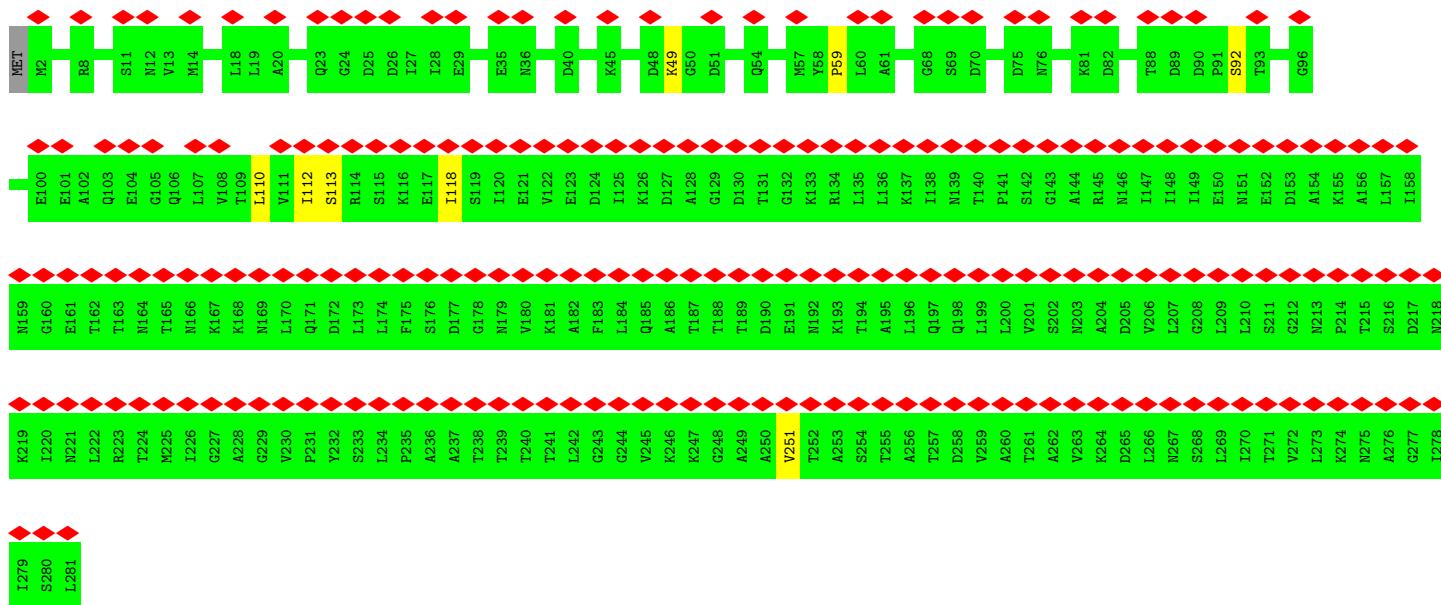
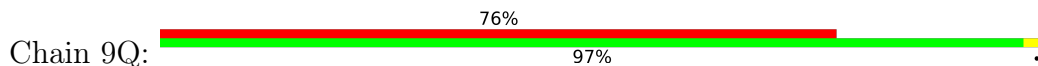


• Molecule 2: Capsid fiber protein

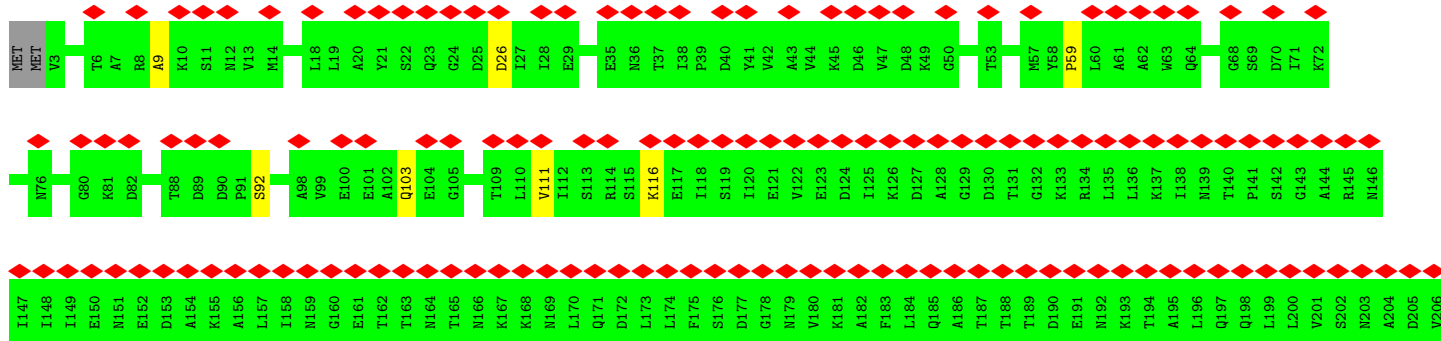
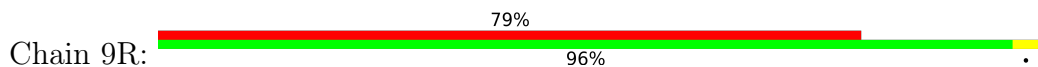


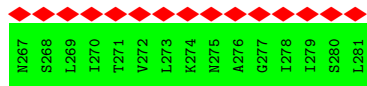
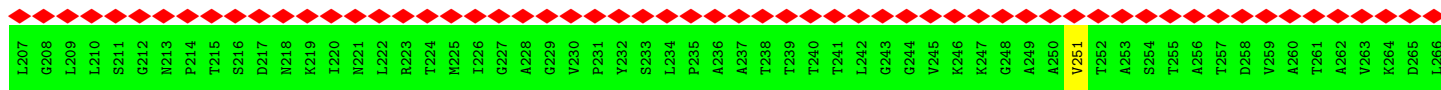


• Molecule 2: Capsid fiber protein

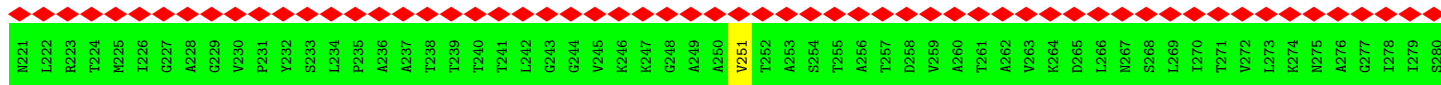
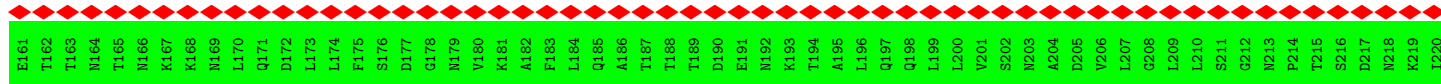
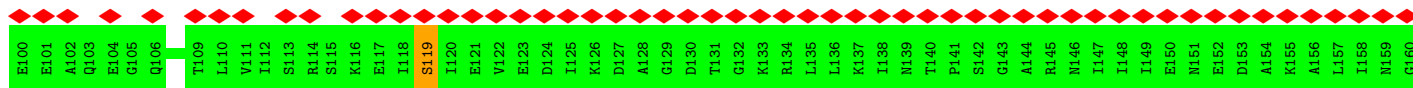
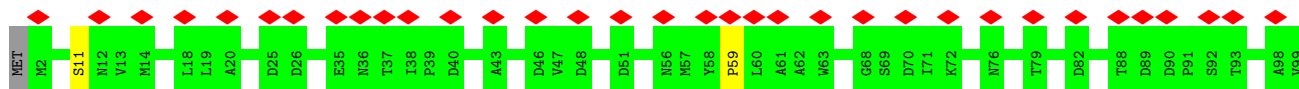
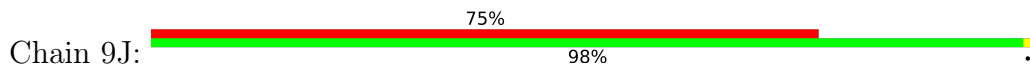


• Molecule 2: Capsid fiber protein





• Molecule 2: Capsid fiber protein



4 Experimental information

| Property | Value | Source |
|--------------------------------------|-------------------------|-----------|
| EM reconstruction method | SINGLE PARTICLE | Depositor |
| Imposed symmetry | POINT, Not provided | |
| Number of particles used | 44059 | Depositor |
| Resolution determination method | FSC 0.143 CUT-OFF | Depositor |
| CTF correction method | PHASE FLIPPING ONLY | Depositor |
| Microscope | FEI TITAN KRIOS | Depositor |
| Voltage (kV) | 300 | Depositor |
| Electron dose ($e^-/\text{\AA}^2$) | 40 | Depositor |
| Minimum defocus (nm) | Not provided | |
| Maximum defocus (nm) | Not provided | |
| Magnification | Not provided | |
| Image detector | FEI FALCON II (4k x 4k) | Depositor |
| Maximum map value | 20.227 | Depositor |
| Minimum map value | -0.429 | Depositor |
| Average map value | 0.109 | Depositor |
| Map value standard deviation | 0.735 | Depositor |
| Recommended contour level | 3.0 | Depositor |
| Map size (\AA) | 734.4, 734.4, 734.4 | wwPDB |
| Map dimensions | 540, 540, 540 | wwPDB |
| Map angles ($^\circ$) | 90.0, 90.0, 90.0 | wwPDB |
| Pixel spacing (\AA) | 1.36, 1.36, 1.36 | Depositor |

5 Model quality i

5.1 Standard geometry i

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 | 0.53 | 0/3460 | 0.60 | 1/4698 (0.0%) |
| 1 | 1B | 0.61 | 0/3551 | 0.66 | 0/4822 |
| 1 | 1C | 0.58 | 0/3551 | 0.62 | 0/4822 |
| 1 | 1D | 0.60 | 0/3551 | 0.66 | 2/4822 (0.0%) |
| 1 | 1E | 0.57 | 0/3489 | 0.59 | 0/4737 |
| 1 | 1F | 0.54 | 0/3513 | 0.64 | 2/4771 (0.0%) |
| 1 | 1G | 0.53 | 0/3460 | 0.60 | 1/4698 (0.0%) |
| 1 | 1H | 0.61 | 0/3551 | 0.66 | 0/4822 |
| 1 | 1I | 0.58 | 0/3551 | 0.62 | 0/4822 |
| 1 | 1J | 0.60 | 0/3551 | 0.66 | 2/4822 (0.0%) |
| 1 | 1K | 0.57 | 0/3489 | 0.59 | 0/4737 |
| 1 | 1L | 0.54 | 0/3513 | 0.64 | 2/4771 (0.0%) |
| 1 | 1M | 0.53 | 0/3460 | 0.60 | 1/4698 (0.0%) |
| 1 | 1N | 0.61 | 0/3551 | 0.66 | 0/4822 |
| 1 | 1O | 0.58 | 0/3551 | 0.62 | 0/4822 |
| 1 | 1P | 0.60 | 0/3551 | 0.66 | 2/4822 (0.0%) |
| 1 | 1Q | 0.57 | 0/3489 | 0.59 | 0/4737 |
| 1 | 1R | 0.54 | 0/3513 | 0.64 | 2/4771 (0.0%) |
| 1 | 1S | 0.53 | 0/3460 | 0.60 | 1/4698 (0.0%) |
| 1 | 1T | 0.61 | 0/3551 | 0.66 | 0/4822 |
| 1 | 1U | 0.58 | 0/3551 | 0.62 | 0/4822 |
| 1 | 1V | 0.60 | 0/3551 | 0.66 | 2/4822 (0.0%) |
| 1 | 1W | 0.57 | 0/3489 | 0.59 | 0/4737 |
| 1 | 1X | 0.54 | 0/3513 | 0.64 | 2/4771 (0.0%) |
| 1 | 1Y | 0.53 | 0/3460 | 0.60 | 1/4698 (0.0%) |
| 1 | 1Z | 0.61 | 0/3551 | 0.66 | 0/4822 |
| 1 | 1a | 0.58 | 0/3551 | 0.62 | 0/4822 |
| 1 | 1b | 0.60 | 0/3551 | 0.66 | 2/4822 (0.0%) |
| 1 | 1c | 0.57 | 0/3489 | 0.59 | 0/4737 |
| 1 | 1d | 0.54 | 0/3513 | 0.64 | 2/4771 (0.0%) |
| 1 | 2A | 0.63 | 1/3493 (0.0%) | 0.64 | 1/4743 (0.0%) |
| 1 | 2B | 0.63 | 0/3551 | 0.63 | 1/4822 (0.0%) |
| 1 | 2C | 0.61 | 0/3551 | 0.61 | 0/4822 |
| 1 | 2D | 0.62 | 0/3551 | 0.61 | 0/4822 |

| Mol | Chain | Bond lengths | | Bond angles | |
|-----|-------|--------------|---------------|-------------|---------------|
| | | RMSZ | # Z >5 | RMSZ | # Z >5 |
| 1 | 2E | 0.62 | 0/3551 | 0.65 | 0/4822 |
| 1 | 2F | 0.63 | 1/3493 (0.0%) | 0.64 | 1/4743 (0.0%) |
| 1 | 2G | 0.63 | 0/3551 | 0.63 | 1/4822 (0.0%) |
| 1 | 2H | 0.61 | 0/3551 | 0.61 | 0/4822 |
| 1 | 2I | 0.62 | 0/3551 | 0.61 | 0/4822 |
| 1 | 2J | 0.62 | 0/3551 | 0.65 | 0/4822 |
| 1 | 2K | 0.63 | 1/3493 (0.0%) | 0.64 | 1/4743 (0.0%) |
| 1 | 2L | 0.63 | 0/3551 | 0.63 | 1/4822 (0.0%) |
| 1 | 2M | 0.61 | 0/3551 | 0.61 | 0/4822 |
| 1 | 2N | 0.62 | 0/3551 | 0.61 | 0/4822 |
| 1 | 2O | 0.62 | 0/3551 | 0.65 | 0/4822 |
| 1 | 2P | 0.63 | 1/3493 (0.0%) | 0.64 | 1/4743 (0.0%) |
| 1 | 2Q | 0.63 | 0/3551 | 0.63 | 1/4822 (0.0%) |
| 1 | 2R | 0.61 | 0/3551 | 0.61 | 0/4822 |
| 1 | 2S | 0.62 | 0/3551 | 0.61 | 0/4822 |
| 1 | 2T | 0.62 | 0/3551 | 0.65 | 0/4822 |
| 1 | 2U | 0.63 | 1/3493 (0.0%) | 0.64 | 1/4743 (0.0%) |
| 1 | 2V | 0.63 | 0/3551 | 0.63 | 1/4822 (0.0%) |
| 1 | 2W | 0.61 | 0/3551 | 0.61 | 0/4822 |
| 1 | 2X | 0.62 | 0/3551 | 0.61 | 0/4822 |
| 1 | 2Y | 0.62 | 0/3551 | 0.65 | 0/4822 |
| 1 | 3A | 0.63 | 0/3485 | 0.64 | 1/4732 (0.0%) |
| 1 | 3B | 0.63 | 0/3489 | 0.67 | 1/4737 (0.0%) |
| 1 | 3C | 0.62 | 0/3547 | 0.63 | 1/4817 (0.0%) |
| 1 | 3D | 0.67 | 2/3551 (0.1%) | 0.65 | 0/4822 |
| 1 | 3E | 0.63 | 0/3551 | 0.62 | 0/4822 |
| 1 | 3F | 0.61 | 0/3551 | 0.63 | 1/4822 (0.0%) |
| 1 | 3G | 0.63 | 0/3485 | 0.64 | 2/4732 (0.0%) |
| 1 | 3H | 0.63 | 0/3489 | 0.67 | 1/4737 (0.0%) |
| 1 | 3I | 0.62 | 0/3547 | 0.63 | 1/4817 (0.0%) |
| 1 | 3J | 0.67 | 2/3551 (0.1%) | 0.65 | 0/4822 |
| 1 | 3K | 0.63 | 0/3551 | 0.62 | 0/4822 |
| 1 | 3L | 0.61 | 0/3551 | 0.63 | 1/4822 (0.0%) |
| 1 | 3M | 0.63 | 0/3485 | 0.64 | 1/4732 (0.0%) |
| 1 | 3N | 0.63 | 0/3489 | 0.67 | 1/4737 (0.0%) |
| 1 | 3O | 0.62 | 0/3547 | 0.63 | 1/4817 (0.0%) |
| 1 | 3P | 0.67 | 2/3551 (0.1%) | 0.65 | 0/4822 |
| 1 | 3Q | 0.63 | 0/3551 | 0.62 | 0/4822 |
| 1 | 3R | 0.61 | 0/3551 | 0.63 | 1/4822 (0.0%) |
| 1 | 3S | 0.63 | 0/3485 | 0.64 | 1/4732 (0.0%) |
| 1 | 3T | 0.63 | 0/3489 | 0.67 | 1/4737 (0.0%) |
| 1 | 3U | 0.62 | 0/3547 | 0.63 | 1/4817 (0.0%) |
| 1 | 3V | 0.67 | 2/3551 (0.1%) | 0.65 | 0/4822 |

| Mol | Chain | Bond lengths | | Bond angles | |
|-----|-------|--------------|---------------|-------------|---------------|
| | | RMSZ | # Z >5 | RMSZ | # Z >5 |
| 1 | 3W | 0.63 | 1/3551 (0.0%) | 0.62 | 0/4822 |
| 1 | 3X | 0.61 | 0/3551 | 0.63 | 1/4822 (0.0%) |
| 1 | 3Y | 0.63 | 0/3485 | 0.64 | 1/4732 (0.0%) |
| 1 | 3Z | 0.63 | 0/3489 | 0.67 | 1/4737 (0.0%) |
| 1 | 3a | 0.62 | 0/3547 | 0.63 | 1/4817 (0.0%) |
| 1 | 3b | 0.67 | 2/3551 (0.1%) | 0.65 | 0/4822 |
| 1 | 3c | 0.63 | 0/3551 | 0.62 | 0/4822 |
| 1 | 3d | 0.61 | 0/3551 | 0.63 | 1/4822 (0.0%) |
| 1 | 4A | 0.63 | 0/3489 | 0.62 | 1/4737 (0.0%) |
| 1 | 4B | 0.61 | 0/3489 | 0.67 | 1/4737 (0.0%) |
| 1 | 4C | 0.65 | 0/3489 | 0.67 | 0/4737 |
| 1 | 4D | 0.65 | 0/3489 | 0.64 | 0/4737 |
| 1 | 4E | 0.63 | 0/3551 | 0.65 | 0/4822 |
| 1 | 4F | 0.64 | 0/3551 | 0.67 | 0/4822 |
| 1 | 4G | 0.63 | 0/3489 | 0.62 | 1/4737 (0.0%) |
| 1 | 4H | 0.61 | 0/3489 | 0.67 | 1/4737 (0.0%) |
| 1 | 4I | 0.65 | 0/3489 | 0.67 | 0/4737 |
| 1 | 4J | 0.65 | 0/3489 | 0.64 | 0/4737 |
| 1 | 4K | 0.63 | 0/3551 | 0.65 | 0/4822 |
| 1 | 4L | 0.64 | 0/3551 | 0.67 | 0/4822 |
| 1 | 4M | 0.63 | 0/3489 | 0.62 | 1/4737 (0.0%) |
| 1 | 4N | 0.61 | 0/3489 | 0.67 | 1/4737 (0.0%) |
| 1 | 4O | 0.65 | 0/3489 | 0.67 | 0/4737 |
| 1 | 4P | 0.65 | 0/3489 | 0.64 | 0/4737 |
| 1 | 4Q | 0.63 | 0/3551 | 0.65 | 0/4822 |
| 1 | 4R | 0.64 | 0/3551 | 0.67 | 0/4822 |
| 1 | 4S | 0.63 | 0/3489 | 0.62 | 1/4737 (0.0%) |
| 1 | 4T | 0.61 | 0/3489 | 0.67 | 1/4737 (0.0%) |
| 1 | 4U | 0.65 | 0/3489 | 0.67 | 0/4737 |
| 1 | 4V | 0.65 | 0/3489 | 0.64 | 0/4737 |
| 1 | 4W | 0.63 | 0/3551 | 0.65 | 0/4822 |
| 1 | 4X | 0.64 | 0/3551 | 0.67 | 0/4822 |
| 1 | 4Y | 0.63 | 0/3489 | 0.62 | 1/4737 (0.0%) |
| 1 | 4Z | 0.61 | 0/3489 | 0.67 | 1/4737 (0.0%) |
| 1 | 4a | 0.65 | 0/3489 | 0.67 | 0/4737 |
| 1 | 4b | 0.65 | 0/3489 | 0.64 | 0/4737 |
| 1 | 4c | 0.63 | 0/3551 | 0.65 | 0/4822 |
| 1 | 4d | 0.64 | 0/3551 | 0.67 | 0/4822 |
| 1 | 5A | 0.64 | 0/3489 | 0.64 | 1/4737 (0.0%) |
| 1 | 5B | 0.62 | 0/3489 | 0.69 | 1/4737 (0.0%) |
| 1 | 5C | 0.63 | 0/3489 | 0.68 | 3/4737 (0.1%) |
| 1 | 5D | 0.62 | 0/3489 | 0.62 | 0/4737 |
| 1 | 5E | 0.60 | 0/3551 | 0.68 | 2/4822 (0.0%) |

| Mol | Chain | Bond lengths | | Bond angles | |
|-----|-------|--------------|---------------|-------------|---------------|
| | | RMSZ | # Z >5 | RMSZ | # Z >5 |
| 1 | 5F | 0.65 | 0/3551 | 0.67 | 0/4822 |
| 1 | 5G | 0.64 | 0/3489 | 0.64 | 1/4737 (0.0%) |
| 1 | 5H | 0.62 | 0/3489 | 0.69 | 1/4737 (0.0%) |
| 1 | 5I | 0.63 | 0/3489 | 0.68 | 3/4737 (0.1%) |
| 1 | 5J | 0.62 | 0/3489 | 0.62 | 0/4737 |
| 1 | 5K | 0.60 | 0/3551 | 0.68 | 2/4822 (0.0%) |
| 1 | 5L | 0.65 | 0/3551 | 0.67 | 0/4822 |
| 1 | 5M | 0.64 | 0/3489 | 0.64 | 1/4737 (0.0%) |
| 1 | 5N | 0.62 | 0/3489 | 0.69 | 1/4737 (0.0%) |
| 1 | 5O | 0.63 | 0/3489 | 0.68 | 3/4737 (0.1%) |
| 1 | 5P | 0.62 | 0/3489 | 0.62 | 0/4737 |
| 1 | 5Q | 0.60 | 0/3551 | 0.68 | 2/4822 (0.0%) |
| 1 | 5R | 0.65 | 0/3551 | 0.67 | 0/4822 |
| 1 | 5S | 0.64 | 0/3489 | 0.64 | 1/4737 (0.0%) |
| 1 | 5T | 0.62 | 0/3489 | 0.69 | 1/4737 (0.0%) |
| 1 | 5U | 0.63 | 0/3489 | 0.68 | 3/4737 (0.1%) |
| 1 | 5V | 0.62 | 0/3489 | 0.62 | 0/4737 |
| 1 | 5W | 0.60 | 0/3551 | 0.68 | 2/4822 (0.0%) |
| 1 | 5X | 0.65 | 0/3551 | 0.67 | 0/4822 |
| 1 | 5Y | 0.64 | 0/3489 | 0.64 | 1/4737 (0.0%) |
| 1 | 5Z | 0.62 | 0/3489 | 0.69 | 1/4737 (0.0%) |
| 1 | 5a | 0.63 | 0/3489 | 0.68 | 3/4737 (0.1%) |
| 1 | 5b | 0.62 | 0/3489 | 0.62 | 0/4737 |
| 1 | 5c | 0.60 | 0/3551 | 0.68 | 2/4822 (0.0%) |
| 1 | 5d | 0.65 | 0/3551 | 0.67 | 0/4822 |
| 1 | 6A | 0.62 | 0/3551 | 0.63 | 0/4822 |
| 1 | 6B | 0.62 | 0/3551 | 0.63 | 0/4822 |
| 1 | 6C | 0.62 | 0/3489 | 0.67 | 1/4737 (0.0%) |
| 1 | 6D | 0.63 | 1/3489 (0.0%) | 0.67 | 1/4737 (0.0%) |
| 1 | 6E | 0.62 | 0/3551 | 0.63 | 0/4822 |
| 1 | 6F | 0.62 | 0/3551 | 0.63 | 1/4822 (0.0%) |
| 1 | 6G | 0.62 | 0/3551 | 0.63 | 0/4822 |
| 1 | 6H | 0.62 | 0/3551 | 0.63 | 0/4822 |
| 1 | 6I | 0.62 | 0/3489 | 0.67 | 1/4737 (0.0%) |
| 1 | 6J | 0.63 | 1/3489 (0.0%) | 0.67 | 1/4737 (0.0%) |
| 1 | 6K | 0.62 | 0/3551 | 0.63 | 0/4822 |
| 1 | 6L | 0.63 | 0/3551 | 0.63 | 1/4822 (0.0%) |
| 1 | 6M | 0.62 | 0/3551 | 0.64 | 0/4822 |
| 1 | 6N | 0.62 | 0/3551 | 0.63 | 0/4822 |
| 1 | 6O | 0.62 | 0/3489 | 0.67 | 1/4737 (0.0%) |
| 1 | 6P | 0.63 | 1/3489 (0.0%) | 0.67 | 1/4737 (0.0%) |
| 1 | 6Q | 0.62 | 0/3551 | 0.63 | 0/4822 |
| 1 | 6R | 0.63 | 0/3551 | 0.63 | 1/4822 (0.0%) |

| Mol | Chain | Bond lengths | | Bond angles | |
|-----|-------|--------------|---------------|-------------|---------------|
| | | RMSZ | # Z >5 | RMSZ | # Z >5 |
| 1 | 6S | 0.62 | 0/3551 | 0.63 | 0/4822 |
| 1 | 6T | 0.62 | 0/3551 | 0.63 | 0/4822 |
| 1 | 6U | 0.62 | 0/3489 | 0.67 | 1/4737 (0.0%) |
| 1 | 6V | 0.63 | 1/3489 (0.0%) | 0.67 | 1/4737 (0.0%) |
| 1 | 6W | 0.62 | 0/3551 | 0.63 | 0/4822 |
| 1 | 6X | 0.63 | 0/3551 | 0.63 | 1/4822 (0.0%) |
| 1 | 6Y | 0.62 | 0/3551 | 0.63 | 0/4822 |
| 1 | 6Z | 0.62 | 0/3551 | 0.63 | 0/4822 |
| 1 | 6a | 0.62 | 0/3489 | 0.67 | 1/4737 (0.0%) |
| 1 | 6b | 0.63 | 1/3489 (0.0%) | 0.67 | 1/4737 (0.0%) |
| 1 | 6c | 0.62 | 0/3551 | 0.63 | 0/4822 |
| 1 | 6d | 0.63 | 0/3551 | 0.63 | 1/4822 (0.0%) |
| 1 | 7A | 0.63 | 0/3551 | 0.63 | 1/4822 (0.0%) |
| 1 | 7B | 0.61 | 0/3551 | 0.62 | 0/4822 |
| 1 | 7C | 0.63 | 0/3551 | 0.62 | 0/4822 |
| 1 | 7D | 0.64 | 0/3551 | 0.65 | 2/4822 (0.0%) |
| 1 | 7E | 0.64 | 2/3551 (0.1%) | 0.66 | 1/4822 (0.0%) |
| 1 | 7F | 0.63 | 0/3551 | 0.63 | 1/4822 (0.0%) |
| 1 | 7G | 0.61 | 0/3551 | 0.62 | 0/4822 |
| 1 | 7H | 0.63 | 0/3551 | 0.62 | 0/4822 |
| 1 | 7I | 0.64 | 0/3551 | 0.65 | 2/4822 (0.0%) |
| 1 | 7J | 0.64 | 2/3551 (0.1%) | 0.66 | 1/4822 (0.0%) |
| 1 | 7K | 0.63 | 0/3551 | 0.63 | 1/4822 (0.0%) |
| 1 | 7L | 0.61 | 0/3551 | 0.62 | 0/4822 |
| 1 | 7M | 0.63 | 0/3551 | 0.62 | 0/4822 |
| 1 | 7N | 0.64 | 0/3551 | 0.65 | 2/4822 (0.0%) |
| 1 | 7O | 0.64 | 2/3551 (0.1%) | 0.66 | 1/4822 (0.0%) |
| 1 | 7P | 0.63 | 0/3551 | 0.63 | 1/4822 (0.0%) |
| 1 | 7Q | 0.61 | 0/3551 | 0.62 | 0/4822 |
| 1 | 7R | 0.63 | 0/3551 | 0.62 | 0/4822 |
| 1 | 7S | 0.64 | 0/3551 | 0.65 | 2/4822 (0.0%) |
| 1 | 7T | 0.64 | 2/3551 (0.1%) | 0.66 | 1/4822 (0.0%) |
| 1 | 7U | 0.63 | 0/3551 | 0.63 | 1/4822 (0.0%) |
| 1 | 7V | 0.61 | 0/3551 | 0.62 | 0/4822 |
| 1 | 7W | 0.63 | 0/3551 | 0.62 | 0/4822 |
| 1 | 7X | 0.64 | 0/3551 | 0.65 | 2/4822 (0.0%) |
| 1 | 7Y | 0.64 | 2/3551 (0.1%) | 0.66 | 1/4822 (0.0%) |
| 1 | 8A | 0.58 | 0/3551 | 0.62 | 0/4822 |
| 1 | 8B | 0.59 | 0/3551 | 0.61 | 0/4822 |
| 1 | 8C | 0.61 | 0/3551 | 0.62 | 1/4822 (0.0%) |
| 1 | 8D | 0.59 | 0/3551 | 0.59 | 1/4822 (0.0%) |
| 1 | 8E | 0.58 | 0/3551 | 0.61 | 0/4822 |
| 1 | 8F | 0.60 | 0/3551 | 0.61 | 1/4822 (0.0%) |

| Mol | Chain | Bond lengths | | Bond angles | |
|-----|-------|--------------|---------------|-------------|---------------|
| | | RMSZ | # Z >5 | RMSZ | # Z >5 |
| 1 | 8G | 0.58 | 0/3551 | 0.62 | 0/4822 |
| 1 | 8H | 0.59 | 0/3551 | 0.61 | 0/4822 |
| 1 | 8I | 0.61 | 0/3551 | 0.62 | 1/4822 (0.0%) |
| 1 | 8J | 0.59 | 0/3551 | 0.59 | 1/4822 (0.0%) |
| 1 | 8K | 0.58 | 0/3551 | 0.61 | 0/4822 |
| 1 | 8L | 0.60 | 0/3551 | 0.61 | 1/4822 (0.0%) |
| 1 | 8M | 0.58 | 0/3551 | 0.62 | 0/4822 |
| 1 | 8N | 0.59 | 0/3551 | 0.61 | 0/4822 |
| 1 | 8O | 0.61 | 0/3551 | 0.62 | 1/4822 (0.0%) |
| 1 | 8P | 0.59 | 0/3551 | 0.59 | 1/4822 (0.0%) |
| 1 | 8Q | 0.58 | 0/3551 | 0.61 | 0/4822 |
| 1 | 8R | 0.60 | 0/3551 | 0.61 | 1/4822 (0.0%) |
| 1 | 8S | 0.58 | 0/3551 | 0.62 | 0/4822 |
| 1 | 8T | 0.59 | 0/3551 | 0.61 | 0/4822 |
| 1 | 8U | 0.61 | 0/3551 | 0.62 | 1/4822 (0.0%) |
| 1 | 8V | 0.59 | 0/3551 | 0.59 | 1/4822 (0.0%) |
| 1 | 8W | 0.58 | 0/3551 | 0.61 | 0/4822 |
| 1 | 8X | 0.60 | 0/3551 | 0.61 | 1/4822 (0.0%) |
| 1 | 8Y | 0.58 | 0/3551 | 0.62 | 0/4822 |
| 1 | 8Z | 0.59 | 0/3551 | 0.61 | 0/4822 |
| 1 | 8a | 0.61 | 0/3551 | 0.62 | 1/4822 (0.0%) |
| 1 | 8b | 0.59 | 0/3551 | 0.59 | 1/4822 (0.0%) |
| 1 | 8c | 0.58 | 0/3551 | 0.61 | 0/4822 |
| 1 | 8d | 0.60 | 0/3551 | 0.61 | 1/4822 (0.0%) |
| 1 | 9A | 0.58 | 0/3551 | 0.63 | 0/4822 |
| 1 | 9B | 0.58 | 0/3551 | 0.64 | 0/4822 |
| 1 | 9C | 0.58 | 0/3551 | 0.63 | 0/4822 |
| 1 | 9D | 0.58 | 0/3551 | 0.63 | 0/4822 |
| 1 | 9E | 0.58 | 0/3551 | 0.63 | 0/4822 |
| 2 | 1e | 0.66 | 0/2150 | 0.67 | 0/2925 |
| 2 | 1f | 0.68 | 1/2142 (0.0%) | 0.69 | 0/2915 |
| 2 | 1g | 0.66 | 0/2150 | 0.67 | 0/2925 |
| 2 | 1h | 0.68 | 1/2142 (0.0%) | 0.69 | 0/2915 |
| 2 | 1i | 0.66 | 0/2150 | 0.67 | 0/2925 |
| 2 | 1j | 0.68 | 1/2142 (0.0%) | 0.69 | 0/2915 |
| 2 | 1k | 0.66 | 0/2150 | 0.67 | 0/2925 |
| 2 | 1l | 0.68 | 1/2142 (0.0%) | 0.69 | 0/2915 |
| 2 | 1m | 0.66 | 0/2150 | 0.67 | 0/2925 |
| 2 | 1n | 0.68 | 1/2142 (0.0%) | 0.69 | 0/2915 |
| 2 | 1o | 0.66 | 0/2150 | 0.67 | 0/2925 |
| 2 | 1p | 0.68 | 1/2142 (0.0%) | 0.69 | 0/2915 |
| 2 | 1q | 0.66 | 0/2150 | 0.67 | 0/2925 |
| 2 | 1r | 0.68 | 1/2142 (0.0%) | 0.69 | 0/2915 |

| Mol | Chain | Bond lengths | | Bond angles | |
|-----|-------|--------------|---------------|-------------|---------|
| | | RMSZ | # Z >5 | RMSZ | # Z >5 |
| 2 | 1s | 0.66 | 0/2150 | 0.67 | 0/2925 |
| 2 | 1t | 0.68 | 1/2142 (0.0%) | 0.69 | 0/2915 |
| 2 | 1u | 0.66 | 0/2150 | 0.67 | 0/2925 |
| 2 | 1v | 0.68 | 1/2142 (0.0%) | 0.69 | 0/2915 |
| 2 | 1w | 0.66 | 0/2150 | 0.67 | 0/2925 |
| 2 | 1x | 0.68 | 1/2142 (0.0%) | 0.69 | 0/2915 |
| 2 | 2Z | 0.67 | 0/2150 | 0.68 | 0/2925 |
| 2 | 2a | 0.67 | 0/2150 | 0.68 | 0/2925 |
| 2 | 2b | 0.67 | 0/2150 | 0.68 | 0/2925 |
| 2 | 2c | 0.67 | 0/2150 | 0.68 | 0/2925 |
| 2 | 2d | 0.67 | 0/2150 | 0.68 | 0/2925 |
| 2 | 2e | 0.67 | 0/2150 | 0.68 | 0/2925 |
| 2 | 2f | 0.67 | 0/2150 | 0.68 | 0/2925 |
| 2 | 2g | 0.67 | 0/2150 | 0.68 | 0/2925 |
| 2 | 2h | 0.67 | 0/2150 | 0.68 | 0/2925 |
| 2 | 2i | 0.67 | 0/2150 | 0.68 | 0/2925 |
| 2 | 2j | 0.67 | 0/2150 | 0.68 | 0/2925 |
| 2 | 2k | 0.67 | 0/2150 | 0.68 | 0/2925 |
| 2 | 2l | 0.67 | 0/2150 | 0.68 | 0/2925 |
| 2 | 2m | 0.67 | 0/2150 | 0.68 | 0/2925 |
| 2 | 2n | 0.67 | 0/2150 | 0.68 | 0/2925 |
| 2 | 2o | 0.67 | 0/2150 | 0.68 | 0/2925 |
| 2 | 2p | 0.67 | 0/2150 | 0.68 | 0/2925 |
| 2 | 2q | 0.67 | 0/2150 | 0.68 | 0/2925 |
| 2 | 2r | 0.67 | 0/2150 | 0.68 | 0/2925 |
| 2 | 2s | 0.67 | 0/2150 | 0.68 | 0/2925 |
| 2 | 2t | 0.67 | 0/2150 | 0.68 | 0/2925 |
| 2 | 2u | 0.67 | 0/2150 | 0.68 | 0/2925 |
| 2 | 2v | 0.67 | 0/2150 | 0.68 | 0/2925 |
| 2 | 2w | 0.67 | 0/2150 | 0.68 | 0/2925 |
| 2 | 2x | 0.67 | 0/2150 | 0.68 | 0/2925 |
| 2 | 3e | 0.68 | 1/2142 (0.0%) | 0.69 | 0/2915 |
| 2 | 3f | 0.66 | 0/2150 | 0.67 | 0/2925 |
| 2 | 3g | 0.68 | 1/2142 (0.0%) | 0.69 | 0/2915 |
| 2 | 3h | 0.66 | 0/2150 | 0.67 | 0/2925 |
| 2 | 3i | 0.68 | 1/2142 (0.0%) | 0.69 | 0/2915 |
| 2 | 3j | 0.66 | 0/2150 | 0.67 | 0/2925 |
| 2 | 3k | 0.68 | 1/2142 (0.0%) | 0.69 | 0/2915 |
| 2 | 3l | 0.66 | 0/2150 | 0.67 | 0/2925 |
| 2 | 3m | 0.68 | 1/2142 (0.0%) | 0.69 | 0/2915 |
| 2 | 3n | 0.66 | 0/2150 | 0.67 | 0/2925 |
| 2 | 3o | 0.68 | 1/2142 (0.0%) | 0.69 | 0/2915 |
| 2 | 3p | 0.66 | 0/2150 | 0.67 | 0/2925 |

| Mol | Chain | Bond lengths | | Bond angles | |
|-----|-------|--------------|---------------|-------------|---------|
| | | RMSZ | # Z >5 | RMSZ | # Z >5 |
| 2 | 3q | 0.68 | 1/2142 (0.0%) | 0.69 | 0/2915 |
| 2 | 3r | 0.66 | 0/2150 | 0.67 | 0/2925 |
| 2 | 3s | 0.68 | 1/2142 (0.0%) | 0.69 | 0/2915 |
| 2 | 3t | 0.66 | 0/2150 | 0.67 | 0/2925 |
| 2 | 3u | 0.68 | 1/2142 (0.0%) | 0.69 | 0/2915 |
| 2 | 3v | 0.66 | 0/2150 | 0.67 | 0/2925 |
| 2 | 3w | 0.68 | 1/2142 (0.0%) | 0.69 | 0/2915 |
| 2 | 3x | 0.66 | 0/2150 | 0.67 | 0/2925 |
| 2 | 4e | 0.66 | 0/2150 | 0.67 | 0/2925 |
| 2 | 4f | 0.68 | 1/2142 (0.0%) | 0.69 | 0/2915 |
| 2 | 4g | 0.66 | 0/2150 | 0.67 | 0/2925 |
| 2 | 4h | 0.68 | 1/2142 (0.0%) | 0.69 | 0/2915 |
| 2 | 4i | 0.66 | 0/2150 | 0.67 | 0/2925 |
| 2 | 4j | 0.68 | 1/2142 (0.0%) | 0.69 | 0/2915 |
| 2 | 4k | 0.66 | 0/2150 | 0.67 | 0/2925 |
| 2 | 4l | 0.68 | 1/2142 (0.0%) | 0.69 | 0/2915 |
| 2 | 4m | 0.66 | 0/2150 | 0.67 | 0/2925 |
| 2 | 4n | 0.68 | 1/2142 (0.0%) | 0.69 | 0/2915 |
| 2 | 5e | 0.66 | 0/2150 | 0.67 | 0/2925 |
| 2 | 5f | 0.68 | 1/2142 (0.0%) | 0.69 | 0/2915 |
| 2 | 5g | 0.66 | 0/2150 | 0.67 | 0/2925 |
| 2 | 5h | 0.68 | 1/2142 (0.0%) | 0.69 | 0/2915 |
| 2 | 5i | 0.66 | 0/2150 | 0.67 | 0/2925 |
| 2 | 5j | 0.68 | 1/2142 (0.0%) | 0.69 | 0/2915 |
| 2 | 5k | 0.66 | 0/2150 | 0.67 | 0/2925 |
| 2 | 5l | 0.68 | 1/2142 (0.0%) | 0.69 | 0/2915 |
| 2 | 5m | 0.66 | 0/2150 | 0.67 | 0/2925 |
| 2 | 5n | 0.68 | 1/2142 (0.0%) | 0.69 | 0/2915 |
| 2 | 6e | 0.68 | 1/2142 (0.0%) | 0.69 | 0/2915 |
| 2 | 6f | 0.66 | 0/2150 | 0.67 | 0/2925 |
| 2 | 6g | 0.68 | 1/2142 (0.0%) | 0.69 | 0/2915 |
| 2 | 6h | 0.66 | 0/2150 | 0.67 | 0/2925 |
| 2 | 6i | 0.68 | 1/2142 (0.0%) | 0.69 | 0/2915 |
| 2 | 6j | 0.66 | 0/2150 | 0.67 | 0/2925 |
| 2 | 6k | 0.68 | 1/2142 (0.0%) | 0.69 | 0/2915 |
| 2 | 6l | 0.66 | 0/2150 | 0.67 | 0/2925 |
| 2 | 6m | 0.68 | 1/2142 (0.0%) | 0.69 | 0/2915 |
| 2 | 6n | 0.66 | 0/2150 | 0.67 | 0/2925 |
| 2 | 6o | 0.68 | 1/2142 (0.0%) | 0.69 | 0/2915 |
| 2 | 6p | 0.66 | 0/2150 | 0.67 | 0/2925 |
| 2 | 6q | 0.68 | 1/2142 (0.0%) | 0.69 | 0/2915 |
| 2 | 6r | 0.66 | 0/2150 | 0.67 | 0/2925 |
| 2 | 6s | 0.68 | 1/2142 (0.0%) | 0.69 | 0/2915 |

| Mol | Chain | Bond lengths | | Bond angles | |
|-----|-------|--------------|---------------|-------------|---------|
| | | RMSZ | # Z >5 | RMSZ | # Z >5 |
| 2 | 6t | 0.66 | 0/2150 | 0.67 | 0/2925 |
| 2 | 6u | 0.68 | 1/2142 (0.0%) | 0.69 | 0/2915 |
| 2 | 6v | 0.66 | 0/2150 | 0.67 | 0/2925 |
| 2 | 6w | 0.68 | 1/2142 (0.0%) | 0.69 | 0/2915 |
| 2 | 6x | 0.66 | 0/2150 | 0.67 | 0/2925 |
| 2 | 7Z | 0.67 | 0/2150 | 0.68 | 0/2925 |
| 2 | 7a | 0.67 | 0/2150 | 0.68 | 0/2925 |
| 2 | 7b | 0.67 | 0/2150 | 0.68 | 0/2925 |
| 2 | 7c | 0.67 | 0/2150 | 0.68 | 0/2925 |
| 2 | 7d | 0.67 | 0/2150 | 0.68 | 0/2925 |
| 2 | 7e | 0.67 | 0/2150 | 0.68 | 0/2925 |
| 2 | 7f | 0.67 | 0/2150 | 0.68 | 0/2925 |
| 2 | 7g | 0.67 | 0/2150 | 0.68 | 0/2925 |
| 2 | 7h | 0.67 | 0/2150 | 0.68 | 0/2925 |
| 2 | 7i | 0.67 | 0/2150 | 0.68 | 0/2925 |
| 2 | 7j | 0.67 | 0/2150 | 0.68 | 0/2925 |
| 2 | 7k | 0.67 | 0/2150 | 0.68 | 0/2925 |
| 2 | 7l | 0.67 | 0/2150 | 0.68 | 0/2925 |
| 2 | 7m | 0.67 | 0/2150 | 0.68 | 0/2925 |
| 2 | 7n | 0.67 | 0/2150 | 0.68 | 0/2925 |
| 2 | 7o | 0.67 | 0/2150 | 0.68 | 0/2925 |
| 2 | 7p | 0.67 | 0/2150 | 0.68 | 0/2925 |
| 2 | 7q | 0.67 | 0/2150 | 0.68 | 0/2925 |
| 2 | 7r | 0.67 | 0/2150 | 0.68 | 0/2925 |
| 2 | 7s | 0.67 | 0/2150 | 0.68 | 0/2925 |
| 2 | 7t | 0.67 | 0/2150 | 0.68 | 0/2925 |
| 2 | 7u | 0.67 | 0/2150 | 0.68 | 0/2925 |
| 2 | 7v | 0.67 | 0/2150 | 0.68 | 0/2925 |
| 2 | 7w | 0.67 | 0/2150 | 0.68 | 0/2925 |
| 2 | 7x | 0.67 | 0/2150 | 0.68 | 0/2925 |
| 2 | 8e | 0.68 | 1/2142 (0.0%) | 0.69 | 0/2915 |
| 2 | 8f | 0.66 | 0/2150 | 0.67 | 0/2925 |
| 2 | 8g | 0.66 | 0/2150 | 0.67 | 0/2925 |
| 2 | 8h | 0.68 | 1/2142 (0.0%) | 0.69 | 0/2915 |
| 2 | 8i | 0.66 | 0/2150 | 0.67 | 0/2925 |
| 2 | 8j | 0.68 | 1/2142 (0.0%) | 0.69 | 0/2915 |
| 2 | 8k | 0.68 | 1/2142 (0.0%) | 0.69 | 0/2915 |
| 2 | 8l | 0.66 | 0/2150 | 0.67 | 0/2925 |
| 2 | 8m | 0.66 | 0/2150 | 0.67 | 0/2925 |
| 2 | 8n | 0.68 | 1/2142 (0.0%) | 0.69 | 0/2915 |
| 2 | 8o | 0.66 | 0/2150 | 0.67 | 0/2925 |
| 2 | 8p | 0.68 | 1/2142 (0.0%) | 0.69 | 0/2915 |
| 2 | 8q | 0.68 | 1/2142 (0.0%) | 0.69 | 0/2915 |

| Mol | Chain | Bond lengths | | Bond angles | |
|-----|-------|--------------|-------------------|-------------|--------------------|
| | | RMSZ | # Z >5 | RMSZ | # Z >5 |
| 2 | 8r | 0.66 | 0/2150 | 0.67 | 0/2925 |
| 2 | 8s | 0.66 | 0/2150 | 0.67 | 0/2925 |
| 2 | 8t | 0.68 | 1/2142 (0.0%) | 0.69 | 0/2915 |
| 2 | 8u | 0.66 | 0/2150 | 0.67 | 0/2925 |
| 2 | 8v | 0.68 | 1/2142 (0.0%) | 0.69 | 0/2915 |
| 2 | 8w | 0.68 | 1/2142 (0.0%) | 0.69 | 0/2915 |
| 2 | 8x | 0.66 | 0/2150 | 0.67 | 0/2925 |
| 2 | 8y | 0.66 | 0/2150 | 0.67 | 0/2925 |
| 2 | 8z | 0.68 | 1/2142 (0.0%) | 0.69 | 0/2915 |
| 2 | 9F | 0.67 | 0/2150 | 0.68 | 0/2925 |
| 2 | 9G | 0.67 | 0/2150 | 0.68 | 0/2925 |
| 2 | 9H | 0.67 | 0/2150 | 0.68 | 0/2925 |
| 2 | 9I | 0.67 | 0/2150 | 0.68 | 0/2925 |
| 2 | 9J | 0.67 | 0/2150 | 0.68 | 0/2925 |
| 2 | 9K | 0.66 | 0/2150 | 0.67 | 0/2925 |
| 2 | 9L | 0.68 | 1/2142 (0.0%) | 0.69 | 0/2915 |
| 2 | 9M | 0.68 | 1/2142 (0.0%) | 0.69 | 0/2915 |
| 2 | 9N | 0.66 | 0/2150 | 0.67 | 0/2925 |
| 2 | 9O | 0.66 | 0/2150 | 0.67 | 0/2925 |
| 2 | 9P | 0.68 | 1/2142 (0.0%) | 0.69 | 0/2915 |
| 2 | 9Q | 0.66 | 0/2150 | 0.67 | 0/2925 |
| 2 | 9R | 0.68 | 1/2142 (0.0%) | 0.69 | 0/2915 |
| All | All | 0.63 | 86/1183790 (0.0%) | 0.65 | 151/1608400 (0.0%) |

