



Full wwPDB EM Validation Report ⓘ

Dec 12, 2022 – 10:05 pm GMT

PDB ID : 6QYD
EMDB ID : EMD-4677
Title : Cryo-EM structure of the head in mature bacteriophage phi29
Authors : Xu, J.W.; Wang, D.H.; Gui, M.; Xiang, Y.
Deposited on : 2019-03-08
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:

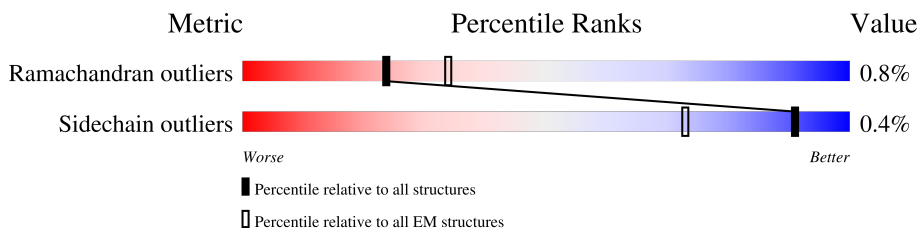
EMDB validation analysis : 0.0.1.dev43
MolProbity : 4.02b-467
Percentile statistics : 20191225.v01 (using entries in the PDB archive December 25th 2019)
MapQ : 1.9.9
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.31.3

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	17% 96% ..
1	1B	448	98% ..
1	1C	448	99% .
1	1D	448	98% ..
1	1E	448	7% 97% .
1	1F	448	6% 97% ..
1	1G	448	18% 96% ..
1	1H	448	98% ..
1	1I	448	99% .

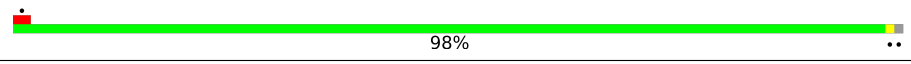
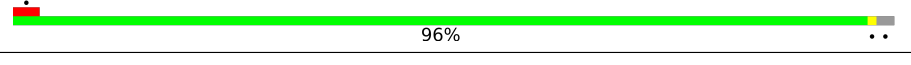
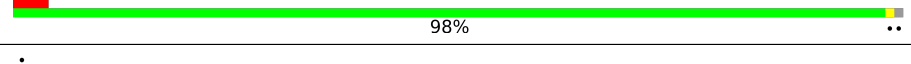
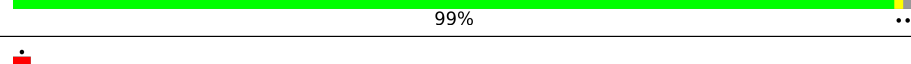
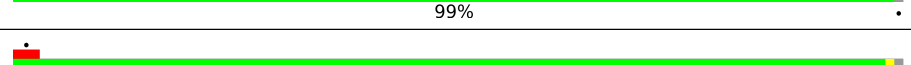
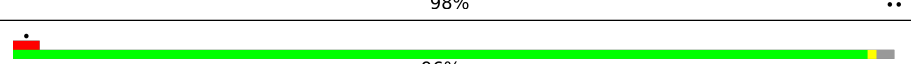
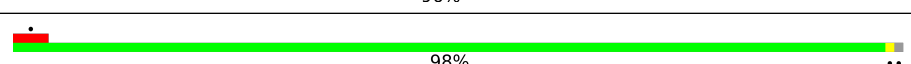
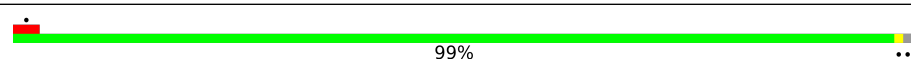
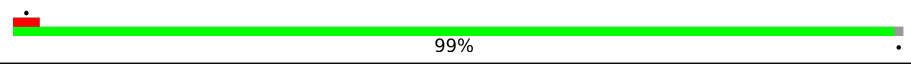
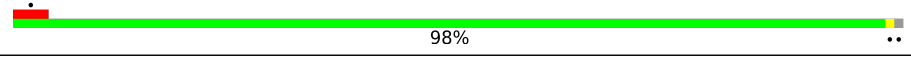
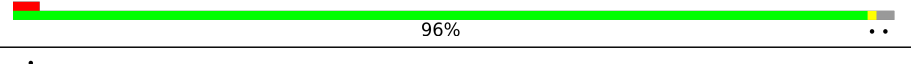
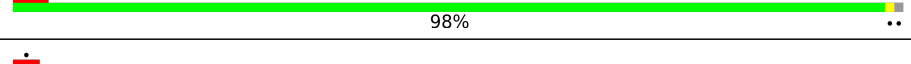
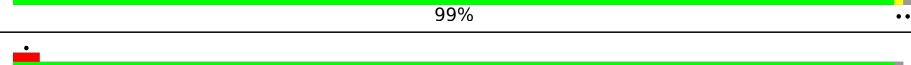
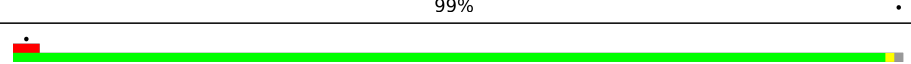
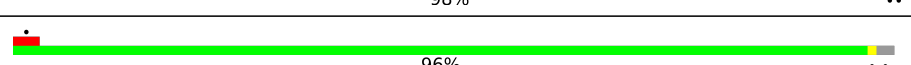
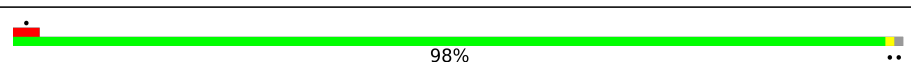
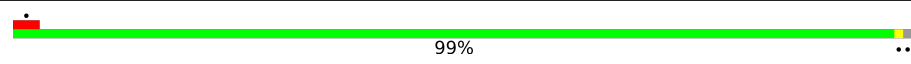
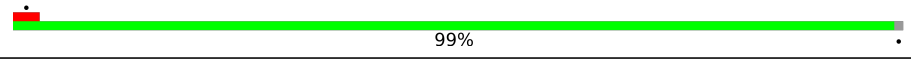
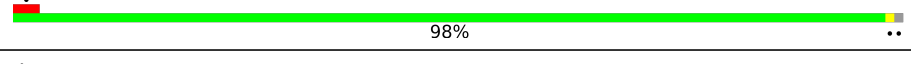
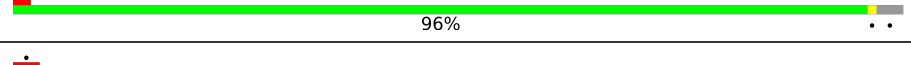
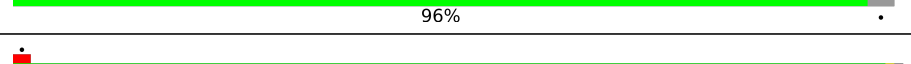
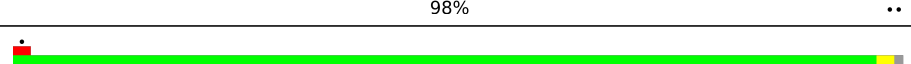
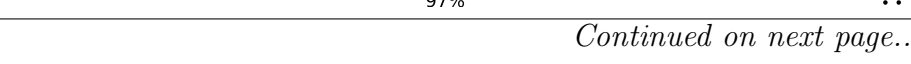


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Mol	Chain	Length	Quality of chain
1	1J	448	5% 98%
1	1K	448	7% 97%
1	1L	448	7% 97%
1	1M	448	18% 96%
1	1N	448	98%
1	1O	448	99%
1	1P	448	98%
1	1Q	448	7% 97%
1	1R	448	6% 97%
1	1S	448	18% 96%
1	1T	448	98%
1	1U	448	99%
1	1V	448	98%
1	1W	448	7% 97%
1	1X	448	6% 97%
1	1Y	448	18% 96%
1	1Z	448	98%
1	1a	448	99%
1	1b	448	98%
1	1c	448	7% 97%
1	1d	448	6% 97%
1	2A	448	96%
1	2B	448	98%
1	2C	448	99%
1	2D	448	99%

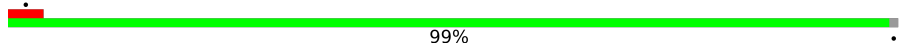
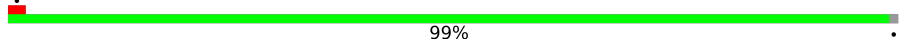
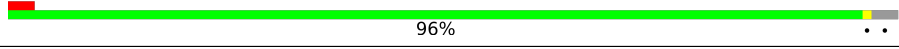
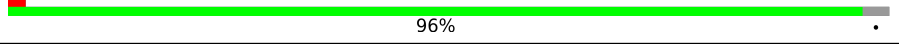
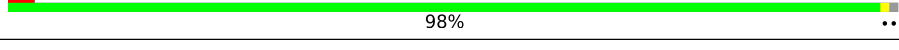
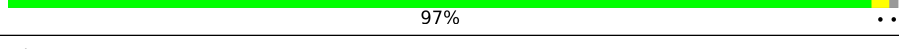
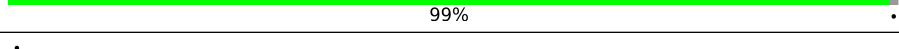
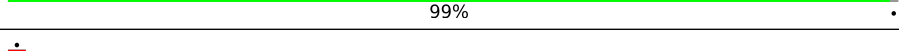
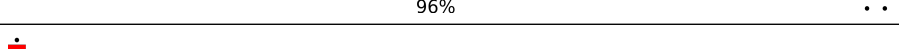
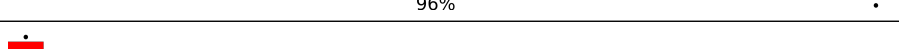
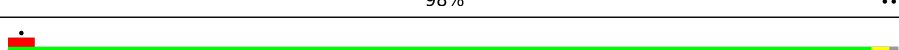
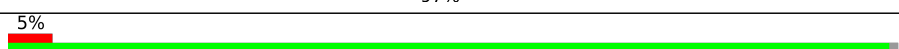
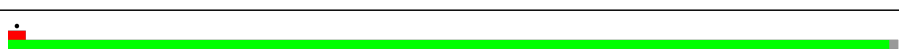
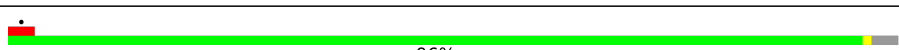
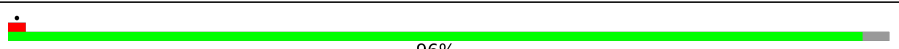


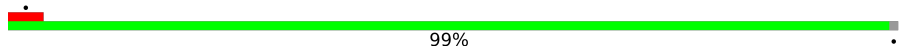
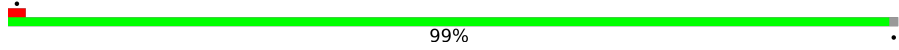
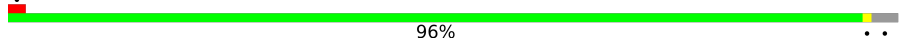
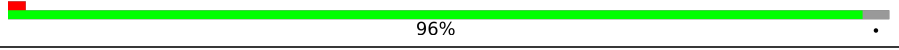
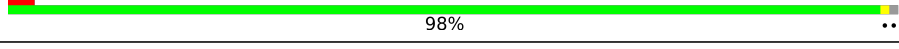
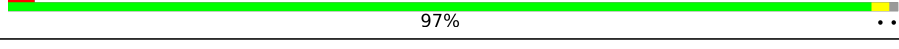
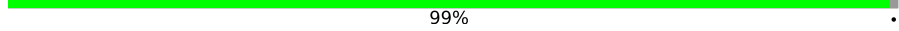

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Mol	Chain	Length	Quality of chain
1	2E	448	 98%
1	2F	448	 96%
1	2G	448	 98%
1	2H	448	 99%
1	2I	448	 99%
1	2J	448	 98%
1	2K	448	 96%
1	2L	448	 98%
1	2M	448	 99%
1	2N	448	 99%
1	2O	448	 98%
1	2P	448	 96%
1	2Q	448	 98%
1	2R	448	 99%
1	2S	448	 99%
1	2T	448	 98%
1	2U	448	 96%
1	2V	448	 98%
1	2W	448	 99%
1	2X	448	 99%
1	2Y	448	 98%
1	3A	448	 96%
1	3B	448	 96%
1	3C	448	 98%
1	3D	448	 97%

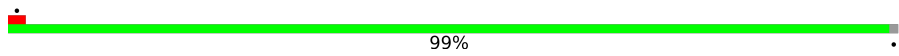
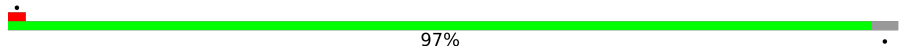
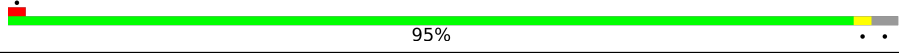
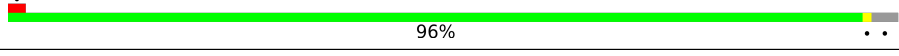
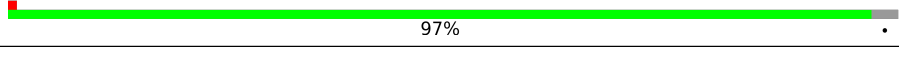
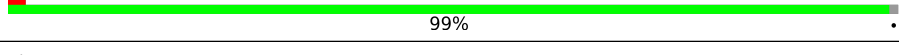
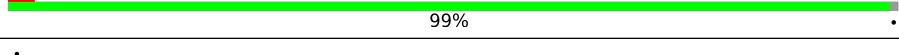
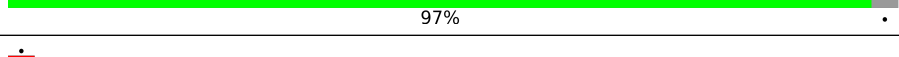
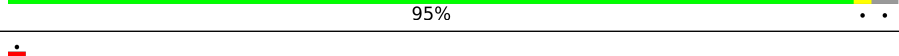
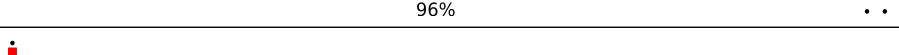
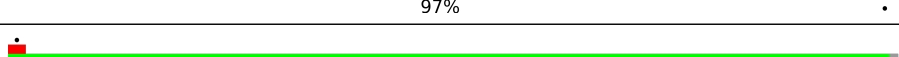
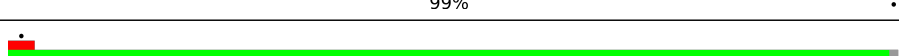
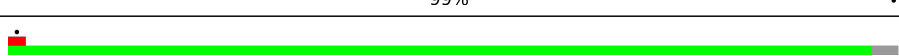
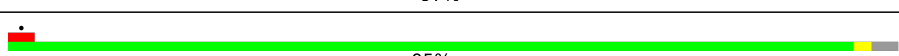
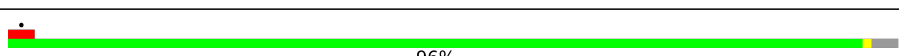
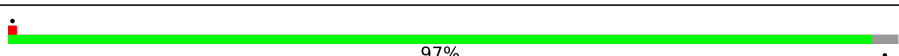
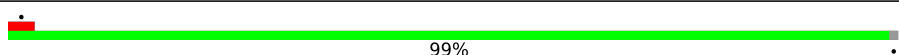
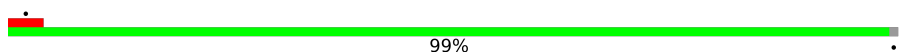
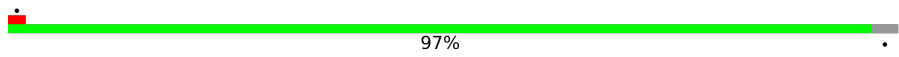
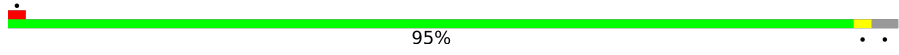
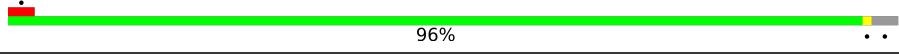
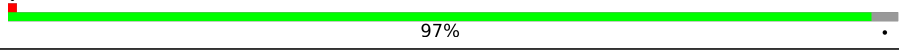
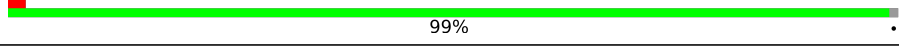
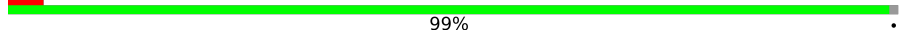

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Mol	Chain	Length	Quality of chain
1	3E	448	 99%
1	3F	448	 99%
1	3G	448	 96%
1	3H	448	 96%
1	3I	448	 98%
1	3J	448	 97%
1	3K	448	 99%
1	3L	448	 99%
1	3M	448	 96%
1	3N	448	 96%
1	3O	448	 98%
1	3P	448	 97%
1	3Q	448	 5% 99%
1	3R	448	 99%
1	3S	448	 96%
1	3T	448	 96%
1	3U	448	 98%
1	3V	448	 97%
1	3W	448	 99%
1	3X	448	 99%
1	3Y	448	 96%
1	3Z	448	 96%
1	3a	448	 98%
1	3b	448	 97%
1	3c	448	 99%

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Mol	Chain	Length	Quality of chain
1	3d	448	 99%
1	4A	448	 97%
1	4B	448	 95%
1	4C	448	 96%
1	4D	448	 97%
1	4E	448	 99%
1	4F	448	 99%
1	4G	448	 97%
1	4H	448	 95%
1	4I	448	 96%
1	4J	448	 97%
1	4K	448	 99%
1	4L	448	 99%
1	4M	448	 97%
1	4N	448	 95%
1	4O	448	 96%
1	4P	448	 97%
1	4Q	448	 99%
1	4R	448	 99%
1	4S	448	 97%
1	4T	448	 95%
1	4U	448	 96%
1	4V	448	 97%
1	4W	448	 99%
1	4X	448	 99%

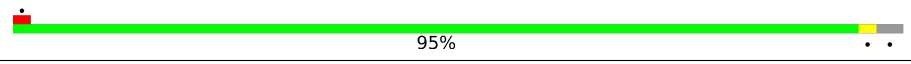
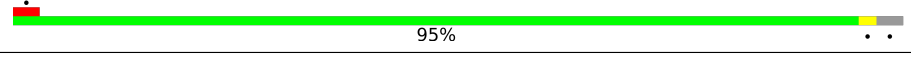
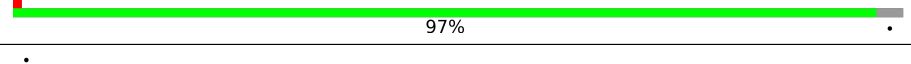
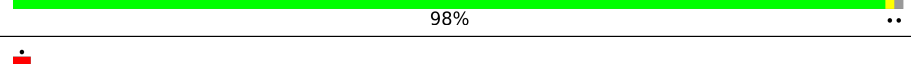
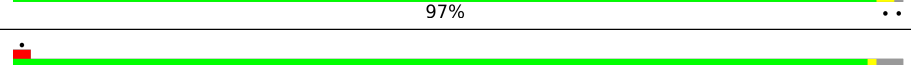
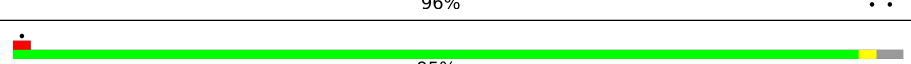
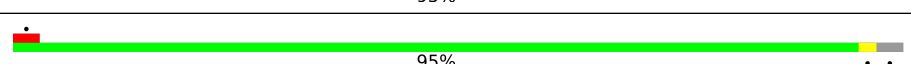
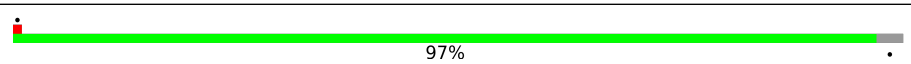
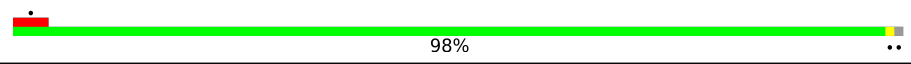
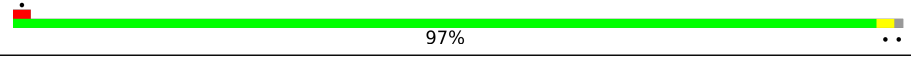
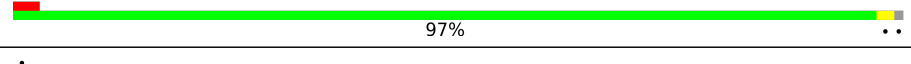
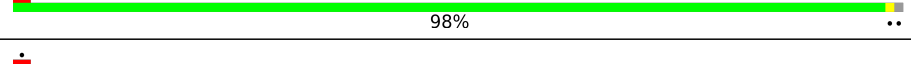
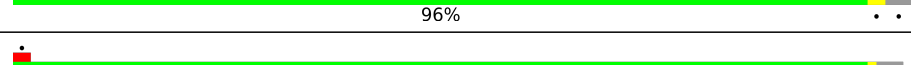
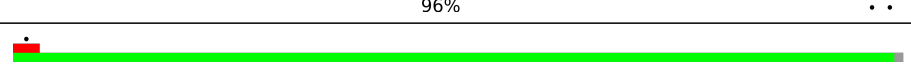
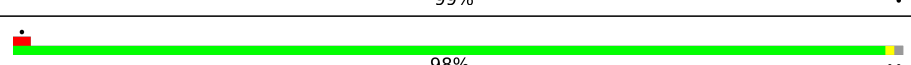
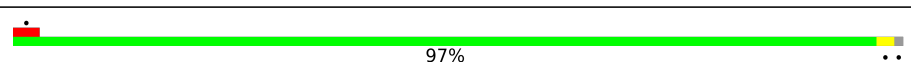
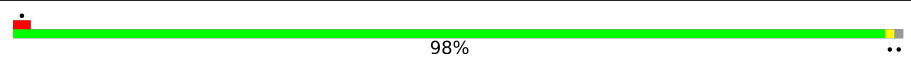
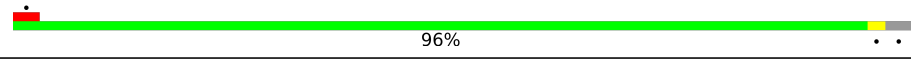
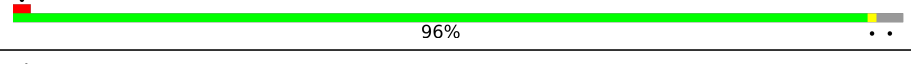
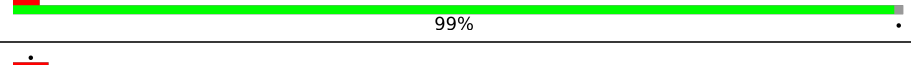
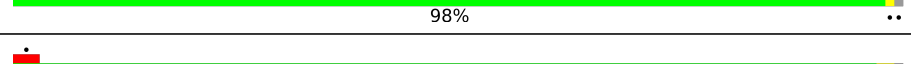
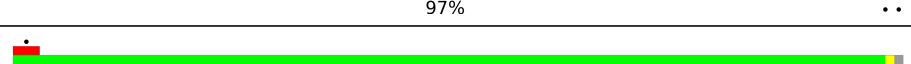
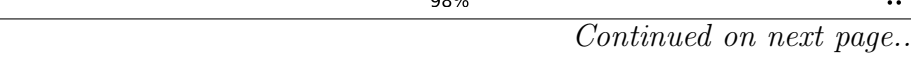


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Mol	Chain	Length	Quality of chain
1	4Y	448	97%
1	4Z	448	95%
1	4a	448	96%
1	4b	448	97%
1	4c	448	99%
1	4d	448	99%
1	5A	448	96%
1	5B	448	95%
1	5C	448	95%
1	5D	448	97%
1	5E	448	98%
1	5F	448	97%
1	5G	448	96%
1	5H	448	95%
1	5I	448	95%
1	5J	448	97%
1	5K	448	98%
1	5L	448	97%
1	5M	448	96%
1	5N	448	95%
1	5O	448	95%
1	5P	448	97%
1	5Q	448	98%
1	5R	448	97%
1	5S	448	96%

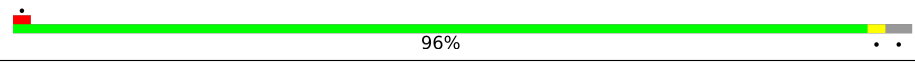
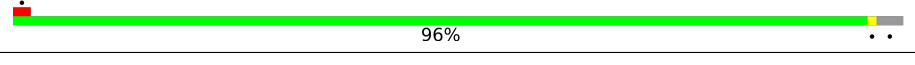
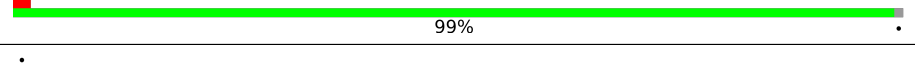
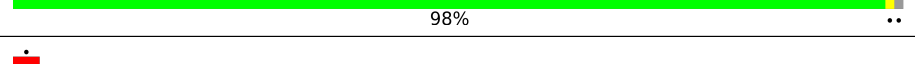
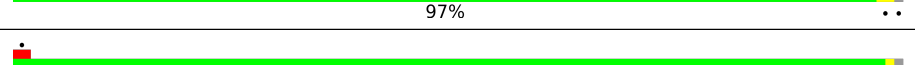
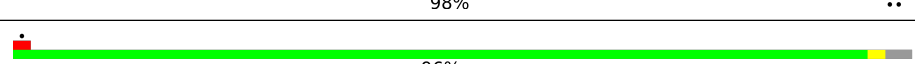
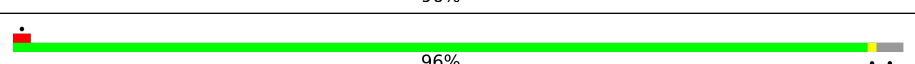
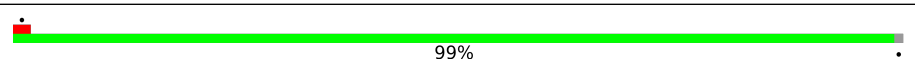
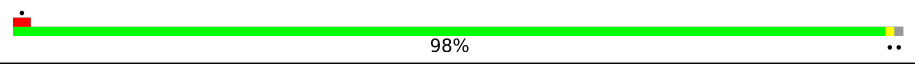
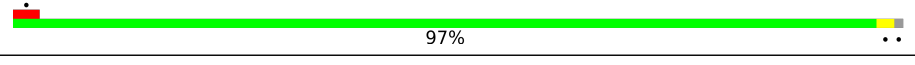
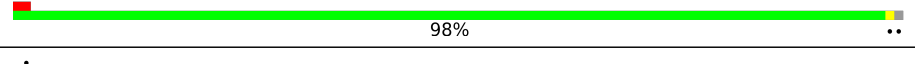
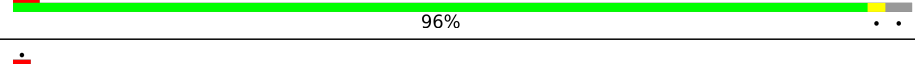
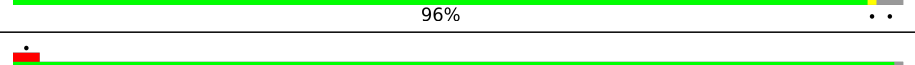
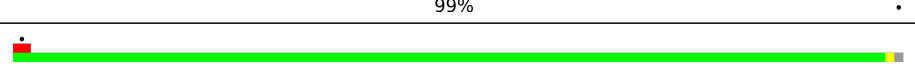
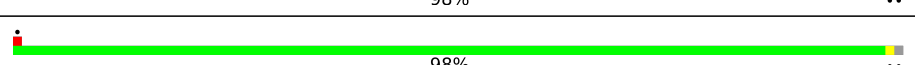
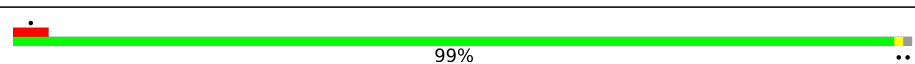
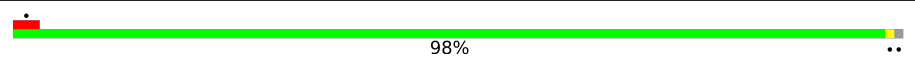
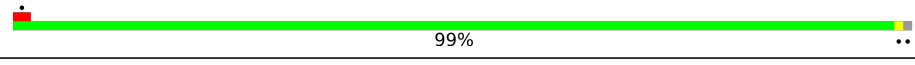
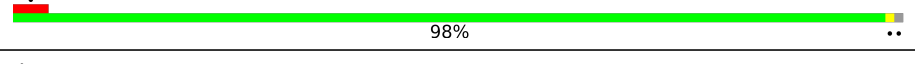
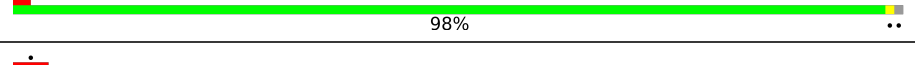
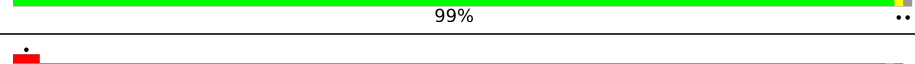
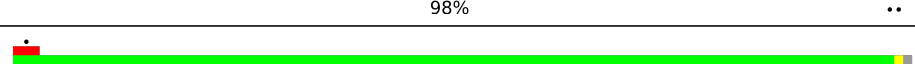
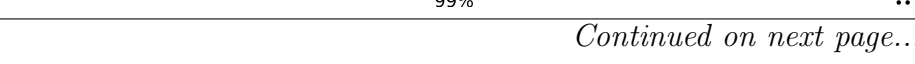


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Mol	Chain	Length	Quality of chain
1	5T	448	 95%
1	5U	448	 95%
1	5V	448	 97%
1	5W	448	 98%
1	5X	448	 97%
1	5Y	448	 96%
1	5Z	448	 95%
1	5a	448	 95%
1	5b	448	 97%
1	5c	448	 98%
1	5d	448	 97%
1	6A	448	 97%
1	6B	448	 98%
1	6C	448	 96%
1	6D	448	 96%
1	6E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

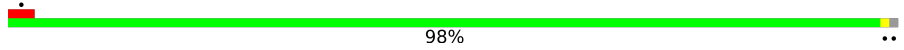
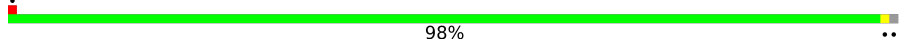
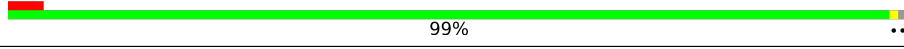
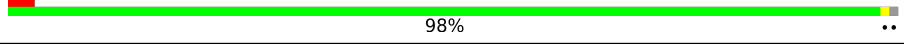
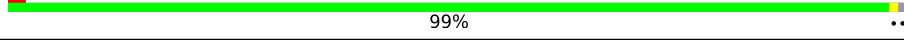
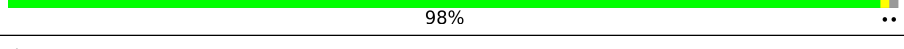
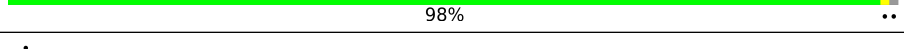
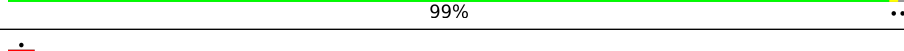
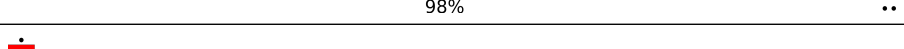
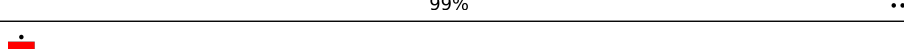
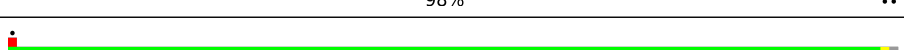
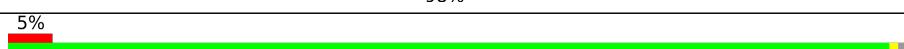
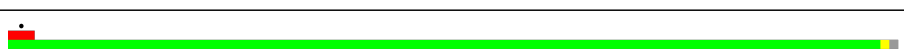
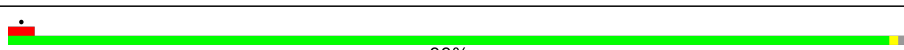
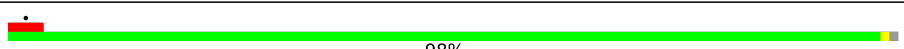


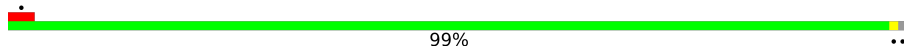
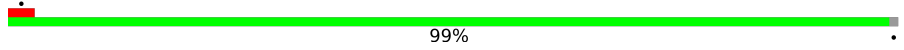
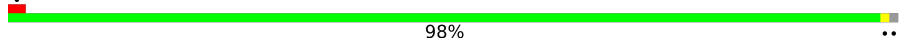
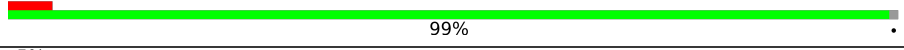
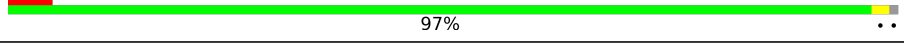
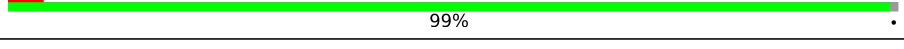
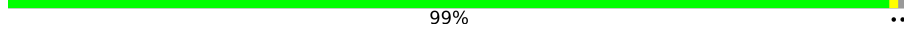

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Mol	Chain	Length	Quality of chain
1	6O	448	 96%
1	6P	448	 96%
1	6Q	448	 99%
1	6R	448	 98%
1	6S	448	 97%
1	6T	448	 98%
1	6U	448	 96%
1	6V	448	 96%
1	6W	448	 99%
1	6X	448	 98%
1	6Y	448	 97%
1	6Z	448	 98%
1	6a	448	 96%
1	6b	448	 96%
1	6c	448	 99%
1	6d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

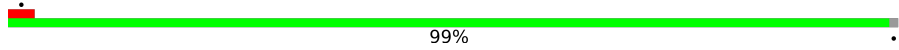
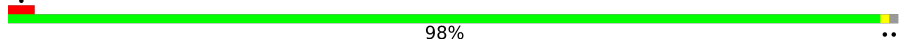
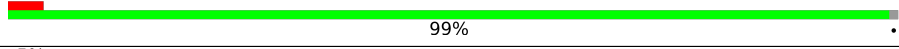
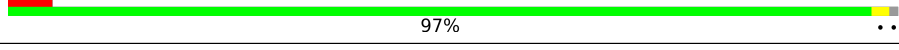
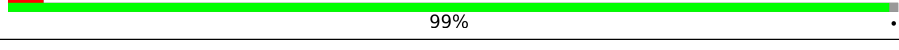
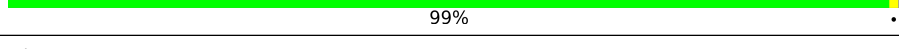
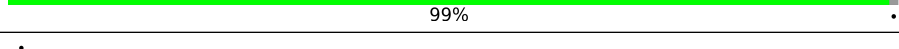
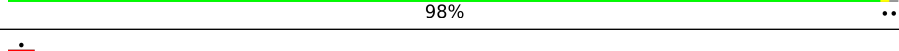
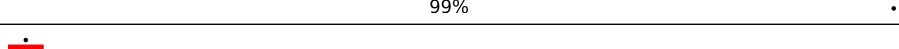
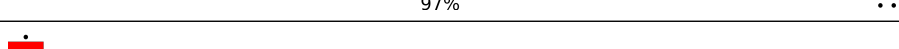
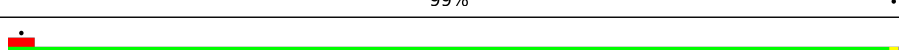
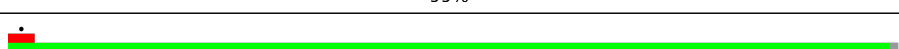
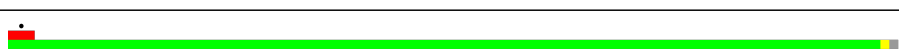
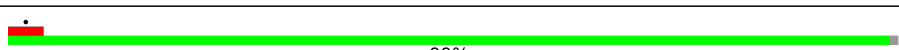
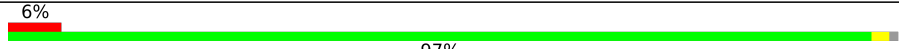
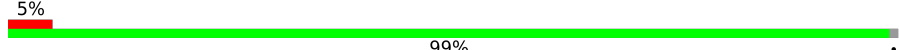
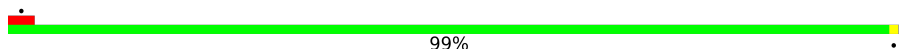
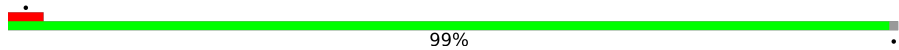
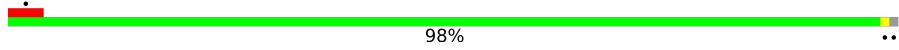
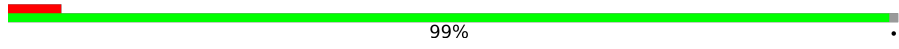
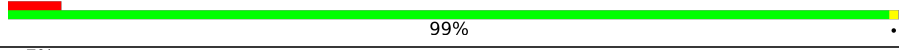
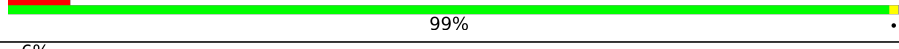
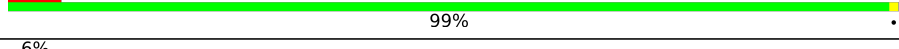
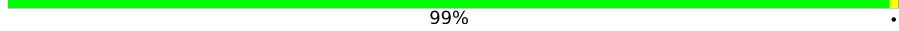

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Mol	Chain	Length	Quality of chain
1	7J	448	 98% ..
1	7K	448	 98% ..
1	7L	448	 99% ..
1	7M	448	 98% ..
1	7N	448	 99% ..
1	7O	448	 98% ..
1	7P	448	 98% ..
1	7Q	448	 99% ..
1	7R	448	 98% ..
1	7S	448	 99% ..
1	7T	448	 98% ..
1	7U	448	 98% ..
1	7V	448	 5% 99% ..
1	7W	448	 98% ..
1	7X	448	 99% ..
1	7Y	448	 98% ..
1	8A	448	 5% 97% ..
1	8B	448	 99% .
1	8C	448	 99% ..
1	8D	448	 99% .
1	8E	448	 98% ..
1	8F	448	 5% 99% .
1	8G	448	 5% 97% ..
1	8H	448	 99% .
1	8I	448	 99% ..

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Mol	Chain	Length	Quality of chain
1	8J	448	 99%
1	8K	448	 98%
1	8L	448	 99%
1	8M	448	 97%
1	8N	448	 99%
1	8O	448	 99%
1	8P	448	 99%
1	8Q	448	 98%
1	8R	448	 99%
1	8S	448	 97%
1	8T	448	 99%
1	8U	448	 99%
1	8V	448	 99%
1	8W	448	 98%
1	8X	448	 99%
1	8Y	448	 97%
1	8Z	448	 99%
1	8a	448	 99%
1	8b	448	 99%
1	8c	448	 98%
1	8d	448	 99%
1	9A	448	 99%
1	9B	448	 99%
1	9C	448	 99%
1	9D	448	 99%

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Mol	Chain	Length	Quality of chain
1	9E	448	5% 99%
2	1e	281	63% 97%
2	1f	281	61% 96%
2	1g	281	64% 97%
2	1h	281	63% 96%
2	1i	281	74% 97%
2	1j	281	71% 96%
2	1k	281	71% 97%
2	1l	281	71% 96%
2	1m	281	73% 97%
2	1n	281	71% 96%
2	1o	281	71% 97%
2	1p	281	72% 96%
2	1q	281	74% 97%
2	1r	281	72% 96%
2	1s	281	72% 97%
2	1t	281	73% 96%
2	1u	281	74% 97%
2	1v	281	70% 96%
2	1w	281	70% 97%
2	1x	281	73% 96%
2	2Z	281	60% 98%
2	2a	281	60% 98%
2	2b	281	62% 98%
2	2c	281	63% 98%

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Mol	Chain	Length	Quality of chain
2	2d	281	61% 98%
2	2e	281	75% 98%
2	2f	281	90% 98%
2	2g	281	92% 98%
2	2h	281	91% 98%
2	2i	281	65% 98%
2	2j	281	75% 98%
2	2k	281	90% 98%
2	2l	281	91% 98%
2	2m	281	91% 98%
2	2n	281	67% 98%
2	2o	281	77% 98%
2	2p	281	91% 98%
2	2q	281	92% 98%
2	2r	281	91% 98%
2	2s	281	67% 98%
2	2t	281	75% 98%
2	2u	281	90% 98%
2	2v	281	92% 98%
2	2w	281	90% 98%
2	2x	281	67% 98%
2	3e	281	61% 96%
2	3f	281	60% 97%
2	3g	281	64% 96%
2	3h	281	65% 97%

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Mol	Chain	Length	Quality of chain
2	3i	281	87% 96%
2	3j	281	70% 97%
2	3k	281	75% 96%
2	3l	281	86% 97%
2	3m	281	88% 96%
2	3n	281	70% 97%
2	3o	281	77% 96%
2	3p	281	85% 97%
2	3q	281	88% 96%
2	3r	281	71% 97%
2	3s	281	79% 96%
2	3t	281	87% 97%
2	3u	281	89% 96%
2	3v	281	70% 97%
2	3w	281	78% 96%
2	3x	281	87% 97%
2	4e	281	62% 97%
2	4f	281	63% 96%
2	4g	281	86% 97%
2	4h	281	90% 96%
2	4i	281	85% 97%
2	4j	281	88% 96%
2	4k	281	86% 97%
2	4l	281	89% 96%
2	4m	281	85% 97%

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Mol	Chain	Length	Quality of chain
2	4n	281	88% 96% ..
2	5e	281	64% 97% .
2	5f	281	63% 96% ..
2	5g	281	89% 97% .
2	5h	281	88% 96% ..
2	5i	281	88% 97% .
2	5j	281	85% 96% ..
2	5k	281	87% 97% .
2	5l	281	86% 96% ..
2	5m	281	85% 97% .
2	5n	281	86% 96% ..
2	6e	281	65% 96% ..
2	6f	281	62% 97% .
2	6g	281	63% 96% ..
2	6h	281	63% 97% .
2	6i	281	91% 96% ..
2	6j	281	93% 97% .
2	6k	281	88% 96% ..
2	6l	281	82% 97% .
2	6m	281	89% 96% ..
2	6n	281	91% 97% .
2	6o	281	83% 96% ..
2	6p	281	81% 97% .
2	6q	281	91% 96% ..
2	6r	281	91% 97% .

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Mol	Chain	Length	Quality of chain
2	6s	281	86% 96% ..
2	6t	281	81% 97% .
2	6u	281	90% 96% ..
2	6v	281	91% 97% .
2	6w	281	86% 96% ..
2	6x	281	78% 97% .
2	7Z	281	62% 98% .
2	7a	281	63% 98% .
2	7b	281	63% 98% .
2	7c	281	63% 98% .
2	7d	281	61% 98% .
2	7e	281	88% 98% .
2	7f	281	85% 98% .
2	7g	281	89% 98% .
2	7h	281	76% 98% .
2	7i	281	89% 98% .
2	7j	281	87% 98% .
2	7k	281	81% 98% .
2	7l	281	85% 98% .
2	7m	281	73% 98% .
2	7n	281	88% 98% .
2	7o	281	88% 98% .
2	7p	281	83% 98% .
2	7q	281	87% 98% .
2	7r	281	74% 98% .

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Mol	Chain	Length	Quality of chain
2	7s	281	88% 98%
2	7t	281	89% 98%
2	7u	281	87% 98%
2	7v	281	85% 98%
2	7w	281	75% 98%
2	7x	281	85% 98%
2	8e	281	64% 96%
2	8f	281	66% 97%
2	8g	281	64% 97%
2	8h	281	64% 96%
2	8i	281	67% 97%
2	8j	281	63% 96%
2	8k	281	64% 96%
2	8l	281	69% 97%
2	8m	281	86% 97%
2	8n	281	91% 96%
2	8o	281	88% 97%
2	8p	281	84% 96%
2	8q	281	65% 96%
2	8r	281	69% 97%
2	8s	281	88% 97%
2	8t	281	92% 96%
2	8u	281	88% 97%
2	8v	281	81% 96%
2	8w	281	65% 96%

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Mol	Chain	Length	Quality of chain
2	8x	281	69% 97% .
2	8y	281	88% 97% .
2	8z	281	90% 96% ..
2	9F	281	65% 98% .
2	9G	281	64% 98% .
2	9H	281	64% 98% .
2	9I	281	64% 98% .
2	9J	281	64% 98% .
2	9K	281	89% 97% .
2	9L	281	82% 96% ..
2	9M	281	64% 96% ..
2	9N	281	69% 97% .
2	9O	281	84% 97% .
2	9P	281	86% 96% ..
2	9Q	281	85% 97% .
2	9R	281	77% 96% ..

2 Entry composition [i](#)

There are 2 unique types of molecules in this entry. The entry contains 1161205 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 3393	C 2144	N 578	O 663	S 8	0	0
1	1B	445	Total 3487	C 2203	N 592	O 684	S 8	0	0
1	1C	445	Total 3483	C 2201	N 592	O 682	S 8	0	0
1	1D	445	Total 3487	C 2203	N 592	O 684	S 8	0	0
1	1E	435	Total 3422	C 2167	N 579	O 668	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 3483	C 2201	N 592	O 682	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
			3422	2167	579	668	8		
1	4B	435	Total	C	N	O	S	0	0
			3422	2167	579	668	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
			3422	2167	579	668	8		
1	4E	445	Total	C	N	O	S	0	0
			3483	2201	592	682	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
			3422	2167	579	668	8		
1	5B	435	Total	C	N	O	S	0	0
			3422	2167	579	668	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
			3422	2167	579	668	8		
1	5E	445	Total	C	N	O	S	0	0
			3483	2201	592	682	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
			3483	2201	592	682	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
			3422	2167	579	668	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
			3483	2201	592	682	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 3483	C 2201	N 592	O 682	S 8	0	0
1	8C	445	Total 3487	C 2203	N 592	O 684	S 8	0	0
1	8D	445	Total 3483	C 2201	N 592	O 682	S 8	0	0
1	8E	445	Total 3487	C 2203	N 592	O 684	S 8	0	0
1	8F	445	Total 3483	C 2201	N 592	O 682	S 8	0	0
1	9A	445	Total 3487	C 2203	N 592	O 684	S 8	0	0
1	1G	433	Total 3393	C 2144	N 578	O 663	S 8	0	0
1	1H	445	Total 3487	C 2203	N 592	O 684	S 8	0	0
1	1I	445	Total 3483	C 2201	N 592	O 682	S 8	0	0
1	1J	445	Total 3487	C 2203	N 592	O 684	S 8	0	0
1	1K	435	Total 3422	C 2167	N 579	O 668	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
			3483	2201	592	682	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
			3422	2167	579	668	8		
1	4H	435	Total	C	N	O	S	0	0
			3422	2167	579	668	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
			3422	2167	579	668	8		
1	4K	445	Total	C	N	O	S	0	0
			3483	2201	592	682	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
			3422	2167	579	668	8		
1	5H	435	Total	C	N	O	S	0	0
			3422	2167	579	668	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
			3422	2167	579	668	8		
1	5K	445	Total	C	N	O	S	0	0
			3483	2201	592	682	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
			3483	2201	592	682	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
			3422	2167	579	668	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 3483	C 2201	N 592	O 682	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 3483	C 2201	N 592	O 682	S 8	0	0
1	8I	445	Total 3487	C 2203	N 592	O 684	S 8	0	0
1	8J	445	Total 3483	C 2201	N 592	O 682	S 8	0	0
1	8K	445	Total 3487	C 2203	N 592	O 684	S 8	0	0
1	8L	445	Total 3483	C 2201	N 592	O 682	S 8	0	0
1	9B	445	Total 3487	C 2203	N 592	O 684	S 8	0	0
1	1M	433	Total 3393	C 2144	N 578	O 663	S 8	0	0
1	1N	445	Total 3487	C 2203	N 592	O 684	S 8	0	0
1	1O	445	Total 3483	C 2201	N 592	O 682	S 8	0	0
1	1P	445	Total 3487	C 2203	N 592	O 684	S 8	0	0
1	1Q	435	Total 3422	C 2167	N 579	O 668	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 3483	C 2201	N 592	O 682	S 8	0	0
1	3R	445	Total 3487	C 2203	N 592	O 684	S 8	0	0
1	4M	435	Total 3422	C 2167	N 579	O 668	S 8	0	0
1	4N	435	Total 3422	C 2167	N 579	O 668	S 8	0	0
1	4O	435	Total 3426	C 2169	N 579	O 670	S 8	0	0
1	4P	435	Total 3422	C 2167	N 579	O 668	S 8	0	0
1	4Q	445	Total 3483	C 2201	N 592	O 682	S 8	0	0
1	4R	445	Total 3487	C 2203	N 592	O 684	S 8	0	0
1	5M	435	Total 3422	C 2167	N 579	O 668	S 8	0	0
1	5N	435	Total 3422	C 2167	N 579	O 668	S 8	0	0
1	5O	435	Total 3426	C 2169	N 579	O 670	S 8	0	0
1	5P	435	Total 3422	C 2167	N 579	O 668	S 8	0	0
1	5Q	445	Total 3483	C 2201	N 592	O 682	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
			3483	2201	592	682	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
			3422	2167	579	668	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
			3483	2201	592	682	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
			3483	2201	592	682	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
			3483	2201	592	682	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
			3483	2201	592	682	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
			3393	2144	578	663	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 3483	C 2201	N 592	O 682	S 8	0	0
1	1V	445	Total 3487	C 2203	N 592	O 684	S 8	0	0
1	1W	435	Total 3422	C 2167	N 579	O 668	S 8	0	0
1	1X	438	Total 3449	C 2182	N 584	O 675	S 8	0	0
1	2P	438	Total 3430	C 2167	N 583	O 672	S 8	0	0
1	2Q	445	Total 3487	C 2203	N 592	O 684	S 8	0	0
1	2R	445	Total 3487	C 2203	N 592	O 684	S 8	0	0
1	2S	445	Total 3487	C 2203	N 592	O 684	S 8	0	0
1	2T	445	Total 3487	C 2203	N 592	O 684	S 8	0	0
1	3S	435	Total 3422	C 2167	N 579	O 668	S 8	0	0
1	3T	435	Total 3426	C 2169	N 579	O 670	S 8	0	0
1	3U	445	Total 3483	C 2201	N 592	O 682	S 8	0	0
1	3V	445	Total 3487	C 2203	N 592	O 684	S 8	0	0
1	3W	445	Total 3483	C 2201	N 592	O 682	S 8	0	0
1	3X	445	Total 3487	C 2203	N 592	O 684	S 8	0	0
1	4S	435	Total 3422	C 2167	N 579	O 668	S 8	0	0
1	4T	435	Total 3422	C 2167	N 579	O 668	S 8	0	0
1	4U	435	Total 3426	C 2169	N 579	O 670	S 8	0	0
1	4V	435	Total 3422	C 2167	N 579	O 668	S 8	0	0
1	4W	445	Total 3483	C 2201	N 592	O 682	S 8	0	0
1	4X	445	Total 3487	C 2203	N 592	O 684	S 8	0	0

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Mol	Chain	Residues	Atoms					AltConf	Trace
1	5S	435	Total	C	N	O	S	0	0
			3422	2167	579	668	8		
1	5T	435	Total	C	N	O	S	0	0
			3422	2167	579	668	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
			3422	2167	579	668	8		
1	5W	445	Total	C	N	O	S	0	0
			3483	2201	592	682	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
			3483	2201	592	682	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
			3422	2167	579	668	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
			3483	2201	592	682	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
			3483	2201	592	682	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
			3483	2201	592	682	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 3483	C 2201	N 592	O 682	S 8	0	0
1	9D	445	Total 3487	C 2203	N 592	O 684	S 8	0	0
1	1Y	433	Total 3393	C 2144	N 578	O 663	S 8	0	0
1	1Z	445	Total 3487	C 2203	N 592	O 684	S 8	0	0
1	1a	445	Total 3483	C 2201	N 592	O 682	S 8	0	0
1	1b	445	Total 3487	C 2203	N 592	O 684	S 8	0	0
1	1c	435	Total 3422	C 2167	N 579	O 668	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 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	4Y	435	Total 3422	C 2167	N 579	O 668	S 8	0	0

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Mol	Chain	Residues	Atoms					AltConf	Trace
1	4Z	435	Total	C	N	O	S	0	0
			3422	2167	579	668	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
			3422	2167	579	668	8		
1	4c	445	Total	C	N	O	S	0	0
			3483	2201	592	682	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
			3422	2167	579	668	8		
1	5Z	435	Total	C	N	O	S	0	0
			3422	2167	579	668	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
			3422	2167	579	668	8		
1	5c	445	Total	C	N	O	S	0	0
			3483	2201	592	682	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
			3483	2201	592	682	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
			3422	2167	579	668	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
			3483	2201	592	682	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
			3483	2201	592	682	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
			3483	2201	592	682	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
			3483	2201	592	682	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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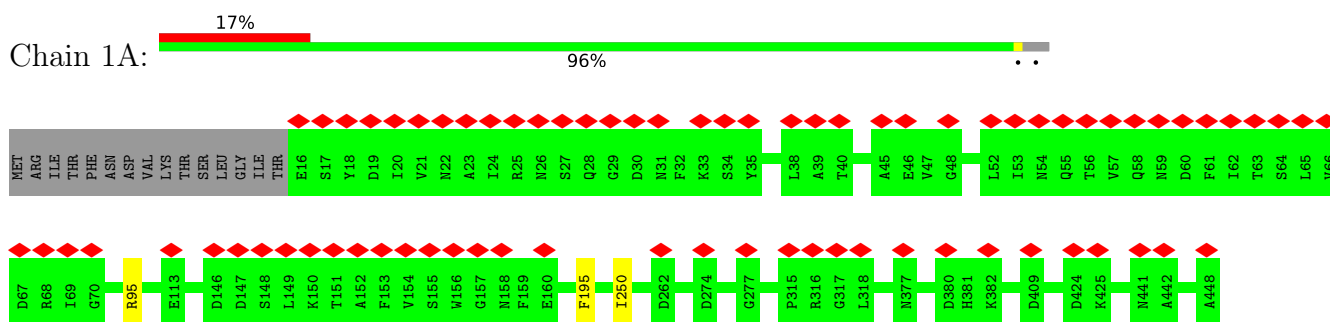
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Chain	Residue	Modelled	Actual	Comment	Reference
9N	281	LEU	-	insertion	UNP B3VMP4
9O	123	GLU	ASP	conflict	UNP B3VMP4
9O	281	LEU	-	insertion	UNP B3VMP4
9P	123	GLU	ASP	conflict	UNP B3VMP4
9P	281	LEU	-	insertion	UNP B3VMP4
9Q	123	GLU	ASP	conflict	UNP 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

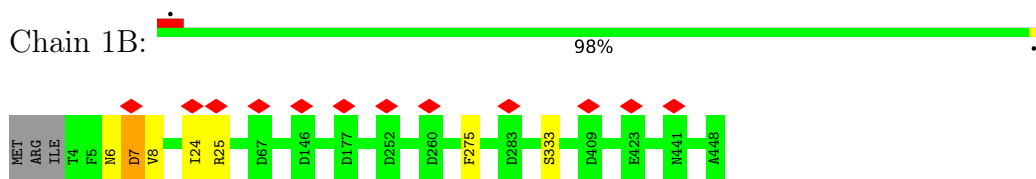
3 Residue-property plots [i](#)

These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and 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.