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

| Mol | Chain | #Chirality outliers | #Planarity outliers |
|-----|-------|---------------------|---------------------|
| 1 | 1B | 0 | 4 |
| 1 | 1C | 0 | 1 |
| 1 | 1D | 0 | 2 |
| 1 | 1H | 0 | 4 |
| 1 | 1I | 0 | 1 |
| 1 | 1J | 0 | 2 |
| 1 | 1N | 0 | 4 |
| 1 | 1O | 0 | 1 |
| 1 | 1P | 0 | 2 |
| 1 | 1T | 0 | 4 |
| 1 | 1U | 0 | 1 |
| 1 | 1V | 0 | 2 |

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| Mol | Chain | #Chirality outliers | #Planarity outliers |
|-----|-------|---------------------|---------------------|
| 1 | 1Z | 0 | 4 |
| 1 | 1a | 0 | 1 |
| 1 | 1b | 0 | 2 |
| 1 | 2A | 0 | 2 |
| 1 | 2B | 0 | 1 |
| 1 | 2C | 0 | 1 |
| 1 | 2D | 0 | 1 |
| 1 | 2E | 0 | 2 |
| 1 | 2F | 0 | 2 |
| 1 | 2G | 0 | 1 |
| 1 | 2H | 0 | 1 |
| 1 | 2I | 0 | 1 |
| 1 | 2J | 0 | 2 |
| 1 | 2K | 0 | 2 |
| 1 | 2L | 0 | 1 |
| 1 | 2M | 0 | 1 |
| 1 | 2N | 0 | 1 |
| 1 | 2O | 0 | 2 |
| 1 | 2P | 0 | 2 |
| 1 | 2Q | 0 | 1 |
| 1 | 2R | 0 | 1 |
| 1 | 2S | 0 | 1 |
| 1 | 2T | 0 | 2 |
| 1 | 2U | 0 | 2 |
| 1 | 2V | 0 | 1 |
| 1 | 2W | 0 | 1 |
| 1 | 2X | 0 | 1 |
| 1 | 2Y | 0 | 2 |
| 1 | 3A | 0 | 1 |
| 1 | 3B | 0 | 1 |
| 1 | 3C | 0 | 3 |
| 1 | 3D | 0 | 4 |
| 1 | 3G | 0 | 1 |
| 1 | 3H | 0 | 1 |
| 1 | 3I | 0 | 3 |
| 1 | 3J | 0 | 4 |
| 1 | 3M | 0 | 1 |
| 1 | 3N | 0 | 1 |
| 1 | 3O | 0 | 3 |
| 1 | 3P | 0 | 4 |
| 1 | 3S | 0 | 1 |
| 1 | 3T | 0 | 1 |

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| Mol | Chain | #Chirality outliers | #Planarity outliers |
|-----|-------|---------------------|---------------------|
| 1 | 3U | 0 | 3 |
| 1 | 3V | 0 | 4 |
| 1 | 3Y | 0 | 1 |
| 1 | 3Z | 0 | 1 |
| 1 | 3a | 0 | 3 |
| 1 | 3b | 0 | 4 |
| 1 | 4A | 0 | 1 |
| 1 | 4B | 0 | 3 |
| 1 | 4C | 0 | 1 |
| 1 | 4D | 0 | 1 |
| 1 | 4E | 0 | 1 |
| 1 | 4G | 0 | 1 |
| 1 | 4H | 0 | 3 |
| 1 | 4I | 0 | 1 |
| 1 | 4J | 0 | 1 |
| 1 | 4K | 0 | 1 |
| 1 | 4M | 0 | 1 |
| 1 | 4N | 0 | 3 |
| 1 | 4O | 0 | 1 |
| 1 | 4P | 0 | 1 |
| 1 | 4Q | 0 | 1 |
| 1 | 4S | 0 | 1 |
| 1 | 4T | 0 | 3 |
| 1 | 4U | 0 | 1 |
| 1 | 4V | 0 | 1 |
| 1 | 4W | 0 | 1 |
| 1 | 4Y | 0 | 1 |
| 1 | 4Z | 0 | 3 |
| 1 | 4a | 0 | 1 |
| 1 | 4b | 0 | 1 |
| 1 | 4c | 0 | 1 |
| 1 | 5A | 0 | 1 |
| 1 | 5B | 0 | 4 |
| 1 | 5C | 0 | 2 |
| 1 | 5D | 0 | 1 |
| 1 | 5E | 0 | 3 |
| 1 | 5F | 0 | 5 |
| 1 | 5G | 0 | 1 |
| 1 | 5H | 0 | 4 |
| 1 | 5I | 0 | 2 |
| 1 | 5J | 0 | 1 |
| 1 | 5K | 0 | 3 |

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| Mol | Chain | #Chirality outliers | #Planarity outliers |
|-----|-------|---------------------|---------------------|
| 1 | 5L | 0 | 5 |
| 1 | 5M | 0 | 1 |
| 1 | 5N | 0 | 4 |
| 1 | 5O | 0 | 2 |
| 1 | 5P | 0 | 1 |
| 1 | 5Q | 0 | 3 |
| 1 | 5R | 0 | 5 |
| 1 | 5S | 0 | 1 |
| 1 | 5T | 0 | 4 |
| 1 | 5U | 0 | 2 |
| 1 | 5V | 0 | 1 |
| 1 | 5W | 0 | 3 |
| 1 | 5X | 0 | 5 |
| 1 | 5Y | 0 | 1 |
| 1 | 5Z | 0 | 4 |
| 1 | 5a | 0 | 2 |
| 1 | 5b | 0 | 1 |
| 1 | 5c | 0 | 3 |
| 1 | 5d | 0 | 5 |
| 1 | 6A | 0 | 4 |
| 1 | 6B | 0 | 4 |
| 1 | 6C | 0 | 3 |
| 1 | 6D | 0 | 3 |
| 1 | 6F | 0 | 4 |
| 1 | 6G | 0 | 4 |
| 1 | 6H | 0 | 4 |
| 1 | 6I | 0 | 3 |
| 1 | 6J | 0 | 3 |
| 1 | 6L | 0 | 4 |
| 1 | 6M | 0 | 4 |
| 1 | 6N | 0 | 4 |
| 1 | 6O | 0 | 3 |
| 1 | 6P | 0 | 3 |
| 1 | 6R | 0 | 4 |
| 1 | 6S | 0 | 4 |
| 1 | 6T | 0 | 4 |
| 1 | 6U | 0 | 3 |
| 1 | 6V | 0 | 3 |
| 1 | 6X | 0 | 4 |
| 1 | 6Y | 0 | 4 |
| 1 | 6Z | 0 | 4 |
| 1 | 6a | 0 | 3 |

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| Mol | Chain | #Chirality outliers | #Planarity outliers |
|-----|-------|---------------------|---------------------|
| 1 | 6b | 0 | 3 |
| 1 | 6d | 0 | 4 |
| 1 | 7A | 0 | 1 |
| 1 | 7B | 0 | 2 |
| 1 | 7C | 0 | 1 |
| 1 | 7D | 0 | 2 |
| 1 | 7F | 0 | 1 |
| 1 | 7G | 0 | 2 |
| 1 | 7H | 0 | 1 |
| 1 | 7I | 0 | 2 |
| 1 | 7K | 0 | 1 |
| 1 | 7L | 0 | 2 |
| 1 | 7M | 0 | 1 |
| 1 | 7N | 0 | 2 |
| 1 | 7P | 0 | 1 |
| 1 | 7Q | 0 | 2 |
| 1 | 7R | 0 | 1 |
| 1 | 7S | 0 | 2 |
| 1 | 7U | 0 | 1 |
| 1 | 7V | 0 | 2 |
| 1 | 7W | 0 | 1 |
| 1 | 7X | 0 | 2 |
| 1 | 8A | 0 | 4 |
| 1 | 8D | 0 | 1 |
| 1 | 8E | 0 | 3 |
| 1 | 8G | 0 | 4 |
| 1 | 8J | 0 | 1 |
| 1 | 8K | 0 | 3 |
| 1 | 8M | 0 | 4 |
| 1 | 8P | 0 | 1 |
| 1 | 8Q | 0 | 3 |
| 1 | 8S | 0 | 4 |
| 1 | 8V | 0 | 1 |
| 1 | 8W | 0 | 3 |
| 1 | 8Y | 0 | 4 |
| 1 | 8b | 0 | 1 |
| 1 | 8c | 0 | 3 |
| 1 | 9A | 0 | 1 |
| 1 | 9B | 0 | 1 |
| 1 | 9C | 0 | 1 |
| 1 | 9D | 0 | 1 |
| 1 | 9E | 0 | 1 |

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| Mol | Chain | #Chirality outliers | #Planarity outliers |
|-----|-------|---------------------|---------------------|
| All | All | 0 | 395 |

All (86) bond length outliers are listed below:

| Mol | Chain | Res | Type | Atoms | Z | Observed(Å) | Ideal(Å) |
|-----|-------|-----|------|-------|-------|-------------|----------|
| 1 | 7T | 137 | GLN | CA-CB | -7.06 | 1.38 | 1.53 |
| 1 | 7O | 137 | GLN | CA-CB | -7.06 | 1.38 | 1.53 |
| 1 | 7J | 137 | GLN | CA-CB | -7.05 | 1.38 | 1.53 |
| 1 | 7E | 137 | GLN | CA-CB | -7.05 | 1.38 | 1.53 |
| 1 | 7Y | 137 | GLN | CA-CB | -7.04 | 1.38 | 1.53 |
| 2 | 5l | 111 | VAL | C-N | -5.72 | 1.20 | 1.34 |
| 2 | 3s | 111 | VAL | C-N | -5.71 | 1.21 | 1.34 |
| 2 | 3q | 111 | VAL | C-N | -5.71 | 1.21 | 1.34 |
| 2 | 1r | 111 | VAL | C-N | -5.70 | 1.21 | 1.34 |
| 2 | 1v | 111 | VAL | C-N | -5.70 | 1.21 | 1.34 |
| 2 | 8k | 111 | VAL | C-N | -5.70 | 1.21 | 1.34 |
| 2 | 8q | 111 | VAL | C-N | -5.70 | 1.21 | 1.34 |
| 2 | 1x | 111 | VAL | C-N | -5.70 | 1.21 | 1.34 |
| 2 | 3g | 111 | VAL | C-N | -5.70 | 1.21 | 1.34 |
| 2 | 5f | 111 | VAL | C-N | -5.70 | 1.21 | 1.34 |
| 2 | 5h | 111 | VAL | C-N | -5.70 | 1.21 | 1.34 |
| 2 | 3u | 111 | VAL | C-N | -5.70 | 1.21 | 1.34 |
| 2 | 3k | 111 | VAL | C-N | -5.69 | 1.21 | 1.34 |
| 2 | 5j | 111 | VAL | C-N | -5.69 | 1.21 | 1.34 |
| 2 | 1f | 111 | VAL | C-N | -5.69 | 1.21 | 1.34 |
| 2 | 1n | 111 | VAL | C-N | -5.69 | 1.21 | 1.34 |
| 2 | 3o | 111 | VAL | C-N | -5.69 | 1.21 | 1.34 |
| 2 | 5n | 111 | VAL | C-N | -5.69 | 1.21 | 1.34 |
| 2 | 3e | 111 | VAL | C-N | -5.68 | 1.21 | 1.34 |
| 2 | 6m | 111 | VAL | C-N | -5.68 | 1.21 | 1.34 |
| 2 | 8e | 111 | VAL | C-N | -5.68 | 1.21 | 1.34 |
| 2 | 1j | 111 | VAL | C-N | -5.68 | 1.21 | 1.34 |
| 2 | 1h | 111 | VAL | C-N | -5.68 | 1.21 | 1.34 |
| 2 | 1t | 111 | VAL | C-N | -5.67 | 1.21 | 1.34 |
| 2 | 4h | 111 | VAL | C-N | -5.67 | 1.21 | 1.34 |
| 2 | 9L | 111 | VAL | C-N | -5.67 | 1.21 | 1.34 |
| 2 | 6u | 111 | VAL | C-N | -5.67 | 1.21 | 1.34 |
| 2 | 6q | 111 | VAL | C-N | -5.67 | 1.21 | 1.34 |
| 2 | 1l | 111 | VAL | C-N | -5.67 | 1.21 | 1.34 |
| 2 | 3m | 111 | VAL | C-N | -5.67 | 1.21 | 1.34 |
| 2 | 1p | 111 | VAL | C-N | -5.67 | 1.21 | 1.34 |
| 2 | 9R | 111 | VAL | C-N | -5.67 | 1.21 | 1.34 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(Å) | Ideal(Å) |
|-----|-------|-----|------|---------|-------|-------------|----------|
| 2 | 4l | 111 | VAL | C-N | -5.67 | 1.21 | 1.34 |
| 2 | 3w | 111 | VAL | C-N | -5.67 | 1.21 | 1.34 |
| 2 | 4f | 111 | VAL | C-N | -5.67 | 1.21 | 1.34 |
| 2 | 6i | 111 | VAL | C-N | -5.67 | 1.21 | 1.34 |
| 2 | 8j | 111 | VAL | C-N | -5.66 | 1.21 | 1.34 |
| 2 | 6s | 111 | VAL | C-N | -5.66 | 1.21 | 1.34 |
| 1 | 2K | 238 | VAL | CB-CG1 | -5.66 | 1.41 | 1.52 |
| 2 | 8w | 111 | VAL | C-N | -5.66 | 1.21 | 1.34 |
| 1 | 2F | 238 | VAL | CB-CG1 | -5.66 | 1.41 | 1.52 |
| 1 | 2P | 238 | VAL | CB-CG1 | -5.66 | 1.41 | 1.52 |
| 1 | 2A | 238 | VAL | CB-CG1 | -5.66 | 1.41 | 1.52 |
| 2 | 6e | 111 | VAL | C-N | -5.66 | 1.21 | 1.34 |
| 2 | 6o | 111 | VAL | C-N | -5.66 | 1.21 | 1.34 |
| 2 | 8t | 111 | VAL | C-N | -5.66 | 1.21 | 1.34 |
| 2 | 4n | 111 | VAL | C-N | -5.66 | 1.21 | 1.34 |
| 2 | 6g | 111 | VAL | C-N | -5.66 | 1.21 | 1.34 |
| 2 | 4j | 111 | VAL | C-N | -5.66 | 1.21 | 1.34 |
| 2 | 3i | 111 | VAL | C-N | -5.66 | 1.21 | 1.34 |
| 2 | 8v | 111 | VAL | C-N | -5.66 | 1.21 | 1.34 |
| 2 | 9M | 111 | VAL | C-N | -5.66 | 1.21 | 1.34 |
| 2 | 6w | 111 | VAL | C-N | -5.65 | 1.21 | 1.34 |
| 2 | 8p | 111 | VAL | C-N | -5.65 | 1.21 | 1.34 |
| 2 | 8h | 111 | VAL | C-N | -5.64 | 1.21 | 1.34 |
| 1 | 2U | 238 | VAL | CB-CG1 | -5.64 | 1.41 | 1.52 |
| 2 | 8z | 111 | VAL | C-N | -5.64 | 1.21 | 1.34 |
| 2 | 8n | 111 | VAL | C-N | -5.63 | 1.21 | 1.34 |
| 2 | 9P | 111 | VAL | C-N | -5.63 | 1.21 | 1.34 |
| 2 | 6k | 111 | VAL | C-N | -5.62 | 1.21 | 1.34 |
| 1 | 3P | 319 | TYR | CD2-CE2 | -5.32 | 1.31 | 1.39 |
| 1 | 3b | 319 | TYR | CD2-CE2 | -5.30 | 1.31 | 1.39 |
| 1 | 3D | 319 | TYR | CD2-CE2 | -5.30 | 1.31 | 1.39 |
| 1 | 3V | 319 | TYR | CD2-CE2 | -5.29 | 1.31 | 1.39 |
| 1 | 3b | 319 | TYR | CB-CG | -5.27 | 1.43 | 1.51 |
| 1 | 3J | 319 | TYR | CB-CG | -5.26 | 1.43 | 1.51 |
| 1 | 3J | 319 | TYR | CD2-CE2 | -5.25 | 1.31 | 1.39 |
| 1 | 3V | 319 | TYR | CB-CG | -5.25 | 1.43 | 1.51 |
| 1 | 3D | 319 | TYR | CB-CG | -5.25 | 1.43 | 1.51 |
| 1 | 3P | 319 | TYR | CB-CG | -5.25 | 1.43 | 1.51 |
| 1 | 6P | 332 | VAL | CB-CG1 | -5.19 | 1.42 | 1.52 |
| 1 | 6J | 332 | VAL | CB-CG1 | -5.17 | 1.42 | 1.52 |
| 1 | 6D | 332 | VAL | CB-CG1 | -5.17 | 1.42 | 1.52 |
| 1 | 6V | 332 | VAL | CB-CG1 | -5.15 | 1.42 | 1.52 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(Å) | Ideal(Å) |
|-----|-------|-----|------|--------|-------|-------------|----------|
| 1 | 6b | 332 | VAL | CB-CG1 | -5.14 | 1.42 | 1.52 |
| 1 | 7J | 437 | ILE | C-N | -5.11 | 1.22 | 1.34 |
| 1 | 7E | 437 | ILE | C-N | -5.11 | 1.22 | 1.34 |
| 1 | 7Y | 437 | ILE | C-N | -5.11 | 1.22 | 1.34 |
| 1 | 7T | 437 | ILE | C-N | -5.09 | 1.22 | 1.34 |
| 1 | 7O | 437 | ILE | C-N | -5.09 | 1.22 | 1.34 |
| 1 | 3W | 269 | ASN | CA-CB | -5.01 | 1.40 | 1.53 |

All (151) bond angle outliers are listed below:

| Mol | Chain | Res | Type | Atoms | Z | Observed(°) | Ideal(°) |
|-----|-------|-----|------|-----------|-------|-------------|----------|
| 1 | 1L | 355 | SER | C-N-CD | -9.96 | 98.69 | 120.60 |
| 1 | 1d | 355 | SER | C-N-CD | -9.96 | 98.70 | 120.60 |
| 1 | 1R | 355 | SER | C-N-CD | -9.95 | 98.71 | 120.60 |
| 1 | 1F | 355 | SER | C-N-CD | -9.95 | 98.71 | 120.60 |
| 1 | 1X | 355 | SER | C-N-CD | -9.95 | 98.71 | 120.60 |
| 1 | 3T | 354 | VAL | C-N-CA | 8.17 | 142.12 | 121.70 |
| 1 | 3B | 354 | VAL | C-N-CA | 8.16 | 142.09 | 121.70 |
| 1 | 3H | 354 | VAL | C-N-CA | 8.16 | 142.10 | 121.70 |
| 1 | 3N | 354 | VAL | C-N-CA | 8.14 | 142.06 | 121.70 |
| 1 | 3Z | 354 | VAL | C-N-CA | 8.14 | 142.06 | 121.70 |
| 1 | 7X | 330 | LEU | CA-CB-CG | 7.60 | 132.77 | 115.30 |
| 1 | 7D | 330 | LEU | CA-CB-CG | 7.59 | 132.77 | 115.30 |
| 1 | 7I | 330 | LEU | CA-CB-CG | 7.59 | 132.75 | 115.30 |
| 1 | 7N | 330 | LEU | CA-CB-CG | 7.59 | 132.75 | 115.30 |
| 1 | 7S | 330 | LEU | CA-CB-CG | 7.58 | 132.75 | 115.30 |
| 1 | 2G | 355 | SER | C-N-CD | -7.05 | 105.09 | 120.60 |
| 1 | 2L | 355 | SER | C-N-CD | -7.05 | 105.10 | 120.60 |
| 1 | 2V | 355 | SER | C-N-CD | -7.04 | 105.10 | 120.60 |
| 1 | 2B | 355 | SER | C-N-CD | -7.04 | 105.11 | 120.60 |
| 1 | 2Q | 355 | SER | C-N-CD | -7.04 | 105.11 | 120.60 |
| 1 | 1J | 330 | LEU | CB-CG-CD1 | -6.80 | 99.44 | 111.00 |
| 1 | 1P | 330 | LEU | CB-CG-CD1 | -6.79 | 99.45 | 111.00 |
| 1 | 1D | 330 | LEU | CB-CG-CD1 | -6.79 | 99.46 | 111.00 |
| 1 | 1b | 330 | LEU | CB-CG-CD1 | -6.78 | 99.47 | 111.00 |
| 1 | 1V | 330 | LEU | CB-CG-CD1 | -6.77 | 99.49 | 111.00 |
| 1 | 4H | 203 | PRO | C-N-CA | 6.70 | 138.44 | 121.70 |
| 1 | 4T | 203 | PRO | C-N-CA | 6.69 | 138.44 | 121.70 |
| 1 | 4B | 203 | PRO | C-N-CA | 6.69 | 138.43 | 121.70 |
| 1 | 4N | 203 | PRO | C-N-CA | 6.69 | 138.43 | 121.70 |
| 1 | 4Z | 203 | PRO | C-N-CA | 6.68 | 138.41 | 121.70 |
| 1 | 5K | 294 | LEU | CA-CB-CG | 6.46 | 130.16 | 115.30 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(°) | Ideal(°) |
|-----|-------|-----|------|-----------|-------|-------------|----------|
| 1 | 5Q | 294 | LEU | CA-CB-CG | 6.46 | 130.16 | 115.30 |
| 1 | 5E | 294 | LEU | CA-CB-CG | 6.46 | 130.16 | 115.30 |
| 1 | 5W | 294 | LEU | CA-CB-CG | 6.45 | 130.14 | 115.30 |
| 1 | 5c | 294 | LEU | CA-CB-CG | 6.45 | 130.13 | 115.30 |
| 1 | 2U | 354 | VAL | C-N-CA | 6.42 | 137.76 | 121.70 |
| 1 | 2K | 354 | VAL | C-N-CA | 6.42 | 137.74 | 121.70 |
| 1 | 2A | 354 | VAL | C-N-CA | 6.41 | 137.73 | 121.70 |
| 1 | 2F | 354 | VAL | C-N-CA | 6.41 | 137.72 | 121.70 |
| 1 | 2P | 354 | VAL | C-N-CA | 6.40 | 137.70 | 121.70 |
| 1 | 5I | 155 | SER | C-N-CA | 6.36 | 137.59 | 121.70 |
| 1 | 5U | 155 | SER | C-N-CA | 6.35 | 137.58 | 121.70 |
| 1 | 5a | 155 | SER | C-N-CA | 6.35 | 137.57 | 121.70 |
| 1 | 5C | 155 | SER | C-N-CA | 6.35 | 137.56 | 121.70 |
| 1 | 5O | 155 | SER | C-N-CA | 6.35 | 137.56 | 121.70 |
| 1 | 5I | 130 | LEU | CB-CG-CD1 | -6.34 | 100.22 | 111.00 |
| 1 | 5U | 130 | LEU | CB-CG-CD1 | -6.33 | 100.23 | 111.00 |
| 1 | 5O | 130 | LEU | CB-CG-CD1 | -6.33 | 100.24 | 111.00 |
| 1 | 5a | 130 | LEU | CB-CG-CD1 | -6.33 | 100.25 | 111.00 |
| 1 | 5C | 130 | LEU | CB-CG-CD1 | -6.32 | 100.25 | 111.00 |
| 1 | 6X | 330 | LEU | CA-CB-CG | 6.21 | 129.59 | 115.30 |
| 1 | 6d | 330 | LEU | CA-CB-CG | 6.21 | 129.59 | 115.30 |
| 1 | 6F | 330 | LEU | CA-CB-CG | 6.21 | 129.58 | 115.30 |
| 1 | 6R | 330 | LEU | CA-CB-CG | 6.21 | 129.57 | 115.30 |
| 1 | 6L | 330 | LEU | CA-CB-CG | 6.20 | 129.56 | 115.30 |
| 1 | 3M | 249 | LEU | CB-CG-CD2 | -6.03 | 100.76 | 111.00 |
| 1 | 3A | 249 | LEU | CB-CG-CD2 | -6.01 | 100.79 | 111.00 |
| 1 | 3G | 249 | LEU | CB-CG-CD2 | -6.00 | 100.80 | 111.00 |
| 1 | 3S | 249 | LEU | CB-CG-CD2 | -5.99 | 100.81 | 111.00 |
| 1 | 3Y | 249 | LEU | CB-CG-CD2 | -5.98 | 100.83 | 111.00 |
| 1 | 7O | 306 | LEU | CA-CB-CG | 5.95 | 128.98 | 115.30 |
| 1 | 7E | 306 | LEU | CA-CB-CG | 5.94 | 128.97 | 115.30 |
| 1 | 7J | 306 | LEU | CA-CB-CG | 5.94 | 128.96 | 115.30 |
| 1 | 7Y | 306 | LEU | CA-CB-CG | 5.93 | 128.94 | 115.30 |
| 1 | 7T | 306 | LEU | CA-CB-CG | 5.93 | 128.93 | 115.30 |
| 1 | 7K | 39 | ALA | C-N-CA | 5.91 | 136.48 | 121.70 |
| 1 | 7A | 39 | ALA | C-N-CA | 5.90 | 136.46 | 121.70 |
| 1 | 7F | 39 | ALA | C-N-CA | 5.90 | 136.44 | 121.70 |
| 1 | 7P | 39 | ALA | C-N-CA | 5.89 | 136.43 | 121.70 |
| 1 | 7U | 39 | ALA | C-N-CA | 5.89 | 136.43 | 121.70 |
| 1 | 8C | 130 | LEU | CA-CB-CG | 5.76 | 128.55 | 115.30 |
| 1 | 8O | 130 | LEU | CA-CB-CG | 5.76 | 128.55 | 115.30 |
| 1 | 8U | 130 | LEU | CA-CB-CG | 5.76 | 128.54 | 115.30 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(°) | Ideal(°) |
|-----|-------|-----|------|------------|-------|-------------|----------|
| 1 | 8I | 130 | LEU | CA-CB-CG | 5.75 | 128.53 | 115.30 |
| 1 | 8a | 130 | LEU | CA-CB-CG | 5.75 | 128.53 | 115.30 |
| 1 | 1Y | 250 | ILE | CG1-CB-CG2 | -5.73 | 98.79 | 111.40 |
| 1 | 1M | 250 | ILE | CG1-CB-CG2 | -5.73 | 98.80 | 111.40 |
| 1 | 1A | 250 | ILE | CG1-CB-CG2 | -5.72 | 98.82 | 111.40 |
| 1 | 1S | 250 | ILE | CG1-CB-CG2 | -5.71 | 98.83 | 111.40 |
| 1 | 1G | 250 | ILE | CG1-CB-CG2 | -5.71 | 98.84 | 111.40 |
| 1 | 6O | 134 | ARG | NE-CZ-NH1 | -5.59 | 117.50 | 120.30 |
| 1 | 6I | 134 | ARG | NE-CZ-NH1 | -5.59 | 117.51 | 120.30 |
| 1 | 6U | 134 | ARG | NE-CZ-NH1 | -5.55 | 117.53 | 120.30 |
| 1 | 1R | 330 | LEU | CB-CG-CD2 | -5.52 | 101.61 | 111.00 |
| 1 | 6C | 134 | ARG | NE-CZ-NH1 | -5.52 | 117.54 | 120.30 |
| 1 | 1L | 330 | LEU | CB-CG-CD2 | -5.52 | 101.61 | 111.00 |
| 1 | 6a | 134 | ARG | NE-CZ-NH1 | -5.51 | 117.54 | 120.30 |
| 1 | 1D | 354 | VAL | C-N-CA | 5.51 | 135.48 | 121.70 |
| 1 | 1F | 330 | LEU | CB-CG-CD2 | -5.51 | 101.63 | 111.00 |
| 1 | 1V | 354 | VAL | C-N-CA | 5.51 | 135.48 | 121.70 |
| 1 | 1J | 354 | VAL | C-N-CA | 5.51 | 135.48 | 121.70 |
| 1 | 1b | 354 | VAL | C-N-CA | 5.51 | 135.47 | 121.70 |
| 1 | 1d | 330 | LEU | CB-CG-CD2 | -5.50 | 101.64 | 111.00 |
| 1 | 1X | 330 | LEU | CB-CG-CD2 | -5.50 | 101.64 | 111.00 |
| 1 | 1P | 354 | VAL | C-N-CA | 5.50 | 135.45 | 121.70 |
| 1 | 5S | 250 | ILE | CG1-CB-CG2 | -5.50 | 99.31 | 111.40 |
| 1 | 5A | 250 | ILE | CG1-CB-CG2 | -5.49 | 99.32 | 111.40 |
| 1 | 5G | 250 | ILE | CG1-CB-CG2 | -5.49 | 99.33 | 111.40 |
| 1 | 5Y | 250 | ILE | CG1-CB-CG2 | -5.49 | 99.33 | 111.40 |
| 1 | 5M | 250 | ILE | CG1-CB-CG2 | -5.48 | 99.34 | 111.40 |
| 1 | 8V | 93 | LEU | CA-CB-CG | 5.44 | 127.81 | 115.30 |
| 1 | 8D | 93 | LEU | CA-CB-CG | 5.44 | 127.81 | 115.30 |
| 1 | 8J | 93 | LEU | CA-CB-CG | 5.44 | 127.80 | 115.30 |
| 1 | 8b | 93 | LEU | CA-CB-CG | 5.43 | 127.79 | 115.30 |
| 1 | 8P | 93 | LEU | CA-CB-CG | 5.43 | 127.78 | 115.30 |
| 1 | 5c | 224 | LEU | CA-CB-CG | 5.41 | 127.75 | 115.30 |
| 1 | 4S | 250 | ILE | CG1-CB-CG2 | -5.41 | 99.50 | 111.40 |
| 1 | 5Q | 224 | LEU | CA-CB-CG | 5.41 | 127.74 | 115.30 |
| 1 | 5W | 224 | LEU | CA-CB-CG | 5.41 | 127.74 | 115.30 |
| 1 | 5E | 224 | LEU | CA-CB-CG | 5.40 | 127.72 | 115.30 |
| 1 | 4A | 250 | ILE | CG1-CB-CG2 | -5.40 | 99.52 | 111.40 |
| 1 | 4G | 250 | ILE | CG1-CB-CG2 | -5.40 | 99.52 | 111.40 |
| 1 | 4M | 250 | ILE | CG1-CB-CG2 | -5.40 | 99.53 | 111.40 |
| 1 | 4Y | 250 | ILE | CG1-CB-CG2 | -5.40 | 99.52 | 111.40 |
| 1 | 5K | 224 | LEU | CA-CB-CG | 5.39 | 127.70 | 115.30 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(°) | Ideal(°) |
|-----|-------|-----|------|------------|-------|-------------|----------|
| 1 | 7S | 330 | LEU | CB-CG-CD1 | -5.35 | 101.91 | 111.00 |
| 1 | 7N | 330 | LEU | CB-CG-CD1 | -5.34 | 101.91 | 111.00 |
| 1 | 7I | 330 | LEU | CB-CG-CD1 | -5.33 | 101.93 | 111.00 |
| 1 | 7D | 330 | LEU | CB-CG-CD1 | -5.33 | 101.94 | 111.00 |
| 1 | 7X | 330 | LEU | CB-CG-CD1 | -5.32 | 101.96 | 111.00 |
| 1 | 5N | 374 | ARG | NE-CZ-NH1 | -5.30 | 117.65 | 120.30 |
| 1 | 5a | 32 | PHE | CB-CG-CD1 | 5.25 | 124.47 | 120.80 |
| 1 | 5I | 32 | PHE | CB-CG-CD1 | 5.24 | 124.47 | 120.80 |
| 1 | 5U | 32 | PHE | CB-CG-CD1 | 5.24 | 124.47 | 120.80 |
| 1 | 5O | 32 | PHE | CB-CG-CD1 | 5.24 | 124.47 | 120.80 |
| 1 | 5C | 32 | PHE | CB-CG-CD1 | 5.23 | 124.46 | 120.80 |
| 1 | 5B | 374 | ARG | NE-CZ-NH1 | -5.23 | 117.69 | 120.30 |
| 1 | 5T | 374 | ARG | NE-CZ-NH1 | -5.21 | 117.70 | 120.30 |
| 1 | 5Z | 374 | ARG | NE-CZ-NH1 | -5.20 | 117.70 | 120.30 |
| 1 | 5H | 374 | ARG | NE-CZ-NH1 | -5.17 | 117.72 | 120.30 |
| 1 | 3I | 250 | ILE | CG1-CB-CG2 | -5.14 | 100.10 | 111.40 |
| 1 | 3a | 250 | ILE | CG1-CB-CG2 | -5.14 | 100.10 | 111.40 |
| 1 | 3C | 250 | ILE | CG1-CB-CG2 | -5.13 | 100.11 | 111.40 |
| 1 | 3U | 250 | ILE | CG1-CB-CG2 | -5.13 | 100.11 | 111.40 |
| 1 | 3O | 250 | ILE | CG1-CB-CG2 | -5.13 | 100.11 | 111.40 |
| 1 | 8X | 250 | ILE | CG1-CB-CG2 | -5.08 | 100.21 | 111.40 |
| 1 | 8d | 250 | ILE | CG1-CB-CG2 | -5.08 | 100.23 | 111.40 |
| 1 | 8F | 250 | ILE | CG1-CB-CG2 | -5.07 | 100.24 | 111.40 |
| 1 | 8L | 250 | ILE | CG1-CB-CG2 | -5.07 | 100.24 | 111.40 |
| 1 | 8R | 250 | ILE | CG1-CB-CG2 | -5.07 | 100.25 | 111.40 |
| 1 | 3L | 249 | LEU | CA-CB-CG | -5.03 | 103.74 | 115.30 |
| 1 | 6P | 317 | GLY | N-CA-C | -5.03 | 100.54 | 113.10 |
| 1 | 3R | 249 | LEU | CA-CB-CG | -5.02 | 103.74 | 115.30 |
| 1 | 6b | 317 | GLY | N-CA-C | -5.02 | 100.54 | 113.10 |
| 1 | 3F | 249 | LEU | CA-CB-CG | -5.02 | 103.76 | 115.30 |
| 1 | 6D | 317 | GLY | N-CA-C | -5.02 | 100.55 | 113.10 |
| 1 | 3d | 249 | LEU | CA-CB-CG | -5.02 | 103.76 | 115.30 |
| 1 | 6V | 317 | GLY | N-CA-C | -5.01 | 100.58 | 113.10 |
| 1 | 6J | 317 | GLY | N-CA-C | -5.01 | 100.58 | 113.10 |
| 1 | 3G | 412 | LEU | CA-CB-CG | -5.00 | 103.79 | 115.30 |
| 1 | 3X | 249 | LEU | CA-CB-CG | -5.00 | 103.80 | 115.30 |

There are no chirality outliers.

All (395) planarity outliers are listed below:

| Mol | Chain | Res | Type | Group |
|-----|-------|-----|------|---------|
| 1 | 1B | 24 | ILE | Peptide |

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| Mol | Chain | Res | Type | Group |
|------------|--------------|------------|-------------|--------------|
| 1 | 1B | 333 | SER | Peptide |
| 1 | 1B | 6 | ASN | Peptide |
| 1 | 1B | 7 | ASP | Peptide |
| 1 | 1C | 425 | LYS | Peptide |
| 1 | 1D | 264 | LEU | Mainchain |
| 1 | 1D | 380 | ASP | Peptide |
| 1 | 1H | 24 | ILE | Peptide |
| 1 | 1H | 333 | SER | Peptide |
| 1 | 1H | 6 | ASN | Peptide |
| 1 | 1H | 7 | ASP | Peptide |
| 1 | 1I | 425 | LYS | Peptide |
| 1 | 1J | 264 | LEU | Mainchain |
| 1 | 1J | 380 | ASP | Peptide |
| 1 | 1N | 24 | ILE | Peptide |
| 1 | 1N | 333 | SER | Peptide |
| 1 | 1N | 6 | ASN | Peptide |
| 1 | 1N | 7 | ASP | Peptide |
| 1 | 1O | 425 | LYS | Peptide |
| 1 | 1P | 264 | LEU | Mainchain |
| 1 | 1P | 380 | ASP | Peptide |
| 1 | 1T | 24 | ILE | Peptide |
| 1 | 1T | 333 | SER | Peptide |
| 1 | 1T | 6 | ASN | Peptide |
| 1 | 1T | 7 | ASP | Peptide |
| 1 | 1U | 425 | LYS | Peptide |
| 1 | 1V | 264 | LEU | Mainchain |
| 1 | 1V | 380 | ASP | Peptide |
| 1 | 1Z | 24 | ILE | Peptide |
| 1 | 1Z | 333 | SER | Peptide |
| 1 | 1Z | 6 | ASN | Peptide |
| 1 | 1Z | 7 | ASP | Peptide |
| 1 | 1a | 425 | LYS | Peptide |
| 1 | 1b | 264 | LEU | Mainchain |
| 1 | 1b | 380 | ASP | Peptide |
| 1 | 2A | 275 | PHE | Peptide |
| 1 | 2A | 355 | SER | Peptide |
| 1 | 2B | 200 | ILE | Peptide |
| 1 | 2C | 355 | SER | Peptide |
| 1 | 2D | 354 | VAL | Peptide |
| 1 | 2E | 336 | ALA | Peptide |
| 1 | 2E | 390 | GLY | Peptide |
| 1 | 2F | 275 | PHE | Peptide |

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| Mol | Chain | Res | Type | Group |
|------------|--------------|------------|-------------|--------------|
| 1 | 2F | 355 | SER | Peptide |
| 1 | 2G | 200 | ILE | Peptide |
| 1 | 2H | 355 | SER | Peptide |
| 1 | 2I | 354 | VAL | Peptide |
| 1 | 2J | 336 | ALA | Peptide |
| 1 | 2J | 390 | GLY | Peptide |
| 1 | 2K | 275 | PHE | Peptide |
| 1 | 2K | 355 | SER | Peptide |
| 1 | 2L | 200 | ILE | Peptide |
| 1 | 2M | 355 | SER | Peptide |
| 1 | 2N | 354 | VAL | Peptide |
| 1 | 2O | 336 | ALA | Peptide |
| 1 | 2O | 390 | GLY | Peptide |
| 1 | 2P | 275 | PHE | Peptide |
| 1 | 2P | 355 | SER | Peptide |
| 1 | 2Q | 200 | ILE | Peptide |
| 1 | 2R | 355 | SER | Peptide |
| 1 | 2S | 354 | VAL | Peptide |
| 1 | 2T | 336 | ALA | Peptide |
| 1 | 2T | 390 | GLY | Peptide |
| 1 | 2U | 275 | PHE | Peptide |
| 1 | 2U | 355 | SER | Peptide |
| 1 | 2V | 200 | ILE | Peptide |
| 1 | 2W | 355 | SER | Peptide |
| 1 | 2X | 354 | VAL | Peptide |
| 1 | 2Y | 336 | ALA | Peptide |
| 1 | 2Y | 390 | GLY | Peptide |
| 1 | 3A | 250 | ILE | Peptide |
| 1 | 3B | 355 | SER | Peptide |
| 1 | 3C | 355 | SER | Peptide |
| 1 | 3C | 377 | ASN | Peptide |
| 1 | 3C | 5 | PHE | Peptide |
| 1 | 3D | 20 | ILE | Peptide |
| 1 | 3D | 267 | ALA | Peptide |
| 1 | 3D | 318 | LEU | Peptide |
| 1 | 3D | 355 | SER | Peptide |
| 1 | 3G | 250 | ILE | Peptide |
| 1 | 3H | 355 | SER | Peptide |
| 1 | 3I | 355 | SER | Peptide |
| 1 | 3I | 377 | ASN | Peptide |
| 1 | 3I | 5 | PHE | Peptide |
| 1 | 3J | 20 | ILE | Peptide |

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| Mol | Chain | Res | Type | Group |
|------------|--------------|------------|-------------|--------------|
| 1 | 3J | 267 | ALA | Peptide |
| 1 | 3J | 318 | LEU | Peptide |
| 1 | 3J | 355 | SER | Peptide |
| 1 | 3M | 250 | ILE | Peptide |
| 1 | 3N | 355 | SER | Peptide |
| 1 | 3O | 355 | SER | Peptide |
| 1 | 3O | 377 | ASN | Peptide |
| 1 | 3O | 5 | PHE | Peptide |
| 1 | 3P | 20 | ILE | Peptide |
| 1 | 3P | 267 | ALA | Peptide |
| 1 | 3P | 318 | LEU | Peptide |
| 1 | 3P | 355 | SER | Peptide |
| 1 | 3S | 250 | ILE | Peptide |
| 1 | 3T | 355 | SER | Peptide |
| 1 | 3U | 355 | SER | Peptide |
| 1 | 3U | 377 | ASN | Peptide |
| 1 | 3U | 5 | PHE | Peptide |
| 1 | 3V | 20 | ILE | Peptide |
| 1 | 3V | 267 | ALA | Peptide |
| 1 | 3V | 318 | LEU | Peptide |
| 1 | 3V | 355 | SER | Peptide |
| 1 | 3Y | 250 | ILE | Peptide |
| 1 | 3Z | 355 | SER | Peptide |
| 1 | 3a | 355 | SER | Peptide |
| 1 | 3a | 377 | ASN | Peptide |
| 1 | 3a | 5 | PHE | Peptide |
| 1 | 3b | 20 | ILE | Peptide |
| 1 | 3b | 267 | ALA | Peptide |
| 1 | 3b | 318 | LEU | Peptide |
| 1 | 3b | 355 | SER | Peptide |
| 1 | 4A | 235 | SER | Peptide |
| 1 | 4B | 118 | LYS | Peptide |
| 1 | 4B | 228 | GLN | Peptide |
| 1 | 4B | 67 | ASP | Peptide |
| 1 | 4C | 355 | SER | Peptide |
| 1 | 4D | 397 | THR | Peptide |
| 1 | 4E | 376 | THR | Peptide |
| 1 | 4G | 235 | SER | Peptide |
| 1 | 4H | 118 | LYS | Peptide |
| 1 | 4H | 228 | GLN | Peptide |
| 1 | 4H | 67 | ASP | Peptide |
| 1 | 4I | 355 | SER | Peptide |

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| Mol | Chain | Res | Type | Group |
|------------|--------------|------------|-------------|--------------|
| 1 | 4J | 397 | THR | Peptide |
| 1 | 4K | 376 | THR | Peptide |
| 1 | 4M | 235 | SER | Peptide |
| 1 | 4N | 118 | LYS | Peptide |
| 1 | 4N | 228 | GLN | Peptide |
| 1 | 4N | 67 | ASP | Peptide |
| 1 | 4O | 355 | SER | Peptide |
| 1 | 4P | 397 | THR | Peptide |
| 1 | 4Q | 376 | THR | Peptide |
| 1 | 4S | 235 | SER | Peptide |
| 1 | 4T | 118 | LYS | Peptide |
| 1 | 4T | 228 | GLN | Peptide |
| 1 | 4T | 67 | ASP | Peptide |
| 1 | 4U | 355 | SER | Peptide |
| 1 | 4V | 397 | THR | Peptide |
| 1 | 4W | 376 | THR | Peptide |
| 1 | 4Y | 235 | SER | Peptide |
| 1 | 4Z | 118 | LYS | Peptide |
| 1 | 4Z | 228 | GLN | Peptide |
| 1 | 4Z | 67 | ASP | Peptide |
| 1 | 4a | 355 | SER | Peptide |
| 1 | 4b | 397 | THR | Peptide |
| 1 | 4c | 376 | THR | Peptide |
| 1 | 5A | 390 | GLY | Peptide |
| 1 | 5B | 231 | ARG | Peptide |
| 1 | 5B | 345 | ASP | Peptide |
| 1 | 5B | 376 | THR | Peptide |
| 1 | 5B | 385 | TRP | Peptide |
| 1 | 5C | 30 | ASP | Peptide |
| 1 | 5C | 355 | SER | Peptide |
| 1 | 5D | 394 | THR | Peptide |
| 1 | 5E | 377 | ASN | Peptide |
| 1 | 5E | 424 | ASP | Peptide |
| 1 | 5E | 94 | GLY | Peptide |
| 1 | 5F | 155 | SER | Peptide |
| 1 | 5F | 156 | TRP | Peptide |
| 1 | 5F | 201 | ASP | Peptide |
| 1 | 5F | 355 | SER | Peptide |
| 1 | 5F | 440 | ASN | Peptide |
| 1 | 5G | 390 | GLY | Peptide |
| 1 | 5H | 231 | ARG | Peptide |
| 1 | 5H | 345 | ASP | Peptide |

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| Mol | Chain | Res | Type | Group |
|------------|--------------|------------|-------------|--------------|
| 1 | 5H | 376 | THR | Peptide |
| 1 | 5H | 385 | TRP | Peptide |
| 1 | 5I | 30 | ASP | Peptide |
| 1 | 5I | 355 | SER | Peptide |
| 1 | 5J | 394 | THR | Peptide |
| 1 | 5K | 377 | ASN | Peptide |
| 1 | 5K | 424 | ASP | Peptide |
| 1 | 5K | 94 | GLY | Peptide |
| 1 | 5L | 155 | SER | Peptide |
| 1 | 5L | 156 | TRP | Peptide |
| 1 | 5L | 201 | ASP | Peptide |
| 1 | 5L | 355 | SER | Peptide |
| 1 | 5L | 440 | ASN | Peptide |
| 1 | 5M | 390 | GLY | Peptide |
| 1 | 5N | 231 | ARG | Peptide |
| 1 | 5N | 345 | ASP | Peptide |
| 1 | 5N | 376 | THR | Peptide |
| 1 | 5N | 385 | TRP | Peptide |
| 1 | 5O | 30 | ASP | Peptide |
| 1 | 5O | 355 | SER | Peptide |
| 1 | 5P | 394 | THR | Peptide |
| 1 | 5Q | 377 | ASN | Peptide |
| 1 | 5Q | 424 | ASP | Peptide |
| 1 | 5Q | 94 | GLY | Peptide |
| 1 | 5R | 155 | SER | Peptide |
| 1 | 5R | 156 | TRP | Peptide |
| 1 | 5R | 201 | ASP | Peptide |
| 1 | 5R | 355 | SER | Peptide |
| 1 | 5R | 440 | ASN | Peptide |
| 1 | 5S | 390 | GLY | Peptide |
| 1 | 5T | 231 | ARG | Peptide |
| 1 | 5T | 345 | ASP | Peptide |
| 1 | 5T | 376 | THR | Peptide |
| 1 | 5T | 385 | TRP | Peptide |
| 1 | 5U | 30 | ASP | Peptide |
| 1 | 5U | 355 | SER | Peptide |
| 1 | 5V | 394 | THR | Peptide |
| 1 | 5W | 377 | ASN | Peptide |
| 1 | 5W | 424 | ASP | Peptide |
| 1 | 5W | 94 | GLY | Peptide |
| 1 | 5X | 155 | SER | Peptide |
| 1 | 5X | 156 | TRP | Peptide |

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| Mol | Chain | Res | Type | Group |
|------------|--------------|------------|-------------|--------------|
| 1 | 5X | 201 | ASP | Peptide |
| 1 | 5X | 355 | SER | Peptide |
| 1 | 5X | 440 | ASN | Peptide |
| 1 | 5Y | 390 | GLY | Peptide |
| 1 | 5Z | 231 | ARG | Peptide |
| 1 | 5Z | 345 | ASP | Peptide |
| 1 | 5Z | 376 | THR | Peptide |
| 1 | 5Z | 385 | TRP | Peptide |
| 1 | 5a | 30 | ASP | Peptide |
| 1 | 5a | 355 | SER | Peptide |
| 1 | 5b | 394 | THR | Peptide |
| 1 | 5c | 377 | ASN | Peptide |
| 1 | 5c | 424 | ASP | Peptide |
| 1 | 5c | 94 | GLY | Peptide |
| 1 | 5d | 155 | SER | Peptide |
| 1 | 5d | 156 | TRP | Peptide |
| 1 | 5d | 201 | ASP | Peptide |
| 1 | 5d | 355 | SER | Peptide |
| 1 | 5d | 440 | ASN | Peptide |
| 1 | 6A | 355 | SER | Peptide |
| 1 | 6A | 377 | ASN | Peptide |
| 1 | 6A | 378 | ALA | Peptide |
| 1 | 6A | 380 | ASP | Peptide |
| 1 | 6B | 155 | SER | Peptide |
| 1 | 6B | 156 | TRP | Peptide |
| 1 | 6B | 333 | SER | Peptide |
| 1 | 6B | 409 | ASP | Peptide |
| 1 | 6C | 201 | ASP | Peptide |
| 1 | 6C | 355 | SER | Peptide |
| 1 | 6C | 404 | VAL | Peptide |
| 1 | 6D | 118 | LYS | Peptide |
| 1 | 6D | 169 | ALA | Peptide |
| 1 | 6D | 7 | ASP | Peptide |
| 1 | 6F | 155 | SER | Peptide |
| 1 | 6F | 17 | SER | Peptide |
| 1 | 6F | 202 | GLU | Peptide |
| 1 | 6F | 355 | SER | Peptide |
| 1 | 6G | 355 | SER | Peptide |
| 1 | 6G | 377 | ASN | Peptide |
| 1 | 6G | 378 | ALA | Peptide |
| 1 | 6G | 380 | ASP | Peptide |
| 1 | 6H | 155 | SER | Peptide |

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| Mol | Chain | Res | Type | Group |
|------------|--------------|------------|-------------|--------------|
| 1 | 6H | 156 | TRP | Peptide |
| 1 | 6H | 333 | SER | Peptide |
| 1 | 6H | 409 | ASP | Peptide |
| 1 | 6I | 201 | ASP | Peptide |
| 1 | 6I | 355 | SER | Peptide |
| 1 | 6I | 404 | VAL | Peptide |
| 1 | 6J | 118 | LYS | Peptide |
| 1 | 6J | 169 | ALA | Peptide |
| 1 | 6J | 7 | ASP | Peptide |
| 1 | 6L | 155 | SER | Peptide |
| 1 | 6L | 17 | SER | Peptide |
| 1 | 6L | 202 | GLU | Peptide |
| 1 | 6L | 355 | SER | Peptide |
| 1 | 6M | 355 | SER | Peptide |
| 1 | 6M | 377 | ASN | Peptide |
| 1 | 6M | 378 | ALA | Peptide |
| 1 | 6M | 380 | ASP | Peptide |
| 1 | 6N | 155 | SER | Peptide |
| 1 | 6N | 156 | TRP | Peptide |
| 1 | 6N | 333 | SER | Peptide |
| 1 | 6N | 409 | ASP | Peptide |
| 1 | 6O | 201 | ASP | Peptide |
| 1 | 6O | 355 | SER | Peptide |
| 1 | 6O | 404 | VAL | Peptide |
| 1 | 6P | 118 | LYS | Peptide |
| 1 | 6P | 169 | ALA | Peptide |
| 1 | 6P | 7 | ASP | Peptide |
| 1 | 6R | 155 | SER | Peptide |
| 1 | 6R | 17 | SER | Peptide |
| 1 | 6R | 202 | GLU | Peptide |
| 1 | 6R | 355 | SER | Peptide |
| 1 | 6S | 355 | SER | Peptide |
| 1 | 6S | 377 | ASN | Peptide |
| 1 | 6S | 378 | ALA | Peptide |
| 1 | 6S | 380 | ASP | Peptide |
| 1 | 6T | 155 | SER | Peptide |
| 1 | 6T | 156 | TRP | Peptide |
| 1 | 6T | 333 | SER | Peptide |
| 1 | 6T | 409 | ASP | Peptide |
| 1 | 6U | 201 | ASP | Peptide |
| 1 | 6U | 355 | SER | Peptide |
| 1 | 6U | 404 | VAL | Peptide |

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| Mol | Chain | Res | Type | Group |
|------------|--------------|------------|-------------|--------------|
| 1 | 6V | 118 | LYS | Peptide |
| 1 | 6V | 169 | ALA | Peptide |
| 1 | 6V | 7 | ASP | Peptide |
| 1 | 6X | 155 | SER | Peptide |
| 1 | 6X | 17 | SER | Peptide |
| 1 | 6X | 202 | GLU | Peptide |
| 1 | 6X | 355 | SER | Peptide |
| 1 | 6Y | 355 | SER | Peptide |
| 1 | 6Y | 377 | ASN | Peptide |
| 1 | 6Y | 378 | ALA | Peptide |
| 1 | 6Y | 380 | ASP | Peptide |
| 1 | 6Z | 155 | SER | Peptide |
| 1 | 6Z | 156 | TRP | Peptide |
| 1 | 6Z | 333 | SER | Peptide |
| 1 | 6Z | 409 | ASP | Peptide |
| 1 | 6a | 201 | ASP | Peptide |
| 1 | 6a | 355 | SER | Peptide |
| 1 | 6a | 404 | VAL | Peptide |
| 1 | 6b | 118 | LYS | Peptide |
| 1 | 6b | 169 | ALA | Peptide |
| 1 | 6b | 7 | ASP | Peptide |
| 1 | 6d | 155 | SER | Peptide |
| 1 | 6d | 17 | SER | Peptide |
| 1 | 6d | 202 | GLU | Peptide |
| 1 | 6d | 355 | SER | Peptide |
| 1 | 7A | 118 | LYS | Peptide |
| 1 | 7B | 39 | ALA | Peptide |
| 1 | 7B | 8 | VAL | Peptide |
| 1 | 7C | 381 | HIS | Peptide |
| 1 | 7D | 334 | ARG | Peptide |
| 1 | 7D | 355 | SER | Peptide |
| 1 | 7F | 118 | LYS | Peptide |
| 1 | 7G | 39 | ALA | Peptide |
| 1 | 7G | 8 | VAL | Peptide |
| 1 | 7H | 381 | HIS | Peptide |
| 1 | 7I | 334 | ARG | Peptide |
| 1 | 7I | 355 | SER | Peptide |
| 1 | 7K | 118 | LYS | Peptide |
| 1 | 7L | 39 | ALA | Peptide |
| 1 | 7L | 8 | VAL | Peptide |
| 1 | 7M | 381 | HIS | Peptide |
| 1 | 7N | 334 | ARG | Peptide |

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| Mol | Chain | Res | Type | Group |
|------------|--------------|------------|-------------|--------------|
| 1 | 7N | 355 | SER | Peptide |
| 1 | 7P | 118 | LYS | Peptide |
| 1 | 7Q | 39 | ALA | Peptide |
| 1 | 7Q | 8 | VAL | Peptide |
| 1 | 7R | 381 | HIS | Peptide |
| 1 | 7S | 334 | ARG | Peptide |
| 1 | 7S | 355 | SER | Peptide |
| 1 | 7U | 118 | LYS | Peptide |
| 1 | 7V | 39 | ALA | Peptide |
| 1 | 7V | 8 | VAL | Peptide |
| 1 | 7W | 381 | HIS | Peptide |
| 1 | 7X | 334 | ARG | Peptide |
| 1 | 7X | 355 | SER | Peptide |
| 1 | 8A | 155 | SER | Peptide |
| 1 | 8A | 250 | ILE | Peptide |
| 1 | 8A | 251 | ILE | Peptide |
| 1 | 8A | 355 | SER | Peptide |
| 1 | 8D | 30 | ASP | Peptide |
| 1 | 8E | 153 | PHE | Peptide |
| 1 | 8E | 355 | SER | Peptide |
| 1 | 8E | 405 | SER | Peptide |
| 1 | 8G | 155 | SER | Peptide |
| 1 | 8G | 250 | ILE | Peptide |
| 1 | 8G | 251 | ILE | Peptide |
| 1 | 8G | 355 | SER | Peptide |
| 1 | 8J | 30 | ASP | Peptide |
| 1 | 8K | 153 | PHE | Peptide |
| 1 | 8K | 355 | SER | Peptide |
| 1 | 8K | 405 | SER | Peptide |
| 1 | 8M | 155 | SER | Peptide |
| 1 | 8M | 250 | ILE | Peptide |
| 1 | 8M | 251 | ILE | Peptide |
| 1 | 8M | 355 | SER | Peptide |
| 1 | 8P | 30 | ASP | Peptide |
| 1 | 8Q | 153 | PHE | Peptide |
| 1 | 8Q | 355 | SER | Peptide |
| 1 | 8Q | 405 | SER | Peptide |
| 1 | 8S | 155 | SER | Peptide |
| 1 | 8S | 250 | ILE | Peptide |
| 1 | 8S | 251 | ILE | Peptide |
| 1 | 8S | 355 | SER | Peptide |
| 1 | 8V | 30 | ASP | Peptide |

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| Mol | Chain | Res | Type | Group |
|-----|-------|-----|------|---------|
| 1 | 8W | 153 | PHE | Peptide |
| 1 | 8W | 355 | SER | Peptide |
| 1 | 8W | 405 | SER | Peptide |
| 1 | 8Y | 155 | SER | Peptide |
| 1 | 8Y | 250 | ILE | Peptide |
| 1 | 8Y | 251 | ILE | Peptide |
| 1 | 8Y | 355 | SER | Peptide |
| 1 | 8b | 30 | ASP | Peptide |
| 1 | 8c | 153 | PHE | Peptide |
| 1 | 8c | 355 | SER | Peptide |
| 1 | 8c | 405 | SER | Peptide |
| 1 | 9A | 333 | SER | Peptide |
| 1 | 9B | 333 | SER | Peptide |
| 1 | 9C | 333 | SER | Peptide |
| 1 | 9D | 333 | SER | Peptide |
| 1 | 9E | 333 | SER | Peptide |

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 PDB entries followed by that with respect to all EM entries.

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

| Mol | Chain | Analysed | Favoured | Allowed | Outliers | Percentiles | |
|-----|-------|---------------|-----------|----------|----------|-------------|-----|
| 1 | 1A | 431/448 (96%) | 401 (93%) | 30 (7%) | 0 | 100 | 100 |
| 1 | 1B | 443/448 (99%) | 400 (90%) | 41 (9%) | 2 (0%) | 29 | 67 |
| 1 | 1C | 443/448 (99%) | 402 (91%) | 40 (9%) | 1 (0%) | 47 | 79 |
| 1 | 1D | 443/448 (99%) | 398 (90%) | 43 (10%) | 2 (0%) | 29 | 67 |
| 1 | 1E | 433/448 (97%) | 406 (94%) | 27 (6%) | 0 | 100 | 100 |
| 1 | 1F | 436/448 (97%) | 399 (92%) | 35 (8%) | 2 (0%) | 29 | 67 |

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| Mol | Chain | Analysed | Favoured | Allowed | Outliers | Percentiles | |
|-----|-------|---------------|-----------|----------|----------|-------------|-----|
| 1 | 1G | 431/448 (96%) | 401 (93%) | 30 (7%) | 0 | 100 | 100 |
| 1 | 1H | 443/448 (99%) | 399 (90%) | 42 (10%) | 2 (0%) | 29 | 67 |
| 1 | 1I | 443/448 (99%) | 402 (91%) | 40 (9%) | 1 (0%) | 47 | 79 |
| 1 | 1J | 443/448 (99%) | 398 (90%) | 43 (10%) | 2 (0%) | 29 | 67 |
| 1 | 1K | 433/448 (97%) | 406 (94%) | 27 (6%) | 0 | 100 | 100 |
| 1 | 1L | 436/448 (97%) | 399 (92%) | 35 (8%) | 2 (0%) | 29 | 67 |
| 1 | 1M | 431/448 (96%) | 401 (93%) | 30 (7%) | 0 | 100 | 100 |
| 1 | 1N | 443/448 (99%) | 399 (90%) | 42 (10%) | 2 (0%) | 29 | 67 |
| 1 | 1O | 443/448 (99%) | 402 (91%) | 40 (9%) | 1 (0%) | 47 | 79 |
| 1 | 1P | 443/448 (99%) | 399 (90%) | 42 (10%) | 2 (0%) | 29 | 67 |
| 1 | 1Q | 433/448 (97%) | 406 (94%) | 27 (6%) | 0 | 100 | 100 |
| 1 | 1R | 436/448 (97%) | 400 (92%) | 34 (8%) | 2 (0%) | 29 | 67 |
| 1 | 1S | 431/448 (96%) | 401 (93%) | 30 (7%) | 0 | 100 | 100 |
| 1 | 1T | 443/448 (99%) | 400 (90%) | 41 (9%) | 2 (0%) | 29 | 67 |
| 1 | 1U | 443/448 (99%) | 401 (90%) | 41 (9%) | 1 (0%) | 47 | 79 |
| 1 | 1V | 443/448 (99%) | 398 (90%) | 43 (10%) | 2 (0%) | 29 | 67 |
| 1 | 1W | 433/448 (97%) | 406 (94%) | 27 (6%) | 0 | 100 | 100 |
| 1 | 1X | 436/448 (97%) | 400 (92%) | 34 (8%) | 2 (0%) | 29 | 67 |
| 1 | 1Y | 431/448 (96%) | 401 (93%) | 30 (7%) | 0 | 100 | 100 |
| 1 | 1Z | 443/448 (99%) | 400 (90%) | 41 (9%) | 2 (0%) | 29 | 67 |
| 1 | 1a | 443/448 (99%) | 401 (90%) | 41 (9%) | 1 (0%) | 47 | 79 |
| 1 | 1b | 443/448 (99%) | 398 (90%) | 43 (10%) | 2 (0%) | 29 | 67 |
| 1 | 1c | 433/448 (97%) | 406 (94%) | 27 (6%) | 0 | 100 | 100 |
| 1 | 1d | 436/448 (97%) | 399 (92%) | 35 (8%) | 2 (0%) | 29 | 67 |
| 1 | 2A | 436/448 (97%) | 411 (94%) | 23 (5%) | 2 (0%) | 29 | 67 |
| 1 | 2B | 443/448 (99%) | 410 (93%) | 30 (7%) | 3 (1%) | 22 | 61 |
| 1 | 2C | 443/448 (99%) | 414 (94%) | 28 (6%) | 1 (0%) | 47 | 79 |
| 1 | 2D | 443/448 (99%) | 407 (92%) | 36 (8%) | 0 | 100 | 100 |
| 1 | 2E | 443/448 (99%) | 402 (91%) | 38 (9%) | 3 (1%) | 22 | 61 |
| 1 | 2F | 436/448 (97%) | 411 (94%) | 23 (5%) | 2 (0%) | 29 | 67 |
| 1 | 2G | 443/448 (99%) | 409 (92%) | 31 (7%) | 3 (1%) | 22 | 61 |

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| Mol | Chain | Analysed | Favoured | Allowed | Outliers | Percentiles | |
|-----|-------|---------------|-----------|----------|----------|-------------|-----|
| 1 | 2H | 443/448 (99%) | 414 (94%) | 28 (6%) | 1 (0%) | 47 | 79 |
| 1 | 2I | 443/448 (99%) | 407 (92%) | 35 (8%) | 1 (0%) | 47 | 79 |
| 1 | 2J | 443/448 (99%) | 402 (91%) | 38 (9%) | 3 (1%) | 22 | 61 |
| 1 | 2K | 436/448 (97%) | 411 (94%) | 23 (5%) | 2 (0%) | 29 | 67 |
| 1 | 2L | 443/448 (99%) | 410 (93%) | 30 (7%) | 3 (1%) | 22 | 61 |
| 1 | 2M | 443/448 (99%) | 414 (94%) | 28 (6%) | 1 (0%) | 47 | 79 |
| 1 | 2N | 443/448 (99%) | 407 (92%) | 36 (8%) | 0 | 100 | 100 |
| 1 | 2O | 443/448 (99%) | 402 (91%) | 38 (9%) | 3 (1%) | 22 | 61 |
| 1 | 2P | 436/448 (97%) | 411 (94%) | 23 (5%) | 2 (0%) | 29 | 67 |
| 1 | 2Q | 443/448 (99%) | 410 (93%) | 30 (7%) | 3 (1%) | 22 | 61 |
| 1 | 2R | 443/448 (99%) | 414 (94%) | 28 (6%) | 1 (0%) | 47 | 79 |
| 1 | 2S | 443/448 (99%) | 407 (92%) | 36 (8%) | 0 | 100 | 100 |
| 1 | 2T | 443/448 (99%) | 402 (91%) | 38 (9%) | 3 (1%) | 22 | 61 |
| 1 | 2U | 436/448 (97%) | 410 (94%) | 24 (6%) | 2 (0%) | 29 | 67 |
| 1 | 2V | 443/448 (99%) | 410 (93%) | 30 (7%) | 3 (1%) | 22 | 61 |
| 1 | 2W | 443/448 (99%) | 414 (94%) | 28 (6%) | 1 (0%) | 47 | 79 |
| 1 | 2X | 443/448 (99%) | 407 (92%) | 36 (8%) | 0 | 100 | 100 |
| 1 | 2Y | 443/448 (99%) | 402 (91%) | 38 (9%) | 3 (1%) | 22 | 61 |
| 1 | 3A | 433/448 (97%) | 389 (90%) | 42 (10%) | 2 (0%) | 29 | 67 |
| 1 | 3B | 433/448 (97%) | 393 (91%) | 39 (9%) | 1 (0%) | 47 | 79 |
| 1 | 3C | 443/448 (99%) | 407 (92%) | 35 (8%) | 1 (0%) | 47 | 79 |
| 1 | 3D | 443/448 (99%) | 398 (90%) | 40 (9%) | 5 (1%) | 14 | 51 |
| 1 | 3E | 443/448 (99%) | 411 (93%) | 32 (7%) | 0 | 100 | 100 |
| 1 | 3F | 443/448 (99%) | 403 (91%) | 40 (9%) | 0 | 100 | 100 |
| 1 | 3G | 433/448 (97%) | 389 (90%) | 42 (10%) | 2 (0%) | 29 | 67 |
| 1 | 3H | 433/448 (97%) | 393 (91%) | 39 (9%) | 1 (0%) | 47 | 79 |
| 1 | 3I | 443/448 (99%) | 407 (92%) | 35 (8%) | 1 (0%) | 47 | 79 |
| 1 | 3J | 443/448 (99%) | 398 (90%) | 40 (9%) | 5 (1%) | 14 | 51 |
| 1 | 3K | 443/448 (99%) | 411 (93%) | 32 (7%) | 0 | 100 | 100 |
| 1 | 3L | 443/448 (99%) | 403 (91%) | 40 (9%) | 0 | 100 | 100 |
| 1 | 3M | 433/448 (97%) | 389 (90%) | 42 (10%) | 2 (0%) | 29 | 67 |

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| Mol | Chain | Analysed | Favoured | Allowed | Outliers | Percentiles | |
|-----|-------|---------------|-----------|----------|----------|-------------|-----|
| 1 | 3N | 433/448 (97%) | 393 (91%) | 39 (9%) | 1 (0%) | 47 | 79 |
| 1 | 3O | 443/448 (99%) | 407 (92%) | 35 (8%) | 1 (0%) | 47 | 79 |
| 1 | 3P | 443/448 (99%) | 398 (90%) | 40 (9%) | 5 (1%) | 14 | 51 |
| 1 | 3Q | 443/448 (99%) | 411 (93%) | 32 (7%) | 0 | 100 | 100 |
| 1 | 3R | 443/448 (99%) | 403 (91%) | 40 (9%) | 0 | 100 | 100 |
| 1 | 3S | 433/448 (97%) | 389 (90%) | 42 (10%) | 2 (0%) | 29 | 67 |
| 1 | 3T | 433/448 (97%) | 393 (91%) | 39 (9%) | 1 (0%) | 47 | 79 |
| 1 | 3U | 443/448 (99%) | 407 (92%) | 35 (8%) | 1 (0%) | 47 | 79 |
| 1 | 3V | 443/448 (99%) | 398 (90%) | 40 (9%) | 5 (1%) | 14 | 51 |
| 1 | 3W | 443/448 (99%) | 411 (93%) | 32 (7%) | 0 | 100 | 100 |
| 1 | 3X | 443/448 (99%) | 403 (91%) | 40 (9%) | 0 | 100 | 100 |
| 1 | 3Y | 433/448 (97%) | 389 (90%) | 42 (10%) | 2 (0%) | 29 | 67 |
| 1 | 3Z | 433/448 (97%) | 393 (91%) | 39 (9%) | 1 (0%) | 47 | 79 |
| 1 | 3a | 443/448 (99%) | 407 (92%) | 35 (8%) | 1 (0%) | 47 | 79 |
| 1 | 3b | 443/448 (99%) | 398 (90%) | 40 (9%) | 5 (1%) | 14 | 51 |
| 1 | 3c | 443/448 (99%) | 411 (93%) | 32 (7%) | 0 | 100 | 100 |
| 1 | 3d | 443/448 (99%) | 403 (91%) | 40 (9%) | 0 | 100 | 100 |
| 1 | 4A | 433/448 (97%) | 400 (92%) | 33 (8%) | 0 | 100 | 100 |
| 1 | 4B | 433/448 (97%) | 379 (88%) | 48 (11%) | 6 (1%) | 11 | 46 |
| 1 | 4C | 433/448 (97%) | 397 (92%) | 34 (8%) | 2 (0%) | 29 | 67 |
| 1 | 4D | 433/448 (97%) | 395 (91%) | 38 (9%) | 0 | 100 | 100 |
| 1 | 4E | 443/448 (99%) | 404 (91%) | 39 (9%) | 0 | 100 | 100 |
| 1 | 4F | 443/448 (99%) | 383 (86%) | 60 (14%) | 0 | 100 | 100 |
| 1 | 4G | 433/448 (97%) | 401 (93%) | 32 (7%) | 0 | 100 | 100 |
| 1 | 4H | 433/448 (97%) | 379 (88%) | 48 (11%) | 6 (1%) | 11 | 46 |
| 1 | 4I | 433/448 (97%) | 397 (92%) | 34 (8%) | 2 (0%) | 29 | 67 |
| 1 | 4J | 433/448 (97%) | 395 (91%) | 38 (9%) | 0 | 100 | 100 |
| 1 | 4K | 443/448 (99%) | 404 (91%) | 39 (9%) | 0 | 100 | 100 |
| 1 | 4L | 443/448 (99%) | 383 (86%) | 60 (14%) | 0 | 100 | 100 |
| 1 | 4M | 433/448 (97%) | 401 (93%) | 32 (7%) | 0 | 100 | 100 |
| 1 | 4N | 433/448 (97%) | 379 (88%) | 48 (11%) | 6 (1%) | 11 | 46 |

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| Mol | Chain | Analysed | Favoured | Allowed | Outliers | Percentiles | |
|-----|-------|---------------|-----------|----------|----------|-------------|-----|
| 1 | 4O | 433/448 (97%) | 397 (92%) | 34 (8%) | 2 (0%) | 29 | 67 |
| 1 | 4P | 433/448 (97%) | 395 (91%) | 38 (9%) | 0 | 100 | 100 |
| 1 | 4Q | 443/448 (99%) | 404 (91%) | 39 (9%) | 0 | 100 | 100 |
| 1 | 4R | 443/448 (99%) | 383 (86%) | 60 (14%) | 0 | 100 | 100 |
| 1 | 4S | 433/448 (97%) | 401 (93%) | 32 (7%) | 0 | 100 | 100 |
| 1 | 4T | 433/448 (97%) | 379 (88%) | 48 (11%) | 6 (1%) | 11 | 46 |
| 1 | 4U | 433/448 (97%) | 397 (92%) | 34 (8%) | 2 (0%) | 29 | 67 |
| 1 | 4V | 433/448 (97%) | 395 (91%) | 38 (9%) | 0 | 100 | 100 |
| 1 | 4W | 443/448 (99%) | 404 (91%) | 39 (9%) | 0 | 100 | 100 |
| 1 | 4X | 443/448 (99%) | 383 (86%) | 60 (14%) | 0 | 100 | 100 |
| 1 | 4Y | 433/448 (97%) | 400 (92%) | 33 (8%) | 0 | 100 | 100 |
| 1 | 4Z | 433/448 (97%) | 378 (87%) | 49 (11%) | 6 (1%) | 11 | 46 |
| 1 | 4a | 433/448 (97%) | 397 (92%) | 34 (8%) | 2 (0%) | 29 | 67 |
| 1 | 4b | 433/448 (97%) | 395 (91%) | 38 (9%) | 0 | 100 | 100 |
| 1 | 4c | 443/448 (99%) | 404 (91%) | 39 (9%) | 0 | 100 | 100 |
| 1 | 4d | 443/448 (99%) | 383 (86%) | 60 (14%) | 0 | 100 | 100 |
| 1 | 5A | 433/448 (97%) | 399 (92%) | 34 (8%) | 0 | 100 | 100 |
| 1 | 5B | 433/448 (97%) | 371 (86%) | 60 (14%) | 2 (0%) | 29 | 67 |
| 1 | 5C | 433/448 (97%) | 385 (89%) | 45 (10%) | 3 (1%) | 22 | 61 |
| 1 | 5D | 433/448 (97%) | 394 (91%) | 38 (9%) | 1 (0%) | 47 | 79 |
| 1 | 5E | 443/448 (99%) | 396 (89%) | 46 (10%) | 1 (0%) | 47 | 79 |
| 1 | 5F | 443/448 (99%) | 396 (89%) | 43 (10%) | 4 (1%) | 17 | 56 |
| 1 | 5G | 433/448 (97%) | 398 (92%) | 35 (8%) | 0 | 100 | 100 |
| 1 | 5H | 433/448 (97%) | 371 (86%) | 60 (14%) | 2 (0%) | 29 | 67 |
| 1 | 5I | 433/448 (97%) | 385 (89%) | 45 (10%) | 3 (1%) | 22 | 61 |
| 1 | 5J | 433/448 (97%) | 394 (91%) | 38 (9%) | 1 (0%) | 47 | 79 |
| 1 | 5K | 443/448 (99%) | 396 (89%) | 46 (10%) | 1 (0%) | 47 | 79 |
| 1 | 5L | 443/448 (99%) | 396 (89%) | 43 (10%) | 4 (1%) | 17 | 56 |
| 1 | 5M | 433/448 (97%) | 398 (92%) | 35 (8%) | 0 | 100 | 100 |
| 1 | 5N | 433/448 (97%) | 371 (86%) | 60 (14%) | 2 (0%) | 29 | 67 |
| 1 | 5O | 433/448 (97%) | 385 (89%) | 45 (10%) | 3 (1%) | 22 | 61 |

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| Mol | Chain | Analysed | Favoured | Allowed | Outliers | Percentiles | |
|-----|-------|---------------|-----------|----------|----------|-------------|-----|
| 1 | 5P | 433/448 (97%) | 394 (91%) | 38 (9%) | 1 (0%) | 47 | 79 |
| 1 | 5Q | 443/448 (99%) | 396 (89%) | 46 (10%) | 1 (0%) | 47 | 79 |
| 1 | 5R | 443/448 (99%) | 396 (89%) | 43 (10%) | 4 (1%) | 17 | 56 |
| 1 | 5S | 433/448 (97%) | 399 (92%) | 34 (8%) | 0 | 100 | 100 |
| 1 | 5T | 433/448 (97%) | 371 (86%) | 60 (14%) | 2 (0%) | 29 | 67 |
| 1 | 5U | 433/448 (97%) | 385 (89%) | 45 (10%) | 3 (1%) | 22 | 61 |
| 1 | 5V | 433/448 (97%) | 394 (91%) | 38 (9%) | 1 (0%) | 47 | 79 |
| 1 | 5W | 443/448 (99%) | 396 (89%) | 46 (10%) | 1 (0%) | 47 | 79 |
| 1 | 5X | 443/448 (99%) | 396 (89%) | 43 (10%) | 4 (1%) | 17 | 56 |
| 1 | 5Y | 433/448 (97%) | 399 (92%) | 34 (8%) | 0 | 100 | 100 |
| 1 | 5Z | 433/448 (97%) | 371 (86%) | 60 (14%) | 2 (0%) | 29 | 67 |
| 1 | 5a | 433/448 (97%) | 385 (89%) | 45 (10%) | 3 (1%) | 22 | 61 |
| 1 | 5b | 433/448 (97%) | 394 (91%) | 38 (9%) | 1 (0%) | 47 | 79 |
| 1 | 5c | 443/448 (99%) | 396 (89%) | 46 (10%) | 1 (0%) | 47 | 79 |
| 1 | 5d | 443/448 (99%) | 396 (89%) | 43 (10%) | 4 (1%) | 17 | 56 |
| 1 | 6A | 443/448 (99%) | 408 (92%) | 29 (6%) | 6 (1%) | 11 | 46 |
| 1 | 6B | 443/448 (99%) | 408 (92%) | 32 (7%) | 3 (1%) | 22 | 61 |
| 1 | 6C | 433/448 (97%) | 391 (90%) | 39 (9%) | 3 (1%) | 22 | 61 |
| 1 | 6D | 433/448 (97%) | 391 (90%) | 42 (10%) | 0 | 100 | 100 |
| 1 | 6E | 443/448 (99%) | 404 (91%) | 39 (9%) | 0 | 100 | 100 |
| 1 | 6F | 443/448 (99%) | 399 (90%) | 43 (10%) | 1 (0%) | 47 | 79 |
| 1 | 6G | 443/448 (99%) | 408 (92%) | 29 (6%) | 6 (1%) | 11 | 46 |
| 1 | 6H | 443/448 (99%) | 407 (92%) | 33 (7%) | 3 (1%) | 22 | 61 |
| 1 | 6I | 433/448 (97%) | 391 (90%) | 39 (9%) | 3 (1%) | 22 | 61 |
| 1 | 6J | 433/448 (97%) | 391 (90%) | 42 (10%) | 0 | 100 | 100 |
| 1 | 6K | 443/448 (99%) | 404 (91%) | 39 (9%) | 0 | 100 | 100 |
| 1 | 6L | 443/448 (99%) | 399 (90%) | 43 (10%) | 1 (0%) | 47 | 79 |
| 1 | 6M | 443/448 (99%) | 408 (92%) | 29 (6%) | 6 (1%) | 11 | 46 |
| 1 | 6N | 443/448 (99%) | 407 (92%) | 33 (7%) | 3 (1%) | 22 | 61 |
| 1 | 6O | 433/448 (97%) | 391 (90%) | 39 (9%) | 3 (1%) | 22 | 61 |
| 1 | 6P | 433/448 (97%) | 391 (90%) | 42 (10%) | 0 | 100 | 100 |

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| Mol | Chain | Analysed | Favoured | Allowed | Outliers | Percentiles | |
|-----|-------|---------------|-----------|----------|----------|-------------|-----|
| 1 | 6Q | 443/448 (99%) | 404 (91%) | 39 (9%) | 0 | 100 | 100 |
| 1 | 6R | 443/448 (99%) | 399 (90%) | 43 (10%) | 1 (0%) | 47 | 79 |
| 1 | 6S | 443/448 (99%) | 408 (92%) | 29 (6%) | 6 (1%) | 11 | 46 |
| 1 | 6T | 443/448 (99%) | 408 (92%) | 32 (7%) | 3 (1%) | 22 | 61 |
| 1 | 6U | 433/448 (97%) | 391 (90%) | 39 (9%) | 3 (1%) | 22 | 61 |
| 1 | 6V | 433/448 (97%) | 391 (90%) | 42 (10%) | 0 | 100 | 100 |
| 1 | 6W | 443/448 (99%) | 404 (91%) | 39 (9%) | 0 | 100 | 100 |
| 1 | 6X | 443/448 (99%) | 398 (90%) | 44 (10%) | 1 (0%) | 47 | 79 |
| 1 | 6Y | 443/448 (99%) | 408 (92%) | 29 (6%) | 6 (1%) | 11 | 46 |
| 1 | 6Z | 443/448 (99%) | 408 (92%) | 32 (7%) | 3 (1%) | 22 | 61 |
| 1 | 6a | 433/448 (97%) | 391 (90%) | 39 (9%) | 3 (1%) | 22 | 61 |
| 1 | 6b | 433/448 (97%) | 391 (90%) | 42 (10%) | 0 | 100 | 100 |
| 1 | 6c | 443/448 (99%) | 404 (91%) | 39 (9%) | 0 | 100 | 100 |
| 1 | 6d | 443/448 (99%) | 399 (90%) | 43 (10%) | 1 (0%) | 47 | 79 |
| 1 | 7A | 443/448 (99%) | 413 (93%) | 29 (6%) | 1 (0%) | 47 | 79 |
| 1 | 7B | 443/448 (99%) | 409 (92%) | 33 (7%) | 1 (0%) | 47 | 79 |
| 1 | 7C | 443/448 (99%) | 408 (92%) | 33 (7%) | 2 (0%) | 29 | 67 |
| 1 | 7D | 443/448 (99%) | 407 (92%) | 36 (8%) | 0 | 100 | 100 |
| 1 | 7E | 443/448 (99%) | 405 (91%) | 37 (8%) | 1 (0%) | 47 | 79 |
| 1 | 7F | 443/448 (99%) | 413 (93%) | 29 (6%) | 1 (0%) | 47 | 79 |
| 1 | 7G | 443/448 (99%) | 409 (92%) | 33 (7%) | 1 (0%) | 47 | 79 |
| 1 | 7H | 443/448 (99%) | 408 (92%) | 33 (7%) | 2 (0%) | 29 | 67 |
| 1 | 7I | 443/448 (99%) | 407 (92%) | 36 (8%) | 0 | 100 | 100 |
| 1 | 7J | 443/448 (99%) | 405 (91%) | 37 (8%) | 1 (0%) | 47 | 79 |
| 1 | 7K | 443/448 (99%) | 413 (93%) | 29 (6%) | 1 (0%) | 47 | 79 |
| 1 | 7L | 443/448 (99%) | 409 (92%) | 33 (7%) | 1 (0%) | 47 | 79 |
| 1 | 7M | 443/448 (99%) | 408 (92%) | 33 (7%) | 2 (0%) | 29 | 67 |
| 1 | 7N | 443/448 (99%) | 407 (92%) | 36 (8%) | 0 | 100 | 100 |
| 1 | 7O | 443/448 (99%) | 405 (91%) | 37 (8%) | 1 (0%) | 47 | 79 |
| 1 | 7P | 443/448 (99%) | 413 (93%) | 29 (6%) | 1 (0%) | 47 | 79 |
| 1 | 7Q | 443/448 (99%) | 409 (92%) | 33 (7%) | 1 (0%) | 47 | 79 |

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| Mol | Chain | Analysed | Favoured | Allowed | Outliers | Percentiles | |
|-----|-------|---------------|-----------|---------|----------|-------------|-----|
| 1 | 7R | 443/448 (99%) | 408 (92%) | 33 (7%) | 2 (0%) | 29 | 67 |
| 1 | 7S | 443/448 (99%) | 407 (92%) | 36 (8%) | 0 | 100 | 100 |
| 1 | 7T | 443/448 (99%) | 405 (91%) | 37 (8%) | 1 (0%) | 47 | 79 |
| 1 | 7U | 443/448 (99%) | 413 (93%) | 29 (6%) | 1 (0%) | 47 | 79 |
| 1 | 7V | 443/448 (99%) | 409 (92%) | 33 (7%) | 1 (0%) | 47 | 79 |
| 1 | 7W | 443/448 (99%) | 408 (92%) | 33 (7%) | 2 (0%) | 29 | 67 |
| 1 | 7X | 443/448 (99%) | 407 (92%) | 36 (8%) | 0 | 100 | 100 |
| 1 | 7Y | 443/448 (99%) | 405 (91%) | 37 (8%) | 1 (0%) | 47 | 79 |
| 1 | 8A | 443/448 (99%) | 407 (92%) | 31 (7%) | 5 (1%) | 14 | 51 |
| 1 | 8B | 443/448 (99%) | 413 (93%) | 30 (7%) | 0 | 100 | 100 |
| 1 | 8C | 443/448 (99%) | 402 (91%) | 41 (9%) | 0 | 100 | 100 |
| 1 | 8D | 443/448 (99%) | 423 (96%) | 20 (4%) | 0 | 100 | 100 |
| 1 | 8E | 443/448 (99%) | 413 (93%) | 28 (6%) | 2 (0%) | 29 | 67 |
| 1 | 8F | 443/448 (99%) | 409 (92%) | 34 (8%) | 0 | 100 | 100 |
| 1 | 8G | 443/448 (99%) | 407 (92%) | 31 (7%) | 5 (1%) | 14 | 51 |
| 1 | 8H | 443/448 (99%) | 413 (93%) | 30 (7%) | 0 | 100 | 100 |
| 1 | 8I | 443/448 (99%) | 402 (91%) | 41 (9%) | 0 | 100 | 100 |
| 1 | 8J | 443/448 (99%) | 423 (96%) | 20 (4%) | 0 | 100 | 100 |
| 1 | 8K | 443/448 (99%) | 414 (94%) | 27 (6%) | 2 (0%) | 29 | 67 |
| 1 | 8L | 443/448 (99%) | 409 (92%) | 34 (8%) | 0 | 100 | 100 |
| 1 | 8M | 443/448 (99%) | 407 (92%) | 31 (7%) | 5 (1%) | 14 | 51 |
| 1 | 8N | 443/448 (99%) | 414 (94%) | 29 (6%) | 0 | 100 | 100 |
| 1 | 8O | 443/448 (99%) | 402 (91%) | 41 (9%) | 0 | 100 | 100 |
| 1 | 8P | 443/448 (99%) | 423 (96%) | 20 (4%) | 0 | 100 | 100 |
| 1 | 8Q | 443/448 (99%) | 413 (93%) | 28 (6%) | 2 (0%) | 29 | 67 |
| 1 | 8R | 443/448 (99%) | 409 (92%) | 34 (8%) | 0 | 100 | 100 |
| 1 | 8S | 443/448 (99%) | 407 (92%) | 31 (7%) | 5 (1%) | 14 | 51 |
| 1 | 8T | 443/448 (99%) | 413 (93%) | 30 (7%) | 0 | 100 | 100 |
| 1 | 8U | 443/448 (99%) | 402 (91%) | 41 (9%) | 0 | 100 | 100 |
| 1 | 8V | 443/448 (99%) | 423 (96%) | 20 (4%) | 0 | 100 | 100 |
| 1 | 8W | 443/448 (99%) | 414 (94%) | 27 (6%) | 2 (0%) | 29 | 67 |

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| Mol | Chain | Analysed | Favoured | Allowed | Outliers | Percentiles | |
|-----|-------|----------------|-----------|---------|----------|-------------|-----|
| 1 | 8X | 443/448 (99%) | 409 (92%) | 34 (8%) | 0 | 100 | 100 |
| 1 | 8Y | 443/448 (99%) | 407 (92%) | 31 (7%) | 5 (1%) | 14 | 51 |
| 1 | 8Z | 443/448 (99%) | 413 (93%) | 30 (7%) | 0 | 100 | 100 |
| 1 | 8a | 443/448 (99%) | 402 (91%) | 41 (9%) | 0 | 100 | 100 |
| 1 | 8b | 443/448 (99%) | 423 (96%) | 20 (4%) | 0 | 100 | 100 |
| 1 | 8c | 443/448 (99%) | 414 (94%) | 27 (6%) | 2 (0%) | 29 | 67 |
| 1 | 8d | 443/448 (99%) | 409 (92%) | 34 (8%) | 0 | 100 | 100 |
| 1 | 9A | 443/448 (99%) | 416 (94%) | 27 (6%) | 0 | 100 | 100 |
| 1 | 9B | 443/448 (99%) | 416 (94%) | 27 (6%) | 0 | 100 | 100 |
| 1 | 9C | 443/448 (99%) | 416 (94%) | 27 (6%) | 0 | 100 | 100 |
| 1 | 9D | 443/448 (99%) | 416 (94%) | 27 (6%) | 0 | 100 | 100 |
| 1 | 9E | 443/448 (99%) | 416 (94%) | 27 (6%) | 0 | 100 | 100 |
| 2 | 1e | 286/281 (102%) | 271 (95%) | 9 (3%) | 6 (2%) | 7 | 37 |
| 2 | 1f | 285/281 (101%) | 268 (94%) | 12 (4%) | 5 (2%) | 8 | 41 |
| 2 | 1g | 286/281 (102%) | 271 (95%) | 9 (3%) | 6 (2%) | 7 | 37 |
| 2 | 1h | 285/281 (101%) | 268 (94%) | 12 (4%) | 5 (2%) | 8 | 41 |
| 2 | 1i | 286/281 (102%) | 271 (95%) | 9 (3%) | 6 (2%) | 7 | 37 |
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| 2 | 1p | 285/281 (101%) | 268 (94%) | 12 (4%) | 5 (2%) | 8 | 41 |
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| 2 | 1r | 285/281 (101%) | 268 (94%) | 12 (4%) | 5 (2%) | 8 | 41 |
| 2 | 1s | 286/281 (102%) | 271 (95%) | 9 (3%) | 6 (2%) | 7 | 37 |
| 2 | 1t | 285/281 (101%) | 268 (94%) | 12 (4%) | 5 (2%) | 8 | 41 |
| 2 | 1u | 286/281 (102%) | 271 (95%) | 9 (3%) | 6 (2%) | 7 | 37 |
| 2 | 1v | 285/281 (101%) | 268 (94%) | 12 (4%) | 5 (2%) | 8 | 41 |
| 2 | 1w | 286/281 (102%) | 271 (95%) | 9 (3%) | 6 (2%) | 7 | 37 |

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| Mol | Chain | Analysed | Favoured | Allowed | Outliers | Percentiles | |
|-----|-------|----------------|-----------|---------|----------|-------------|----|
| 2 | 1x | 285/281 (101%) | 268 (94%) | 12 (4%) | 5 (2%) | 8 | 41 |
| 2 | 2Z | 286/281 (102%) | 267 (93%) | 16 (6%) | 3 (1%) | 15 | 54 |
| 2 | 2a | 286/281 (102%) | 267 (93%) | 16 (6%) | 3 (1%) | 15 | 54 |
| 2 | 2b | 286/281 (102%) | 267 (93%) | 16 (6%) | 3 (1%) | 15 | 54 |
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| 2 | 2h | 286/281 (102%) | 267 (93%) | 16 (6%) | 3 (1%) | 15 | 54 |
| 2 | 2i | 286/281 (102%) | 267 (93%) | 16 (6%) | 3 (1%) | 15 | 54 |
| 2 | 2j | 286/281 (102%) | 267 (93%) | 16 (6%) | 3 (1%) | 15 | 54 |
| 2 | 2k | 286/281 (102%) | 267 (93%) | 16 (6%) | 3 (1%) | 15 | 54 |
| 2 | 2l | 286/281 (102%) | 267 (93%) | 16 (6%) | 3 (1%) | 15 | 54 |
| 2 | 2m | 286/281 (102%) | 267 (93%) | 16 (6%) | 3 (1%) | 15 | 54 |
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| 2 | 2u | 286/281 (102%) | 267 (93%) | 16 (6%) | 3 (1%) | 15 | 54 |
| 2 | 2v | 286/281 (102%) | 267 (93%) | 16 (6%) | 3 (1%) | 15 | 54 |
| 2 | 2w | 286/281 (102%) | 267 (93%) | 16 (6%) | 3 (1%) | 15 | 54 |
| 2 | 2x | 286/281 (102%) | 267 (93%) | 16 (6%) | 3 (1%) | 15 | 54 |
| 2 | 3e | 285/281 (101%) | 268 (94%) | 12 (4%) | 5 (2%) | 8 | 41 |
| 2 | 3f | 286/281 (102%) | 271 (95%) | 9 (3%) | 6 (2%) | 7 | 37 |
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| 2 | 3h | 286/281 (102%) | 271 (95%) | 9 (3%) | 6 (2%) | 7 | 37 |
| 2 | 3i | 285/281 (101%) | 268 (94%) | 12 (4%) | 5 (2%) | 8 | 41 |

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| Mol | Chain | Analysed | Favoured | Allowed | Outliers | Percentiles | |
|-----|-------|----------------|-----------|---------|----------|-------------|----|
| 2 | 3j | 286/281 (102%) | 271 (95%) | 9 (3%) | 6 (2%) | 7 | 37 |
| 2 | 3k | 285/281 (101%) | 268 (94%) | 12 (4%) | 5 (2%) | 8 | 41 |
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| Mol | Chain | Analysed | Favoured | Allowed | Outliers | Percentiles | |
|-----|-------|----------------|-----------|---------|----------|-------------|----|
| 2 | 5k | 286/281 (102%) | 271 (95%) | 9 (3%) | 6 (2%) | 7 | 37 |
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| 2 | 6h | 286/281 (102%) | 271 (95%) | 9 (3%) | 6 (2%) | 7 | 37 |
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| 2 | 7e | 286/281 (102%) | 267 (93%) | 16 (6%) | 3 (1%) | 15 | 54 |
| 2 | 7f | 286/281 (102%) | 267 (93%) | 16 (6%) | 3 (1%) | 15 | 54 |