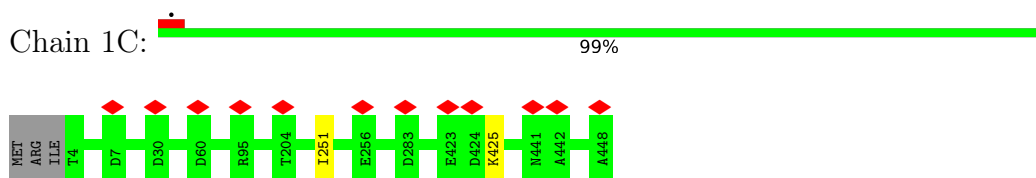
- Molecule 1: Major capsid protein



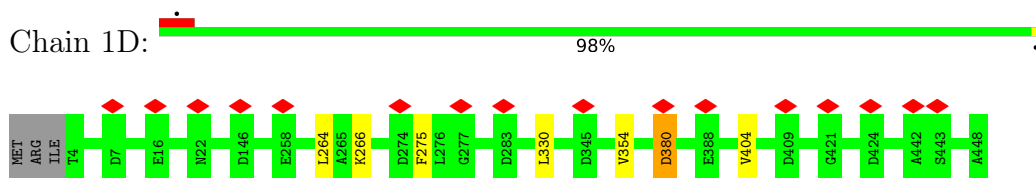
- Molecule 1: Major capsid protein



- Molecule 1: Major capsid protein

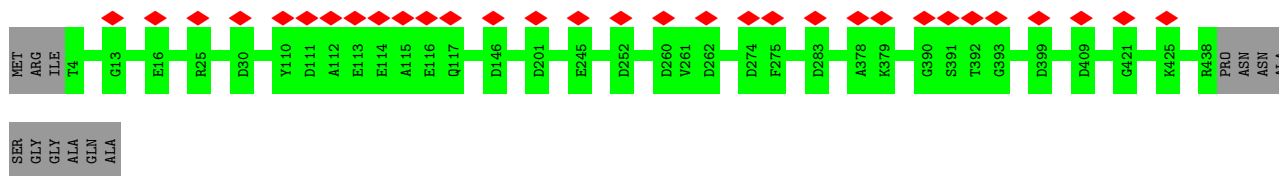


- Molecule 1: Major capsid protein

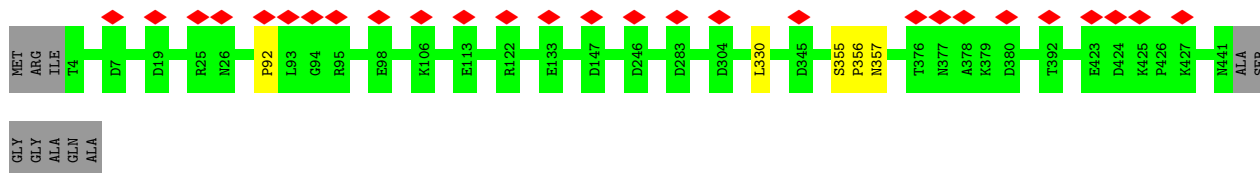


- Molecule 1: Major capsid protein

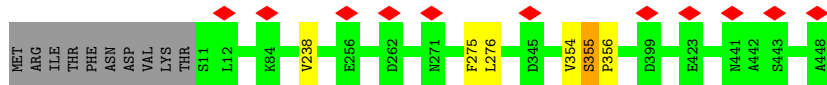




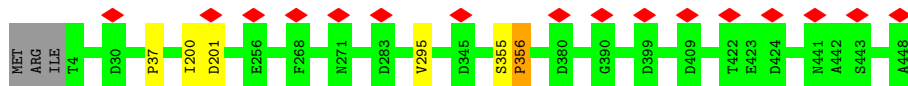
● Molecule 1: Major capsid protein



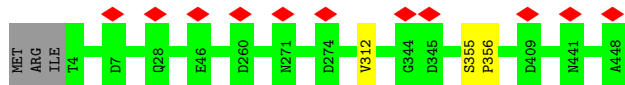
● Molecule 1: Major capsid protein



● Molecule 1: Major capsid protein



● Molecule 1: Major capsid protein



● Molecule 1: Major capsid protein

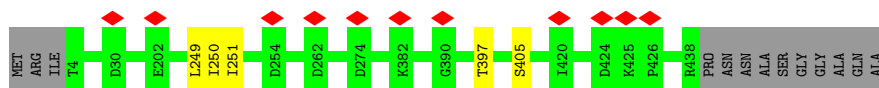


● Molecule 1: Major capsid protein

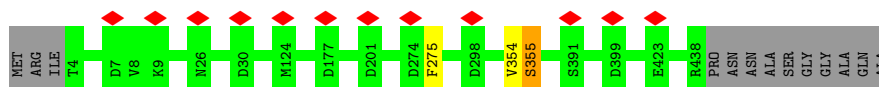




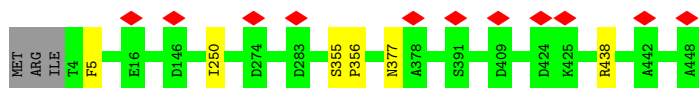
- Molecule 1: Major capsid protein



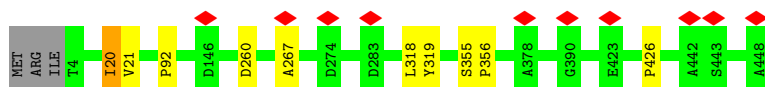
- Molecule 1: Major capsid protein



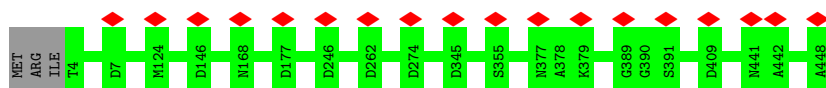
- Molecule 1: Major capsid protein



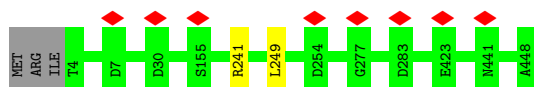
- Molecule 1: Major capsid protein



- Molecule 1: Major capsid protein

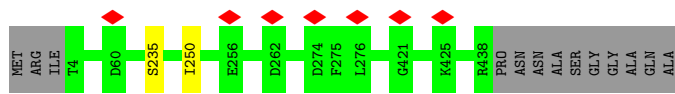


- Molecule 1: Major capsid protein



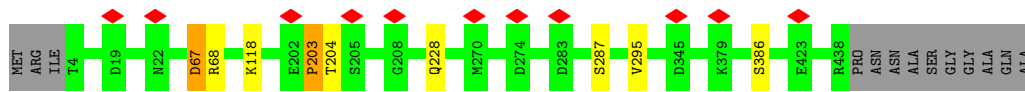
- Molecule 1: Major capsid protein

Chain 4A:  97%



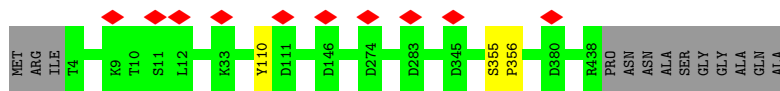
• Molecule 1: Major capsid protein

Chain 4B:  95%



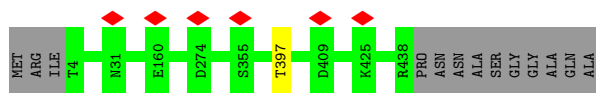
• Molecule 1: Major capsid protein

Chain 4C:  96%



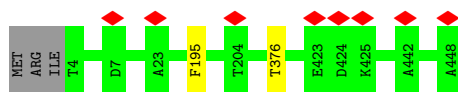
• Molecule 1: Major capsid protein

Chain 4D:  97%



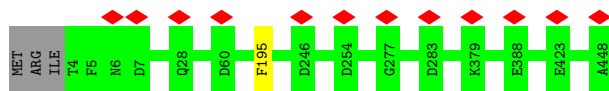
• Molecule 1: Major capsid protein

Chain 4E:  99%



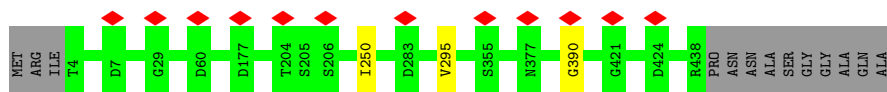
• Molecule 1: Major capsid protein

Chain 4F:  99%

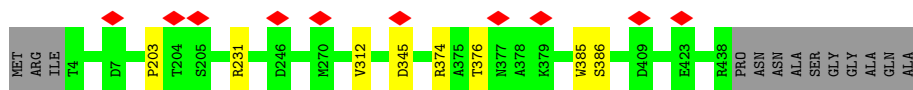


• Molecule 1: Major capsid protein

Chain 5A:  96%



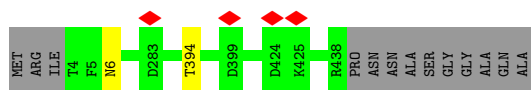
- Molecule 1: Major capsid protein



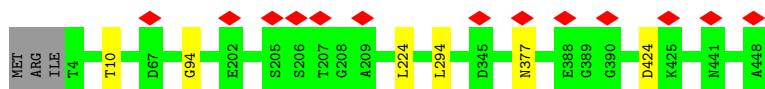
- Molecule 1: Major capsid protein



- Molecule 1: Major capsid protein



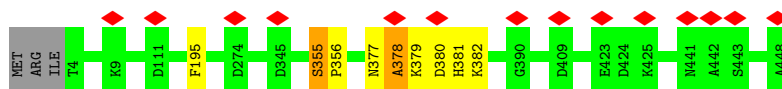
- Molecule 1: Major capsid protein



- Molecule 1: Major capsid protein

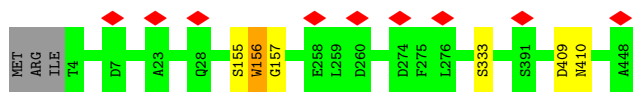


- Molecule 1: Major capsid protein

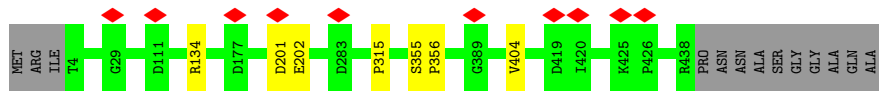


- Molecule 1: Major capsid protein

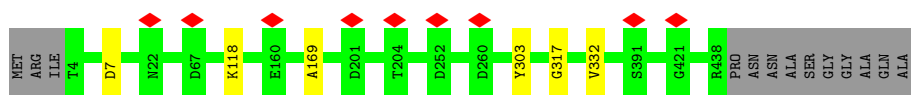




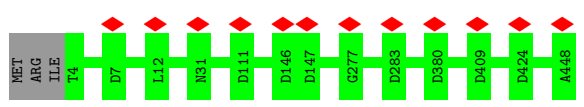
• Molecule 1: Major capsid protein



• Molecule 1: Major capsid protein



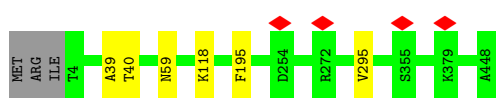
• Molecule 1: Major capsid protein



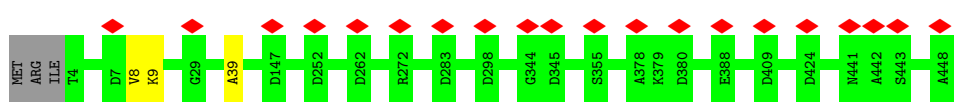
• Molecule 1: Major capsid protein



• Molecule 1: Major capsid protein

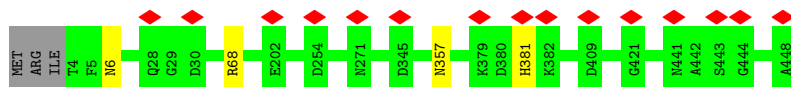


• Molecule 1: Major capsid protein



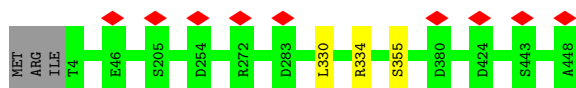
• Molecule 1: Major capsid protein

Chain 7C:  98%



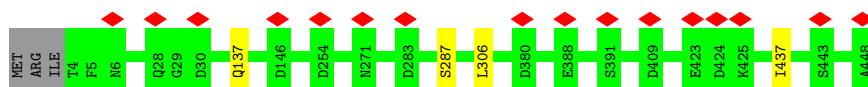
- Molecule 1: Major capsid protein

Chain 7D:  99%



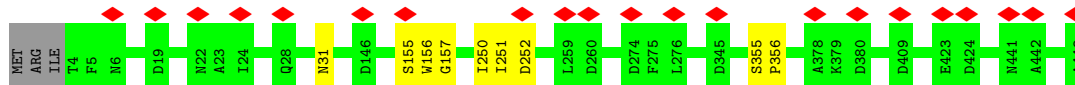
- Molecule 1: Major capsid protein

Chain 7E:  98%



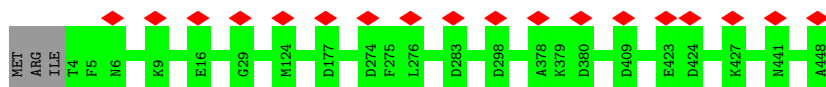
- Molecule 1: Major capsid protein

Chain 8A:  97%



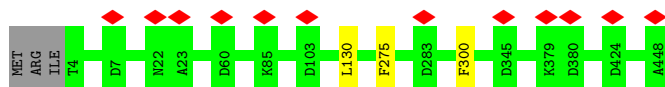
- Molecule 1: Major capsid protein

Chain 8B:  99%



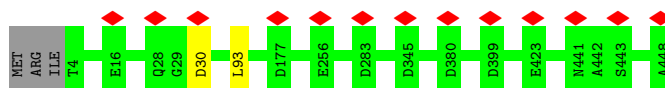
- Molecule 1: Major capsid protein

Chain 8C:  99%

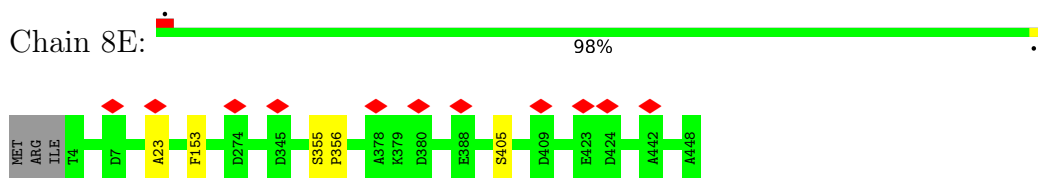


- Molecule 1: Major capsid protein

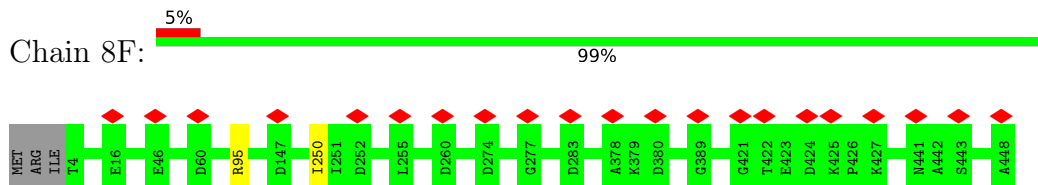
Chain 8D:  99%



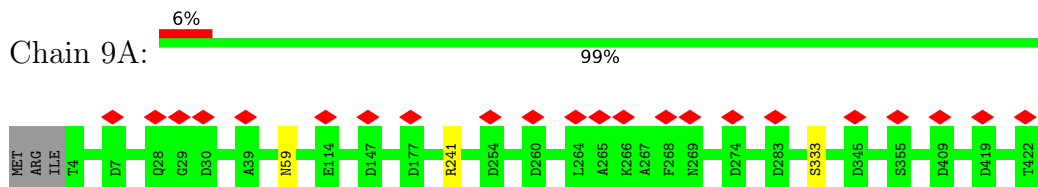
- Molecule 1: Major capsid protein



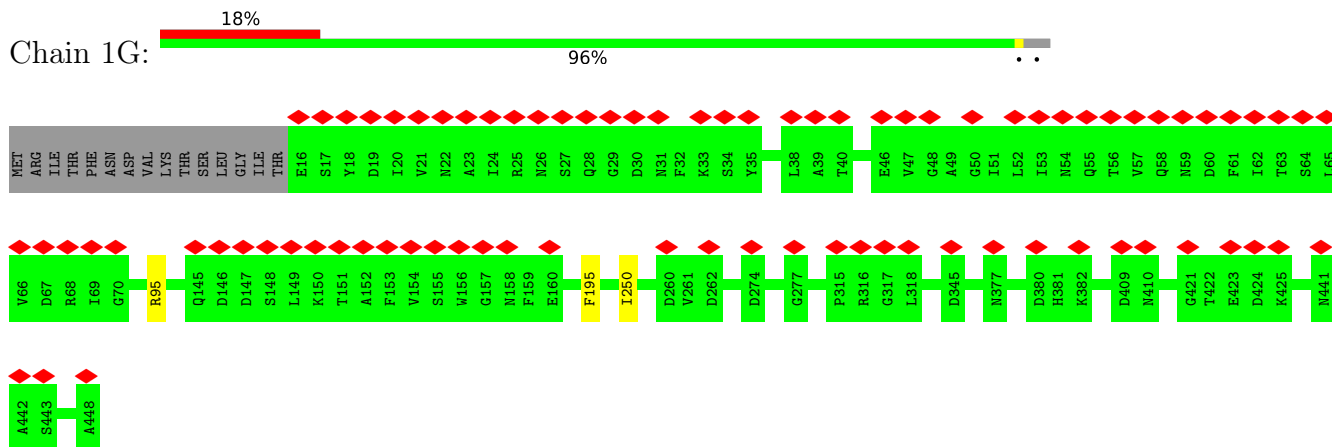
- Molecule 1: Major capsid protein



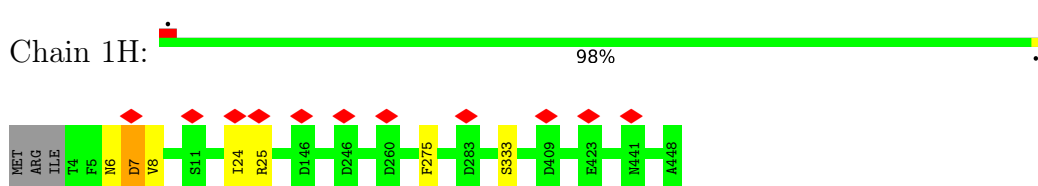
- Molecule 1: Major capsid protein



- Molecule 1: Major capsid protein

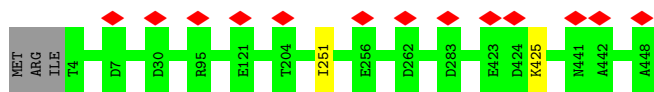


- Molecule 1: Major capsid protein

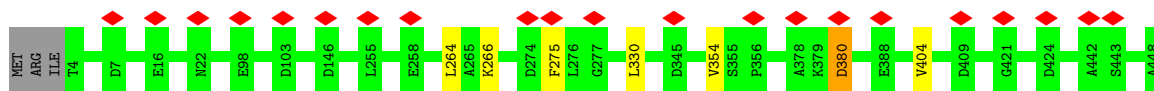


- Molecule 1: Major capsid protein

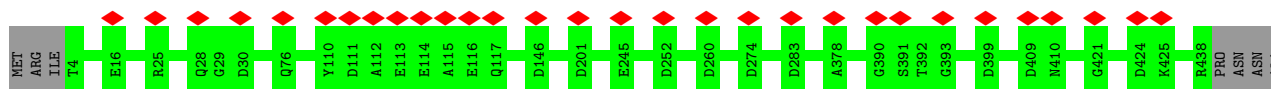




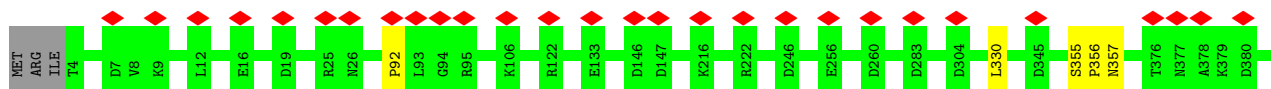
• Molecule 1: Major capsid protein



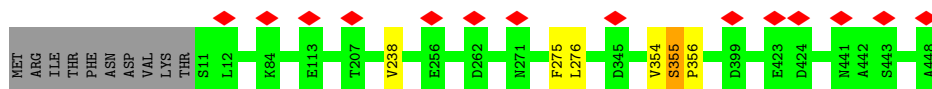
• Molecule 1: Major capsid protein



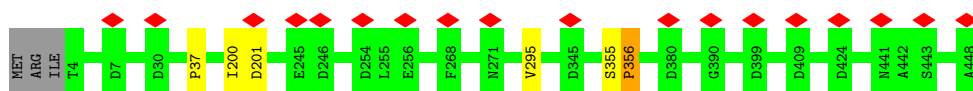
• Molecule 1: Major capsid protein



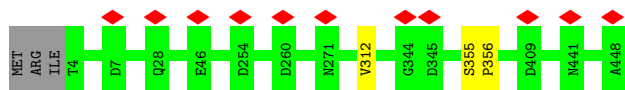
• Molecule 1: Major capsid protein



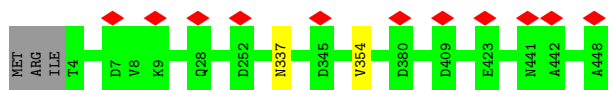
• Molecule 1: Major capsid protein



• Molecule 1: Major capsid protein



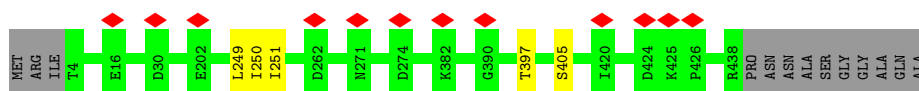
• Molecule 1: Major capsid protein



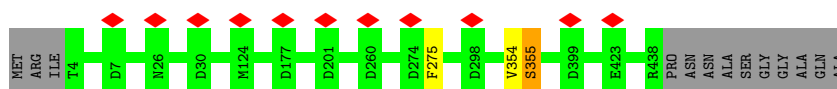
• Molecule 1: Major capsid protein



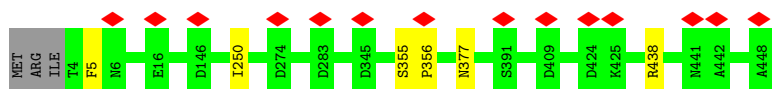
• Molecule 1: Major capsid protein



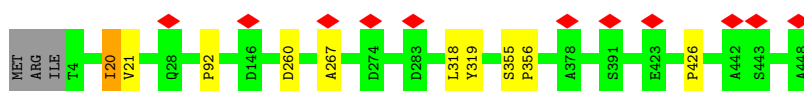
• Molecule 1: Major capsid protein



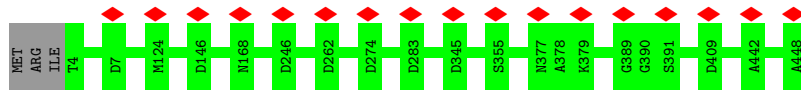
• Molecule 1: Major capsid protein



• Molecule 1: Major capsid protein



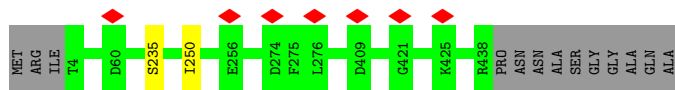
- Molecule 1: Major capsid protein



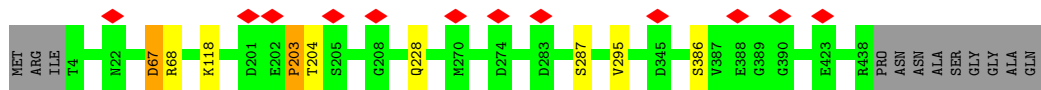
- Molecule 1: Major capsid protein



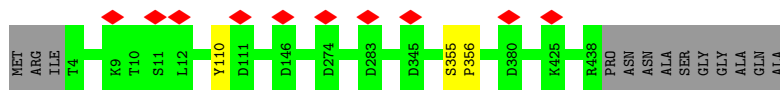
- Molecule 1: Major capsid protein



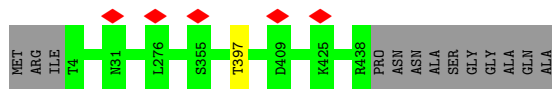
- Molecule 1: Major capsid protein



- Molecule 1: Major capsid protein



- Molecule 1: Major capsid protein

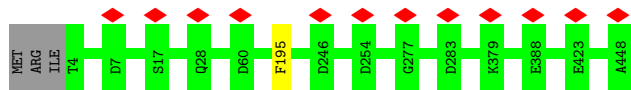


- Molecule 1: Major capsid protein

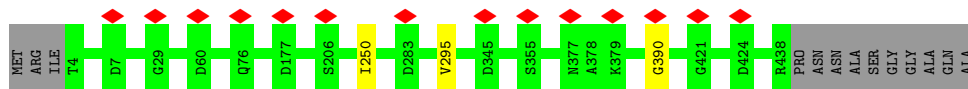




• Molecule 1: Major capsid protein



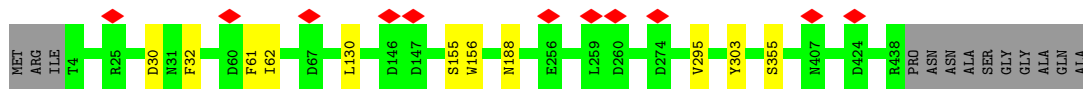
• Molecule 1: Major capsid protein



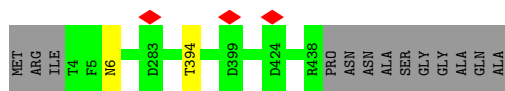
• Molecule 1: Major capsid protein



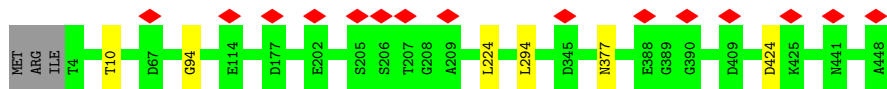
• Molecule 1: Major capsid protein



• Molecule 1: Major capsid protein



• Molecule 1: Major capsid protein



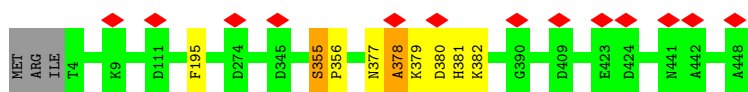
• Molecule 1: Major capsid protein

Chain 5L:  97%



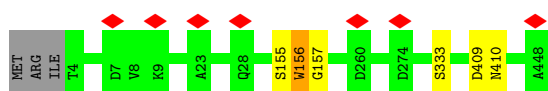
• Molecule 1: Major capsid protein

Chain 6G:  97%



• Molecule 1: Major capsid protein

Chain 6H:  98%



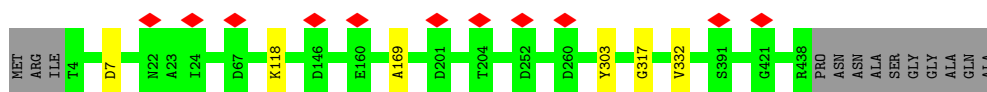
• Molecule 1: Major capsid protein

Chain 6I:  96%



• Molecule 1: Major capsid protein

Chain 6J:  96%



• Molecule 1: Major capsid protein

Chain 6K:  99%

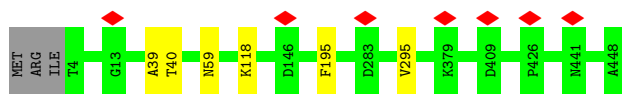


• Molecule 1: Major capsid protein

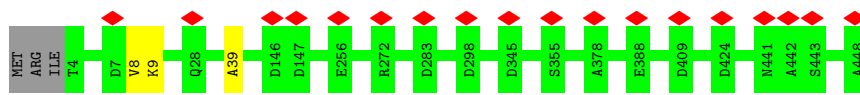
Chain 6L:  98%



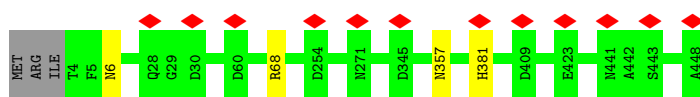
- Molecule 1: Major capsid protein



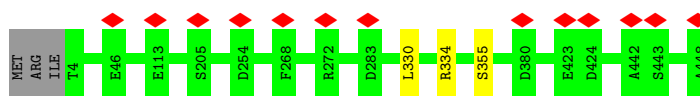
- Molecule 1: Major capsid protein



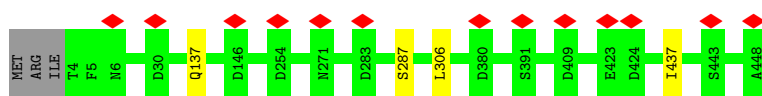
- Molecule 1: Major capsid protein



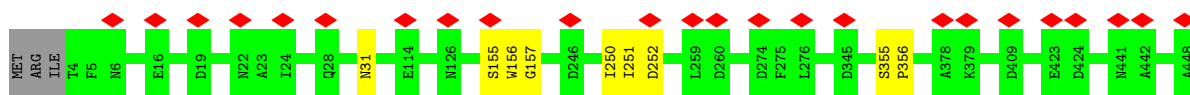
- Molecule 1: Major capsid protein



- Molecule 1: Major capsid protein

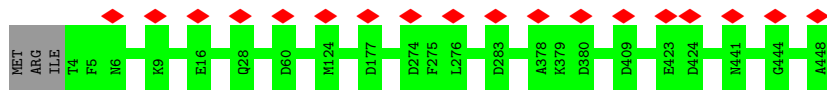


- Molecule 1: Major capsid protein

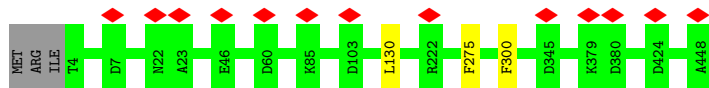


- Molecule 1: Major capsid protein





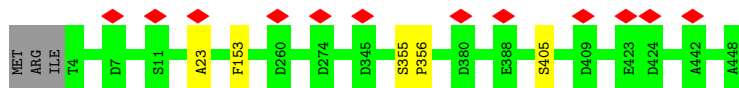
• Molecule 1: Major capsid protein



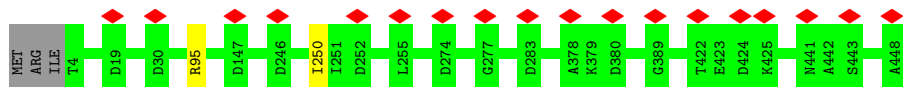
• Molecule 1: Major capsid protein



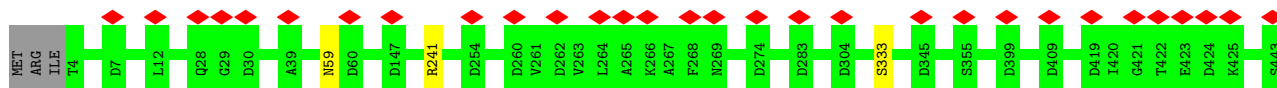
• Molecule 1: Major capsid protein



• Molecule 1: Major capsid protein

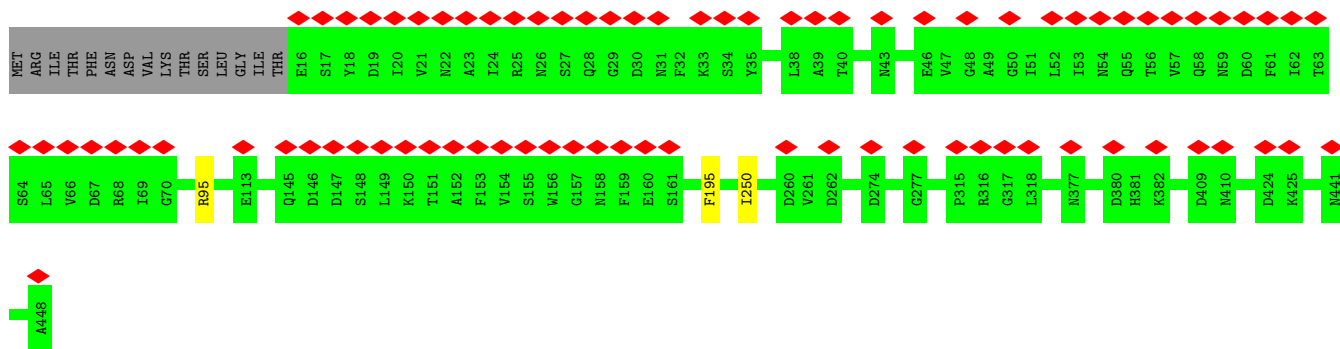


• Molecule 1: Major capsid protein

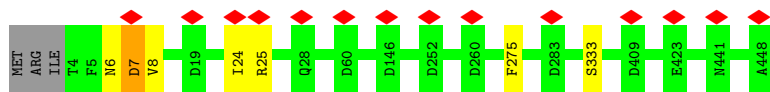


• Molecule 1: Major capsid protein





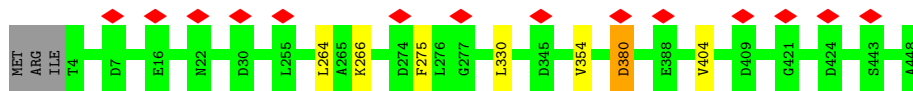
• Molecule 1: Major capsid protein



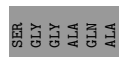
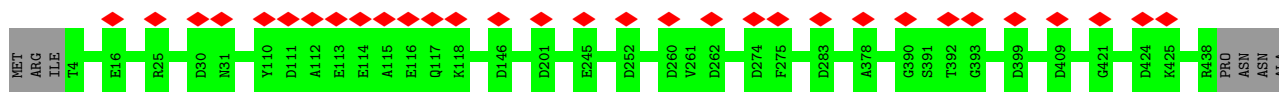
• Molecule 1: Major capsid protein



• Molecule 1: Major capsid protein

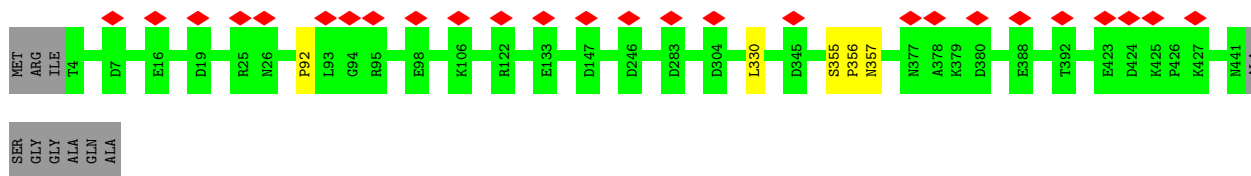


• Molecule 1: Major capsid protein

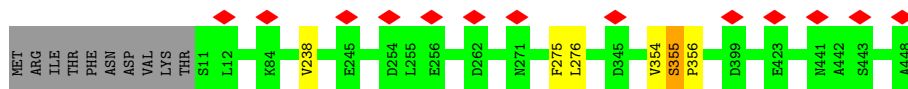


• Molecule 1: Major capsid protein

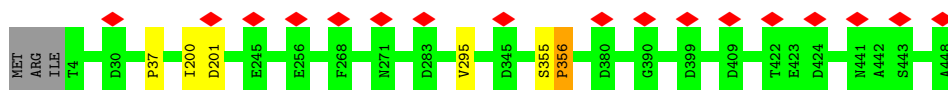




• Molecule 1: Major capsid protein



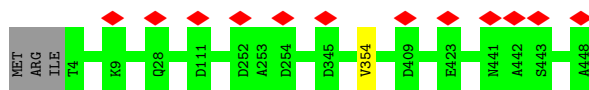
• Molecule 1: Major capsid protein



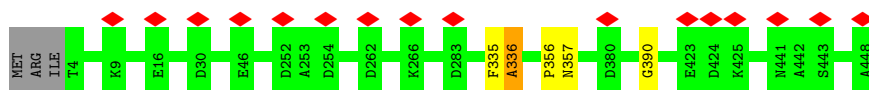
• Molecule 1: Major capsid protein



• Molecule 1: Major capsid protein

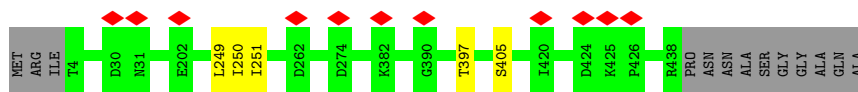


• Molecule 1: Major capsid protein

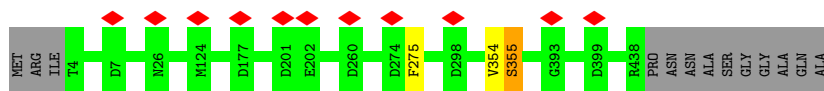


• Molecule 1: Major capsid protein





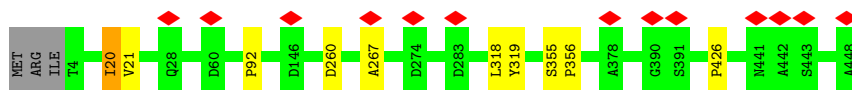
- Molecule 1: Major capsid protein



- Molecule 1: Major capsid protein



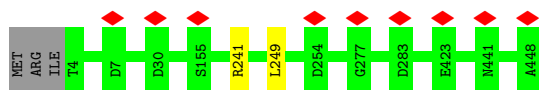
- Molecule 1: Major capsid protein



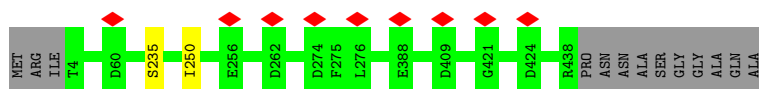
- Molecule 1: Major capsid protein



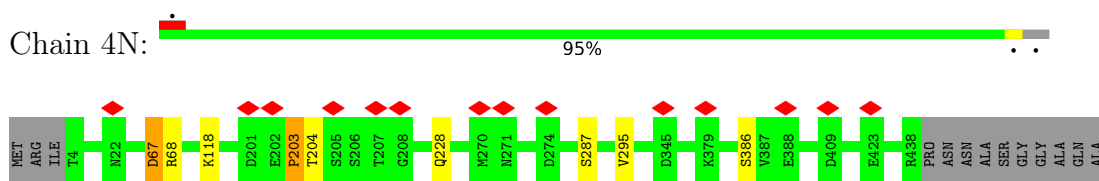
- Molecule 1: Major capsid protein



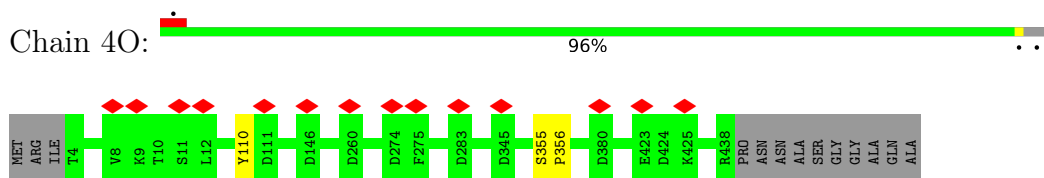
- Molecule 1: Major capsid protein



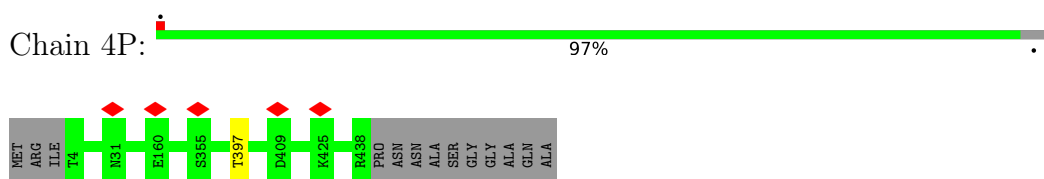
- Molecule 1: Major capsid protein



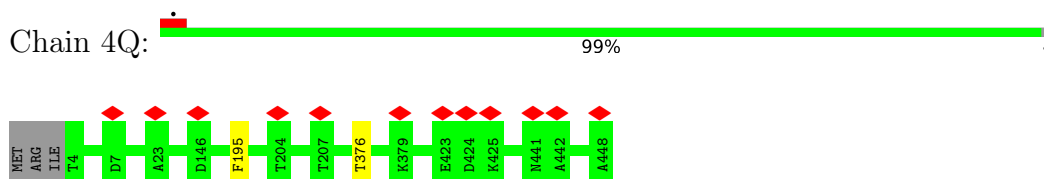
• Molecule 1: Major capsid protein



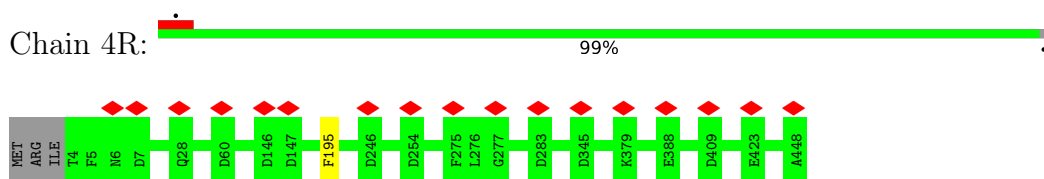
• Molecule 1: Major capsid protein



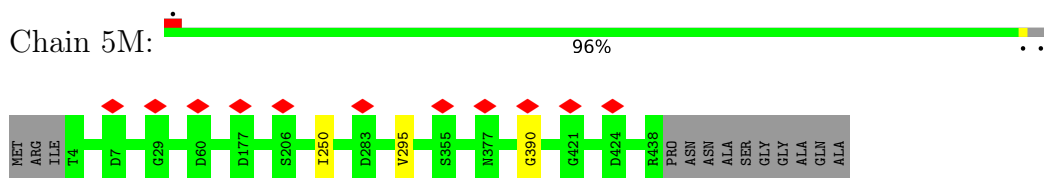
• Molecule 1: Major capsid protein



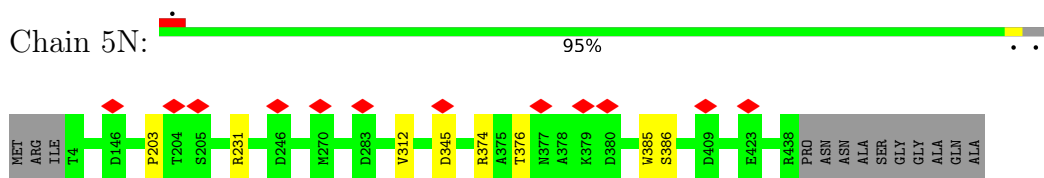
• Molecule 1: Major capsid protein



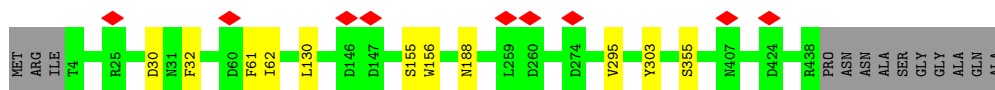
• Molecule 1: Major capsid protein



• Molecule 1: Major capsid protein



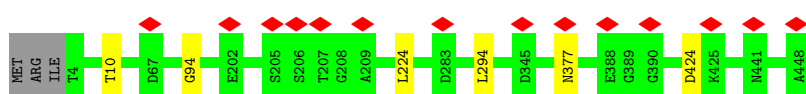
- Molecule 1: Major capsid protein



- Molecule 1: Major capsid protein



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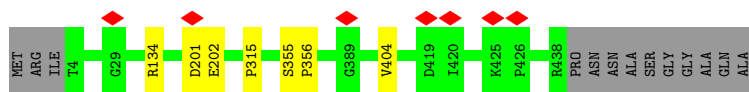