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| Mol | Chain | Analysed | Favoured | Allowed | Outliers | Percentiles | |
|-----|-------|----------------|-----------|---------|----------|-------------|----|
| 2 | 7g | 286/281 (102%) | 267 (93%) | 16 (6%) | 3 (1%) | 15 | 54 |
| 2 | 7h | 286/281 (102%) | 267 (93%) | 16 (6%) | 3 (1%) | 15 | 54 |
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| Mol | Chain | Analysed | Favoured | Allowed | Outliers | Percentiles | |
|-----|-------|---------------------|--------------|------------|-----------|-------------|----|
| 2 | 8r | 286/281 (102%) | 271 (95%) | 9 (3%) | 6 (2%) | 7 | 37 |
| 2 | 8s | 286/281 (102%) | 271 (95%) | 9 (3%) | 6 (2%) | 7 | 37 |
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| 2 | 9R | 285/281 (101%) | 268 (94%) | 12 (4%) | 5 (2%) | 8 | 41 |
| All | All | 150460/151645 (99%) | 138708 (92%) | 10636 (7%) | 1116 (1%) | 26 | 61 |

All (1116) Ramachandran outliers are listed below:

| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1 | 1B | 7 | ASP |
| 1 | 1F | 356 | PRO |
| 1 | 2A | 276 | LEU |
| 1 | 2B | 356 | PRO |
| 1 | 3B | 355 | SER |
| 1 | 3D | 21 | VAL |
| 1 | 5B | 386 | SER |

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| Mol | Chain | Res | Type |
|------------|--------------|------------|-------------|
| 1 | 6A | 356 | PRO |
| 1 | 6A | 378 | ALA |
| 1 | 6A | 379 | LYS |
| 1 | 6A | 381 | HIS |
| 1 | 1H | 7 | ASP |
| 1 | 1L | 356 | PRO |
| 1 | 2F | 276 | LEU |
| 1 | 2G | 356 | PRO |
| 1 | 3H | 355 | SER |
| 1 | 3J | 21 | VAL |
| 1 | 5H | 386 | SER |
| 1 | 6G | 356 | PRO |
| 1 | 6G | 378 | ALA |
| 1 | 6G | 379 | LYS |
| 1 | 6G | 381 | HIS |
| 1 | 1N | 7 | ASP |
| 1 | 1R | 356 | PRO |
| 1 | 2K | 276 | LEU |
| 1 | 2L | 356 | PRO |
| 1 | 3N | 355 | SER |
| 1 | 3P | 21 | VAL |
| 1 | 5N | 386 | SER |
| 1 | 6M | 356 | PRO |
| 1 | 6M | 378 | ALA |
| 1 | 6M | 379 | LYS |
| 1 | 6M | 381 | HIS |
| 1 | 1T | 7 | ASP |
| 1 | 1X | 356 | PRO |
| 1 | 2P | 276 | LEU |
| 1 | 2Q | 356 | PRO |
| 1 | 3T | 355 | SER |
| 1 | 3V | 21 | VAL |
| 1 | 5T | 386 | SER |
| 1 | 6S | 356 | PRO |
| 1 | 6S | 378 | ALA |
| 1 | 6S | 379 | LYS |
| 1 | 6S | 381 | HIS |
| 1 | 1Z | 7 | ASP |
| 1 | 1d | 356 | PRO |
| 1 | 2U | 276 | LEU |
| 1 | 2V | 356 | PRO |
| 1 | 3Z | 355 | SER |

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| Mol | Chain | Res | Type |
|------------|--------------|------------|-------------|
| 1 | 3b | 21 | VAL |
| 1 | 5Z | 386 | SER |
| 1 | 6Y | 356 | PRO |
| 1 | 6Y | 378 | ALA |
| 1 | 6Y | 379 | LYS |
| 1 | 6Y | 381 | HIS |
| 2 | 1e | 112 | ILE |
| 2 | 1g | 112 | ILE |
| 2 | 3f | 112 | ILE |
| 2 | 3h | 112 | ILE |
| 2 | 4e | 112 | ILE |
| 2 | 5e | 112 | ILE |
| 2 | 6f | 112 | ILE |
| 2 | 6h | 112 | ILE |
| 2 | 8f | 112 | ILE |
| 2 | 8g | 112 | ILE |
| 2 | 8i | 112 | ILE |
| 2 | 1i | 112 | ILE |
| 2 | 1k | 112 | ILE |
| 2 | 3j | 112 | ILE |
| 2 | 3l | 112 | ILE |
| 2 | 4g | 112 | ILE |
| 2 | 5g | 112 | ILE |
| 2 | 6j | 112 | ILE |
| 2 | 6l | 112 | ILE |
| 2 | 8l | 112 | ILE |
| 2 | 8m | 112 | ILE |
| 2 | 8o | 112 | ILE |
| 2 | 1m | 112 | ILE |
| 2 | 1o | 112 | ILE |
| 2 | 3n | 112 | ILE |
| 2 | 3p | 112 | ILE |
| 2 | 4i | 112 | ILE |
| 2 | 5i | 112 | ILE |
| 2 | 6n | 112 | ILE |
| 2 | 6p | 112 | ILE |
| 2 | 8r | 112 | ILE |
| 2 | 8s | 112 | ILE |
| 2 | 8u | 112 | ILE |
| 2 | 1q | 112 | ILE |
| 2 | 1s | 112 | ILE |
| 2 | 3r | 112 | ILE |

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| Mol | Chain | Res | Type |
|------------|--------------|------------|-------------|
| 2 | 3t | 112 | ILE |
| 2 | 4k | 112 | ILE |
| 2 | 5k | 112 | ILE |
| 2 | 6r | 112 | ILE |
| 2 | 6t | 112 | ILE |
| 2 | 8x | 112 | ILE |
| 2 | 8y | 112 | ILE |
| 2 | 9K | 112 | ILE |
| 2 | 1u | 112 | ILE |
| 2 | 1w | 112 | ILE |
| 2 | 3v | 112 | ILE |
| 2 | 3x | 112 | ILE |
| 2 | 4m | 112 | ILE |
| 2 | 5m | 112 | ILE |
| 2 | 6v | 112 | ILE |
| 2 | 6x | 112 | ILE |
| 2 | 9N | 112 | ILE |
| 2 | 9O | 112 | ILE |
| 2 | 9Q | 112 | ILE |
| 1 | 1B | 8 | VAL |
| 1 | 1C | 251 | ILE |
| 1 | 2A | 355 | SER |
| 1 | 2E | 356 | PRO |
| 1 | 3A | 251 | ILE |
| 1 | 4B | 67 | ASP |
| 1 | 4B | 68 | ARG |
| 1 | 4B | 386 | SER |
| 1 | 4C | 110 | TYR |
| 1 | 5C | 62 | ILE |
| 1 | 7A | 40 | THR |
| 1 | 8A | 156 | TRP |
| 1 | 8A | 157 | GLY |
| 1 | 8A | 252 | ASP |
| 1 | 8E | 23 | ALA |
| 1 | 1H | 8 | VAL |
| 1 | 1I | 251 | ILE |
| 1 | 2F | 355 | SER |
| 1 | 2J | 356 | PRO |
| 1 | 3G | 251 | ILE |
| 1 | 4H | 67 | ASP |
| 1 | 4H | 68 | ARG |
| 1 | 4H | 386 | SER |

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| Mol | Chain | Res | Type |
|------------|--------------|------------|-------------|
| 1 | 4I | 110 | TYR |
| 1 | 5I | 62 | ILE |
| 1 | 7F | 40 | THR |
| 1 | 8G | 156 | TRP |
| 1 | 8G | 157 | GLY |
| 1 | 8G | 252 | ASP |
| 1 | 8K | 23 | ALA |
| 1 | 1N | 8 | VAL |
| 1 | 1O | 251 | ILE |
| 1 | 2K | 355 | SER |
| 1 | 2O | 356 | PRO |
| 1 | 3M | 251 | ILE |
| 1 | 4N | 67 | ASP |
| 1 | 4N | 68 | ARG |
| 1 | 4N | 386 | SER |
| 1 | 4O | 110 | TYR |
| 1 | 5O | 62 | ILE |
| 1 | 7K | 40 | THR |
| 1 | 8M | 156 | TRP |
| 1 | 8M | 157 | GLY |
| 1 | 8M | 252 | ASP |
| 1 | 8Q | 23 | ALA |
| 1 | 1T | 8 | VAL |
| 1 | 1U | 251 | ILE |
| 1 | 2P | 355 | SER |
| 1 | 2T | 356 | PRO |
| 1 | 3S | 251 | ILE |
| 1 | 4T | 67 | ASP |
| 1 | 4T | 68 | ARG |
| 1 | 4T | 386 | SER |
| 1 | 4U | 110 | TYR |
| 1 | 5U | 62 | ILE |
| 1 | 7P | 40 | THR |
| 1 | 8S | 156 | TRP |
| 1 | 8S | 157 | GLY |
| 1 | 8S | 252 | ASP |
| 1 | 8W | 23 | ALA |
| 1 | 1Z | 8 | VAL |
| 1 | 1a | 251 | ILE |
| 1 | 2U | 355 | SER |
| 1 | 2Y | 356 | PRO |
| 1 | 3Y | 251 | ILE |

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| Mol | Chain | Res | Type |
|------------|--------------|------------|-------------|
| 1 | 4Z | 67 | ASP |
| 1 | 4Z | 68 | ARG |
| 1 | 4Z | 386 | SER |
| 1 | 4a | 110 | TYR |
| 1 | 5a | 62 | ILE |
| 1 | 7U | 40 | THR |
| 1 | 8Y | 156 | TRP |
| 1 | 8Y | 157 | GLY |
| 1 | 8Y | 252 | ASP |
| 1 | 8c | 23 | ALA |
| 2 | 1e | 92 | SER |
| 2 | 1f | 26 | ASP |
| 2 | 1g | 92 | SER |
| 2 | 1h | 26 | ASP |
| 2 | 3e | 26 | ASP |
| 2 | 3f | 92 | SER |
| 2 | 3g | 26 | ASP |
| 2 | 3h | 92 | SER |
| 2 | 4e | 92 | SER |
| 2 | 4f | 26 | ASP |
| 2 | 5e | 92 | SER |
| 2 | 5f | 26 | ASP |
| 2 | 6e | 26 | ASP |
| 2 | 6f | 92 | SER |
| 2 | 6g | 26 | ASP |
| 2 | 6h | 92 | SER |
| 2 | 8e | 26 | ASP |
| 2 | 8f | 92 | SER |
| 2 | 8g | 92 | SER |
| 2 | 8h | 26 | ASP |
| 2 | 8i | 92 | SER |
| 2 | 8j | 26 | ASP |
| 2 | 1i | 92 | SER |
| 2 | 1j | 26 | ASP |
| 2 | 1k | 92 | SER |
| 2 | 1l | 26 | ASP |
| 2 | 3i | 26 | ASP |
| 2 | 3j | 92 | SER |
| 2 | 3k | 26 | ASP |
| 2 | 3l | 92 | SER |
| 2 | 4g | 92 | SER |
| 2 | 4h | 26 | ASP |

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| Mol | Chain | Res | Type |
|------------|--------------|------------|-------------|
| 2 | 5g | 92 | SER |
| 2 | 5h | 26 | ASP |
| 2 | 6i | 26 | ASP |
| 2 | 6j | 92 | SER |
| 2 | 6k | 26 | ASP |
| 2 | 6l | 92 | SER |
| 2 | 8k | 26 | ASP |
| 2 | 8l | 92 | SER |
| 2 | 8m | 92 | SER |
| 2 | 8n | 26 | ASP |
| 2 | 8o | 92 | SER |
| 2 | 8p | 26 | ASP |
| 2 | 1m | 92 | SER |
| 2 | 1n | 26 | ASP |
| 2 | 1o | 92 | SER |
| 2 | 1p | 26 | ASP |
| 2 | 3m | 26 | ASP |
| 2 | 3n | 92 | SER |
| 2 | 3o | 26 | ASP |
| 2 | 3p | 92 | SER |
| 2 | 4i | 92 | SER |
| 2 | 4j | 26 | ASP |
| 2 | 5i | 92 | SER |
| 2 | 5j | 26 | ASP |
| 2 | 6m | 26 | ASP |
| 2 | 6n | 92 | SER |
| 2 | 6o | 26 | ASP |
| 2 | 6p | 92 | SER |
| 2 | 8q | 26 | ASP |
| 2 | 8r | 92 | SER |
| 2 | 8s | 92 | SER |
| 2 | 8t | 26 | ASP |
| 2 | 8u | 92 | SER |
| 2 | 8v | 26 | ASP |
| 2 | 1q | 92 | SER |
| 2 | 1r | 26 | ASP |
| 2 | 1s | 92 | SER |
| 2 | 1t | 26 | ASP |
| 2 | 3q | 26 | ASP |
| 2 | 3r | 92 | SER |
| 2 | 3s | 26 | ASP |
| 2 | 3t | 92 | SER |

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| Mol | Chain | Res | Type |
|------------|--------------|------------|-------------|
| 2 | 4k | 92 | SER |
| 2 | 4l | 26 | ASP |
| 2 | 5k | 92 | SER |
| 2 | 5l | 26 | ASP |
| 2 | 6q | 26 | ASP |
| 2 | 6r | 92 | SER |
| 2 | 6s | 26 | ASP |
| 2 | 6t | 92 | SER |
| 2 | 8w | 26 | ASP |
| 2 | 8x | 92 | SER |
| 2 | 8y | 92 | SER |
| 2 | 8z | 26 | ASP |
| 2 | 9K | 92 | SER |
| 2 | 9L | 26 | ASP |
| 2 | 1u | 92 | SER |
| 2 | 1v | 26 | ASP |
| 2 | 1w | 92 | SER |
| 2 | 1x | 26 | ASP |
| 2 | 3u | 26 | ASP |
| 2 | 3v | 92 | SER |
| 2 | 3w | 26 | ASP |
| 2 | 3x | 92 | SER |
| 2 | 4m | 92 | SER |
| 2 | 4n | 26 | ASP |
| 2 | 5m | 92 | SER |
| 2 | 5n | 26 | ASP |
| 2 | 6u | 26 | ASP |
| 2 | 6v | 92 | SER |
| 2 | 6w | 26 | ASP |
| 2 | 6x | 92 | SER |
| 2 | 9M | 26 | ASP |
| 2 | 9N | 92 | SER |
| 2 | 9O | 92 | SER |
| 2 | 9P | 26 | ASP |
| 2 | 9Q | 92 | SER |
| 2 | 9R | 26 | ASP |
| 1 | 1D | 404 | VAL |
| 1 | 2B | 201 | ASP |
| 1 | 2E | 336 | ALA |
| 1 | 3A | 405 | SER |
| 1 | 3D | 92 | PRO |
| 1 | 4B | 203 | PRO |

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| Mol | Chain | Res | Type |
|------------|--------------|------------|-------------|
| 1 | 5D | 6 | ASN |
| 1 | 5E | 10 | THR |
| 1 | 5F | 31 | ASN |
| 1 | 6B | 410 | ASN |
| 1 | 7B | 9 | LYS |
| 1 | 7C | 6 | ASN |
| 1 | 1J | 404 | VAL |
| 1 | 2G | 201 | ASP |
| 1 | 2J | 336 | ALA |
| 1 | 3G | 405 | SER |
| 1 | 3J | 92 | PRO |
| 1 | 4H | 203 | PRO |
| 1 | 5J | 6 | ASN |
| 1 | 5K | 10 | THR |
| 1 | 5L | 31 | ASN |
| 1 | 6H | 410 | ASN |
| 1 | 7G | 9 | LYS |
| 1 | 7H | 6 | ASN |
| 1 | 1P | 404 | VAL |
| 1 | 2L | 201 | ASP |
| 1 | 2O | 336 | ALA |
| 1 | 3M | 405 | SER |
| 1 | 3P | 92 | PRO |
| 1 | 4N | 203 | PRO |
| 1 | 5P | 6 | ASN |
| 1 | 5Q | 10 | THR |
| 1 | 5R | 31 | ASN |
| 1 | 6N | 410 | ASN |
| 1 | 7L | 9 | LYS |
| 1 | 7M | 6 | ASN |
| 1 | 1V | 404 | VAL |
| 1 | 2Q | 201 | ASP |
| 1 | 2T | 336 | ALA |
| 1 | 3S | 405 | SER |
| 1 | 3V | 92 | PRO |
| 1 | 4T | 203 | PRO |
| 1 | 5V | 6 | ASN |
| 1 | 5W | 10 | THR |
| 1 | 5X | 31 | ASN |
| 1 | 6T | 410 | ASN |
| 1 | 7Q | 9 | LYS |
| 1 | 7R | 6 | ASN |

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| Mol | Chain | Res | Type |
|------------|--------------|------------|-------------|
| 1 | 1b | 404 | VAL |
| 1 | 2V | 201 | ASP |
| 1 | 2Y | 336 | ALA |
| 1 | 3Y | 405 | SER |
| 1 | 3b | 92 | PRO |
| 1 | 4Z | 203 | PRO |
| 1 | 5b | 6 | ASN |
| 1 | 5c | 10 | THR |
| 1 | 5d | 31 | ASN |
| 1 | 6Z | 410 | ASN |
| 1 | 7V | 9 | LYS |
| 1 | 7W | 6 | ASN |
| 2 | 1e | 118 | ILE |
| 2 | 1f | 9 | ALA |
| 2 | 1f | 59 | PRO |
| 2 | 1f | 92 | SER |
| 2 | 1f | 103 | GLN |
| 2 | 1g | 118 | ILE |
| 2 | 1h | 9 | ALA |
| 2 | 1h | 59 | PRO |
| 2 | 1h | 92 | SER |
| 2 | 1h | 103 | GLN |
| 2 | 3e | 9 | ALA |
| 2 | 3e | 59 | PRO |
| 2 | 3e | 92 | SER |
| 2 | 3e | 103 | GLN |
| 2 | 3f | 118 | ILE |
| 2 | 3g | 9 | ALA |
| 2 | 3g | 59 | PRO |
| 2 | 3g | 92 | SER |
| 2 | 3g | 103 | GLN |
| 2 | 3h | 118 | ILE |
| 2 | 4e | 118 | ILE |
| 2 | 4f | 9 | ALA |
| 2 | 4f | 59 | PRO |
| 2 | 4f | 92 | SER |
| 2 | 4f | 103 | GLN |
| 2 | 5e | 118 | ILE |
| 2 | 5f | 9 | ALA |
| 2 | 5f | 59 | PRO |
| 2 | 5f | 92 | SER |
| 2 | 5f | 103 | GLN |

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| Mol | Chain | Res | Type |
|------------|--------------|------------|-------------|
| 2 | 6e | 9 | ALA |
| 2 | 6e | 59 | PRO |
| 2 | 6e | 92 | SER |
| 2 | 6e | 103 | GLN |
| 2 | 6f | 118 | ILE |
| 2 | 6g | 9 | ALA |
| 2 | 6g | 59 | PRO |
| 2 | 6g | 92 | SER |
| 2 | 6g | 103 | GLN |
| 2 | 6h | 118 | ILE |
| 2 | 8e | 9 | ALA |
| 2 | 8e | 59 | PRO |
| 2 | 8e | 92 | SER |
| 2 | 8e | 103 | GLN |
| 2 | 8f | 118 | ILE |
| 2 | 8g | 118 | ILE |
| 2 | 8h | 9 | ALA |
| 2 | 8h | 59 | PRO |
| 2 | 8h | 92 | SER |
| 2 | 8h | 103 | GLN |
| 2 | 8i | 118 | ILE |
| 2 | 8j | 9 | ALA |
| 2 | 8j | 59 | PRO |
| 2 | 8j | 92 | SER |
| 2 | 8j | 103 | GLN |
| 2 | 1i | 118 | ILE |
| 2 | 1j | 9 | ALA |
| 2 | 1j | 59 | PRO |
| 2 | 1j | 92 | SER |
| 2 | 1j | 103 | GLN |
| 2 | 1k | 118 | ILE |
| 2 | 1l | 9 | ALA |
| 2 | 1l | 59 | PRO |
| 2 | 1l | 92 | SER |
| 2 | 1l | 103 | GLN |
| 2 | 3i | 9 | ALA |
| 2 | 3i | 59 | PRO |
| 2 | 3i | 92 | SER |
| 2 | 3i | 103 | GLN |
| 2 | 3j | 118 | ILE |
| 2 | 3k | 9 | ALA |
| 2 | 3k | 59 | PRO |

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| Mol | Chain | Res | Type |
|------------|--------------|------------|-------------|
| 2 | 3k | 92 | SER |
| 2 | 3k | 103 | GLN |
| 2 | 3l | 118 | ILE |
| 2 | 4g | 118 | ILE |
| 2 | 4h | 9 | ALA |
| 2 | 4h | 59 | PRO |
| 2 | 4h | 92 | SER |
| 2 | 4h | 103 | GLN |
| 2 | 5g | 118 | ILE |
| 2 | 5h | 9 | ALA |
| 2 | 5h | 59 | PRO |
| 2 | 5h | 92 | SER |
| 2 | 5h | 103 | GLN |
| 2 | 6i | 9 | ALA |
| 2 | 6i | 59 | PRO |
| 2 | 6i | 92 | SER |
| 2 | 6i | 103 | GLN |
| 2 | 6j | 118 | ILE |
| 2 | 6k | 9 | ALA |
| 2 | 6k | 59 | PRO |
| 2 | 6k | 92 | SER |
| 2 | 6k | 103 | GLN |
| 2 | 6l | 118 | ILE |
| 2 | 8k | 9 | ALA |
| 2 | 8k | 59 | PRO |
| 2 | 8k | 92 | SER |
| 2 | 8k | 103 | GLN |
| 2 | 8l | 118 | ILE |
| 2 | 8m | 118 | ILE |
| 2 | 8n | 9 | ALA |
| 2 | 8n | 59 | PRO |
| 2 | 8n | 92 | SER |
| 2 | 8n | 103 | GLN |
| 2 | 8o | 118 | ILE |
| 2 | 8p | 9 | ALA |
| 2 | 8p | 59 | PRO |
| 2 | 8p | 92 | SER |
| 2 | 8p | 103 | GLN |
| 2 | 1m | 118 | ILE |
| 2 | 1n | 9 | ALA |
| 2 | 1n | 59 | PRO |
| 2 | 1n | 92 | SER |

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| Mol | Chain | Res | Type |
|------------|--------------|------------|-------------|
| 2 | 1n | 103 | GLN |
| 2 | 1o | 118 | ILE |
| 2 | 1p | 9 | ALA |
| 2 | 1p | 59 | PRO |
| 2 | 1p | 92 | SER |
| 2 | 1p | 103 | GLN |
| 2 | 3m | 9 | ALA |
| 2 | 3m | 59 | PRO |
| 2 | 3m | 92 | SER |
| 2 | 3m | 103 | GLN |
| 2 | 3n | 118 | ILE |
| 2 | 3o | 9 | ALA |
| 2 | 3o | 59 | PRO |
| 2 | 3o | 92 | SER |
| 2 | 3o | 103 | GLN |
| 2 | 3p | 118 | ILE |
| 2 | 4i | 118 | ILE |
| 2 | 4j | 9 | ALA |
| 2 | 4j | 59 | PRO |
| 2 | 4j | 92 | SER |
| 2 | 4j | 103 | GLN |
| 2 | 5i | 118 | ILE |
| 2 | 5j | 9 | ALA |
| 2 | 5j | 59 | PRO |
| 2 | 5j | 92 | SER |
| 2 | 5j | 103 | GLN |
| 2 | 6m | 9 | ALA |
| 2 | 6m | 59 | PRO |
| 2 | 6m | 92 | SER |
| 2 | 6m | 103 | GLN |
| 2 | 6n | 118 | ILE |
| 2 | 6o | 9 | ALA |
| 2 | 6o | 59 | PRO |
| 2 | 6o | 92 | SER |
| 2 | 6o | 103 | GLN |
| 2 | 6p | 118 | ILE |
| 2 | 8q | 9 | ALA |
| 2 | 8q | 59 | PRO |
| 2 | 8q | 92 | SER |
| 2 | 8q | 103 | GLN |
| 2 | 8r | 118 | ILE |
| 2 | 8s | 118 | ILE |

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| Mol | Chain | Res | Type |
|------------|--------------|------------|-------------|
| 2 | 8t | 9 | ALA |
| 2 | 8t | 59 | PRO |
| 2 | 8t | 92 | SER |
| 2 | 8t | 103 | GLN |
| 2 | 8u | 118 | ILE |
| 2 | 8v | 9 | ALA |
| 2 | 8v | 59 | PRO |
| 2 | 8v | 92 | SER |
| 2 | 8v | 103 | GLN |
| 2 | 1q | 118 | ILE |
| 2 | 1r | 9 | ALA |
| 2 | 1r | 59 | PRO |
| 2 | 1r | 92 | SER |
| 2 | 1r | 103 | GLN |
| 2 | 1s | 118 | ILE |
| 2 | 1t | 9 | ALA |
| 2 | 1t | 59 | PRO |
| 2 | 1t | 92 | SER |
| 2 | 1t | 103 | GLN |
| 2 | 3q | 9 | ALA |
| 2 | 3q | 59 | PRO |
| 2 | 3q | 92 | SER |
| 2 | 3q | 103 | GLN |
| 2 | 3r | 118 | ILE |
| 2 | 3s | 9 | ALA |
| 2 | 3s | 59 | PRO |
| 2 | 3s | 92 | SER |
| 2 | 3s | 103 | GLN |
| 2 | 3t | 118 | ILE |
| 2 | 4k | 118 | ILE |
| 2 | 4l | 9 | ALA |
| 2 | 4l | 59 | PRO |
| 2 | 4l | 92 | SER |
| 2 | 4l | 103 | GLN |
| 2 | 5k | 118 | ILE |
| 2 | 5l | 9 | ALA |
| 2 | 5l | 59 | PRO |
| 2 | 5l | 92 | SER |
| 2 | 5l | 103 | GLN |
| 2 | 6q | 9 | ALA |
| 2 | 6q | 59 | PRO |
| 2 | 6q | 92 | SER |

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| Mol | Chain | Res | Type |
|------------|--------------|------------|-------------|
| 2 | 6q | 103 | GLN |
| 2 | 6r | 118 | ILE |
| 2 | 6s | 9 | ALA |
| 2 | 6s | 59 | PRO |
| 2 | 6s | 92 | SER |
| 2 | 6s | 103 | GLN |
| 2 | 6t | 118 | ILE |
| 2 | 8w | 9 | ALA |
| 2 | 8w | 59 | PRO |
| 2 | 8w | 92 | SER |
| 2 | 8w | 103 | GLN |
| 2 | 8x | 118 | ILE |
| 2 | 8y | 118 | ILE |
| 2 | 8z | 9 | ALA |
| 2 | 8z | 59 | PRO |
| 2 | 8z | 92 | SER |
| 2 | 8z | 103 | GLN |
| 2 | 9K | 118 | ILE |
| 2 | 9L | 9 | ALA |
| 2 | 9L | 59 | PRO |
| 2 | 9L | 92 | SER |
| 2 | 9L | 103 | GLN |
| 2 | 1u | 118 | ILE |
| 2 | 1v | 9 | ALA |
| 2 | 1v | 59 | PRO |
| 2 | 1v | 92 | SER |
| 2 | 1v | 103 | GLN |
| 2 | 1w | 118 | ILE |
| 2 | 1x | 9 | ALA |
| 2 | 1x | 59 | PRO |
| 2 | 1x | 92 | SER |
| 2 | 1x | 103 | GLN |
| 2 | 3u | 9 | ALA |
| 2 | 3u | 59 | PRO |
| 2 | 3u | 92 | SER |
| 2 | 3u | 103 | GLN |
| 2 | 3v | 118 | ILE |
| 2 | 3w | 9 | ALA |
| 2 | 3w | 59 | PRO |
| 2 | 3w | 92 | SER |
| 2 | 3w | 103 | GLN |
| 2 | 3x | 118 | ILE |

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| Mol | Chain | Res | Type |
|------------|--------------|------------|-------------|
| 2 | 4m | 118 | ILE |
| 2 | 4n | 9 | ALA |
| 2 | 4n | 59 | PRO |
| 2 | 4n | 92 | SER |
| 2 | 4n | 103 | GLN |
| 2 | 5m | 118 | ILE |
| 2 | 5n | 9 | ALA |
| 2 | 5n | 59 | PRO |
| 2 | 5n | 92 | SER |
| 2 | 5n | 103 | GLN |
| 2 | 6u | 9 | ALA |
| 2 | 6u | 59 | PRO |
| 2 | 6u | 92 | SER |
| 2 | 6u | 103 | GLN |
| 2 | 6v | 118 | ILE |
| 2 | 6w | 9 | ALA |
| 2 | 6w | 59 | PRO |
| 2 | 6w | 92 | SER |
| 2 | 6w | 103 | GLN |
| 2 | 6x | 118 | ILE |
| 2 | 9M | 9 | ALA |
| 2 | 9M | 59 | PRO |
| 2 | 9M | 92 | SER |
| 2 | 9M | 103 | GLN |
| 2 | 9N | 118 | ILE |
| 2 | 9O | 118 | ILE |
| 2 | 9P | 9 | ALA |
| 2 | 9P | 59 | PRO |
| 2 | 9P | 92 | SER |
| 2 | 9P | 103 | GLN |
| 2 | 9Q | 118 | ILE |
| 2 | 9R | 9 | ALA |
| 2 | 9R | 59 | PRO |
| 2 | 9R | 92 | SER |
| 2 | 9R | 103 | GLN |
| 1 | 1D | 380 | ASP |
| 1 | 2E | 335 | PHE |
| 1 | 4B | 287 | SER |
| 1 | 5C | 156 | TRP |
| 1 | 5F | 157 | GLY |
| 1 | 5F | 440 | ASN |
| 1 | 6B | 157 | GLY |

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| Mol | Chain | Res | Type |
|------------|--------------|------------|-------------|
| 1 | 8A | 31 | ASN |
| 1 | 1J | 380 | ASP |
| 1 | 2J | 335 | PHE |
| 1 | 4H | 287 | SER |
| 1 | 5I | 156 | TRP |
| 1 | 5L | 157 | GLY |
| 1 | 5L | 440 | ASN |
| 1 | 6H | 157 | GLY |
| 1 | 8G | 31 | ASN |
| 1 | 1P | 380 | ASP |
| 1 | 2M | 356 | PRO |
| 1 | 2O | 335 | PHE |
| 1 | 4N | 287 | SER |
| 1 | 5O | 156 | TRP |
| 1 | 5R | 157 | GLY |
| 1 | 5R | 440 | ASN |
| 1 | 6N | 157 | GLY |
| 1 | 8M | 31 | ASN |
| 1 | 1V | 380 | ASP |
| 1 | 2T | 335 | PHE |
| 1 | 4T | 287 | SER |
| 1 | 5U | 156 | TRP |
| 1 | 5X | 157 | GLY |
| 1 | 5X | 440 | ASN |
| 1 | 6T | 157 | GLY |
| 1 | 8S | 31 | ASN |
| 1 | 1b | 380 | ASP |
| 1 | 2W | 356 | PRO |
| 1 | 2Y | 335 | PHE |
| 1 | 4Z | 287 | SER |
| 1 | 5a | 156 | TRP |
| 1 | 5d | 157 | GLY |
| 1 | 5d | 440 | ASN |
| 1 | 6Z | 157 | GLY |
| 2 | 1e | 49 | LYS |
| 2 | 1e | 59 | PRO |
| 2 | 1g | 49 | LYS |
| 2 | 1g | 59 | PRO |
| 2 | 2Z | 11 | SER |
| 2 | 2a | 11 | SER |
| 2 | 2b | 11 | SER |
| 2 | 2c | 11 | SER |

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| Mol | Chain | Res | Type |
|------------|--------------|------------|-------------|
| 2 | 2d | 11 | SER |
| 2 | 3f | 49 | LYS |
| 2 | 3f | 59 | PRO |
| 2 | 3h | 49 | LYS |
| 2 | 3h | 59 | PRO |
| 2 | 4e | 49 | LYS |
| 2 | 4e | 59 | PRO |
| 2 | 5e | 49 | LYS |
| 2 | 5e | 59 | PRO |
| 2 | 6f | 49 | LYS |
| 2 | 6f | 59 | PRO |
| 2 | 6h | 49 | LYS |
| 2 | 6h | 59 | PRO |
| 2 | 7Z | 11 | SER |
| 2 | 7a | 11 | SER |
| 2 | 7b | 11 | SER |
| 2 | 7c | 11 | SER |
| 2 | 7d | 11 | SER |
| 2 | 8f | 49 | LYS |
| 2 | 8f | 59 | PRO |
| 2 | 8g | 49 | LYS |
| 2 | 8g | 59 | PRO |
| 2 | 8i | 49 | LYS |
| 2 | 8i | 59 | PRO |
| 2 | 9F | 11 | SER |
| 2 | 1i | 49 | LYS |
| 2 | 1i | 59 | PRO |
| 2 | 1k | 49 | LYS |
| 2 | 1k | 59 | PRO |
| 2 | 2e | 11 | SER |
| 2 | 2f | 11 | SER |
| 2 | 2g | 11 | SER |
| 2 | 2h | 11 | SER |
| 2 | 2i | 11 | SER |
| 2 | 3j | 49 | LYS |
| 2 | 3j | 59 | PRO |
| 2 | 3l | 49 | LYS |
| 2 | 3l | 59 | PRO |
| 2 | 4g | 49 | LYS |
| 2 | 4g | 59 | PRO |
| 2 | 5g | 49 | LYS |
| 2 | 5g | 59 | PRO |

Continued on next page...

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| Mol | Chain | Res | Type |
|------------|--------------|------------|-------------|
| 2 | 6j | 49 | LYS |
| 2 | 6j | 59 | PRO |
| 2 | 6l | 49 | LYS |
| 2 | 6l | 59 | PRO |
| 2 | 7e | 11 | SER |
| 2 | 7f | 11 | SER |
| 2 | 7g | 11 | SER |
| 2 | 7h | 11 | SER |
| 2 | 7i | 11 | SER |
| 2 | 8l | 49 | LYS |
| 2 | 8l | 59 | PRO |
| 2 | 8m | 49 | LYS |
| 2 | 8m | 59 | PRO |
| 2 | 8o | 49 | LYS |
| 2 | 8o | 59 | PRO |
| 2 | 9G | 11 | SER |
| 2 | 1m | 49 | LYS |
| 2 | 1m | 59 | PRO |
| 2 | 1o | 49 | LYS |
| 2 | 1o | 59 | PRO |
| 2 | 2j | 11 | SER |
| 2 | 2k | 11 | SER |
| 2 | 2l | 11 | SER |
| 2 | 2m | 11 | SER |
| 2 | 2n | 11 | SER |
| 2 | 3n | 49 | LYS |
| 2 | 3n | 59 | PRO |
| 2 | 3p | 49 | LYS |
| 2 | 3p | 59 | PRO |
| 2 | 4i | 49 | LYS |
| 2 | 4i | 59 | PRO |
| 2 | 5i | 49 | LYS |
| 2 | 5i | 59 | PRO |
| 2 | 6n | 49 | LYS |
| 2 | 6n | 59 | PRO |
| 2 | 6p | 49 | LYS |
| 2 | 6p | 59 | PRO |
| 2 | 7j | 11 | SER |
| 2 | 7k | 11 | SER |
| 2 | 7l | 11 | SER |
| 2 | 7m | 11 | SER |
| 2 | 7n | 11 | SER |

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| Mol | Chain | Res | Type |
|------------|--------------|------------|-------------|
| 2 | 8r | 49 | LYS |
| 2 | 8r | 59 | PRO |
| 2 | 8s | 49 | LYS |
| 2 | 8s | 59 | PRO |
| 2 | 8u | 49 | LYS |
| 2 | 8u | 59 | PRO |
| 2 | 9H | 11 | SER |
| 2 | 1q | 49 | LYS |
| 2 | 1q | 59 | PRO |
| 2 | 1s | 49 | LYS |
| 2 | 1s | 59 | PRO |
| 2 | 2o | 11 | SER |
| 2 | 2p | 11 | SER |
| 2 | 2q | 11 | SER |
| 2 | 2r | 11 | SER |
| 2 | 2s | 11 | SER |
| 2 | 3r | 49 | LYS |
| 2 | 3r | 59 | PRO |
| 2 | 3t | 49 | LYS |
| 2 | 3t | 59 | PRO |
| 2 | 4k | 49 | LYS |
| 2 | 4k | 59 | PRO |
| 2 | 5k | 49 | LYS |
| 2 | 5k | 59 | PRO |
| 2 | 6r | 49 | LYS |
| 2 | 6r | 59 | PRO |
| 2 | 6t | 49 | LYS |
| 2 | 6t | 59 | PRO |
| 2 | 7o | 11 | SER |
| 2 | 7p | 11 | SER |
| 2 | 7q | 11 | SER |
| 2 | 7r | 11 | SER |
| 2 | 7s | 11 | SER |
| 2 | 8x | 49 | LYS |
| 2 | 8x | 59 | PRO |
| 2 | 8y | 49 | LYS |
| 2 | 8y | 59 | PRO |
| 2 | 9K | 49 | LYS |
| 2 | 9K | 59 | PRO |
| 2 | 9I | 11 | SER |
| 2 | 1u | 49 | LYS |
| 2 | 1u | 59 | PRO |

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| Mol | Chain | Res | Type |
|------------|--------------|------------|-------------|
| 2 | 1w | 49 | LYS |
| 2 | 1w | 59 | PRO |
| 2 | 2t | 11 | SER |
| 2 | 2u | 11 | SER |
| 2 | 2v | 11 | SER |
| 2 | 2w | 11 | SER |
| 2 | 2x | 11 | SER |
| 2 | 3v | 49 | LYS |
| 2 | 3v | 59 | PRO |
| 2 | 3x | 49 | LYS |
| 2 | 3x | 59 | PRO |
| 2 | 4m | 49 | LYS |
| 2 | 4m | 59 | PRO |
| 2 | 5m | 49 | LYS |
| 2 | 5m | 59 | PRO |
| 2 | 6v | 49 | LYS |
| 2 | 6v | 59 | PRO |
| 2 | 6x | 49 | LYS |
| 2 | 6x | 59 | PRO |
| 2 | 7t | 11 | SER |
| 2 | 7u | 11 | SER |
| 2 | 7v | 11 | SER |
| 2 | 7w | 11 | SER |
| 2 | 7x | 11 | SER |
| 2 | 9N | 49 | LYS |
| 2 | 9N | 59 | PRO |
| 2 | 9O | 49 | LYS |
| 2 | 9O | 59 | PRO |
| 2 | 9Q | 49 | LYS |
| 2 | 9Q | 59 | PRO |
| 2 | 9J | 11 | SER |
| 1 | 1F | 92 | PRO |
| 1 | 2C | 356 | PRO |
| 1 | 5C | 61 | PHE |
| 1 | 6A | 382 | LYS |
| 1 | 6B | 156 | TRP |
| 1 | 6C | 356 | PRO |
| 1 | 7E | 287 | SER |
| 1 | 8A | 356 | PRO |
| 1 | 1L | 92 | PRO |
| 1 | 2H | 356 | PRO |
| 1 | 5I | 61 | PHE |

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| Mol | Chain | Res | Type |
|------------|--------------|------------|-------------|
| 1 | 6G | 382 | LYS |
| 1 | 6H | 156 | TRP |
| 1 | 6I | 356 | PRO |
| 1 | 7J | 287 | SER |
| 1 | 8G | 356 | PRO |
| 1 | 1R | 92 | PRO |
| 1 | 5O | 61 | PHE |
| 1 | 6M | 382 | LYS |
| 1 | 6N | 156 | TRP |
| 1 | 6O | 356 | PRO |
| 1 | 7O | 287 | SER |
| 1 | 1X | 92 | PRO |
| 1 | 2R | 356 | PRO |
| 1 | 5U | 61 | PHE |
| 1 | 6S | 382 | LYS |
| 1 | 6T | 156 | TRP |
| 1 | 6U | 356 | PRO |
| 1 | 7T | 287 | SER |
| 1 | 8S | 356 | PRO |
| 1 | 1d | 92 | PRO |
| 1 | 5a | 61 | PHE |
| 1 | 6Y | 382 | LYS |
| 1 | 6Z | 156 | TRP |
| 1 | 6a | 356 | PRO |
| 1 | 7Y | 287 | SER |
| 1 | 8Y | 31 | ASN |
| 1 | 8Y | 356 | PRO |
| 2 | 1e | 113 | SER |
| 2 | 1g | 113 | SER |
| 2 | 2Z | 119 | SER |
| 2 | 2a | 119 | SER |
| 2 | 2b | 119 | SER |
| 2 | 2c | 119 | SER |
| 2 | 2d | 119 | SER |
| 2 | 3f | 113 | SER |
| 2 | 3h | 113 | SER |
| 2 | 4e | 113 | SER |
| 2 | 5e | 113 | SER |
| 2 | 6f | 113 | SER |
| 2 | 6h | 113 | SER |
| 2 | 7Z | 119 | SER |
| 2 | 7a | 119 | SER |

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| Mol | Chain | Res | Type |
|------------|--------------|------------|-------------|
| 2 | 7b | 119 | SER |
| 2 | 7c | 119 | SER |
| 2 | 7d | 119 | SER |
| 2 | 8f | 113 | SER |
| 2 | 8g | 113 | SER |
| 2 | 8i | 113 | SER |
| 2 | 9F | 119 | SER |
| 2 | 1i | 113 | SER |
| 2 | 1k | 113 | SER |
| 2 | 2e | 119 | SER |
| 2 | 2f | 119 | SER |
| 2 | 2g | 119 | SER |
| 2 | 2h | 119 | SER |
| 2 | 2i | 119 | SER |
| 2 | 3j | 113 | SER |
| 2 | 3l | 113 | SER |
| 2 | 4g | 113 | SER |
| 2 | 5g | 113 | SER |
| 2 | 6j | 113 | SER |
| 2 | 6l | 113 | SER |
| 2 | 7e | 119 | SER |
| 2 | 7f | 119 | SER |
| 2 | 7g | 119 | SER |
| 2 | 7h | 119 | SER |
| 2 | 7i | 119 | SER |
| 2 | 8l | 113 | SER |
| 2 | 8m | 113 | SER |
| 2 | 8o | 113 | SER |
| 2 | 9G | 119 | SER |
| 2 | 1m | 113 | SER |
| 2 | 1o | 113 | SER |
| 2 | 2j | 119 | SER |
| 2 | 2k | 119 | SER |
| 2 | 2l | 119 | SER |
| 2 | 2m | 119 | SER |
| 2 | 2n | 119 | SER |
| 2 | 3n | 113 | SER |
| 2 | 3p | 113 | SER |
| 2 | 4i | 113 | SER |
| 2 | 5i | 113 | SER |
| 2 | 6n | 113 | SER |
| 2 | 6p | 113 | SER |

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| Mol | Chain | Res | Type |
|------------|--------------|------------|-------------|
| 2 | 7j | 119 | SER |
| 2 | 7k | 119 | SER |
| 2 | 7l | 119 | SER |
| 2 | 7m | 119 | SER |
| 2 | 7n | 119 | SER |
| 2 | 8r | 113 | SER |
| 2 | 8s | 113 | SER |
| 2 | 8u | 113 | SER |
| 2 | 9H | 119 | SER |
| 2 | 1q | 113 | SER |
| 2 | 1s | 113 | SER |
| 2 | 2o | 119 | SER |
| 2 | 2p | 119 | SER |
| 2 | 2q | 119 | SER |
| 2 | 2r | 119 | SER |
| 2 | 2s | 119 | SER |
| 2 | 3r | 113 | SER |
| 2 | 3t | 113 | SER |
| 2 | 4k | 113 | SER |
| 2 | 5k | 113 | SER |
| 2 | 6r | 113 | SER |
| 2 | 6t | 113 | SER |
| 2 | 7o | 119 | SER |
| 2 | 7p | 119 | SER |
| 2 | 7q | 119 | SER |
| 2 | 7r | 119 | SER |
| 2 | 7s | 119 | SER |
| 2 | 8x | 113 | SER |
| 2 | 8y | 113 | SER |
| 2 | 9K | 113 | SER |
| 2 | 9I | 119 | SER |
| 2 | 1u | 113 | SER |
| 2 | 1w | 113 | SER |
| 2 | 2t | 119 | SER |
| 2 | 2u | 119 | SER |
| 2 | 2v | 119 | SER |
| 2 | 2w | 119 | SER |
| 2 | 2x | 119 | SER |
| 2 | 3v | 113 | SER |
| 2 | 3x | 113 | SER |
| 2 | 4m | 113 | SER |
| 2 | 5m | 113 | SER |

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| Mol | Chain | Res | Type |
|------------|--------------|------------|-------------|
| 2 | 6v | 113 | SER |
| 2 | 6x | 113 | SER |
| 2 | 7t | 119 | SER |
| 2 | 7u | 119 | SER |
| 2 | 7v | 119 | SER |
| 2 | 7w | 119 | SER |
| 2 | 7x | 119 | SER |
| 2 | 9N | 113 | SER |
| 2 | 9O | 113 | SER |
| 2 | 9Q | 113 | SER |
| 2 | 9J | 119 | SER |
| 1 | 2B | 37 | PRO |
| 1 | 3D | 426 | PRO |
| 1 | 4B | 204 | THR |
| 1 | 7C | 68 | ARG |
| 1 | 2G | 37 | PRO |
| 1 | 2I | 337 | ASN |
| 1 | 3J | 426 | PRO |
| 1 | 4H | 204 | THR |
| 1 | 7H | 68 | ARG |
| 1 | 2L | 37 | PRO |
| 1 | 3P | 426 | PRO |
| 1 | 4N | 204 | THR |
| 1 | 7M | 68 | ARG |
| 1 | 8M | 356 | PRO |
| 1 | 2Q | 37 | PRO |
| 1 | 3V | 426 | PRO |
| 1 | 4T | 204 | THR |
| 1 | 7R | 68 | ARG |
| 1 | 2V | 37 | PRO |
| 1 | 3b | 426 | PRO |
| 1 | 4Z | 204 | THR |
| 1 | 7W | 68 | ARG |
| 1 | 3D | 20 | ILE |
| 1 | 6C | 202 | GLU |
| 1 | 3J | 20 | ILE |
| 1 | 3J | 356 | PRO |
| 1 | 6I | 202 | GLU |
| 1 | 3P | 20 | ILE |
| 1 | 6O | 202 | GLU |
| 1 | 3V | 20 | ILE |
| 1 | 6U | 202 | GLU |

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| Mol | Chain | Res | Type |
|------------|--------------|------------|-------------|
| 1 | 3b | 20 | ILE |
| 1 | 6a | 202 | GLU |
| 2 | 2c | 59 | PRO |
| 2 | 7a | 59 | PRO |
| 2 | 9F | 59 | PRO |
| 2 | 2f | 59 | PRO |
| 2 | 2h | 59 | PRO |
| 2 | 2m | 59 | PRO |
| 2 | 7k | 59 | PRO |
| 2 | 2p | 59 | PRO |
| 2 | 2q | 59 | PRO |
| 2 | 2r | 59 | PRO |
| 2 | 9I | 59 | PRO |
| 2 | 2u | 59 | PRO |
| 2 | 2w | 59 | PRO |
| 2 | 7v | 59 | PRO |
| 2 | 7w | 59 | PRO |
| 1 | 3D | 356 | PRO |
| 1 | 6F | 356 | PRO |
| 1 | 8E | 356 | PRO |
| 1 | 6L | 356 | PRO |
| 1 | 8K | 356 | PRO |
| 1 | 3P | 356 | PRO |
| 1 | 6R | 356 | PRO |
| 1 | 8Q | 356 | PRO |
| 1 | 3V | 356 | PRO |
| 1 | 6X | 356 | PRO |
| 1 | 8W | 356 | PRO |
| 1 | 3b | 356 | PRO |
| 1 | 6d | 356 | PRO |
| 1 | 8c | 356 | PRO |
| 2 | 2Z | 59 | PRO |
| 2 | 2a | 59 | PRO |
| 2 | 2b | 59 | PRO |
| 2 | 2d | 59 | PRO |
| 2 | 7Z | 59 | PRO |
| 2 | 7b | 59 | PRO |
| 2 | 7c | 59 | PRO |
| 2 | 7d | 59 | PRO |
| 2 | 2e | 59 | PRO |
| 2 | 2g | 59 | PRO |
| 2 | 2i | 59 | PRO |

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| Mol | Chain | Res | Type |
|------------|--------------|------------|-------------|
| 2 | 7e | 59 | PRO |
| 2 | 7f | 59 | PRO |
| 2 | 7g | 59 | PRO |
| 2 | 7h | 59 | PRO |
| 2 | 7i | 59 | PRO |
| 2 | 9G | 59 | PRO |
| 2 | 2j | 59 | PRO |
| 2 | 2k | 59 | PRO |
| 2 | 2l | 59 | PRO |
| 2 | 2n | 59 | PRO |
| 2 | 7j | 59 | PRO |
| 2 | 7l | 59 | PRO |
| 2 | 7m | 59 | PRO |
| 2 | 7n | 59 | PRO |
| 2 | 9H | 59 | PRO |
| 2 | 2o | 59 | PRO |
| 2 | 2s | 59 | PRO |
| 2 | 7o | 59 | PRO |
| 2 | 7p | 59 | PRO |
| 2 | 7q | 59 | PRO |
| 2 | 7r | 59 | PRO |
| 2 | 7s | 59 | PRO |
| 2 | 2t | 59 | PRO |
| 2 | 2v | 59 | PRO |
| 2 | 2x | 59 | PRO |
| 2 | 7t | 59 | PRO |
| 2 | 7u | 59 | PRO |
| 2 | 7x | 59 | PRO |
| 2 | 9J | 59 | PRO |
| 1 | 3C | 356 | PRO |
| 1 | 5F | 425 | LYS |
| 1 | 6A | 355 | SER |
| 1 | 3I | 356 | PRO |
| 1 | 5L | 425 | LYS |
| 1 | 6G | 355 | SER |
| 1 | 3O | 356 | PRO |
| 1 | 5R | 425 | LYS |
| 1 | 6M | 355 | SER |
| 1 | 3U | 356 | PRO |
| 1 | 5X | 425 | LYS |
| 1 | 6S | 355 | SER |
| 1 | 3a | 356 | PRO |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1 | 5d | 425 | LYS |
| 1 | 6Y | 355 | SER |
| 1 | 4C | 356 | PRO |
| 1 | 6C | 315 | PRO |
| 1 | 4I | 356 | PRO |
| 1 | 6I | 315 | PRO |
| 1 | 4O | 356 | PRO |
| 1 | 6O | 315 | PRO |
| 1 | 4U | 356 | PRO |
| 1 | 6U | 315 | PRO |
| 1 | 4a | 356 | PRO |
| 1 | 6a | 315 | PRO |
| 1 | 5B | 203 | PRO |
| 1 | 5H | 203 | PRO |
| 1 | 5N | 203 | PRO |
| 1 | 5T | 203 | PRO |
| 1 | 5Z | 203 | PRO |

5.3.2 Protein sidechains [i](#)

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

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

| Mol | Chain | Analysed | Rotameric | Outliers | Percentiles | |
|-----|-------|---------------|------------|----------|-------------|-----|
| 1 | 1A | 370/384 (96%) | 368 (100%) | 2 (0%) | 88 | 95 |
| 1 | 1B | 381/384 (99%) | 379 (100%) | 2 (0%) | 88 | 95 |
| 1 | 1C | 381/384 (99%) | 381 (100%) | 0 | 100 | 100 |
| 1 | 1D | 381/384 (99%) | 379 (100%) | 2 (0%) | 88 | 95 |
| 1 | 1E | 376/384 (98%) | 376 (100%) | 0 | 100 | 100 |
| 1 | 1F | 379/384 (99%) | 378 (100%) | 1 (0%) | 92 | 96 |
| 1 | 1G | 370/384 (96%) | 368 (100%) | 2 (0%) | 88 | 95 |
| 1 | 1H | 381/384 (99%) | 379 (100%) | 2 (0%) | 88 | 95 |
| 1 | 1I | 381/384 (99%) | 381 (100%) | 0 | 100 | 100 |
| 1 | 1J | 381/384 (99%) | 378 (99%) | 3 (1%) | 81 | 93 |
| 1 | 1K | 376/384 (98%) | 376 (100%) | 0 | 100 | 100 |

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| Mol | Chain | Analysed | Rotameric | Outliers | Percentiles | |
|-----|-------|---------------|------------|----------|-------------|-----|
| 1 | 1L | 379/384 (99%) | 378 (100%) | 1 (0%) | 92 | 96 |
| 1 | 1M | 370/384 (96%) | 368 (100%) | 2 (0%) | 88 | 95 |
| 1 | 1N | 381/384 (99%) | 379 (100%) | 2 (0%) | 88 | 95 |
| 1 | 1O | 381/384 (99%) | 381 (100%) | 0 | 100 | 100 |
| 1 | 1P | 381/384 (99%) | 379 (100%) | 2 (0%) | 88 | 95 |
| 1 | 1Q | 376/384 (98%) | 376 (100%) | 0 | 100 | 100 |
| 1 | 1R | 379/384 (99%) | 378 (100%) | 1 (0%) | 92 | 96 |
| 1 | 1S | 370/384 (96%) | 368 (100%) | 2 (0%) | 88 | 95 |
| 1 | 1T | 381/384 (99%) | 379 (100%) | 2 (0%) | 88 | 95 |
| 1 | 1U | 381/384 (99%) | 381 (100%) | 0 | 100 | 100 |
| 1 | 1V | 381/384 (99%) | 378 (99%) | 3 (1%) | 81 | 93 |
| 1 | 1W | 376/384 (98%) | 376 (100%) | 0 | 100 | 100 |
| 1 | 1X | 379/384 (99%) | 378 (100%) | 1 (0%) | 92 | 96 |
| 1 | 1Y | 370/384 (96%) | 368 (100%) | 2 (0%) | 88 | 95 |
| 1 | 1Z | 381/384 (99%) | 379 (100%) | 2 (0%) | 88 | 95 |
| 1 | 1a | 381/384 (99%) | 381 (100%) | 0 | 100 | 100 |
| 1 | 1b | 381/384 (99%) | 378 (99%) | 3 (1%) | 81 | 93 |
| 1 | 1c | 376/384 (98%) | 376 (100%) | 0 | 100 | 100 |
| 1 | 1d | 379/384 (99%) | 378 (100%) | 1 (0%) | 92 | 96 |
| 1 | 2A | 374/384 (97%) | 373 (100%) | 1 (0%) | 92 | 96 |
| 1 | 2B | 381/384 (99%) | 379 (100%) | 2 (0%) | 88 | 95 |
| 1 | 2C | 381/384 (99%) | 380 (100%) | 1 (0%) | 92 | 96 |
| 1 | 2D | 381/384 (99%) | 381 (100%) | 0 | 100 | 100 |
| 1 | 2E | 381/384 (99%) | 380 (100%) | 1 (0%) | 92 | 96 |
| 1 | 2F | 374/384 (97%) | 373 (100%) | 1 (0%) | 92 | 96 |
| 1 | 2G | 381/384 (99%) | 379 (100%) | 2 (0%) | 88 | 95 |
| 1 | 2H | 381/384 (99%) | 380 (100%) | 1 (0%) | 92 | 96 |
| 1 | 2I | 381/384 (99%) | 381 (100%) | 0 | 100 | 100 |
| 1 | 2J | 381/384 (99%) | 380 (100%) | 1 (0%) | 92 | 96 |
| 1 | 2K | 374/384 (97%) | 373 (100%) | 1 (0%) | 92 | 96 |
| 1 | 2L | 381/384 (99%) | 379 (100%) | 2 (0%) | 88 | 95 |

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| Mol | Chain | Analysed | Rotameric | Outliers | Percentiles | |
|-----|-------|---------------|------------|----------|-------------|-----|
| 1 | 2M | 381/384 (99%) | 380 (100%) | 1 (0%) | 92 | 96 |
| 1 | 2N | 381/384 (99%) | 381 (100%) | 0 | 100 | 100 |
| 1 | 2O | 381/384 (99%) | 380 (100%) | 1 (0%) | 92 | 96 |
| 1 | 2P | 374/384 (97%) | 373 (100%) | 1 (0%) | 92 | 96 |
| 1 | 2Q | 381/384 (99%) | 379 (100%) | 2 (0%) | 88 | 95 |
| 1 | 2R | 381/384 (99%) | 380 (100%) | 1 (0%) | 92 | 96 |
| 1 | 2S | 381/384 (99%) | 381 (100%) | 0 | 100 | 100 |
| 1 | 2T | 381/384 (99%) | 380 (100%) | 1 (0%) | 92 | 96 |
| 1 | 2U | 374/384 (97%) | 373 (100%) | 1 (0%) | 92 | 96 |
| 1 | 2V | 381/384 (99%) | 379 (100%) | 2 (0%) | 88 | 95 |
| 1 | 2W | 381/384 (99%) | 380 (100%) | 1 (0%) | 92 | 96 |
| 1 | 2X | 381/384 (99%) | 381 (100%) | 0 | 100 | 100 |
| 1 | 2Y | 381/384 (99%) | 380 (100%) | 1 (0%) | 92 | 96 |
| 1 | 3A | 375/384 (98%) | 374 (100%) | 1 (0%) | 92 | 96 |
| 1 | 3B | 376/384 (98%) | 375 (100%) | 1 (0%) | 92 | 96 |
| 1 | 3C | 380/384 (99%) | 379 (100%) | 1 (0%) | 92 | 96 |
| 1 | 3D | 381/384 (99%) | 380 (100%) | 1 (0%) | 92 | 96 |
| 1 | 3E | 381/384 (99%) | 381 (100%) | 0 | 100 | 100 |
| 1 | 3F | 381/384 (99%) | 380 (100%) | 1 (0%) | 92 | 96 |
| 1 | 3G | 375/384 (98%) | 374 (100%) | 1 (0%) | 92 | 96 |
| 1 | 3H | 376/384 (98%) | 375 (100%) | 1 (0%) | 92 | 96 |
| 1 | 3I | 380/384 (99%) | 379 (100%) | 1 (0%) | 92 | 96 |
| 1 | 3J | 381/384 (99%) | 380 (100%) | 1 (0%) | 92 | 96 |
| 1 | 3K | 381/384 (99%) | 381 (100%) | 0 | 100 | 100 |
| 1 | 3L | 381/384 (99%) | 380 (100%) | 1 (0%) | 92 | 96 |
| 1 | 3M | 375/384 (98%) | 374 (100%) | 1 (0%) | 92 | 96 |
| 1 | 3N | 376/384 (98%) | 375 (100%) | 1 (0%) | 92 | 96 |
| 1 | 3O | 380/384 (99%) | 379 (100%) | 1 (0%) | 92 | 96 |
| 1 | 3P | 381/384 (99%) | 380 (100%) | 1 (0%) | 92 | 96 |
| 1 | 3Q | 381/384 (99%) | 381 (100%) | 0 | 100 | 100 |
| 1 | 3R | 381/384 (99%) | 380 (100%) | 1 (0%) | 92 | 96 |

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| Mol | Chain | Analysed | Rotameric | Outliers | Percentiles | |
|-----|-------|---------------|------------|----------|-------------|-----|
| 1 | 3S | 375/384 (98%) | 374 (100%) | 1 (0%) | 92 | 96 |
| 1 | 3T | 376/384 (98%) | 375 (100%) | 1 (0%) | 92 | 96 |
| 1 | 3U | 380/384 (99%) | 379 (100%) | 1 (0%) | 92 | 96 |
| 1 | 3V | 381/384 (99%) | 380 (100%) | 1 (0%) | 92 | 96 |
| 1 | 3W | 381/384 (99%) | 381 (100%) | 0 | 100 | 100 |
| 1 | 3X | 381/384 (99%) | 380 (100%) | 1 (0%) | 92 | 96 |
| 1 | 3Y | 375/384 (98%) | 374 (100%) | 1 (0%) | 92 | 96 |
| 1 | 3Z | 376/384 (98%) | 375 (100%) | 1 (0%) | 92 | 96 |
| 1 | 3a | 380/384 (99%) | 379 (100%) | 1 (0%) | 92 | 96 |
| 1 | 3b | 381/384 (99%) | 380 (100%) | 1 (0%) | 92 | 96 |
| 1 | 3c | 381/384 (99%) | 381 (100%) | 0 | 100 | 100 |
| 1 | 3d | 381/384 (99%) | 380 (100%) | 1 (0%) | 92 | 96 |
| 1 | 4A | 376/384 (98%) | 376 (100%) | 0 | 100 | 100 |
| 1 | 4B | 376/384 (98%) | 375 (100%) | 1 (0%) | 92 | 96 |
| 1 | 4C | 376/384 (98%) | 376 (100%) | 0 | 100 | 100 |
| 1 | 4D | 376/384 (98%) | 376 (100%) | 0 | 100 | 100 |
| 1 | 4E | 381/384 (99%) | 380 (100%) | 1 (0%) | 92 | 96 |
| 1 | 4F | 381/384 (99%) | 380 (100%) | 1 (0%) | 92 | 96 |
| 1 | 4G | 376/384 (98%) | 376 (100%) | 0 | 100 | 100 |
| 1 | 4H | 376/384 (98%) | 375 (100%) | 1 (0%) | 92 | 96 |
| 1 | 4I | 376/384 (98%) | 376 (100%) | 0 | 100 | 100 |
| 1 | 4J | 376/384 (98%) | 376 (100%) | 0 | 100 | 100 |
| 1 | 4K | 381/384 (99%) | 380 (100%) | 1 (0%) | 92 | 96 |
| 1 | 4L | 381/384 (99%) | 380 (100%) | 1 (0%) | 92 | 96 |
| 1 | 4M | 376/384 (98%) | 376 (100%) | 0 | 100 | 100 |
| 1 | 4N | 376/384 (98%) | 375 (100%) | 1 (0%) | 92 | 96 |
| 1 | 4O | 376/384 (98%) | 376 (100%) | 0 | 100 | 100 |
| 1 | 4P | 376/384 (98%) | 376 (100%) | 0 | 100 | 100 |
| 1 | 4Q | 381/384 (99%) | 380 (100%) | 1 (0%) | 92 | 96 |
| 1 | 4R | 381/384 (99%) | 380 (100%) | 1 (0%) | 92 | 96 |
| 1 | 4S | 376/384 (98%) | 376 (100%) | 0 | 100 | 100 |

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| Mol | Chain | Analysed | Rotameric | Outliers | Percentiles | |
|-----|-------|---------------|------------|----------|-------------|-----|
| 1 | 4T | 376/384 (98%) | 375 (100%) | 1 (0%) | 92 | 96 |
| 1 | 4U | 376/384 (98%) | 376 (100%) | 0 | 100 | 100 |
| 1 | 4V | 376/384 (98%) | 376 (100%) | 0 | 100 | 100 |
| 1 | 4W | 381/384 (99%) | 380 (100%) | 1 (0%) | 92 | 96 |
| 1 | 4X | 381/384 (99%) | 380 (100%) | 1 (0%) | 92 | 96 |
| 1 | 4Y | 376/384 (98%) | 376 (100%) | 0 | 100 | 100 |
| 1 | 4Z | 376/384 (98%) | 375 (100%) | 1 (0%) | 92 | 96 |
| 1 | 4a | 376/384 (98%) | 376 (100%) | 0 | 100 | 100 |
| 1 | 4b | 376/384 (98%) | 376 (100%) | 0 | 100 | 100 |
| 1 | 4c | 381/384 (99%) | 380 (100%) | 1 (0%) | 92 | 96 |
| 1 | 4d | 381/384 (99%) | 380 (100%) | 1 (0%) | 92 | 96 |
| 1 | 5A | 376/384 (98%) | 375 (100%) | 1 (0%) | 92 | 96 |
| 1 | 5B | 376/384 (98%) | 375 (100%) | 1 (0%) | 92 | 96 |
| 1 | 5C | 376/384 (98%) | 373 (99%) | 3 (1%) | 81 | 93 |
| 1 | 5D | 376/384 (98%) | 376 (100%) | 0 | 100 | 100 |
| 1 | 5E | 381/384 (99%) | 381 (100%) | 0 | 100 | 100 |
| 1 | 5F | 381/384 (99%) | 378 (99%) | 3 (1%) | 81 | 93 |
| 1 | 5G | 376/384 (98%) | 375 (100%) | 1 (0%) | 92 | 96 |
| 1 | 5H | 376/384 (98%) | 375 (100%) | 1 (0%) | 92 | 96 |
| 1 | 5I | 376/384 (98%) | 373 (99%) | 3 (1%) | 81 | 93 |
| 1 | 5J | 376/384 (98%) | 376 (100%) | 0 | 100 | 100 |
| 1 | 5K | 381/384 (99%) | 381 (100%) | 0 | 100 | 100 |
| 1 | 5L | 381/384 (99%) | 378 (99%) | 3 (1%) | 81 | 93 |
| 1 | 5M | 376/384 (98%) | 375 (100%) | 1 (0%) | 92 | 96 |
| 1 | 5N | 376/384 (98%) | 375 (100%) | 1 (0%) | 92 | 96 |
| 1 | 5O | 376/384 (98%) | 373 (99%) | 3 (1%) | 81 | 93 |
| 1 | 5P | 376/384 (98%) | 376 (100%) | 0 | 100 | 100 |
| 1 | 5Q | 381/384 (99%) | 381 (100%) | 0 | 100 | 100 |
| 1 | 5R | 381/384 (99%) | 378 (99%) | 3 (1%) | 81 | 93 |
| 1 | 5S | 376/384 (98%) | 375 (100%) | 1 (0%) | 92 | 96 |
| 1 | 5T | 376/384 (98%) | 375 (100%) | 1 (0%) | 92 | 96 |

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| Mol | Chain | Analysed | Rotameric | Outliers | Percentiles | |
|-----|-------|---------------|------------|----------|-------------|-----|
| 1 | 5U | 376/384 (98%) | 372 (99%) | 4 (1%) | 73 | 88 |
| 1 | 5V | 376/384 (98%) | 376 (100%) | 0 | 100 | 100 |
| 1 | 5W | 381/384 (99%) | 381 (100%) | 0 | 100 | 100 |
| 1 | 5X | 381/384 (99%) | 378 (99%) | 3 (1%) | 81 | 93 |
| 1 | 5Y | 376/384 (98%) | 375 (100%) | 1 (0%) | 92 | 96 |
| 1 | 5Z | 376/384 (98%) | 375 (100%) | 1 (0%) | 92 | 96 |
| 1 | 5a | 376/384 (98%) | 373 (99%) | 3 (1%) | 81 | 93 |
| 1 | 5b | 376/384 (98%) | 376 (100%) | 0 | 100 | 100 |
| 1 | 5c | 381/384 (99%) | 381 (100%) | 0 | 100 | 100 |
| 1 | 5d | 381/384 (99%) | 378 (99%) | 3 (1%) | 81 | 93 |
| 1 | 6A | 381/384 (99%) | 380 (100%) | 1 (0%) | 92 | 96 |
| 1 | 6B | 381/384 (99%) | 381 (100%) | 0 | 100 | 100 |
| 1 | 6C | 376/384 (98%) | 376 (100%) | 0 | 100 | 100 |
| 1 | 6D | 376/384 (98%) | 375 (100%) | 1 (0%) | 92 | 96 |
| 1 | 6E | 381/384 (99%) | 381 (100%) | 0 | 100 | 100 |
| 1 | 6F | 381/384 (99%) | 381 (100%) | 0 | 100 | 100 |
| 1 | 6G | 381/384 (99%) | 380 (100%) | 1 (0%) | 92 | 96 |
| 1 | 6H | 381/384 (99%) | 381 (100%) | 0 | 100 | 100 |
| 1 | 6I | 376/384 (98%) | 376 (100%) | 0 | 100 | 100 |
| 1 | 6J | 376/384 (98%) | 375 (100%) | 1 (0%) | 92 | 96 |
| 1 | 6K | 381/384 (99%) | 381 (100%) | 0 | 100 | 100 |
| 1 | 6L | 381/384 (99%) | 381 (100%) | 0 | 100 | 100 |
| 1 | 6M | 381/384 (99%) | 380 (100%) | 1 (0%) | 92 | 96 |
| 1 | 6N | 381/384 (99%) | 381 (100%) | 0 | 100 | 100 |
| 1 | 6O | 376/384 (98%) | 376 (100%) | 0 | 100 | 100 |
| 1 | 6P | 376/384 (98%) | 375 (100%) | 1 (0%) | 92 | 96 |
| 1 | 6Q | 381/384 (99%) | 381 (100%) | 0 | 100 | 100 |
| 1 | 6R | 381/384 (99%) | 381 (100%) | 0 | 100 | 100 |
| 1 | 6S | 381/384 (99%) | 380 (100%) | 1 (0%) | 92 | 96 |
| 1 | 6T | 381/384 (99%) | 381 (100%) | 0 | 100 | 100 |
| 1 | 6U | 376/384 (98%) | 376 (100%) | 0 | 100 | 100 |

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| Mol | Chain | Analysed | Rotameric | Outliers | Percentiles | |
|-----|-------|---------------|------------|----------|-------------|-----|
| 1 | 6V | 376/384 (98%) | 375 (100%) | 1 (0%) | 92 | 96 |
| 1 | 6W | 381/384 (99%) | 381 (100%) | 0 | 100 | 100 |
| 1 | 6X | 381/384 (99%) | 381 (100%) | 0 | 100 | 100 |
| 1 | 6Y | 381/384 (99%) | 380 (100%) | 1 (0%) | 92 | 96 |
| 1 | 6Z | 381/384 (99%) | 381 (100%) | 0 | 100 | 100 |
| 1 | 6a | 376/384 (98%) | 376 (100%) | 0 | 100 | 100 |
| 1 | 6b | 376/384 (98%) | 375 (100%) | 1 (0%) | 92 | 96 |
| 1 | 6c | 381/384 (99%) | 381 (100%) | 0 | 100 | 100 |
| 1 | 6d | 381/384 (99%) | 381 (100%) | 0 | 100 | 100 |
| 1 | 7A | 381/384 (99%) | 378 (99%) | 3 (1%) | 81 | 93 |
| 1 | 7B | 381/384 (99%) | 381 (100%) | 0 | 100 | 100 |
| 1 | 7C | 381/384 (99%) | 380 (100%) | 1 (0%) | 92 | 96 |
| 1 | 7D | 381/384 (99%) | 381 (100%) | 0 | 100 | 100 |
| 1 | 7E | 381/384 (99%) | 381 (100%) | 0 | 100 | 100 |
| 1 | 7F | 381/384 (99%) | 378 (99%) | 3 (1%) | 81 | 93 |
| 1 | 7G | 381/384 (99%) | 381 (100%) | 0 | 100 | 100 |
| 1 | 7H | 381/384 (99%) | 380 (100%) | 1 (0%) | 92 | 96 |
| 1 | 7I | 381/384 (99%) | 381 (100%) | 0 | 100 | 100 |
| 1 | 7J | 381/384 (99%) | 381 (100%) | 0 | 100 | 100 |
| 1 | 7K | 381/384 (99%) | 378 (99%) | 3 (1%) | 81 | 93 |
| 1 | 7L | 381/384 (99%) | 381 (100%) | 0 | 100 | 100 |
| 1 | 7M | 381/384 (99%) | 380 (100%) | 1 (0%) | 92 | 96 |
| 1 | 7N | 381/384 (99%) | 381 (100%) | 0 | 100 | 100 |
| 1 | 7O | 381/384 (99%) | 381 (100%) | 0 | 100 | 100 |
| 1 | 7P | 381/384 (99%) | 378 (99%) | 3 (1%) | 81 | 93 |
| 1 | 7Q | 381/384 (99%) | 381 (100%) | 0 | 100 | 100 |
| 1 | 7R | 381/384 (99%) | 380 (100%) | 1 (0%) | 92 | 96 |
| 1 | 7S | 381/384 (99%) | 381 (100%) | 0 | 100 | 100 |
| 1 | 7T | 381/384 (99%) | 381 (100%) | 0 | 100 | 100 |
| 1 | 7U | 381/384 (99%) | 378 (99%) | 3 (1%) | 81 | 93 |
| 1 | 7V | 381/384 (99%) | 381 (100%) | 0 | 100 | 100 |

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| Mol | Chain | Analysed | Rotameric | Outliers | Percentiles | |
|-----|-------|---------------|------------|----------|-------------|-----|
| 1 | 7W | 381/384 (99%) | 380 (100%) | 1 (0%) | 92 | 96 |
| 1 | 7X | 381/384 (99%) | 381 (100%) | 0 | 100 | 100 |
| 1 | 7Y | 381/384 (99%) | 381 (100%) | 0 | 100 | 100 |
| 1 | 8A | 381/384 (99%) | 381 (100%) | 0 | 100 | 100 |
| 1 | 8B | 381/384 (99%) | 381 (100%) | 0 | 100 | 100 |
| 1 | 8C | 381/384 (99%) | 379 (100%) | 2 (0%) | 88 | 95 |
| 1 | 8D | 381/384 (99%) | 381 (100%) | 0 | 100 | 100 |
| 1 | 8E | 381/384 (99%) | 381 (100%) | 0 | 100 | 100 |
| 1 | 8F | 381/384 (99%) | 380 (100%) | 1 (0%) | 92 | 96 |
| 1 | 8G | 381/384 (99%) | 381 (100%) | 0 | 100 | 100 |
| 1 | 8H | 381/384 (99%) | 381 (100%) | 0 | 100 | 100 |
| 1 | 8I | 381/384 (99%) | 379 (100%) | 2 (0%) | 88 | 95 |
| 1 | 8J | 381/384 (99%) | 381 (100%) | 0 | 100 | 100 |
| 1 | 8K | 381/384 (99%) | 381 (100%) | 0 | 100 | 100 |
| 1 | 8L | 381/384 (99%) | 380 (100%) | 1 (0%) | 92 | 96 |
| 1 | 8M | 381/384 (99%) | 381 (100%) | 0 | 100 | 100 |
| 1 | 8N | 381/384 (99%) | 381 (100%) | 0 | 100 | 100 |
| 1 | 8O | 381/384 (99%) | 379 (100%) | 2 (0%) | 88 | 95 |
| 1 | 8P | 381/384 (99%) | 381 (100%) | 0 | 100 | 100 |
| 1 | 8Q | 381/384 (99%) | 381 (100%) | 0 | 100 | 100 |
| 1 | 8R | 381/384 (99%) | 380 (100%) | 1 (0%) | 92 | 96 |
| 1 | 8S | 381/384 (99%) | 381 (100%) | 0 | 100 | 100 |
| 1 | 8T | 381/384 (99%) | 381 (100%) | 0 | 100 | 100 |
| 1 | 8U | 381/384 (99%) | 379 (100%) | 2 (0%) | 88 | 95 |
| 1 | 8V | 381/384 (99%) | 381 (100%) | 0 | 100 | 100 |
| 1 | 8W | 381/384 (99%) | 381 (100%) | 0 | 100 | 100 |
| 1 | 8X | 381/384 (99%) | 380 (100%) | 1 (0%) | 92 | 96 |
| 1 | 8Y | 381/384 (99%) | 381 (100%) | 0 | 100 | 100 |
| 1 | 8Z | 381/384 (99%) | 381 (100%) | 0 | 100 | 100 |
| 1 | 8a | 381/384 (99%) | 379 (100%) | 2 (0%) | 88 | 95 |
| 1 | 8b | 381/384 (99%) | 381 (100%) | 0 | 100 | 100 |

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| Mol | Chain | Analysed | Rotameric | Outliers | Percentiles | |
|-----|-------|----------------|------------|----------|-------------|-----|
| 1 | 8c | 381/384 (99%) | 381 (100%) | 0 | 100 | 100 |
| 1 | 8d | 381/384 (99%) | 380 (100%) | 1 (0%) | 92 | 96 |
| 1 | 9A | 381/384 (99%) | 379 (100%) | 2 (0%) | 88 | 95 |
| 1 | 9B | 381/384 (99%) | 379 (100%) | 2 (0%) | 88 | 95 |
| 1 | 9C | 381/384 (99%) | 379 (100%) | 2 (0%) | 88 | 95 |
| 1 | 9D | 381/384 (99%) | 379 (100%) | 2 (0%) | 88 | 95 |
| 1 | 9E | 381/384 (99%) | 379 (100%) | 2 (0%) | 88 | 95 |
| 2 | 1e | 236/229 (103%) | 234 (99%) | 2 (1%) | 81 | 93 |
| 2 | 1f | 235/229 (103%) | 233 (99%) | 2 (1%) | 78 | 91 |
| 2 | 1g | 236/229 (103%) | 234 (99%) | 2 (1%) | 81 | 93 |
| 2 | 1h | 235/229 (103%) | 233 (99%) | 2 (1%) | 78 | 91 |
| 2 | 1i | 236/229 (103%) | 234 (99%) | 2 (1%) | 81 | 93 |
| 2 | 1j | 235/229 (103%) | 233 (99%) | 2 (1%) | 78 | 91 |
| 2 | 1k | 236/229 (103%) | 234 (99%) | 2 (1%) | 81 | 93 |
| 2 | 1l | 235/229 (103%) | 233 (99%) | 2 (1%) | 78 | 91 |
| 2 | 1m | 236/229 (103%) | 234 (99%) | 2 (1%) | 81 | 93 |
| 2 | 1n | 235/229 (103%) | 233 (99%) | 2 (1%) | 78 | 91 |
| 2 | 1o | 236/229 (103%) | 234 (99%) | 2 (1%) | 81 | 93 |
| 2 | 1p | 235/229 (103%) | 233 (99%) | 2 (1%) | 78 | 91 |
| 2 | 1q | 236/229 (103%) | 234 (99%) | 2 (1%) | 81 | 93 |
| 2 | 1r | 235/229 (103%) | 233 (99%) | 2 (1%) | 78 | 91 |
| 2 | 1s | 236/229 (103%) | 234 (99%) | 2 (1%) | 81 | 93 |
| 2 | 1t | 235/229 (103%) | 233 (99%) | 2 (1%) | 78 | 91 |
| 2 | 1u | 236/229 (103%) | 234 (99%) | 2 (1%) | 81 | 93 |
| 2 | 1v | 235/229 (103%) | 233 (99%) | 2 (1%) | 78 | 91 |
| 2 | 1w | 236/229 (103%) | 234 (99%) | 2 (1%) | 81 | 93 |
| 2 | 1x | 235/229 (103%) | 233 (99%) | 2 (1%) | 78 | 91 |
| 2 | 2Z | 236/229 (103%) | 234 (99%) | 2 (1%) | 81 | 93 |
| 2 | 2a | 236/229 (103%) | 234 (99%) | 2 (1%) | 81 | 93 |
| 2 | 2b | 236/229 (103%) | 234 (99%) | 2 (1%) | 81 | 93 |
| 2 | 2c | 236/229 (103%) | 234 (99%) | 2 (1%) | 81 | 93 |

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| Mol | Chain | Analysed | Rotameric | Outliers | Percentiles | |
|-----|-------|----------------|-----------|----------|-------------|----|
| 2 | 2d | 236/229 (103%) | 234 (99%) | 2 (1%) | 81 | 93 |
| 2 | 2e | 236/229 (103%) | 234 (99%) | 2 (1%) | 81 | 93 |
| 2 | 2f | 236/229 (103%) | 234 (99%) | 2 (1%) | 81 | 93 |
| 2 | 2g | 236/229 (103%) | 234 (99%) | 2 (1%) | 81 | 93 |
| 2 | 2h | 236/229 (103%) | 234 (99%) | 2 (1%) | 81 | 93 |
| 2 | 2i | 236/229 (103%) | 234 (99%) | 2 (1%) | 81 | 93 |
| 2 | 2j | 236/229 (103%) | 234 (99%) | 2 (1%) | 81 | 93 |
| 2 | 2k | 236/229 (103%) | 234 (99%) | 2 (1%) | 81 | 93 |
| 2 | 2l | 236/229 (103%) | 234 (99%) | 2 (1%) | 81 | 93 |
| 2 | 2m | 236/229 (103%) | 234 (99%) | 2 (1%) | 81 | 93 |
| 2 | 2n | 236/229 (103%) | 234 (99%) | 2 (1%) | 81 | 93 |
| 2 | 2o | 236/229 (103%) | 234 (99%) | 2 (1%) | 81 | 93 |
| 2 | 2p | 236/229 (103%) | 234 (99%) | 2 (1%) | 81 | 93 |
| 2 | 2q | 236/229 (103%) | 234 (99%) | 2 (1%) | 81 | 93 |
| 2 | 2r | 236/229 (103%) | 234 (99%) | 2 (1%) | 81 | 93 |
| 2 | 2s | 236/229 (103%) | 234 (99%) | 2 (1%) | 81 | 93 |
| 2 | 2t | 236/229 (103%) | 234 (99%) | 2 (1%) | 81 | 93 |
| 2 | 2u | 236/229 (103%) | 234 (99%) | 2 (1%) | 81 | 93 |
| 2 | 2v | 236/229 (103%) | 234 (99%) | 2 (1%) | 81 | 93 |
| 2 | 2w | 236/229 (103%) | 234 (99%) | 2 (1%) | 81 | 93 |
| 2 | 2x | 236/229 (103%) | 234 (99%) | 2 (1%) | 81 | 93 |
| 2 | 3e | 235/229 (103%) | 233 (99%) | 2 (1%) | 78 | 91 |
| 2 | 3f | 236/229 (103%) | 234 (99%) | 2 (1%) | 81 | 93 |
| 2 | 3g | 235/229 (103%) | 233 (99%) | 2 (1%) | 78 | 91 |
| 2 | 3h | 236/229 (103%) | 234 (99%) | 2 (1%) | 81 | 93 |
| 2 | 3i | 235/229 (103%) | 233 (99%) | 2 (1%) | 78 | 91 |
| 2 | 3j | 236/229 (103%) | 234 (99%) | 2 (1%) | 81 | 93 |
| 2 | 3k | 235/229 (103%) | 233 (99%) | 2 (1%) | 78 | 91 |
| 2 | 3l | 236/229 (103%) | 234 (99%) | 2 (1%) | 81 | 93 |
| 2 | 3m | 235/229 (103%) | 233 (99%) | 2 (1%) | 78 | 91 |
| 2 | 3n | 236/229 (103%) | 234 (99%) | 2 (1%) | 81 | 93 |

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| Mol | Chain | Analysed | Rotameric | Outliers | Percentiles | |
|-----|-------|----------------|-----------|----------|-------------|----|
| 2 | 3o | 235/229 (103%) | 233 (99%) | 2 (1%) | 78 | 91 |
| 2 | 3p | 236/229 (103%) | 234 (99%) | 2 (1%) | 81 | 93 |
| 2 | 3q | 235/229 (103%) | 233 (99%) | 2 (1%) | 78 | 91 |
| 2 | 3r | 236/229 (103%) | 234 (99%) | 2 (1%) | 81 | 93 |
| 2 | 3s | 235/229 (103%) | 233 (99%) | 2 (1%) | 78 | 91 |
| 2 | 3t | 236/229 (103%) | 234 (99%) | 2 (1%) | 81 | 93 |
| 2 | 3u | 235/229 (103%) | 233 (99%) | 2 (1%) | 78 | 91 |
| 2 | 3v | 236/229 (103%) | 234 (99%) | 2 (1%) | 81 | 93 |
| 2 | 3w | 235/229 (103%) | 233 (99%) | 2 (1%) | 78 | 91 |
| 2 | 3x | 236/229 (103%) | 234 (99%) | 2 (1%) | 81 | 93 |
| 2 | 4e | 236/229 (103%) | 234 (99%) | 2 (1%) | 81 | 93 |
| 2 | 4f | 235/229 (103%) | 233 (99%) | 2 (1%) | 78 | 91 |
| 2 | 4g | 236/229 (103%) | 234 (99%) | 2 (1%) | 81 | 93 |
| 2 | 4h | 235/229 (103%) | 233 (99%) | 2 (1%) | 78 | 91 |
| 2 | 4i | 236/229 (103%) | 234 (99%) | 2 (1%) | 81 | 93 |
| 2 | 4j | 235/229 (103%) | 233 (99%) | 2 (1%) | 78 | 91 |
| 2 | 4k | 236/229 (103%) | 234 (99%) | 2 (1%) | 81 | 93 |
| 2 | 4l | 235/229 (103%) | 233 (99%) | 2 (1%) | 78 | 91 |
| 2 | 4m | 236/229 (103%) | 234 (99%) | 2 (1%) | 81 | 93 |
| 2 | 4n | 235/229 (103%) | 233 (99%) | 2 (1%) | 78 | 91 |
| 2 | 5e | 236/229 (103%) | 234 (99%) | 2 (1%) | 81 | 93 |
| 2 | 5f | 235/229 (103%) | 233 (99%) | 2 (1%) | 78 | 91 |
| 2 | 5g | 236/229 (103%) | 234 (99%) | 2 (1%) | 81 | 93 |
| 2 | 5h | 235/229 (103%) | 233 (99%) | 2 (1%) | 78 | 91 |
| 2 | 5i | 236/229 (103%) | 234 (99%) | 2 (1%) | 81 | 93 |
| 2 | 5j | 235/229 (103%) | 233 (99%) | 2 (1%) | 78 | 91 |
| 2 | 5k | 236/229 (103%) | 234 (99%) | 2 (1%) | 81 | 93 |
| 2 | 5l | 235/229 (103%) | 233 (99%) | 2 (1%) | 78 | 91 |
| 2 | 5m | 236/229 (103%) | 234 (99%) | 2 (1%) | 81 | 93 |
| 2 | 5n | 235/229 (103%) | 233 (99%) | 2 (1%) | 78 | 91 |
| 2 | 6e | 235/229 (103%) | 233 (99%) | 2 (1%) | 78 | 91 |

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| Mol | Chain | Analysed | Rotameric | Outliers | Percentiles | |
|-----|-------|----------------|-----------|----------|-------------|----|
| 2 | 6f | 236/229 (103%) | 234 (99%) | 2 (1%) | 81 | 93 |
| 2 | 6g | 235/229 (103%) | 233 (99%) | 2 (1%) | 78 | 91 |
| 2 | 6h | 236/229 (103%) | 234 (99%) | 2 (1%) | 81 | 93 |
| 2 | 6i | 235/229 (103%) | 233 (99%) | 2 (1%) | 78 | 91 |
| 2 | 6j | 236/229 (103%) | 234 (99%) | 2 (1%) | 81 | 93 |
| 2 | 6k | 235/229 (103%) | 233 (99%) | 2 (1%) | 78 | 91 |
| 2 | 6l | 236/229 (103%) | 234 (99%) | 2 (1%) | 81 | 93 |
| 2 | 6m | 235/229 (103%) | 233 (99%) | 2 (1%) | 78 | 91 |
| 2 | 6n | 236/229 (103%) | 234 (99%) | 2 (1%) | 81 | 93 |
| 2 | 6o | 235/229 (103%) | 233 (99%) | 2 (1%) | 78 | 91 |
| 2 | 6p | 236/229 (103%) | 234 (99%) | 2 (1%) | 81 | 93 |
| 2 | 6q | 235/229 (103%) | 233 (99%) | 2 (1%) | 78 | 91 |
| 2 | 6r | 236/229 (103%) | 234 (99%) | 2 (1%) | 81 | 93 |
| 2 | 6s | 235/229 (103%) | 233 (99%) | 2 (1%) | 78 | 91 |
| 2 | 6t | 236/229 (103%) | 234 (99%) | 2 (1%) | 81 | 93 |
| 2 | 6u | 235/229 (103%) | 233 (99%) | 2 (1%) | 78 | 91 |
| 2 | 6v | 236/229 (103%) | 234 (99%) | 2 (1%) | 81 | 93 |
| 2 | 6w | 235/229 (103%) | 233 (99%) | 2 (1%) | 78 | 91 |
| 2 | 6x | 236/229 (103%) | 234 (99%) | 2 (1%) | 81 | 93 |
| 2 | 7Z | 236/229 (103%) | 234 (99%) | 2 (1%) | 81 | 93 |
| 2 | 7a | 236/229 (103%) | 234 (99%) | 2 (1%) | 81 | 93 |
| 2 | 7b | 236/229 (103%) | 234 (99%) | 2 (1%) | 81 | 93 |
| 2 | 7c | 236/229 (103%) | 234 (99%) | 2 (1%) | 81 | 93 |
| 2 | 7d | 236/229 (103%) | 234 (99%) | 2 (1%) | 81 | 93 |
| 2 | 7e | 236/229 (103%) | 234 (99%) | 2 (1%) | 81 | 93 |
| 2 | 7f | 236/229 (103%) | 234 (99%) | 2 (1%) | 81 | 93 |
| 2 | 7g | 236/229 (103%) | 234 (99%) | 2 (1%) | 81 | 93 |
| 2 | 7h | 236/229 (103%) | 234 (99%) | 2 (1%) | 81 | 93 |
| 2 | 7i | 236/229 (103%) | 234 (99%) | 2 (1%) | 81 | 93 |
| 2 | 7j | 236/229 (103%) | 234 (99%) | 2 (1%) | 81 | 93 |
| 2 | 7k | 236/229 (103%) | 234 (99%) | 2 (1%) | 81 | 93 |

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| Mol | Chain | Analysed | Rotameric | Outliers | Percentiles | |
|-----|-------|----------------|-----------|----------|-------------|----|
| 2 | 7l | 236/229 (103%) | 234 (99%) | 2 (1%) | 81 | 93 |
| 2 | 7m | 236/229 (103%) | 234 (99%) | 2 (1%) | 81 | 93 |
| 2 | 7n | 236/229 (103%) | 234 (99%) | 2 (1%) | 81 | 93 |
| 2 | 7o | 236/229 (103%) | 234 (99%) | 2 (1%) | 81 | 93 |
| 2 | 7p | 236/229 (103%) | 234 (99%) | 2 (1%) | 81 | 93 |
| 2 | 7q | 236/229 (103%) | 234 (99%) | 2 (1%) | 81 | 93 |
| 2 | 7r | 236/229 (103%) | 234 (99%) | 2 (1%) | 81 | 93 |
| 2 | 7s | 236/229 (103%) | 234 (99%) | 2 (1%) | 81 | 93 |
| 2 | 7t | 236/229 (103%) | 234 (99%) | 2 (1%) | 81 | 93 |
| 2 | 7u | 236/229 (103%) | 234 (99%) | 2 (1%) | 81 | 93 |
| 2 | 7v | 236/229 (103%) | 234 (99%) | 2 (1%) | 81 | 93 |
| 2 | 7w | 236/229 (103%) | 234 (99%) | 2 (1%) | 81 | 93 |
| 2 | 7x | 236/229 (103%) | 234 (99%) | 2 (1%) | 81 | 93 |
| 2 | 8e | 235/229 (103%) | 233 (99%) | 2 (1%) | 78 | 91 |
| 2 | 8f | 236/229 (103%) | 234 (99%) | 2 (1%) | 81 | 93 |
| 2 | 8g | 236/229 (103%) | 234 (99%) | 2 (1%) | 81 | 93 |
| 2 | 8h | 235/229 (103%) | 233 (99%) | 2 (1%) | 78 | 91 |
| 2 | 8i | 236/229 (103%) | 234 (99%) | 2 (1%) | 81 | 93 |
| 2 | 8j | 235/229 (103%) | 233 (99%) | 2 (1%) | 78 | 91 |
| 2 | 8k | 235/229 (103%) | 233 (99%) | 2 (1%) | 78 | 91 |
| 2 | 8l | 236/229 (103%) | 234 (99%) | 2 (1%) | 81 | 93 |
| 2 | 8m | 236/229 (103%) | 234 (99%) | 2 (1%) | 81 | 93 |
| 2 | 8n | 235/229 (103%) | 233 (99%) | 2 (1%) | 78 | 91 |
| 2 | 8o | 236/229 (103%) | 234 (99%) | 2 (1%) | 81 | 93 |
| 2 | 8p | 235/229 (103%) | 233 (99%) | 2 (1%) | 78 | 91 |
| 2 | 8q | 235/229 (103%) | 233 (99%) | 2 (1%) | 78 | 91 |
| 2 | 8r | 236/229 (103%) | 234 (99%) | 2 (1%) | 81 | 93 |
| 2 | 8s | 236/229 (103%) | 234 (99%) | 2 (1%) | 81 | 93 |
| 2 | 8t | 235/229 (103%) | 233 (99%) | 2 (1%) | 78 | 91 |
| 2 | 8u | 236/229 (103%) | 234 (99%) | 2 (1%) | 81 | 93 |
| 2 | 8v | 235/229 (103%) | 233 (99%) | 2 (1%) | 78 | 91 |

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| Mol | Chain | Analysed | Rotameric | Outliers | Percentiles | |
|-----|-------|----------------------|---------------|----------|-------------|----|
| 2 | 8w | 235/229 (103%) | 233 (99%) | 2 (1%) | 78 | 91 |
| 2 | 8x | 236/229 (103%) | 234 (99%) | 2 (1%) | 81 | 93 |
| 2 | 8y | 236/229 (103%) | 234 (99%) | 2 (1%) | 81 | 93 |
| 2 | 8z | 235/229 (103%) | 233 (99%) | 2 (1%) | 78 | 91 |
| 2 | 9F | 236/229 (103%) | 234 (99%) | 2 (1%) | 81 | 93 |
| 2 | 9G | 236/229 (103%) | 234 (99%) | 2 (1%) | 81 | 93 |
| 2 | 9H | 236/229 (103%) | 234 (99%) | 2 (1%) | 81 | 93 |
| 2 | 9I | 236/229 (103%) | 234 (99%) | 2 (1%) | 81 | 93 |
| 2 | 9J | 236/229 (103%) | 234 (99%) | 2 (1%) | 81 | 93 |
| 2 | 9K | 236/229 (103%) | 234 (99%) | 2 (1%) | 81 | 93 |
| 2 | 9L | 235/229 (103%) | 233 (99%) | 2 (1%) | 78 | 91 |
| 2 | 9M | 235/229 (103%) | 233 (99%) | 2 (1%) | 78 | 91 |
| 2 | 9N | 236/229 (103%) | 234 (99%) | 2 (1%) | 81 | 93 |
| 2 | 9O | 236/229 (103%) | 234 (99%) | 2 (1%) | 81 | 93 |
| 2 | 9P | 235/229 (103%) | 233 (99%) | 2 (1%) | 78 | 91 |
| 2 | 9Q | 236/229 (103%) | 234 (99%) | 2 (1%) | 81 | 93 |
| 2 | 9R | 235/229 (103%) | 233 (99%) | 2 (1%) | 78 | 91 |
| All | All | 127985/128025 (100%) | 127456 (100%) | 529 (0%) | 91 | 95 |