- Molecule 1: Major capsid protein

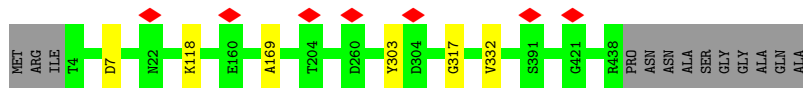


- Molecule 1: Major capsid protein

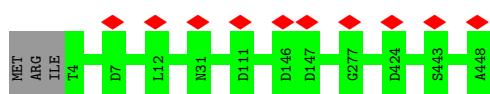




• Molecule 1: Major capsid protein



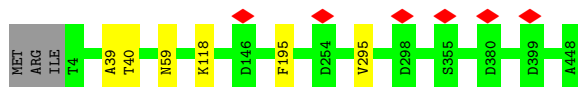
• Molecule 1: Major capsid protein



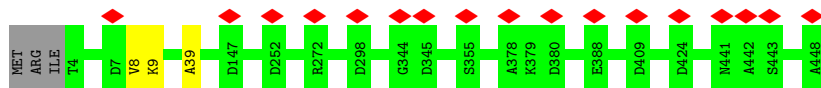
• Molecule 1: Major capsid protein



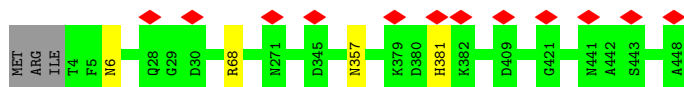
• Molecule 1: Major capsid protein



• Molecule 1: Major capsid protein

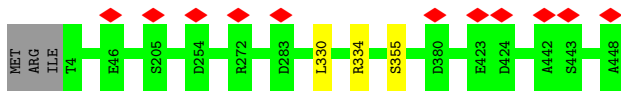


• Molecule 1: Major capsid protein



• Molecule 1: Major capsid protein

Chain 7N:  99%



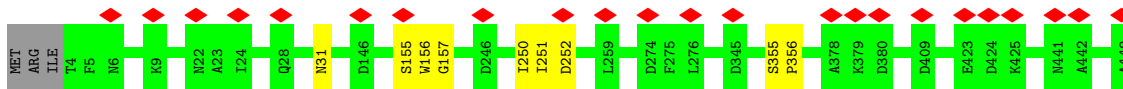
• Molecule 1: Major capsid protein

Chain 7O:  98%



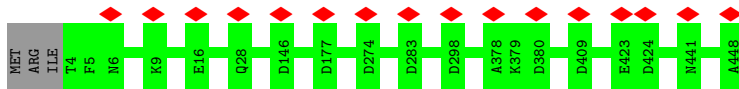
• Molecule 1: Major capsid protein

Chain 8M:  97%



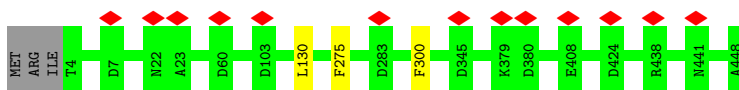
• Molecule 1: Major capsid protein

Chain 8N:  99%



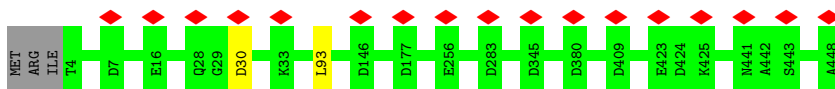
• Molecule 1: Major capsid protein

Chain 8O:  99%



• Molecule 1: Major capsid protein

Chain 8P:  99%

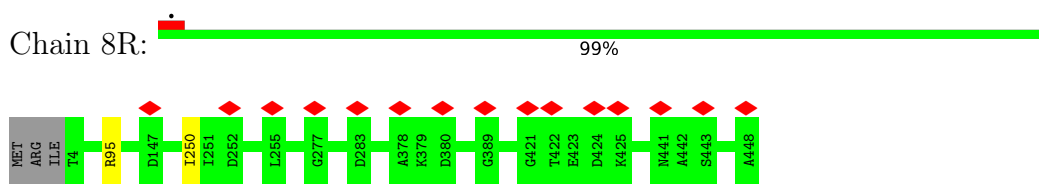


• Molecule 1: Major capsid protein

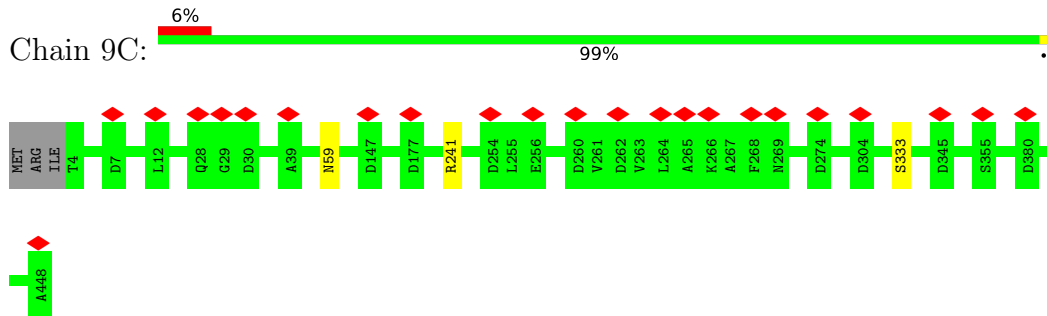
Chain 8Q:  98%



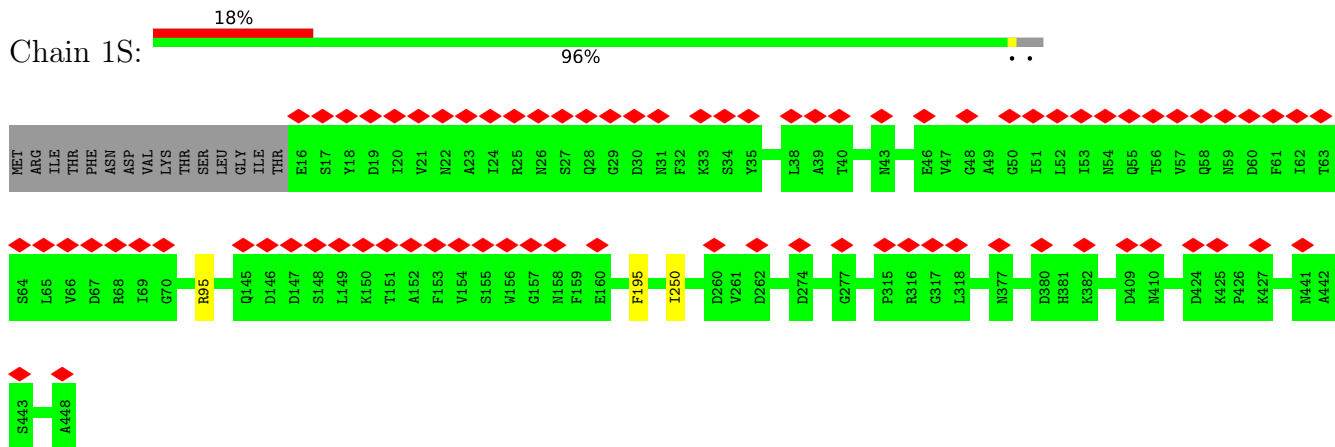
- Molecule 1: Major capsid protein



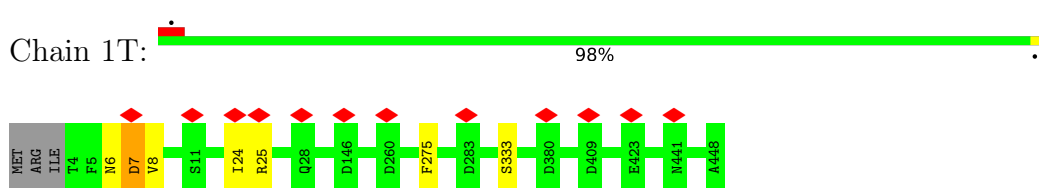
- Molecule 1: Major capsid protein



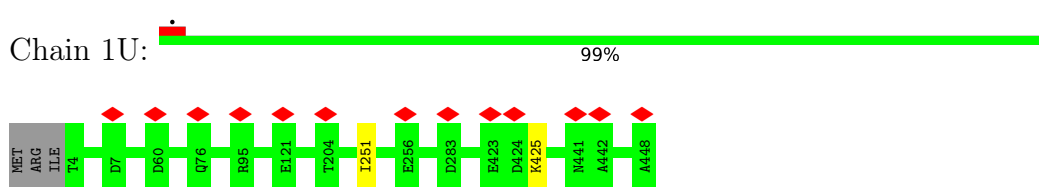
- Molecule 1: Major capsid protein



- Molecule 1: Major capsid protein

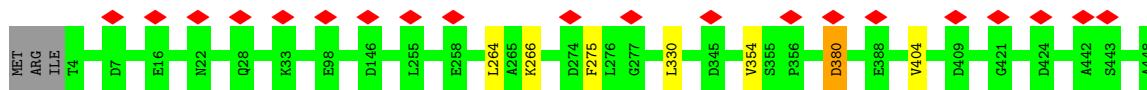


- Molecule 1: Major capsid protein



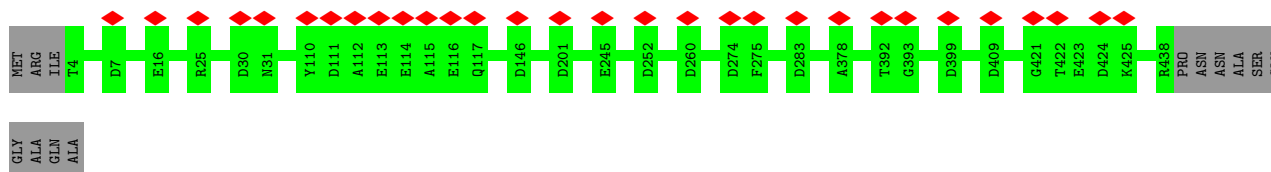
- Molecule 1: Major capsid protein

Chain 1V:  98%



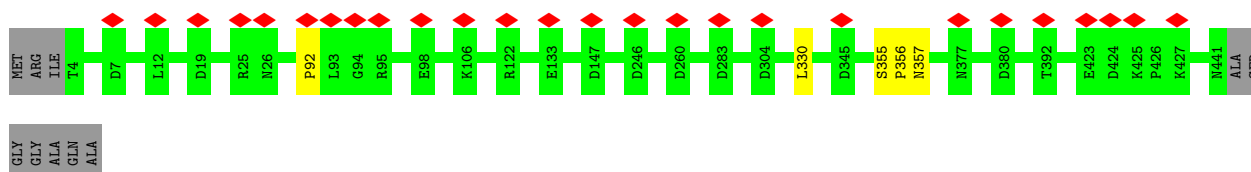
• Molecule 1: Major capsid protein

Chain 1W:  97%



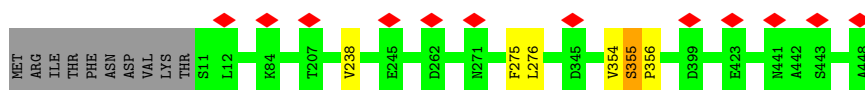
• Molecule 1: Major capsid protein

Chain 1X:  97%



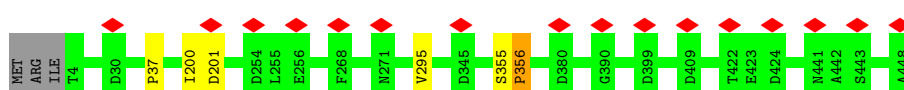
• Molecule 1: Major capsid protein

Chain 2P:  96%



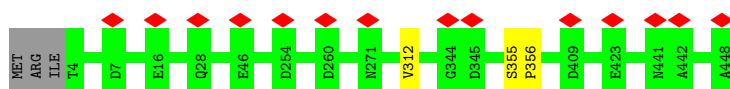
• Molecule 1: Major capsid protein

Chain 2Q:  98%



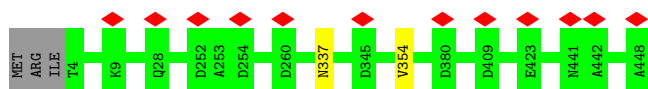
• Molecule 1: Major capsid protein

Chain 2R:  99%



• Molecule 1: Major capsid protein

Chain 2S:  99%



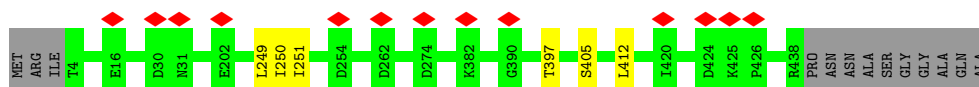
• Molecule 1: Major capsid protein

Chain 2T:  98%



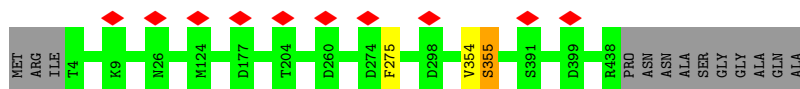
• Molecule 1: Major capsid protein

Chain 3S:  96%



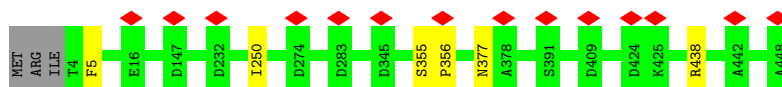
• Molecule 1: Major capsid protein

Chain 3T:  96%



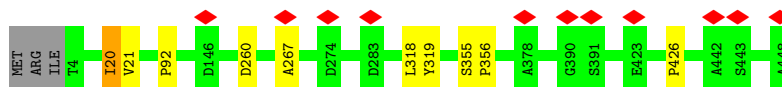
• Molecule 1: Major capsid protein

Chain 3U:  98%



• Molecule 1: Major capsid protein

Chain 3V:  97%

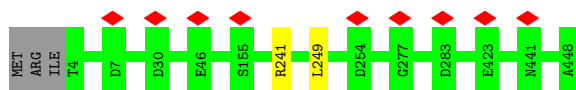


• Molecule 1: Major capsid protein

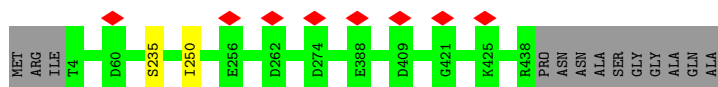
Chain 3W:  99%



- Molecule 1: Major capsid protein



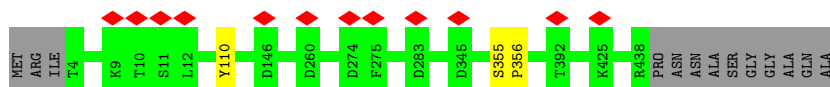
- Molecule 1: Major capsid protein



- Molecule 1: Major capsid protein



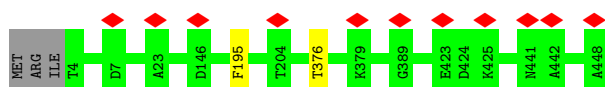
- Molecule 1: Major capsid protein



- Molecule 1: Major capsid protein

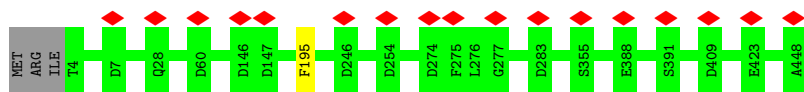


- Molecule 1: Major capsid protein

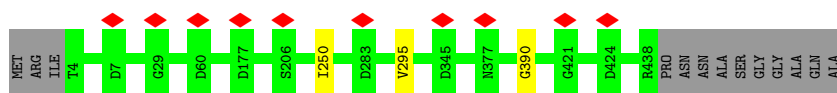


- Molecule 1: Major capsid protein

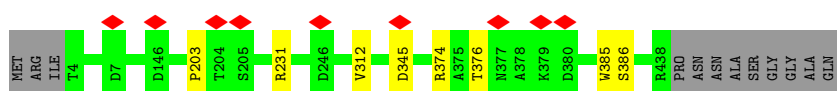




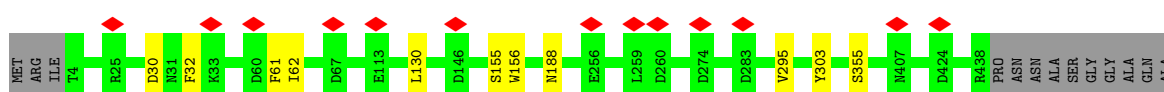
• Molecule 1: Major capsid protein



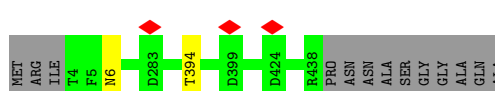
• Molecule 1: Major capsid protein



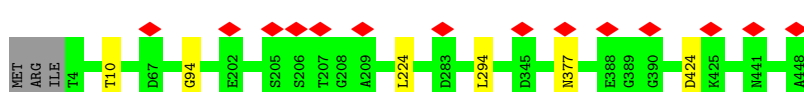
• Molecule 1: Major capsid protein



• Molecule 1: Major capsid protein



• Molecule 1: Major capsid protein



• Molecule 1: Major capsid protein



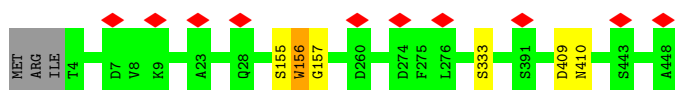
• Molecule 1: Major capsid protein

Chain 6S:  97%



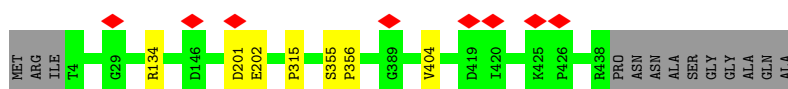
- Molecule 1: Major capsid protein

Chain 6T:  98%



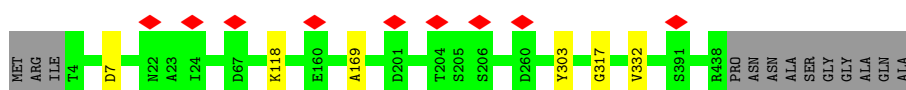
- Molecule 1: Major capsid protein

Chain 6U:  96%



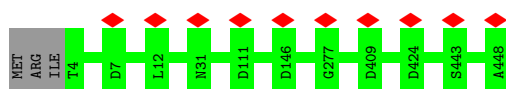
- Molecule 1: Major capsid protein

Chain 6V:  96%



- Molecule 1: Major capsid protein

Chain 6W:  99%



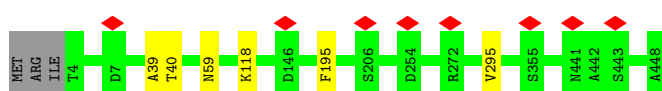
- Molecule 1: Major capsid protein

Chain 6X:  98%

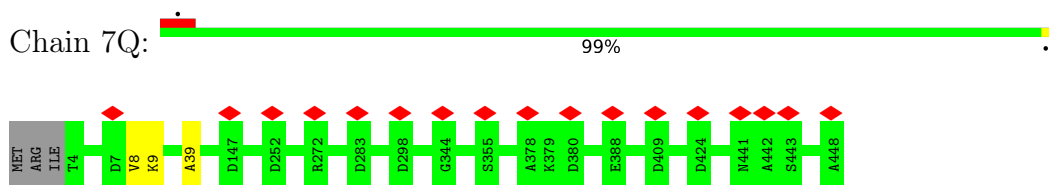


- Molecule 1: Major capsid protein

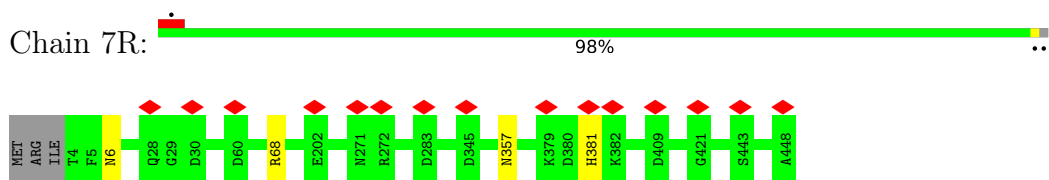
Chain 7P:  98%



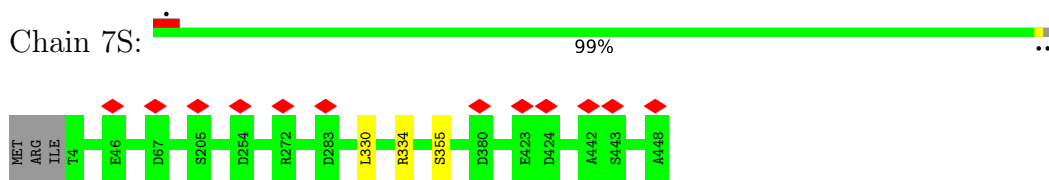
- Molecule 1: Major capsid protein



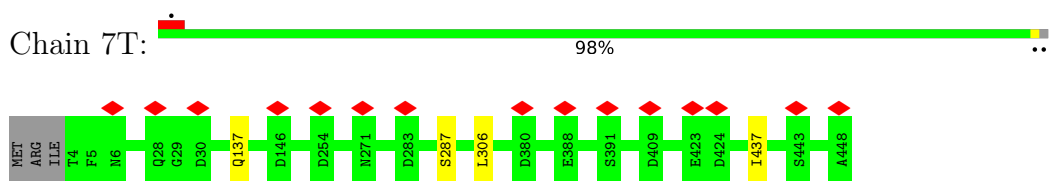
- Molecule 1: Major capsid protein



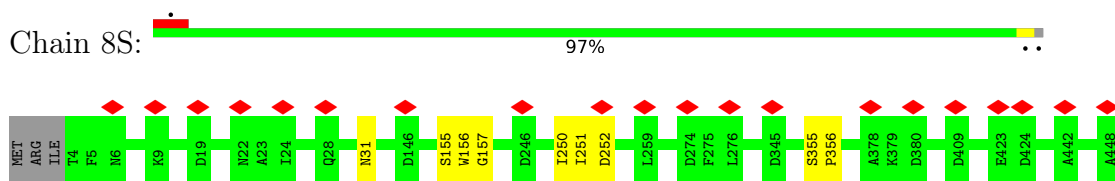
- Molecule 1: Major capsid protein



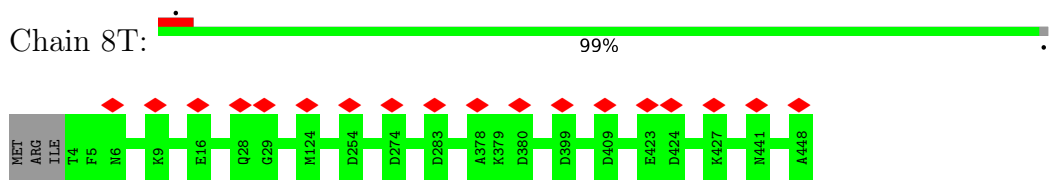
- Molecule 1: Major capsid protein



- Molecule 1: Major capsid protein



- Molecule 1: Major capsid protein

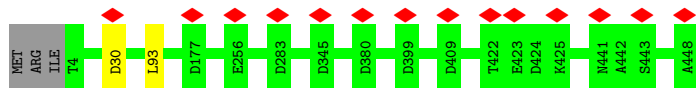


- Molecule 1: Major capsid protein

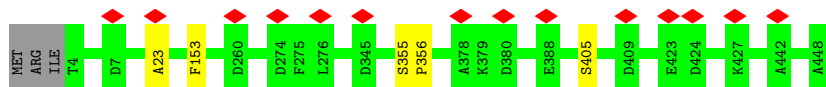




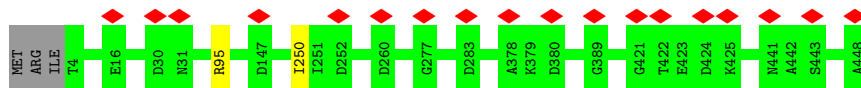
• Molecule 1: Major capsid protein



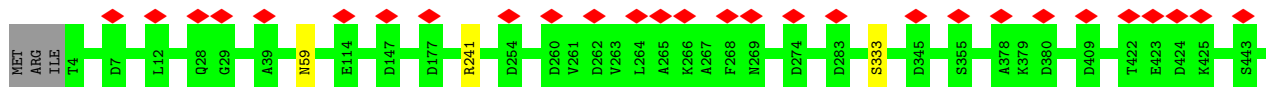
• Molecule 1: Major capsid protein



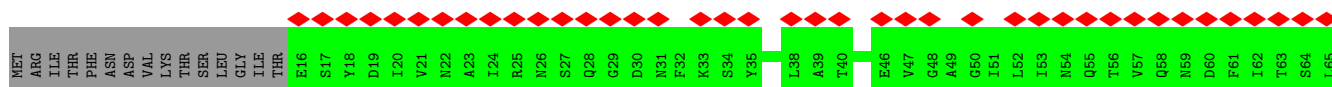
• Molecule 1: Major capsid protein



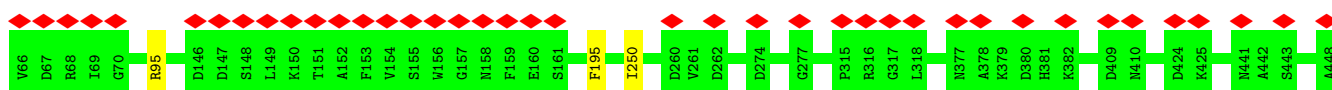
• Molecule 1: Major capsid protein



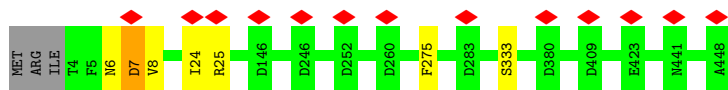
• Molecule 1: Major capsid protein



• Molecule 1: Major capsid protein

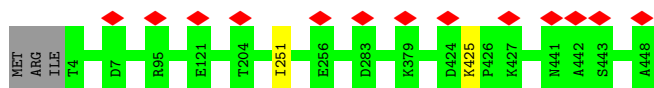


Chain 1Z:  98%



• Molecule 1: Major capsid protein

Chain 1a:  99%



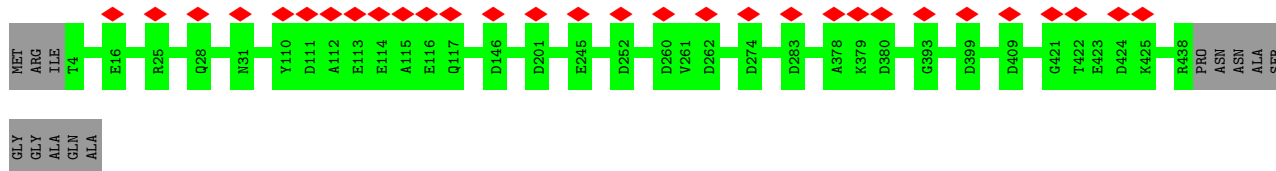
• Molecule 1: Major capsid protein

Chain 1b:  98%



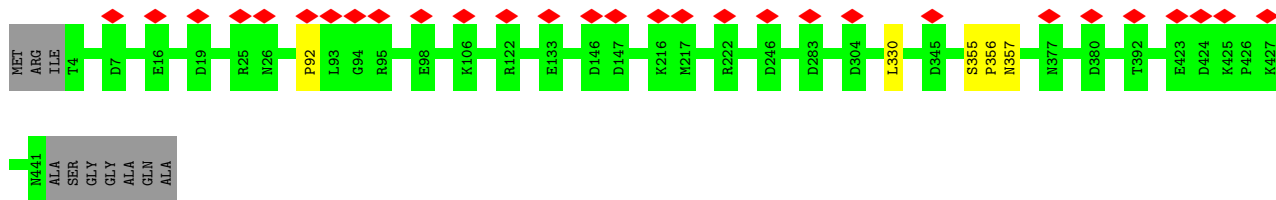
• Molecule 1: Major capsid protein

Chain 1c:  97%



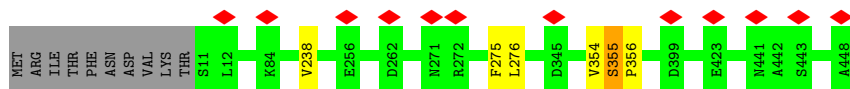
• Molecule 1: Major capsid protein

Chain 1d:  97%



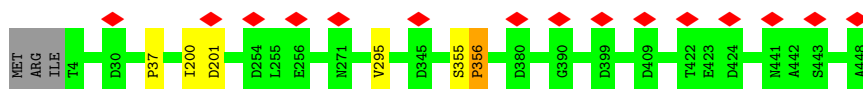
• Molecule 1: Major capsid protein

Chain 2U:  96%



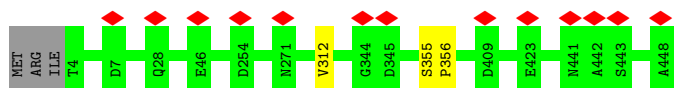
• Molecule 1: Major capsid protein

Chain 2V:  98%



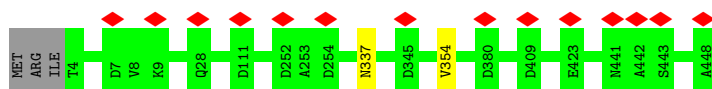
• Molecule 1: Major capsid protein

Chain 2W:  99%



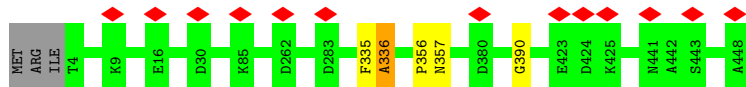
• Molecule 1: Major capsid protein

Chain 2X:  99%



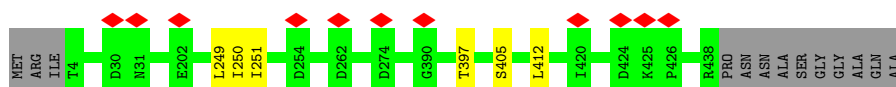
• Molecule 1: Major capsid protein

Chain 2Y:  98%



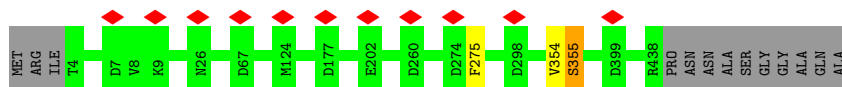
• Molecule 1: Major capsid protein

Chain 3Y:  96%



• Molecule 1: Major capsid protein

Chain 3Z:  96%

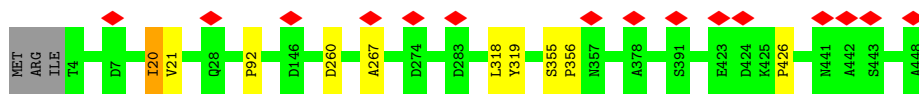


• Molecule 1: Major capsid protein

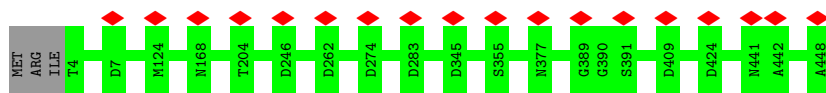
Chain 3a:  98%



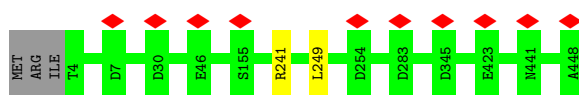
- Molecule 1: Major capsid protein



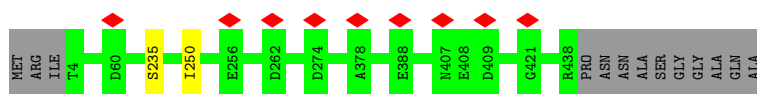
- Molecule 1: Major capsid protein



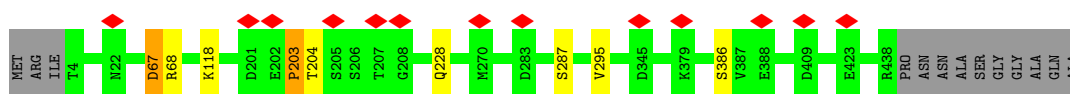
- Molecule 1: Major capsid protein



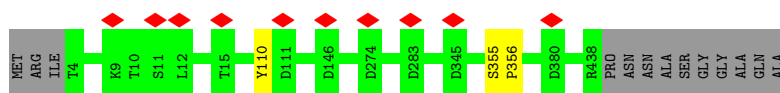
- Molecule 1: Major capsid protein



- Molecule 1: Major capsid protein

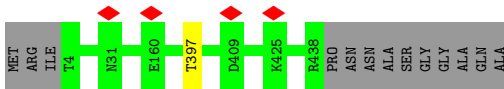


- Molecule 1: Major capsid protein



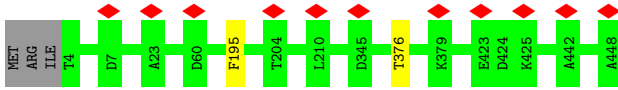
- Molecule 1: Major capsid protein





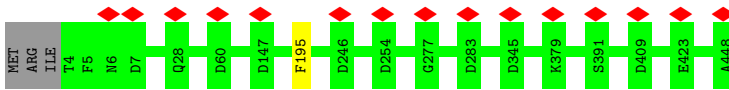
- Molecule 1: Major capsid protein

Chain 4c: 99%



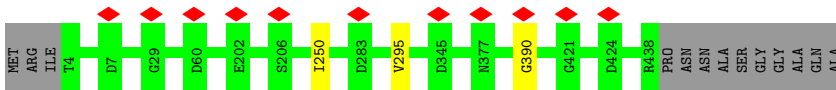
- Molecule 1: Major capsid protein

Chain 4d: 99%



- Molecule 1: Major capsid protein

Chain 5Y: 96%



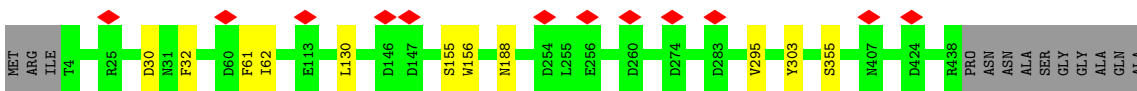
- Molecule 1: Major capsid protein

Chain 5Z: 95%



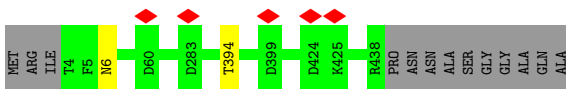
- Molecule 1: Major capsid protein

Chain 5a: 95%



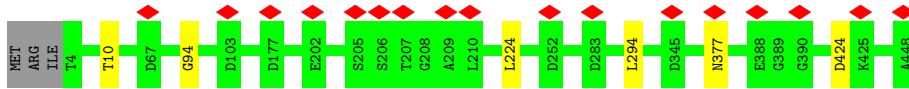
- Molecule 1: Major capsid protein

Chain 5b: 97%



- Molecule 1: Major capsid protein

Chain 5c:  98%



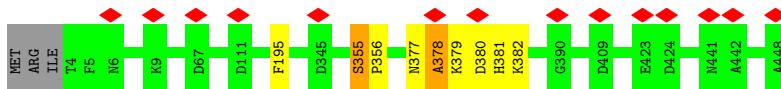
• Molecule 1: Major capsid protein

Chain 5d:  97%



• Molecule 1: Major capsid protein

Chain 6Y:  97%



• Molecule 1: Major capsid protein

Chain 6Z:  98%



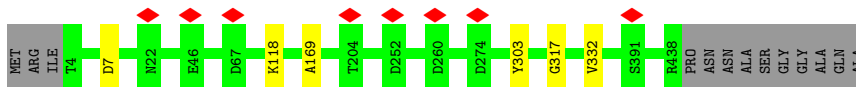
• Molecule 1: Major capsid protein

Chain 6a:  96%



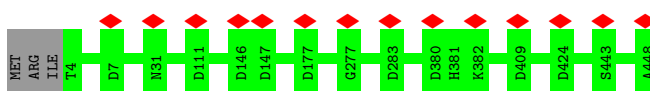
• Molecule 1: Major capsid protein

Chain 6b:  96%

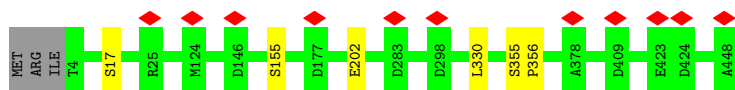


• Molecule 1: Major capsid protein

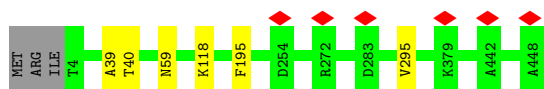
Chain 6c:  99%



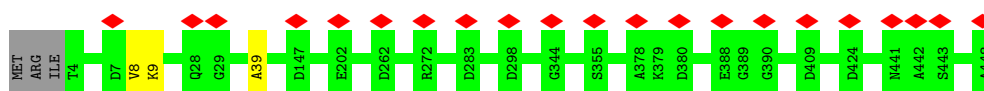
- Molecule 1: Major capsid protein



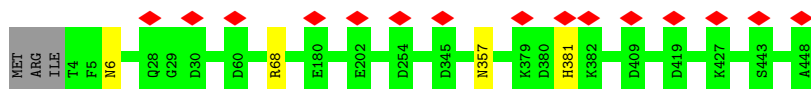
- Molecule 1: Major capsid protein



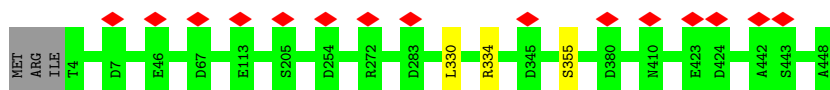
- Molecule 1: Major capsid protein



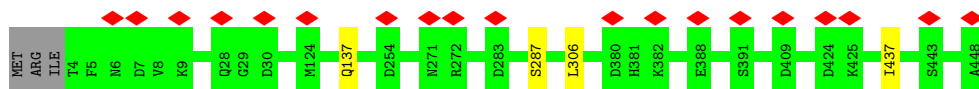
- Molecule 1: Major capsid protein



- Molecule 1: Major capsid protein

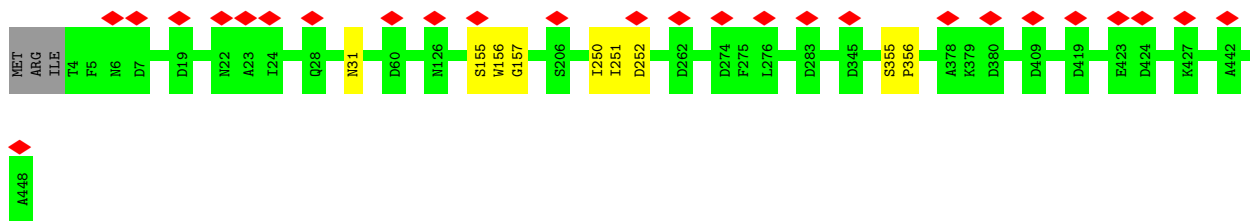


- Molecule 1: Major capsid protein

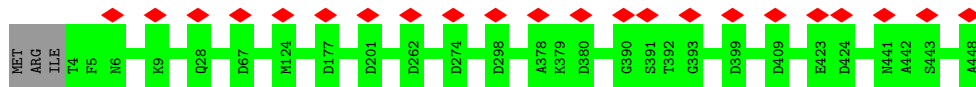


- Molecule 1: Major capsid protein





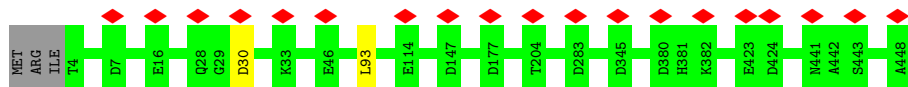
• Molecule 1: Major capsid protein



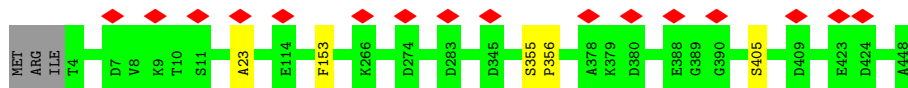
• Molecule 1: Major capsid protein



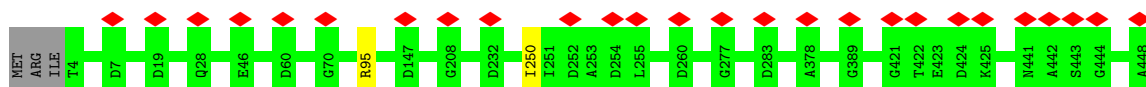
• Molecule 1: Major capsid protein



• Molecule 1: Major capsid protein

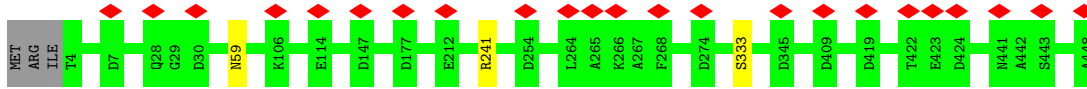


• Molecule 1: Major capsid protein



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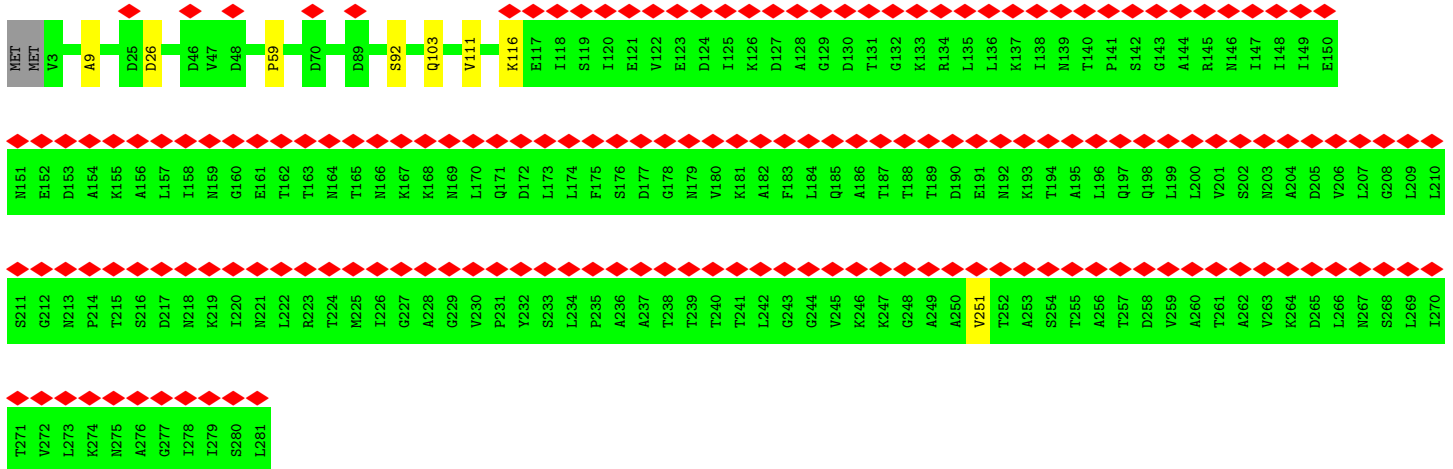




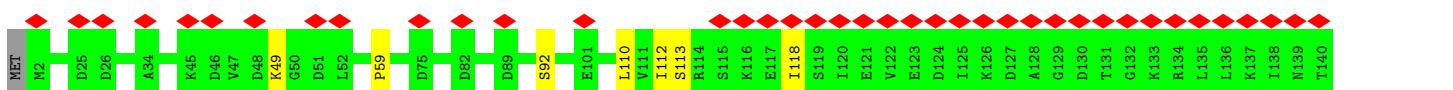
• Molecule 2: Capsid fiber protein



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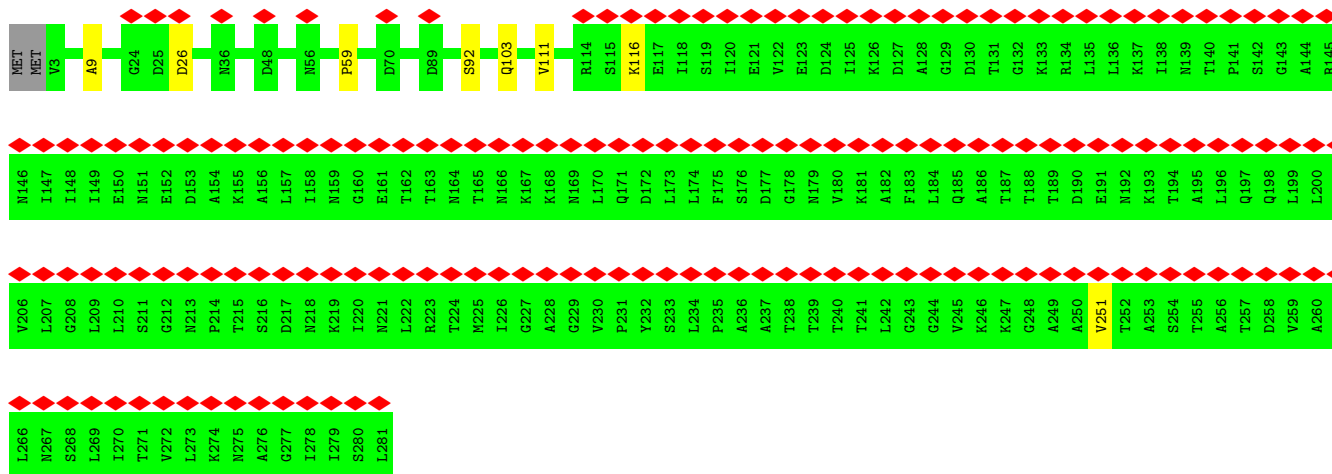


• Molecule 2: Capsid fiber protein

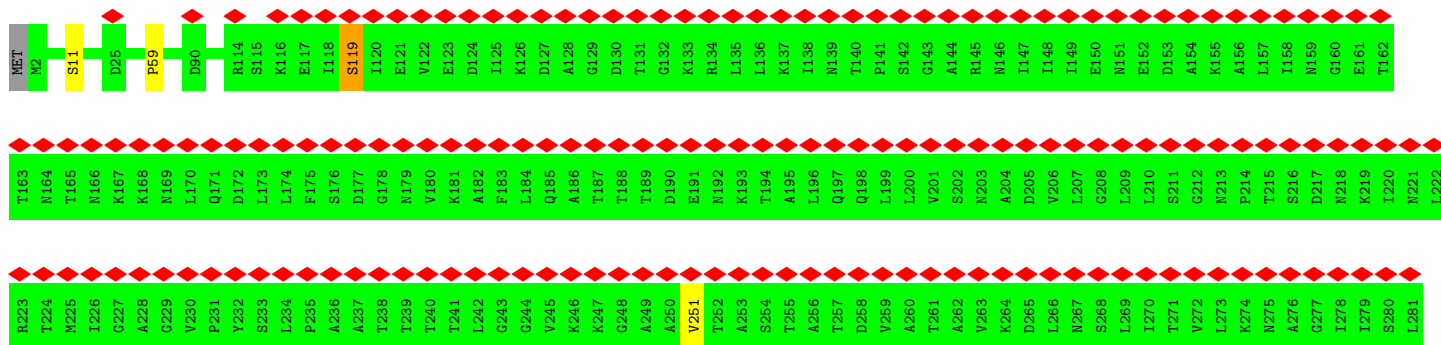




• Molecule 2: Capsid fiber protein

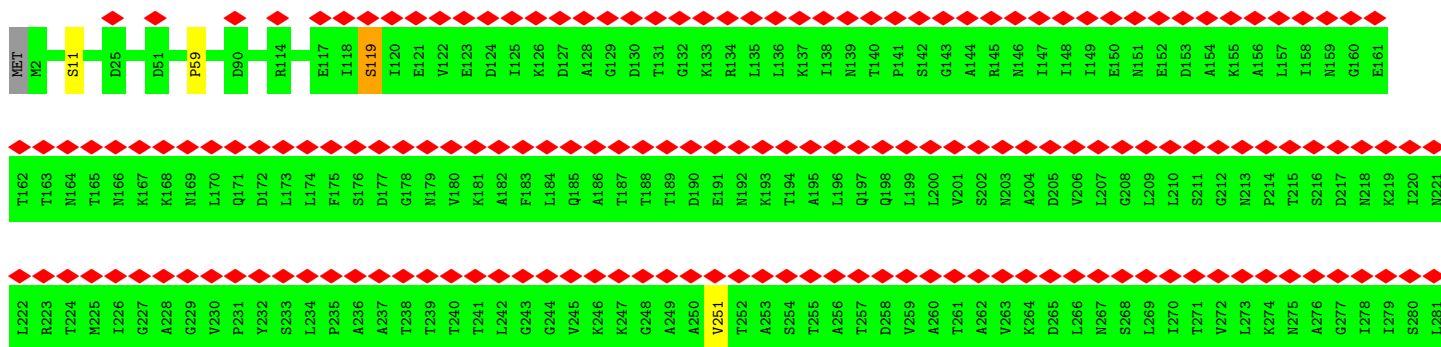


• Molecule 2: Capsid fiber protein

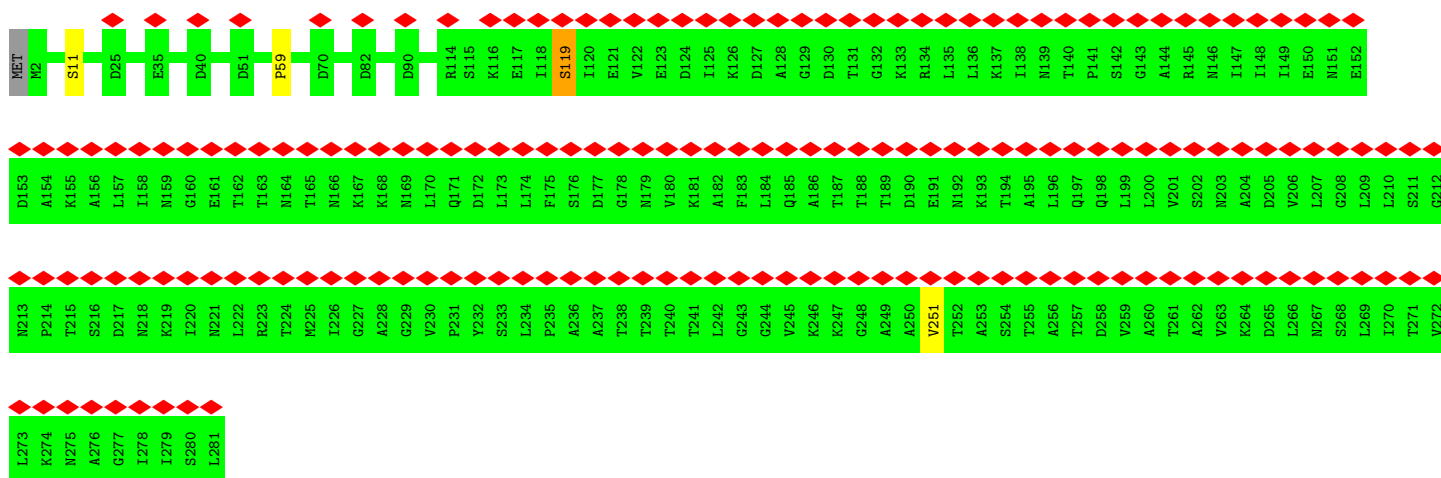


• Molecule 2: Capsid fiber protein

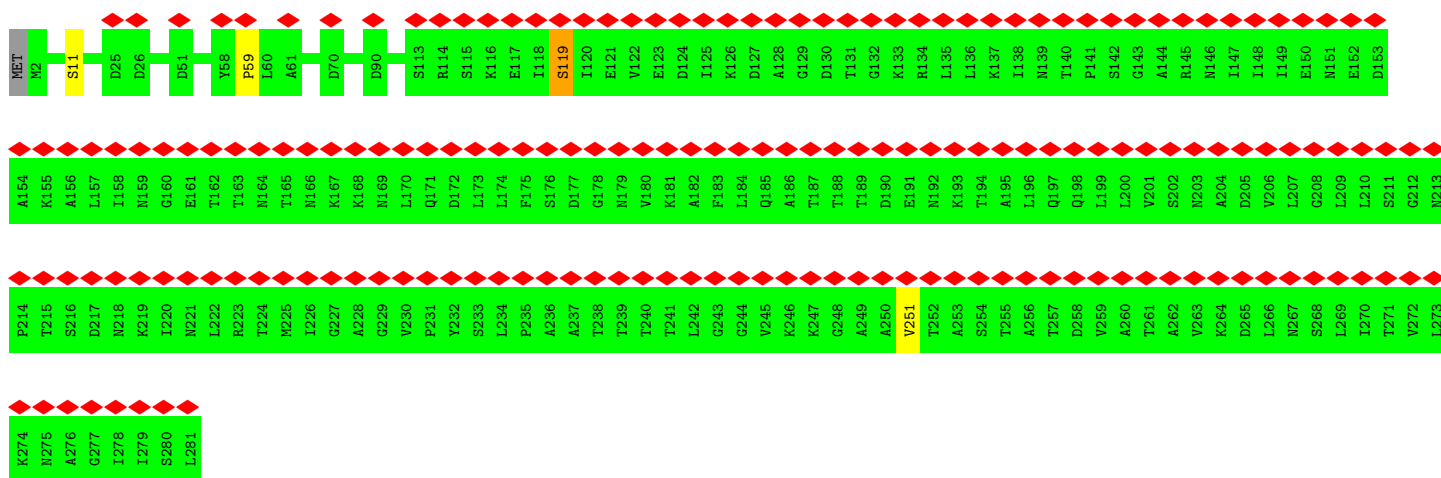




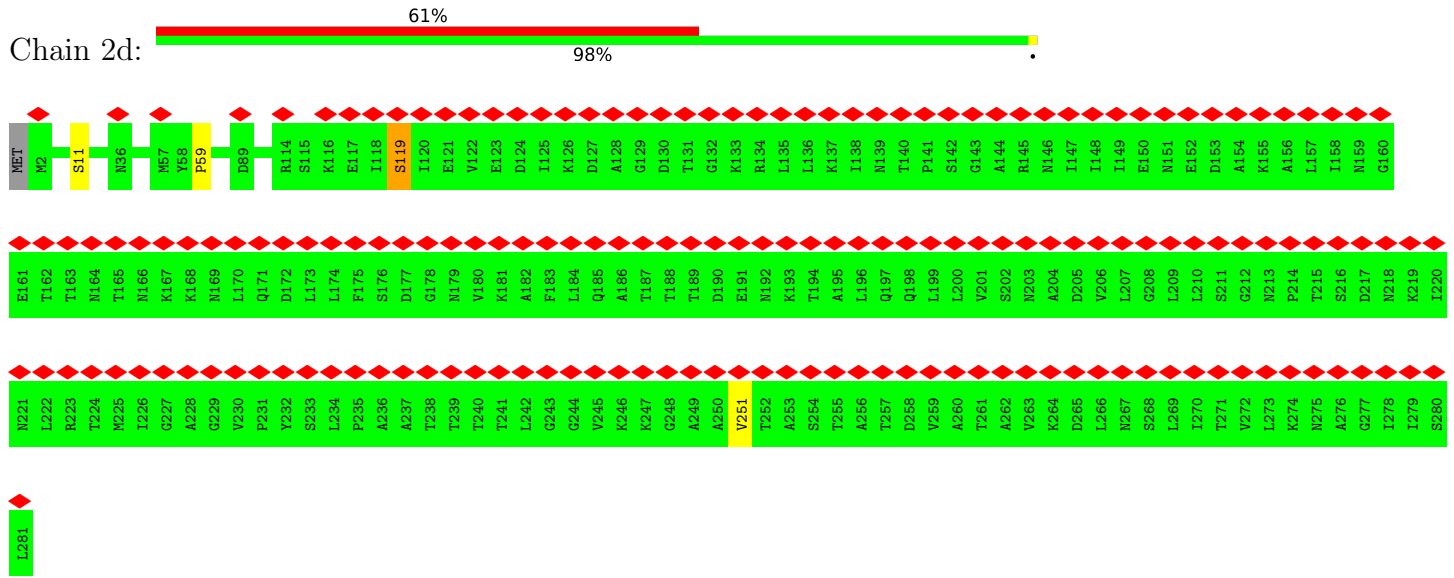
• Molecule 2: Capsid fiber protein



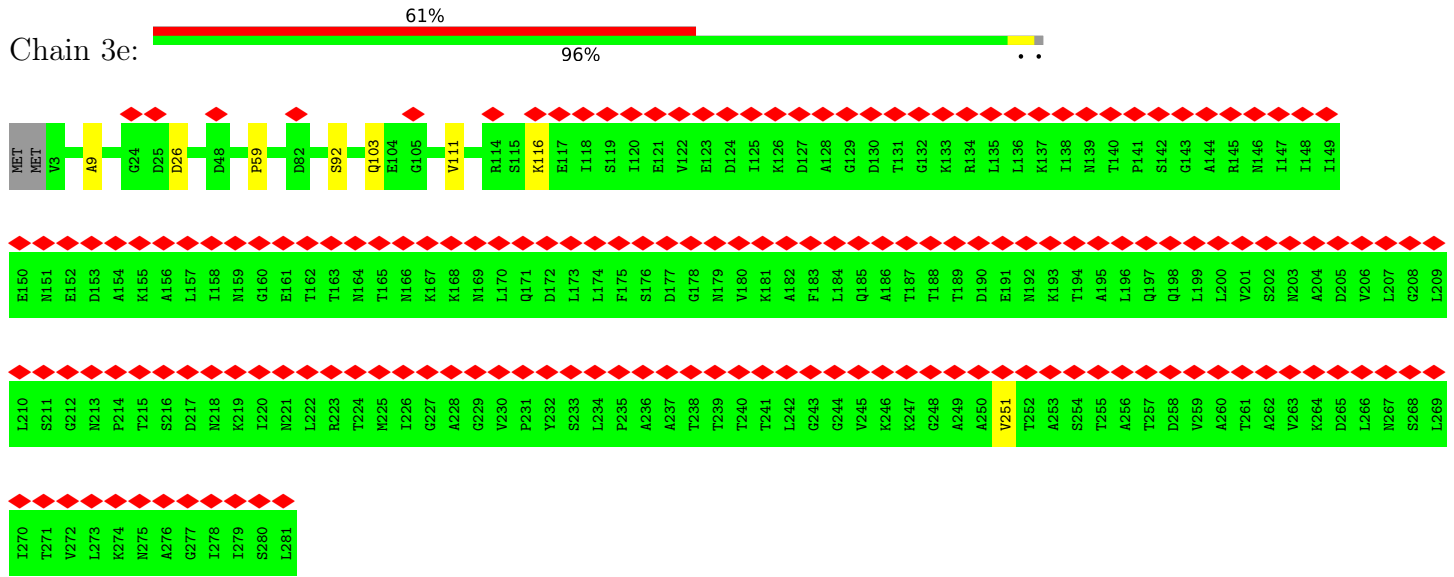
• Molecule 2: Capsid fiber protein



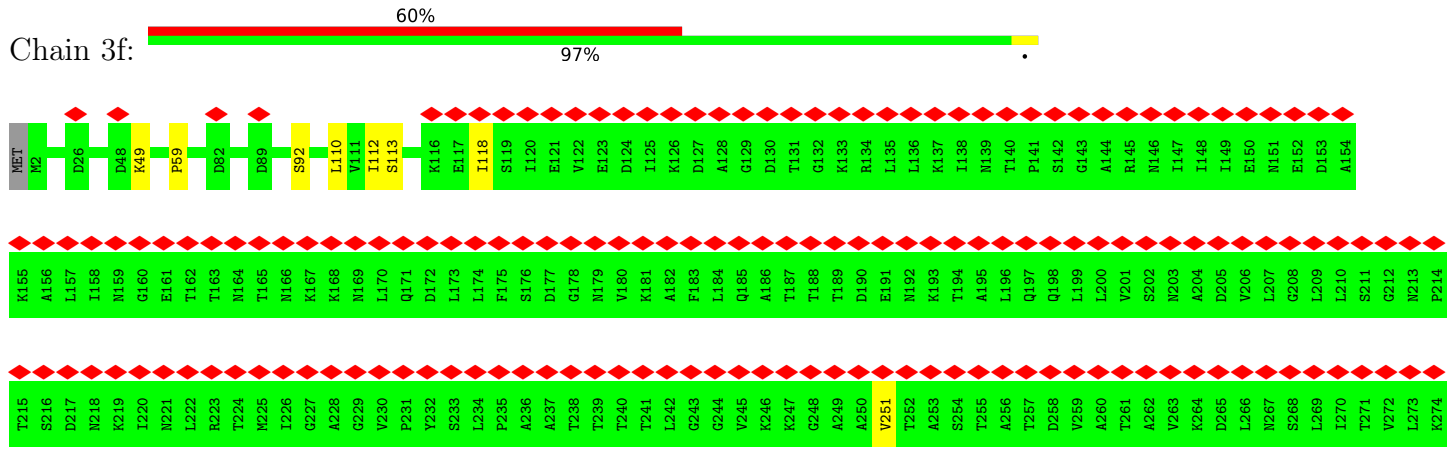
• Molecule 2: Capsid fiber protein

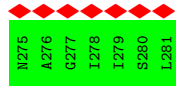


• Molecule 2: Capsid fiber protein

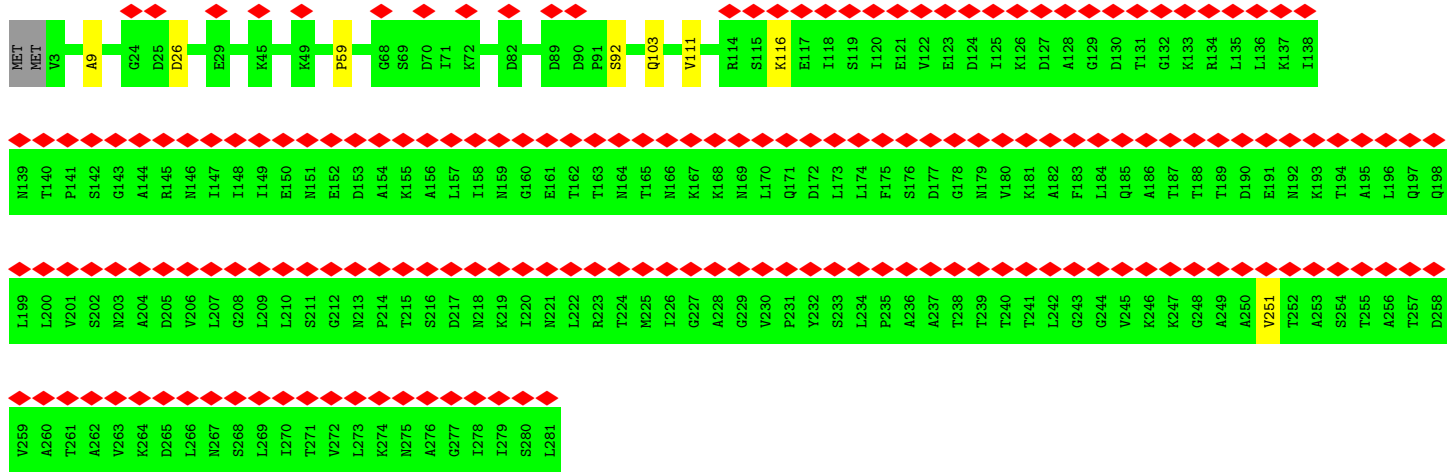


• Molecule 2: Capsid fiber protein

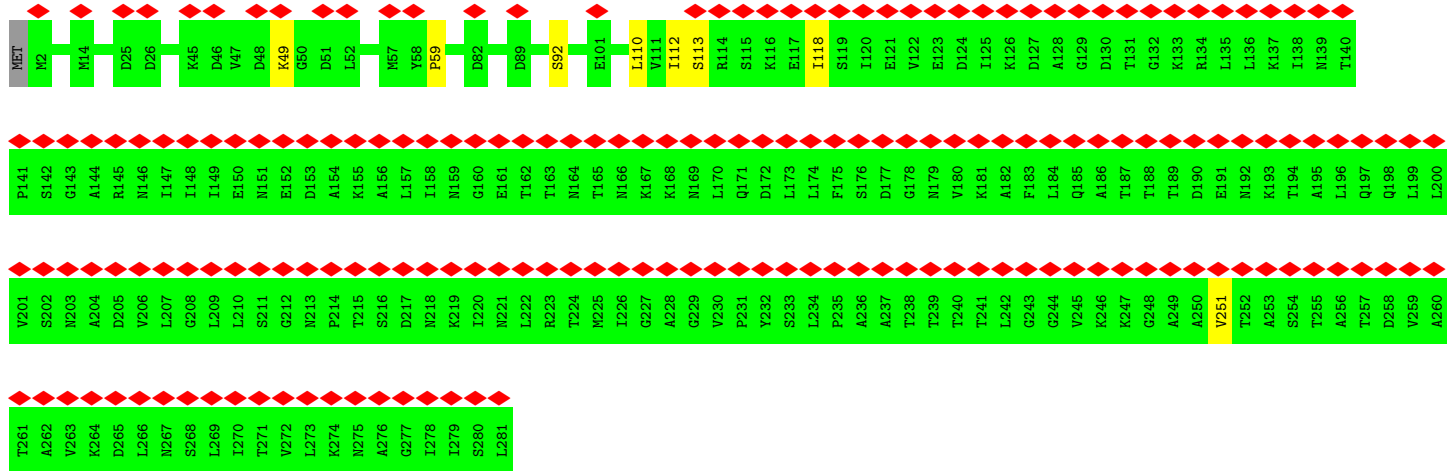




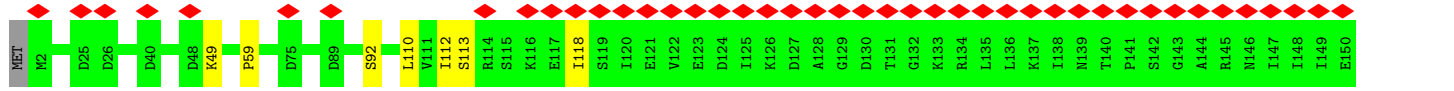
• Molecule 2: Capsid fiber protein

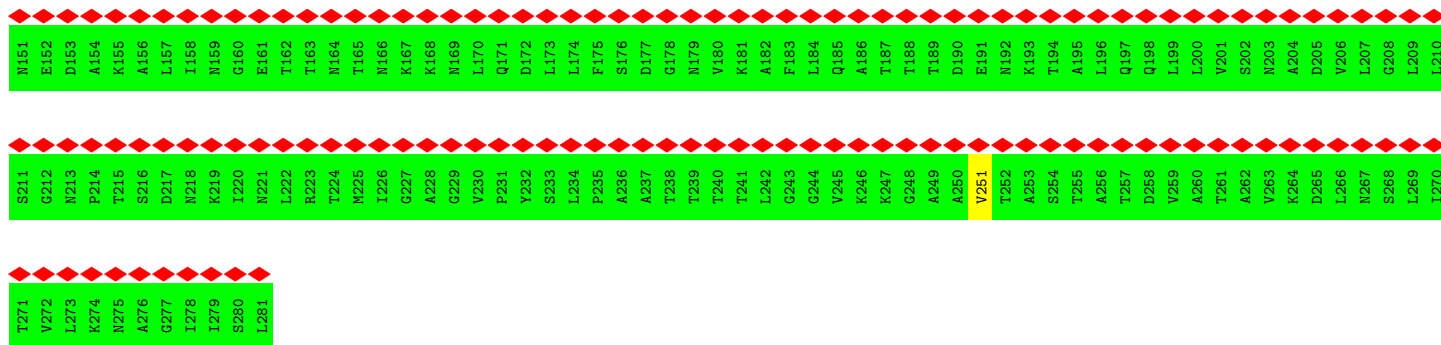


• Molecule 2: Capsid fiber protein

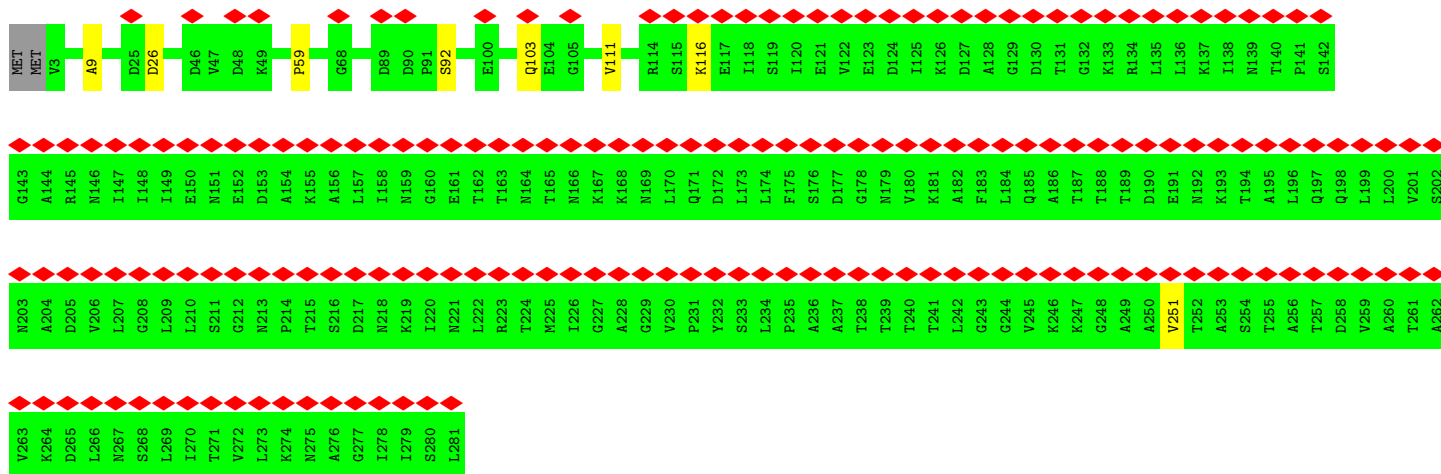


• Molecule 2: Capsid fiber protein





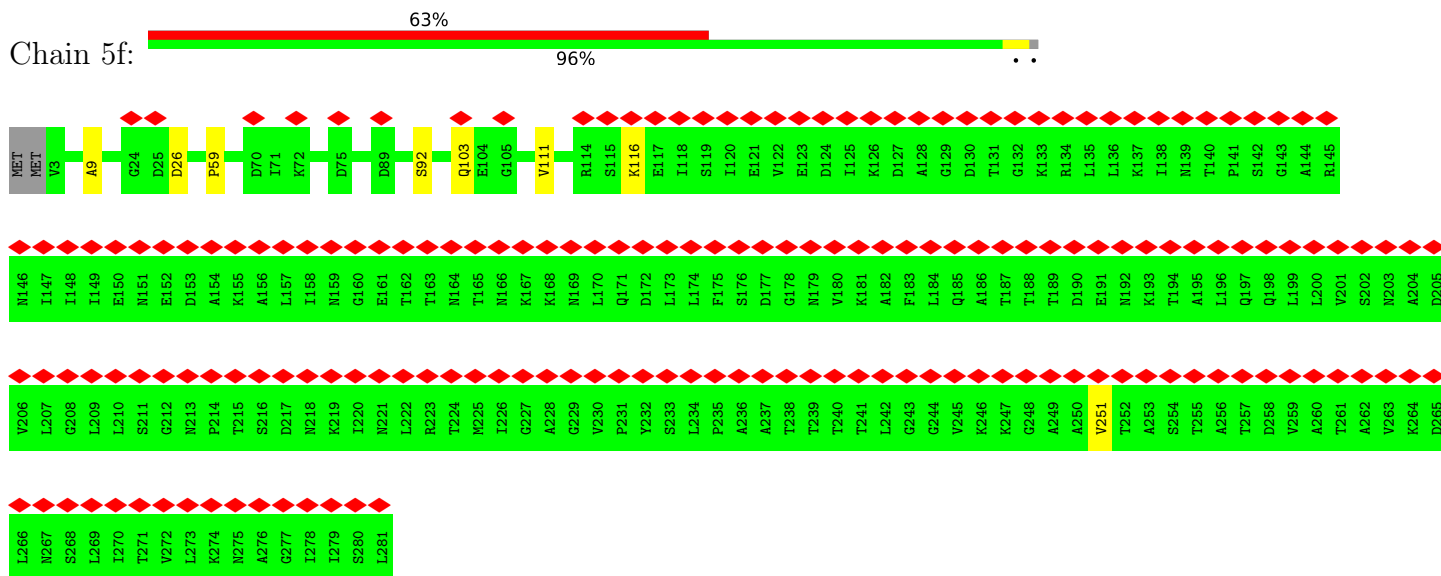
• Molecule 2: Capsid fiber protein



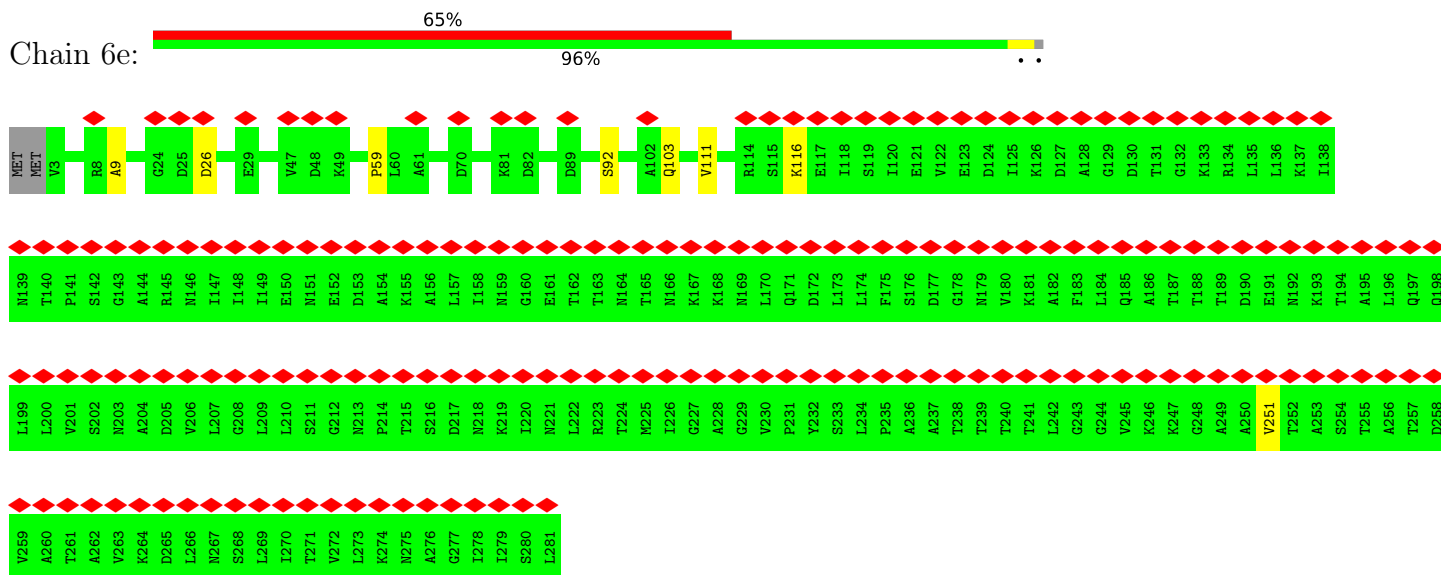
• Molecule 2: Capsid fiber protein



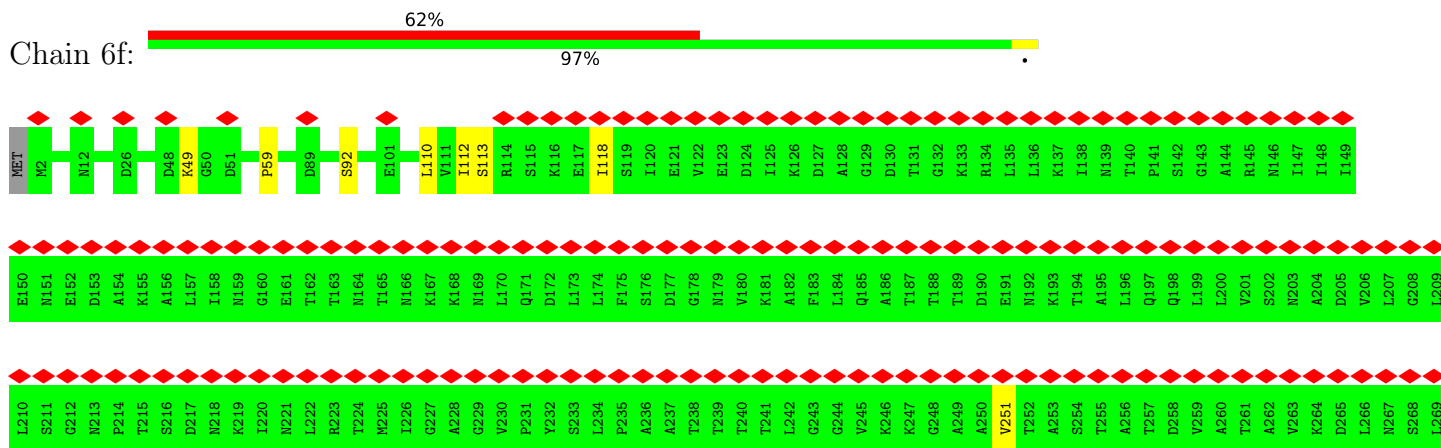
• Molecule 2: Capsid fiber protein

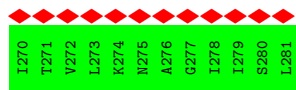


● Molecule 2: Capsid fiber protein

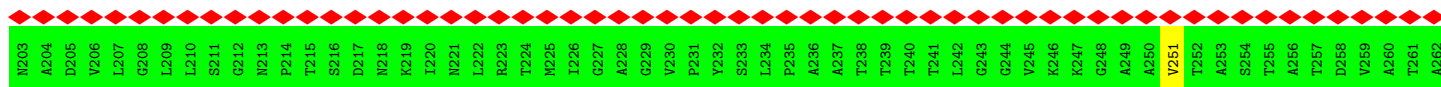
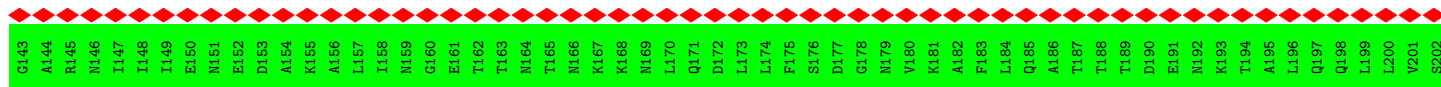
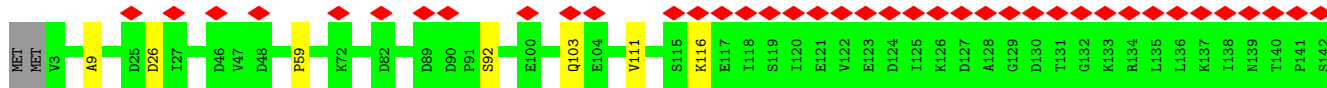


● Molecule 2: Capsid fiber protein

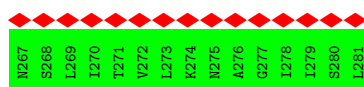
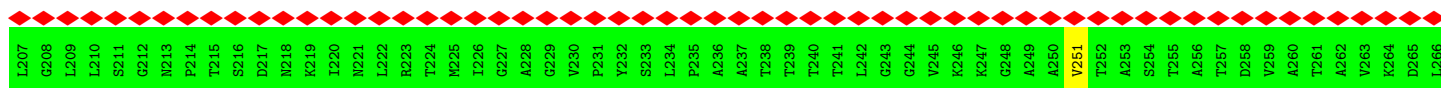
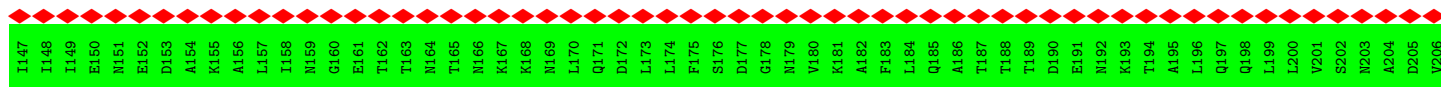




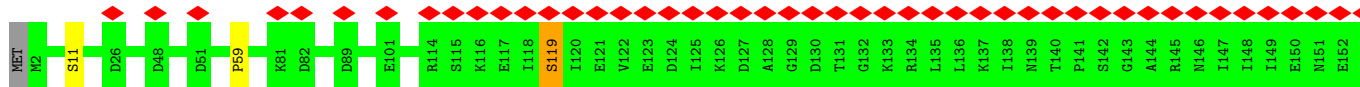
• Molecule 2: Capsid fiber protein

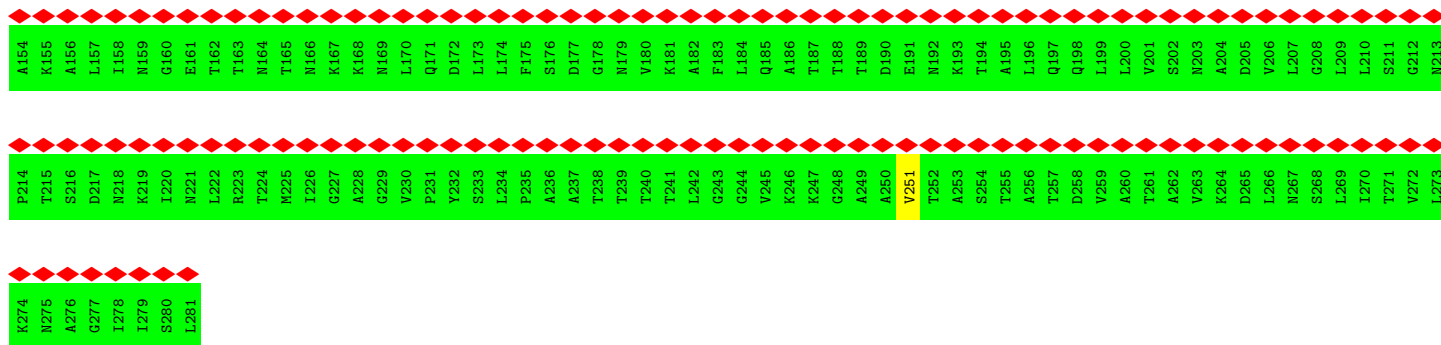


• Molecule 2: Capsid fiber protein



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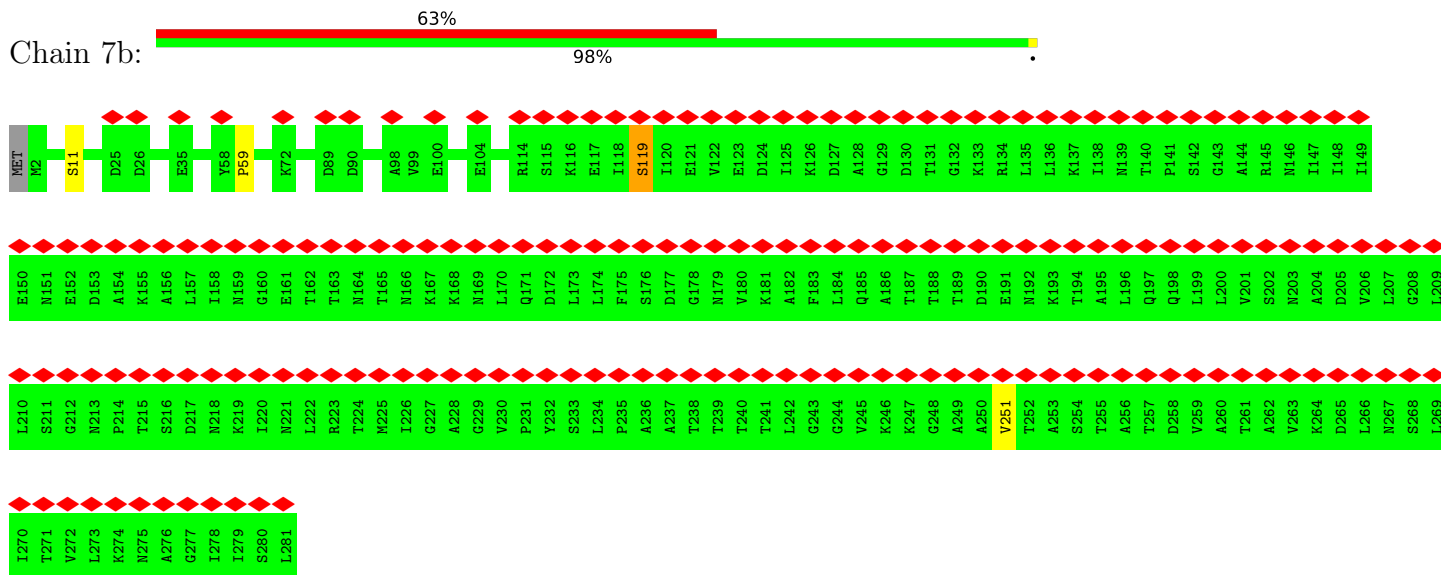