All (529) residues with a non-rotameric sidechain are listed below:

| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1 | 1A | 95 | ARG |
| 1 | 1A | 195 | PHE |
| 1 | 1B | 25 | ARG |
| 1 | 1B | 275 | PHE |
| 1 | 1D | 266 | LYS |
| 1 | 1D | 275 | PHE |
| 1 | 1F | 357 | ASN |
| 1 | 2A | 356 | PRO |
| 1 | 2B | 295 | VAL |
| 1 | 2B | 356 | PRO |
| 1 | 2C | 312 | VAL |
| 1 | 2E | 357 | ASN |
| 1 | 3A | 397 | THR |
| 1 | 3B | 275 | PHE |

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| Mol | Chain | Res | Type |
|------------|--------------|------------|-------------|
| 1 | 3C | 438 | ARG |
| 1 | 3D | 260 | ASP |
| 1 | 3F | 241 | ARG |
| 1 | 4B | 295 | VAL |
| 1 | 4E | 195 | PHE |
| 1 | 4F | 195 | PHE |
| 1 | 5A | 295 | VAL |
| 1 | 5B | 312 | VAL |
| 1 | 5C | 188 | ASN |
| 1 | 5C | 295 | VAL |
| 1 | 5C | 303 | TYR |
| 1 | 5F | 241 | ARG |
| 1 | 5F | 303 | TYR |
| 1 | 5F | 425 | LYS |
| 1 | 6A | 195 | PHE |
| 1 | 6D | 303 | TYR |
| 1 | 7A | 59 | ASN |
| 1 | 7A | 195 | PHE |
| 1 | 7A | 295 | VAL |
| 1 | 7C | 357 | ASN |
| 1 | 8C | 275 | PHE |
| 1 | 8C | 300 | PHE |
| 1 | 8F | 95 | ARG |
| 1 | 9A | 59 | ASN |
| 1 | 9A | 241 | ARG |
| 1 | 1G | 95 | ARG |
| 1 | 1G | 195 | PHE |
| 1 | 1H | 25 | ARG |
| 1 | 1H | 275 | PHE |
| 1 | 1J | 266 | LYS |
| 1 | 1J | 275 | PHE |
| 1 | 1J | 387 | VAL |
| 1 | 1L | 357 | ASN |
| 1 | 2F | 356 | PRO |
| 1 | 2G | 295 | VAL |
| 1 | 2G | 356 | PRO |
| 1 | 2H | 312 | VAL |
| 1 | 2J | 357 | ASN |
| 1 | 3G | 397 | THR |
| 1 | 3H | 275 | PHE |
| 1 | 3I | 438 | ARG |
| 1 | 3J | 260 | ASP |

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| Mol | Chain | Res | Type |
|------------|--------------|------------|-------------|
| 1 | 3L | 241 | ARG |
| 1 | 4H | 295 | VAL |
| 1 | 4K | 195 | PHE |
| 1 | 4L | 195 | PHE |
| 1 | 5G | 295 | VAL |
| 1 | 5H | 312 | VAL |
| 1 | 5I | 188 | ASN |
| 1 | 5I | 295 | VAL |
| 1 | 5I | 303 | TYR |
| 1 | 5L | 241 | ARG |
| 1 | 5L | 303 | TYR |
| 1 | 5L | 425 | LYS |
| 1 | 6G | 195 | PHE |
| 1 | 6J | 303 | TYR |
| 1 | 7F | 59 | ASN |
| 1 | 7F | 195 | PHE |
| 1 | 7F | 295 | VAL |
| 1 | 7H | 357 | ASN |
| 1 | 8I | 275 | PHE |
| 1 | 8I | 300 | PHE |
| 1 | 8L | 95 | ARG |
| 1 | 9B | 59 | ASN |
| 1 | 9B | 241 | ARG |
| 1 | 1M | 95 | ARG |
| 1 | 1M | 195 | PHE |
| 1 | 1N | 25 | ARG |
| 1 | 1N | 275 | PHE |
| 1 | 1P | 266 | LYS |
| 1 | 1P | 275 | PHE |
| 1 | 1R | 357 | ASN |
| 1 | 2K | 356 | PRO |
| 1 | 2L | 295 | VAL |
| 1 | 2L | 356 | PRO |
| 1 | 2M | 312 | VAL |
| 1 | 2O | 357 | ASN |
| 1 | 3M | 397 | THR |
| 1 | 3N | 275 | PHE |
| 1 | 3O | 438 | ARG |
| 1 | 3P | 260 | ASP |
| 1 | 3R | 241 | ARG |
| 1 | 4N | 295 | VAL |
| 1 | 4Q | 195 | PHE |

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Continued from previous page...

| Mol | Chain | Res | Type |
|------------|--------------|------------|-------------|
| 1 | 4R | 195 | PHE |
| 1 | 5M | 295 | VAL |
| 1 | 5N | 312 | VAL |
| 1 | 5O | 188 | ASN |
| 1 | 5O | 295 | VAL |
| 1 | 5O | 303 | TYR |
| 1 | 5R | 241 | ARG |
| 1 | 5R | 303 | TYR |
| 1 | 5R | 425 | LYS |
| 1 | 6M | 195 | PHE |
| 1 | 6P | 303 | TYR |
| 1 | 7K | 59 | ASN |
| 1 | 7K | 195 | PHE |
| 1 | 7K | 295 | VAL |
| 1 | 7M | 357 | ASN |
| 1 | 8O | 275 | PHE |
| 1 | 8O | 300 | PHE |
| 1 | 8R | 95 | ARG |
| 1 | 9C | 59 | ASN |
| 1 | 9C | 241 | ARG |
| 1 | 1S | 95 | ARG |
| 1 | 1S | 195 | PHE |
| 1 | 1T | 25 | ARG |
| 1 | 1T | 275 | PHE |
| 1 | 1V | 266 | LYS |
| 1 | 1V | 275 | PHE |
| 1 | 1V | 387 | VAL |
| 1 | 1X | 357 | ASN |
| 1 | 2P | 356 | PRO |
| 1 | 2Q | 295 | VAL |
| 1 | 2Q | 356 | PRO |
| 1 | 2R | 312 | VAL |
| 1 | 2T | 357 | ASN |
| 1 | 3S | 397 | THR |
| 1 | 3T | 275 | PHE |
| 1 | 3U | 438 | ARG |
| 1 | 3V | 260 | ASP |
| 1 | 3X | 241 | ARG |
| 1 | 4T | 295 | VAL |
| 1 | 4W | 195 | PHE |
| 1 | 4X | 195 | PHE |
| 1 | 5S | 295 | VAL |

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| Mol | Chain | Res | Type |
|------------|--------------|------------|-------------|
| 1 | 5T | 312 | VAL |
| 1 | 5U | 188 | ASN |
| 1 | 5U | 295 | VAL |
| 1 | 5U | 300 | PHE |
| 1 | 5U | 303 | TYR |
| 1 | 5X | 241 | ARG |
| 1 | 5X | 303 | TYR |
| 1 | 5X | 425 | LYS |
| 1 | 6S | 195 | PHE |
| 1 | 6V | 303 | TYR |
| 1 | 7P | 59 | ASN |
| 1 | 7P | 195 | PHE |
| 1 | 7P | 295 | VAL |
| 1 | 7R | 357 | ASN |
| 1 | 8U | 275 | PHE |
| 1 | 8U | 300 | PHE |
| 1 | 8X | 95 | ARG |
| 1 | 9D | 59 | ASN |
| 1 | 9D | 241 | ARG |
| 1 | 1Y | 95 | ARG |
| 1 | 1Y | 195 | PHE |
| 1 | 1Z | 25 | ARG |
| 1 | 1Z | 275 | PHE |
| 1 | 1b | 266 | LYS |
| 1 | 1b | 275 | PHE |
| 1 | 1b | 387 | VAL |
| 1 | 1d | 357 | ASN |
| 1 | 2U | 356 | PRO |
| 1 | 2V | 295 | VAL |
| 1 | 2V | 356 | PRO |
| 1 | 2W | 312 | VAL |
| 1 | 2Y | 357 | ASN |
| 1 | 3Y | 397 | THR |
| 1 | 3Z | 275 | PHE |
| 1 | 3a | 438 | ARG |
| 1 | 3b | 260 | ASP |
| 1 | 3d | 241 | ARG |
| 1 | 4Z | 295 | VAL |
| 1 | 4c | 195 | PHE |
| 1 | 4d | 195 | PHE |
| 1 | 5Y | 295 | VAL |
| 1 | 5Z | 312 | VAL |

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| Mol | Chain | Res | Type |
|------------|--------------|------------|-------------|
| 1 | 5a | 188 | ASN |
| 1 | 5a | 295 | VAL |
| 1 | 5a | 303 | TYR |
| 1 | 5d | 241 | ARG |
| 1 | 5d | 303 | TYR |
| 1 | 5d | 425 | LYS |
| 1 | 6Y | 195 | PHE |
| 1 | 6b | 303 | TYR |
| 1 | 7U | 59 | ASN |
| 1 | 7U | 195 | PHE |
| 1 | 7U | 295 | VAL |
| 1 | 7W | 357 | ASN |
| 1 | 8a | 275 | PHE |
| 1 | 8a | 300 | PHE |
| 1 | 8d | 95 | ARG |
| 1 | 9E | 59 | ASN |
| 1 | 9E | 241 | ARG |
| 2 | 1e | 110 | LEU |
| 2 | 1e | 251 | VAL |
| 2 | 1f | 116 | LYS |
| 2 | 1f | 251 | VAL |
| 2 | 1g | 110 | LEU |
| 2 | 1g | 251 | VAL |
| 2 | 1h | 116 | LYS |
| 2 | 1h | 251 | VAL |
| 2 | 2Z | 119 | SER |
| 2 | 2Z | 251 | VAL |
| 2 | 2a | 119 | SER |
| 2 | 2a | 251 | VAL |
| 2 | 2b | 119 | SER |
| 2 | 2b | 251 | VAL |
| 2 | 2c | 119 | SER |
| 2 | 2c | 251 | VAL |
| 2 | 2d | 119 | SER |
| 2 | 2d | 251 | VAL |
| 2 | 3e | 116 | LYS |
| 2 | 3e | 251 | VAL |
| 2 | 3f | 110 | LEU |
| 2 | 3f | 251 | VAL |
| 2 | 3g | 116 | LYS |
| 2 | 3g | 251 | VAL |
| 2 | 3h | 110 | LEU |

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| Mol | Chain | Res | Type |
|------------|--------------|------------|-------------|
| 2 | 3h | 251 | VAL |
| 2 | 4e | 110 | LEU |
| 2 | 4e | 251 | VAL |
| 2 | 4f | 116 | LYS |
| 2 | 4f | 251 | VAL |
| 2 | 5e | 110 | LEU |
| 2 | 5e | 251 | VAL |
| 2 | 5f | 116 | LYS |
| 2 | 5f | 251 | VAL |
| 2 | 6e | 116 | LYS |
| 2 | 6e | 251 | VAL |
| 2 | 6f | 110 | LEU |
| 2 | 6f | 251 | VAL |
| 2 | 6g | 116 | LYS |
| 2 | 6g | 251 | VAL |
| 2 | 6h | 110 | LEU |
| 2 | 6h | 251 | VAL |
| 2 | 7Z | 119 | SER |
| 2 | 7Z | 251 | VAL |
| 2 | 7a | 119 | SER |
| 2 | 7a | 251 | VAL |
| 2 | 7b | 119 | SER |
| 2 | 7b | 251 | VAL |
| 2 | 7c | 119 | SER |
| 2 | 7c | 251 | VAL |
| 2 | 7d | 119 | SER |
| 2 | 7d | 251 | VAL |
| 2 | 8e | 116 | LYS |
| 2 | 8e | 251 | VAL |
| 2 | 8f | 110 | LEU |
| 2 | 8f | 251 | VAL |
| 2 | 8g | 110 | LEU |
| 2 | 8g | 251 | VAL |
| 2 | 8h | 116 | LYS |
| 2 | 8h | 251 | VAL |
| 2 | 8i | 110 | LEU |
| 2 | 8i | 251 | VAL |
| 2 | 8j | 116 | LYS |
| 2 | 8j | 251 | VAL |
| 2 | 9F | 119 | SER |
| 2 | 9F | 251 | VAL |
| 2 | 1i | 110 | LEU |

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| Mol | Chain | Res | Type |
|------------|--------------|------------|-------------|
| 2 | 1i | 251 | VAL |
| 2 | 1j | 116 | LYS |
| 2 | 1j | 251 | VAL |
| 2 | 1k | 110 | LEU |
| 2 | 1k | 251 | VAL |
| 2 | 1l | 116 | LYS |
| 2 | 1l | 251 | VAL |
| 2 | 2e | 119 | SER |
| 2 | 2e | 251 | VAL |
| 2 | 2f | 119 | SER |
| 2 | 2f | 251 | VAL |
| 2 | 2g | 119 | SER |
| 2 | 2g | 251 | VAL |
| 2 | 2h | 119 | SER |
| 2 | 2h | 251 | VAL |
| 2 | 2i | 119 | SER |
| 2 | 2i | 251 | VAL |
| 2 | 3i | 116 | LYS |
| 2 | 3i | 251 | VAL |
| 2 | 3j | 110 | LEU |
| 2 | 3j | 251 | VAL |
| 2 | 3k | 116 | LYS |
| 2 | 3k | 251 | VAL |
| 2 | 3l | 110 | LEU |
| 2 | 3l | 251 | VAL |
| 2 | 4g | 110 | LEU |
| 2 | 4g | 251 | VAL |
| 2 | 4h | 116 | LYS |
| 2 | 4h | 251 | VAL |
| 2 | 5g | 110 | LEU |
| 2 | 5g | 251 | VAL |
| 2 | 5h | 116 | LYS |
| 2 | 5h | 251 | VAL |
| 2 | 6i | 116 | LYS |
| 2 | 6i | 251 | VAL |
| 2 | 6j | 110 | LEU |
| 2 | 6j | 251 | VAL |
| 2 | 6k | 116 | LYS |
| 2 | 6k | 251 | VAL |
| 2 | 6l | 110 | LEU |
| 2 | 6l | 251 | VAL |
| 2 | 7e | 119 | SER |

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Continued from previous page...

| Mol | Chain | Res | Type |
|------------|--------------|------------|-------------|
| 2 | 7e | 251 | VAL |
| 2 | 7f | 119 | SER |
| 2 | 7f | 251 | VAL |
| 2 | 7g | 119 | SER |
| 2 | 7g | 251 | VAL |
| 2 | 7h | 119 | SER |
| 2 | 7h | 251 | VAL |
| 2 | 7i | 119 | SER |
| 2 | 7i | 251 | VAL |
| 2 | 8k | 116 | LYS |
| 2 | 8k | 251 | VAL |
| 2 | 8l | 110 | LEU |
| 2 | 8l | 251 | VAL |
| 2 | 8m | 110 | LEU |
| 2 | 8m | 251 | VAL |
| 2 | 8n | 116 | LYS |
| 2 | 8n | 251 | VAL |
| 2 | 8o | 110 | LEU |
| 2 | 8o | 251 | VAL |
| 2 | 8p | 116 | LYS |
| 2 | 8p | 251 | VAL |
| 2 | 9G | 119 | SER |
| 2 | 9G | 251 | VAL |
| 2 | 1m | 110 | LEU |
| 2 | 1m | 251 | VAL |
| 2 | 1n | 116 | LYS |
| 2 | 1n | 251 | VAL |
| 2 | 1o | 110 | LEU |
| 2 | 1o | 251 | VAL |
| 2 | 1p | 116 | LYS |
| 2 | 1p | 251 | VAL |
| 2 | 2j | 119 | SER |
| 2 | 2j | 251 | VAL |
| 2 | 2k | 119 | SER |
| 2 | 2k | 251 | VAL |
| 2 | 2l | 119 | SER |
| 2 | 2l | 251 | VAL |
| 2 | 2m | 119 | SER |
| 2 | 2m | 251 | VAL |
| 2 | 2n | 119 | SER |
| 2 | 2n | 251 | VAL |
| 2 | 3m | 116 | LYS |

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Continued from previous page...

| Mol | Chain | Res | Type |
|------------|--------------|------------|-------------|
| 2 | 3m | 251 | VAL |
| 2 | 3n | 110 | LEU |
| 2 | 3n | 251 | VAL |
| 2 | 3o | 116 | LYS |
| 2 | 3o | 251 | VAL |
| 2 | 3p | 110 | LEU |
| 2 | 3p | 251 | VAL |
| 2 | 4i | 110 | LEU |
| 2 | 4i | 251 | VAL |
| 2 | 4j | 116 | LYS |
| 2 | 4j | 251 | VAL |
| 2 | 5i | 110 | LEU |
| 2 | 5i | 251 | VAL |
| 2 | 5j | 116 | LYS |
| 2 | 5j | 251 | VAL |
| 2 | 6m | 116 | LYS |
| 2 | 6m | 251 | VAL |
| 2 | 6n | 110 | LEU |
| 2 | 6n | 251 | VAL |
| 2 | 6o | 116 | LYS |
| 2 | 6o | 251 | VAL |
| 2 | 6p | 110 | LEU |
| 2 | 6p | 251 | VAL |
| 2 | 7j | 119 | SER |
| 2 | 7j | 251 | VAL |
| 2 | 7k | 119 | SER |
| 2 | 7k | 251 | VAL |
| 2 | 7l | 119 | SER |
| 2 | 7l | 251 | VAL |
| 2 | 7m | 119 | SER |
| 2 | 7m | 251 | VAL |
| 2 | 7n | 119 | SER |
| 2 | 7n | 251 | VAL |
| 2 | 8q | 116 | LYS |
| 2 | 8q | 251 | VAL |
| 2 | 8r | 110 | LEU |
| 2 | 8r | 251 | VAL |
| 2 | 8s | 110 | LEU |
| 2 | 8s | 251 | VAL |
| 2 | 8t | 116 | LYS |
| 2 | 8t | 251 | VAL |
| 2 | 8u | 110 | LEU |

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Continued from previous page...

| Mol | Chain | Res | Type |
|------------|--------------|------------|-------------|
| 2 | 8u | 251 | VAL |
| 2 | 8v | 116 | LYS |
| 2 | 8v | 251 | VAL |
| 2 | 9H | 119 | SER |
| 2 | 9H | 251 | VAL |
| 2 | 1q | 110 | LEU |
| 2 | 1q | 251 | VAL |
| 2 | 1r | 116 | LYS |
| 2 | 1r | 251 | VAL |
| 2 | 1s | 110 | LEU |
| 2 | 1s | 251 | VAL |
| 2 | 1t | 116 | LYS |
| 2 | 1t | 251 | VAL |
| 2 | 2o | 119 | SER |
| 2 | 2o | 251 | VAL |
| 2 | 2p | 119 | SER |
| 2 | 2p | 251 | VAL |
| 2 | 2q | 119 | SER |
| 2 | 2q | 251 | VAL |
| 2 | 2r | 119 | SER |
| 2 | 2r | 251 | VAL |
| 2 | 2s | 119 | SER |
| 2 | 2s | 251 | VAL |
| 2 | 3q | 116 | LYS |
| 2 | 3q | 251 | VAL |
| 2 | 3r | 110 | LEU |
| 2 | 3r | 251 | VAL |
| 2 | 3s | 116 | LYS |
| 2 | 3s | 251 | VAL |
| 2 | 3t | 110 | LEU |
| 2 | 3t | 251 | VAL |
| 2 | 4k | 110 | LEU |
| 2 | 4k | 251 | VAL |
| 2 | 4l | 116 | LYS |
| 2 | 4l | 251 | VAL |
| 2 | 5k | 110 | LEU |
| 2 | 5k | 251 | VAL |
| 2 | 5l | 116 | LYS |
| 2 | 5l | 251 | VAL |
| 2 | 6q | 116 | LYS |
| 2 | 6q | 251 | VAL |
| 2 | 6r | 110 | LEU |

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Continued from previous page...

| Mol | Chain | Res | Type |
|------------|--------------|------------|-------------|
| 2 | 6r | 251 | VAL |
| 2 | 6s | 116 | LYS |
| 2 | 6s | 251 | VAL |
| 2 | 6t | 110 | LEU |
| 2 | 6t | 251 | VAL |
| 2 | 7o | 119 | SER |
| 2 | 7o | 251 | VAL |
| 2 | 7p | 119 | SER |
| 2 | 7p | 251 | VAL |
| 2 | 7q | 119 | SER |
| 2 | 7q | 251 | VAL |
| 2 | 7r | 119 | SER |
| 2 | 7r | 251 | VAL |
| 2 | 7s | 119 | SER |
| 2 | 7s | 251 | VAL |
| 2 | 8w | 116 | LYS |
| 2 | 8w | 251 | VAL |
| 2 | 8x | 110 | LEU |
| 2 | 8x | 251 | VAL |
| 2 | 8y | 110 | LEU |
| 2 | 8y | 251 | VAL |
| 2 | 8z | 116 | LYS |
| 2 | 8z | 251 | VAL |
| 2 | 9K | 110 | LEU |
| 2 | 9K | 251 | VAL |
| 2 | 9L | 116 | LYS |
| 2 | 9L | 251 | VAL |
| 2 | 9I | 119 | SER |
| 2 | 9I | 251 | VAL |
| 2 | 1u | 110 | LEU |
| 2 | 1u | 251 | VAL |
| 2 | 1v | 116 | LYS |
| 2 | 1v | 251 | VAL |
| 2 | 1w | 110 | LEU |
| 2 | 1w | 251 | VAL |
| 2 | 1x | 116 | LYS |
| 2 | 1x | 251 | VAL |
| 2 | 2t | 119 | SER |
| 2 | 2t | 251 | VAL |
| 2 | 2u | 119 | SER |
| 2 | 2u | 251 | VAL |
| 2 | 2v | 119 | SER |

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| Mol | Chain | Res | Type |
|------------|--------------|------------|-------------|
| 2 | 2v | 251 | VAL |
| 2 | 2w | 119 | SER |
| 2 | 2w | 251 | VAL |
| 2 | 2x | 119 | SER |
| 2 | 2x | 251 | VAL |
| 2 | 3u | 116 | LYS |
| 2 | 3u | 251 | VAL |
| 2 | 3v | 110 | LEU |
| 2 | 3v | 251 | VAL |
| 2 | 3w | 116 | LYS |
| 2 | 3w | 251 | VAL |
| 2 | 3x | 110 | LEU |
| 2 | 3x | 251 | VAL |
| 2 | 4m | 110 | LEU |
| 2 | 4m | 251 | VAL |
| 2 | 4n | 116 | LYS |
| 2 | 4n | 251 | VAL |
| 2 | 5m | 110 | LEU |
| 2 | 5m | 251 | VAL |
| 2 | 5n | 116 | LYS |
| 2 | 5n | 251 | VAL |
| 2 | 6u | 116 | LYS |
| 2 | 6u | 251 | VAL |
| 2 | 6v | 110 | LEU |
| 2 | 6v | 251 | VAL |
| 2 | 6w | 116 | LYS |
| 2 | 6w | 251 | VAL |
| 2 | 6x | 110 | LEU |
| 2 | 6x | 251 | VAL |
| 2 | 7t | 119 | SER |
| 2 | 7t | 251 | VAL |
| 2 | 7u | 119 | SER |
| 2 | 7u | 251 | VAL |
| 2 | 7v | 119 | SER |
| 2 | 7v | 251 | VAL |
| 2 | 7w | 119 | SER |
| 2 | 7w | 251 | VAL |
| 2 | 7x | 119 | SER |
| 2 | 7x | 251 | VAL |
| 2 | 9M | 116 | LYS |
| 2 | 9M | 251 | VAL |
| 2 | 9N | 110 | LEU |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 2 | 9N | 251 | VAL |
| 2 | 9O | 110 | LEU |
| 2 | 9O | 251 | VAL |
| 2 | 9P | 116 | LYS |
| 2 | 9P | 251 | VAL |
| 2 | 9Q | 110 | LEU |
| 2 | 9Q | 251 | VAL |
| 2 | 9R | 116 | LYS |
| 2 | 9R | 251 | VAL |
| 2 | 9J | 119 | SER |
| 2 | 9J | 251 | VAL |

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (1524) such sidechains are listed below:

| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1 | 1A | 168 | ASN |
| 1 | 1A | 234 | ASN |
| 1 | 1A | 328 | GLN |
| 1 | 1A | 357 | ASN |
| 1 | 1B | 55 | GLN |
| 1 | 1B | 228 | GLN |
| 1 | 1C | 234 | ASN |
| 1 | 1C | 328 | GLN |
| 1 | 1D | 117 | GLN |
| 1 | 1D | 141 | HIS |
| 1 | 1D | 142 | GLN |
| 1 | 1D | 145 | GLN |
| 1 | 1E | 328 | GLN |
| 1 | 1E | 337 | ASN |
| 1 | 1F | 278 | ASN |
| 1 | 1F | 351 | GLN |
| 1 | 1F | 410 | ASN |
| 1 | 2A | 26 | ASN |
| 1 | 2A | 43 | ASN |
| 1 | 2A | 305 | ASN |
| 1 | 2B | 278 | ASN |
| 1 | 2C | 28 | GLN |
| 1 | 2C | 135 | ASN |
| 1 | 2C | 168 | ASN |
| 1 | 2C | 278 | ASN |
| 1 | 2C | 351 | GLN |
| 1 | 2D | 28 | GLN |

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| Mol | Chain | Res | Type |
|------------|--------------|------------|-------------|
| 1 | 2E | 76 | GLN |
| 1 | 2E | 168 | ASN |
| 1 | 2E | 407 | ASN |
| 1 | 2E | 410 | ASN |
| 1 | 3A | 54 | ASN |
| 1 | 3A | 55 | GLN |
| 1 | 3A | 269 | ASN |
| 1 | 3B | 26 | ASN |
| 1 | 3B | 76 | GLN |
| 1 | 3B | 135 | ASN |
| 1 | 3B | 142 | GLN |
| 1 | 3B | 357 | ASN |
| 1 | 3C | 137 | GLN |
| 1 | 3C | 328 | GLN |
| 1 | 3C | 337 | ASN |
| 1 | 3D | 305 | ASN |
| 1 | 3D | 337 | ASN |
| 1 | 3E | 269 | ASN |
| 1 | 3E | 337 | ASN |
| 1 | 3E | 407 | ASN |
| 1 | 3F | 22 | ASN |
| 1 | 3F | 43 | ASN |
| 1 | 3F | 337 | ASN |
| 1 | 3F | 381 | HIS |
| 1 | 3F | 447 | GLN |
| 1 | 4A | 76 | GLN |
| 1 | 4A | 135 | ASN |
| 1 | 4A | 141 | HIS |
| 1 | 4A | 168 | ASN |
| 1 | 4A | 278 | ASN |
| 1 | 4B | 76 | GLN |
| 1 | 4B | 278 | ASN |
| 1 | 4B | 305 | ASN |
| 1 | 4B | 411 | GLN |
| 1 | 4C | 363 | GLN |
| 1 | 4C | 407 | ASN |
| 1 | 4D | 141 | HIS |
| 1 | 4D | 328 | GLN |
| 1 | 4D | 337 | ASN |
| 1 | 4E | 135 | ASN |
| 1 | 4E | 168 | ASN |
| 1 | 4E | 278 | ASN |

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| Mol | Chain | Res | Type |
|------------|--------------|------------|-------------|
| 1 | 4F | 142 | GLN |
| 1 | 4F | 407 | ASN |
| 1 | 5A | 145 | GLN |
| 1 | 5A | 234 | ASN |
| 1 | 5A | 328 | GLN |
| 1 | 5A | 337 | ASN |
| 1 | 5A | 363 | GLN |
| 1 | 5A | 407 | ASN |
| 1 | 5C | 168 | ASN |
| 1 | 5C | 188 | ASN |
| 1 | 5C | 278 | ASN |
| 1 | 5C | 305 | ASN |
| 1 | 5C | 366 | GLN |
| 1 | 5D | 168 | ASN |
| 1 | 5D | 278 | ASN |
| 1 | 5D | 328 | GLN |
| 1 | 5E | 22 | ASN |
| 1 | 5E | 26 | ASN |
| 1 | 5E | 76 | GLN |
| 1 | 5E | 234 | ASN |
| 1 | 5E | 269 | ASN |
| 1 | 5E | 278 | ASN |
| 1 | 5E | 328 | GLN |
| 1 | 5E | 410 | ASN |
| 1 | 5F | 76 | GLN |
| 1 | 5F | 145 | GLN |
| 1 | 5F | 328 | GLN |
| 1 | 5F | 337 | ASN |
| 1 | 6A | 278 | ASN |
| 1 | 6A | 328 | GLN |
| 1 | 6B | 305 | ASN |
| 1 | 6C | 135 | ASN |
| 1 | 6D | 142 | GLN |
| 1 | 6E | 278 | ASN |
| 1 | 6E | 321 | ASN |
| 1 | 7A | 28 | GLN |
| 1 | 7A | 59 | ASN |
| 1 | 7A | 76 | GLN |
| 1 | 7A | 168 | ASN |
| 1 | 7A | 328 | GLN |
| 1 | 7B | 26 | ASN |
| 1 | 7B | 43 | ASN |

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| Mol | Chain | Res | Type |
|------------|--------------|------------|-------------|
| 1 | 7B | 321 | ASN |
| 1 | 7C | 22 | ASN |
| 1 | 7C | 28 | GLN |
| 1 | 7C | 248 | HIS |
| 1 | 7D | 26 | ASN |
| 1 | 7D | 137 | GLN |
| 1 | 7D | 168 | ASN |
| 1 | 7D | 234 | ASN |
| 1 | 7D | 366 | GLN |
| 1 | 7D | 447 | GLN |
| 1 | 8A | 305 | ASN |
| 1 | 8A | 337 | ASN |
| 1 | 8B | 234 | ASN |
| 1 | 8B | 278 | ASN |
| 1 | 8B | 328 | GLN |
| 1 | 8C | 76 | GLN |
| 1 | 8C | 337 | ASN |
| 1 | 8C | 363 | GLN |
| 1 | 8D | 22 | ASN |
| 1 | 8D | 328 | GLN |
| 1 | 8E | 141 | HIS |
| 1 | 8E | 168 | ASN |
| 1 | 8E | 278 | ASN |
| 1 | 8E | 328 | GLN |
| 1 | 8E | 363 | GLN |
| 1 | 8F | 168 | ASN |
| 1 | 8F | 234 | ASN |
| 1 | 8F | 278 | ASN |
| 1 | 8F | 328 | GLN |
| 1 | 8F | 407 | ASN |
| 1 | 9A | 28 | GLN |
| 1 | 9A | 59 | ASN |
| 1 | 9A | 76 | GLN |
| 1 | 9A | 142 | GLN |
| 1 | 9A | 168 | ASN |
| 1 | 9A | 269 | ASN |
| 1 | 9A | 357 | ASN |
| 1 | 1G | 168 | ASN |
| 1 | 1G | 234 | ASN |
| 1 | 1G | 328 | GLN |
| 1 | 1G | 357 | ASN |
| 1 | 1H | 55 | GLN |

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Continued from previous page...

| Mol | Chain | Res | Type |
|------------|--------------|------------|-------------|
| 1 | 1H | 228 | GLN |
| 1 | 1I | 234 | ASN |
| 1 | 1I | 328 | GLN |
| 1 | 1J | 117 | GLN |
| 1 | 1J | 141 | HIS |
| 1 | 1J | 142 | GLN |
| 1 | 1J | 145 | GLN |
| 1 | 1K | 328 | GLN |
| 1 | 1L | 278 | ASN |
| 1 | 1L | 351 | GLN |
| 1 | 1L | 410 | ASN |
| 1 | 2F | 26 | ASN |
| 1 | 2F | 43 | ASN |
| 1 | 2F | 305 | ASN |
| 1 | 2G | 278 | ASN |
| 1 | 2H | 28 | GLN |
| 1 | 2H | 135 | ASN |
| 1 | 2H | 168 | ASN |
| 1 | 2H | 278 | ASN |
| 1 | 2H | 351 | GLN |
| 1 | 2I | 28 | GLN |
| 1 | 2J | 76 | GLN |
| 1 | 2J | 168 | ASN |
| 1 | 2J | 407 | ASN |
| 1 | 3G | 54 | ASN |
| 1 | 3G | 55 | GLN |
| 1 | 3G | 269 | ASN |
| 1 | 3H | 26 | ASN |
| 1 | 3H | 76 | GLN |
| 1 | 3H | 135 | ASN |
| 1 | 3H | 142 | GLN |
| 1 | 3H | 357 | ASN |
| 1 | 3I | 137 | GLN |
| 1 | 3I | 328 | GLN |
| 1 | 3I | 337 | ASN |
| 1 | 3J | 305 | ASN |
| 1 | 3J | 337 | ASN |
| 1 | 3K | 337 | ASN |
| 1 | 3K | 407 | ASN |
| 1 | 3L | 22 | ASN |
| 1 | 3L | 43 | ASN |
| 1 | 3L | 337 | ASN |

Continued on next page...

Continued from previous page...

| Mol | Chain | Res | Type |
|------------|--------------|------------|-------------|
| 1 | 3L | 381 | HIS |
| 1 | 3L | 447 | GLN |
| 1 | 4G | 76 | GLN |
| 1 | 4G | 135 | ASN |
| 1 | 4G | 141 | HIS |
| 1 | 4G | 142 | GLN |
| 1 | 4G | 168 | ASN |
| 1 | 4G | 278 | ASN |
| 1 | 4H | 76 | GLN |
| 1 | 4H | 278 | ASN |
| 1 | 4H | 305 | ASN |
| 1 | 4H | 411 | GLN |
| 1 | 4I | 363 | GLN |
| 1 | 4I | 407 | ASN |
| 1 | 4J | 141 | HIS |
| 1 | 4J | 328 | GLN |
| 1 | 4J | 337 | ASN |
| 1 | 4K | 135 | ASN |
| 1 | 4K | 168 | ASN |
| 1 | 4K | 278 | ASN |
| 1 | 4L | 142 | GLN |
| 1 | 4L | 407 | ASN |
| 1 | 5G | 145 | GLN |
| 1 | 5G | 234 | ASN |
| 1 | 5G | 328 | GLN |
| 1 | 5G | 363 | GLN |
| 1 | 5G | 407 | ASN |
| 1 | 5I | 168 | ASN |
| 1 | 5I | 188 | ASN |
| 1 | 5I | 278 | ASN |
| 1 | 5I | 305 | ASN |
| 1 | 5I | 366 | GLN |
| 1 | 5J | 168 | ASN |
| 1 | 5J | 278 | ASN |
| 1 | 5J | 328 | GLN |
| 1 | 5J | 351 | GLN |
| 1 | 5K | 22 | ASN |
| 1 | 5K | 26 | ASN |
| 1 | 5K | 76 | GLN |
| 1 | 5K | 234 | ASN |
| 1 | 5K | 269 | ASN |
| 1 | 5K | 278 | ASN |

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Continued from previous page...

| Mol | Chain | Res | Type |
|------------|--------------|------------|-------------|
| 1 | 5K | 328 | GLN |
| 1 | 5K | 410 | ASN |
| 1 | 5L | 76 | GLN |
| 1 | 5L | 145 | GLN |
| 1 | 5L | 328 | GLN |
| 1 | 5L | 337 | ASN |
| 1 | 6G | 278 | ASN |
| 1 | 6G | 328 | GLN |
| 1 | 6H | 305 | ASN |
| 1 | 6I | 135 | ASN |
| 1 | 6J | 142 | GLN |
| 1 | 6K | 278 | ASN |
| 1 | 6K | 321 | ASN |
| 1 | 7F | 28 | GLN |
| 1 | 7F | 59 | ASN |
| 1 | 7F | 76 | GLN |
| 1 | 7F | 168 | ASN |
| 1 | 7F | 328 | GLN |
| 1 | 7G | 26 | ASN |
| 1 | 7G | 43 | ASN |
| 1 | 7G | 321 | ASN |
| 1 | 7H | 22 | ASN |
| 1 | 7H | 28 | GLN |
| 1 | 7H | 248 | HIS |
| 1 | 7I | 137 | GLN |
| 1 | 7I | 168 | ASN |
| 1 | 7I | 234 | ASN |
| 1 | 7I | 366 | GLN |
| 1 | 7I | 447 | GLN |
| 1 | 8G | 145 | GLN |
| 1 | 8G | 305 | ASN |
| 1 | 8G | 337 | ASN |
| 1 | 8H | 234 | ASN |
| 1 | 8H | 278 | ASN |
| 1 | 8H | 328 | GLN |
| 1 | 8I | 76 | GLN |
| 1 | 8I | 337 | ASN |
| 1 | 8I | 363 | GLN |
| 1 | 8J | 22 | ASN |
| 1 | 8J | 328 | GLN |
| 1 | 8K | 141 | HIS |
| 1 | 8K | 168 | ASN |

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| Mol | Chain | Res | Type |
|------------|--------------|------------|-------------|
| 1 | 8K | 278 | ASN |
| 1 | 8K | 328 | GLN |
| 1 | 8K | 363 | GLN |
| 1 | 8L | 168 | ASN |
| 1 | 8L | 234 | ASN |
| 1 | 8L | 278 | ASN |
| 1 | 8L | 328 | GLN |
| 1 | 8L | 407 | ASN |
| 1 | 9B | 28 | GLN |
| 1 | 9B | 59 | ASN |
| 1 | 9B | 76 | GLN |
| 1 | 9B | 142 | GLN |
| 1 | 9B | 168 | ASN |
| 1 | 9B | 269 | ASN |
| 1 | 9B | 357 | ASN |
| 1 | 1M | 168 | ASN |
| 1 | 1M | 234 | ASN |
| 1 | 1M | 328 | GLN |
| 1 | 1M | 357 | ASN |
| 1 | 1M | 377 | ASN |
| 1 | 1N | 55 | GLN |
| 1 | 1N | 228 | GLN |
| 1 | 1O | 234 | ASN |
| 1 | 1O | 328 | GLN |
| 1 | 1P | 117 | GLN |
| 1 | 1P | 141 | HIS |
| 1 | 1P | 142 | GLN |
| 1 | 1P | 145 | GLN |
| 1 | 1Q | 328 | GLN |
| 1 | 1R | 278 | ASN |
| 1 | 1R | 351 | GLN |
| 1 | 1R | 410 | ASN |
| 1 | 2K | 26 | ASN |
| 1 | 2K | 43 | ASN |
| 1 | 2K | 305 | ASN |
| 1 | 2L | 278 | ASN |
| 1 | 2M | 28 | GLN |
| 1 | 2M | 135 | ASN |
| 1 | 2M | 168 | ASN |
| 1 | 2M | 278 | ASN |
| 1 | 2M | 351 | GLN |
| 1 | 2N | 28 | GLN |

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| Mol | Chain | Res | Type |
|------------|--------------|------------|-------------|
| 1 | 2O | 76 | GLN |
| 1 | 2O | 168 | ASN |
| 1 | 2O | 407 | ASN |
| 1 | 2O | 410 | ASN |
| 1 | 3M | 54 | ASN |
| 1 | 3M | 55 | GLN |
| 1 | 3M | 269 | ASN |
| 1 | 3N | 26 | ASN |
| 1 | 3N | 76 | GLN |
| 1 | 3N | 135 | ASN |
| 1 | 3N | 142 | GLN |
| 1 | 3O | 137 | GLN |
| 1 | 3O | 328 | GLN |
| 1 | 3O | 337 | ASN |
| 1 | 3P | 305 | ASN |
| 1 | 3P | 337 | ASN |
| 1 | 3Q | 269 | ASN |
| 1 | 3Q | 337 | ASN |
| 1 | 3Q | 407 | ASN |
| 1 | 3R | 22 | ASN |
| 1 | 3R | 43 | ASN |
| 1 | 3R | 337 | ASN |
| 1 | 3R | 381 | HIS |
| 1 | 3R | 447 | GLN |
| 1 | 4M | 76 | GLN |
| 1 | 4M | 135 | ASN |
| 1 | 4M | 141 | HIS |
| 1 | 4M | 142 | GLN |
| 1 | 4M | 168 | ASN |
| 1 | 4M | 278 | ASN |
| 1 | 4N | 76 | GLN |
| 1 | 4N | 278 | ASN |
| 1 | 4N | 305 | ASN |
| 1 | 4N | 411 | GLN |
| 1 | 4O | 363 | GLN |
| 1 | 4O | 407 | ASN |
| 1 | 4P | 141 | HIS |
| 1 | 4P | 328 | GLN |
| 1 | 4P | 337 | ASN |
| 1 | 4Q | 135 | ASN |
| 1 | 4Q | 168 | ASN |
| 1 | 4Q | 278 | ASN |

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| Mol | Chain | Res | Type |
|------------|--------------|------------|-------------|
| 1 | 4R | 142 | GLN |
| 1 | 4R | 407 | ASN |
| 1 | 5M | 145 | GLN |
| 1 | 5M | 234 | ASN |
| 1 | 5M | 328 | GLN |
| 1 | 5M | 363 | GLN |
| 1 | 5M | 407 | ASN |
| 1 | 5O | 168 | ASN |
| 1 | 5O | 188 | ASN |
| 1 | 5O | 278 | ASN |
| 1 | 5O | 305 | ASN |
| 1 | 5O | 366 | GLN |
| 1 | 5P | 168 | ASN |
| 1 | 5P | 278 | ASN |
| 1 | 5P | 328 | GLN |
| 1 | 5P | 363 | GLN |
| 1 | 5Q | 22 | ASN |
| 1 | 5Q | 26 | ASN |
| 1 | 5Q | 76 | GLN |
| 1 | 5Q | 234 | ASN |
| 1 | 5Q | 269 | ASN |
| 1 | 5Q | 278 | ASN |
| 1 | 5Q | 328 | GLN |
| 1 | 5Q | 410 | ASN |
| 1 | 5R | 76 | GLN |
| 1 | 5R | 145 | GLN |
| 1 | 5R | 328 | GLN |
| 1 | 5R | 337 | ASN |
| 1 | 6M | 278 | ASN |
| 1 | 6M | 328 | GLN |
| 1 | 6N | 305 | ASN |
| 1 | 6O | 135 | ASN |
| 1 | 6P | 142 | GLN |
| 1 | 6Q | 168 | ASN |
| 1 | 6Q | 278 | ASN |
| 1 | 6Q | 321 | ASN |
| 1 | 7K | 28 | GLN |
| 1 | 7K | 59 | ASN |
| 1 | 7K | 76 | GLN |
| 1 | 7K | 168 | ASN |
| 1 | 7K | 328 | GLN |
| 1 | 7L | 26 | ASN |

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Continued from previous page...

| Mol | Chain | Res | Type |
|------------|--------------|------------|-------------|
| 1 | 7L | 43 | ASN |
| 1 | 7L | 269 | ASN |
| 1 | 7L | 321 | ASN |
| 1 | 7M | 22 | ASN |
| 1 | 7M | 28 | GLN |
| 1 | 7M | 248 | HIS |
| 1 | 7N | 26 | ASN |
| 1 | 7N | 137 | GLN |
| 1 | 7N | 168 | ASN |
| 1 | 7N | 234 | ASN |
| 1 | 7N | 366 | GLN |
| 1 | 7N | 447 | GLN |
| 1 | 8M | 305 | ASN |
| 1 | 8M | 337 | ASN |
| 1 | 8N | 234 | ASN |
| 1 | 8N | 278 | ASN |
| 1 | 8N | 328 | GLN |
| 1 | 8O | 76 | GLN |
| 1 | 8O | 337 | ASN |
| 1 | 8O | 363 | GLN |
| 1 | 8P | 22 | ASN |
| 1 | 8P | 328 | GLN |
| 1 | 8Q | 141 | HIS |
| 1 | 8Q | 168 | ASN |
| 1 | 8Q | 278 | ASN |
| 1 | 8Q | 328 | GLN |
| 1 | 8Q | 363 | GLN |
| 1 | 8R | 168 | ASN |
| 1 | 8R | 234 | ASN |
| 1 | 8R | 278 | ASN |
| 1 | 8R | 328 | GLN |
| 1 | 8R | 407 | ASN |
| 1 | 9C | 28 | GLN |
| 1 | 9C | 59 | ASN |
| 1 | 9C | 76 | GLN |
| 1 | 9C | 142 | GLN |
| 1 | 9C | 168 | ASN |
| 1 | 9C | 269 | ASN |
| 1 | 9C | 357 | ASN |
| 1 | 1S | 168 | ASN |
| 1 | 1S | 234 | ASN |
| 1 | 1S | 328 | GLN |

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Continued from previous page...

| Mol | Chain | Res | Type |
|------------|--------------|------------|-------------|
| 1 | 1S | 357 | ASN |
| 1 | 1S | 377 | ASN |
| 1 | 1T | 55 | GLN |
| 1 | 1T | 228 | GLN |
| 1 | 1U | 234 | ASN |
| 1 | 1U | 328 | GLN |
| 1 | 1V | 117 | GLN |
| 1 | 1V | 141 | HIS |
| 1 | 1V | 142 | GLN |
| 1 | 1V | 145 | GLN |
| 1 | 1W | 328 | GLN |
| 1 | 1X | 278 | ASN |
| 1 | 1X | 351 | GLN |
| 1 | 1X | 410 | ASN |
| 1 | 2P | 26 | ASN |
| 1 | 2P | 43 | ASN |
| 1 | 2P | 305 | ASN |
| 1 | 2P | 337 | ASN |
| 1 | 2Q | 278 | ASN |
| 1 | 2R | 28 | GLN |
| 1 | 2R | 135 | ASN |
| 1 | 2R | 278 | ASN |
| 1 | 2R | 351 | GLN |
| 1 | 2S | 28 | GLN |
| 1 | 2T | 76 | GLN |
| 1 | 2T | 168 | ASN |
| 1 | 2T | 407 | ASN |
| 1 | 2T | 410 | ASN |
| 1 | 3S | 55 | GLN |
| 1 | 3S | 269 | ASN |
| 1 | 3T | 26 | ASN |
| 1 | 3T | 76 | GLN |
| 1 | 3T | 135 | ASN |
| 1 | 3T | 142 | GLN |
| 1 | 3T | 357 | ASN |
| 1 | 3U | 137 | GLN |
| 1 | 3U | 328 | GLN |
| 1 | 3U | 337 | ASN |
| 1 | 3V | 305 | ASN |
| 1 | 3V | 337 | ASN |
| 1 | 3W | 269 | ASN |
| 1 | 3W | 328 | GLN |

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| Mol | Chain | Res | Type |
|------------|--------------|------------|-------------|
| 1 | 3W | 407 | ASN |
| 1 | 3X | 22 | ASN |
| 1 | 3X | 43 | ASN |
| 1 | 3X | 337 | ASN |
| 1 | 3X | 381 | HIS |
| 1 | 3X | 447 | GLN |
| 1 | 4S | 76 | GLN |
| 1 | 4S | 135 | ASN |
| 1 | 4S | 141 | HIS |
| 1 | 4S | 142 | GLN |
| 1 | 4S | 168 | ASN |
| 1 | 4S | 278 | ASN |
| 1 | 4T | 76 | GLN |
| 1 | 4T | 278 | ASN |
| 1 | 4T | 305 | ASN |
| 1 | 4T | 411 | GLN |
| 1 | 4U | 363 | GLN |
| 1 | 4U | 407 | ASN |
| 1 | 4V | 141 | HIS |
| 1 | 4V | 328 | GLN |
| 1 | 4V | 337 | ASN |
| 1 | 4W | 135 | ASN |
| 1 | 4W | 168 | ASN |
| 1 | 4W | 278 | ASN |
| 1 | 4X | 142 | GLN |
| 1 | 4X | 407 | ASN |
| 1 | 5S | 145 | GLN |
| 1 | 5S | 234 | ASN |
| 1 | 5S | 328 | GLN |
| 1 | 5S | 357 | ASN |
| 1 | 5S | 363 | GLN |
| 1 | 5S | 407 | ASN |
| 1 | 5U | 168 | ASN |
| 1 | 5U | 188 | ASN |
| 1 | 5U | 278 | ASN |
| 1 | 5U | 305 | ASN |
| 1 | 5U | 366 | GLN |
| 1 | 5V | 278 | ASN |
| 1 | 5V | 328 | GLN |
| 1 | 5W | 22 | ASN |
| 1 | 5W | 26 | ASN |
| 1 | 5W | 76 | GLN |