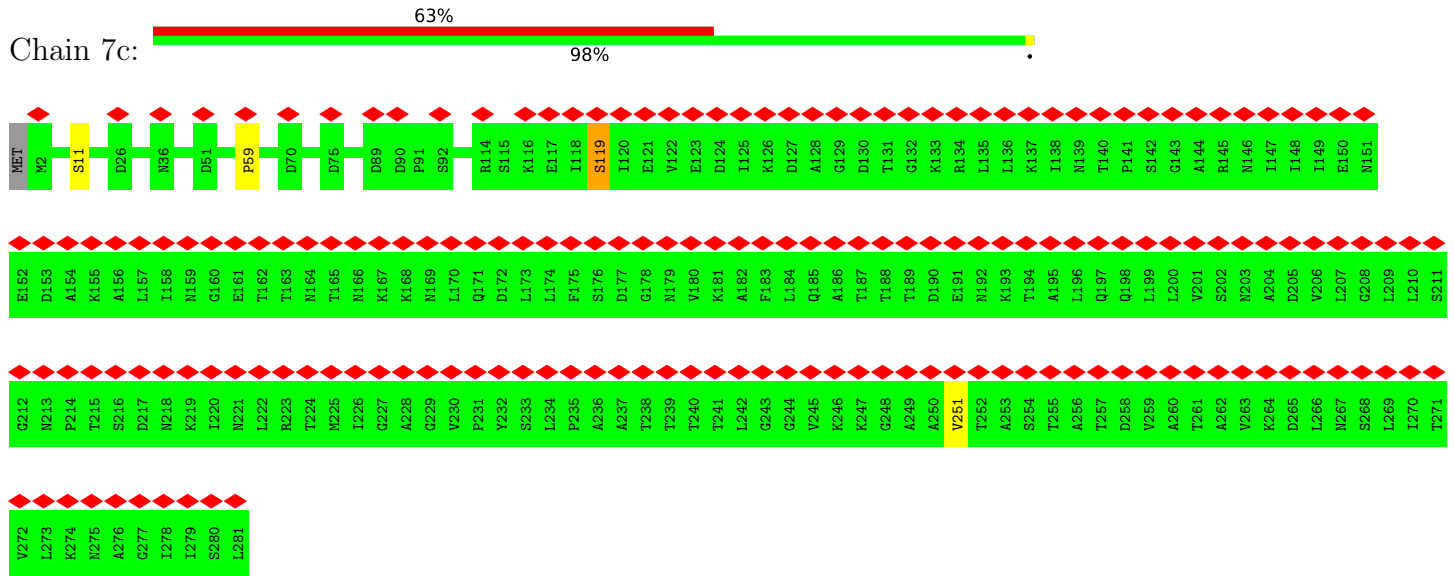
• Molecule 2: Capsid fiber protein



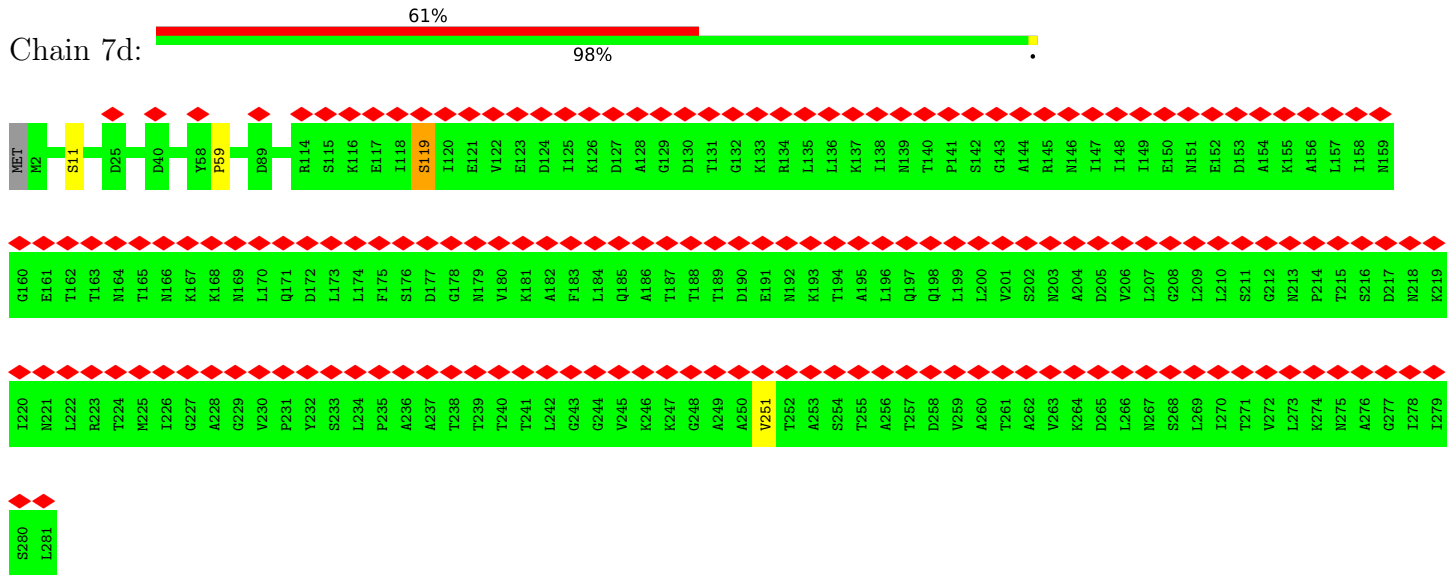
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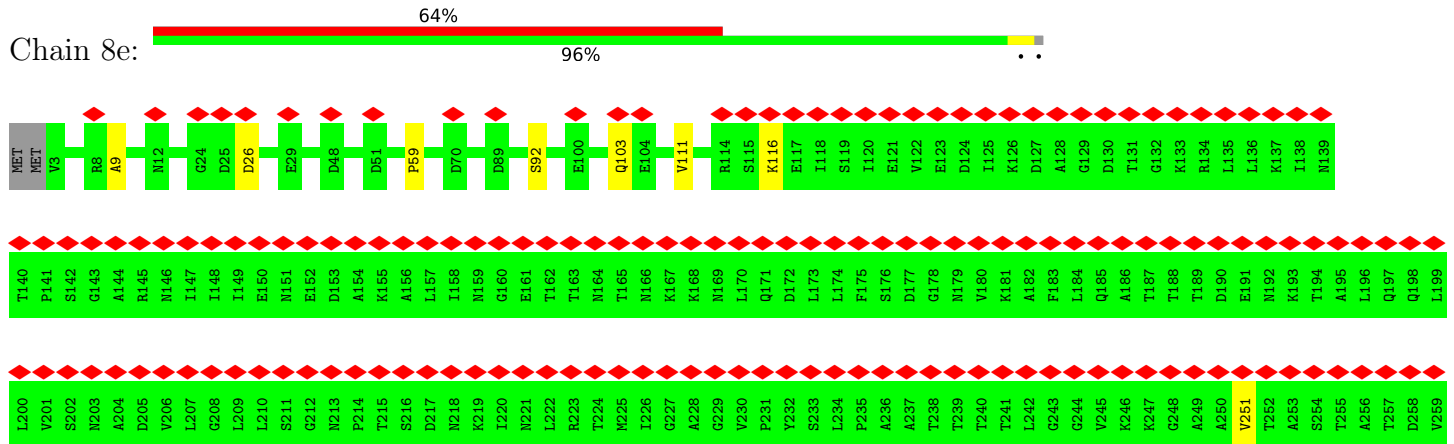
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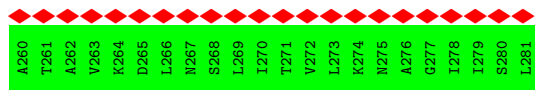


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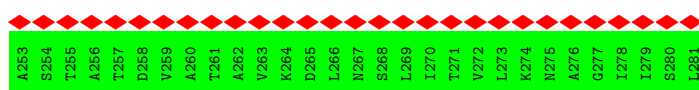
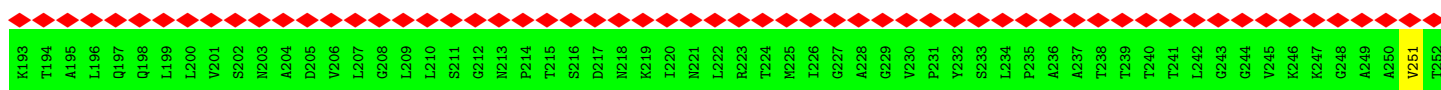
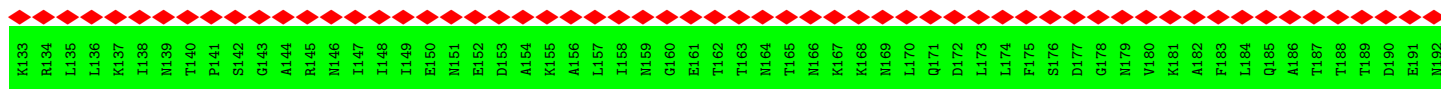
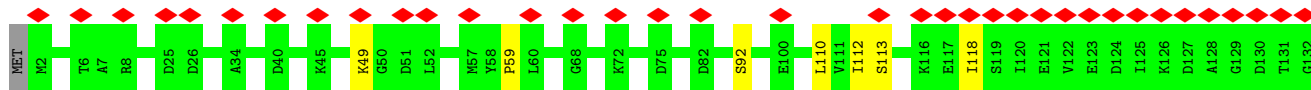


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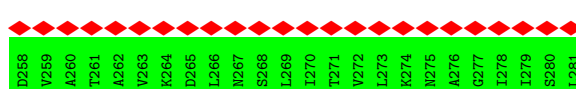
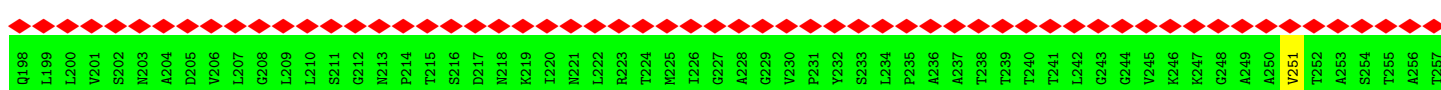
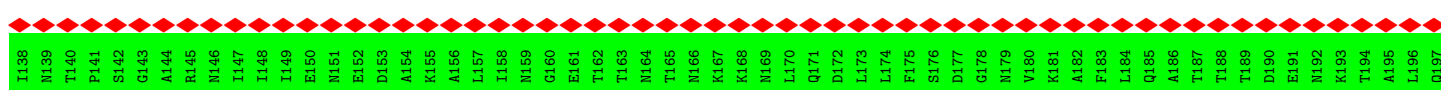
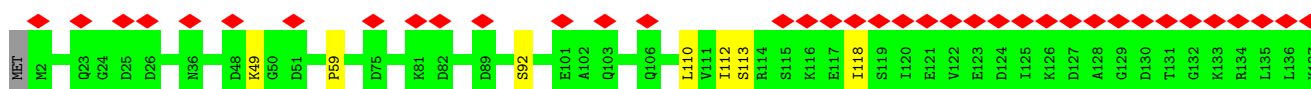




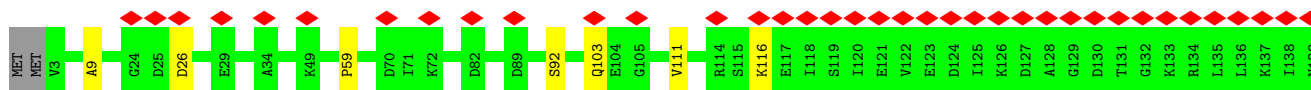
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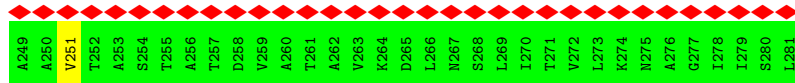
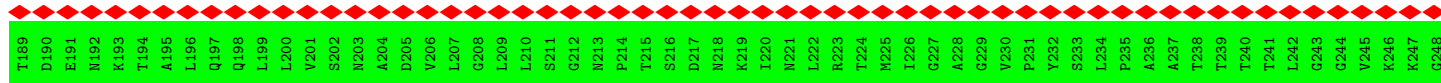
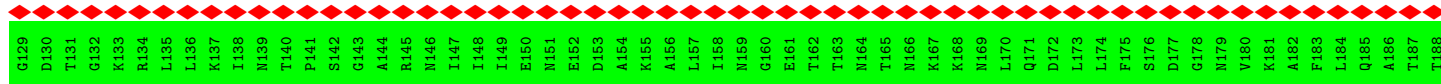
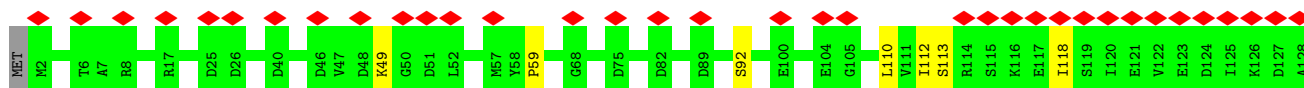


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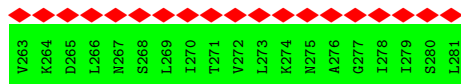
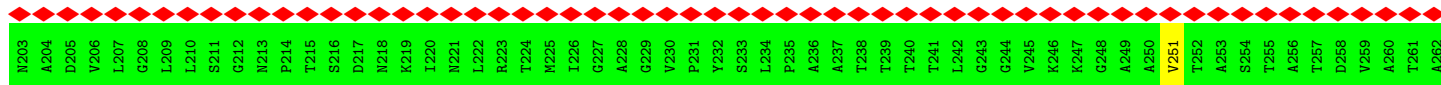
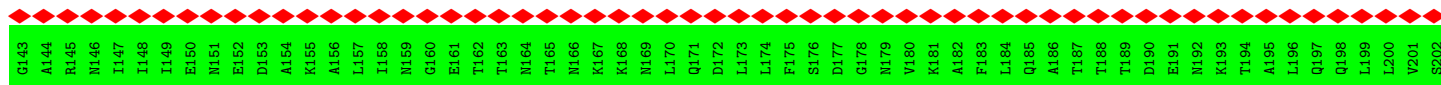
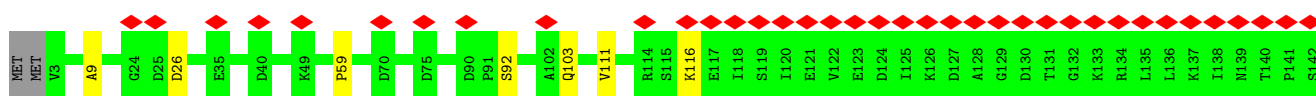




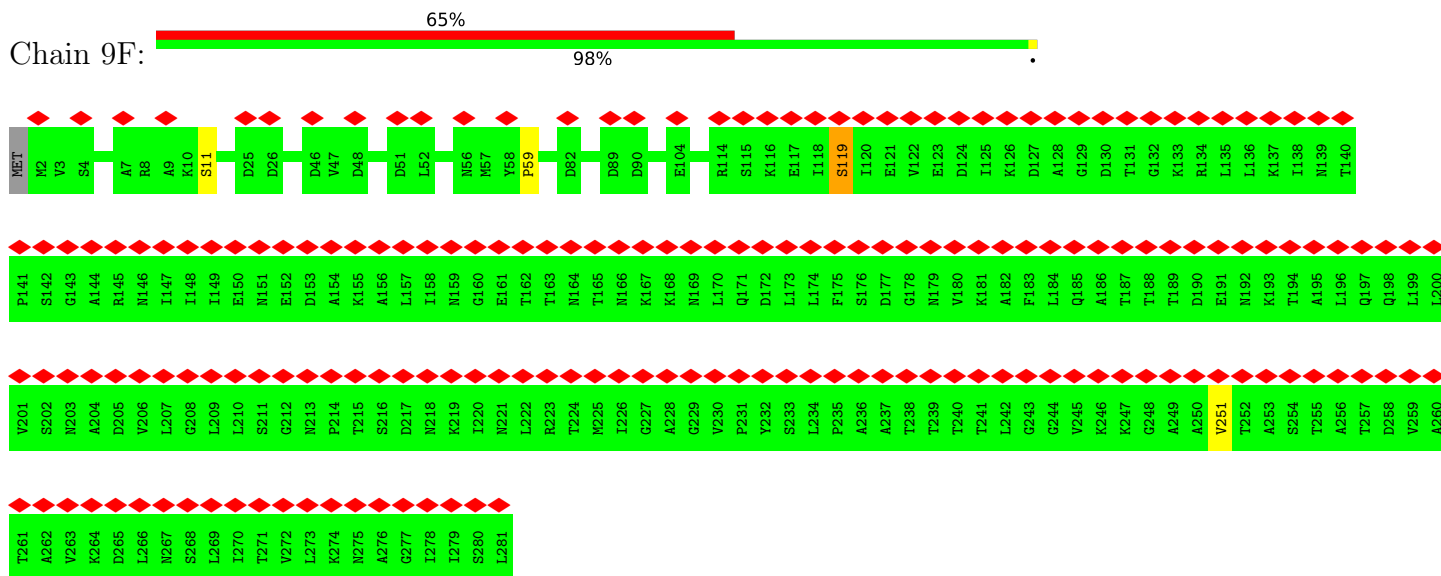
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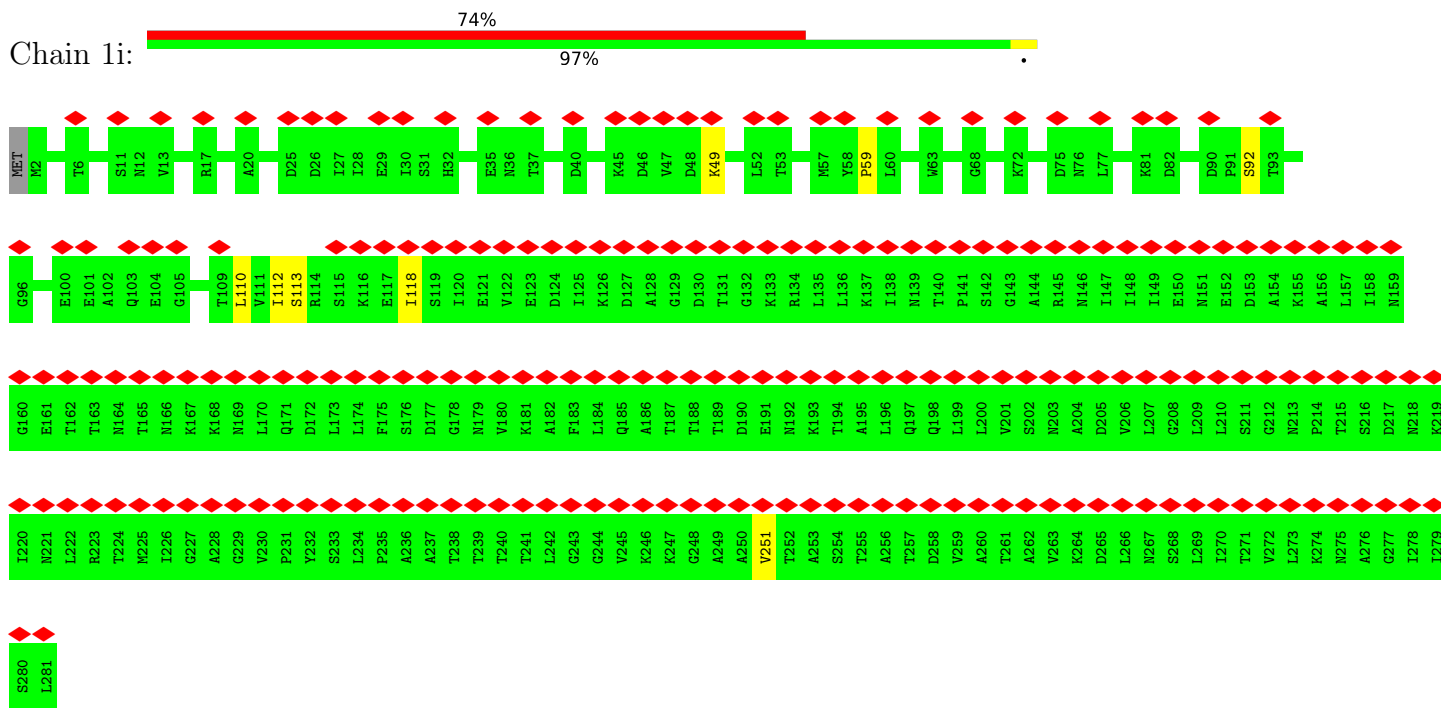
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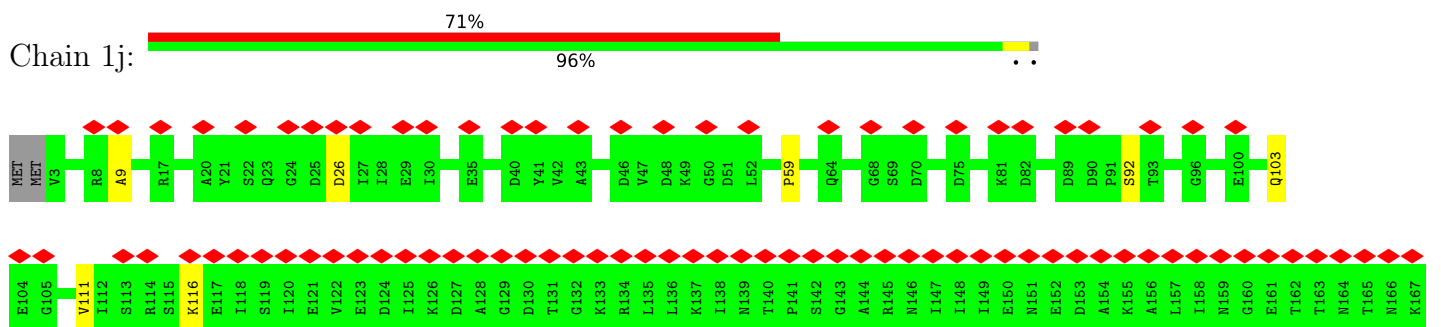
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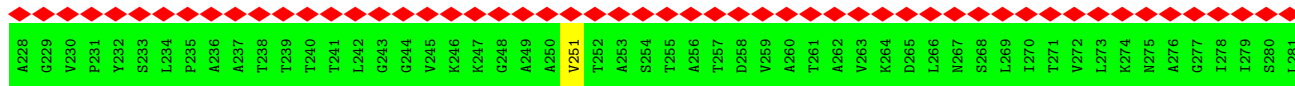
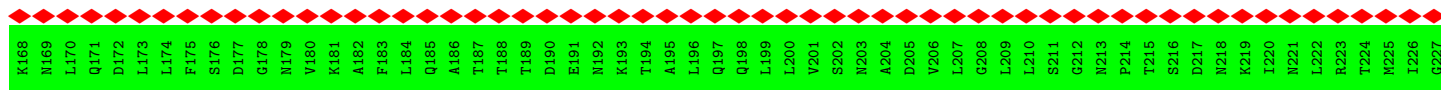


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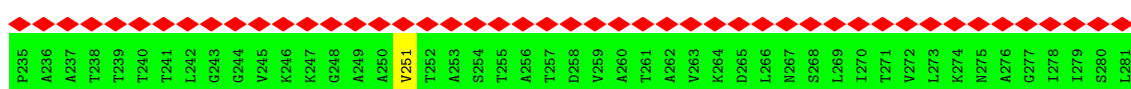
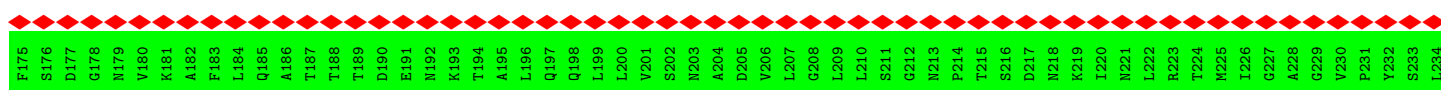
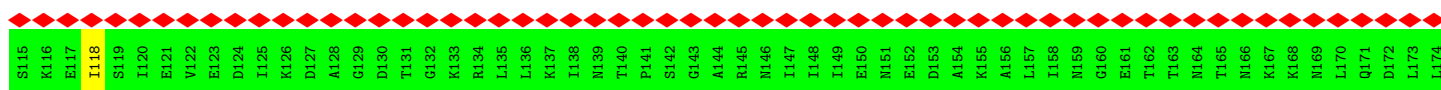
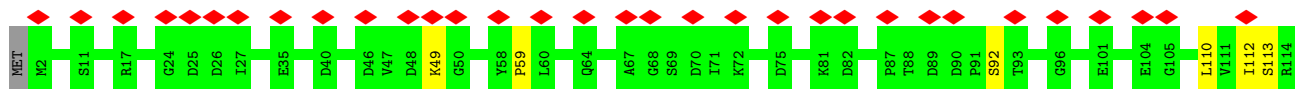
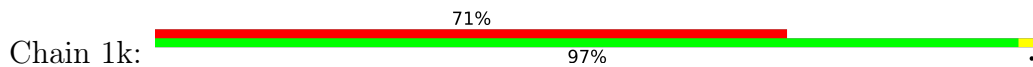


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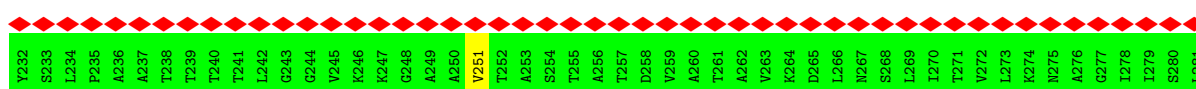
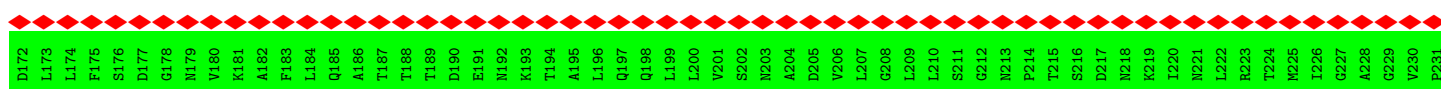
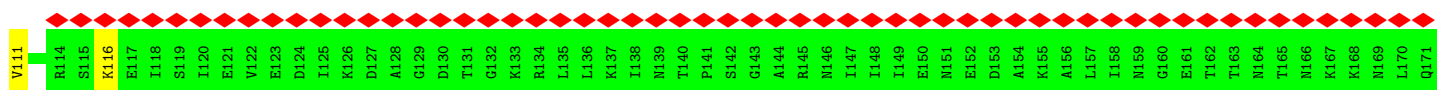
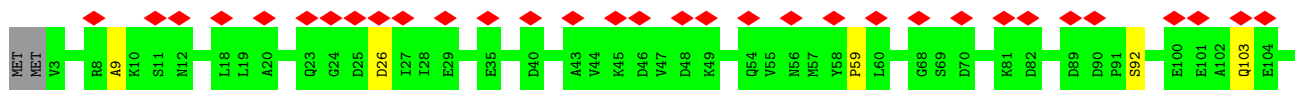




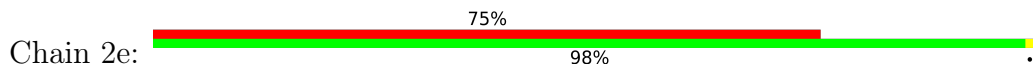
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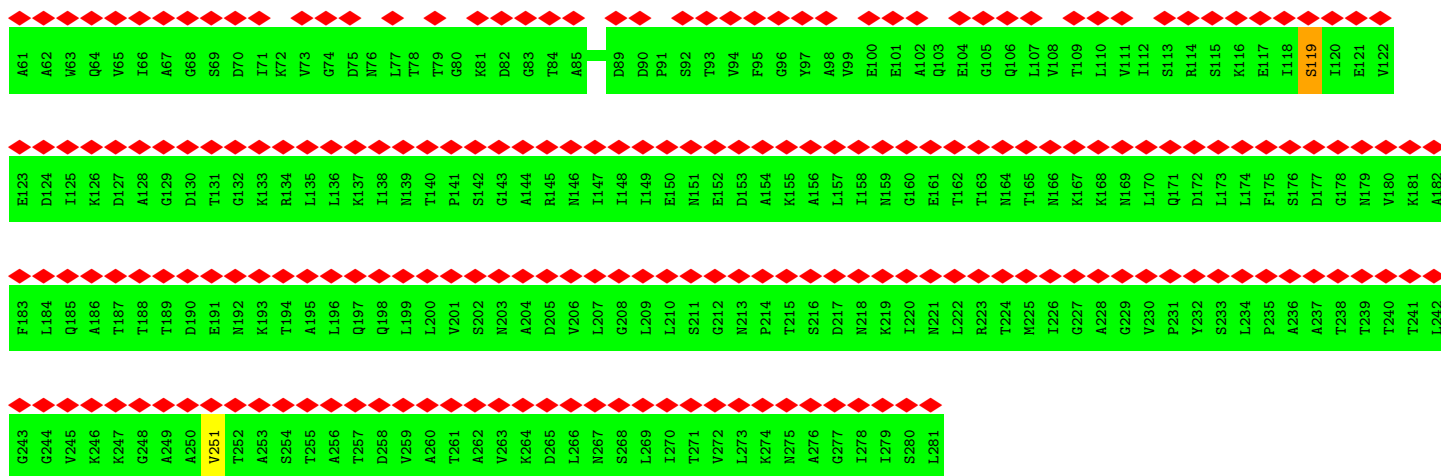


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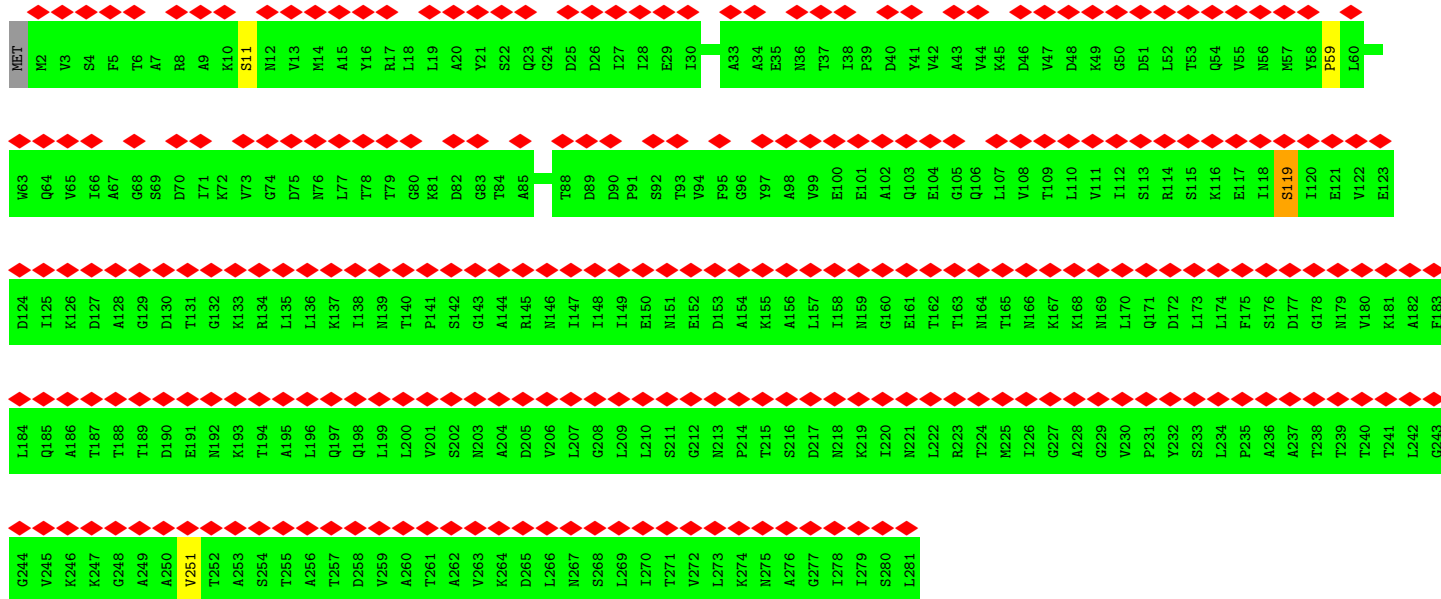


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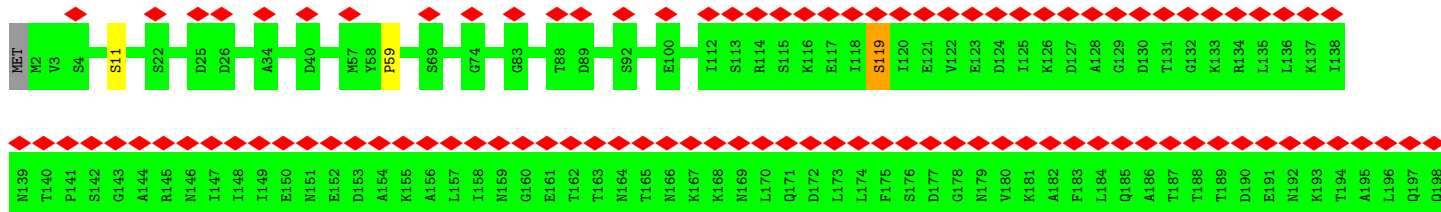


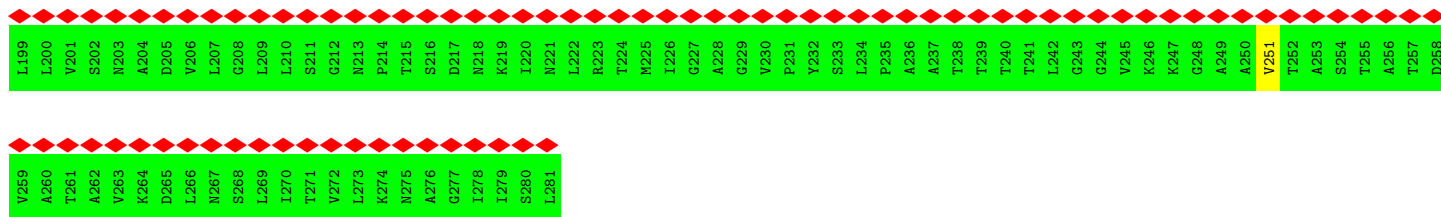


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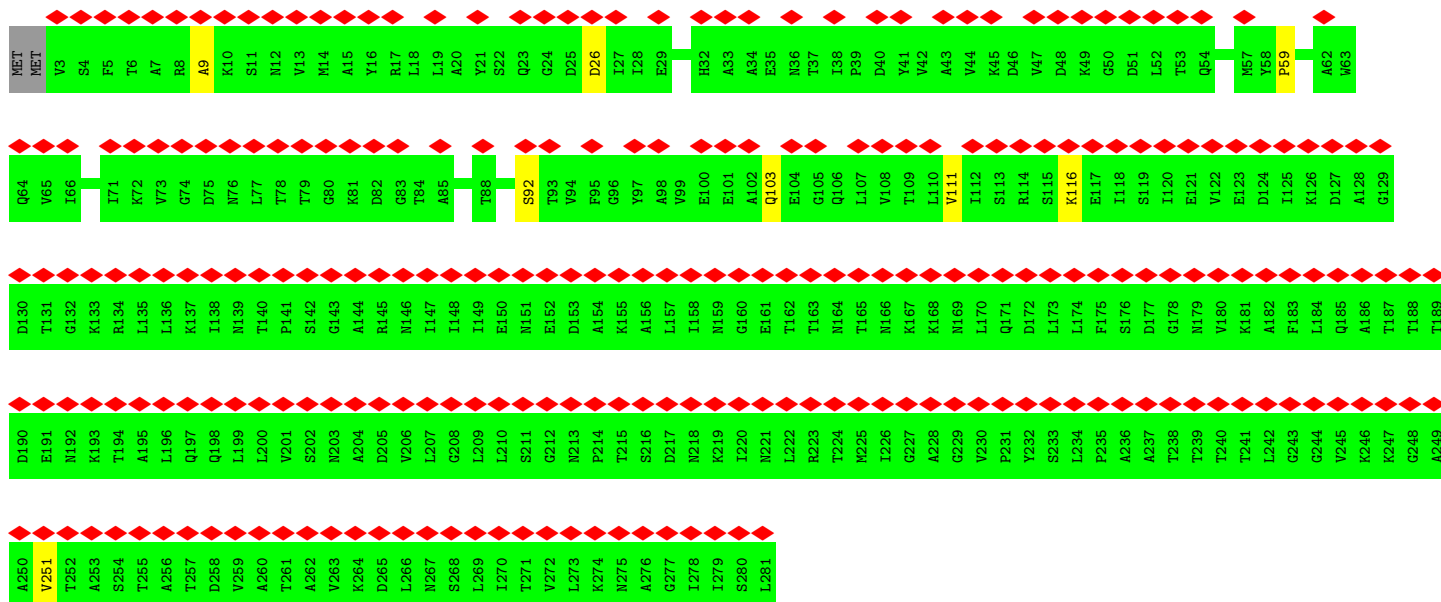
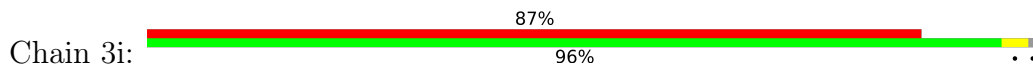


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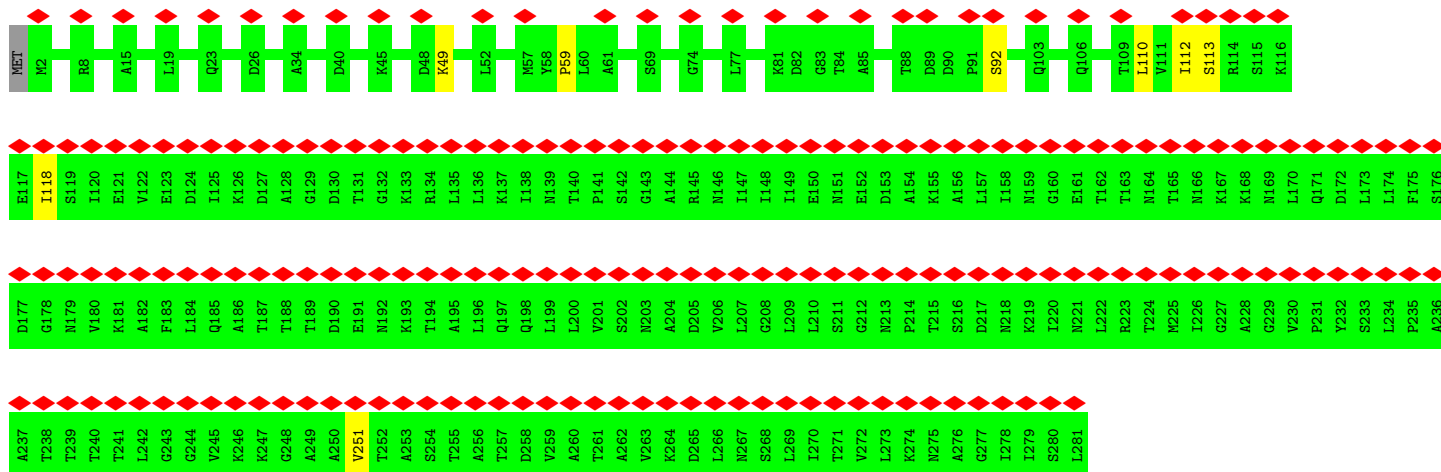




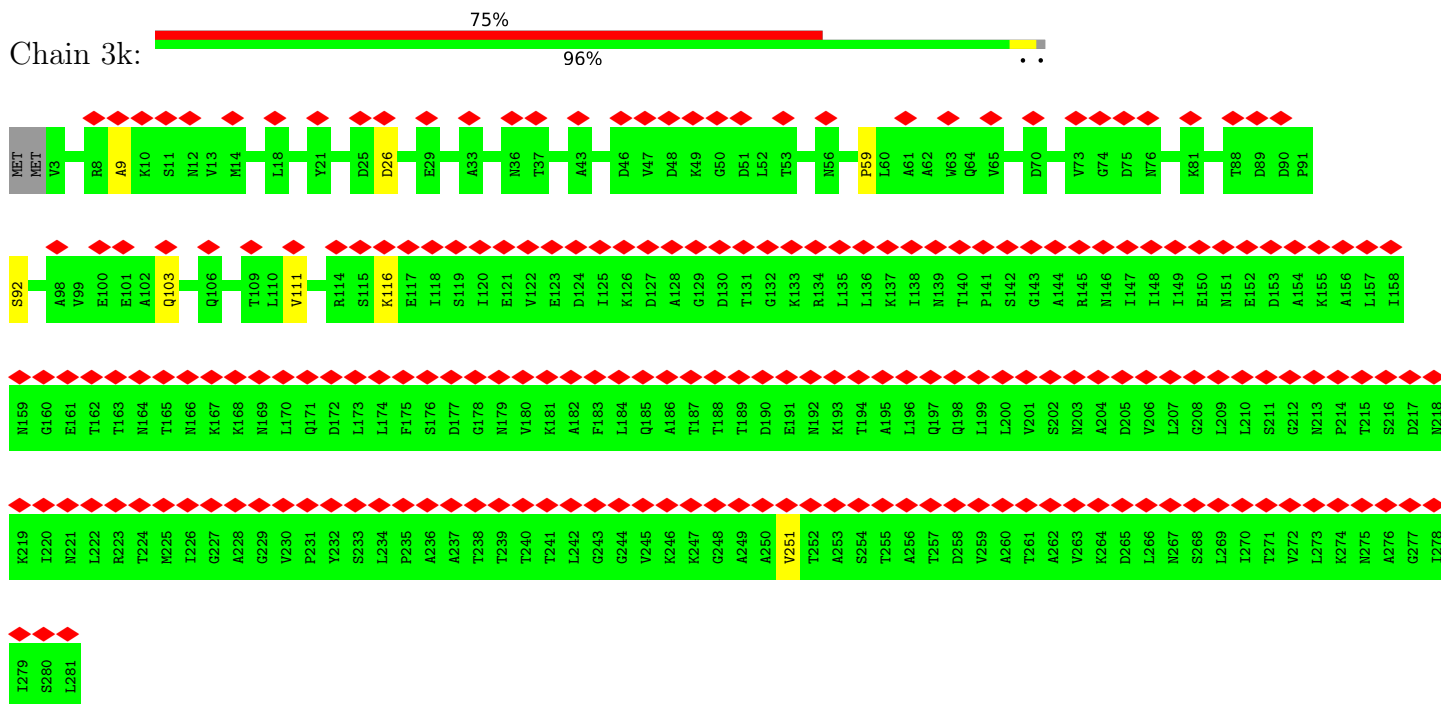
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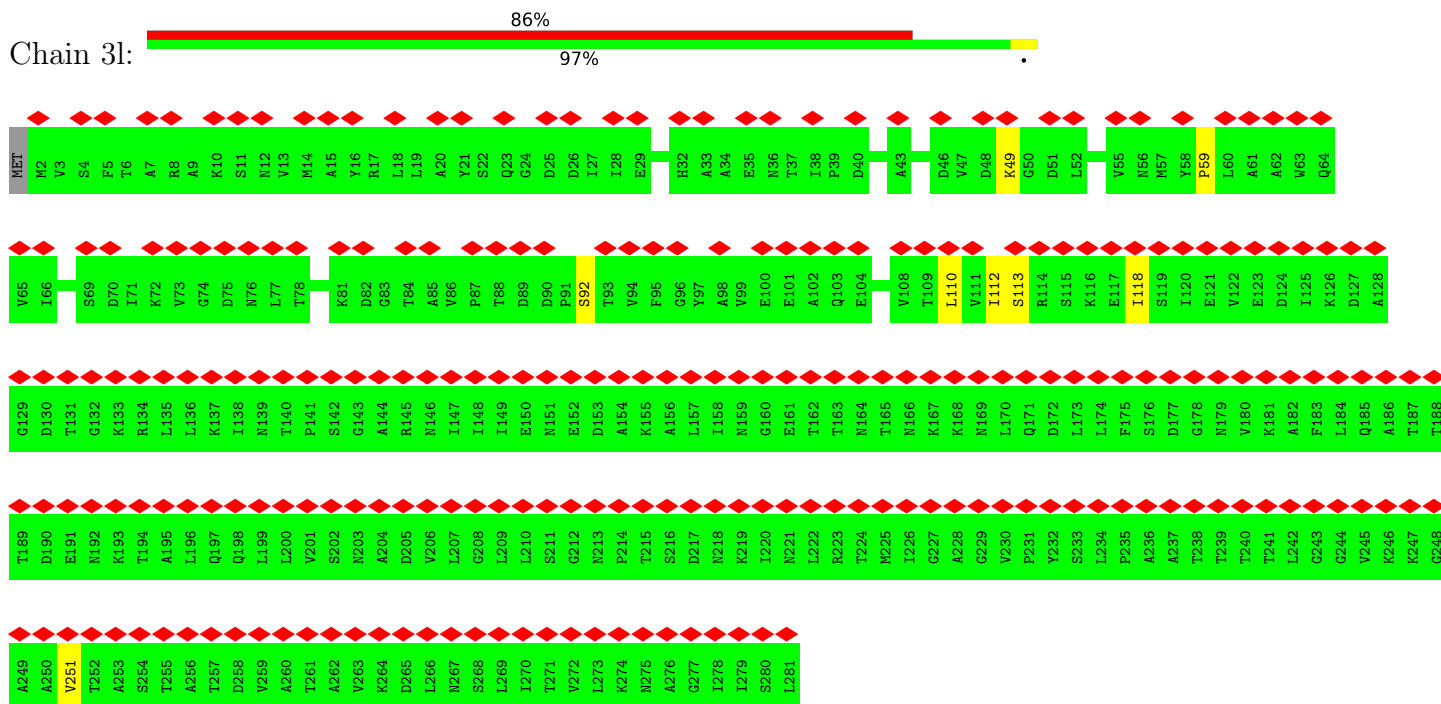
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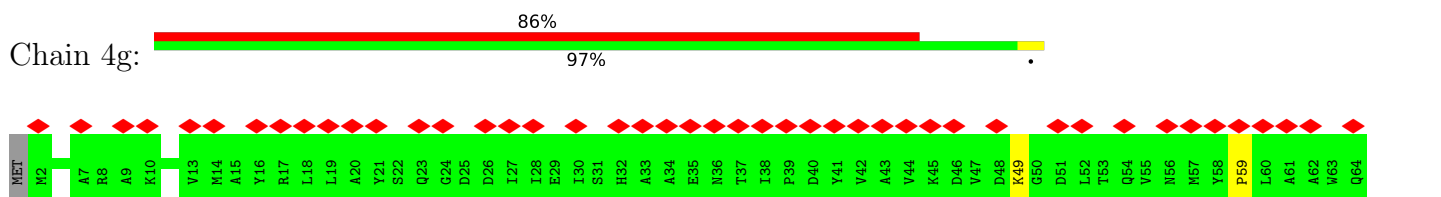
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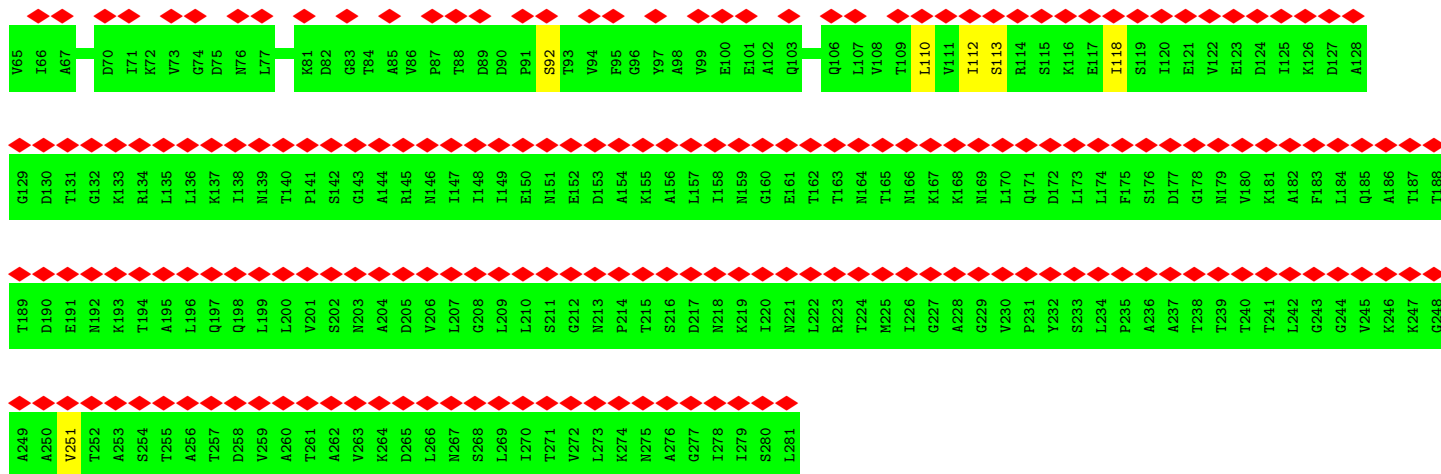


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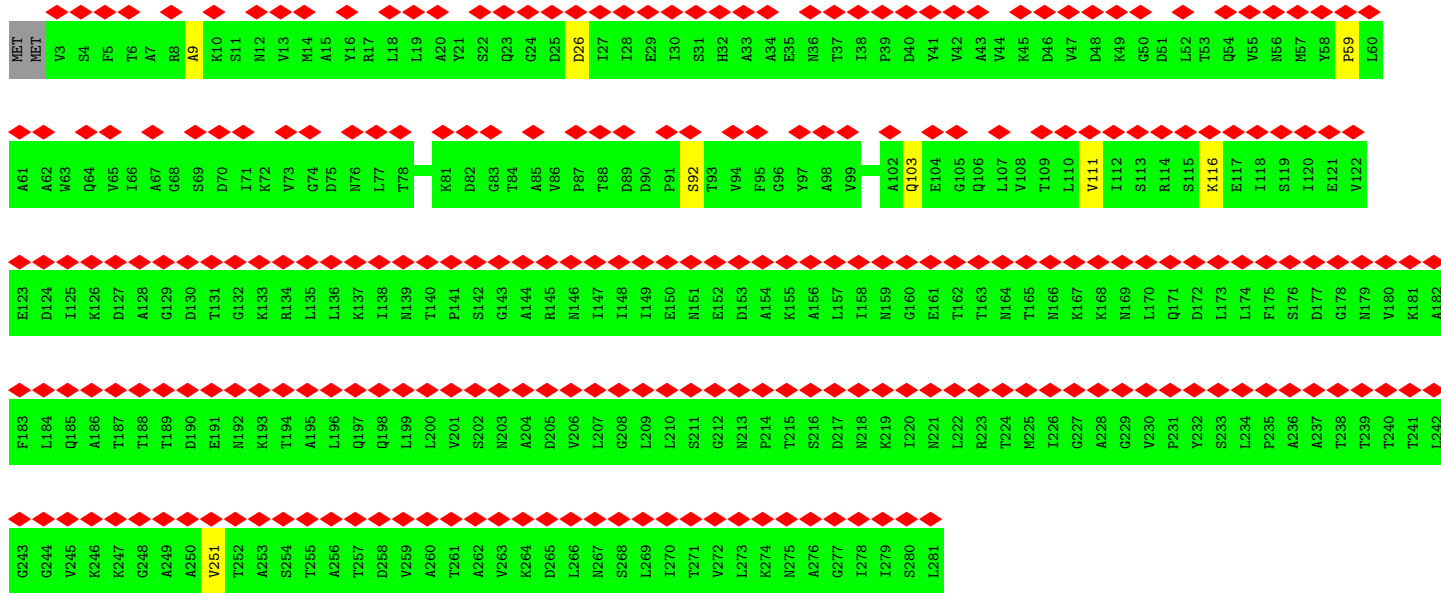


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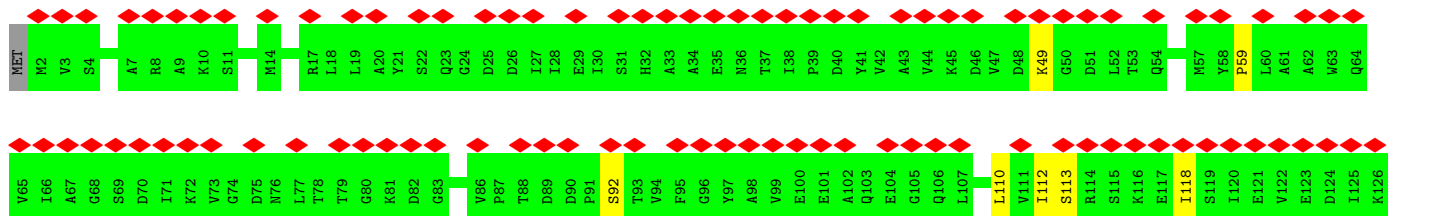
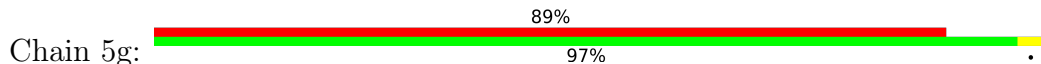


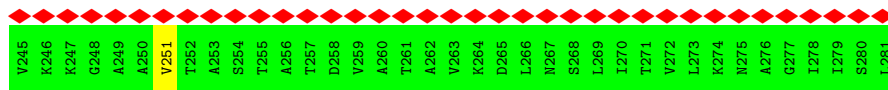


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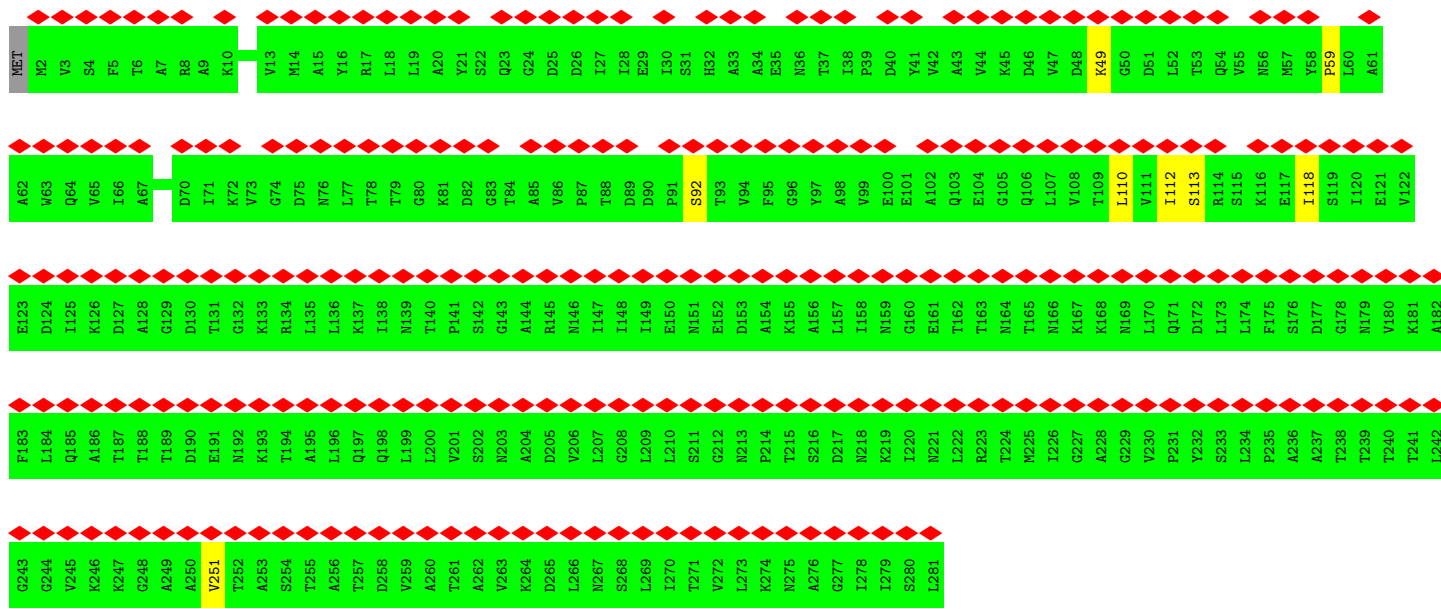
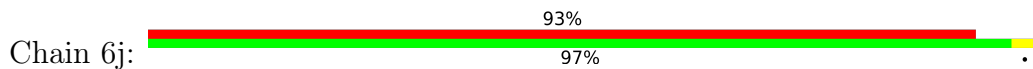


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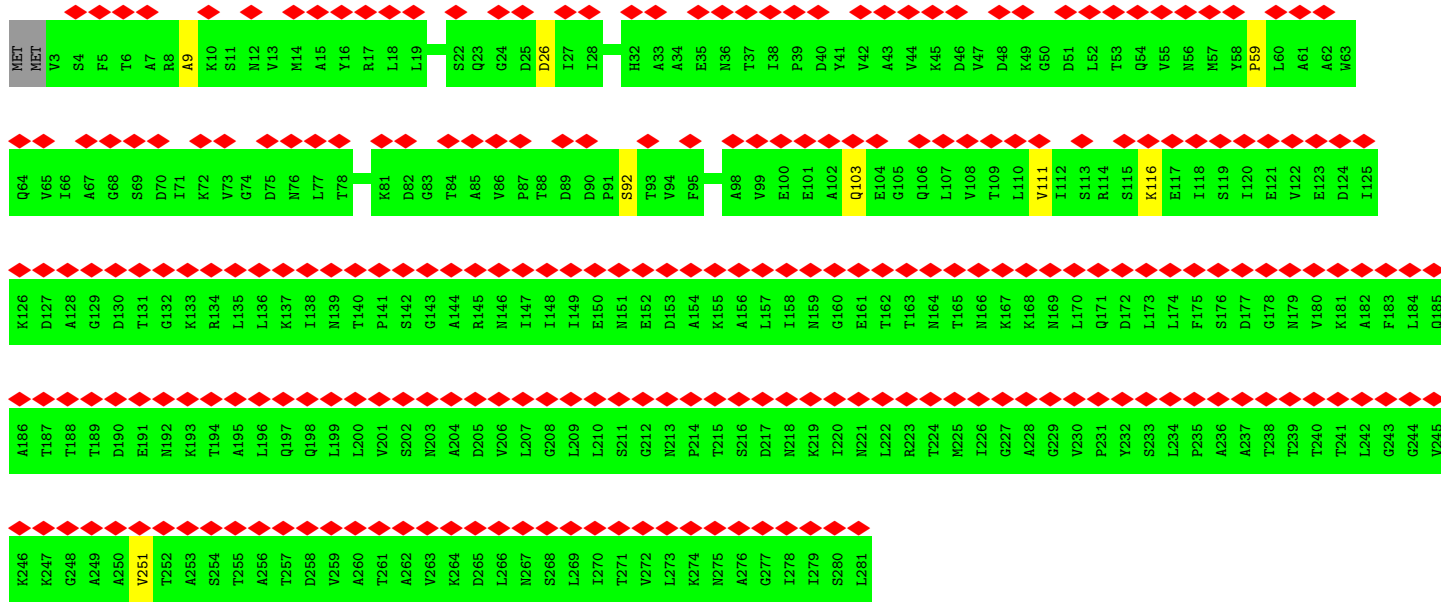
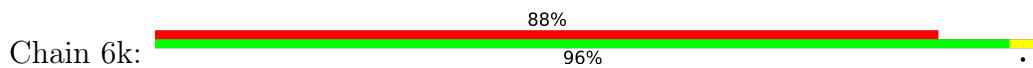




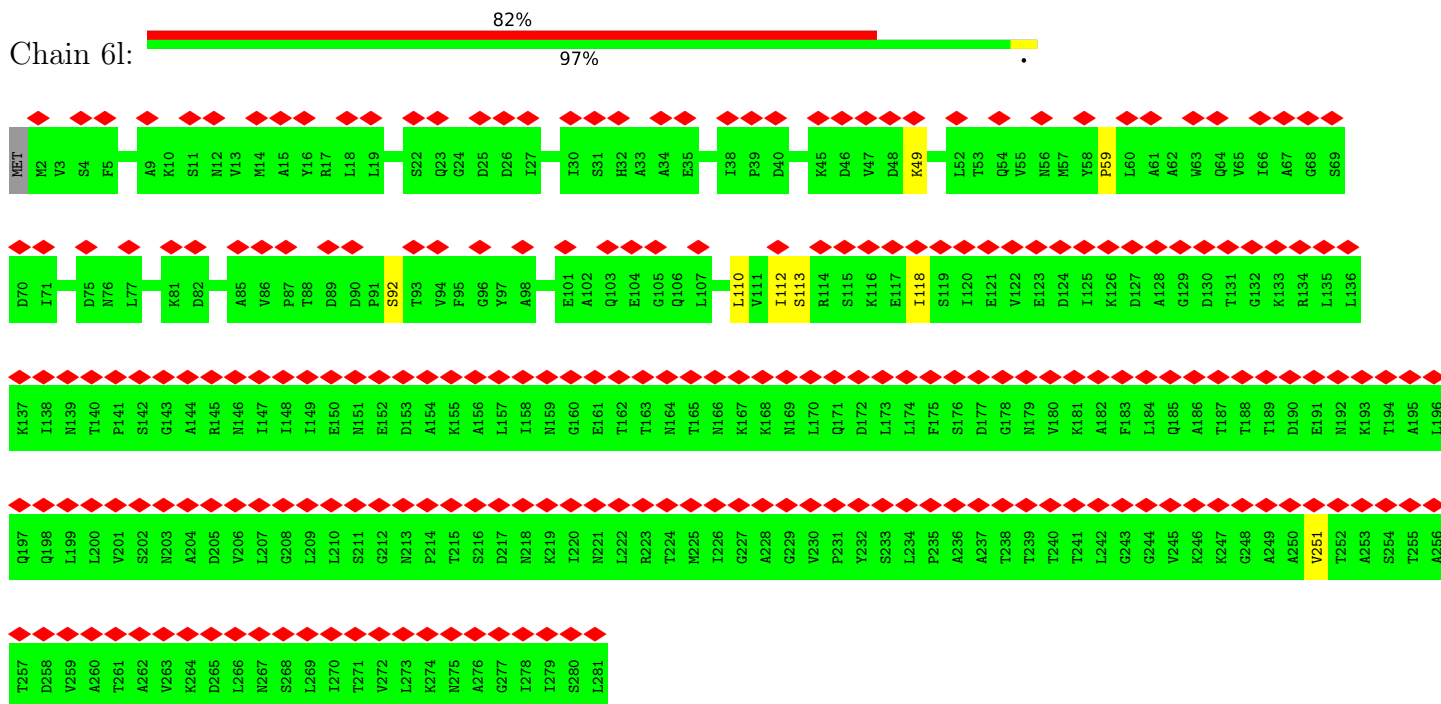
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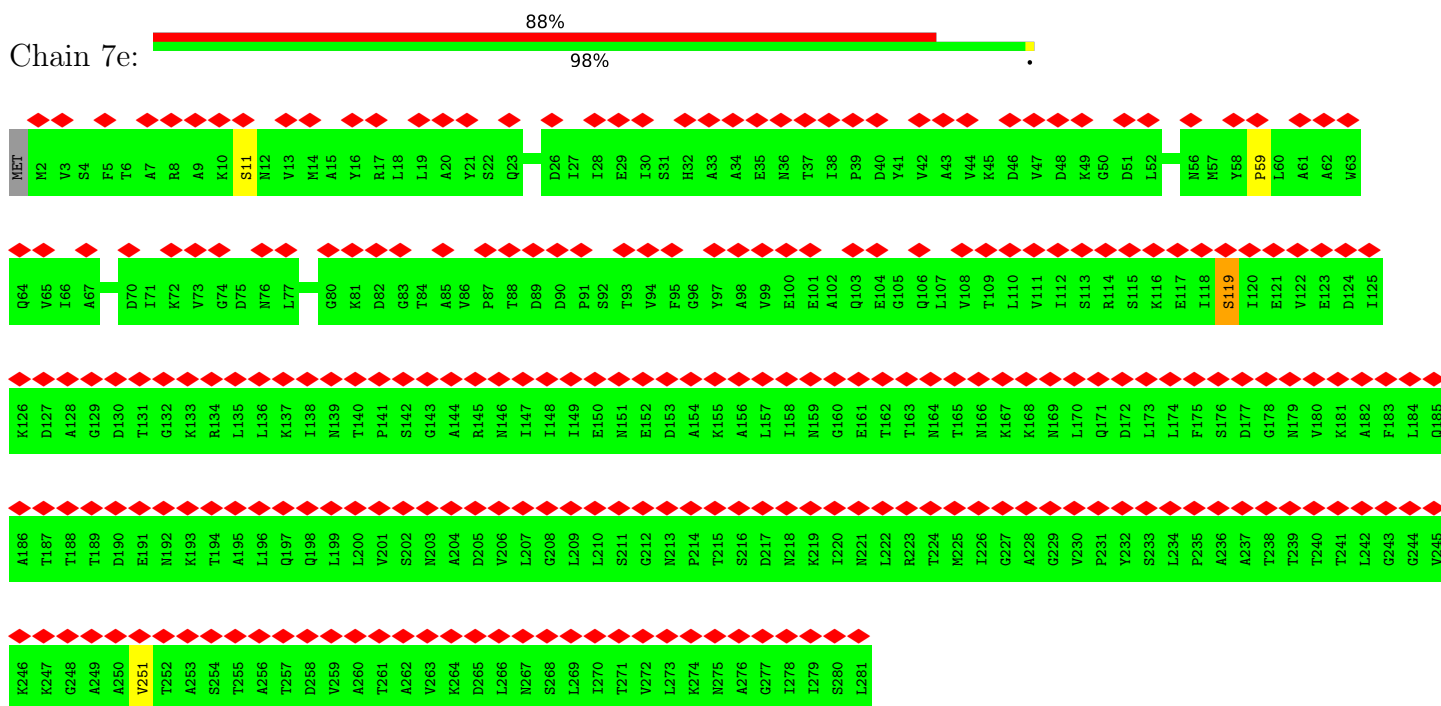
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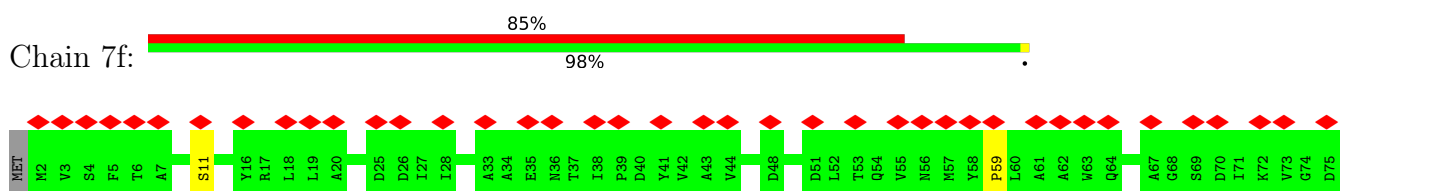
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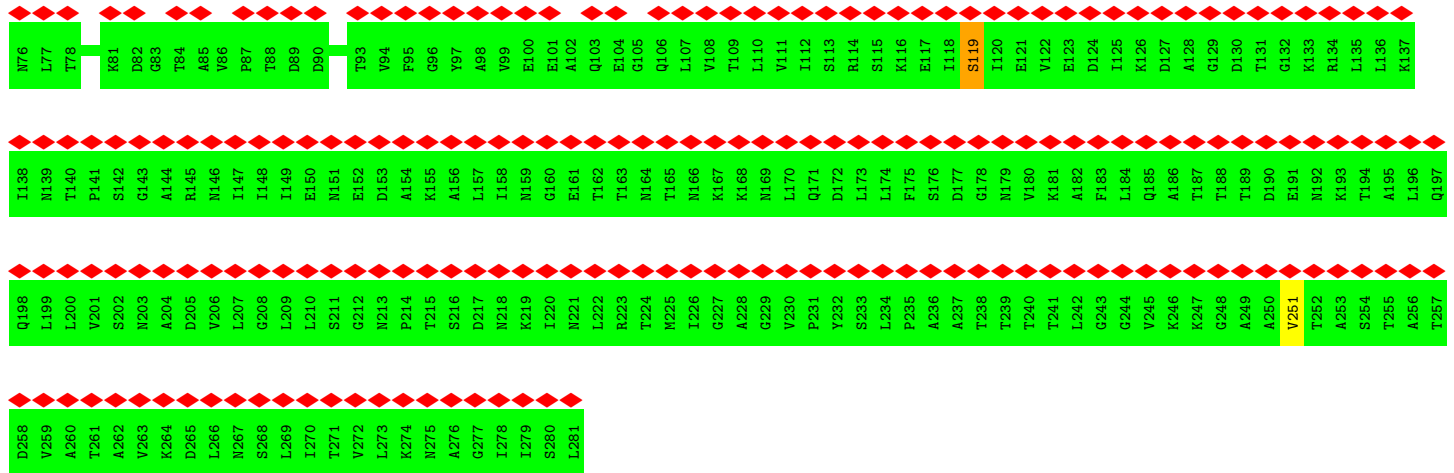


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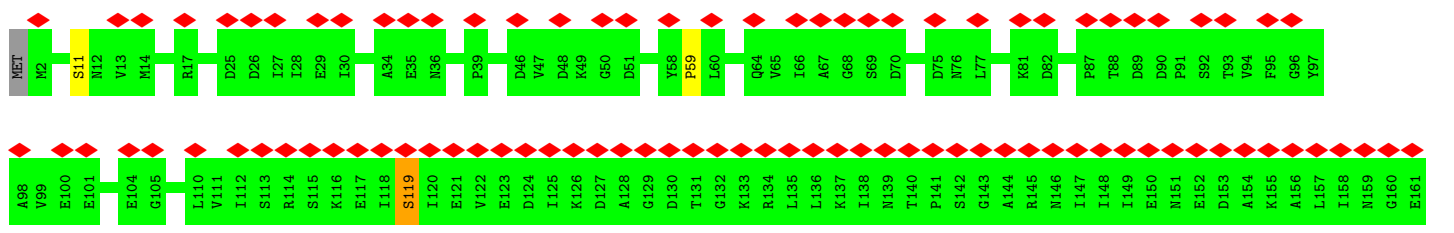
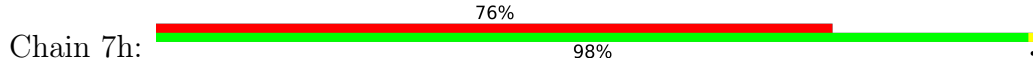


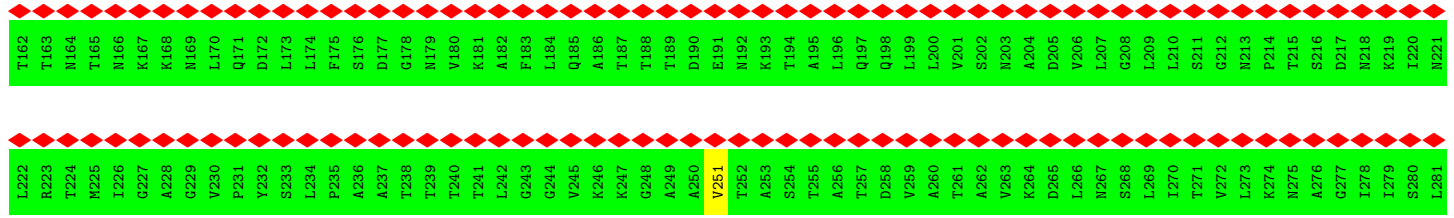


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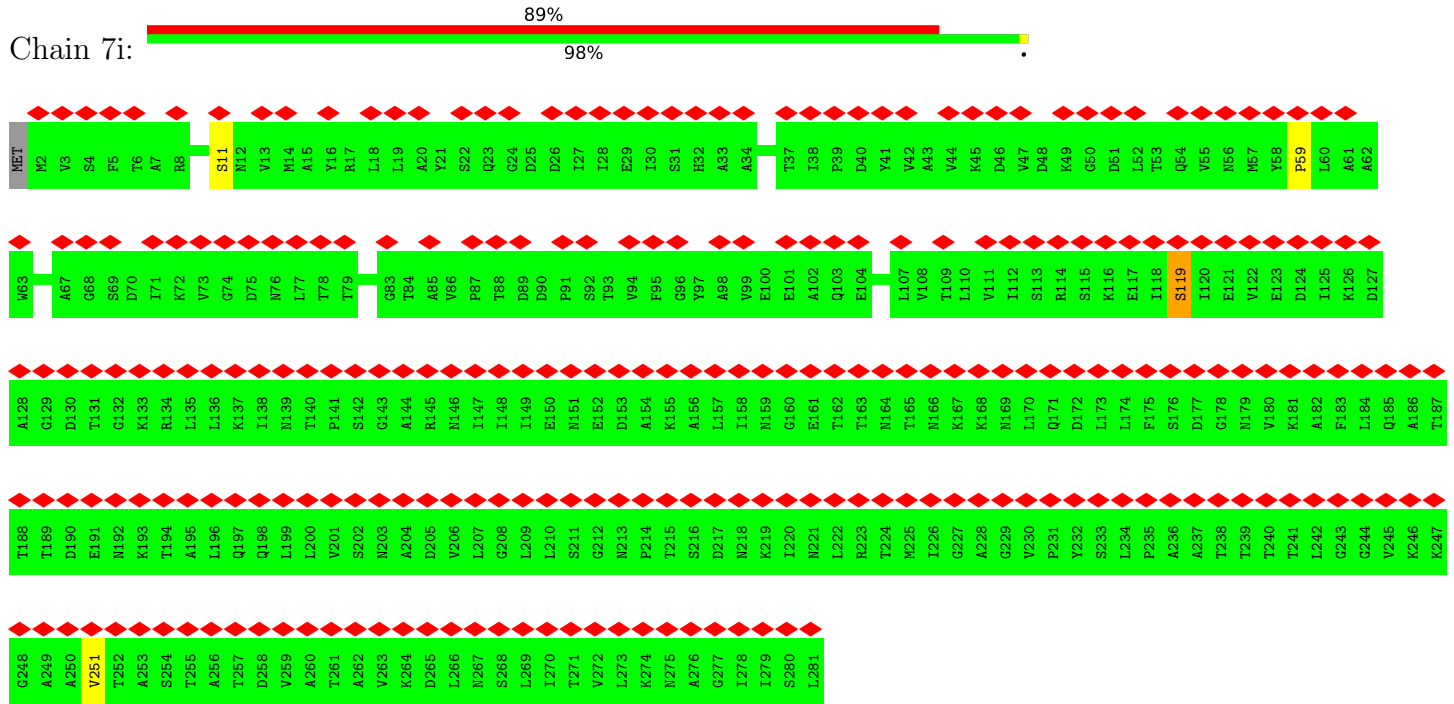


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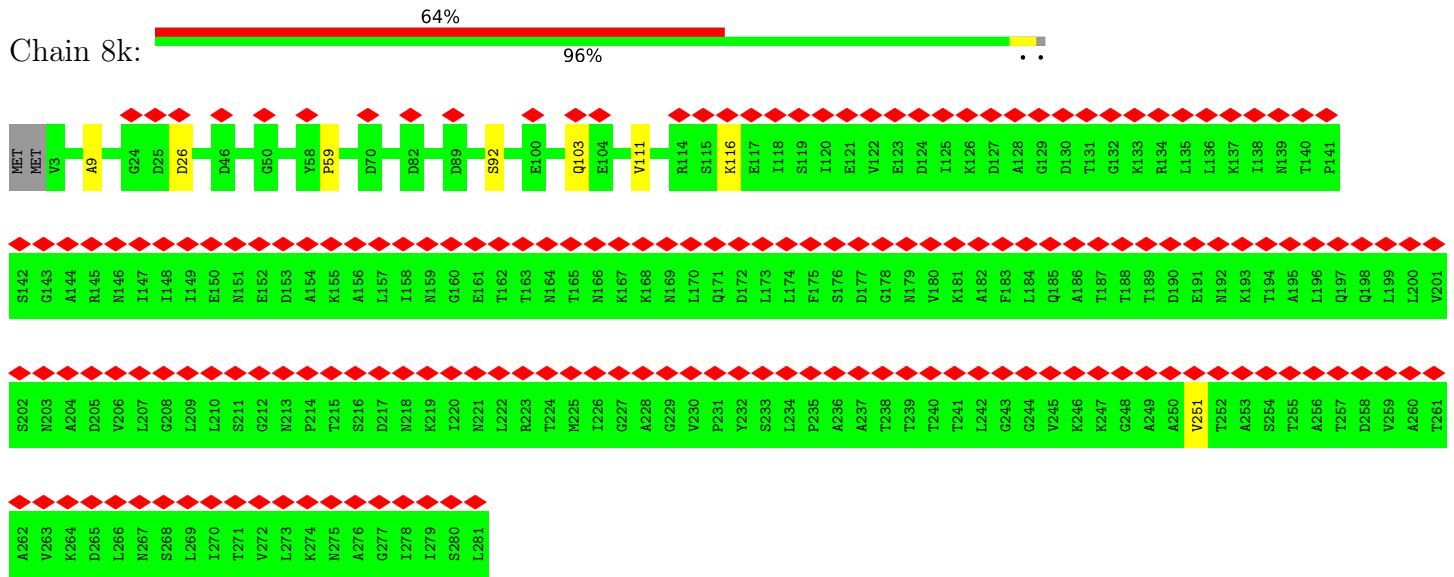




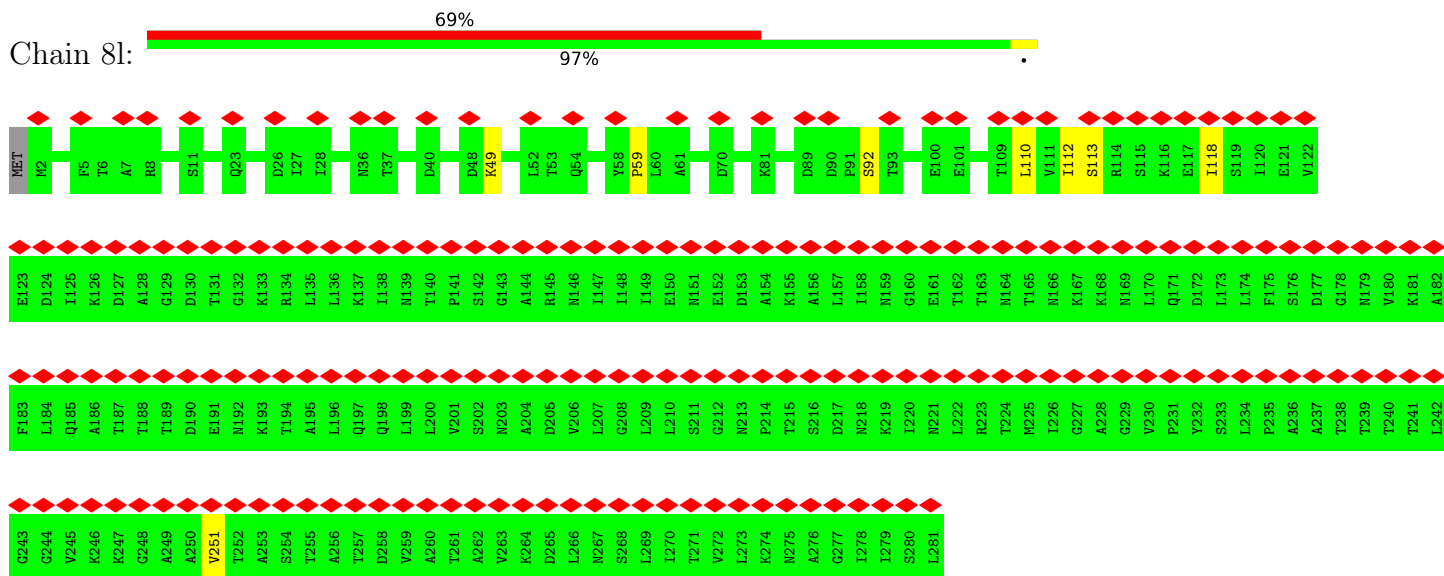
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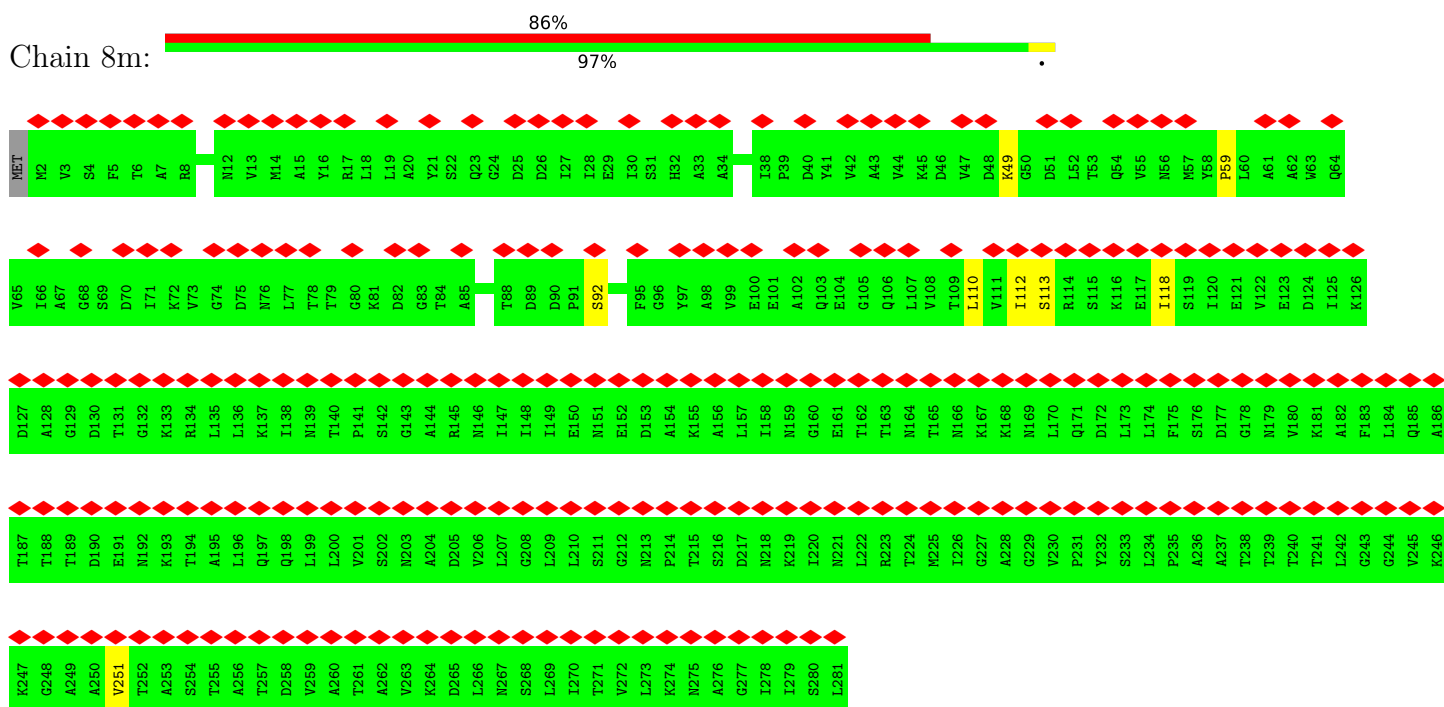
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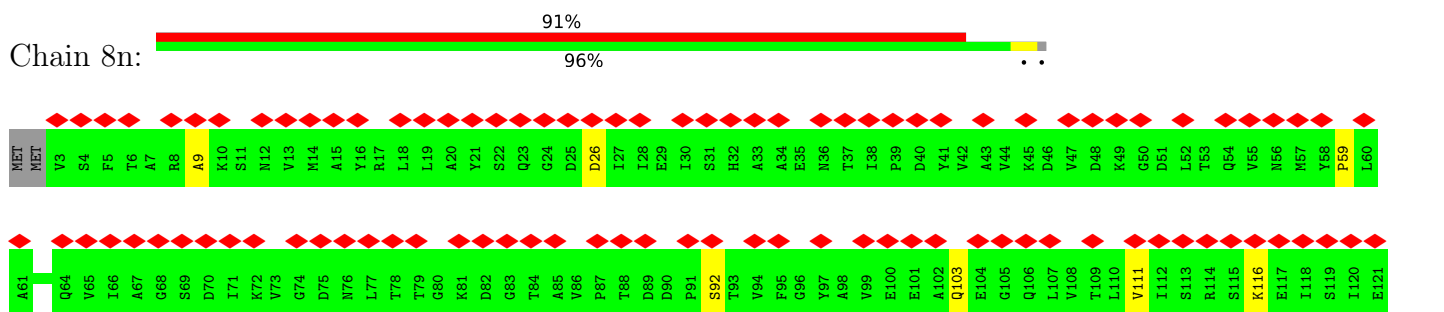
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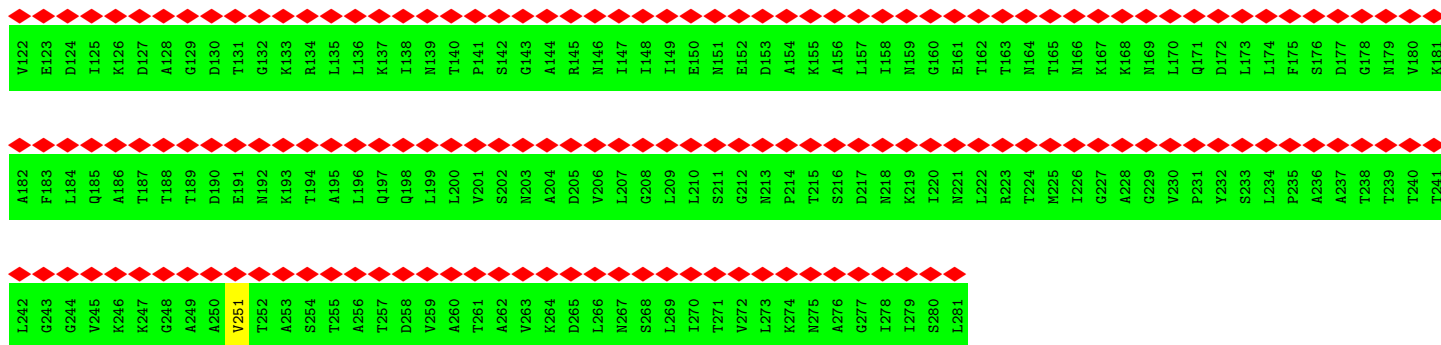


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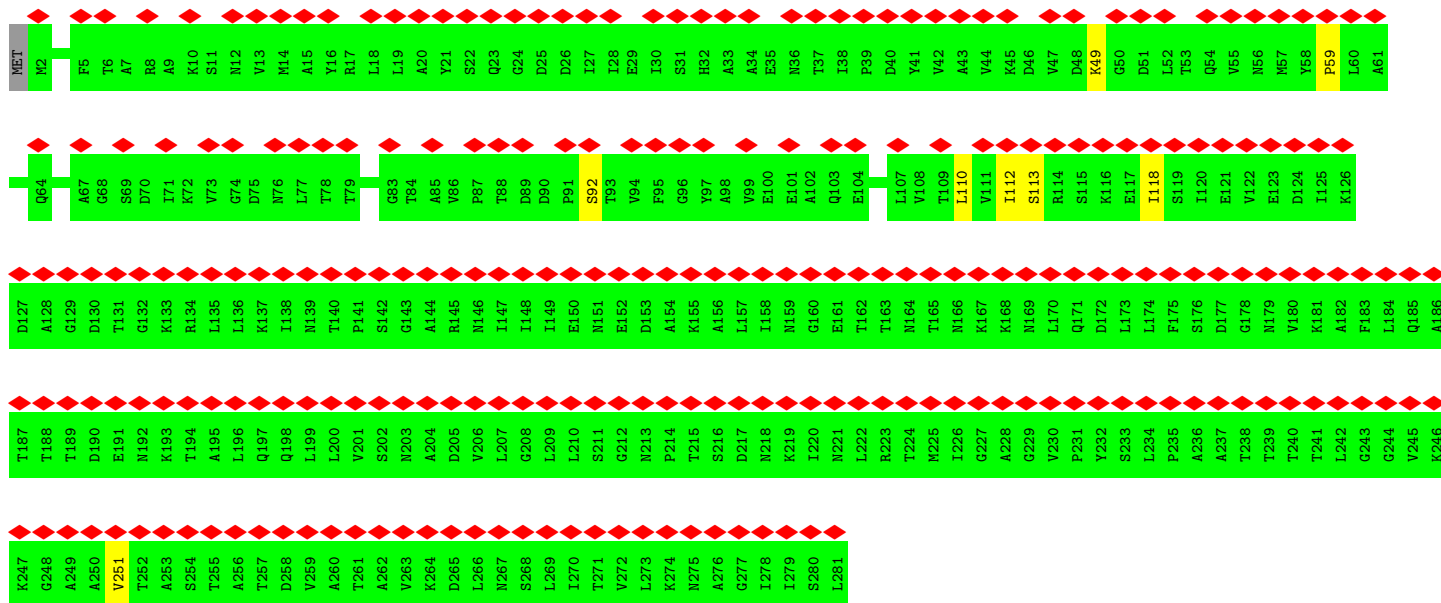


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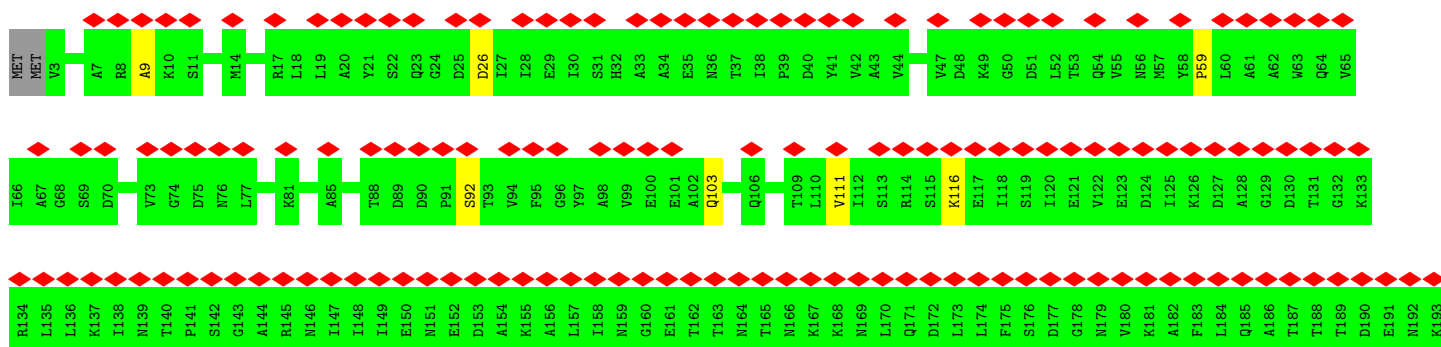
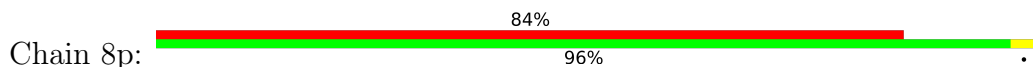


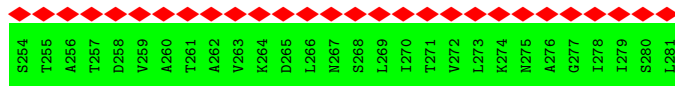
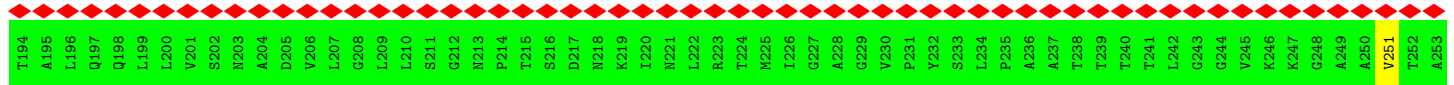


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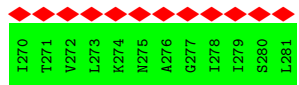
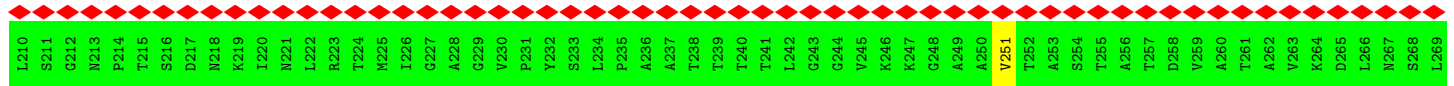
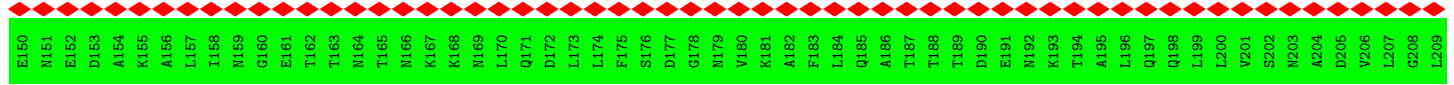
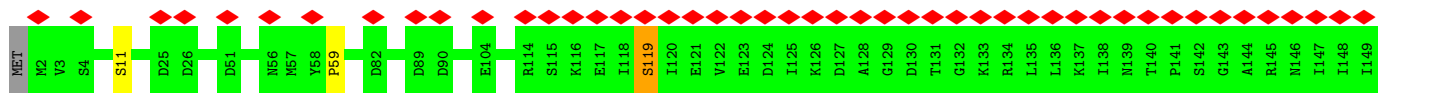


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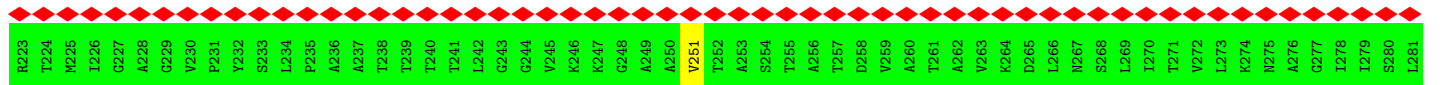
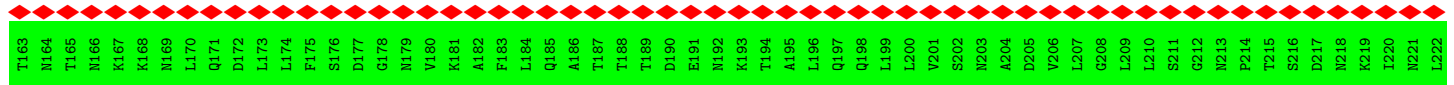
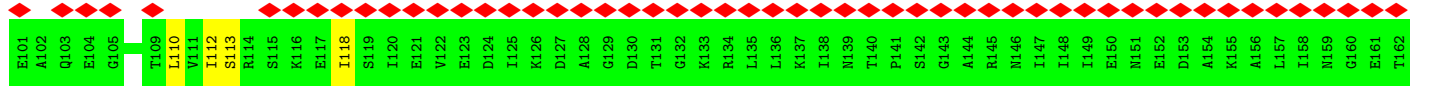
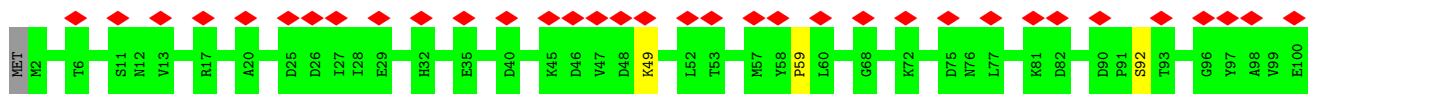
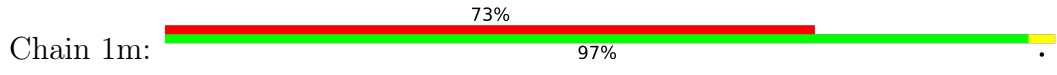




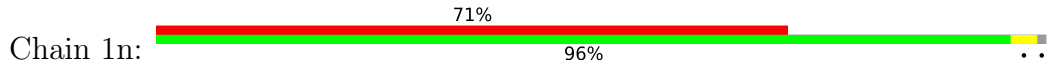
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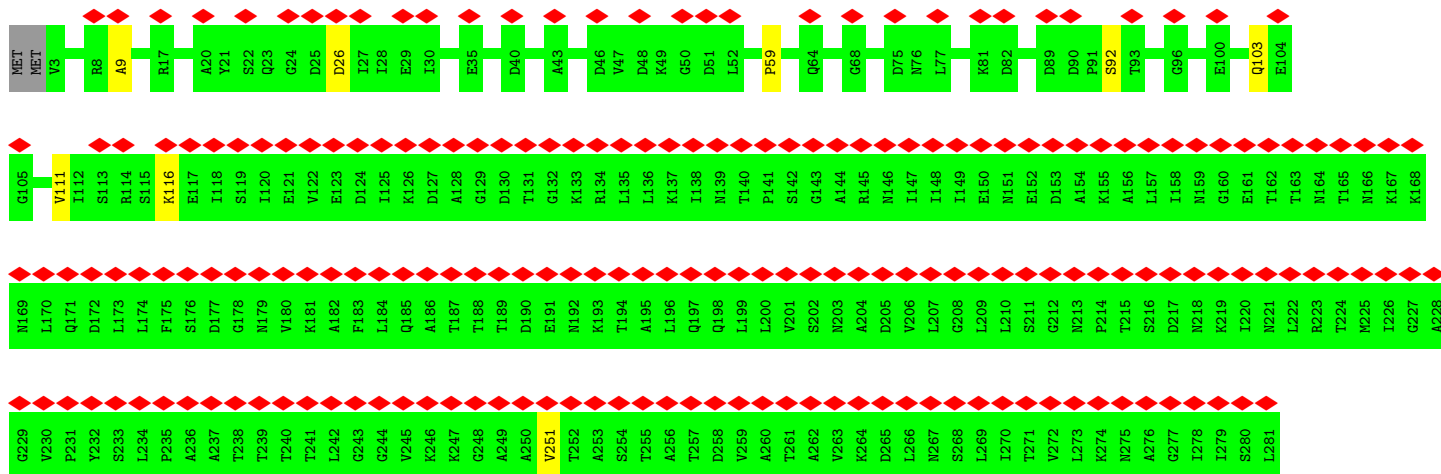


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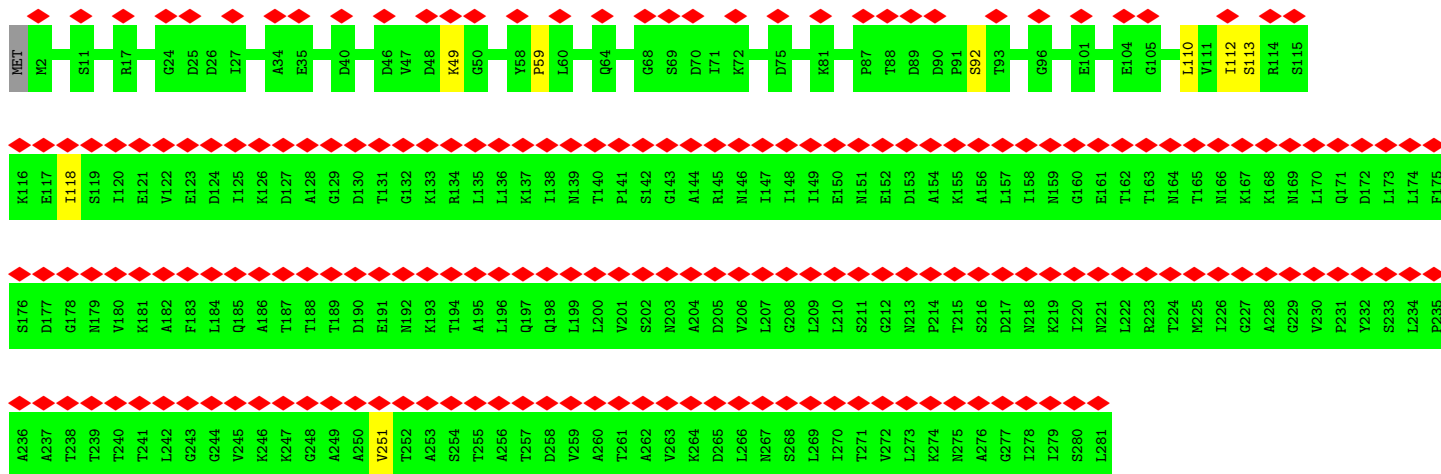


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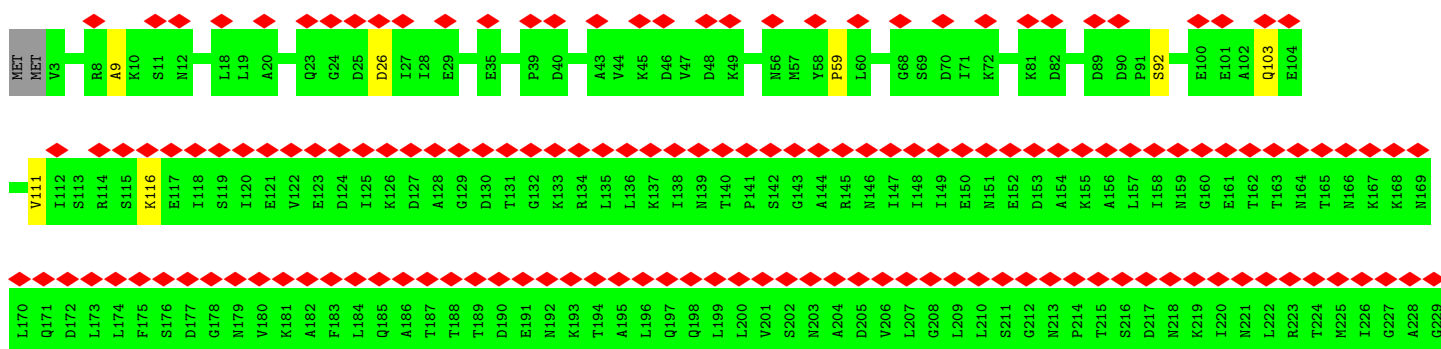
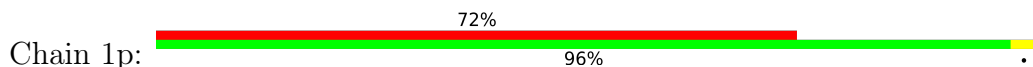


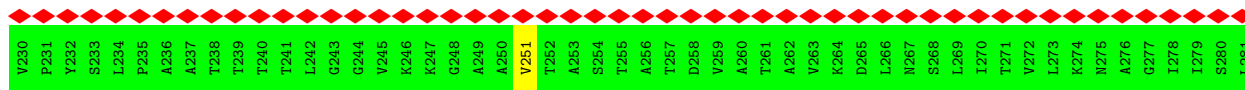


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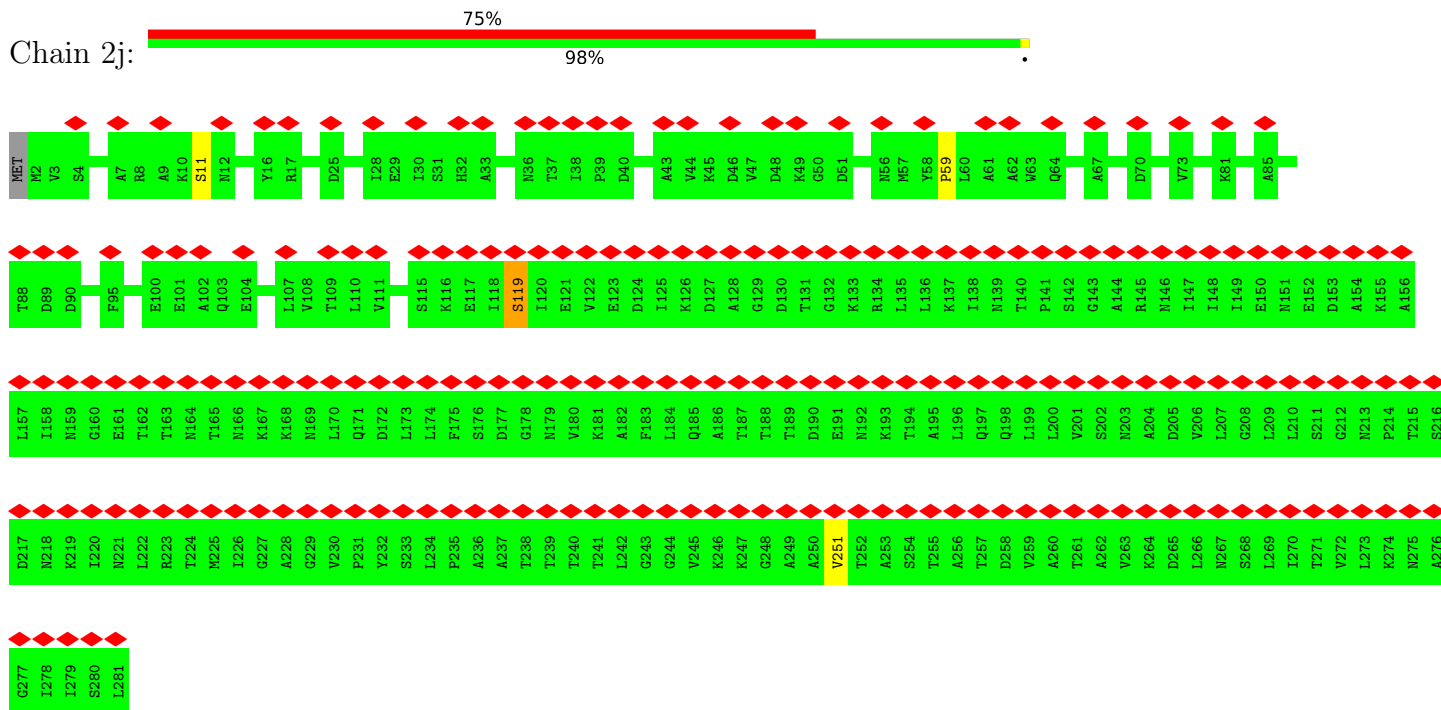


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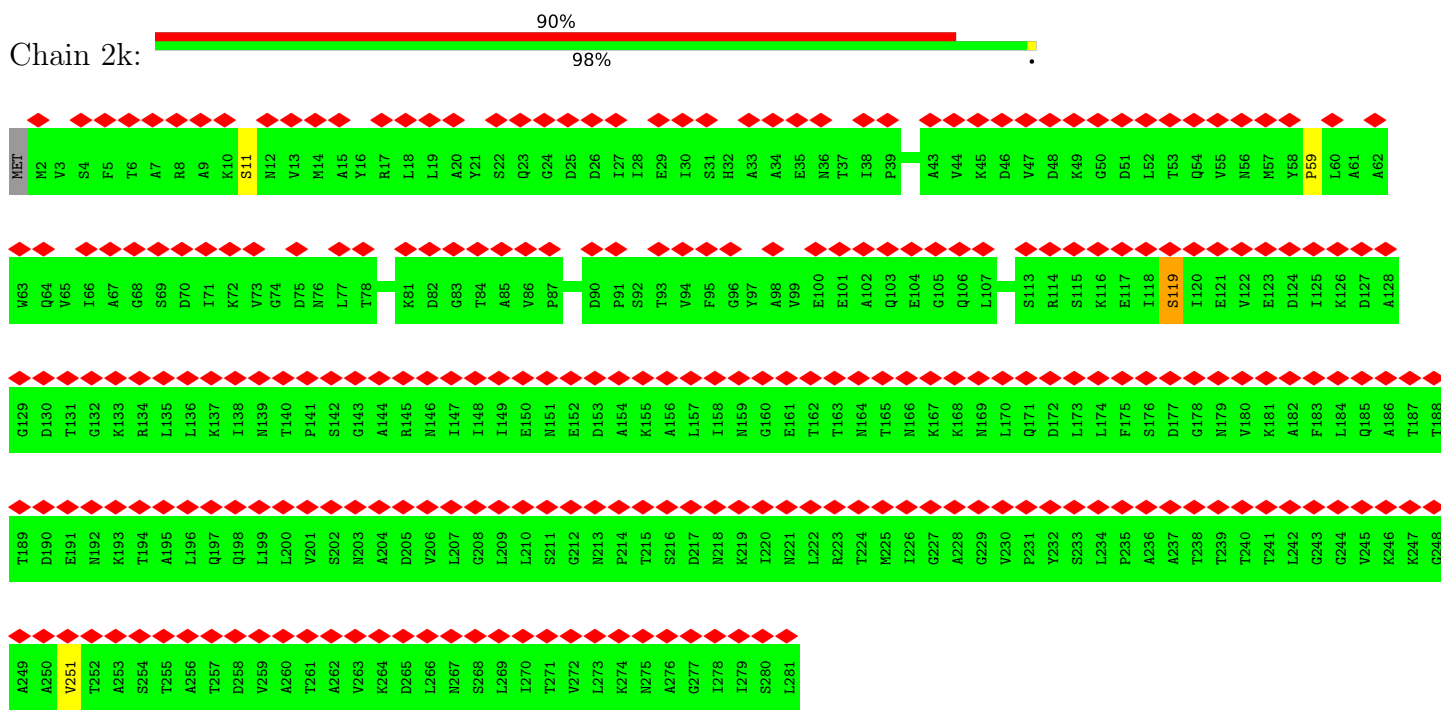




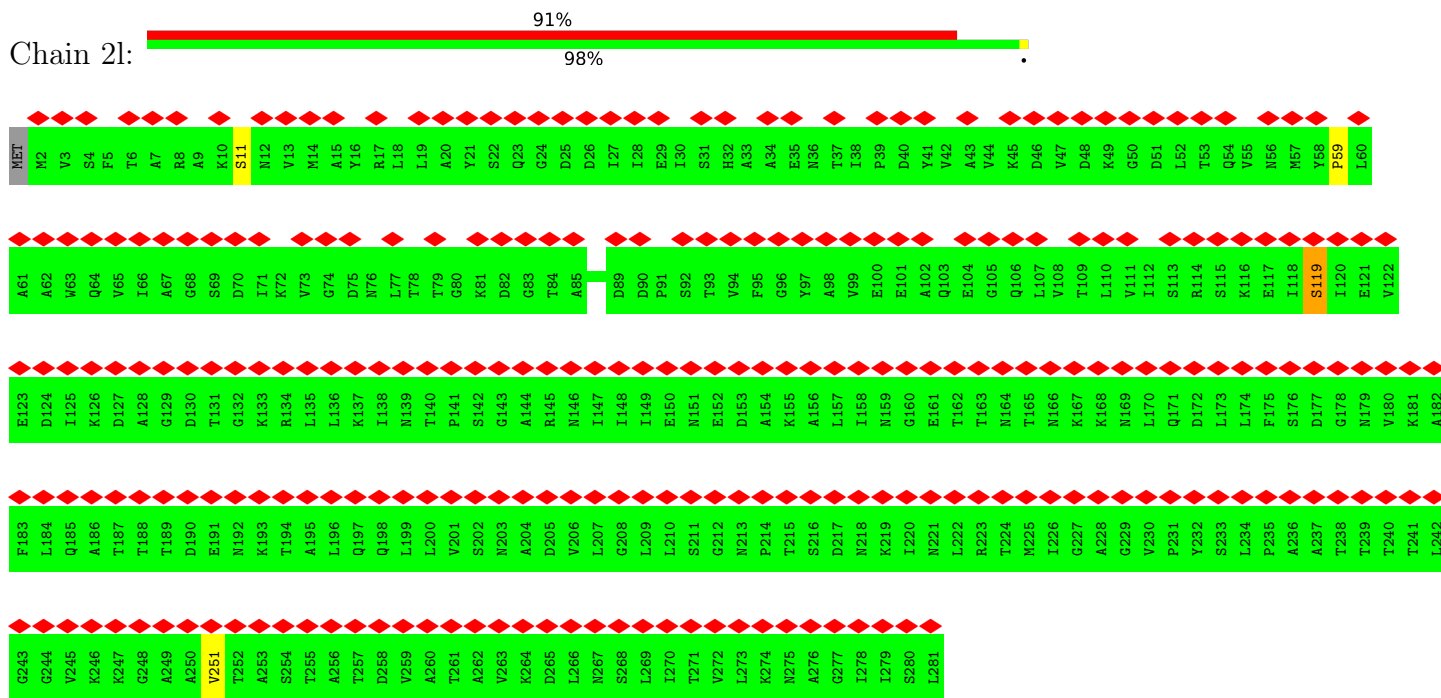
• Molecule 2: Capsid fiber protein



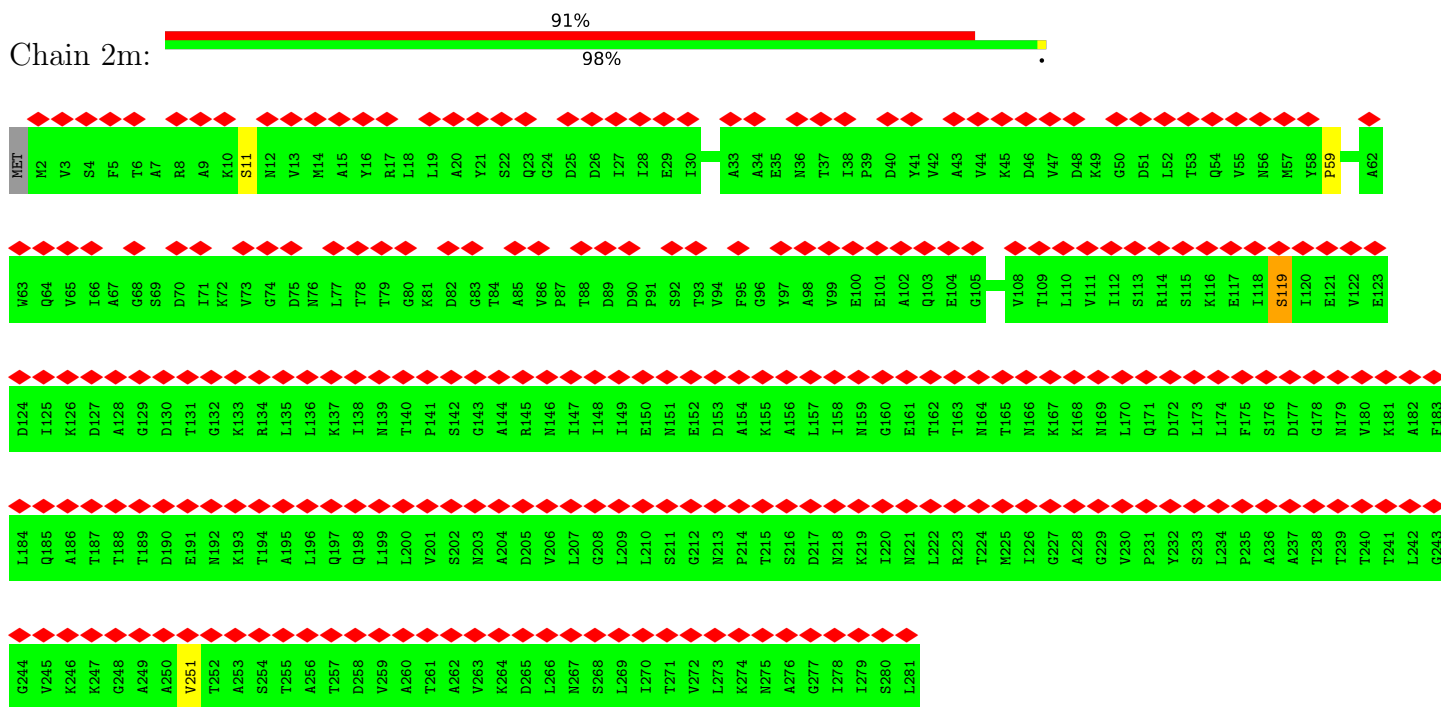
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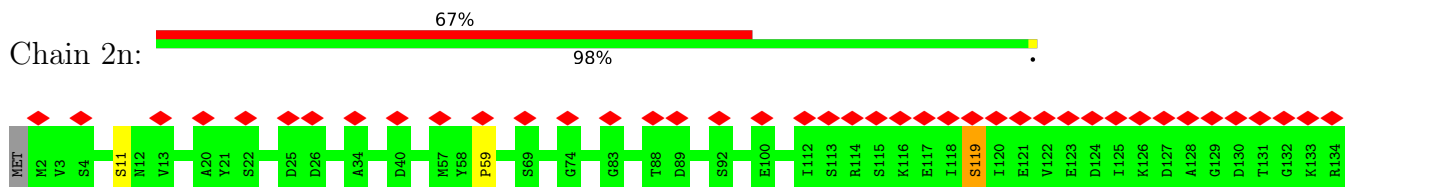
• Molecule 2: Capsid fiber protein



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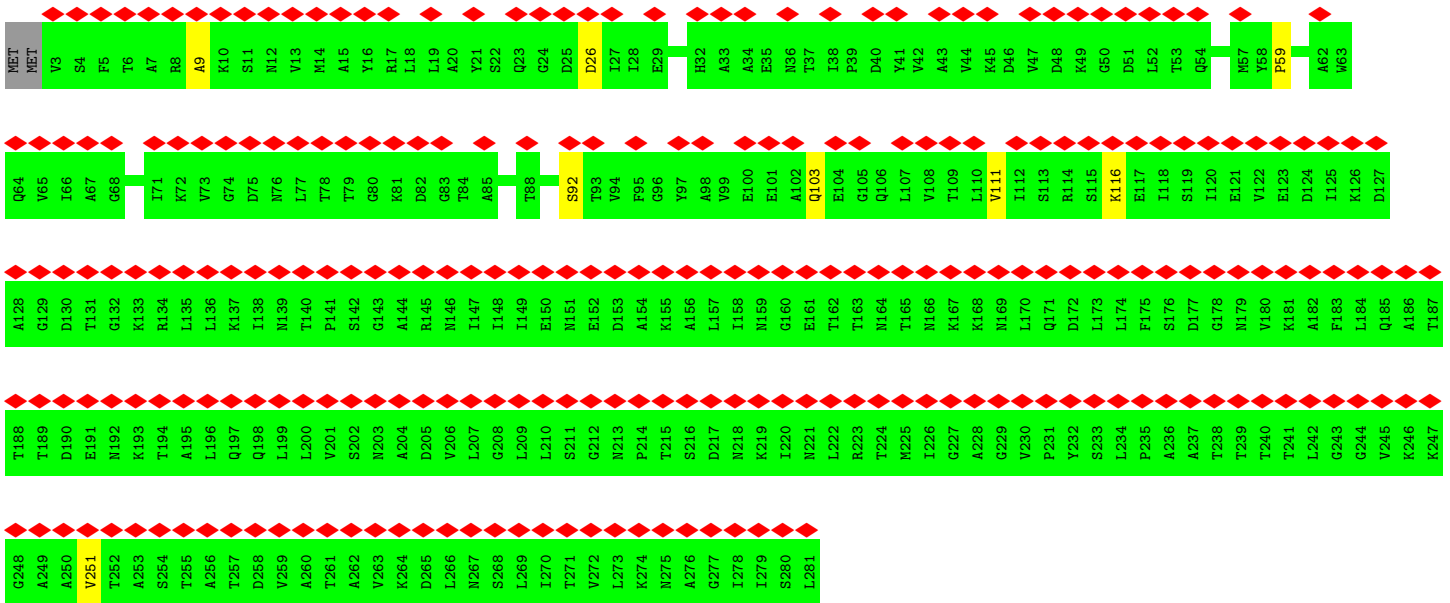


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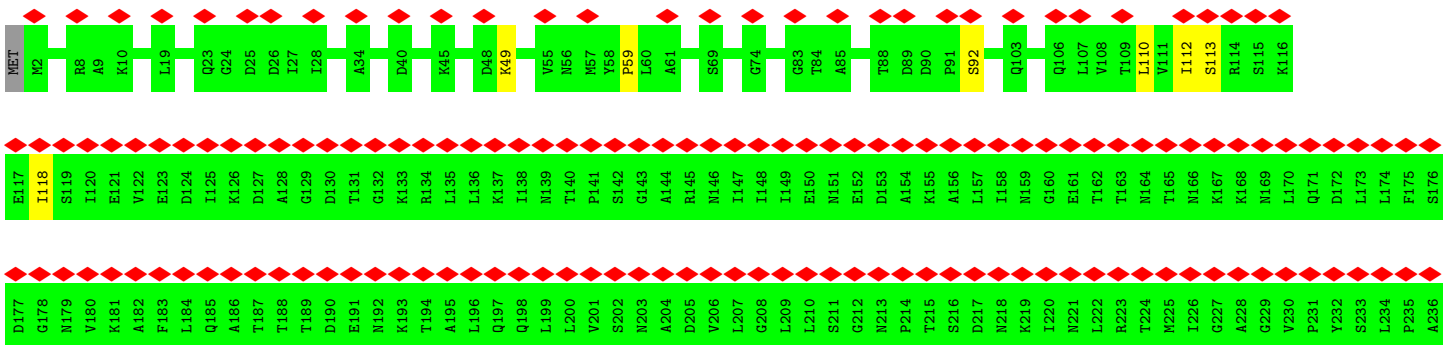