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| Mol | Chain | Res | Type |
|------------|--------------|------------|-------------|
| 1 | 5W | 234 | ASN |
| 1 | 5W | 269 | ASN |
| 1 | 5W | 278 | ASN |
| 1 | 5W | 328 | GLN |
| 1 | 5W | 410 | ASN |
| 1 | 5X | 76 | GLN |
| 1 | 5X | 145 | GLN |
| 1 | 5X | 328 | GLN |
| 1 | 5X | 337 | ASN |
| 1 | 6S | 278 | ASN |
| 1 | 6S | 328 | GLN |
| 1 | 6T | 305 | ASN |
| 1 | 6U | 135 | ASN |
| 1 | 6V | 142 | GLN |
| 1 | 6W | 168 | ASN |
| 1 | 6W | 278 | ASN |
| 1 | 6W | 321 | ASN |
| 1 | 7P | 28 | GLN |
| 1 | 7P | 59 | ASN |
| 1 | 7P | 76 | GLN |
| 1 | 7P | 168 | ASN |
| 1 | 7P | 328 | GLN |
| 1 | 7Q | 26 | ASN |
| 1 | 7Q | 43 | ASN |
| 1 | 7Q | 269 | ASN |
| 1 | 7Q | 321 | ASN |
| 1 | 7R | 22 | ASN |
| 1 | 7R | 28 | GLN |
| 1 | 7R | 248 | HIS |
| 1 | 7S | 137 | GLN |
| 1 | 7S | 168 | ASN |
| 1 | 7S | 234 | ASN |
| 1 | 7S | 366 | GLN |
| 1 | 7S | 447 | GLN |
| 1 | 8S | 305 | ASN |
| 1 | 8S | 337 | ASN |
| 1 | 8T | 234 | ASN |
| 1 | 8T | 278 | ASN |
| 1 | 8T | 328 | GLN |
| 1 | 8U | 76 | GLN |
| 1 | 8U | 337 | ASN |
| 1 | 8U | 363 | GLN |

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| Mol | Chain | Res | Type |
|------------|--------------|------------|-------------|
| 1 | 8V | 22 | ASN |
| 1 | 8V | 328 | GLN |
| 1 | 8W | 141 | HIS |
| 1 | 8W | 168 | ASN |
| 1 | 8W | 278 | ASN |
| 1 | 8W | 328 | GLN |
| 1 | 8W | 337 | ASN |
| 1 | 8W | 363 | GLN |
| 1 | 8X | 168 | ASN |
| 1 | 8X | 234 | ASN |
| 1 | 8X | 278 | ASN |
| 1 | 8X | 328 | GLN |
| 1 | 8X | 407 | ASN |
| 1 | 9D | 28 | GLN |
| 1 | 9D | 59 | ASN |
| 1 | 9D | 76 | GLN |
| 1 | 9D | 142 | GLN |
| 1 | 9D | 168 | ASN |
| 1 | 9D | 357 | ASN |
| 1 | 1Y | 168 | ASN |
| 1 | 1Y | 234 | ASN |
| 1 | 1Y | 328 | GLN |
| 1 | 1Y | 357 | ASN |
| 1 | 1Z | 55 | GLN |
| 1 | 1Z | 228 | GLN |
| 1 | 1a | 234 | ASN |
| 1 | 1a | 328 | GLN |
| 1 | 1b | 117 | GLN |
| 1 | 1b | 141 | HIS |
| 1 | 1b | 142 | GLN |
| 1 | 1b | 145 | GLN |
| 1 | 1c | 328 | GLN |
| 1 | 1d | 278 | ASN |
| 1 | 1d | 351 | GLN |
| 1 | 1d | 410 | ASN |
| 1 | 2U | 26 | ASN |
| 1 | 2U | 43 | ASN |
| 1 | 2U | 305 | ASN |
| 1 | 2V | 278 | ASN |
| 1 | 2W | 28 | GLN |
| 1 | 2W | 135 | ASN |
| 1 | 2W | 168 | ASN |

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| Mol | Chain | Res | Type |
|------------|--------------|------------|-------------|
| 1 | 2W | 278 | ASN |
| 1 | 2W | 351 | GLN |
| 1 | 2X | 28 | GLN |
| 1 | 2Y | 76 | GLN |
| 1 | 2Y | 168 | ASN |
| 1 | 2Y | 407 | ASN |
| 1 | 2Y | 410 | ASN |
| 1 | 3Y | 54 | ASN |
| 1 | 3Y | 55 | GLN |
| 1 | 3Y | 269 | ASN |
| 1 | 3Z | 26 | ASN |
| 1 | 3Z | 76 | GLN |
| 1 | 3Z | 135 | ASN |
| 1 | 3Z | 142 | GLN |
| 1 | 3Z | 357 | ASN |
| 1 | 3a | 137 | GLN |
| 1 | 3a | 328 | GLN |
| 1 | 3a | 337 | ASN |
| 1 | 3b | 305 | ASN |
| 1 | 3b | 337 | ASN |
| 1 | 3c | 269 | ASN |
| 1 | 3c | 337 | ASN |
| 1 | 3c | 407 | ASN |
| 1 | 3d | 22 | ASN |
| 1 | 3d | 43 | ASN |
| 1 | 3d | 337 | ASN |
| 1 | 3d | 381 | HIS |
| 1 | 3d | 447 | GLN |
| 1 | 4Y | 76 | GLN |
| 1 | 4Y | 135 | ASN |
| 1 | 4Y | 141 | HIS |
| 1 | 4Y | 168 | ASN |
| 1 | 4Y | 278 | ASN |
| 1 | 4Z | 76 | GLN |
| 1 | 4Z | 278 | ASN |
| 1 | 4Z | 305 | ASN |
| 1 | 4Z | 411 | GLN |
| 1 | 4a | 363 | GLN |
| 1 | 4a | 407 | ASN |
| 1 | 4b | 141 | HIS |
| 1 | 4b | 328 | GLN |
| 1 | 4b | 337 | ASN |

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| Mol | Chain | Res | Type |
|------------|--------------|------------|-------------|
| 1 | 4c | 135 | ASN |
| 1 | 4c | 168 | ASN |
| 1 | 4c | 278 | ASN |
| 1 | 4d | 142 | GLN |
| 1 | 4d | 407 | ASN |
| 1 | 5Y | 234 | ASN |
| 1 | 5Y | 328 | GLN |
| 1 | 5Y | 363 | GLN |
| 1 | 5Y | 407 | ASN |
| 1 | 5a | 168 | ASN |
| 1 | 5a | 188 | ASN |
| 1 | 5a | 278 | ASN |
| 1 | 5a | 305 | ASN |
| 1 | 5a | 366 | GLN |
| 1 | 5b | 168 | ASN |
| 1 | 5b | 278 | ASN |
| 1 | 5b | 328 | GLN |
| 1 | 5c | 22 | ASN |
| 1 | 5c | 26 | ASN |
| 1 | 5c | 76 | GLN |
| 1 | 5c | 234 | ASN |
| 1 | 5c | 269 | ASN |
| 1 | 5c | 278 | ASN |
| 1 | 5c | 328 | GLN |
| 1 | 5c | 410 | ASN |
| 1 | 5d | 76 | GLN |
| 1 | 5d | 145 | GLN |
| 1 | 5d | 328 | GLN |
| 1 | 5d | 337 | ASN |
| 1 | 6Y | 278 | ASN |
| 1 | 6Y | 328 | GLN |
| 1 | 6Z | 305 | ASN |
| 1 | 6a | 135 | ASN |
| 1 | 6b | 142 | GLN |
| 1 | 6c | 278 | ASN |
| 1 | 6c | 321 | ASN |
| 1 | 7U | 28 | GLN |
| 1 | 7U | 59 | ASN |
| 1 | 7U | 76 | GLN |
| 1 | 7U | 168 | ASN |
| 1 | 7U | 328 | GLN |
| 1 | 7V | 26 | ASN |

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| Mol | Chain | Res | Type |
|------------|--------------|------------|-------------|
| 1 | 7V | 43 | ASN |
| 1 | 7V | 269 | ASN |
| 1 | 7V | 321 | ASN |
| 1 | 7W | 22 | ASN |
| 1 | 7W | 28 | GLN |
| 1 | 7W | 248 | HIS |
| 1 | 7X | 26 | ASN |
| 1 | 7X | 137 | GLN |
| 1 | 7X | 168 | ASN |
| 1 | 7X | 234 | ASN |
| 1 | 7X | 366 | GLN |
| 1 | 7X | 447 | GLN |
| 1 | 8Y | 145 | GLN |
| 1 | 8Y | 305 | ASN |
| 1 | 8Y | 337 | ASN |
| 1 | 8Z | 234 | ASN |
| 1 | 8Z | 278 | ASN |
| 1 | 8Z | 328 | GLN |
| 1 | 8a | 76 | GLN |
| 1 | 8a | 337 | ASN |
| 1 | 8a | 363 | GLN |
| 1 | 8b | 22 | ASN |
| 1 | 8b | 328 | GLN |
| 1 | 8b | 337 | ASN |
| 1 | 8c | 141 | HIS |
| 1 | 8c | 168 | ASN |
| 1 | 8c | 278 | ASN |
| 1 | 8c | 328 | GLN |
| 1 | 8c | 363 | GLN |
| 1 | 8d | 168 | ASN |
| 1 | 8d | 234 | ASN |
| 1 | 8d | 278 | ASN |
| 1 | 8d | 328 | GLN |
| 1 | 8d | 407 | ASN |
| 1 | 9E | 28 | GLN |
| 1 | 9E | 59 | ASN |
| 1 | 9E | 76 | GLN |
| 1 | 9E | 142 | GLN |
| 1 | 9E | 168 | ASN |
| 1 | 9E | 269 | ASN |
| 1 | 9E | 357 | ASN |
| 1 | 9E | 411 | GLN |

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| Mol | Chain | Res | Type |
|------------|--------------|------------|-------------|
| 2 | 1e | 159 | ASN |
| 2 | 1e | 166 | ASN |
| 2 | 1e | 179 | ASN |
| 2 | 1e | 218 | ASN |
| 2 | 1f | 76 | ASN |
| 2 | 1f | 159 | ASN |
| 2 | 1f | 166 | ASN |
| 2 | 1f | 179 | ASN |
| 2 | 1f | 218 | ASN |
| 2 | 1g | 56 | ASN |
| 2 | 1g | 159 | ASN |
| 2 | 1g | 166 | ASN |
| 2 | 1g | 179 | ASN |
| 2 | 1g | 218 | ASN |
| 2 | 1h | 56 | ASN |
| 2 | 1h | 76 | ASN |
| 2 | 1h | 159 | ASN |
| 2 | 1h | 166 | ASN |
| 2 | 1h | 179 | ASN |
| 2 | 1h | 218 | ASN |
| 2 | 2Z | 159 | ASN |
| 2 | 2Z | 166 | ASN |
| 2 | 2Z | 179 | ASN |
| 2 | 2Z | 218 | ASN |
| 2 | 2a | 159 | ASN |
| 2 | 2a | 166 | ASN |
| 2 | 2a | 179 | ASN |
| 2 | 2a | 218 | ASN |
| 2 | 2b | 103 | GLN |
| 2 | 2b | 159 | ASN |
| 2 | 2b | 166 | ASN |
| 2 | 2b | 179 | ASN |
| 2 | 2b | 218 | ASN |
| 2 | 2c | 103 | GLN |
| 2 | 2c | 159 | ASN |
| 2 | 2c | 166 | ASN |
| 2 | 2c | 179 | ASN |
| 2 | 2c | 218 | ASN |
| 2 | 2d | 159 | ASN |
| 2 | 2d | 166 | ASN |
| 2 | 2d | 179 | ASN |
| 2 | 2d | 218 | ASN |

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| Mol | Chain | Res | Type |
|------------|--------------|------------|-------------|
| 2 | 3e | 56 | ASN |
| 2 | 3e | 76 | ASN |
| 2 | 3e | 159 | ASN |
| 2 | 3e | 166 | ASN |
| 2 | 3e | 179 | ASN |
| 2 | 3e | 218 | ASN |
| 2 | 3f | 159 | ASN |
| 2 | 3f | 166 | ASN |
| 2 | 3f | 179 | ASN |
| 2 | 3f | 218 | ASN |
| 2 | 3g | 56 | ASN |
| 2 | 3g | 76 | ASN |
| 2 | 3g | 159 | ASN |
| 2 | 3g | 166 | ASN |
| 2 | 3g | 179 | ASN |
| 2 | 3g | 218 | ASN |
| 2 | 3h | 159 | ASN |
| 2 | 3h | 166 | ASN |
| 2 | 3h | 179 | ASN |
| 2 | 3h | 218 | ASN |
| 2 | 4e | 159 | ASN |
| 2 | 4e | 166 | ASN |
| 2 | 4e | 179 | ASN |
| 2 | 4e | 218 | ASN |
| 2 | 4f | 76 | ASN |
| 2 | 4f | 159 | ASN |
| 2 | 4f | 166 | ASN |
| 2 | 4f | 179 | ASN |
| 2 | 4f | 218 | ASN |
| 2 | 5e | 159 | ASN |
| 2 | 5e | 166 | ASN |
| 2 | 5e | 179 | ASN |
| 2 | 5e | 218 | ASN |
| 2 | 5f | 56 | ASN |
| 2 | 5f | 76 | ASN |
| 2 | 5f | 159 | ASN |
| 2 | 5f | 166 | ASN |
| 2 | 5f | 179 | ASN |
| 2 | 5f | 218 | ASN |
| 2 | 6e | 23 | GLN |
| 2 | 6e | 76 | ASN |
| 2 | 6e | 159 | ASN |

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| Mol | Chain | Res | Type |
|------------|--------------|------------|-------------|
| 2 | 6e | 166 | ASN |
| 2 | 6e | 179 | ASN |
| 2 | 6e | 218 | ASN |
| 2 | 6f | 159 | ASN |
| 2 | 6f | 166 | ASN |
| 2 | 6f | 179 | ASN |
| 2 | 6f | 218 | ASN |
| 2 | 6g | 56 | ASN |
| 2 | 6g | 76 | ASN |
| 2 | 6g | 159 | ASN |
| 2 | 6g | 166 | ASN |
| 2 | 6g | 179 | ASN |
| 2 | 6g | 218 | ASN |
| 2 | 6h | 56 | ASN |
| 2 | 6h | 159 | ASN |
| 2 | 6h | 166 | ASN |
| 2 | 6h | 179 | ASN |
| 2 | 6h | 218 | ASN |
| 2 | 7Z | 64 | GLN |
| 2 | 7Z | 159 | ASN |
| 2 | 7Z | 166 | ASN |
| 2 | 7Z | 179 | ASN |
| 2 | 7Z | 218 | ASN |
| 2 | 7a | 159 | ASN |
| 2 | 7a | 166 | ASN |
| 2 | 7a | 179 | ASN |
| 2 | 7a | 218 | ASN |
| 2 | 7b | 23 | GLN |
| 2 | 7b | 159 | ASN |
| 2 | 7b | 166 | ASN |
| 2 | 7b | 179 | ASN |
| 2 | 7b | 218 | ASN |
| 2 | 7c | 159 | ASN |
| 2 | 7c | 166 | ASN |
| 2 | 7c | 179 | ASN |
| 2 | 7c | 218 | ASN |
| 2 | 7d | 159 | ASN |
| 2 | 7d | 166 | ASN |
| 2 | 7d | 179 | ASN |
| 2 | 7d | 218 | ASN |
| 2 | 8e | 76 | ASN |
| 2 | 8e | 159 | ASN |

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| Mol | Chain | Res | Type |
|------------|--------------|------------|-------------|
| 2 | 8e | 166 | ASN |
| 2 | 8e | 179 | ASN |
| 2 | 8e | 218 | ASN |
| 2 | 8f | 159 | ASN |
| 2 | 8f | 166 | ASN |
| 2 | 8f | 179 | ASN |
| 2 | 8f | 218 | ASN |
| 2 | 8g | 159 | ASN |
| 2 | 8g | 166 | ASN |
| 2 | 8g | 179 | ASN |
| 2 | 8g | 218 | ASN |
| 2 | 8h | 76 | ASN |
| 2 | 8h | 159 | ASN |
| 2 | 8h | 166 | ASN |
| 2 | 8h | 179 | ASN |
| 2 | 8h | 218 | ASN |
| 2 | 8i | 56 | ASN |
| 2 | 8i | 159 | ASN |
| 2 | 8i | 166 | ASN |
| 2 | 8i | 179 | ASN |
| 2 | 8i | 218 | ASN |
| 2 | 8j | 76 | ASN |
| 2 | 8j | 159 | ASN |
| 2 | 8j | 166 | ASN |
| 2 | 8j | 179 | ASN |
| 2 | 8j | 218 | ASN |
| 2 | 9F | 103 | GLN |
| 2 | 9F | 159 | ASN |
| 2 | 9F | 166 | ASN |
| 2 | 9F | 179 | ASN |
| 2 | 9F | 218 | ASN |
| 2 | 1i | 159 | ASN |
| 2 | 1i | 166 | ASN |
| 2 | 1i | 179 | ASN |
| 2 | 1i | 218 | ASN |
| 2 | 1j | 76 | ASN |
| 2 | 1j | 159 | ASN |
| 2 | 1j | 166 | ASN |
| 2 | 1j | 179 | ASN |
| 2 | 1j | 218 | ASN |
| 2 | 1k | 56 | ASN |
| 2 | 1k | 159 | ASN |

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| Mol | Chain | Res | Type |
|------------|--------------|------------|-------------|
| 2 | 1k | 166 | ASN |
| 2 | 1k | 179 | ASN |
| 2 | 1k | 218 | ASN |
| 2 | 1l | 56 | ASN |
| 2 | 1l | 76 | ASN |
| 2 | 1l | 159 | ASN |
| 2 | 1l | 166 | ASN |
| 2 | 1l | 179 | ASN |
| 2 | 1l | 218 | ASN |
| 2 | 2e | 159 | ASN |
| 2 | 2e | 166 | ASN |
| 2 | 2e | 179 | ASN |
| 2 | 2e | 218 | ASN |
| 2 | 2f | 159 | ASN |
| 2 | 2f | 166 | ASN |
| 2 | 2f | 179 | ASN |
| 2 | 2f | 218 | ASN |
| 2 | 2g | 103 | GLN |
| 2 | 2g | 159 | ASN |
| 2 | 2g | 166 | ASN |
| 2 | 2g | 179 | ASN |
| 2 | 2g | 218 | ASN |
| 2 | 2h | 103 | GLN |
| 2 | 2h | 159 | ASN |
| 2 | 2h | 166 | ASN |
| 2 | 2h | 179 | ASN |
| 2 | 2h | 218 | ASN |
| 2 | 2i | 159 | ASN |
| 2 | 2i | 166 | ASN |
| 2 | 2i | 179 | ASN |
| 2 | 2i | 218 | ASN |
| 2 | 3i | 56 | ASN |
| 2 | 3i | 76 | ASN |
| 2 | 3i | 159 | ASN |
| 2 | 3i | 166 | ASN |
| 2 | 3i | 179 | ASN |
| 2 | 3i | 218 | ASN |
| 2 | 3j | 159 | ASN |
| 2 | 3j | 166 | ASN |
| 2 | 3j | 179 | ASN |
| 2 | 3j | 218 | ASN |
| 2 | 3k | 56 | ASN |

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| Mol | Chain | Res | Type |
|------------|--------------|------------|-------------|
| 2 | 3k | 76 | ASN |
| 2 | 3k | 159 | ASN |
| 2 | 3k | 166 | ASN |
| 2 | 3k | 179 | ASN |
| 2 | 3k | 218 | ASN |
| 2 | 3l | 159 | ASN |
| 2 | 3l | 166 | ASN |
| 2 | 3l | 179 | ASN |
| 2 | 3l | 218 | ASN |
| 2 | 4g | 159 | ASN |
| 2 | 4g | 166 | ASN |
| 2 | 4g | 179 | ASN |
| 2 | 4g | 218 | ASN |
| 2 | 4h | 76 | ASN |
| 2 | 4h | 159 | ASN |
| 2 | 4h | 166 | ASN |
| 2 | 4h | 179 | ASN |
| 2 | 4h | 218 | ASN |
| 2 | 5g | 159 | ASN |
| 2 | 5g | 166 | ASN |
| 2 | 5g | 179 | ASN |
| 2 | 5g | 218 | ASN |
| 2 | 5h | 56 | ASN |
| 2 | 5h | 76 | ASN |
| 2 | 5h | 159 | ASN |
| 2 | 5h | 166 | ASN |
| 2 | 5h | 179 | ASN |
| 2 | 5h | 218 | ASN |
| 2 | 6i | 23 | GLN |
| 2 | 6i | 76 | ASN |
| 2 | 6i | 159 | ASN |
| 2 | 6i | 166 | ASN |
| 2 | 6i | 179 | ASN |
| 2 | 6i | 218 | ASN |
| 2 | 6j | 159 | ASN |
| 2 | 6j | 166 | ASN |
| 2 | 6j | 179 | ASN |
| 2 | 6j | 218 | ASN |
| 2 | 6k | 56 | ASN |
| 2 | 6k | 76 | ASN |
| 2 | 6k | 159 | ASN |
| 2 | 6k | 166 | ASN |

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| Mol | Chain | Res | Type |
|------------|--------------|------------|-------------|
| 2 | 6k | 179 | ASN |
| 2 | 6k | 218 | ASN |
| 2 | 6l | 56 | ASN |
| 2 | 6l | 159 | ASN |
| 2 | 6l | 166 | ASN |
| 2 | 6l | 179 | ASN |
| 2 | 6l | 218 | ASN |
| 2 | 7e | 64 | GLN |
| 2 | 7e | 159 | ASN |
| 2 | 7e | 166 | ASN |
| 2 | 7e | 179 | ASN |
| 2 | 7e | 218 | ASN |
| 2 | 7f | 159 | ASN |
| 2 | 7f | 166 | ASN |
| 2 | 7f | 179 | ASN |
| 2 | 7f | 218 | ASN |
| 2 | 7g | 159 | ASN |
| 2 | 7g | 166 | ASN |
| 2 | 7g | 179 | ASN |
| 2 | 7g | 218 | ASN |
| 2 | 7h | 159 | ASN |
| 2 | 7h | 166 | ASN |
| 2 | 7h | 179 | ASN |
| 2 | 7h | 218 | ASN |
| 2 | 7i | 159 | ASN |
| 2 | 7i | 166 | ASN |
| 2 | 7i | 179 | ASN |
| 2 | 7i | 218 | ASN |
| 2 | 8k | 76 | ASN |
| 2 | 8k | 159 | ASN |
| 2 | 8k | 166 | ASN |
| 2 | 8k | 179 | ASN |
| 2 | 8k | 218 | ASN |
| 2 | 8l | 159 | ASN |
| 2 | 8l | 166 | ASN |
| 2 | 8l | 179 | ASN |
| 2 | 8l | 218 | ASN |
| 2 | 8m | 159 | ASN |
| 2 | 8m | 166 | ASN |
| 2 | 8m | 179 | ASN |
| 2 | 8m | 218 | ASN |
| 2 | 8n | 76 | ASN |

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| Mol | Chain | Res | Type |
|------------|--------------|------------|-------------|
| 2 | 8n | 159 | ASN |
| 2 | 8n | 166 | ASN |
| 2 | 8n | 179 | ASN |
| 2 | 8n | 218 | ASN |
| 2 | 8o | 56 | ASN |
| 2 | 8o | 159 | ASN |
| 2 | 8o | 166 | ASN |
| 2 | 8o | 179 | ASN |
| 2 | 8o | 218 | ASN |
| 2 | 8p | 76 | ASN |
| 2 | 8p | 159 | ASN |
| 2 | 8p | 166 | ASN |
| 2 | 8p | 179 | ASN |
| 2 | 8p | 218 | ASN |
| 2 | 9G | 103 | GLN |
| 2 | 9G | 159 | ASN |
| 2 | 9G | 166 | ASN |
| 2 | 9G | 179 | ASN |
| 2 | 9G | 218 | ASN |
| 2 | 1m | 159 | ASN |
| 2 | 1m | 166 | ASN |
| 2 | 1m | 179 | ASN |
| 2 | 1m | 218 | ASN |
| 2 | 1n | 76 | ASN |
| 2 | 1n | 159 | ASN |
| 2 | 1n | 166 | ASN |
| 2 | 1n | 179 | ASN |
| 2 | 1n | 218 | ASN |
| 2 | 1o | 56 | ASN |
| 2 | 1o | 159 | ASN |
| 2 | 1o | 166 | ASN |
| 2 | 1o | 179 | ASN |
| 2 | 1o | 218 | ASN |
| 2 | 1p | 56 | ASN |
| 2 | 1p | 76 | ASN |
| 2 | 1p | 159 | ASN |
| 2 | 1p | 166 | ASN |
| 2 | 1p | 179 | ASN |
| 2 | 1p | 218 | ASN |
| 2 | 2j | 159 | ASN |
| 2 | 2j | 166 | ASN |
| 2 | 2j | 179 | ASN |

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| Mol | Chain | Res | Type |
|------------|--------------|------------|-------------|
| 2 | 2j | 218 | ASN |
| 2 | 2k | 159 | ASN |
| 2 | 2k | 166 | ASN |
| 2 | 2k | 179 | ASN |
| 2 | 2k | 218 | ASN |
| 2 | 2l | 103 | GLN |
| 2 | 2l | 159 | ASN |
| 2 | 2l | 166 | ASN |
| 2 | 2l | 179 | ASN |
| 2 | 2l | 218 | ASN |
| 2 | 2m | 103 | GLN |
| 2 | 2m | 159 | ASN |
| 2 | 2m | 166 | ASN |
| 2 | 2m | 179 | ASN |
| 2 | 2m | 218 | ASN |
| 2 | 2n | 159 | ASN |
| 2 | 2n | 166 | ASN |
| 2 | 2n | 179 | ASN |
| 2 | 2n | 218 | ASN |
| 2 | 3m | 56 | ASN |
| 2 | 3m | 76 | ASN |
| 2 | 3m | 159 | ASN |
| 2 | 3m | 166 | ASN |
| 2 | 3m | 179 | ASN |
| 2 | 3m | 218 | ASN |
| 2 | 3n | 159 | ASN |
| 2 | 3n | 166 | ASN |
| 2 | 3n | 179 | ASN |
| 2 | 3n | 218 | ASN |
| 2 | 3o | 56 | ASN |
| 2 | 3o | 76 | ASN |
| 2 | 3o | 159 | ASN |
| 2 | 3o | 166 | ASN |
| 2 | 3o | 179 | ASN |
| 2 | 3o | 218 | ASN |
| 2 | 3p | 159 | ASN |
| 2 | 3p | 166 | ASN |
| 2 | 3p | 179 | ASN |
| 2 | 3p | 218 | ASN |
| 2 | 4i | 159 | ASN |
| 2 | 4i | 166 | ASN |
| 2 | 4i | 179 | ASN |

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| Mol | Chain | Res | Type |
|------------|--------------|------------|-------------|
| 2 | 4i | 218 | ASN |
| 2 | 4j | 76 | ASN |
| 2 | 4j | 159 | ASN |
| 2 | 4j | 166 | ASN |
| 2 | 4j | 179 | ASN |
| 2 | 4j | 218 | ASN |
| 2 | 5i | 159 | ASN |
| 2 | 5i | 166 | ASN |
| 2 | 5i | 179 | ASN |
| 2 | 5i | 218 | ASN |
| 2 | 5j | 56 | ASN |
| 2 | 5j | 76 | ASN |
| 2 | 5j | 159 | ASN |
| 2 | 5j | 166 | ASN |
| 2 | 5j | 179 | ASN |
| 2 | 5j | 218 | ASN |
| 2 | 6m | 23 | GLN |
| 2 | 6m | 76 | ASN |
| 2 | 6m | 159 | ASN |
| 2 | 6m | 166 | ASN |
| 2 | 6m | 179 | ASN |
| 2 | 6m | 218 | ASN |
| 2 | 6n | 159 | ASN |
| 2 | 6n | 166 | ASN |
| 2 | 6n | 179 | ASN |
| 2 | 6n | 218 | ASN |
| 2 | 6o | 56 | ASN |
| 2 | 6o | 76 | ASN |
| 2 | 6o | 159 | ASN |
| 2 | 6o | 166 | ASN |
| 2 | 6o | 179 | ASN |
| 2 | 6o | 218 | ASN |
| 2 | 6p | 56 | ASN |
| 2 | 6p | 159 | ASN |
| 2 | 6p | 166 | ASN |
| 2 | 6p | 179 | ASN |
| 2 | 6p | 218 | ASN |
| 2 | 7j | 64 | GLN |
| 2 | 7j | 159 | ASN |
| 2 | 7j | 166 | ASN |
| 2 | 7j | 179 | ASN |
| 2 | 7j | 218 | ASN |

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| Mol | Chain | Res | Type |
|------------|--------------|------------|-------------|
| 2 | 7k | 159 | ASN |
| 2 | 7k | 166 | ASN |
| 2 | 7k | 179 | ASN |
| 2 | 7k | 218 | ASN |
| 2 | 7l | 23 | GLN |
| 2 | 7l | 159 | ASN |
| 2 | 7l | 166 | ASN |
| 2 | 7l | 179 | ASN |
| 2 | 7l | 218 | ASN |
| 2 | 7m | 159 | ASN |
| 2 | 7m | 166 | ASN |
| 2 | 7m | 179 | ASN |
| 2 | 7m | 218 | ASN |
| 2 | 7n | 159 | ASN |
| 2 | 7n | 166 | ASN |
| 2 | 7n | 179 | ASN |
| 2 | 7n | 218 | ASN |
| 2 | 8q | 76 | ASN |
| 2 | 8q | 159 | ASN |
| 2 | 8q | 166 | ASN |
| 2 | 8q | 179 | ASN |
| 2 | 8q | 218 | ASN |
| 2 | 8r | 159 | ASN |
| 2 | 8r | 166 | ASN |
| 2 | 8r | 179 | ASN |
| 2 | 8r | 218 | ASN |
| 2 | 8s | 159 | ASN |
| 2 | 8s | 166 | ASN |
| 2 | 8s | 179 | ASN |
| 2 | 8s | 218 | ASN |
| 2 | 8t | 76 | ASN |
| 2 | 8t | 159 | ASN |
| 2 | 8t | 166 | ASN |
| 2 | 8t | 179 | ASN |
| 2 | 8t | 218 | ASN |
| 2 | 8u | 56 | ASN |
| 2 | 8u | 159 | ASN |
| 2 | 8u | 166 | ASN |
| 2 | 8u | 179 | ASN |
| 2 | 8u | 218 | ASN |
| 2 | 8v | 76 | ASN |
| 2 | 8v | 159 | ASN |

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| Mol | Chain | Res | Type |
|------------|--------------|------------|-------------|
| 2 | 8v | 166 | ASN |
| 2 | 8v | 179 | ASN |
| 2 | 8v | 218 | ASN |
| 2 | 9H | 103 | GLN |
| 2 | 9H | 159 | ASN |
| 2 | 9H | 166 | ASN |
| 2 | 9H | 179 | ASN |
| 2 | 9H | 218 | ASN |
| 2 | 1q | 159 | ASN |
| 2 | 1q | 166 | ASN |
| 2 | 1q | 179 | ASN |
| 2 | 1q | 218 | ASN |
| 2 | 1r | 76 | ASN |
| 2 | 1r | 159 | ASN |
| 2 | 1r | 166 | ASN |
| 2 | 1r | 179 | ASN |
| 2 | 1r | 218 | ASN |
| 2 | 1s | 56 | ASN |
| 2 | 1s | 159 | ASN |
| 2 | 1s | 166 | ASN |
| 2 | 1s | 179 | ASN |
| 2 | 1s | 218 | ASN |
| 2 | 1t | 56 | ASN |
| 2 | 1t | 76 | ASN |
| 2 | 1t | 159 | ASN |
| 2 | 1t | 166 | ASN |
| 2 | 1t | 179 | ASN |
| 2 | 1t | 218 | ASN |
| 2 | 2o | 159 | ASN |
| 2 | 2o | 166 | ASN |
| 2 | 2o | 179 | ASN |
| 2 | 2o | 218 | ASN |
| 2 | 2p | 159 | ASN |
| 2 | 2p | 166 | ASN |
| 2 | 2p | 179 | ASN |
| 2 | 2p | 218 | ASN |
| 2 | 2q | 103 | GLN |
| 2 | 2q | 159 | ASN |
| 2 | 2q | 166 | ASN |
| 2 | 2q | 179 | ASN |
| 2 | 2q | 218 | ASN |
| 2 | 2r | 103 | GLN |

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| Mol | Chain | Res | Type |
|------------|--------------|------------|-------------|
| 2 | 2r | 159 | ASN |
| 2 | 2r | 166 | ASN |
| 2 | 2r | 179 | ASN |
| 2 | 2r | 218 | ASN |
| 2 | 2s | 159 | ASN |
| 2 | 2s | 166 | ASN |
| 2 | 2s | 179 | ASN |
| 2 | 2s | 218 | ASN |
| 2 | 3q | 56 | ASN |
| 2 | 3q | 76 | ASN |
| 2 | 3q | 159 | ASN |
| 2 | 3q | 166 | ASN |
| 2 | 3q | 179 | ASN |
| 2 | 3q | 218 | ASN |
| 2 | 3r | 159 | ASN |
| 2 | 3r | 166 | ASN |
| 2 | 3r | 179 | ASN |
| 2 | 3r | 218 | ASN |
| 2 | 3s | 56 | ASN |
| 2 | 3s | 76 | ASN |
| 2 | 3s | 159 | ASN |
| 2 | 3s | 166 | ASN |
| 2 | 3s | 179 | ASN |
| 2 | 3s | 218 | ASN |
| 2 | 3t | 159 | ASN |
| 2 | 3t | 166 | ASN |
| 2 | 3t | 179 | ASN |
| 2 | 3t | 218 | ASN |
| 2 | 4k | 159 | ASN |
| 2 | 4k | 166 | ASN |
| 2 | 4k | 179 | ASN |
| 2 | 4k | 218 | ASN |
| 2 | 4l | 76 | ASN |
| 2 | 4l | 159 | ASN |
| 2 | 4l | 166 | ASN |
| 2 | 4l | 179 | ASN |
| 2 | 4l | 218 | ASN |
| 2 | 5k | 159 | ASN |
| 2 | 5k | 166 | ASN |
| 2 | 5k | 179 | ASN |
| 2 | 5k | 218 | ASN |
| 2 | 5l | 56 | ASN |

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| Mol | Chain | Res | Type |
|------------|--------------|------------|-------------|
| 2 | 5l | 76 | ASN |
| 2 | 5l | 159 | ASN |
| 2 | 5l | 166 | ASN |
| 2 | 5l | 179 | ASN |
| 2 | 5l | 218 | ASN |
| 2 | 6q | 23 | GLN |
| 2 | 6q | 76 | ASN |
| 2 | 6q | 159 | ASN |
| 2 | 6q | 166 | ASN |
| 2 | 6q | 179 | ASN |
| 2 | 6q | 218 | ASN |
| 2 | 6r | 159 | ASN |
| 2 | 6r | 166 | ASN |
| 2 | 6r | 179 | ASN |
| 2 | 6r | 218 | ASN |
| 2 | 6s | 56 | ASN |
| 2 | 6s | 76 | ASN |
| 2 | 6s | 159 | ASN |
| 2 | 6s | 166 | ASN |
| 2 | 6s | 179 | ASN |
| 2 | 6s | 218 | ASN |
| 2 | 6t | 56 | ASN |
| 2 | 6t | 159 | ASN |
| 2 | 6t | 166 | ASN |
| 2 | 6t | 179 | ASN |
| 2 | 6t | 218 | ASN |
| 2 | 7o | 64 | GLN |
| 2 | 7o | 159 | ASN |
| 2 | 7o | 166 | ASN |
| 2 | 7o | 179 | ASN |
| 2 | 7o | 218 | ASN |
| 2 | 7p | 159 | ASN |
| 2 | 7p | 166 | ASN |
| 2 | 7p | 179 | ASN |
| 2 | 7p | 218 | ASN |
| 2 | 7q | 159 | ASN |
| 2 | 7q | 166 | ASN |
| 2 | 7q | 179 | ASN |
| 2 | 7q | 218 | ASN |
| 2 | 7r | 159 | ASN |
| 2 | 7r | 166 | ASN |
| 2 | 7r | 179 | ASN |

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| Mol | Chain | Res | Type |
|------------|--------------|------------|-------------|
| 2 | 7r | 218 | ASN |
| 2 | 7s | 159 | ASN |
| 2 | 7s | 166 | ASN |
| 2 | 7s | 179 | ASN |
| 2 | 7s | 218 | ASN |
| 2 | 8w | 76 | ASN |
| 2 | 8w | 159 | ASN |
| 2 | 8w | 166 | ASN |
| 2 | 8w | 179 | ASN |
| 2 | 8w | 218 | ASN |
| 2 | 8x | 159 | ASN |
| 2 | 8x | 166 | ASN |
| 2 | 8x | 179 | ASN |
| 2 | 8x | 218 | ASN |
| 2 | 8y | 159 | ASN |
| 2 | 8y | 166 | ASN |
| 2 | 8y | 179 | ASN |
| 2 | 8y | 218 | ASN |
| 2 | 8z | 76 | ASN |
| 2 | 8z | 159 | ASN |
| 2 | 8z | 166 | ASN |
| 2 | 8z | 179 | ASN |
| 2 | 8z | 218 | ASN |
| 2 | 9K | 56 | ASN |
| 2 | 9K | 159 | ASN |
| 2 | 9K | 166 | ASN |
| 2 | 9K | 179 | ASN |
| 2 | 9K | 218 | ASN |
| 2 | 9L | 76 | ASN |
| 2 | 9L | 159 | ASN |
| 2 | 9L | 166 | ASN |
| 2 | 9L | 179 | ASN |
| 2 | 9L | 218 | ASN |
| 2 | 9I | 103 | GLN |
| 2 | 9I | 159 | ASN |
| 2 | 9I | 166 | ASN |
| 2 | 9I | 179 | ASN |
| 2 | 9I | 218 | ASN |
| 2 | 1u | 159 | ASN |
| 2 | 1u | 166 | ASN |
| 2 | 1u | 179 | ASN |
| 2 | 1u | 218 | ASN |

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| Mol | Chain | Res | Type |
|------------|--------------|------------|-------------|
| 2 | 1v | 76 | ASN |
| 2 | 1v | 159 | ASN |
| 2 | 1v | 166 | ASN |
| 2 | 1v | 179 | ASN |
| 2 | 1v | 218 | ASN |
| 2 | 1w | 56 | ASN |
| 2 | 1w | 159 | ASN |
| 2 | 1w | 166 | ASN |
| 2 | 1w | 179 | ASN |
| 2 | 1w | 218 | ASN |
| 2 | 1x | 56 | ASN |
| 2 | 1x | 76 | ASN |
| 2 | 1x | 159 | ASN |
| 2 | 1x | 166 | ASN |
| 2 | 1x | 179 | ASN |
| 2 | 1x | 218 | ASN |
| 2 | 2t | 159 | ASN |
| 2 | 2t | 166 | ASN |
| 2 | 2t | 179 | ASN |
| 2 | 2t | 218 | ASN |
| 2 | 2u | 159 | ASN |
| 2 | 2u | 166 | ASN |
| 2 | 2u | 179 | ASN |
| 2 | 2u | 218 | ASN |
| 2 | 2v | 103 | GLN |
| 2 | 2v | 159 | ASN |
| 2 | 2v | 166 | ASN |
| 2 | 2v | 179 | ASN |
| 2 | 2v | 218 | ASN |
| 2 | 2w | 103 | GLN |
| 2 | 2w | 159 | ASN |
| 2 | 2w | 166 | ASN |
| 2 | 2w | 179 | ASN |
| 2 | 2w | 218 | ASN |
| 2 | 2x | 159 | ASN |
| 2 | 2x | 166 | ASN |
| 2 | 2x | 179 | ASN |
| 2 | 2x | 218 | ASN |
| 2 | 3u | 56 | ASN |
| 2 | 3u | 76 | ASN |
| 2 | 3u | 159 | ASN |
| 2 | 3u | 166 | ASN |

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| Mol | Chain | Res | Type |
|------------|--------------|------------|-------------|
| 2 | 3u | 179 | ASN |
| 2 | 3u | 218 | ASN |
| 2 | 3v | 159 | ASN |
| 2 | 3v | 166 | ASN |
| 2 | 3v | 179 | ASN |
| 2 | 3v | 218 | ASN |
| 2 | 3w | 56 | ASN |
| 2 | 3w | 76 | ASN |
| 2 | 3w | 159 | ASN |
| 2 | 3w | 166 | ASN |
| 2 | 3w | 179 | ASN |
| 2 | 3w | 218 | ASN |
| 2 | 3x | 159 | ASN |
| 2 | 3x | 166 | ASN |
| 2 | 3x | 179 | ASN |
| 2 | 3x | 218 | ASN |
| 2 | 4m | 159 | ASN |
| 2 | 4m | 166 | ASN |
| 2 | 4m | 179 | ASN |
| 2 | 4m | 218 | ASN |
| 2 | 4n | 76 | ASN |
| 2 | 4n | 159 | ASN |
| 2 | 4n | 166 | ASN |
| 2 | 4n | 179 | ASN |
| 2 | 4n | 218 | ASN |
| 2 | 5m | 159 | ASN |
| 2 | 5m | 166 | ASN |
| 2 | 5m | 179 | ASN |
| 2 | 5m | 218 | ASN |
| 2 | 5n | 56 | ASN |
| 2 | 5n | 76 | ASN |
| 2 | 5n | 159 | ASN |
| 2 | 5n | 166 | ASN |
| 2 | 5n | 179 | ASN |
| 2 | 5n | 218 | ASN |
| 2 | 6u | 23 | GLN |
| 2 | 6u | 76 | ASN |
| 2 | 6u | 159 | ASN |
| 2 | 6u | 166 | ASN |
| 2 | 6u | 179 | ASN |
| 2 | 6u | 218 | ASN |
| 2 | 6v | 159 | ASN |

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| Mol | Chain | Res | Type |
|------------|--------------|------------|-------------|
| 2 | 6v | 166 | ASN |
| 2 | 6v | 179 | ASN |
| 2 | 6v | 218 | ASN |
| 2 | 6w | 56 | ASN |
| 2 | 6w | 76 | ASN |
| 2 | 6w | 159 | ASN |
| 2 | 6w | 166 | ASN |
| 2 | 6w | 179 | ASN |
| 2 | 6w | 218 | ASN |
| 2 | 6x | 56 | ASN |
| 2 | 6x | 159 | ASN |
| 2 | 6x | 166 | ASN |
| 2 | 6x | 179 | ASN |
| 2 | 6x | 218 | ASN |
| 2 | 7t | 64 | GLN |
| 2 | 7t | 159 | ASN |
| 2 | 7t | 166 | ASN |
| 2 | 7t | 179 | ASN |
| 2 | 7t | 218 | ASN |
| 2 | 7u | 159 | ASN |
| 2 | 7u | 166 | ASN |
| 2 | 7u | 179 | ASN |
| 2 | 7u | 218 | ASN |
| 2 | 7v | 23 | GLN |
| 2 | 7v | 159 | ASN |
| 2 | 7v | 166 | ASN |
| 2 | 7v | 179 | ASN |
| 2 | 7v | 218 | ASN |
| 2 | 7w | 159 | ASN |
| 2 | 7w | 166 | ASN |
| 2 | 7w | 179 | ASN |
| 2 | 7w | 218 | ASN |
| 2 | 7x | 159 | ASN |
| 2 | 7x | 166 | ASN |
| 2 | 7x | 179 | ASN |
| 2 | 7x | 218 | ASN |
| 2 | 9M | 76 | ASN |
| 2 | 9M | 159 | ASN |
| 2 | 9M | 166 | ASN |
| 2 | 9M | 179 | ASN |
| 2 | 9M | 218 | ASN |
| 2 | 9N | 159 | ASN |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 2 | 9N | 166 | ASN |
| 2 | 9N | 179 | ASN |
| 2 | 9N | 218 | ASN |
| 2 | 9O | 159 | ASN |
| 2 | 9O | 166 | ASN |
| 2 | 9O | 179 | ASN |
| 2 | 9O | 218 | ASN |
| 2 | 9P | 76 | ASN |
| 2 | 9P | 159 | ASN |
| 2 | 9P | 166 | ASN |
| 2 | 9P | 179 | ASN |
| 2 | 9P | 218 | ASN |
| 2 | 9Q | 56 | ASN |
| 2 | 9Q | 159 | ASN |
| 2 | 9Q | 166 | ASN |
| 2 | 9Q | 179 | ASN |
| 2 | 9Q | 218 | ASN |
| 2 | 9R | 76 | ASN |
| 2 | 9R | 159 | ASN |
| 2 | 9R | 166 | ASN |
| 2 | 9R | 179 | ASN |
| 2 | 9R | 218 | ASN |
| 2 | 9J | 103 | GLN |
| 2 | 9J | 159 | ASN |
| 2 | 9J | 166 | ASN |
| 2 | 9J | 179 | ASN |
| 2 | 9J | 218 | ASN |

5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates [i](#)

There are no monosaccharides in this entry.

5.6 Ligand geometry [i](#)

There are no ligands in this entry.

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.

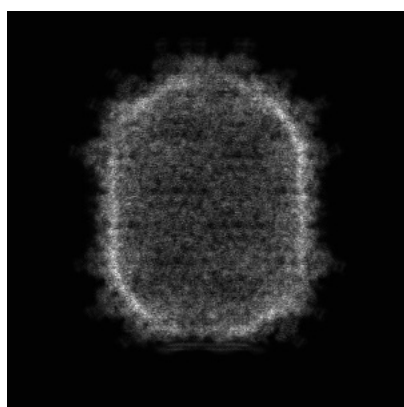
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-4681. These allow visual inspection of the internal detail of the map and identification of artifacts.

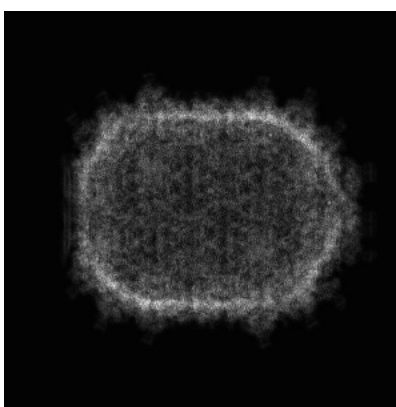
No raw map or half-maps were deposited for this entry and therefore no images, graphs, etc. pertaining to the raw map can be shown.