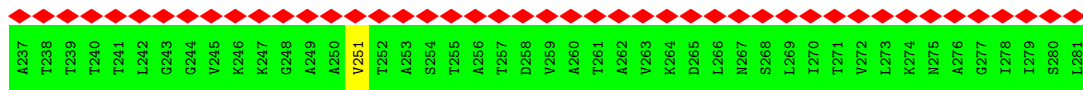


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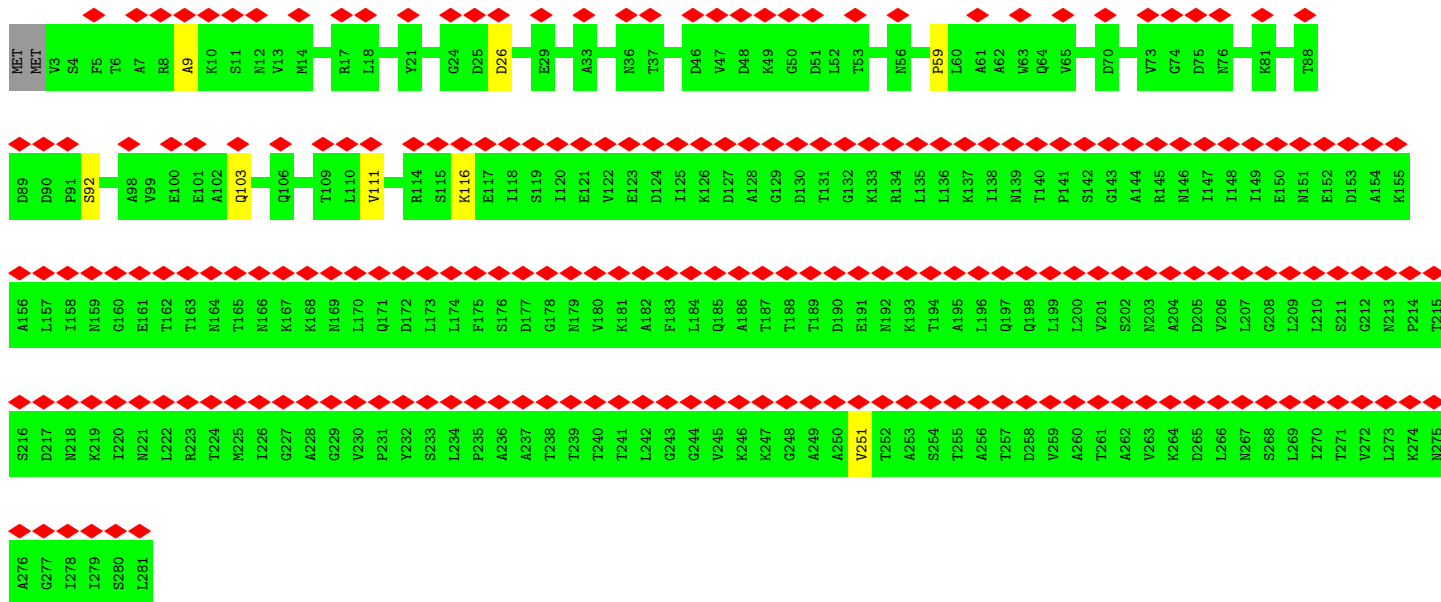
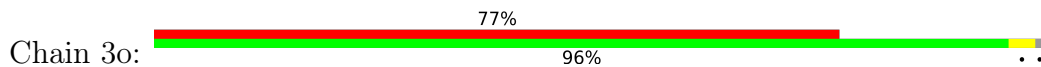


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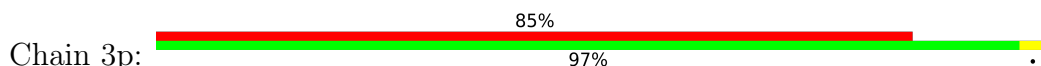




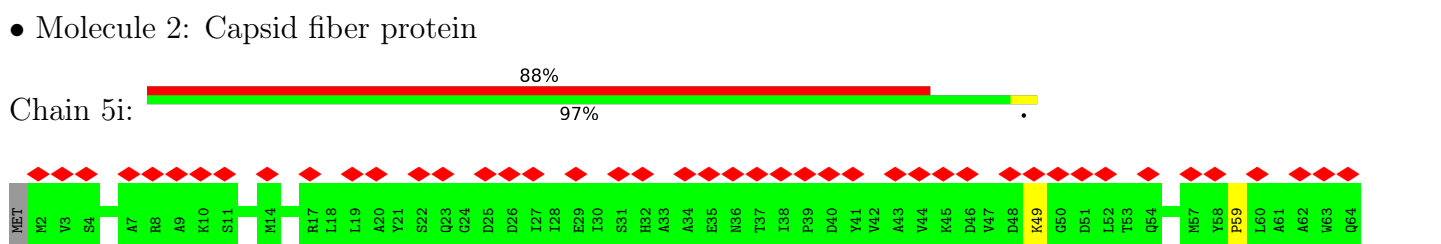
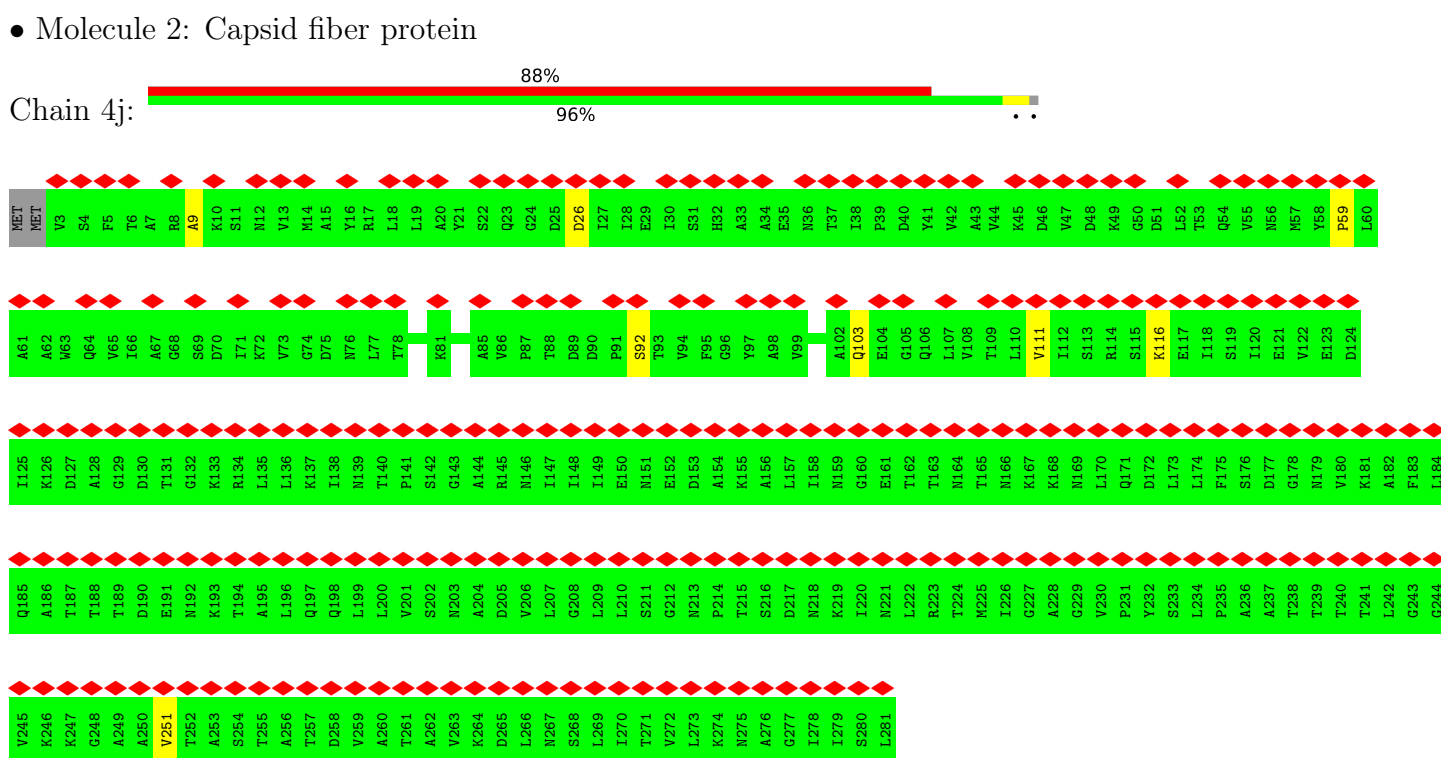
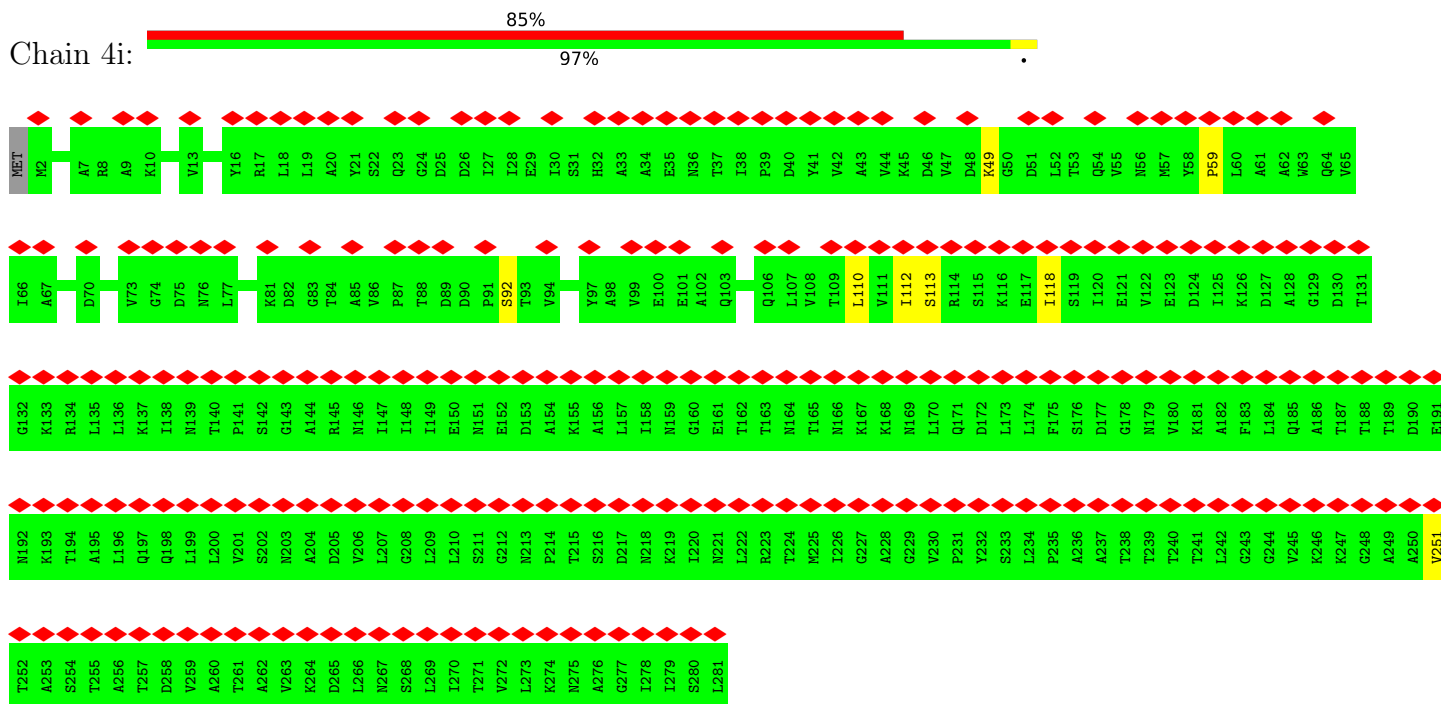
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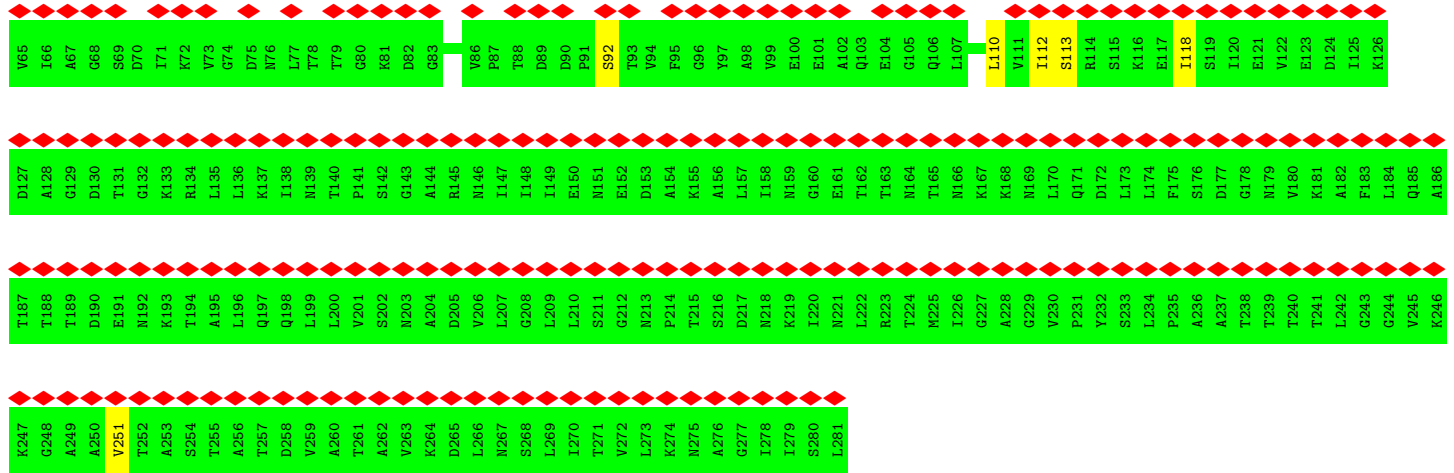


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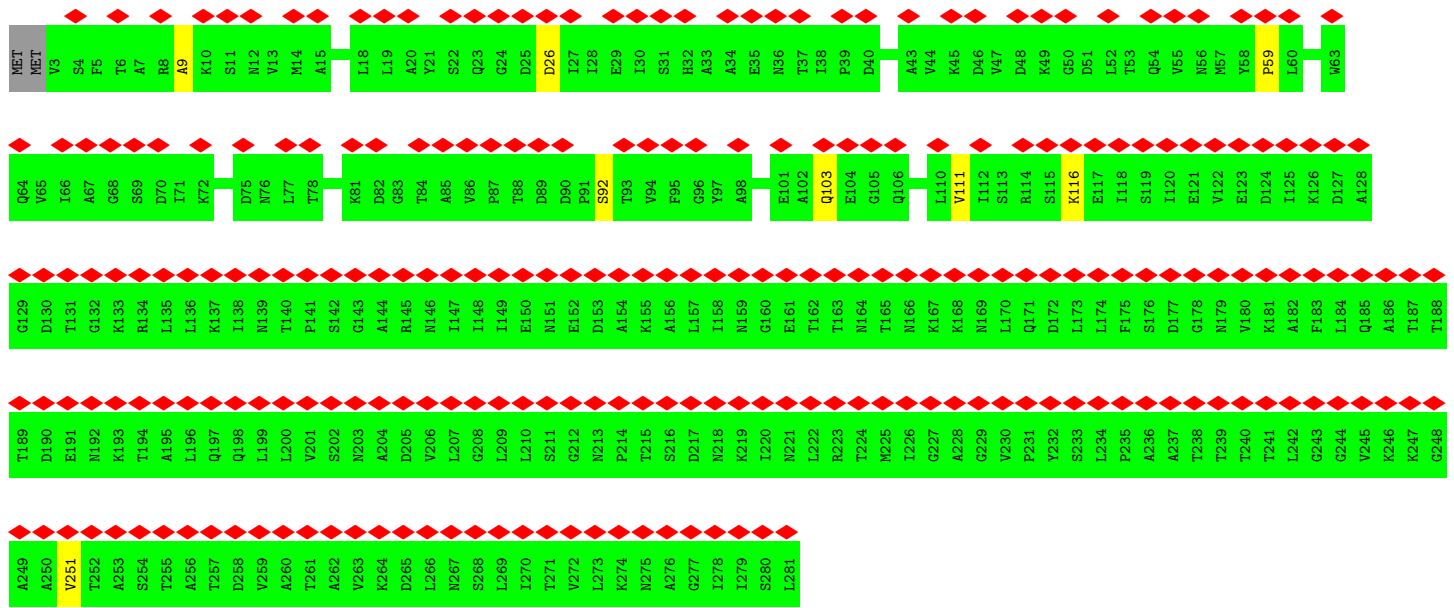
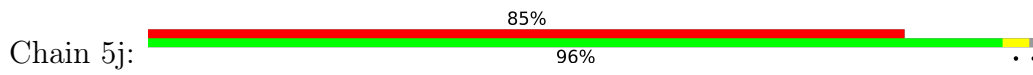


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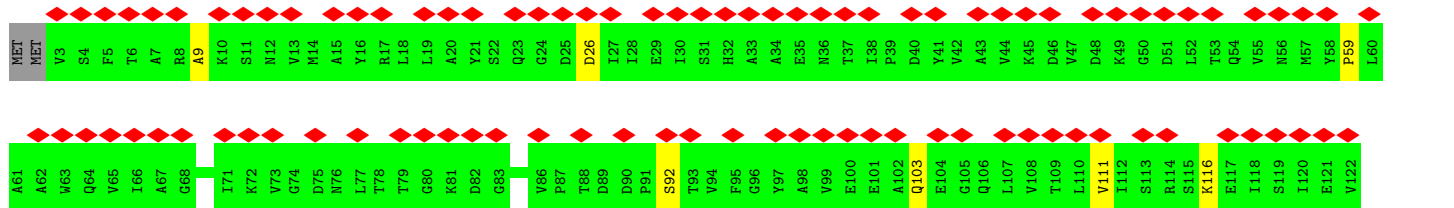
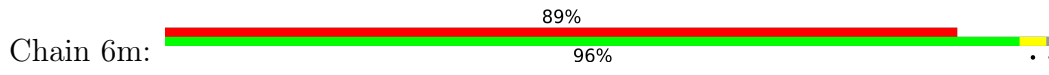


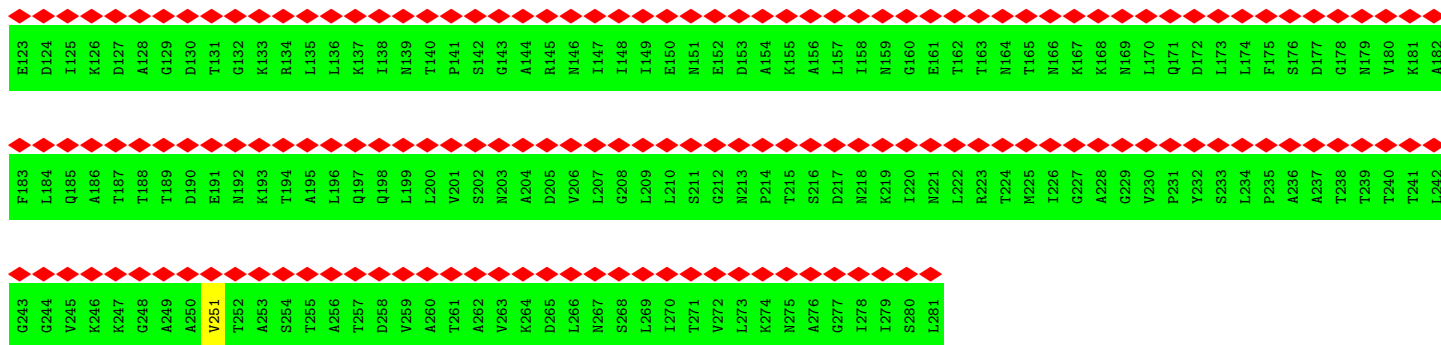


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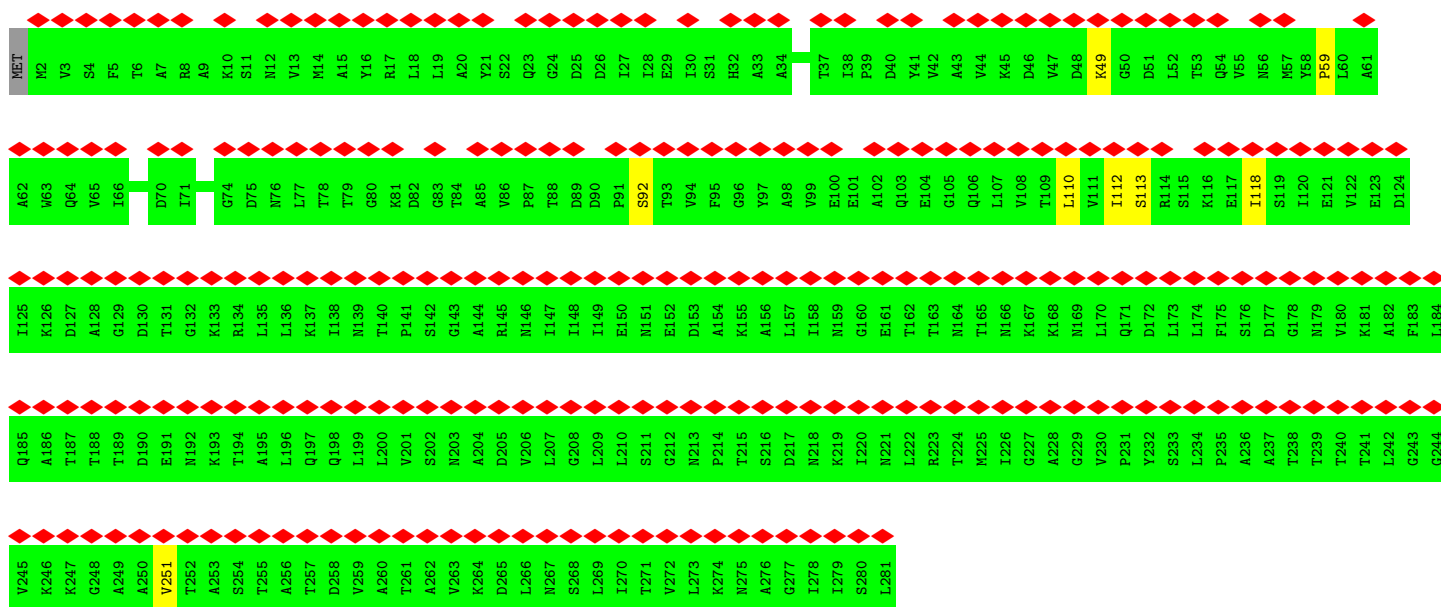


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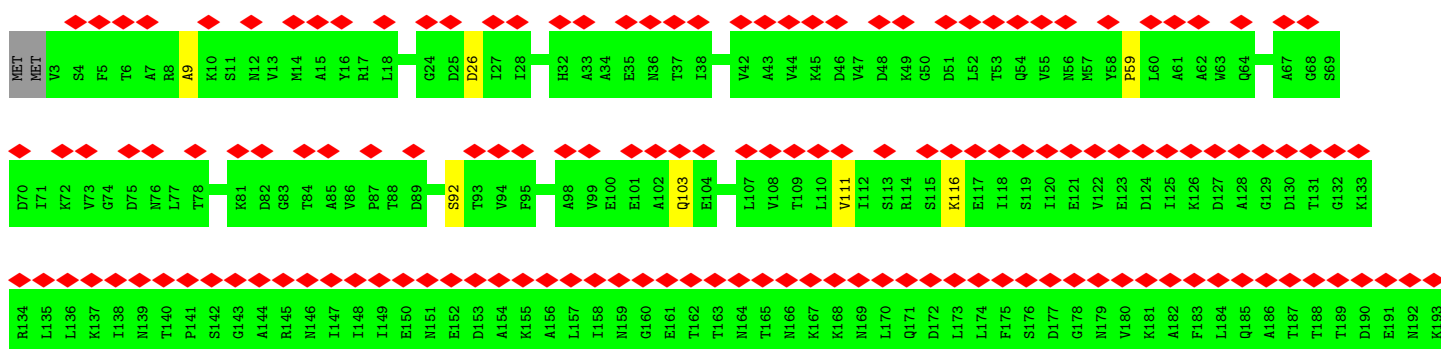
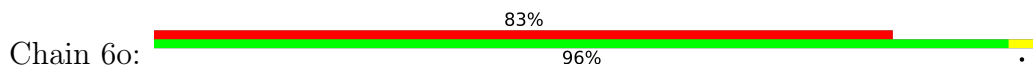


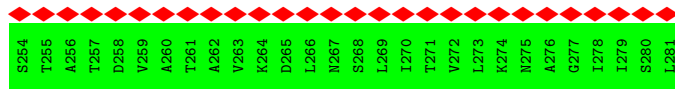
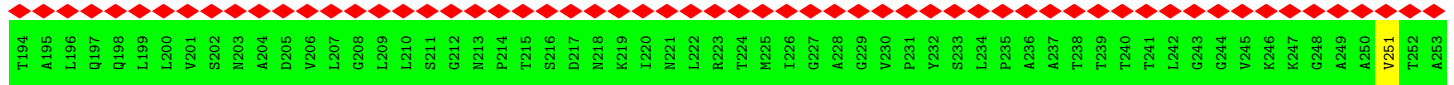


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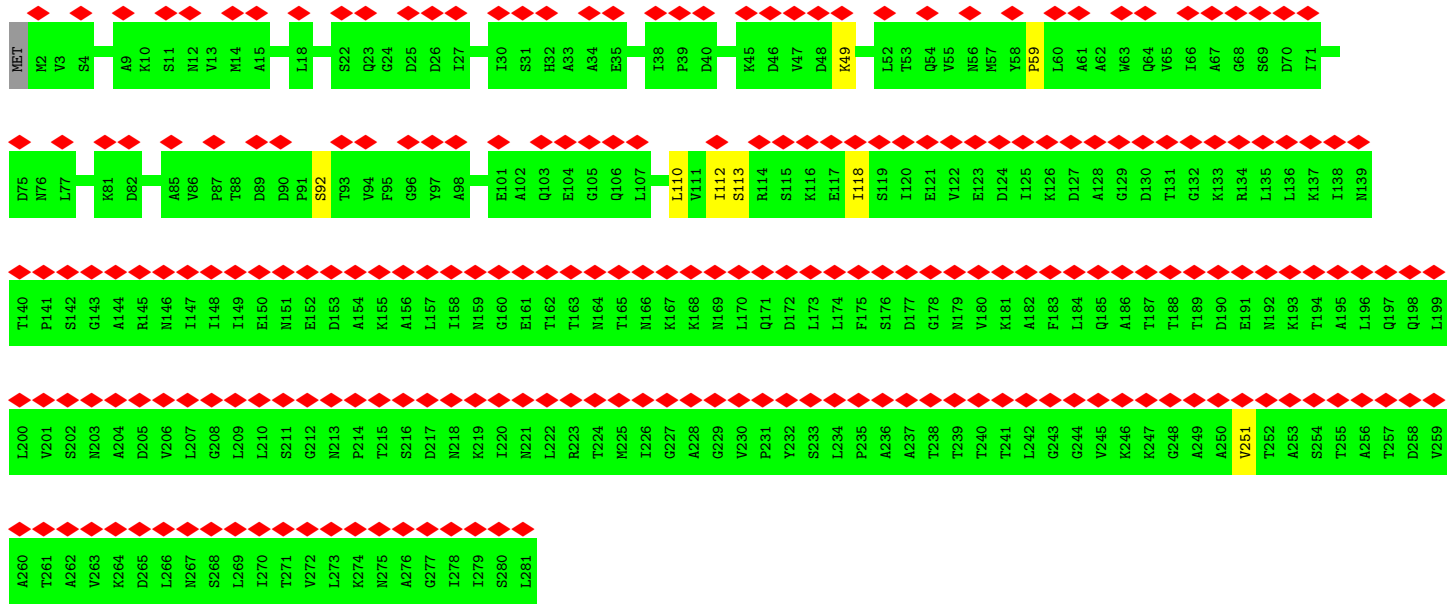
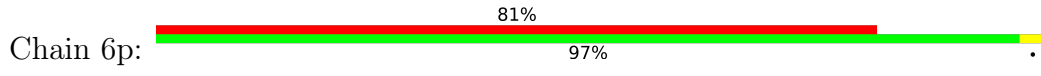


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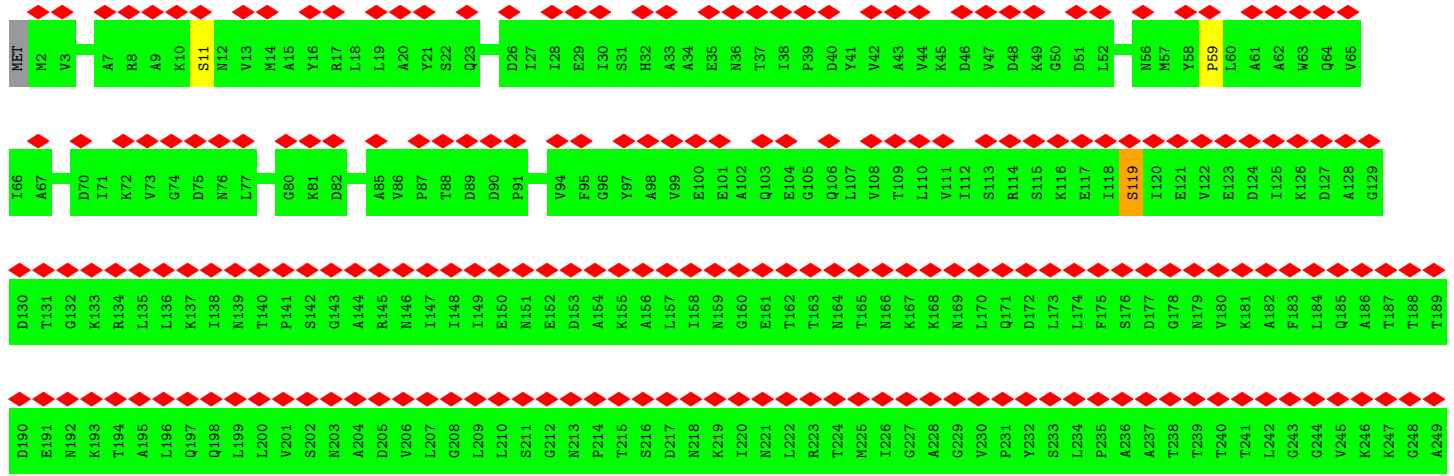
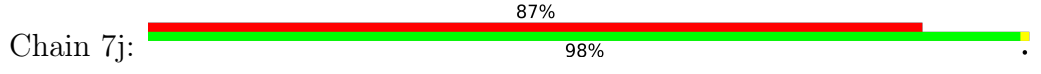


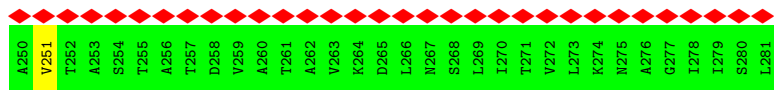


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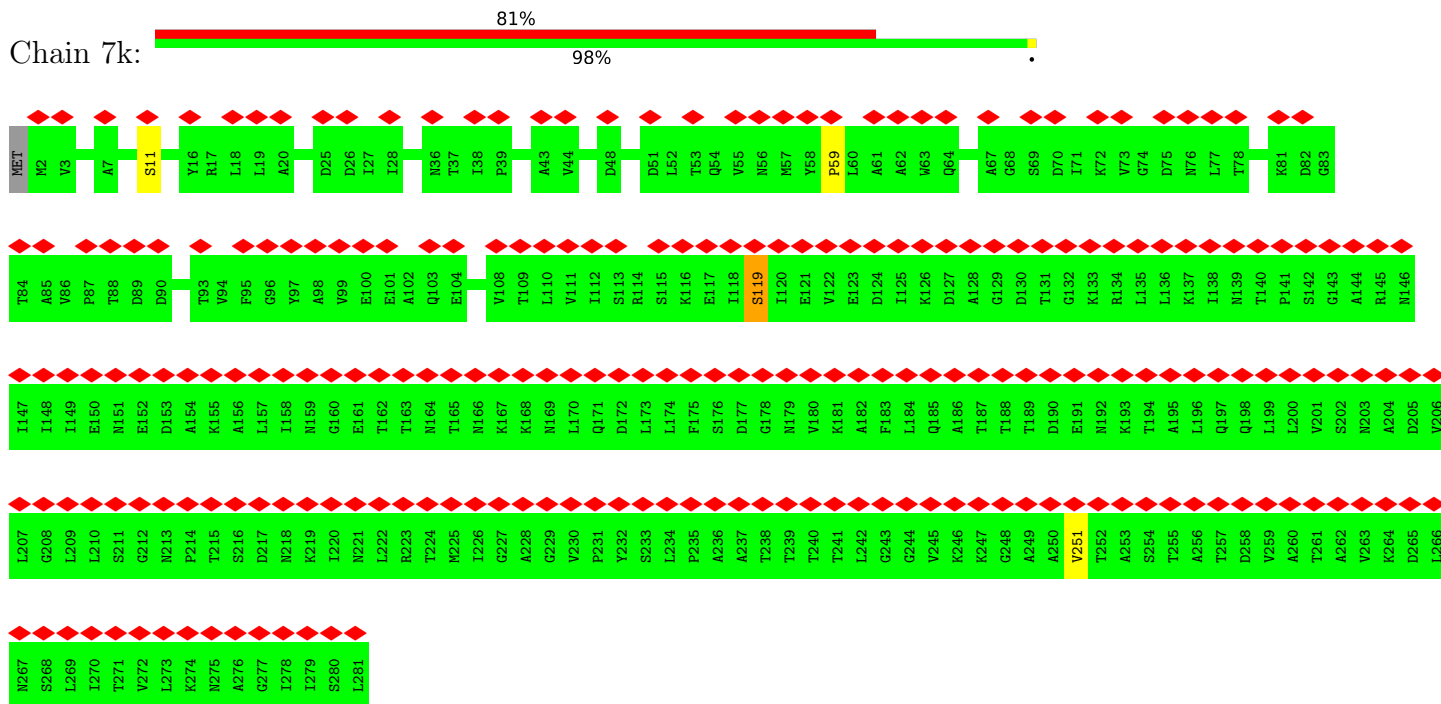


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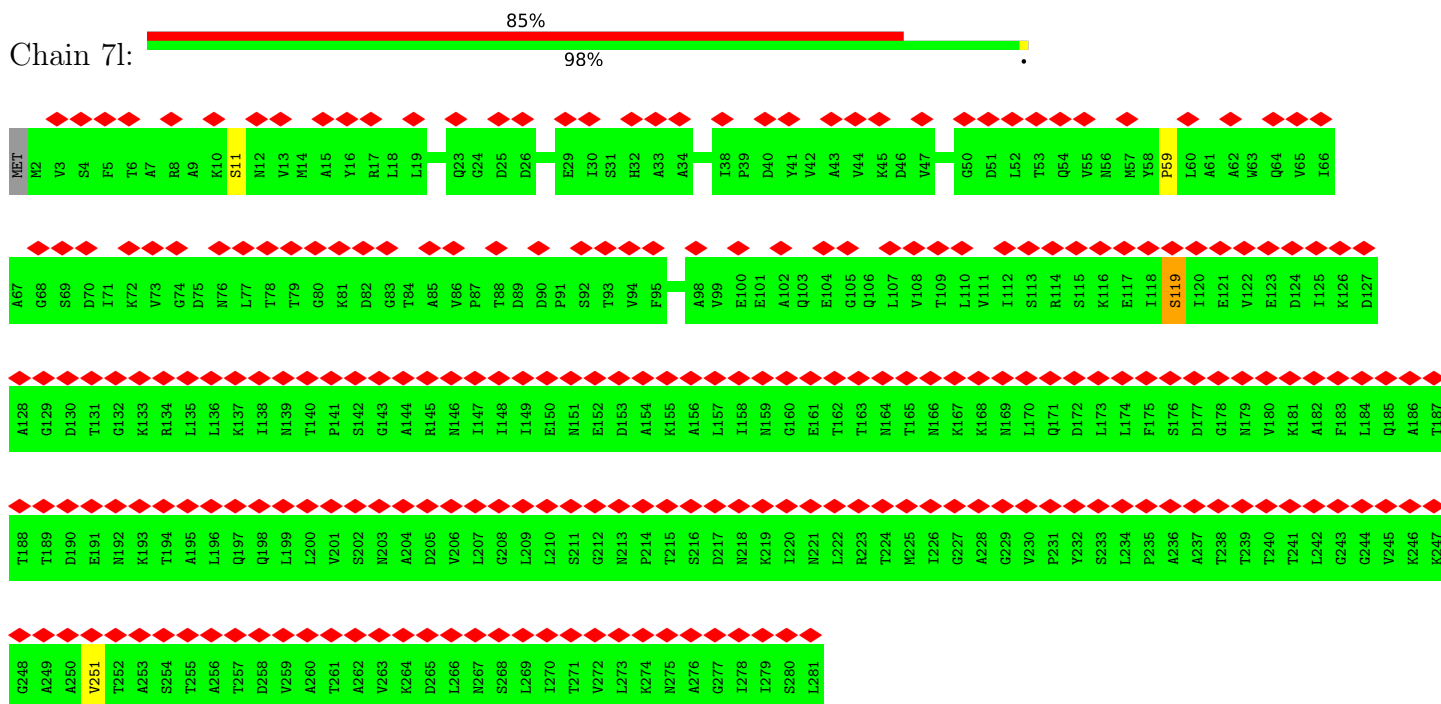




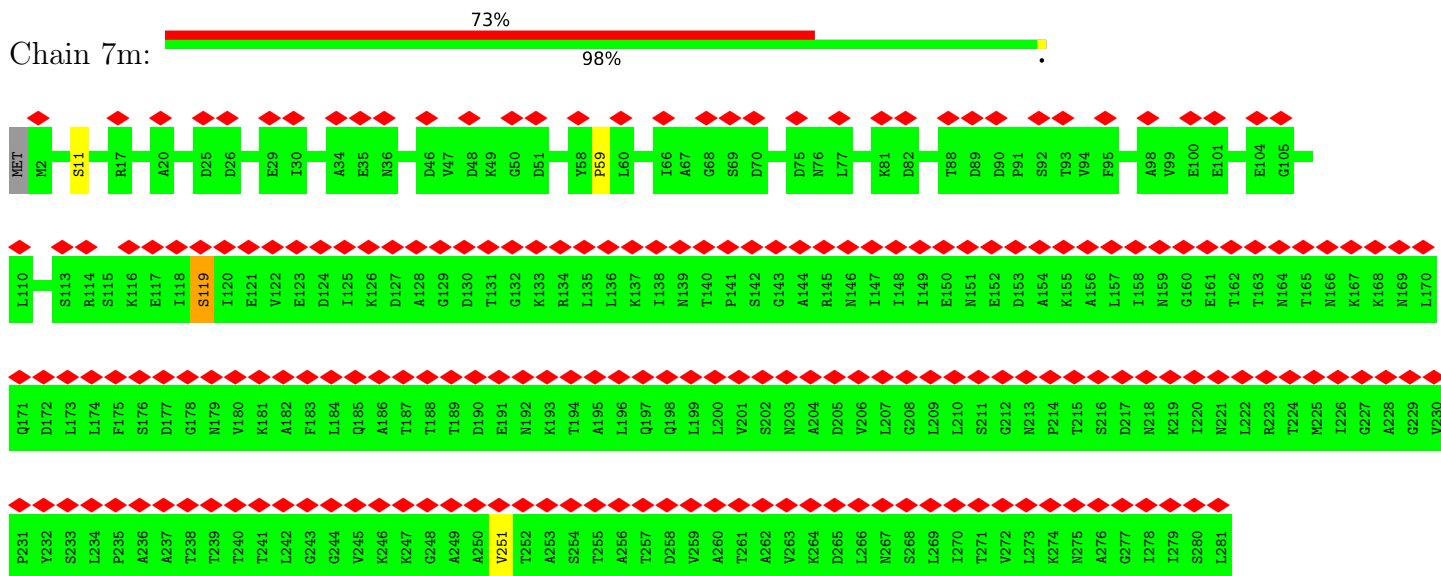
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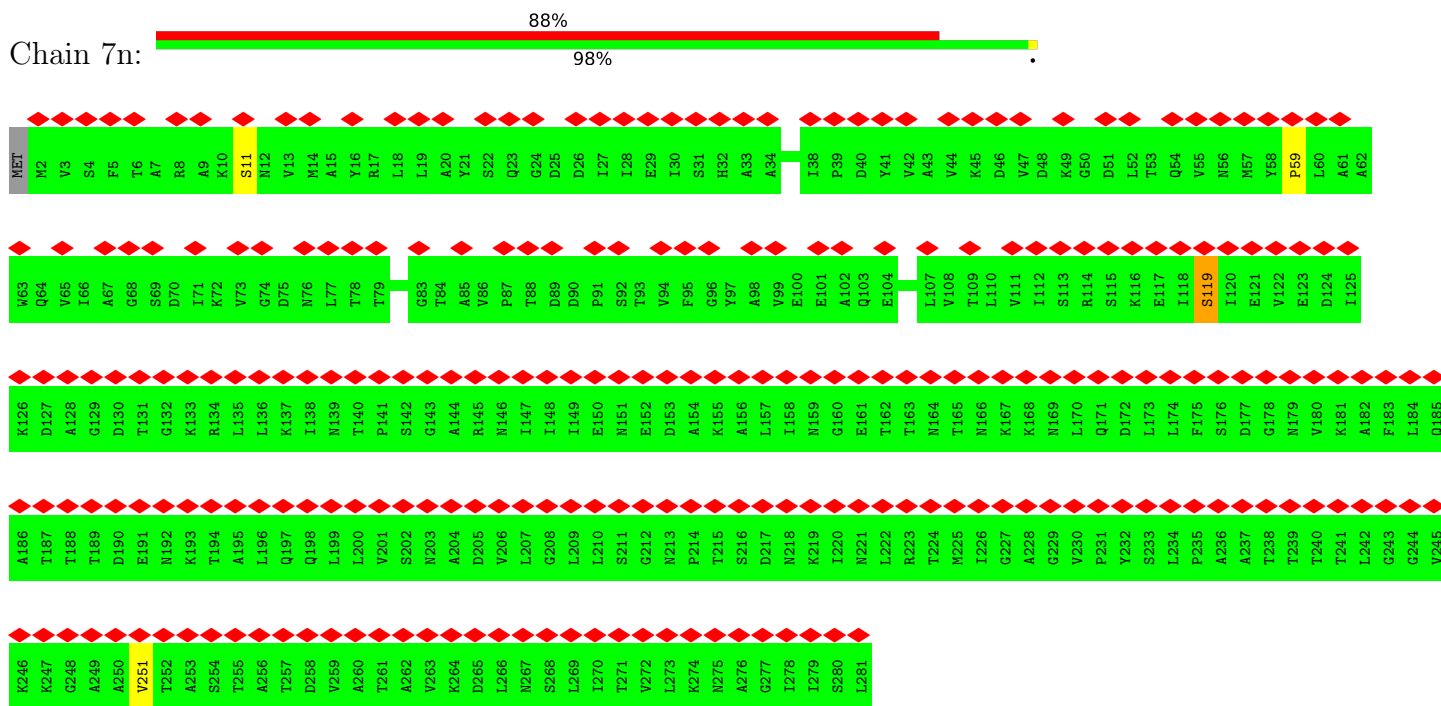
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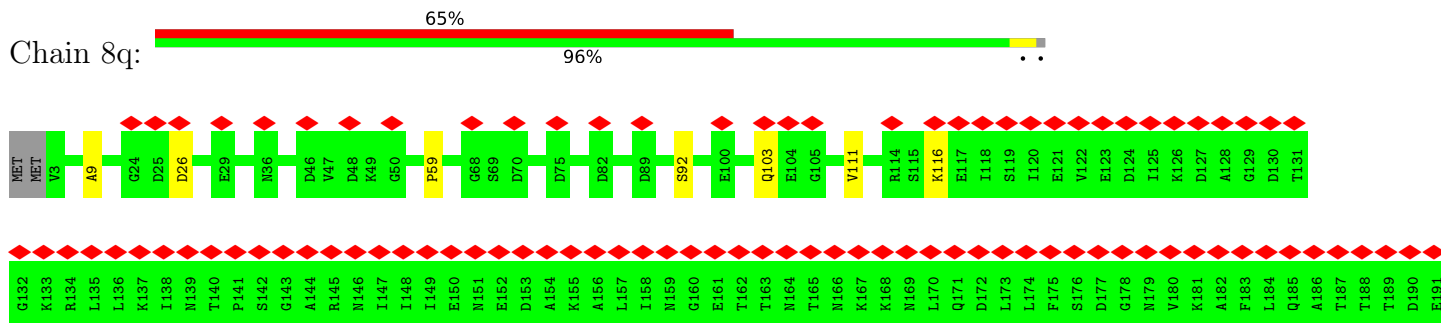
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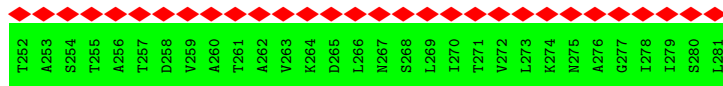
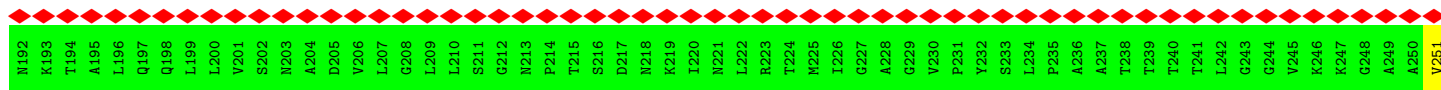


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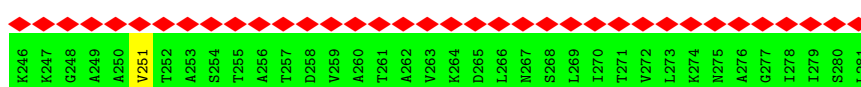
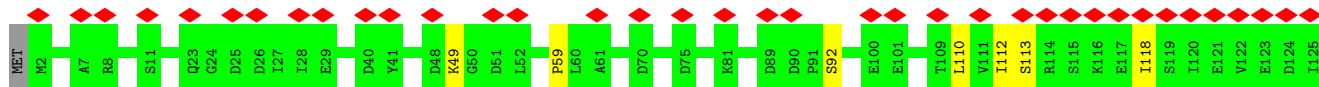


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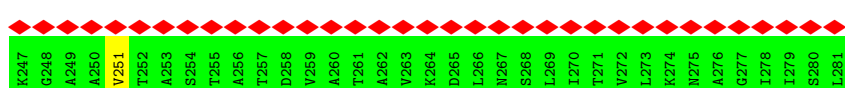
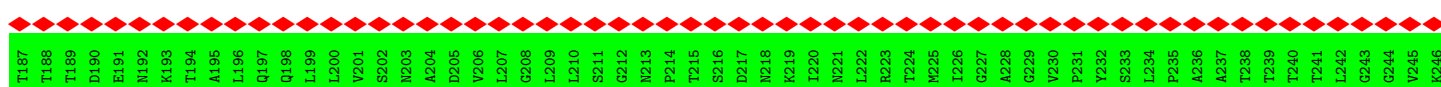
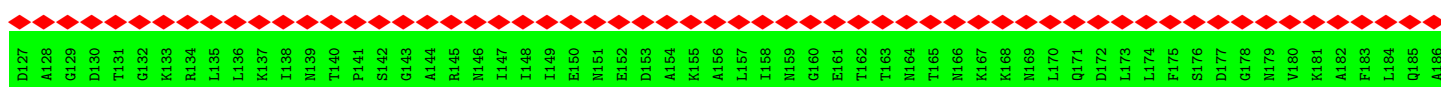
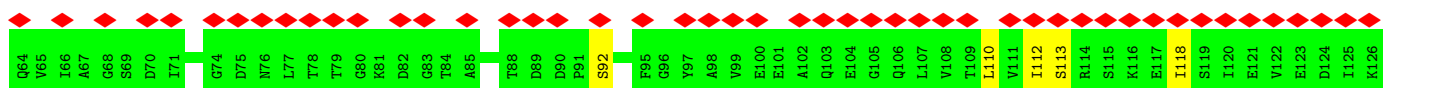
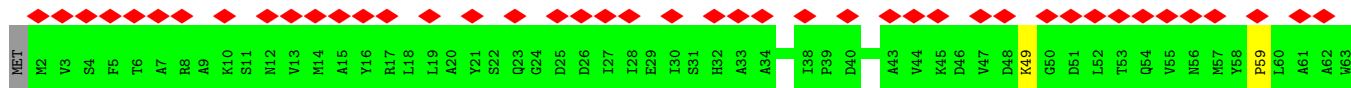
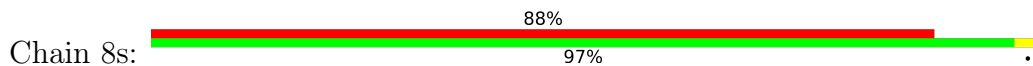




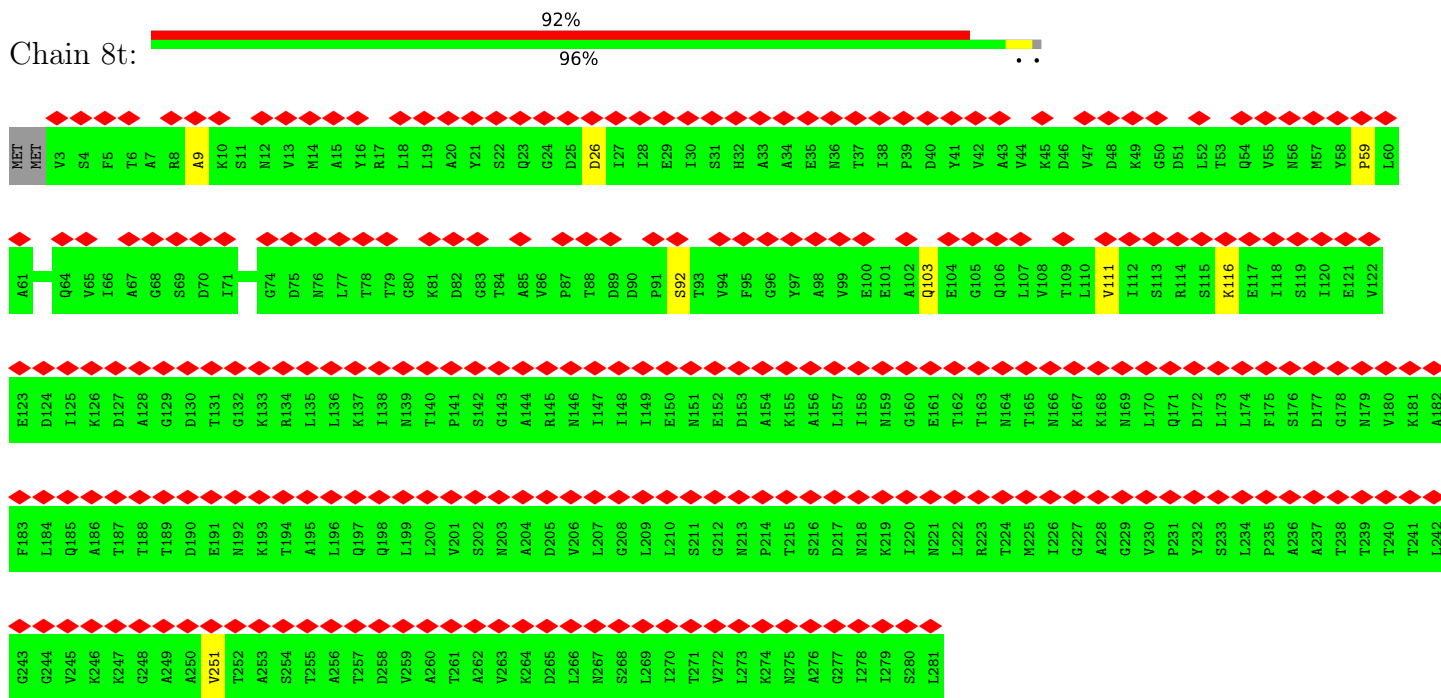
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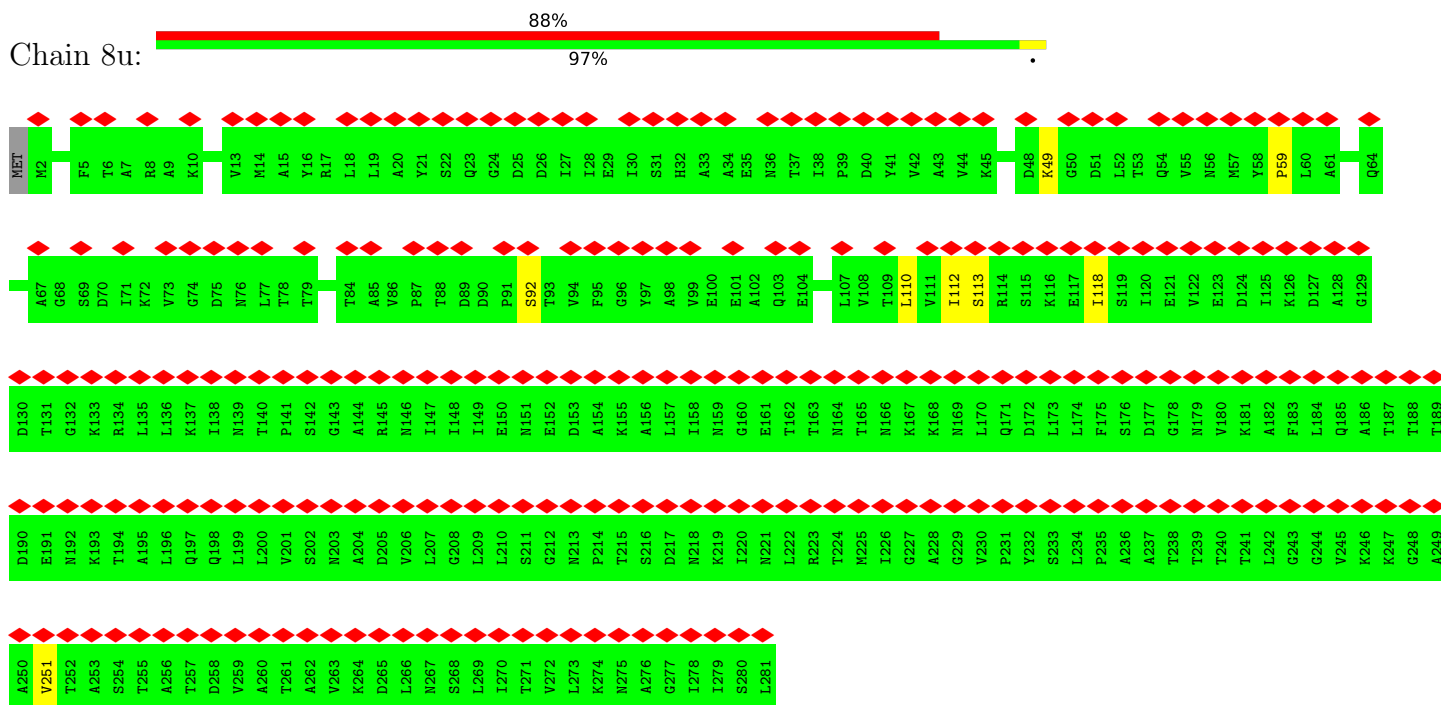
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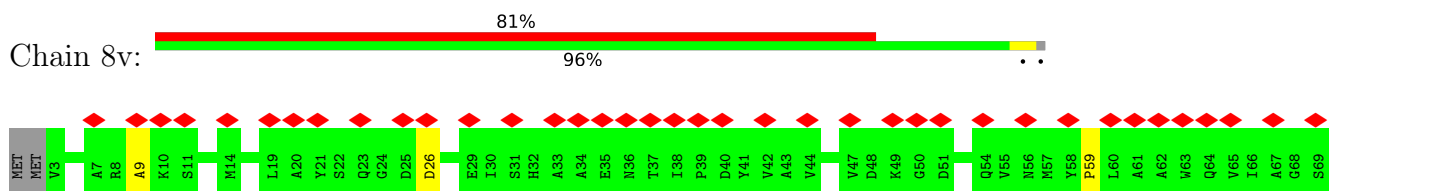
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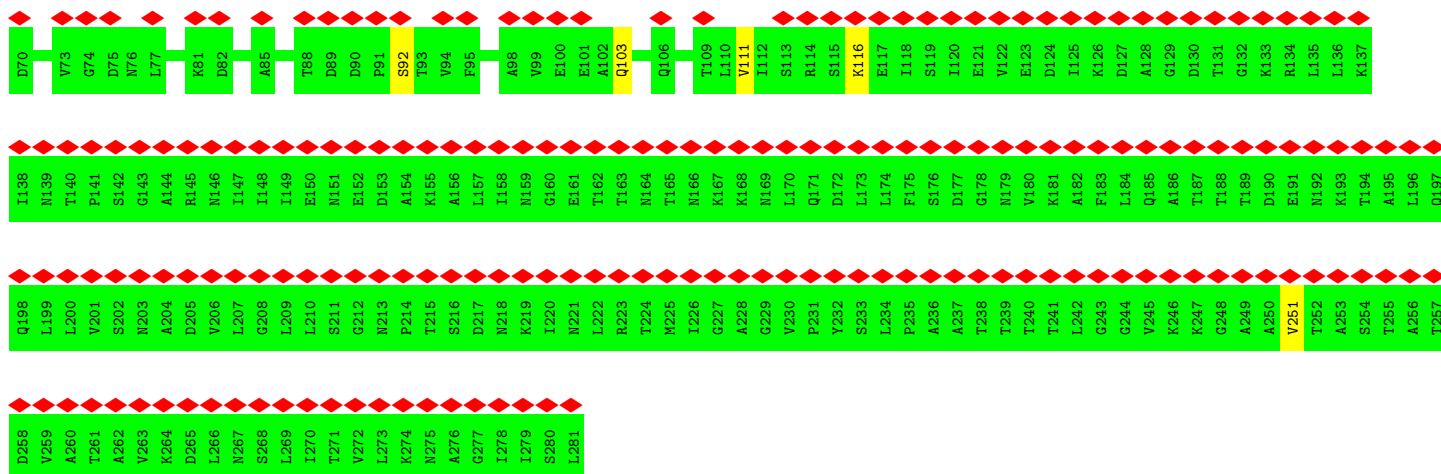


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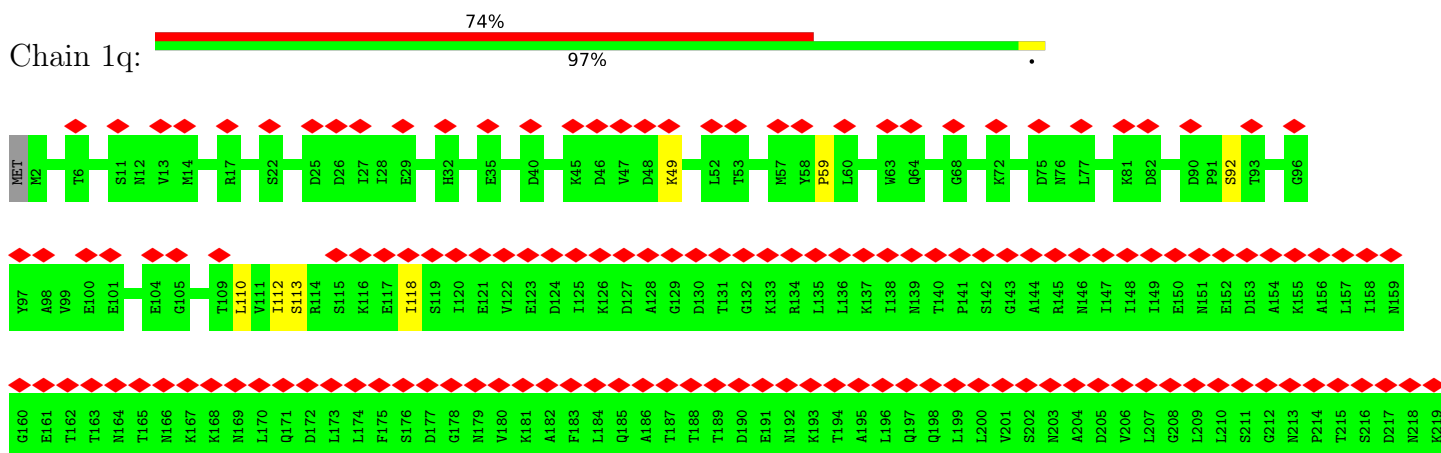


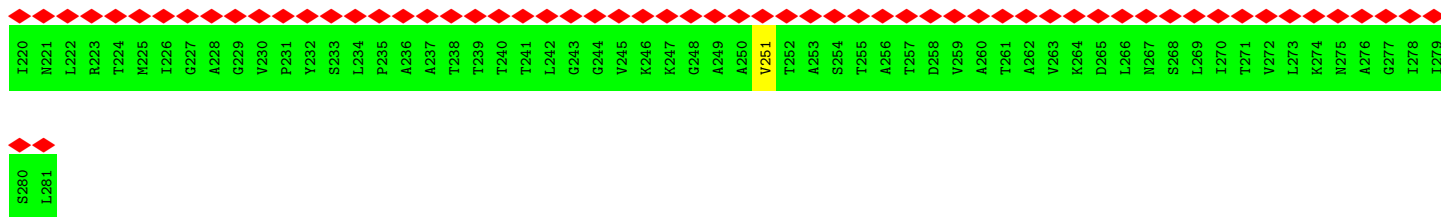


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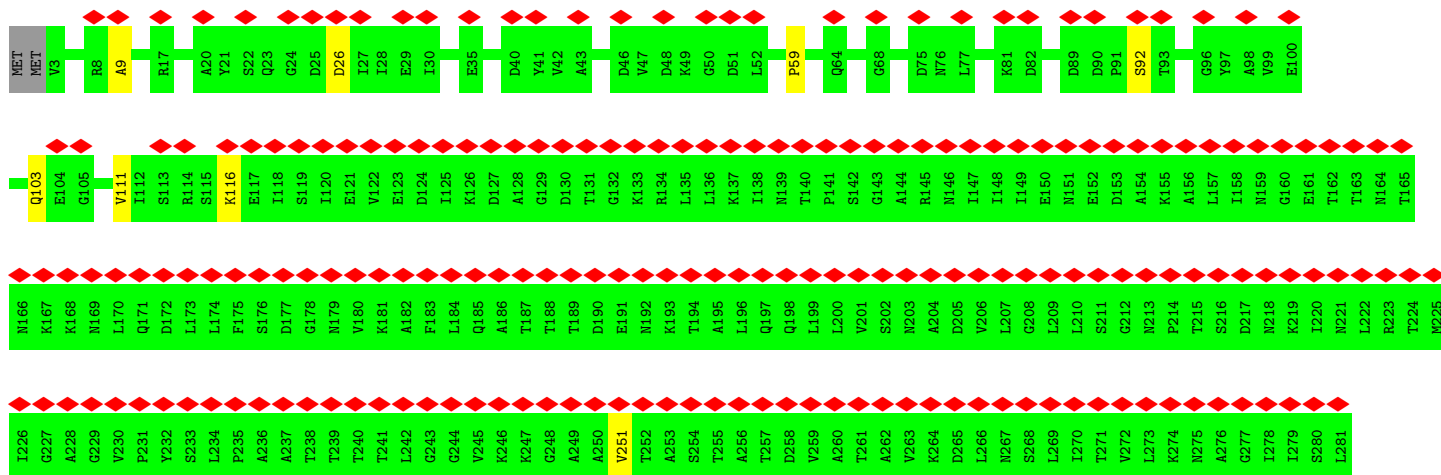
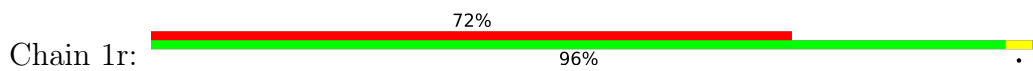


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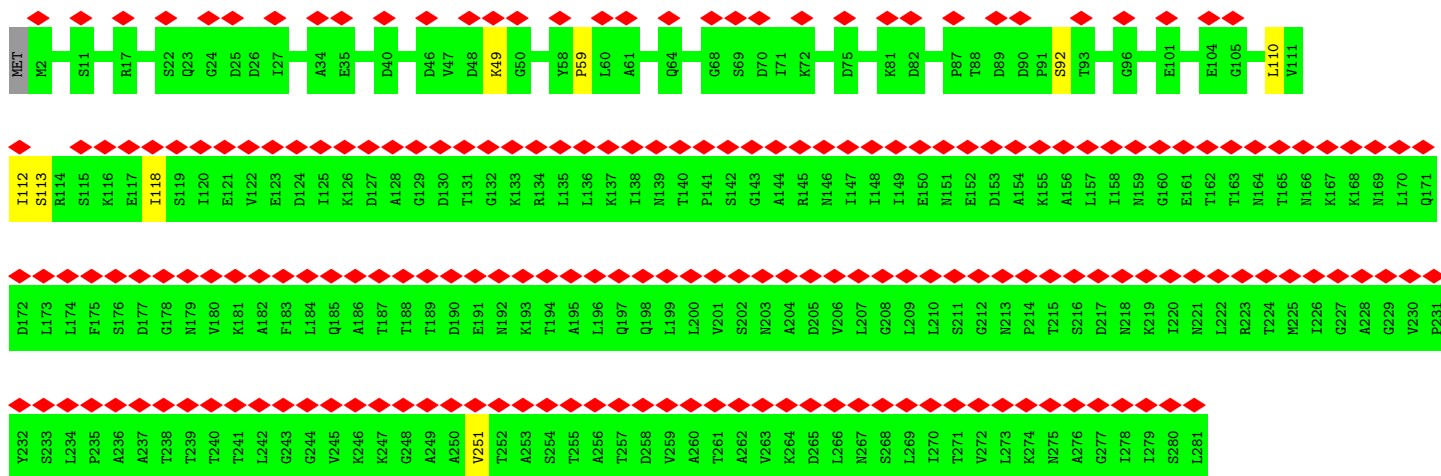
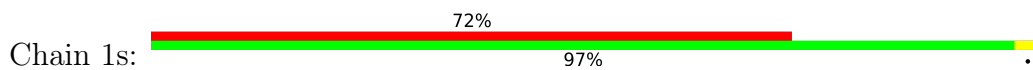




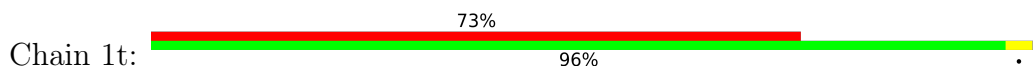
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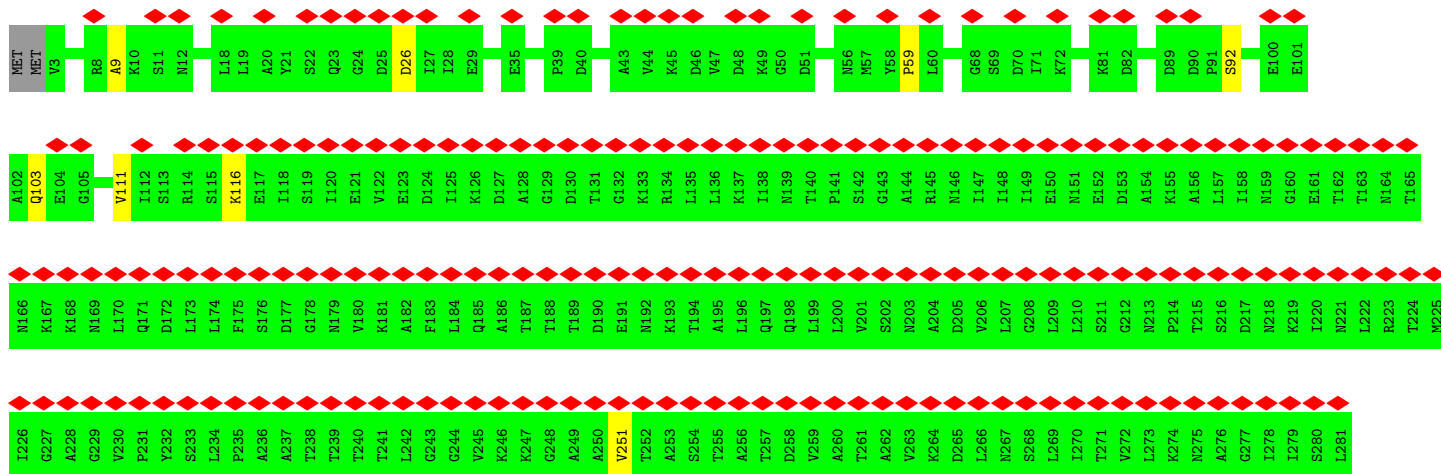


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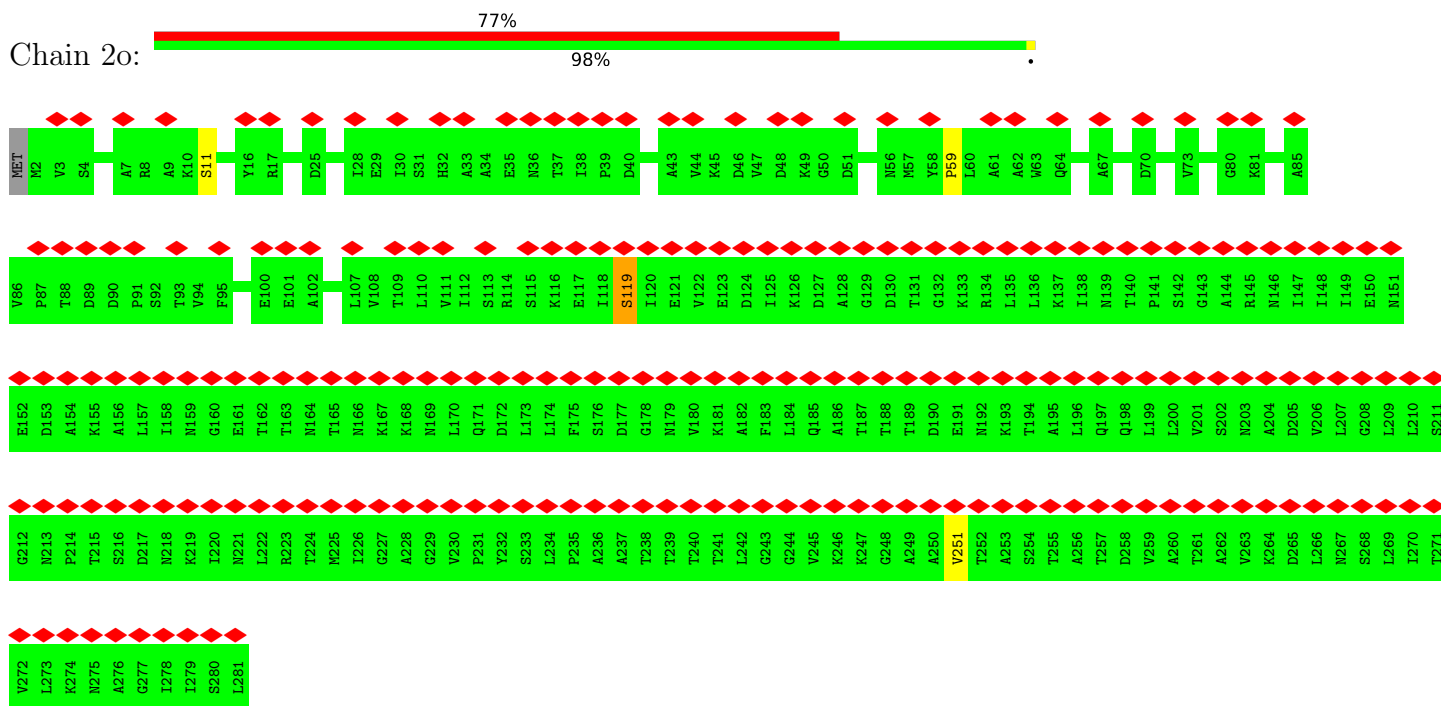


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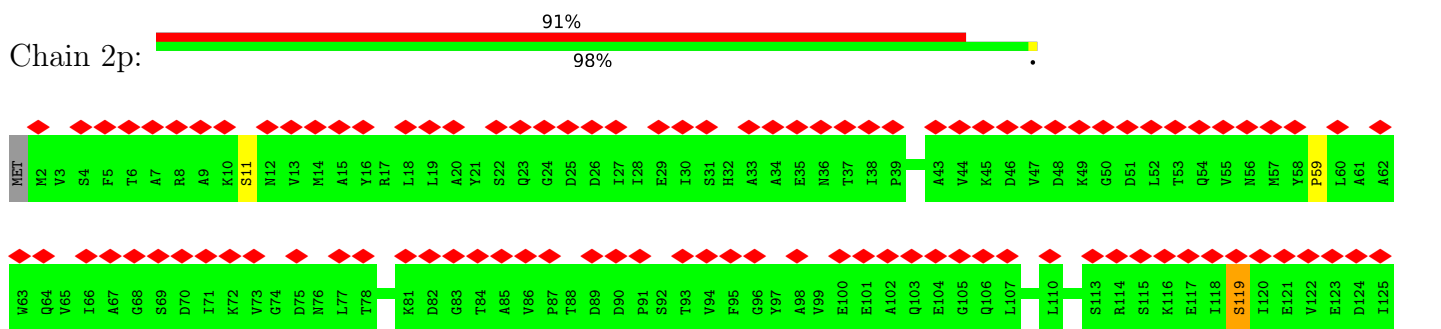


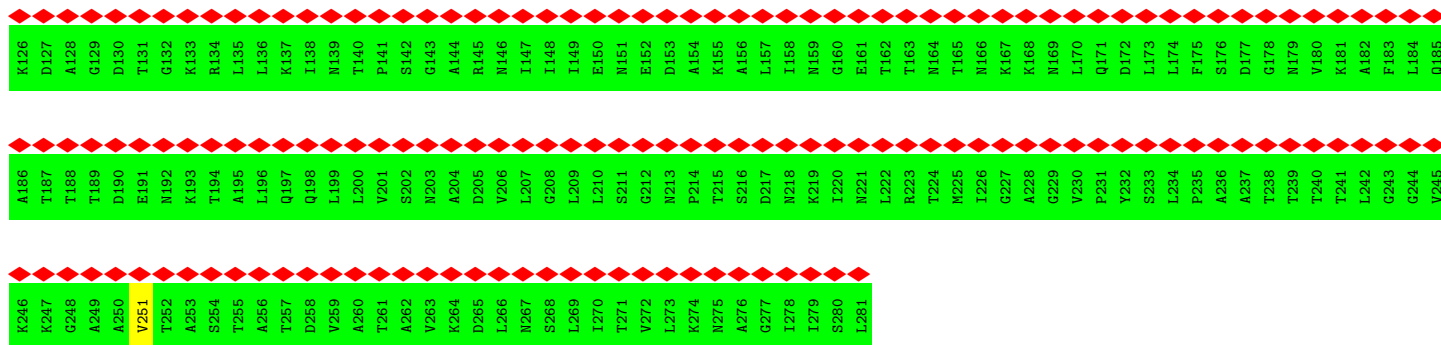


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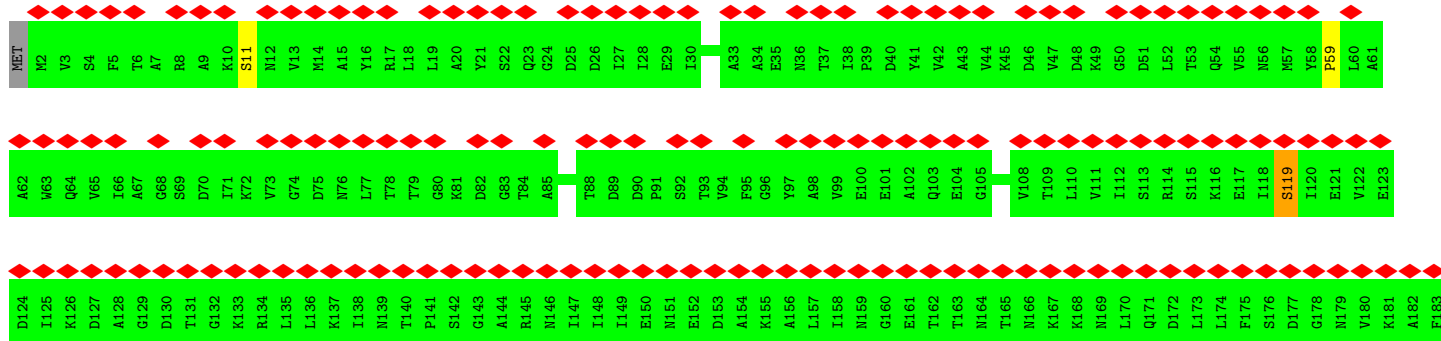


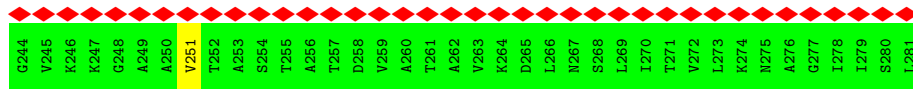
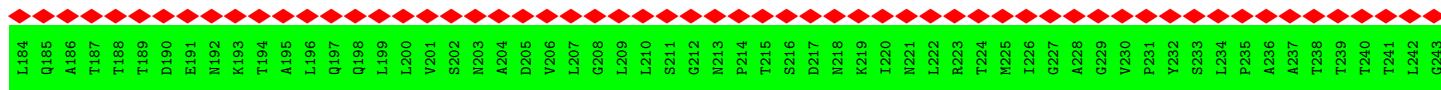


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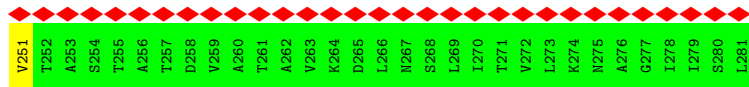
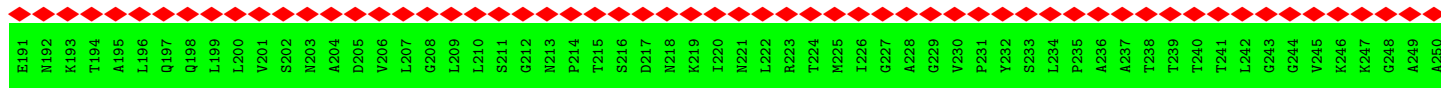
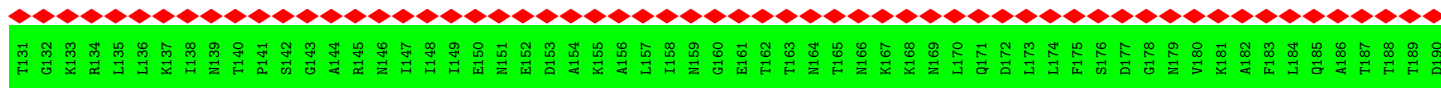
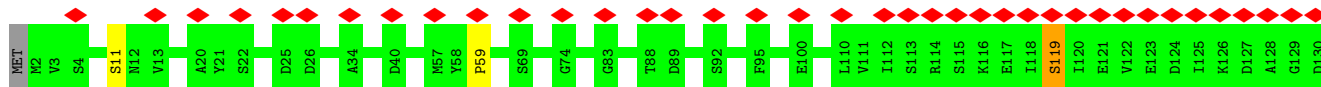


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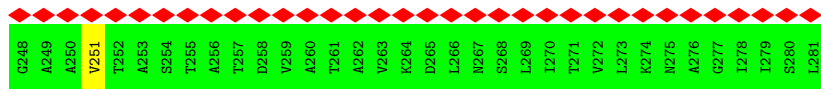
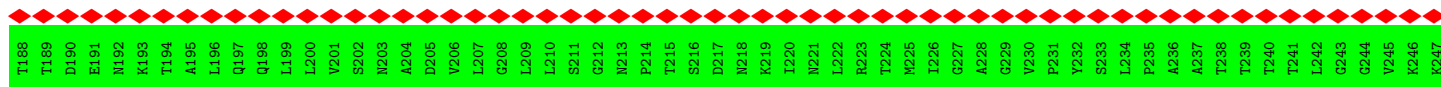
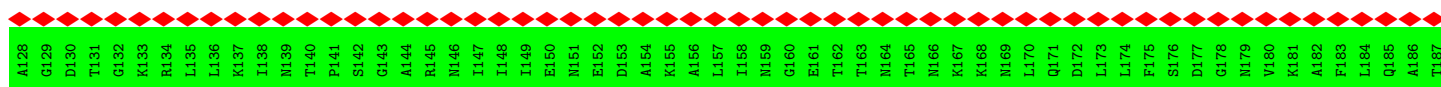
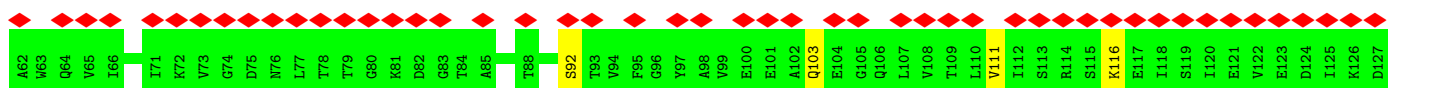
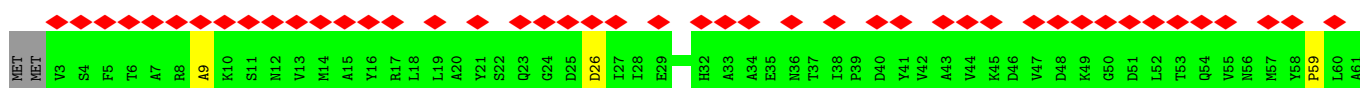
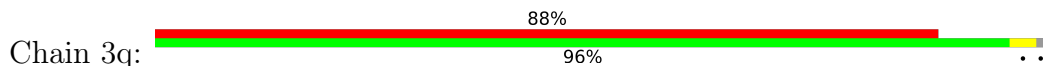




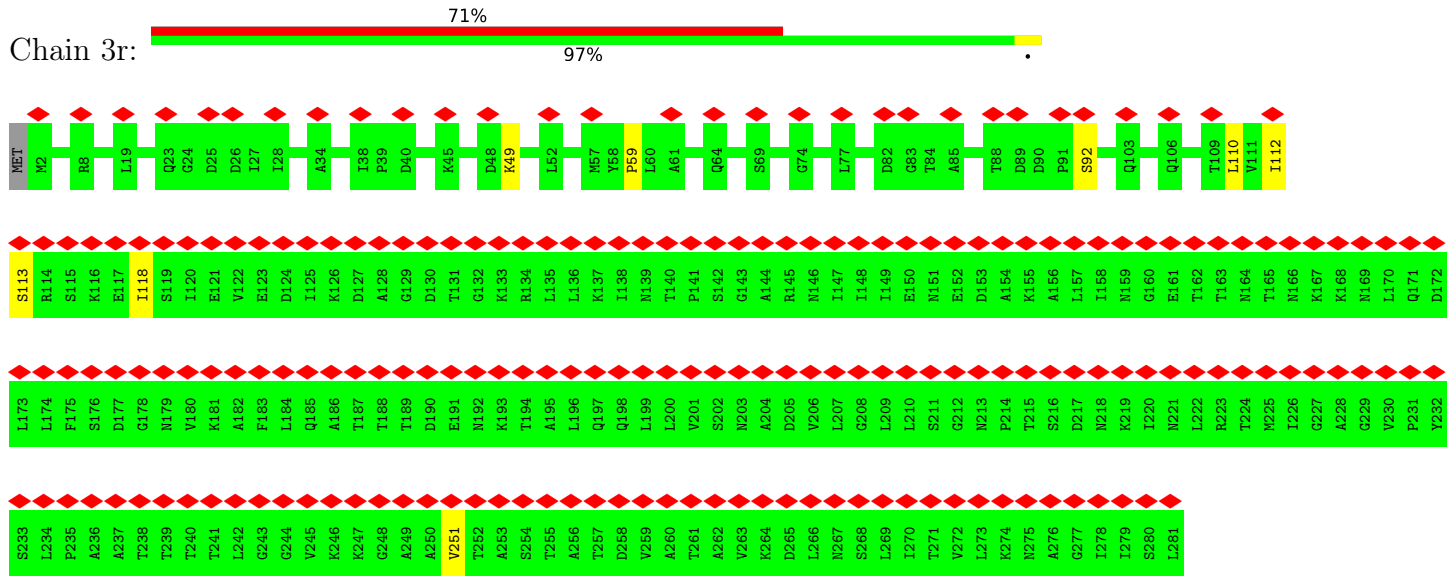
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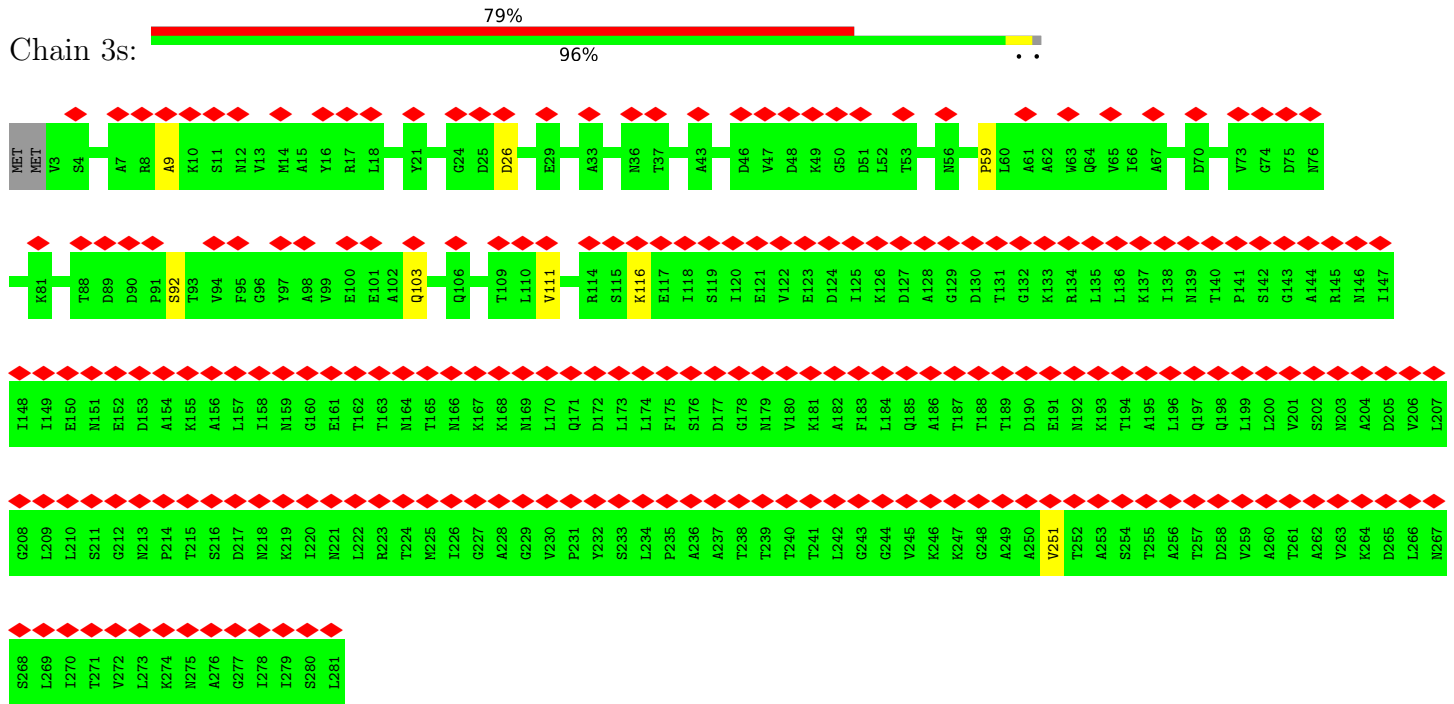
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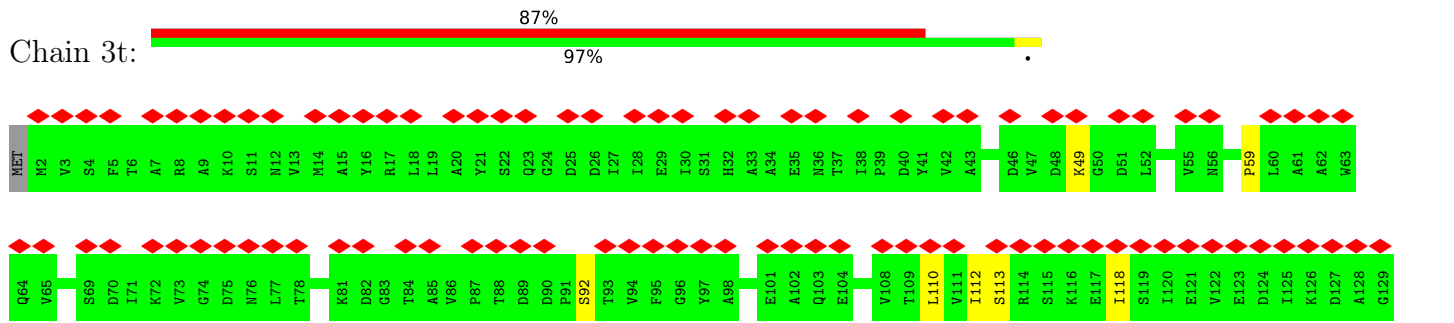
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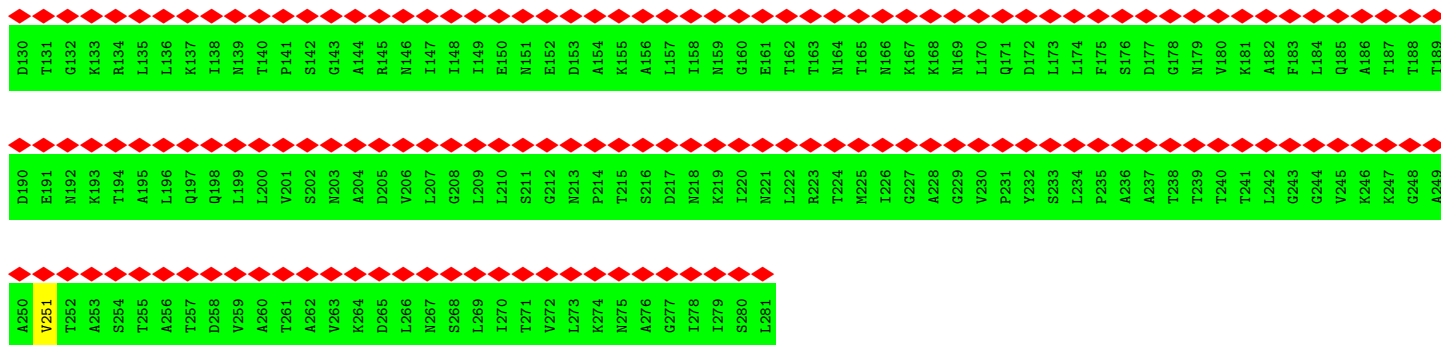


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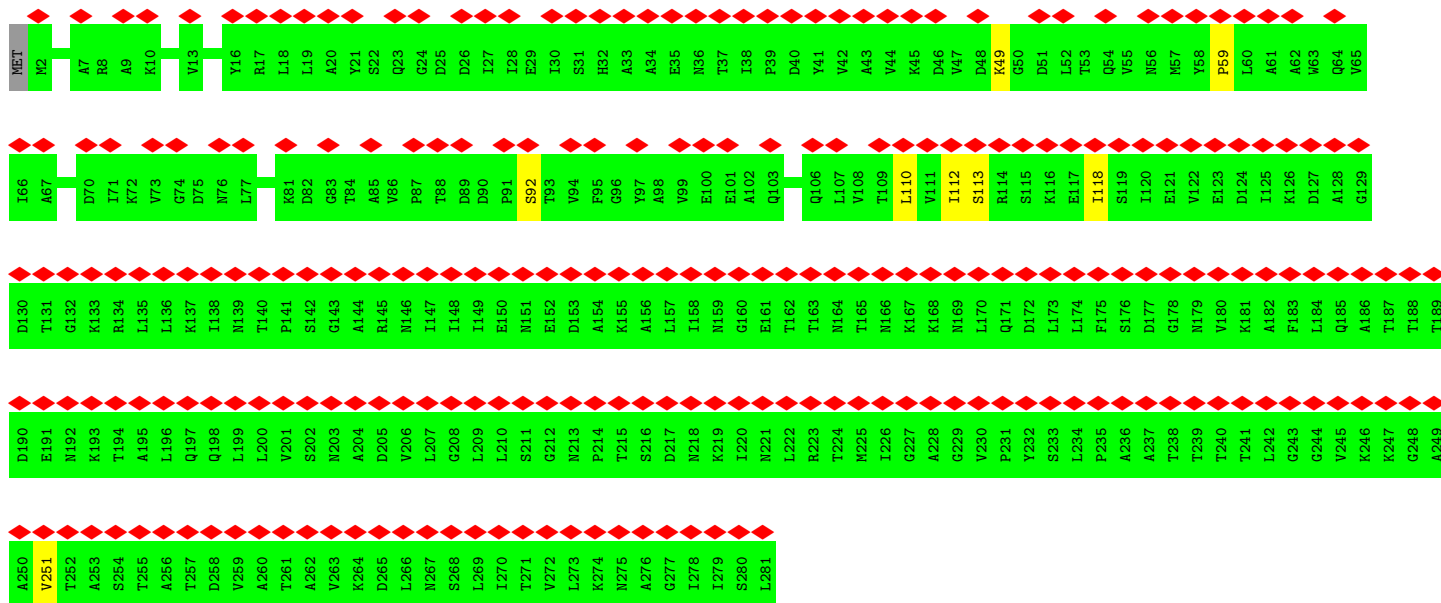
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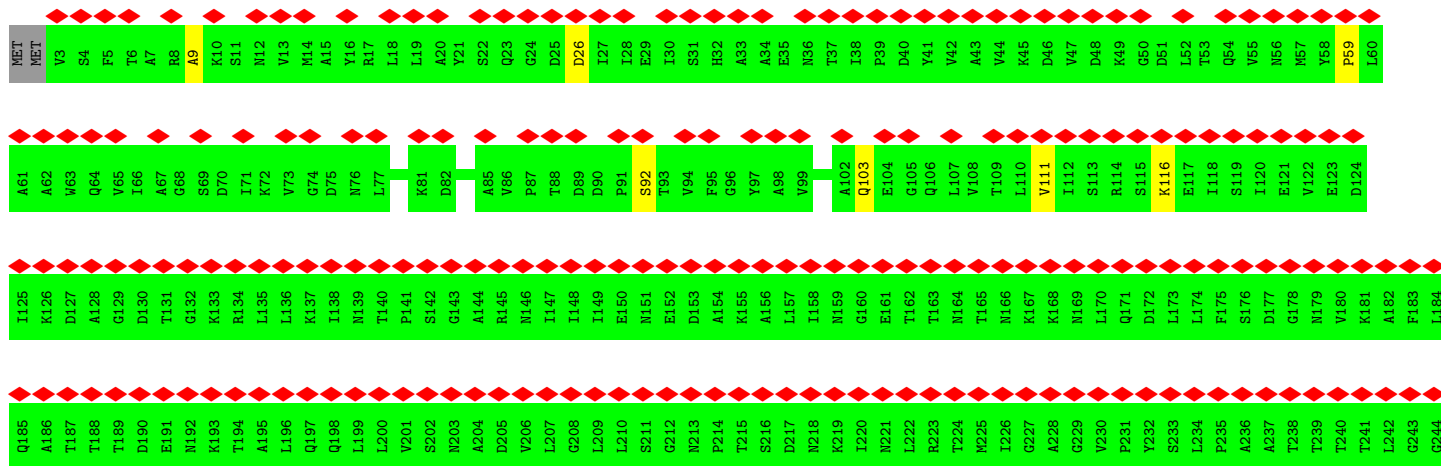
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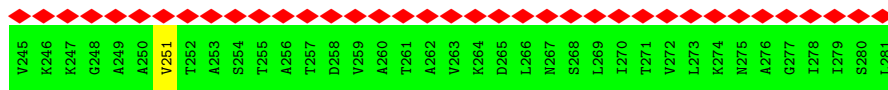
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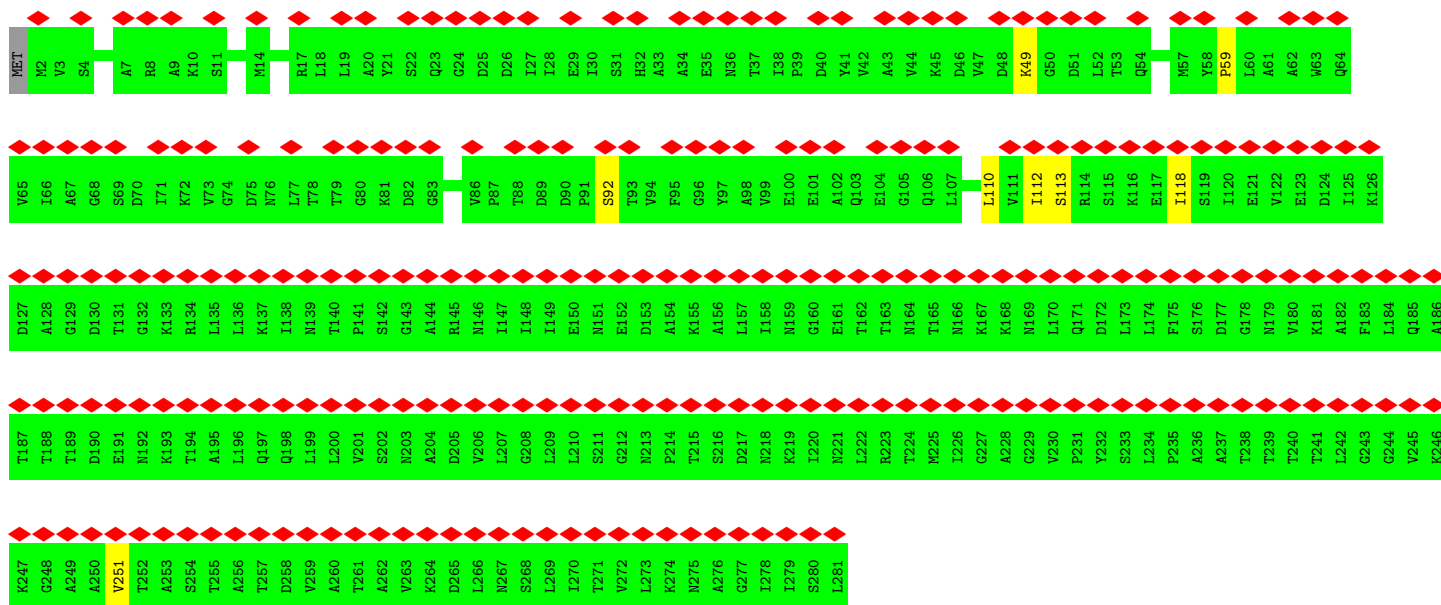
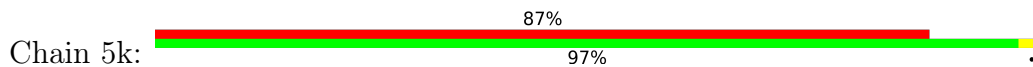
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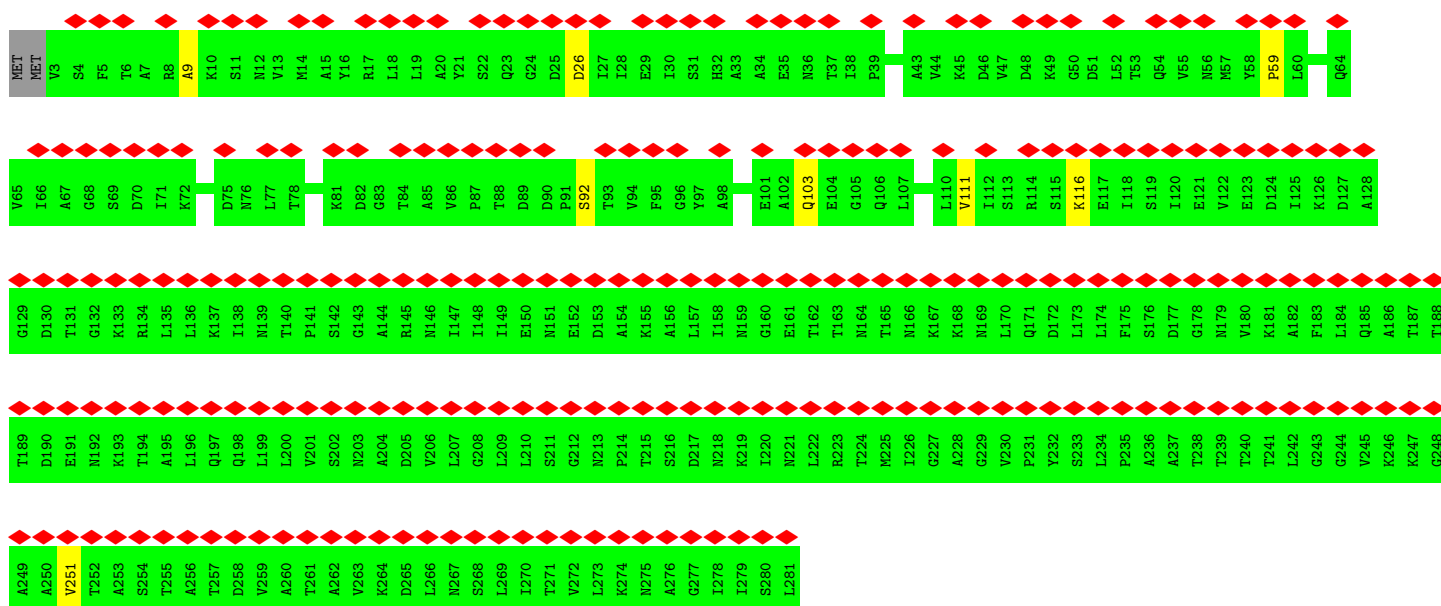
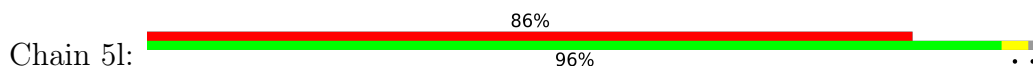




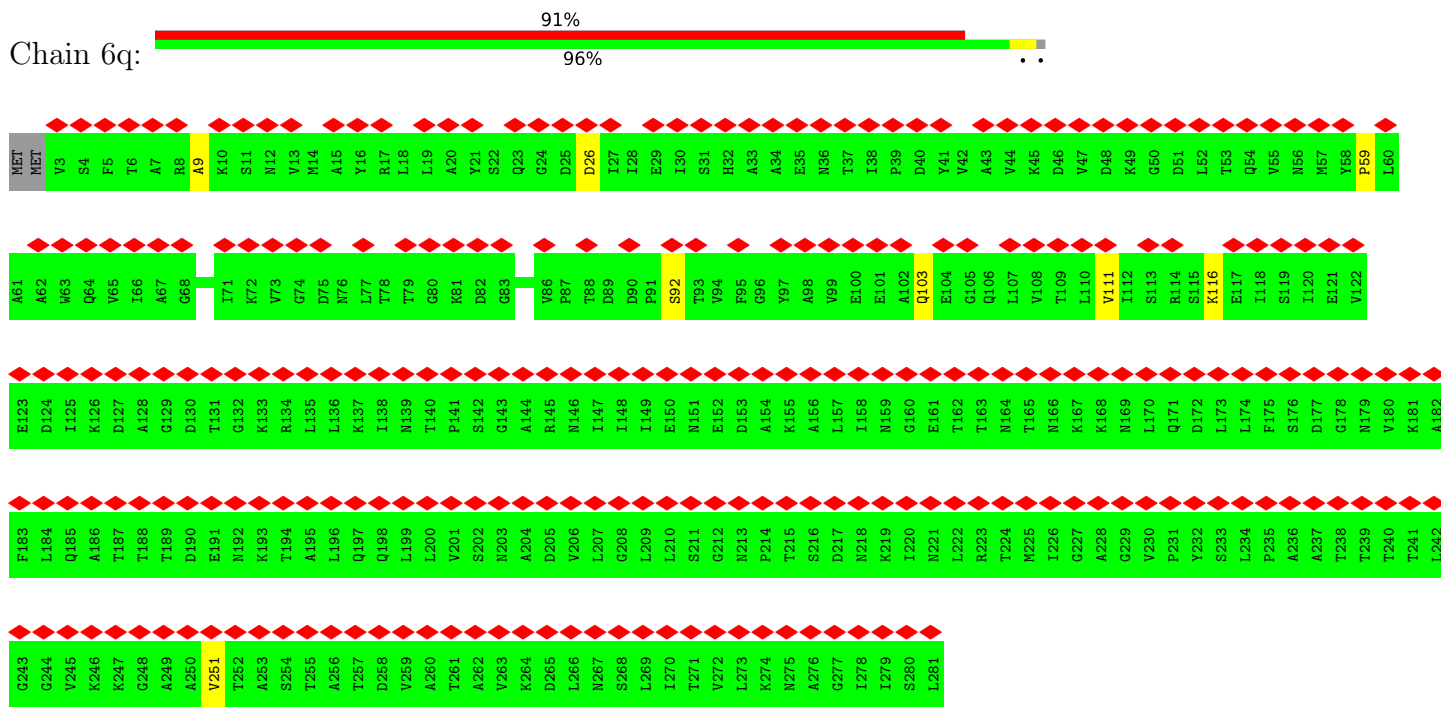
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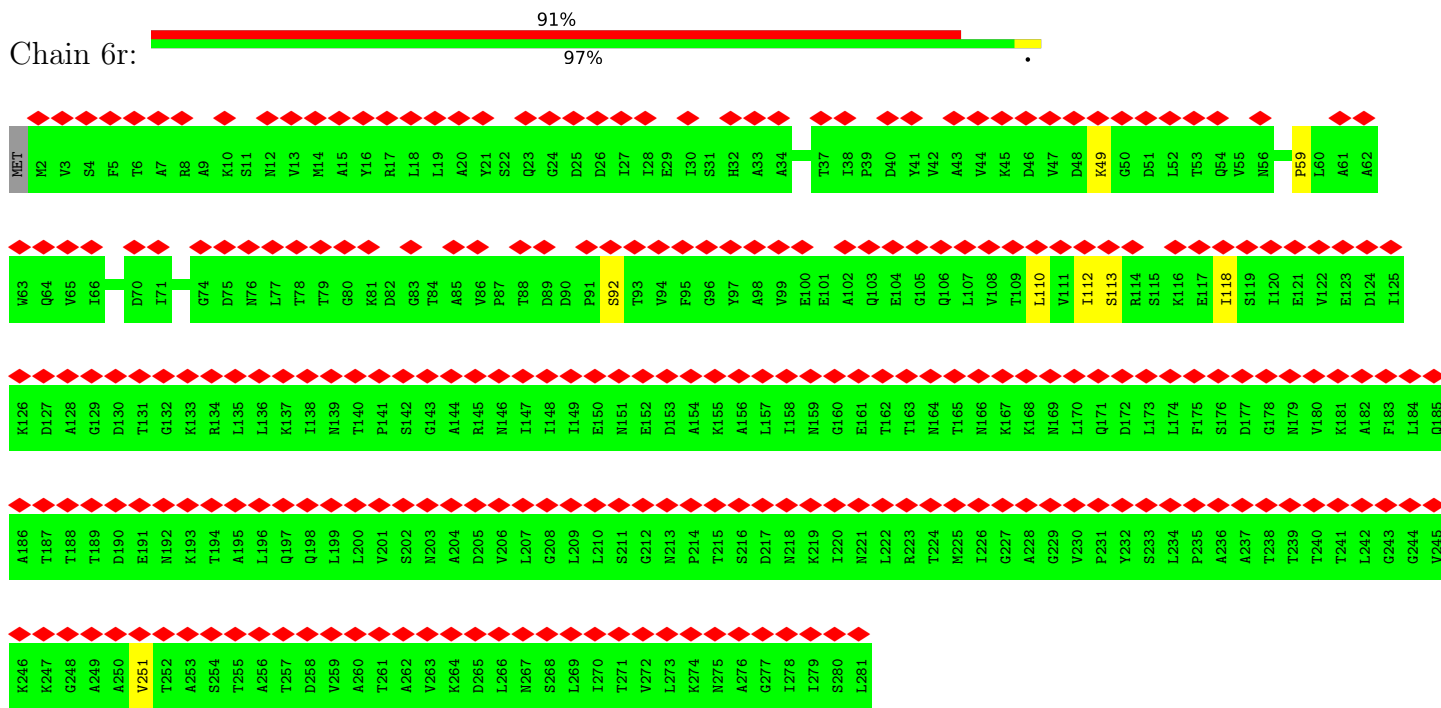
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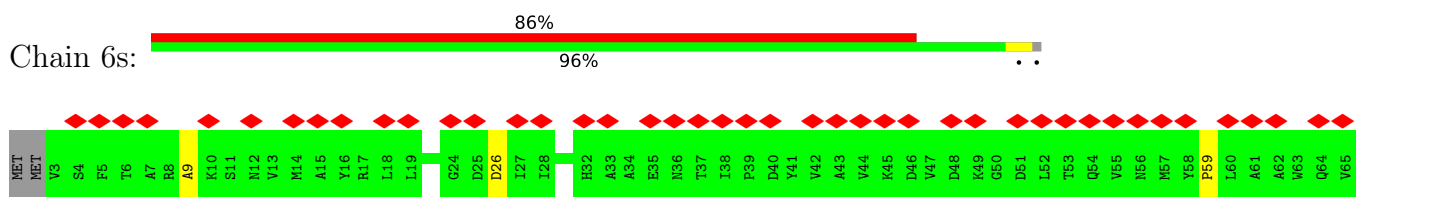
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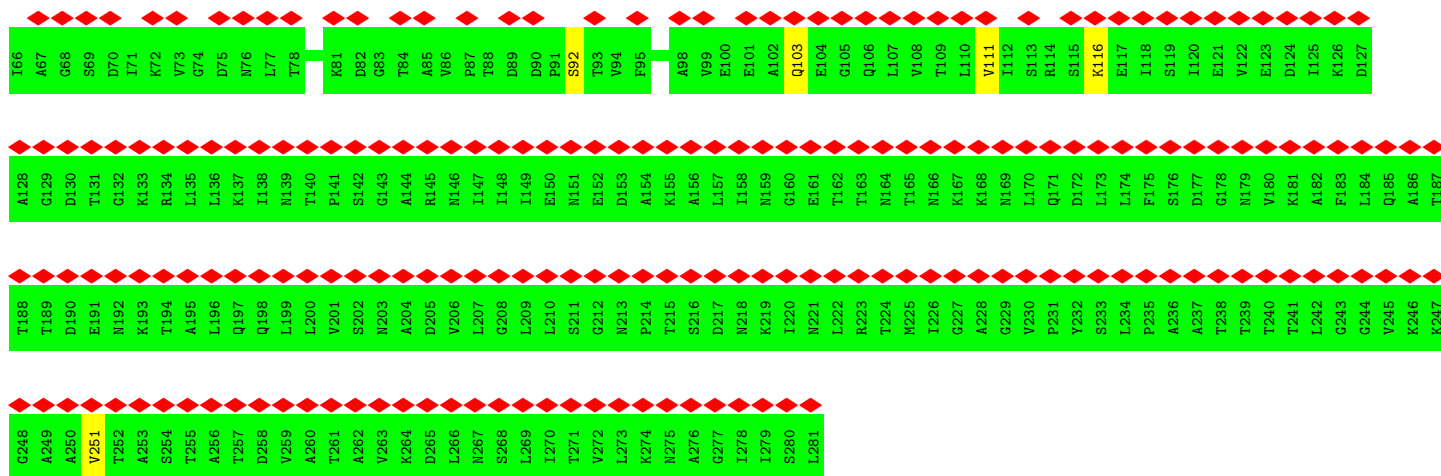


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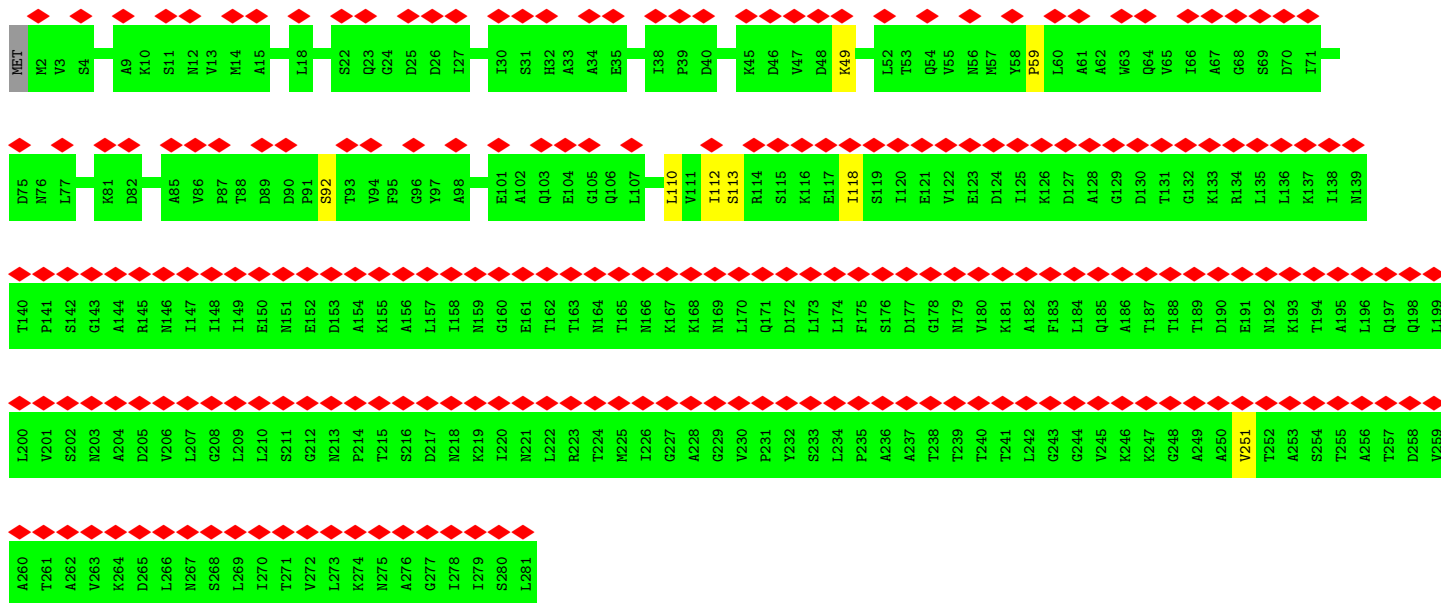
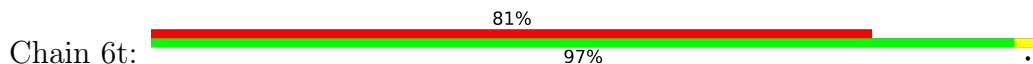


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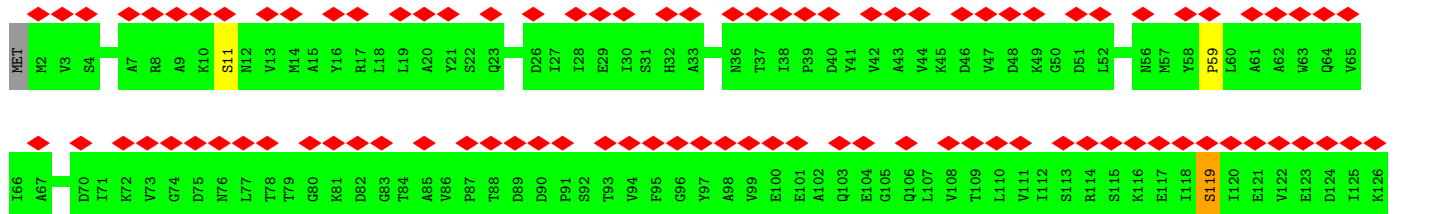
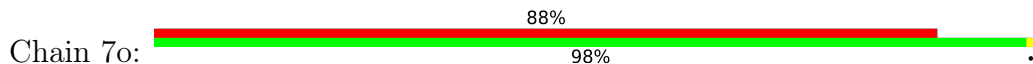




• Molecule 2: Capsid fiber protein

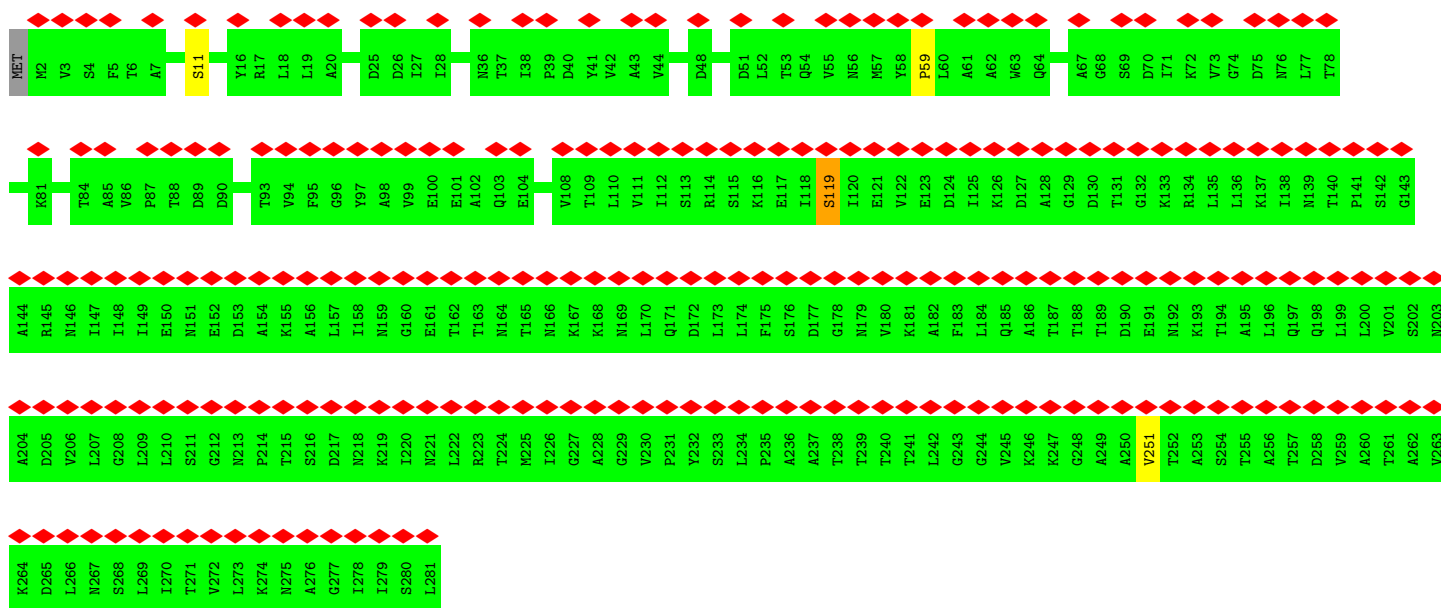
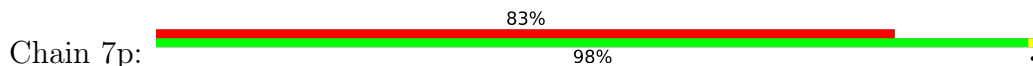


• Molecule 2: Capsid fiber protein

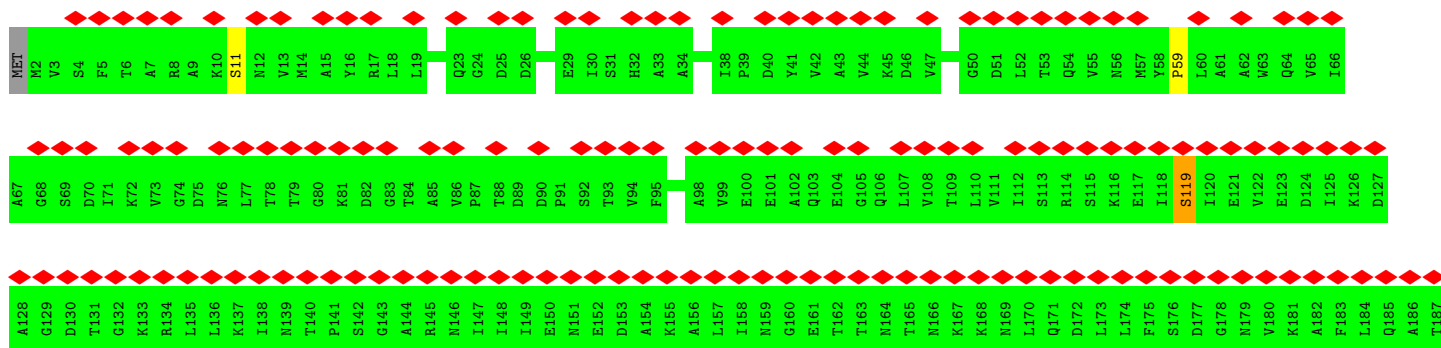
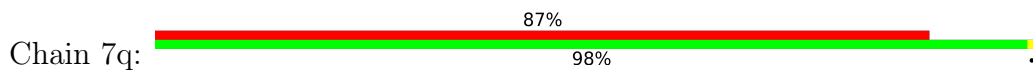


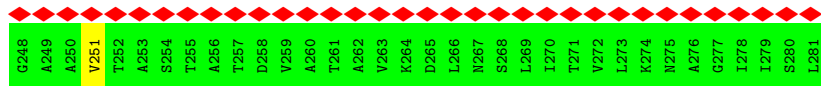
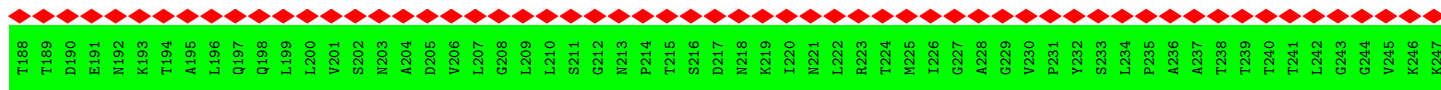


• Molecule 2: Capsid fiber protein

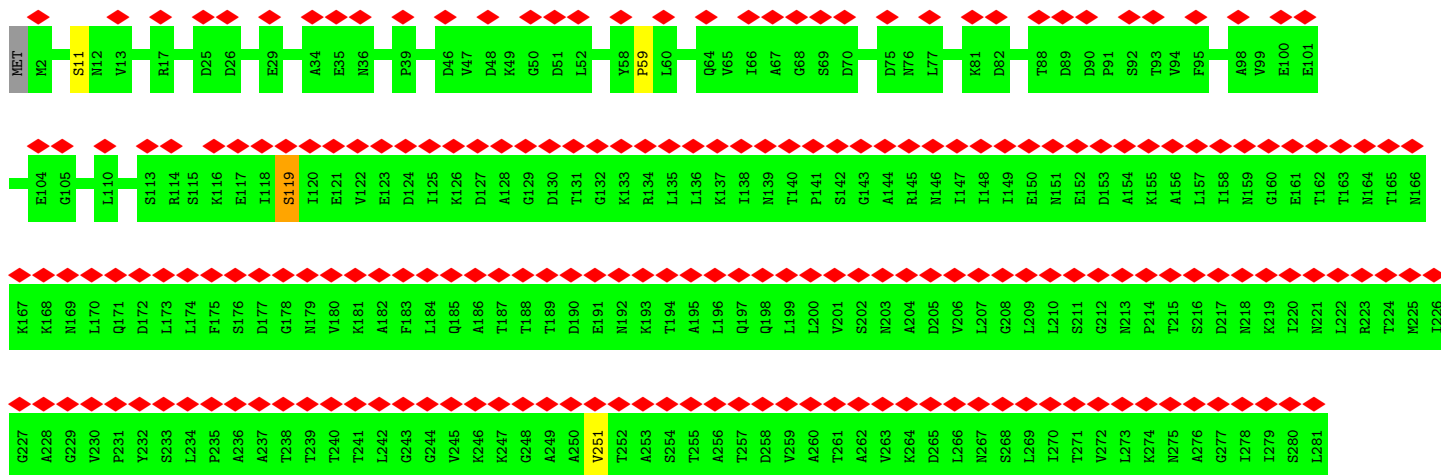
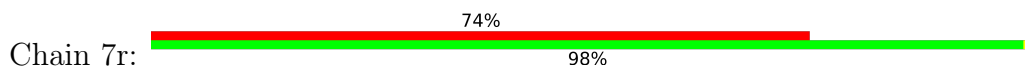