6.1 Orthogonal projections [i](#)

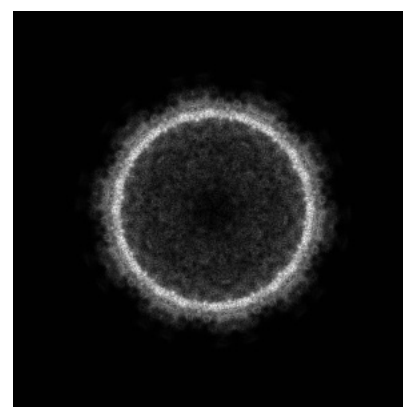
6.1.1 Primary map



X



Y



Z

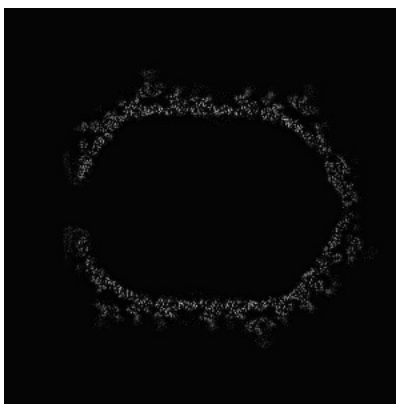
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

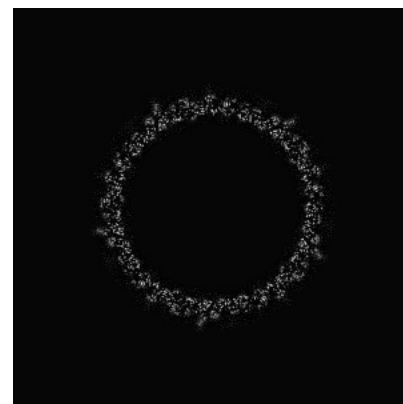
6.2.1 Primary map



X Index: 270



Y Index: 270

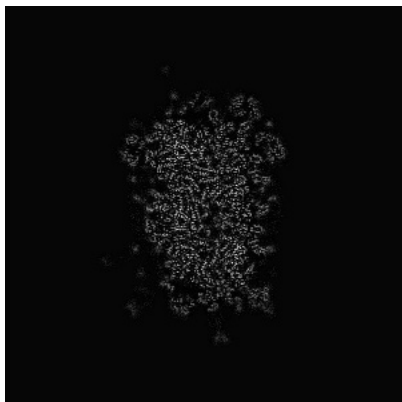


Z Index: 270

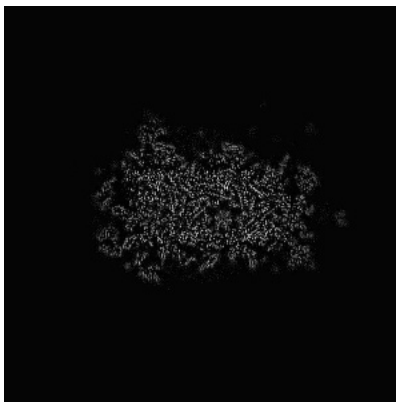
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

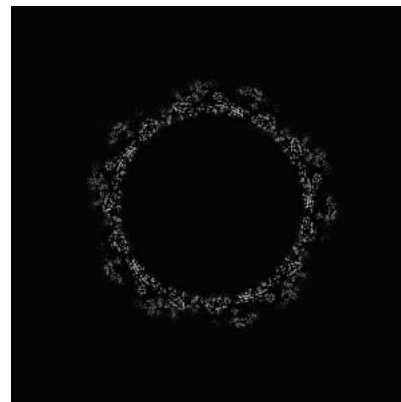
6.3.1 Primary map



X Index: 396



Y Index: 143

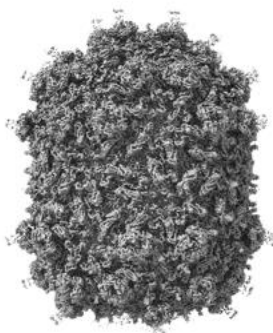


Z Index: 212

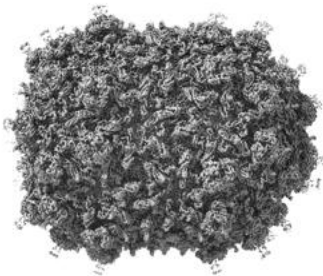
The images above show the largest variance slices of the map in three orthogonal directions.

6.4 Orthogonal surface views [i](#)

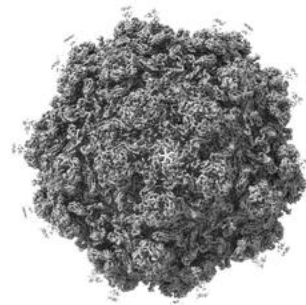
6.4.1 Primary map



X



Y



Z

The images above show the 3D surface view of the map at the recommended contour level 3.0. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

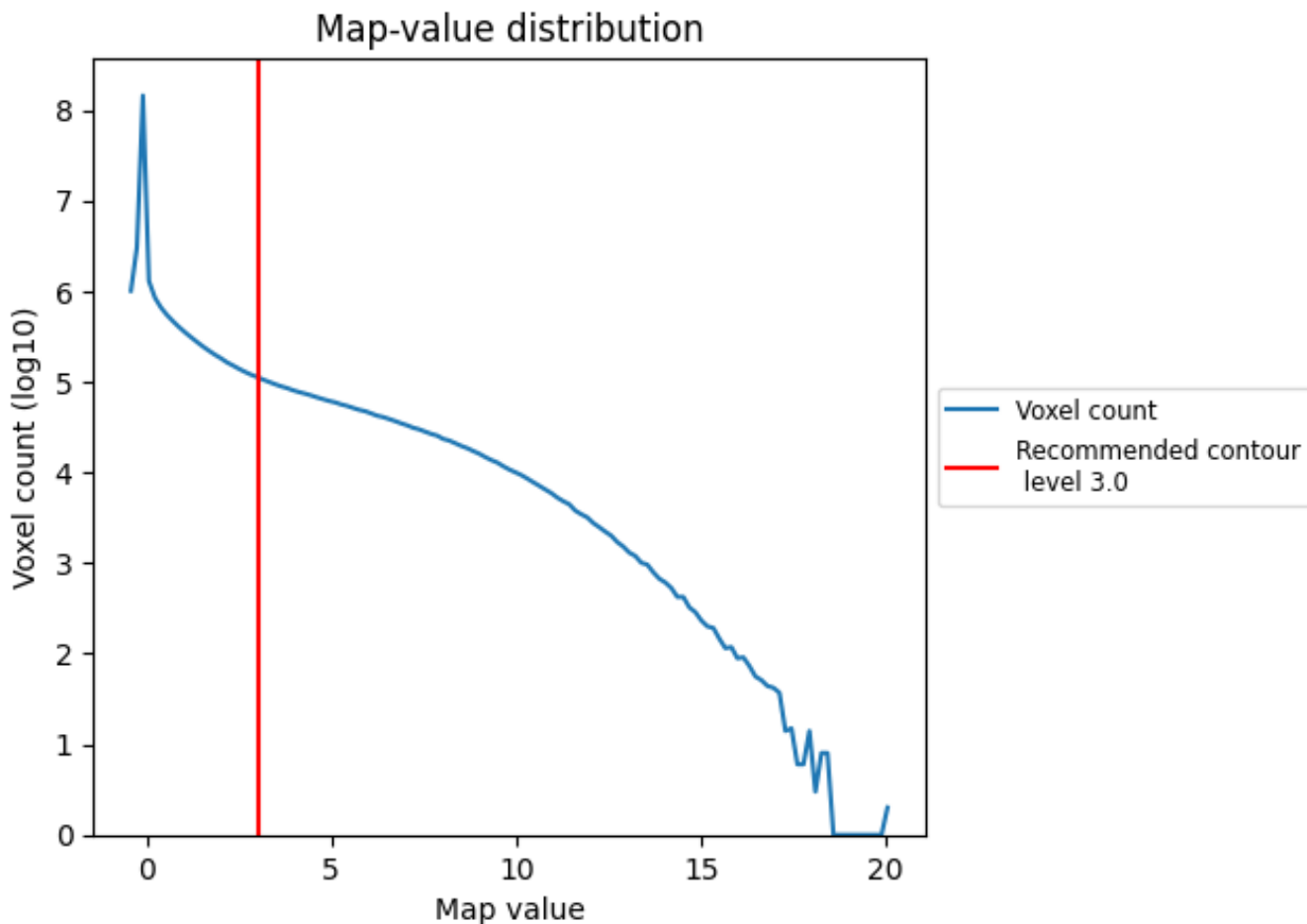
6.5 Mask visualisation

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

7 Map analysis [i](#)

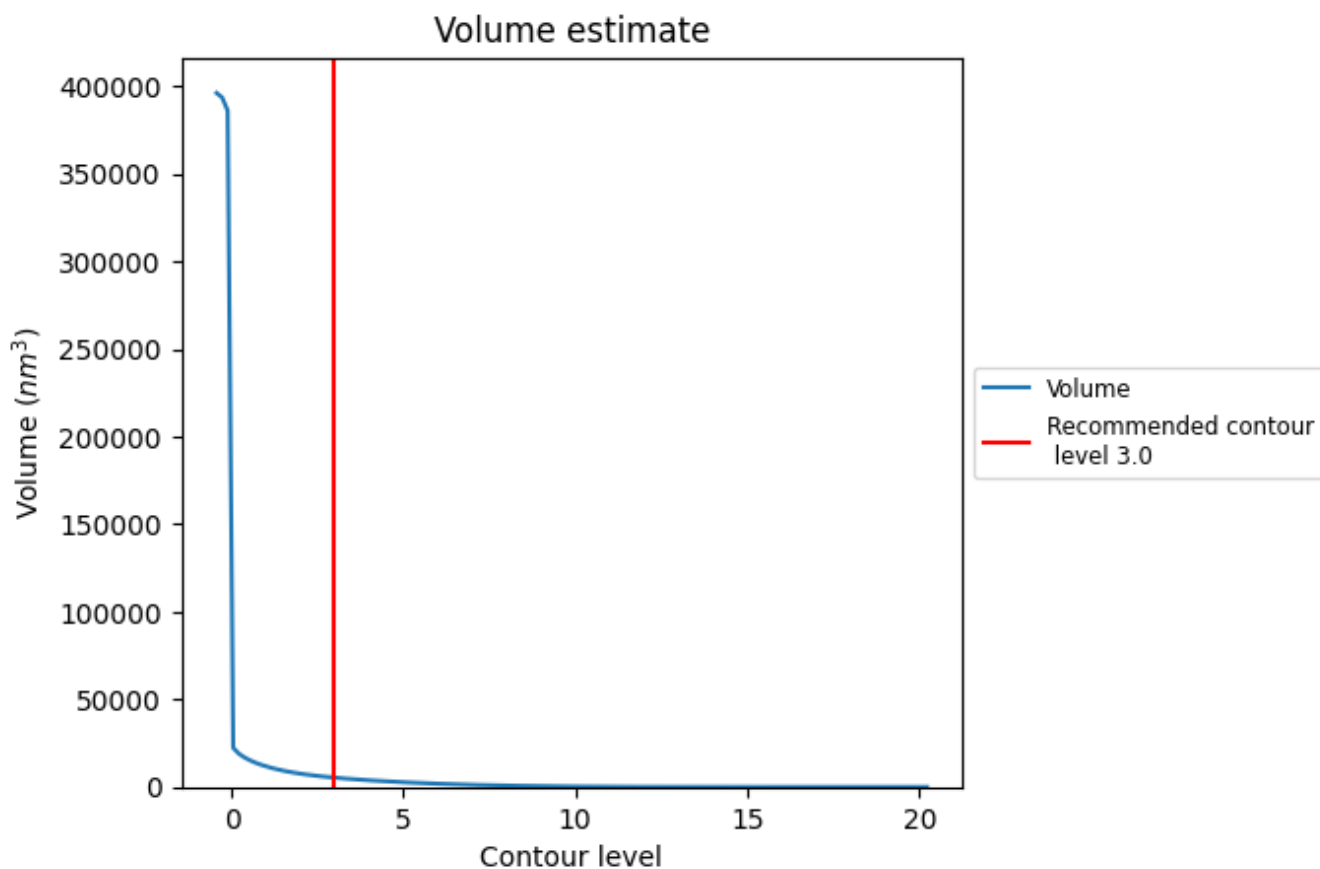
This section contains the results of statistical analysis of the map.

7.1 Map-value distribution [i](#)



The map-value distribution is plotted in 128 intervals along the x-axis. The y-axis is logarithmic. A spike in this graph at zero usually indicates that the volume has been masked.

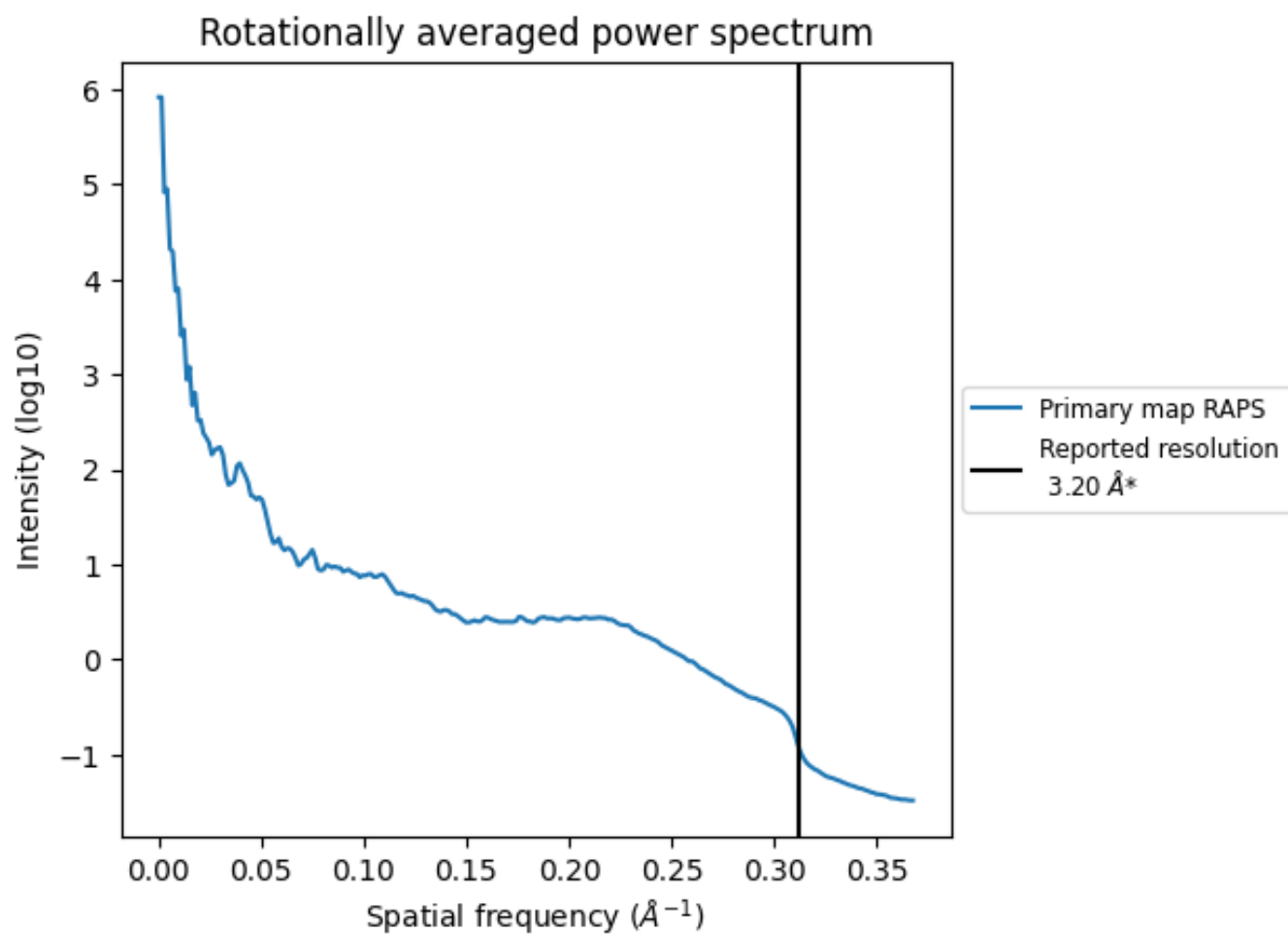
7.2 Volume estimate [\(i\)](#)



The volume at the recommended contour level is 5310 nm³; this corresponds to an approximate mass of 4796 kDa.

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

7.3 Rotationally averaged power spectrum [i](#)



*Reported resolution corresponds to spatial frequency of 0.312 Å⁻¹

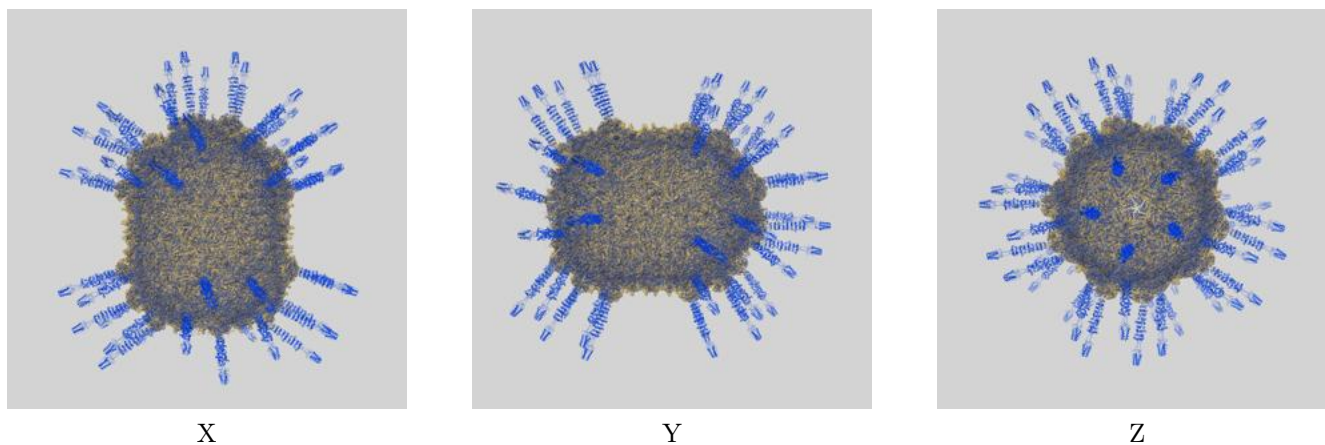
8 Fourier-Shell correlation

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

9 Map-model fit [i](#)

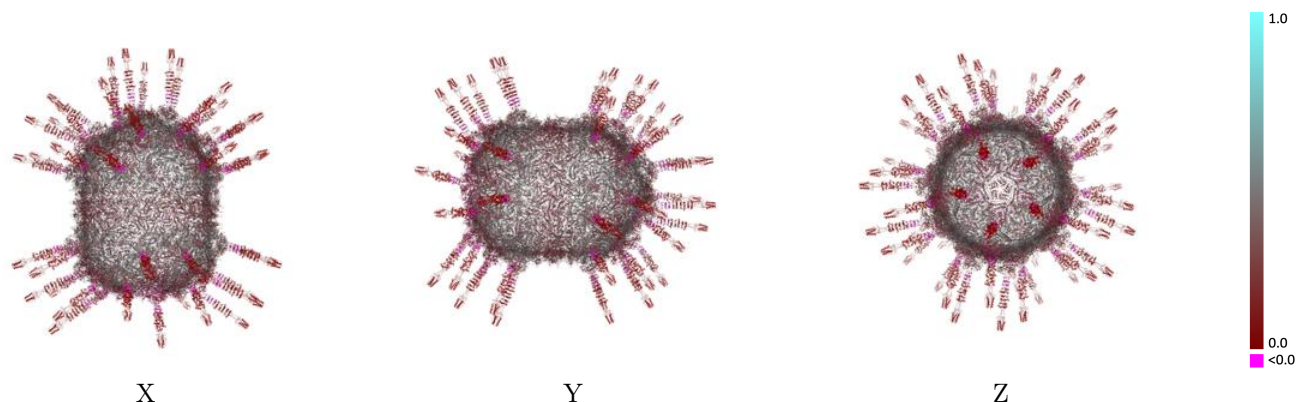
This section contains information regarding the fit between EMDB map EMD-4681 and PDB model 6QZ0. Per-residue inclusion information can be found in section 3 on page 47.

9.1 Map-model overlay [i](#)



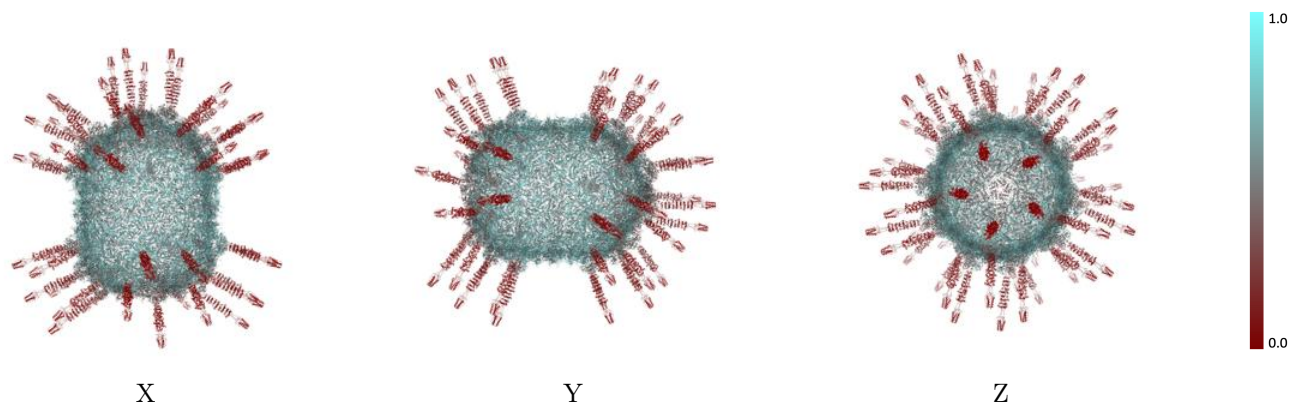
The images above show the 3D surface view of the map at the recommended contour level 3.0 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

9.2 Q-score mapped to coordinate model [i](#)



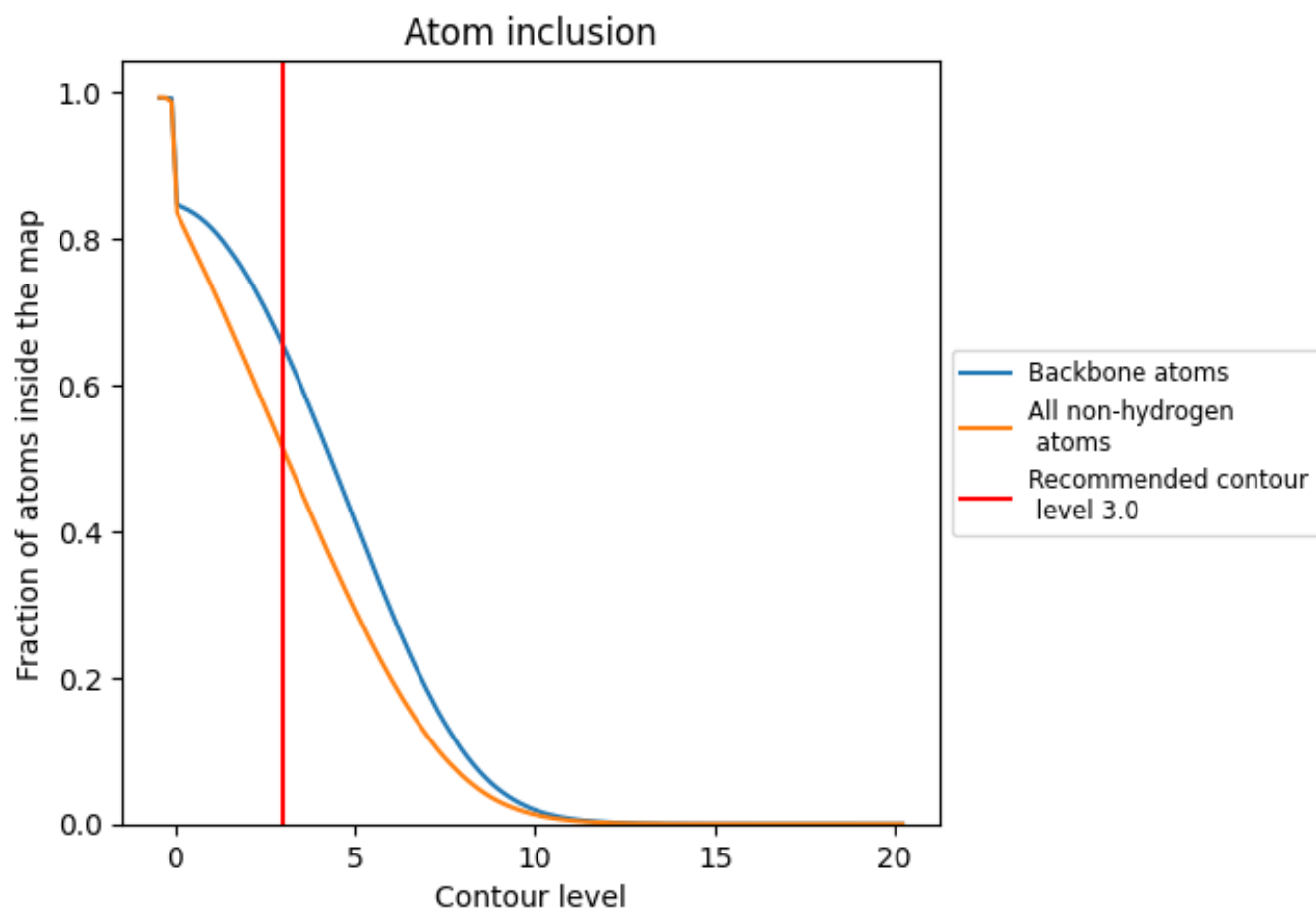
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions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

9.3 Atom inclusion mapped to coordinate model [i](#)



The images above show the model with each residue coloured according to its atom inclusion. This shows to what extent they are inside the map at the recommended contour level (3.0).

9.4 Atom inclusion [i](#)



At the recommended contour level, 65% of all backbone atoms, 51% of all non-hydrogen atoms, are inside the map.

9.5 Map-model fit summary

The table lists the average atom inclusion at the recommended contour level (3.0) and Q-score for the entire model and for each chain.

| Chain | Atom inclusion | Q-score |
|-------|----------------|---------|
| All | 0.5121 | 0.2750 |
| 1A | 0.4473 | 0.2090 |
| 1B | 0.6278 | 0.3420 |
| 1C | 0.6613 | 0.3890 |
| 1D | 0.6406 | 0.3550 |
| 1E | 0.5524 | 0.2730 |
| 1F | 0.4681 | 0.2010 |
| 1G | 0.4479 | 0.2130 |
| 1H | 0.6281 | 0.3460 |
| 1I | 0.6657 | 0.3930 |
| 1J | 0.6444 | 0.3590 |
| 1K | 0.5509 | 0.2790 |
| 1L | 0.4720 | 0.2070 |
| 1M | 0.4482 | 0.2110 |
| 1N | 0.6272 | 0.3440 |
| 1O | 0.6648 | 0.3920 |
| 1P | 0.6426 | 0.3580 |
| 1Q | 0.5518 | 0.2750 |
| 1R | 0.4732 | 0.2060 |
| 1S | 0.4482 | 0.2160 |
| 1T | 0.6313 | 0.3480 |
| 1U | 0.6625 | 0.3950 |
| 1V | 0.6444 | 0.3610 |
| 1W | 0.5569 | 0.2810 |
| 1X | 0.4755 | 0.2110 |
| 1Y | 0.4545 | 0.2150 |
| 1Z | 0.6301 | 0.3470 |
| 1a | 0.6637 | 0.3950 |
| 1b | 0.6441 | 0.3590 |
| 1c | 0.5587 | 0.2790 |
| 1d | 0.4720 | 0.2070 |
| 1e | 0.1585 | 0.0540 |
| 1f | 0.2008 | 0.1110 |
| 1g | 0.2107 | 0.1150 |
| 1h | 0.1890 | 0.0780 |



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| Chain | Atom inclusion | Q-score |
|-------|----------------|---------|
| 1i | 0.1580 | 0.0540 |
| 1j | 0.2003 | 0.1090 |
| 1k | 0.2156 | 0.1160 |
| 1l | 0.1895 | 0.0820 |
| 1m | 0.1590 | 0.0550 |
| 1n | 0.2003 | 0.1080 |
| 1o | 0.2141 | 0.1150 |
| 1p | 0.1915 | 0.0830 |
| 1q | 0.1629 | 0.0570 |
| 1r | 0.2042 | 0.1120 |
| 1s | 0.2132 | 0.1150 |
| 1t | 0.1920 | 0.0840 |
| 1u | 0.1551 | 0.0540 |
| 1v | 0.2037 | 0.1110 |
| 1w | 0.2117 | 0.1150 |
| 1x | 0.1929 | 0.0820 |
| 2A | 0.6422 | 0.3340 |
| 2B | 0.6418 | 0.3330 |
| 2C | 0.6429 | 0.3330 |
| 2D | 0.6056 | 0.2920 |
| 2E | 0.6027 | 0.2890 |
| 2F | 0.6416 | 0.3380 |
| 2G | 0.6397 | 0.3320 |
| 2H | 0.6424 | 0.3350 |
| 2I | 0.6068 | 0.2960 |
| 2J | 0.6012 | 0.2920 |
| 2K | 0.6440 | 0.3360 |
| 2L | 0.6403 | 0.3310 |
| 2M | 0.6438 | 0.3360 |
| 2N | 0.6079 | 0.2920 |
| 2O | 0.6065 | 0.2870 |
| 2P | 0.6452 | 0.3370 |
| 2Q | 0.6426 | 0.3350 |
| 2R | 0.6473 | 0.3400 |
| 2S | 0.6068 | 0.2950 |
| 2T | 0.6030 | 0.2910 |
| 2U | 0.6479 | 0.3390 |
| 2V | 0.6397 | 0.3360 |
| 2W | 0.6453 | 0.3380 |
| 2X | 0.6056 | 0.2980 |
| 2Y | 0.6021 | 0.2900 |
| 2Z | 0.1668 | 0.0600 |
























































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| Chain | Atom inclusion | Q-score |
|-------|----------------|---------|
| 2a | 0.2215 | 0.1300 |
| 2b | 0.2395 | 0.1480 |
| 2c | 0.2273 | 0.1320 |
| 2d | 0.1956 | 0.1060 |
| 2e | 0.1717 | 0.0620 |
| 2f | 0.2200 | 0.1320 |
| 2g | 0.2400 | 0.1480 |
| 2h | 0.2293 | 0.1330 |
| 2i | 0.1937 | 0.1060 |
| 2j | 0.1683 | 0.0590 |
| 2k | 0.2224 | 0.1310 |
| 2l | 0.2405 | 0.1480 |
| 2m | 0.2298 | 0.1330 |
| 2n | 0.1946 | 0.1050 |
| 2o | 0.1746 | 0.0630 |
| 2p | 0.2229 | 0.1330 |
| 2q | 0.2385 | 0.1450 |
| 2r | 0.2298 | 0.1370 |
| 2s | 0.1971 | 0.1060 |
| 2t | 0.1693 | 0.0620 |
| 2u | 0.2229 | 0.1320 |
| 2v | 0.2380 | 0.1470 |
| 2w | 0.2337 | 0.1350 |
| 2x | 0.1937 | 0.1070 |
| 3A | 0.6958 | 0.3770 |
| 3B | 0.6656 | 0.3320 |
| 3C | 0.6764 | 0.3530 |
| 3D | 0.6960 | 0.3950 |
| 3E | 0.6998 | 0.4120 |
| 3F | 0.6969 | 0.4160 |
| 3G | 0.6961 | 0.3790 |
| 3H | 0.6647 | 0.3320 |
| 3I | 0.6764 | 0.3540 |
| 3J | 0.6954 | 0.3960 |
| 3K | 0.6954 | 0.4120 |
| 3L | 0.6969 | 0.4190 |
| 3M | 0.6961 | 0.3780 |
| 3N | 0.6656 | 0.3330 |
| 3O | 0.6761 | 0.3510 |
| 3P | 0.6998 | 0.3940 |
| 3Q | 0.6975 | 0.4120 |
| 3R | 0.6984 | 0.4170 |





















































































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| Chain | Atom inclusion | Q-score |
|-------|--|--|
| 3S |  0.6970 |  0.3790 |
| 3T |  0.6656 |  0.3360 |
| 3U |  0.6787 |  0.3550 |
| 3V |  0.6914 |  0.3950 |
| 3W |  0.6966 |  0.4130 |
| 3X |  0.6975 |  0.4170 |
| 3Y |  0.6952 |  0.3790 |
| 3Z |  0.6647 |  0.3330 |
| 3a |  0.6764 |  0.3520 |
| 3b |  0.6978 |  0.3950 |
| 3c |  0.6966 |  0.4120 |
| 3d |  0.6987 |  0.4170 |
| 3e |  0.2370 |  0.1470 |
| 3f |  0.2029 |  0.1140 |
| 3g |  0.1743 |  0.0650 |
| 3h |  0.2273 |  0.1450 |
| 3i |  0.2375 |  0.1450 |
| 3j |  0.2049 |  0.1130 |
| 3k |  0.1748 |  0.0640 |
| 3l |  0.2293 |  0.1450 |
| 3m |  0.2365 |  0.1460 |
| 3n |  0.2083 |  0.1150 |
| 3o |  0.1738 |  0.0650 |
| 3p |  0.2278 |  0.1450 |
| 3q |  0.2346 |  0.1490 |
| 3r |  0.2034 |  0.1130 |
| 3s |  0.1758 |  0.0660 |
| 3t |  0.2317 |  0.1440 |
| 3u |  0.2380 |  0.1450 |
| 3v |  0.2054 |  0.1120 |
| 3w |  0.1783 |  0.0660 |
| 3x |  0.2298 |  0.1450 |
| 4A |  0.6879 |  0.3560 |
| 4B |  0.6314 |  0.2680 |
| 4C |  0.6386 |  0.2720 |
| 4D |  0.6537 |  0.2930 |
| 4E |  0.6587 |  0.3310 |
| 4F |  0.6917 |  0.3860 |
| 4G |  0.6926 |  0.3610 |
| 4H |  0.6341 |  0.2710 |
| 4I |  0.6403 |  0.2740 |
| 4J |  0.6576 |  0.2950 |





















































































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| Chain | Atom inclusion | Q-score |
|-------|--|--|
| 4K |  0.6593 |  0.3330 |
| 4L |  0.6960 |  0.3860 |
| 4M |  0.6899 |  0.3590 |
| 4N |  0.6359 |  0.2730 |
| 4O |  0.6415 |  0.2780 |
| 4P |  0.6549 |  0.2980 |
| 4Q |  0.6578 |  0.3340 |
| 4R |  0.6934 |  0.3830 |
| 4S |  0.6876 |  0.3580 |
| 4T |  0.6359 |  0.2720 |
| 4U |  0.6430 |  0.2770 |
| 4V |  0.6567 |  0.3000 |
| 4W |  0.6587 |  0.3350 |
| 4X |  0.6952 |  0.3860 |
| 4Y |  0.6884 |  0.3570 |
| 4Z |  0.6350 |  0.2700 |
| 4a |  0.6400 |  0.2730 |
| 4b |  0.6546 |  0.2940 |
| 4c |  0.6593 |  0.3350 |
| 4d |  0.6972 |  0.3860 |
| 4e |  0.2449 |  0.1530 |
| 4f |  0.2199 |  0.1210 |
| 4g |  0.2415 |  0.1510 |
| 4h |  0.2174 |  0.1220 |
| 4i |  0.2420 |  0.1500 |
| 4j |  0.2179 |  0.1200 |
| 4k |  0.2415 |  0.1500 |
| 4l |  0.2179 |  0.1210 |
| 4m |  0.2429 |  0.1490 |
| 4n |  0.2169 |  0.1210 |
| 5A |  0.6920 |  0.3650 |
| 5B |  0.6273 |  0.2610 |
| 5C |  0.6261 |  0.2670 |
| 5D |  0.6504 |  0.2900 |
| 5E |  0.6672 |  0.3390 |
| 5F |  0.6995 |  0.3900 |
| 5G |  0.6902 |  0.3670 |
| 5H |  0.6222 |  0.2610 |
| 5I |  0.6305 |  0.2660 |
| 5J |  0.6504 |  0.2910 |
| 5K |  0.6689 |  0.3390 |
| 5L |  0.6960 |  0.3910 |





















































































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| Chain | Atom inclusion | Q-score |
|-------|--|--|
| 5M |  0.6899 |  0.3680 |
| 5N |  0.6246 |  0.2610 |
| 5O |  0.6290 |  0.2670 |
| 5P |  0.6516 |  0.2940 |
| 5Q |  0.6666 |  0.3410 |
| 5R |  0.6981 |  0.3920 |
| 5S |  0.6890 |  0.3680 |
| 5T |  0.6282 |  0.2650 |
| 5U |  0.6267 |  0.2660 |
| 5V |  0.6522 |  0.2950 |
| 5W |  0.6674 |  0.3390 |
| 5X |  0.6946 |  0.3900 |
| 5Y |  0.6890 |  0.3660 |
| 5Z |  0.6264 |  0.2630 |
| 5a |  0.6261 |  0.2670 |
| 5b |  0.6486 |  0.2930 |
| 5c |  0.6695 |  0.3380 |
| 5d |  0.6969 |  0.3900 |
| 5e |  0.2332 |  0.1310 |
| 5f |  0.2076 |  0.1240 |
| 5g |  0.2317 |  0.1320 |
| 5h |  0.2096 |  0.1240 |
| 5i |  0.2312 |  0.1310 |
| 5j |  0.2071 |  0.1230 |
| 5k |  0.2322 |  0.1300 |
| 5l |  0.2067 |  0.1210 |
| 5m |  0.2337 |  0.1330 |
| 5n |  0.2067 |  0.1230 |
| 6A |  0.6937 |  0.4210 |
| 6B |  0.6984 |  0.4200 |
| 6C |  0.6965 |  0.3790 |
| 6D |  0.6656 |  0.3380 |
| 6E |  0.6882 |  0.3680 |
| 6F |  0.6989 |  0.4040 |
| 6G |  0.6919 |  0.4200 |
| 6H |  0.7022 |  0.4210 |
| 6I |  0.6935 |  0.3800 |
| 6J |  0.6671 |  0.3400 |
| 6K |  0.6884 |  0.3700 |
| 6L |  0.6966 |  0.4020 |
| 6M |  0.6952 |  0.4220 |
| 6N |  0.7033 |  0.4210 |





















































































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| Chain | Atom inclusion | Q-score |
|-------|--|--|
| 6O |  0.6938 |  0.3830 |
| 6P |  0.6691 |  0.3430 |
| 6Q |  0.6884 |  0.3710 |
| 6R |  0.6978 |  0.4030 |
| 6S |  0.6925 |  0.4200 |
| 6T |  0.7013 |  0.4190 |
| 6U |  0.6908 |  0.3780 |
| 6V |  0.6709 |  0.3410 |
| 6W |  0.6890 |  0.3700 |
| 6X |  0.6957 |  0.4010 |
| 6Y |  0.6952 |  0.4200 |
| 6Z |  0.7022 |  0.4210 |
| 6a |  0.6956 |  0.3780 |
| 6b |  0.6691 |  0.3380 |
| 6c |  0.6893 |  0.3660 |
| 6d |  0.6998 |  0.4020 |
| 6e |  0.1670 |  0.0700 |
| 6f |  0.2288 |  0.1280 |
| 6g |  0.1954 |  0.0980 |
| 6h |  0.1966 |  0.1110 |
| 6i |  0.1655 |  0.0640 |
| 6j |  0.2283 |  0.1260 |
| 6k |  0.1929 |  0.0950 |
| 6l |  0.1966 |  0.1070 |
| 6m |  0.1645 |  0.0660 |
| 6n |  0.2298 |  0.1270 |
| 6o |  0.1988 |  0.0960 |
| 6p |  0.1971 |  0.1090 |
| 6q |  0.1626 |  0.0640 |
| 6r |  0.2283 |  0.1250 |
| 6s |  0.1954 |  0.0920 |
| 6t |  0.1946 |  0.1070 |
| 6u |  0.1655 |  0.0680 |
| 6v |  0.2263 |  0.1250 |
| 6w |  0.1988 |  0.0930 |
| 6x |  0.1941 |  0.1090 |
| 7A |  0.6076 |  0.3200 |
| 7B |  0.6138 |  0.3320 |
| 7C |  0.6313 |  0.3390 |
| 7D |  0.6330 |  0.3350 |
| 7E |  0.6278 |  0.3240 |
| 7F |  0.6071 |  0.3120 |





















































































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| Chain | Atom inclusion | Q-score |
|-------|--|--|
| 7G |  0.6103 |  0.3220 |
| 7H |  0.6286 |  0.3330 |
| 7I |  0.6354 |  0.3310 |
| 7J |  0.6246 |  0.3140 |
| 7K |  0.6047 |  0.3080 |
| 7L |  0.6120 |  0.3200 |
| 7M |  0.6286 |  0.3320 |
| 7N |  0.6333 |  0.3290 |
| 7O |  0.6286 |  0.3140 |
| 7P |  0.6021 |  0.3050 |
| 7Q |  0.6071 |  0.3170 |
| 7R |  0.6286 |  0.3270 |
| 7S |  0.6348 |  0.3250 |
| 7T |  0.6257 |  0.3110 |
| 7U |  0.6047 |  0.3120 |
| 7V |  0.6091 |  0.3210 |
| 7W |  0.6269 |  0.3320 |
| 7X |  0.6327 |  0.3300 |
| 7Y |  0.6237 |  0.3160 |
| 7Z |  0.2454 |  0.1540 |
| 7a |  0.2351 |  0.1430 |
| 7b |  0.2005 |  0.1180 |
| 7c |  0.1668 |  0.0710 |
| 7d |  0.1849 |  0.0880 |
| 7e |  0.2488 |  0.1540 |
| 7f |  0.2332 |  0.1430 |
| 7g |  0.1966 |  0.1160 |
| 7h |  0.1654 |  0.0680 |
| 7i |  0.1820 |  0.0850 |
| 7j |  0.2444 |  0.1530 |
| 7k |  0.2351 |  0.1420 |
| 7l |  0.1966 |  0.1170 |
| 7m |  0.1702 |  0.0670 |
| 7n |  0.1815 |  0.0870 |
| 7o |  0.2434 |  0.1510 |
| 7p |  0.2302 |  0.1410 |
| 7q |  0.1961 |  0.1130 |
| 7r |  0.1634 |  0.0690 |
| 7s |  0.1795 |  0.0830 |
| 7t |  0.2468 |  0.1530 |
| 7u |  0.2327 |  0.1410 |
| 7v |  0.1976 |  0.1130 |

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| Chain | Atom inclusion | Q-score |
|-------|--|--|
| 7w |  0.1639 |  0.0690 |
| 7x |  0.1824 |  0.0850 |
| 8A |  0.6313 |  0.4070 |
| 8B |  0.6330 |  0.4110 |
| 8C |  0.6604 |  0.4030 |
| 8D |  0.6680 |  0.4140 |
| 8E |  0.6698 |  0.4070 |
| 8F |  0.6453 |  0.4170 |
| 8G |  0.6237 |  0.4040 |
| 8H |  0.6336 |  0.4070 |
| 8I |  0.6587 |  0.4010 |
| 8J |  0.6654 |  0.4100 |
| 8K |  0.6712 |  0.4040 |
| 8L |  0.6432 |  0.4130 |
| 8M |  0.6234 |  0.4060 |
| 8N |  0.6313 |  0.4090 |
| 8O |  0.6631 |  0.4020 |
| 8P |  0.6695 |  0.4080 |
| 8Q |  0.6698 |  0.4040 |
| 8R |  0.6470 |  0.4160 |
| 8S |  0.6260 |  0.4030 |
| 8T |  0.6292 |  0.4060 |
| 8U |  0.6599 |  0.4020 |
| 8V |  0.6666 |  0.4060 |
| 8W |  0.6672 |  0.4010 |
| 8X |  0.6435 |  0.4150 |
| 8Y |  0.6246 |  0.4070 |
| 8Z |  0.6301 |  0.4090 |
| 8a |  0.6599 |  0.4010 |
| 8b |  0.6666 |  0.4080 |
| 8c |  0.6701 |  0.4040 |
| 8d |  0.6456 |  0.4170 |
| 8e |  0.1401 |  0.0880 |
| 8f |  0.1927 |  0.0900 |
| 8g |  0.1610 |  0.1190 |
| 8h |  0.1513 |  0.0570 |
| 8i |  0.1976 |  0.1080 |
| 8j |  0.1626 |  0.0820 |
| 8k |  0.1381 |  0.0850 |
| 8l |  0.1927 |  0.0870 |
| 8m |  0.1590 |  0.1160 |
| 8n |  0.1464 |  0.0500 |

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| Chain | Atom inclusion | Q-score |
|-------|----------------|----------|
| 8o | ■ 0.1976 | ■ 0.1030 |
| 8p | ■ 0.1611 | ■ 0.0800 |
| 8q | ■ 0.1405 | ■ 0.0850 |
| 8r | ■ 0.1956 | ■ 0.0860 |
| 8s | ■ 0.1590 | ■ 0.1170 |
| 8t | ■ 0.1484 | ■ 0.0530 |
| 8u | ■ 0.1990 | ■ 0.1050 |
| 8v | ■ 0.1655 | ■ 0.0810 |
| 8w | ■ 0.1332 | ■ 0.0830 |
| 8x | ■ 0.1912 | ■ 0.0820 |
| 8y | ■ 0.1566 | ■ 0.1140 |
| 8z | ■ 0.1440 | ■ 0.0540 |
| 9A | ■ 0.5295 | ■ 0.3160 |
| 9B | ■ 0.5251 | ■ 0.3080 |
| 9C | ■ 0.5245 | ■ 0.3110 |
| 9D | ■ 0.5233 | ■ 0.3030 |
| 9E | ■ 0.5193 | ■ 0.3070 |
| 9F | ■ 0.1761 | ■ 0.1410 |
| 9G | ■ 0.1785 | ■ 0.1400 |
| 9H | ■ 0.1746 | ■ 0.1400 |
| 9I | ■ 0.1746 | ■ 0.1360 |
| 9J | ■ 0.1776 | ■ 0.1380 |
| 9K | ■ 0.1971 | ■ 0.1020 |
| 9L | ■ 0.1650 | ■ 0.0800 |
| 9M | ■ 0.1366 | ■ 0.0850 |
| 9N | ■ 0.1922 | ■ 0.0860 |
| 9O | ■ 0.1585 | ■ 0.1150 |
| 9P | ■ 0.1464 | ■ 0.0560 |
| 9Q | ■ 0.1971 | ■ 0.1060 |
| 9R | ■ 0.1670 | ■ 0.0830 |