• Molecule 2: Capsid fiber protein

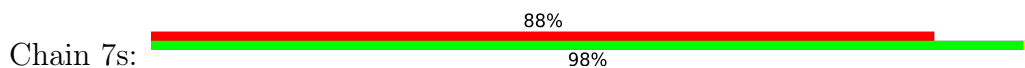




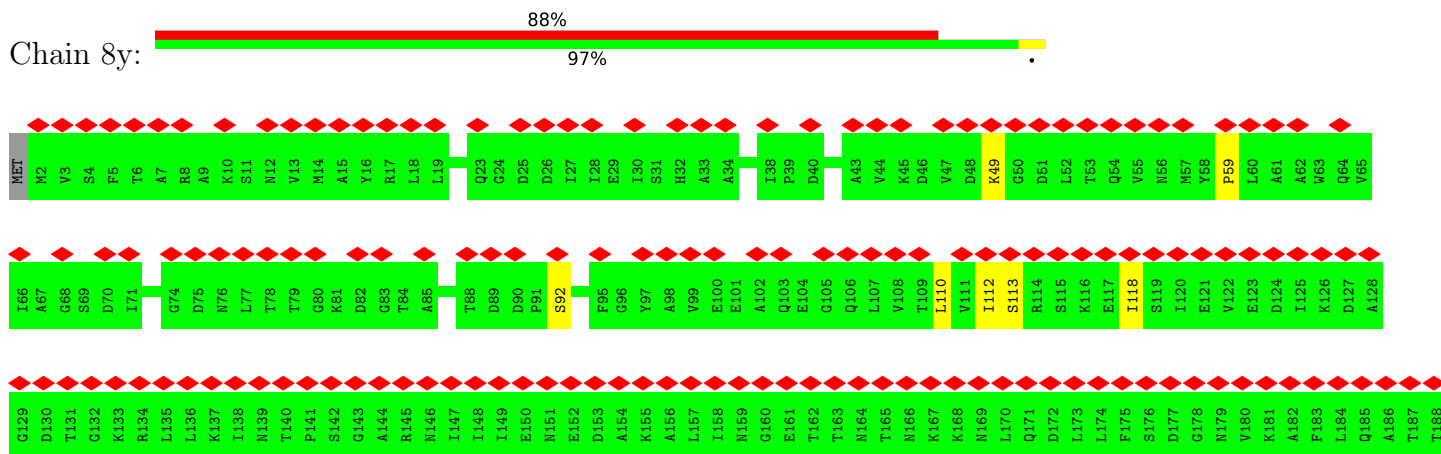
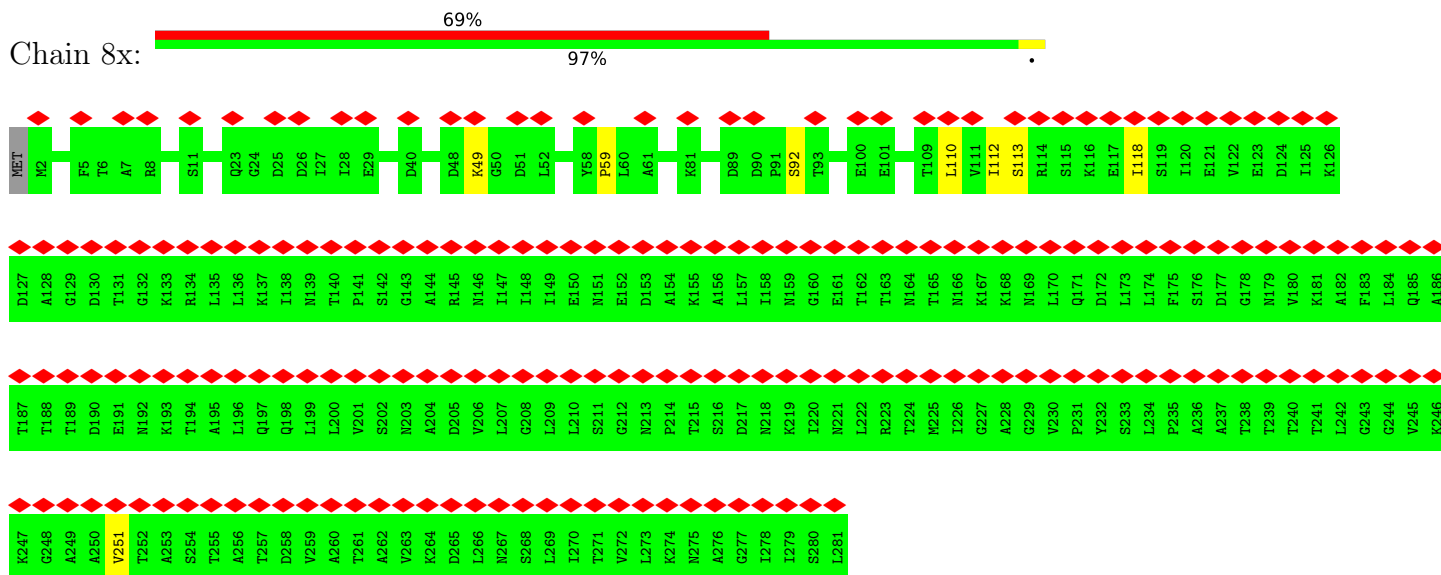
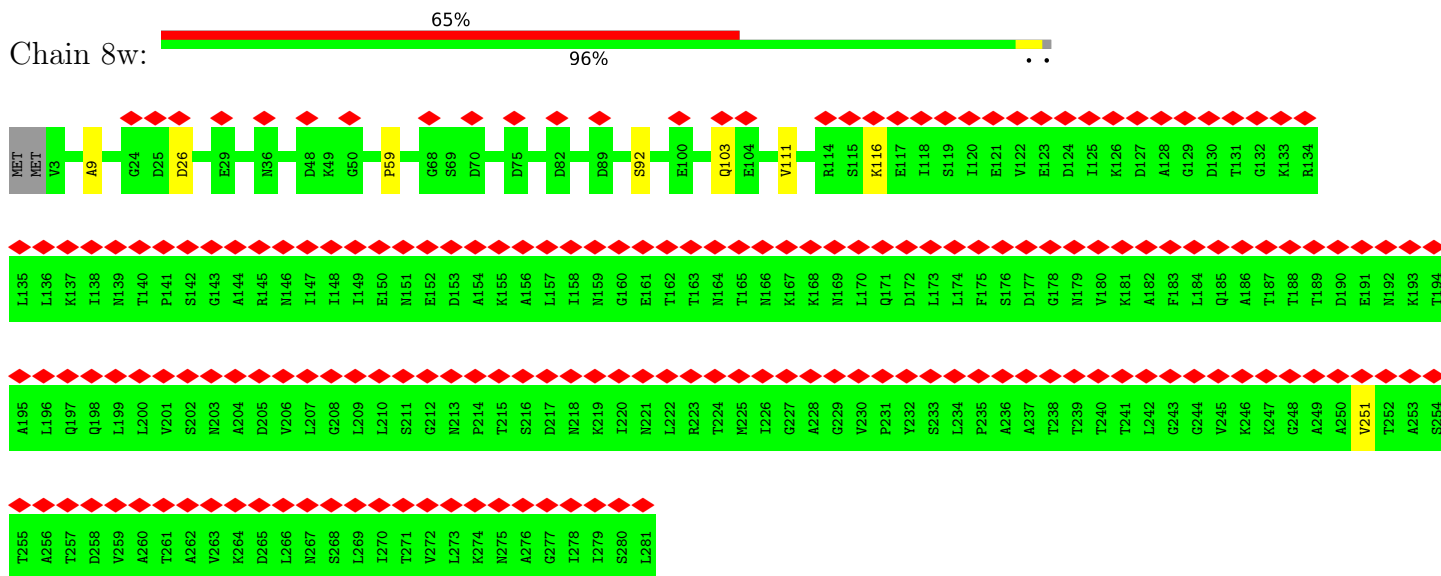
• Molecule 2: Capsid fiber protein



• Molecule 2: Capsid fiber protein

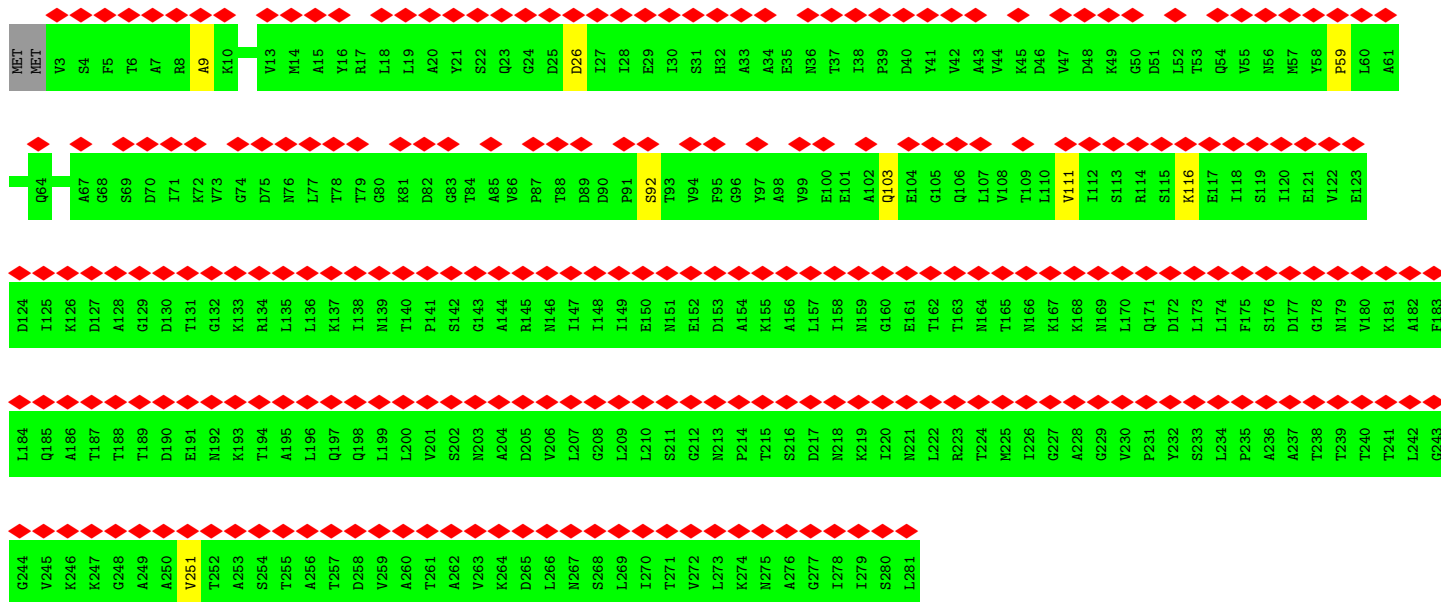
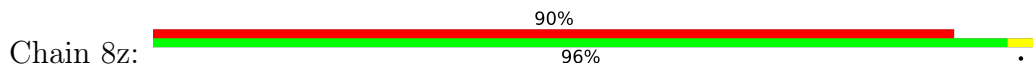


• Molecule 2: Capsid fiber protein

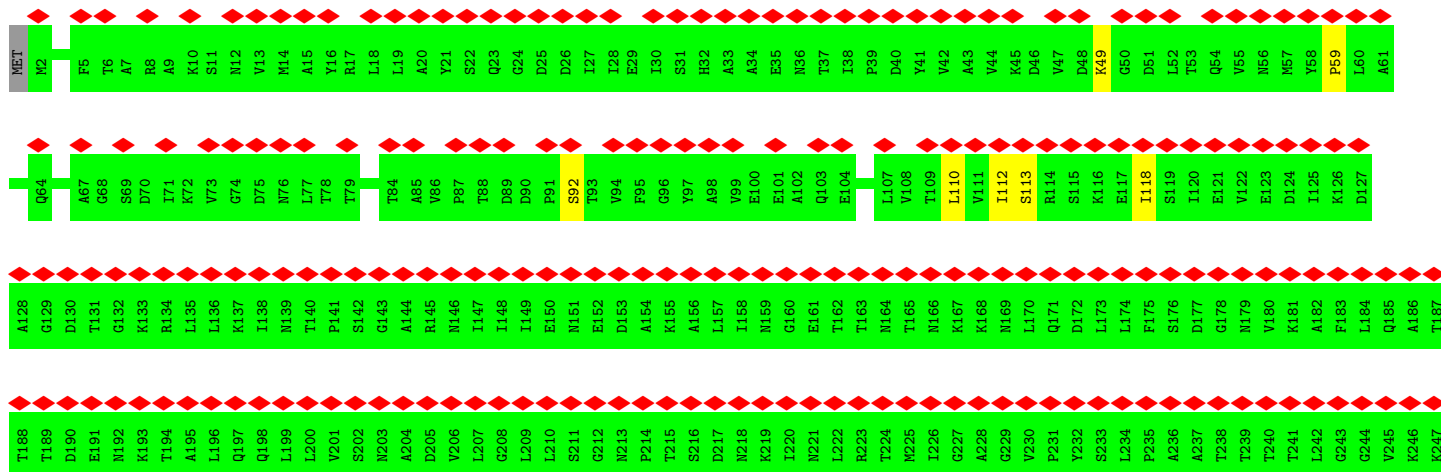


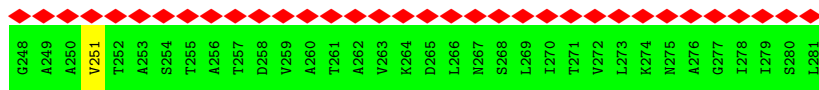


• Molecule 2: Capsid fiber protein

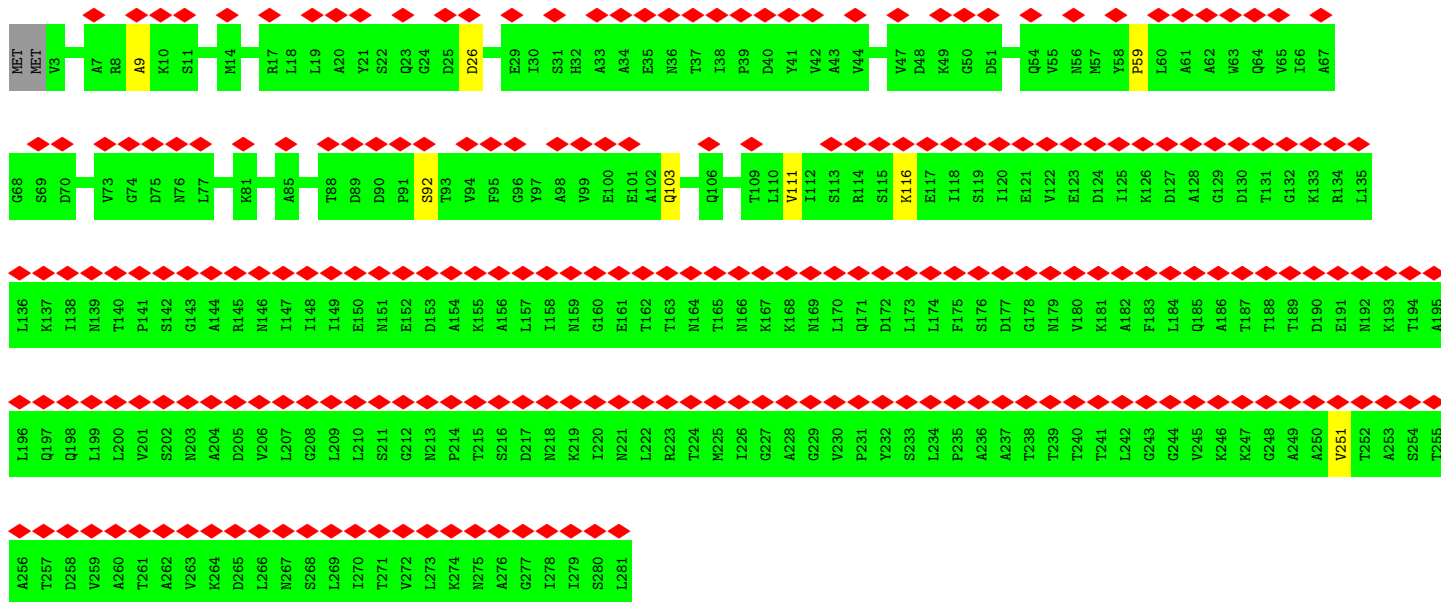
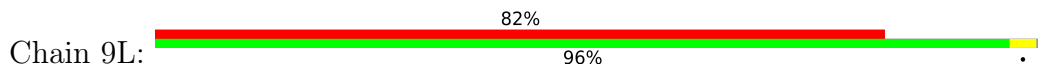


• Molecule 2: Capsid fiber protein

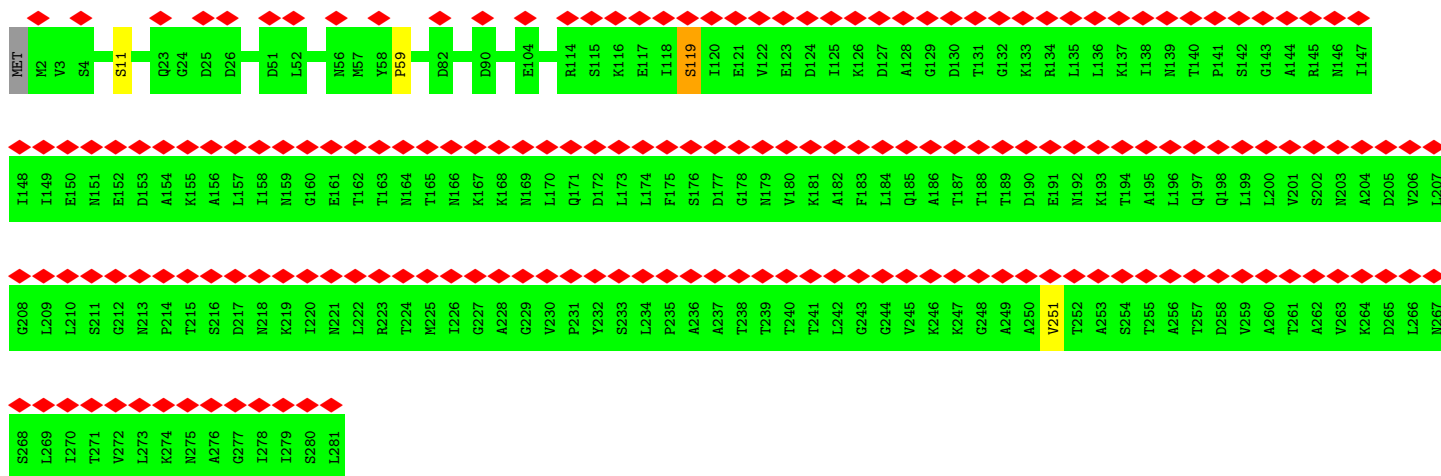




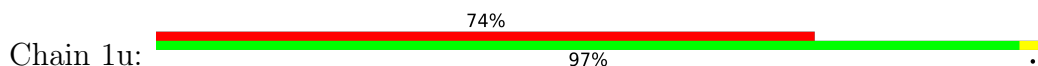
• Molecule 2: Capsid fiber protein

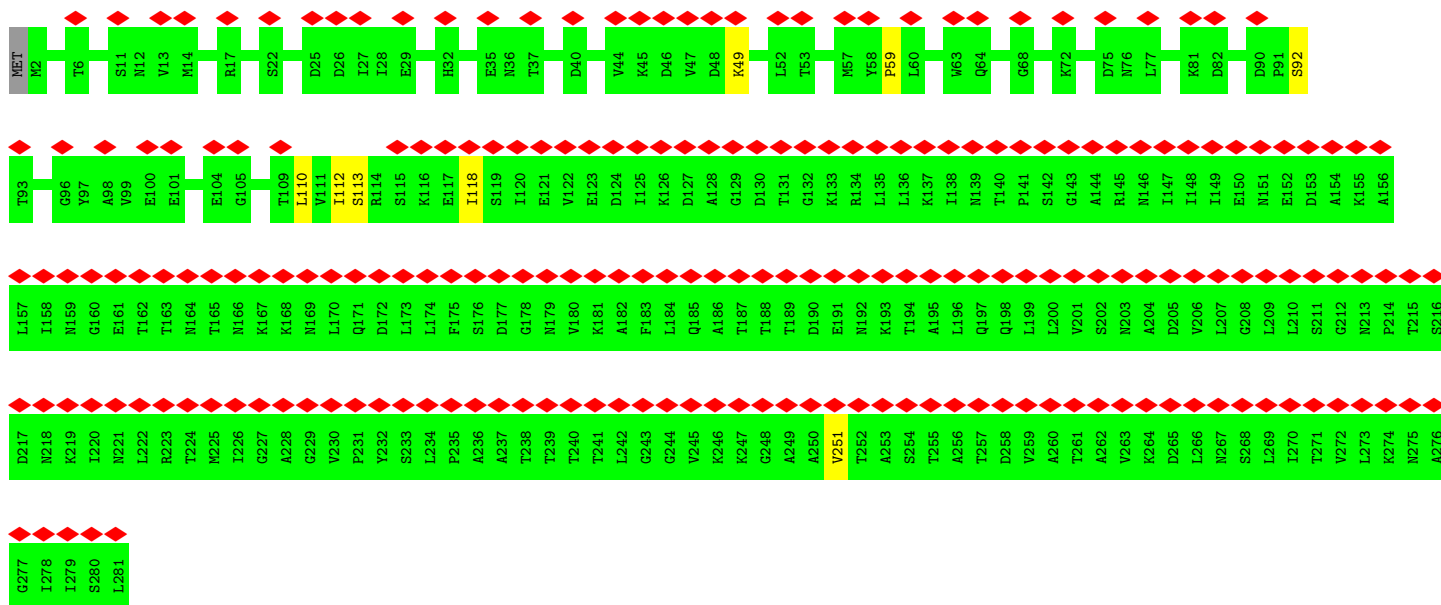


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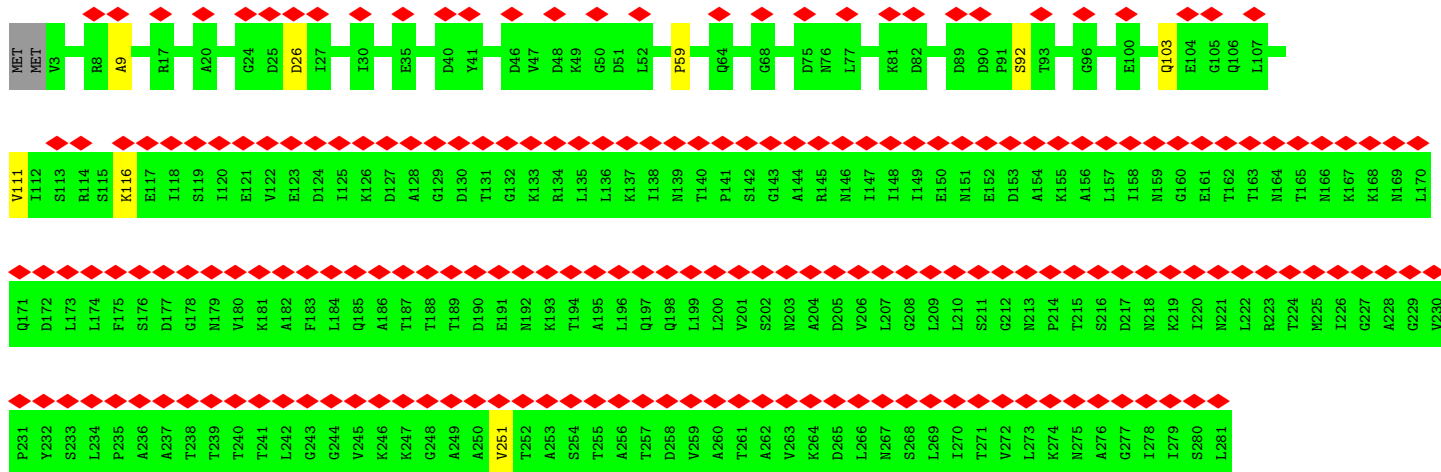


• Molecule 2: Capsid fiber protein

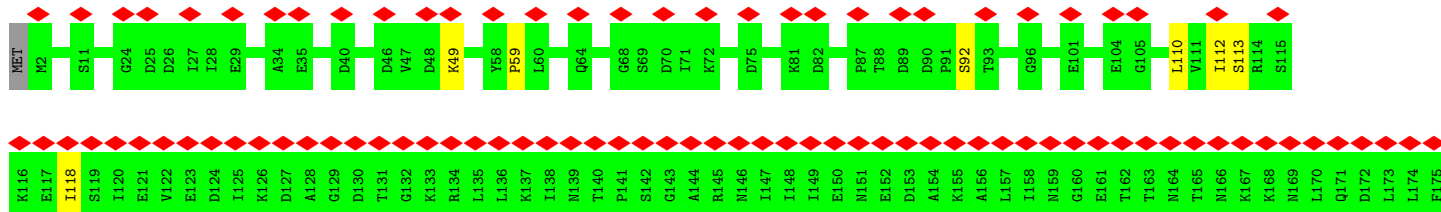


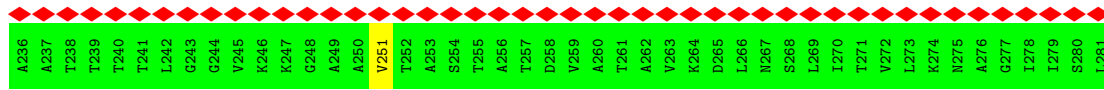


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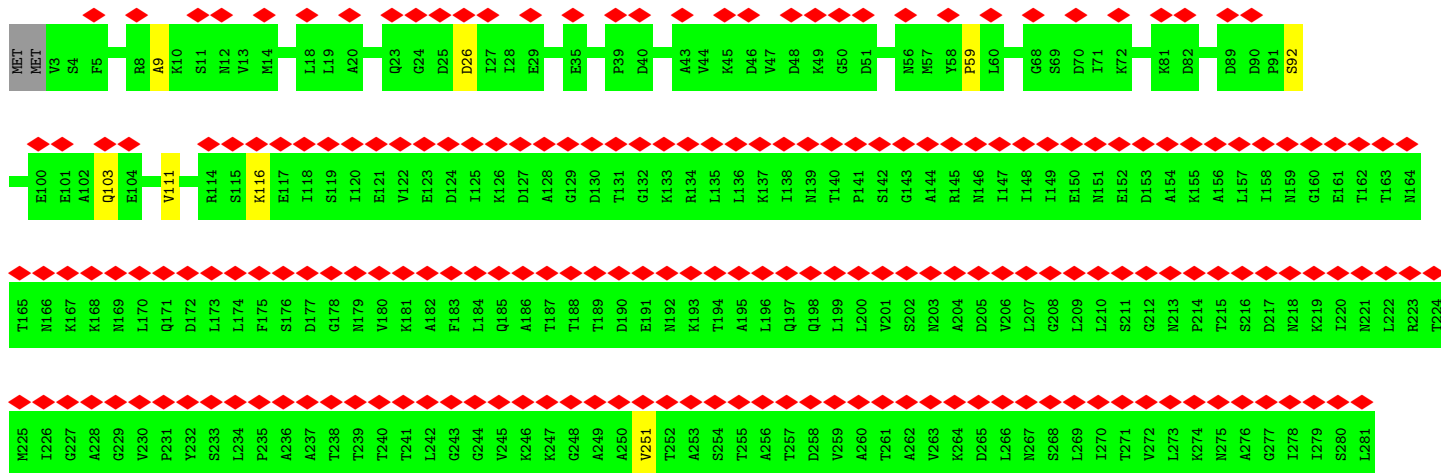
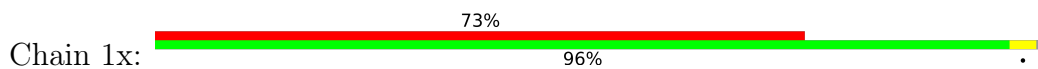


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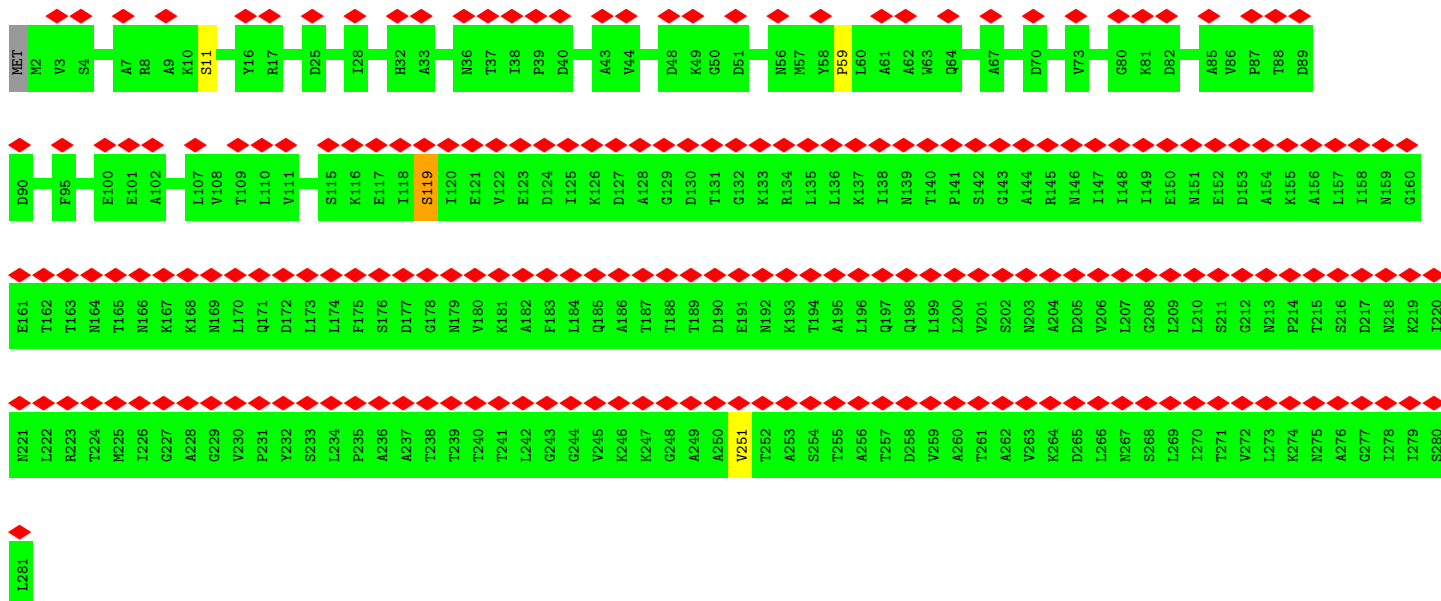
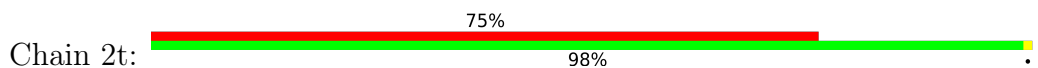




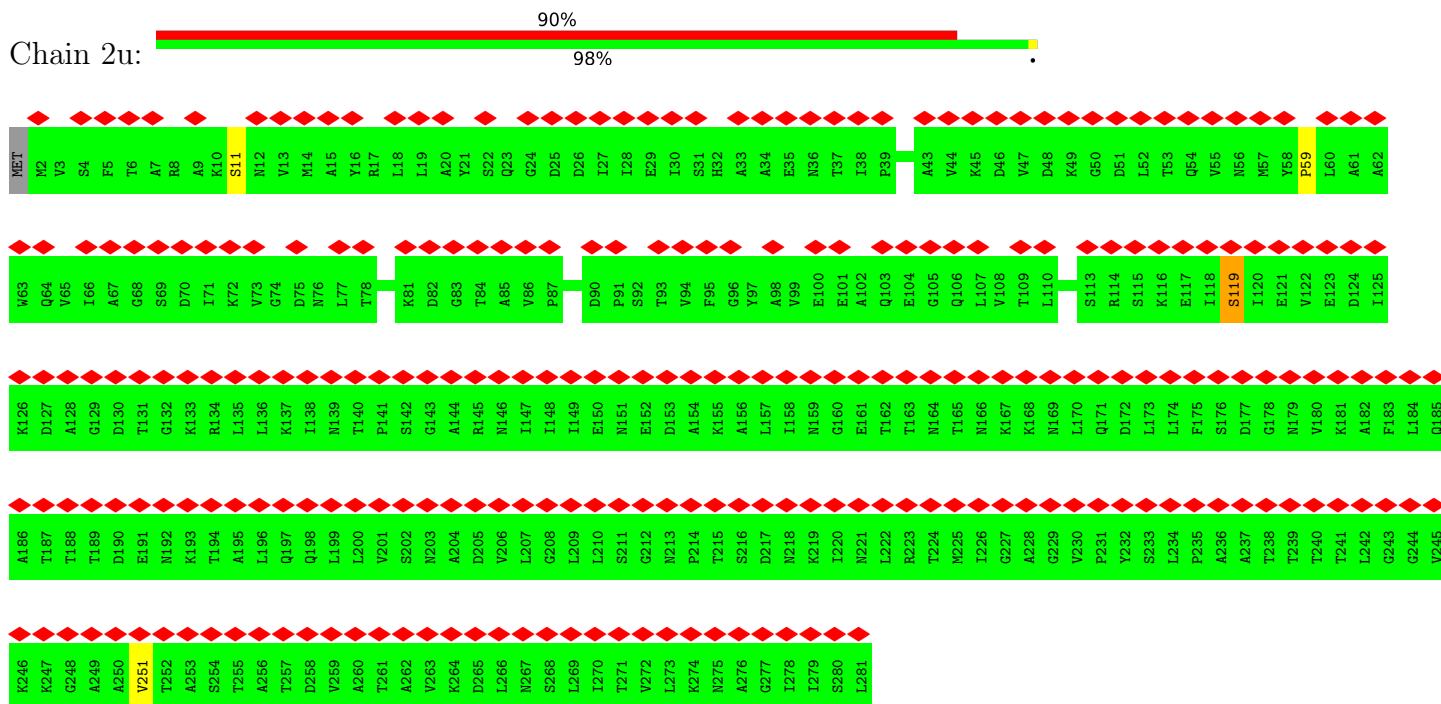
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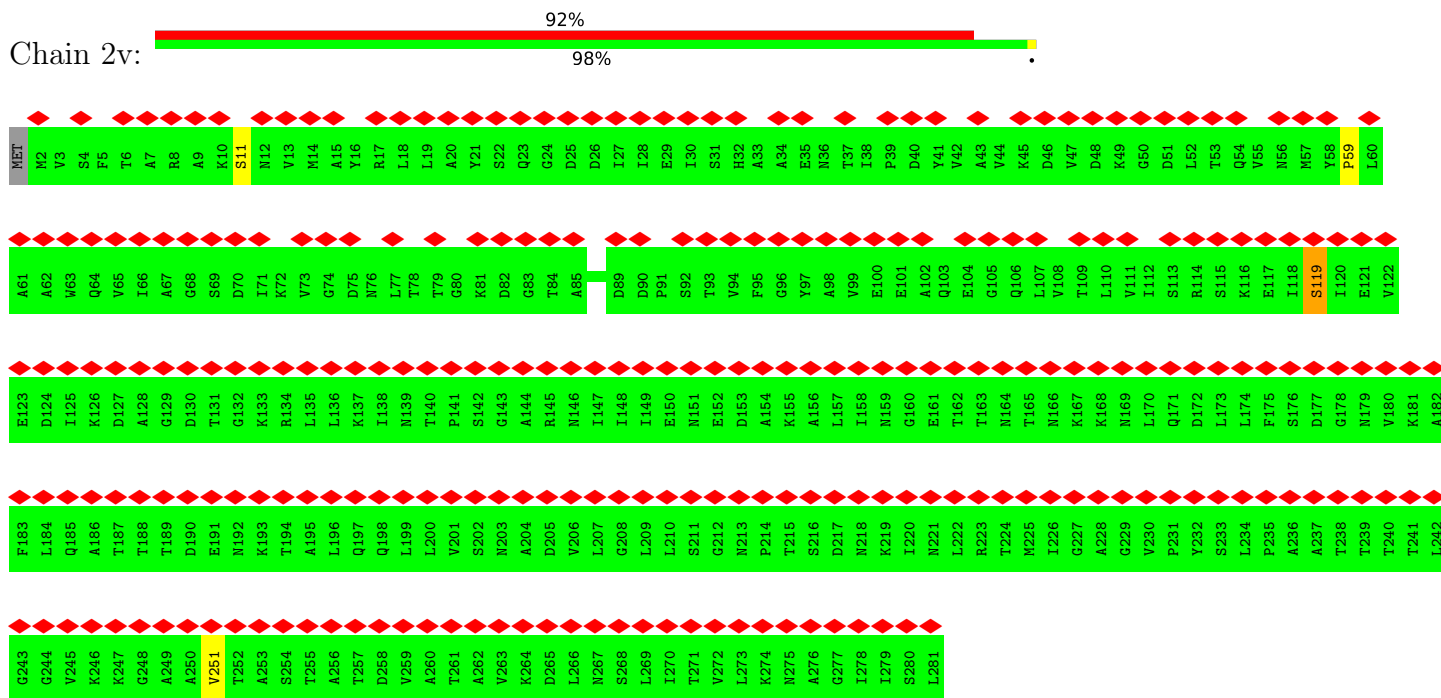
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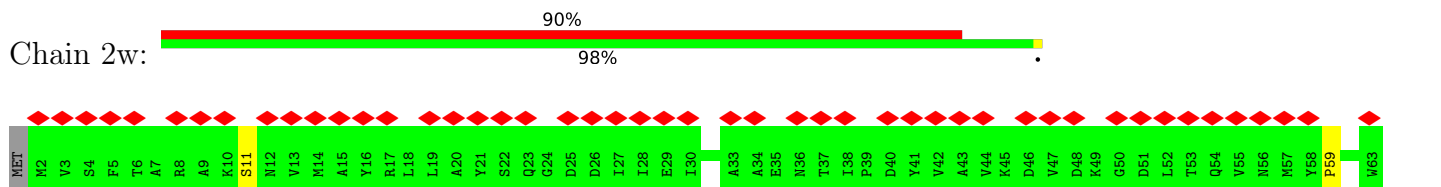
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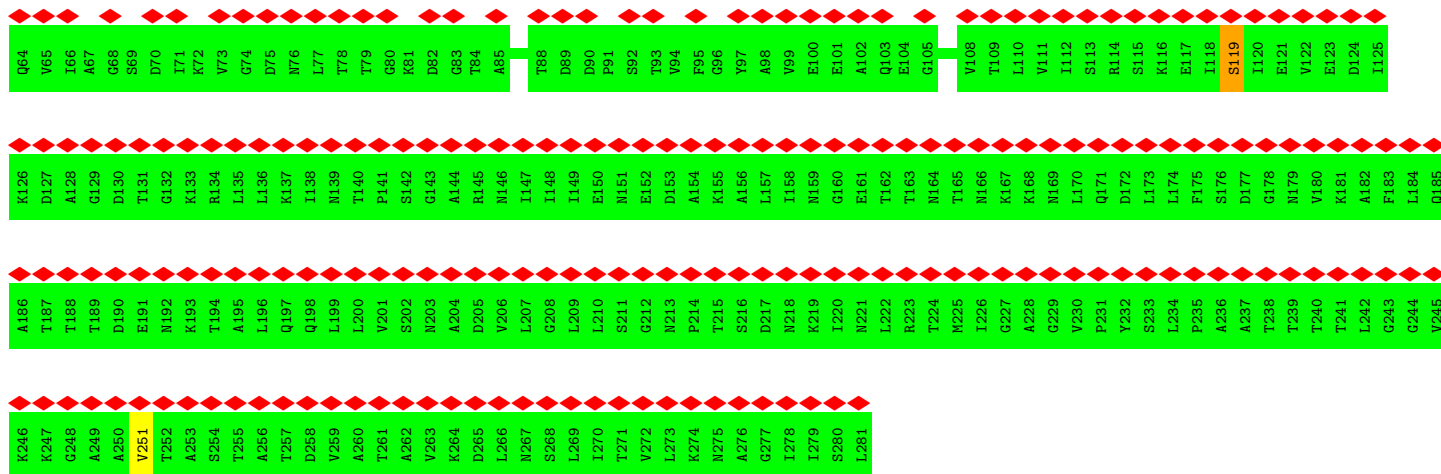


• Molecule 2: Capsid fiber protein



• Molecule 2: Capsid fiber protein

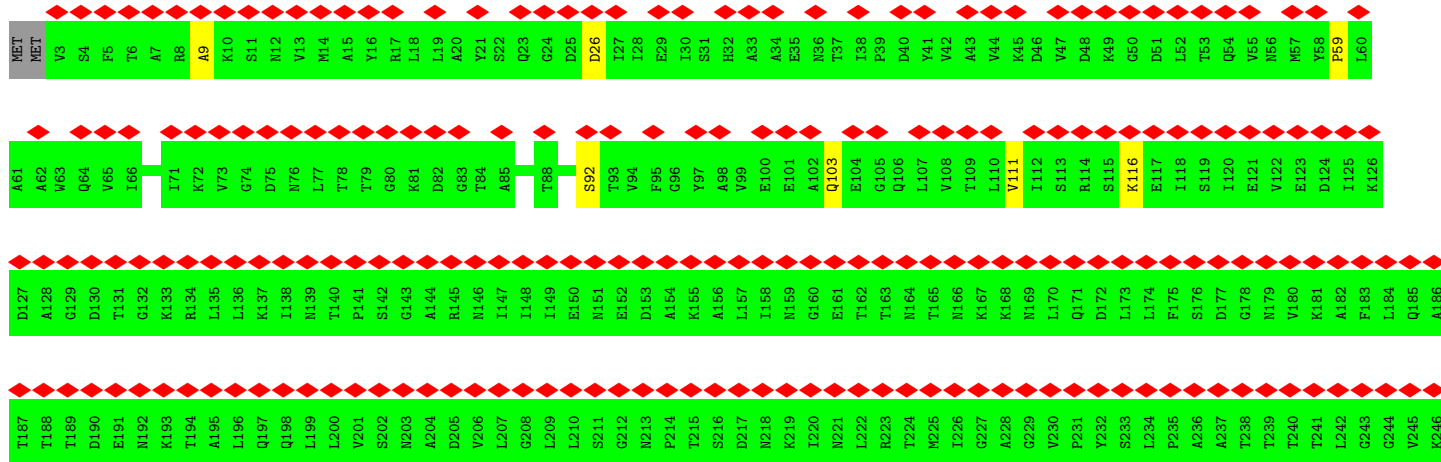
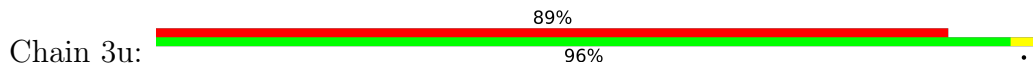


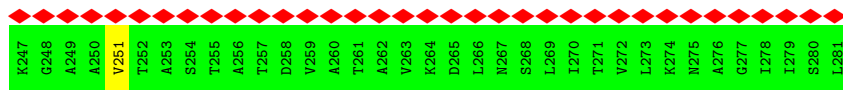


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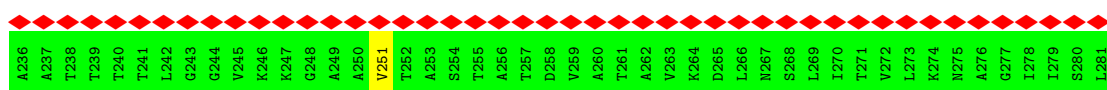
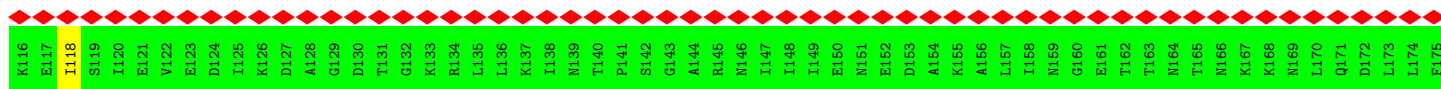
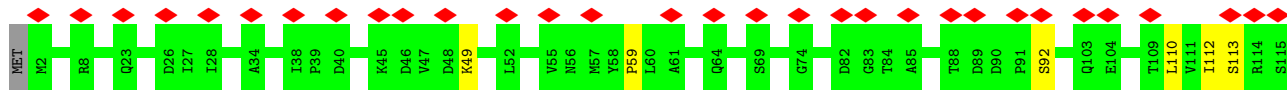


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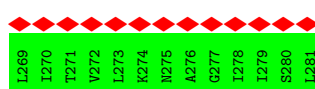
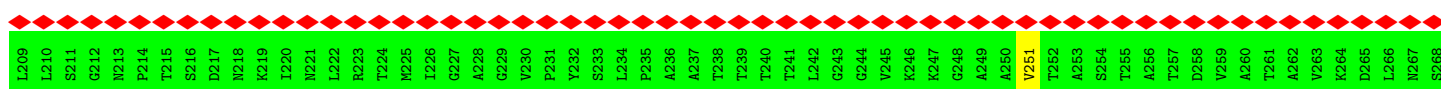
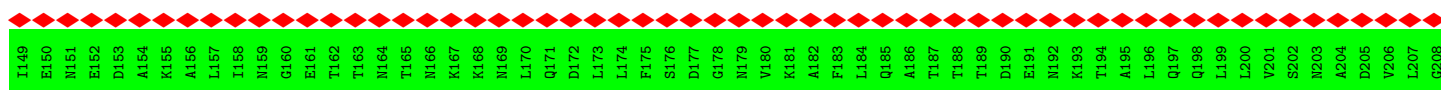
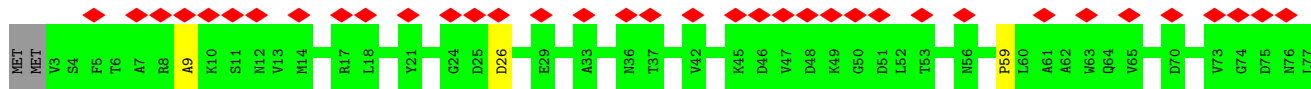
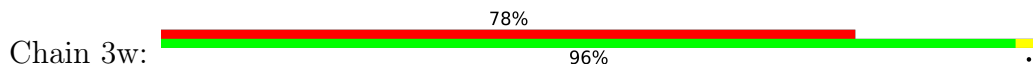




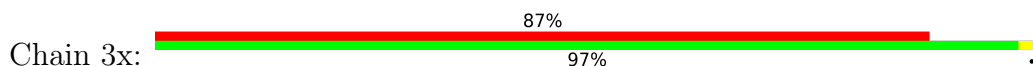
• Molecule 2: Capsid fiber protein



• Molecule 2: Capsid fiber protein

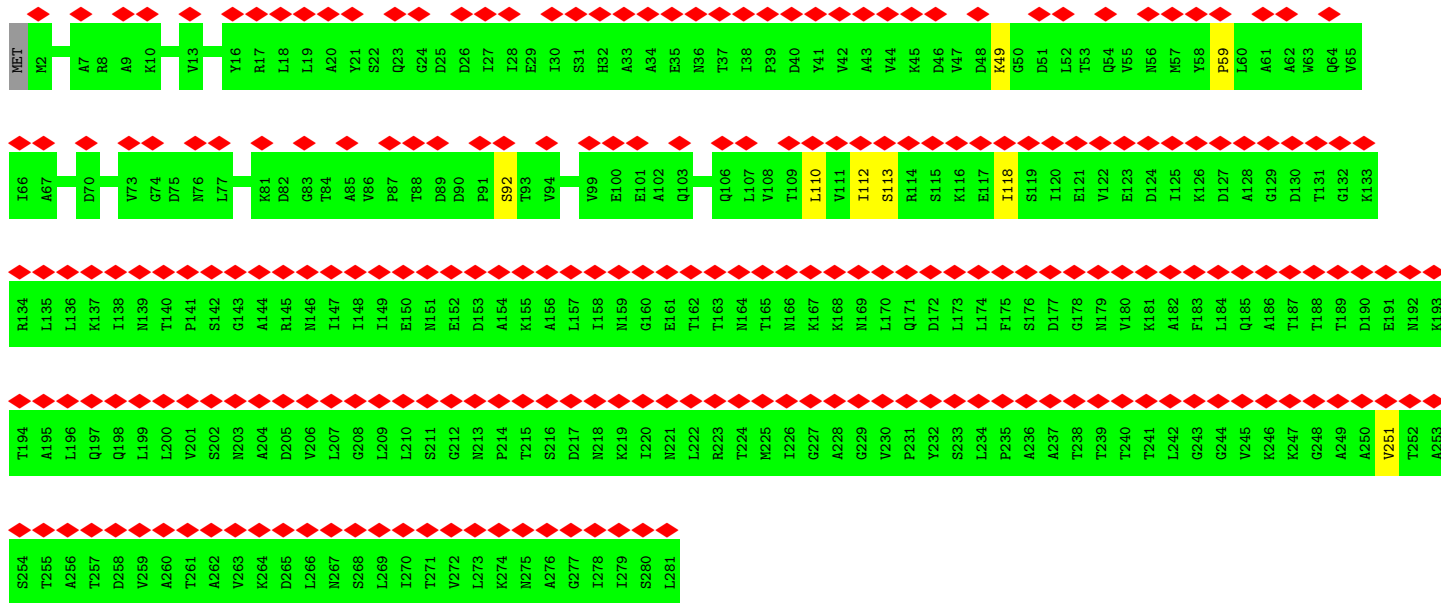
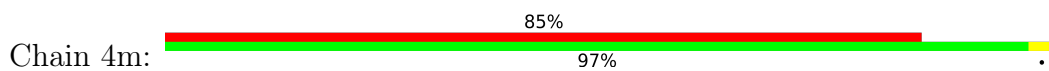


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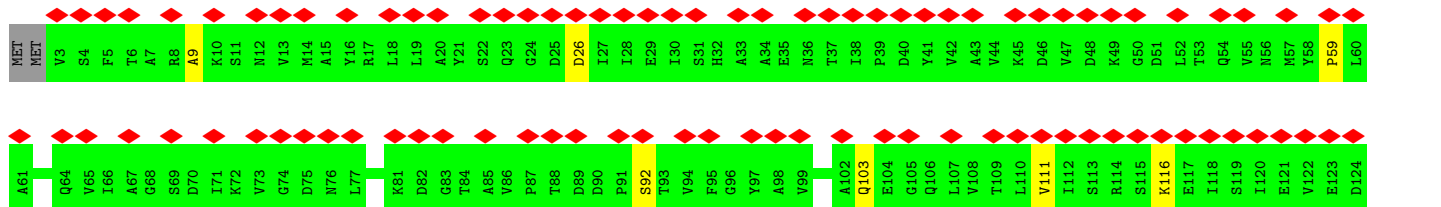
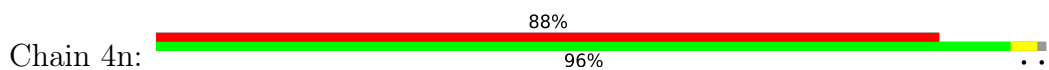


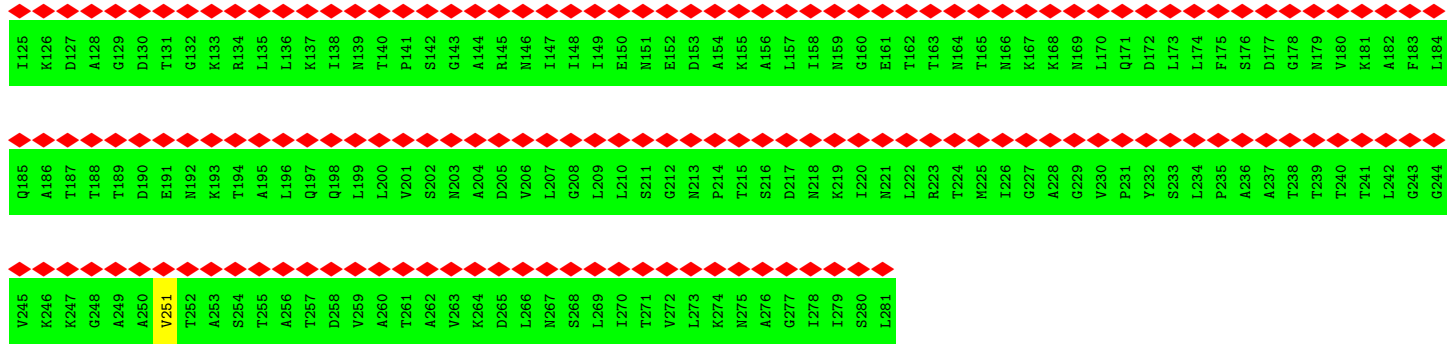


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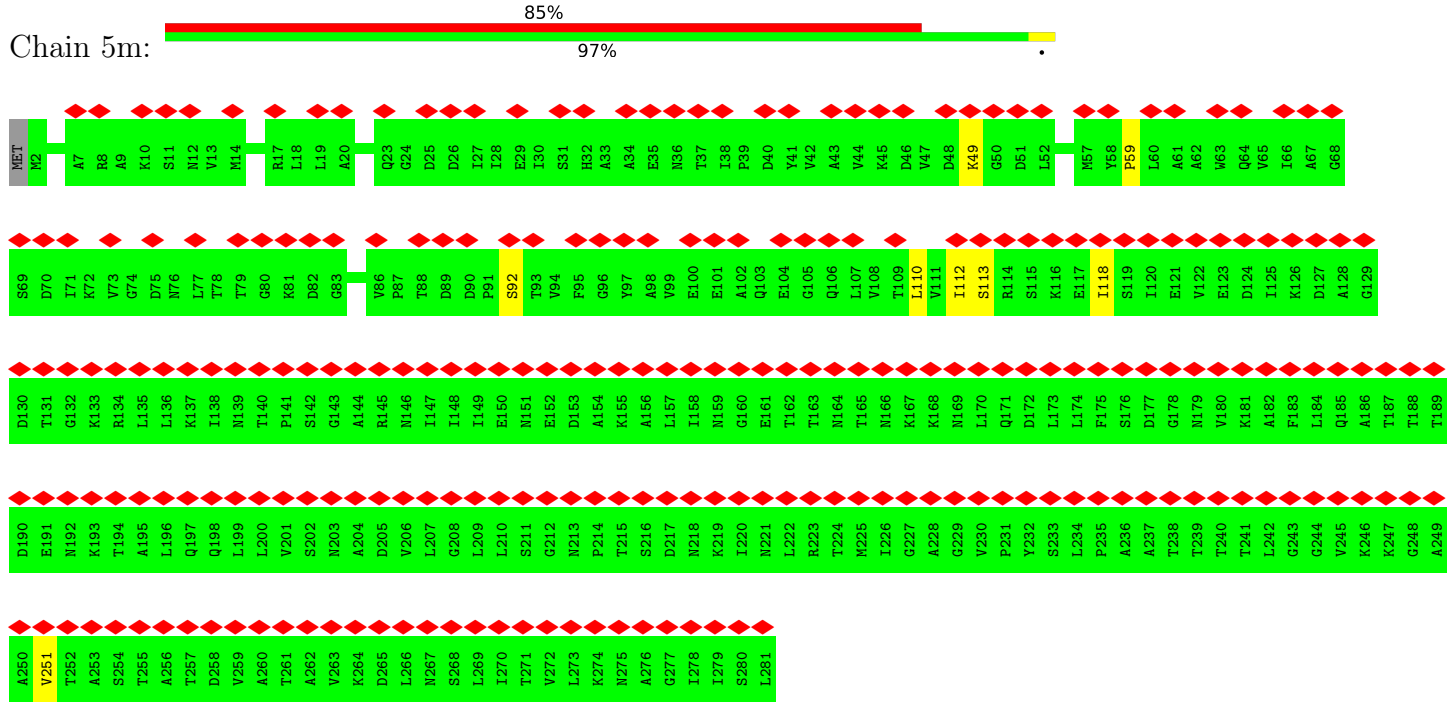


• Molecule 2: Capsid fiber protein

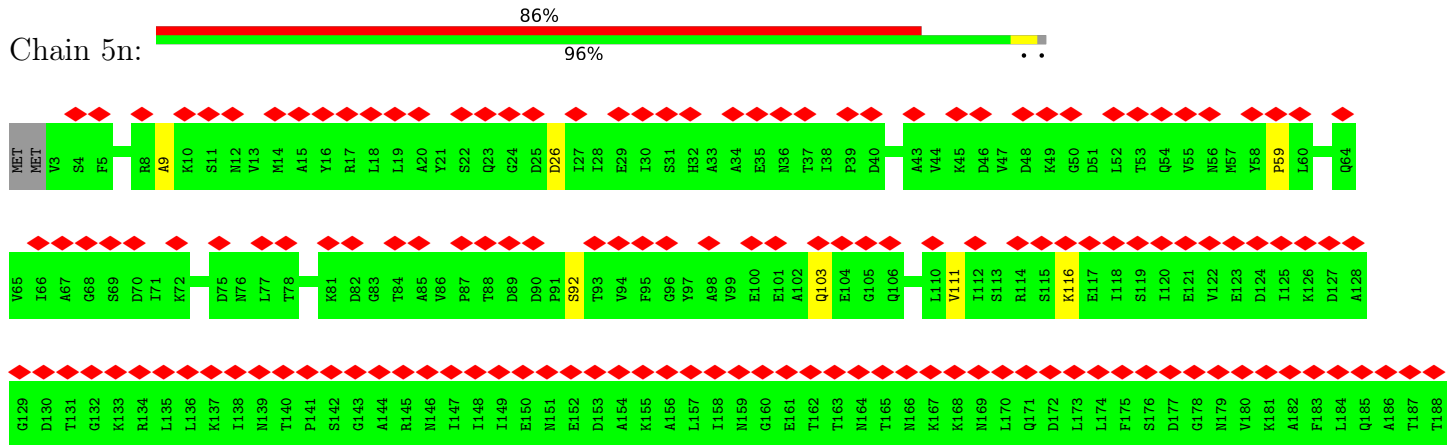




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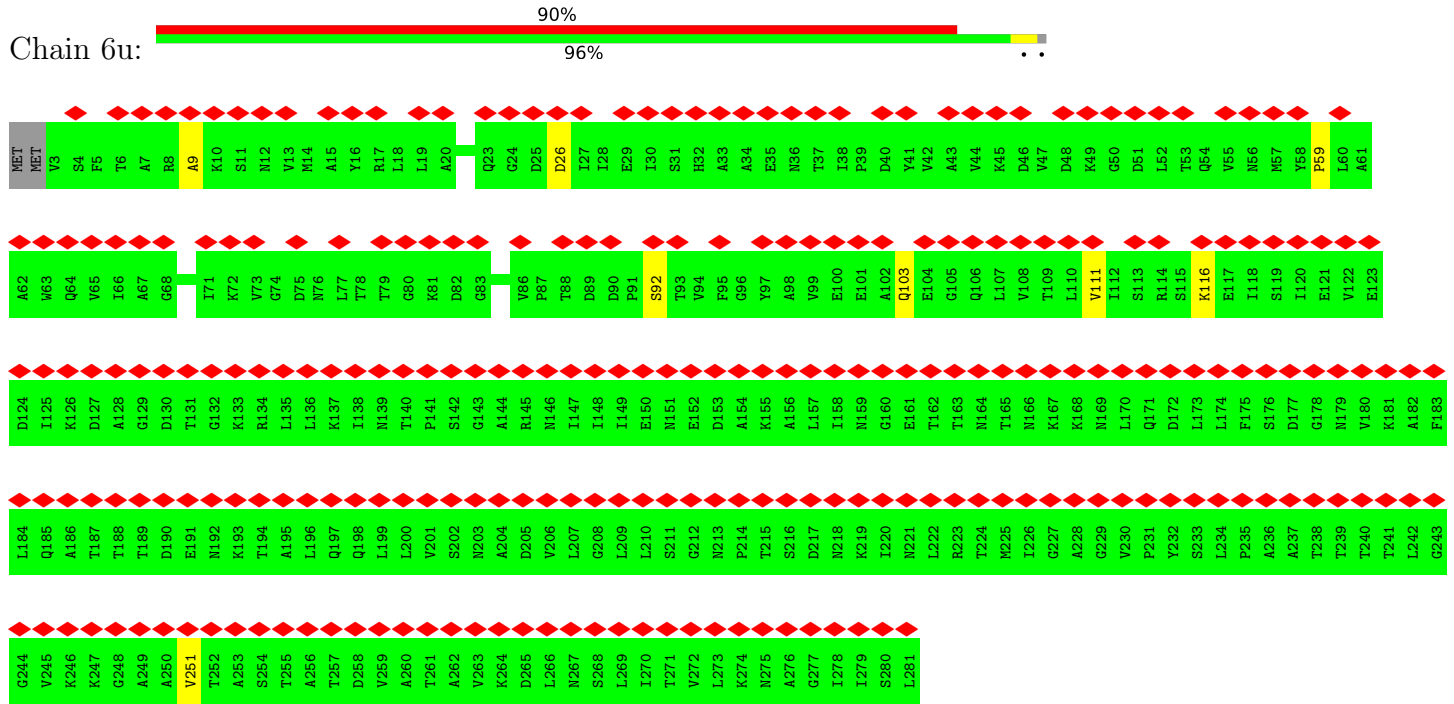


• Molecule 2: Capsid fiber protein

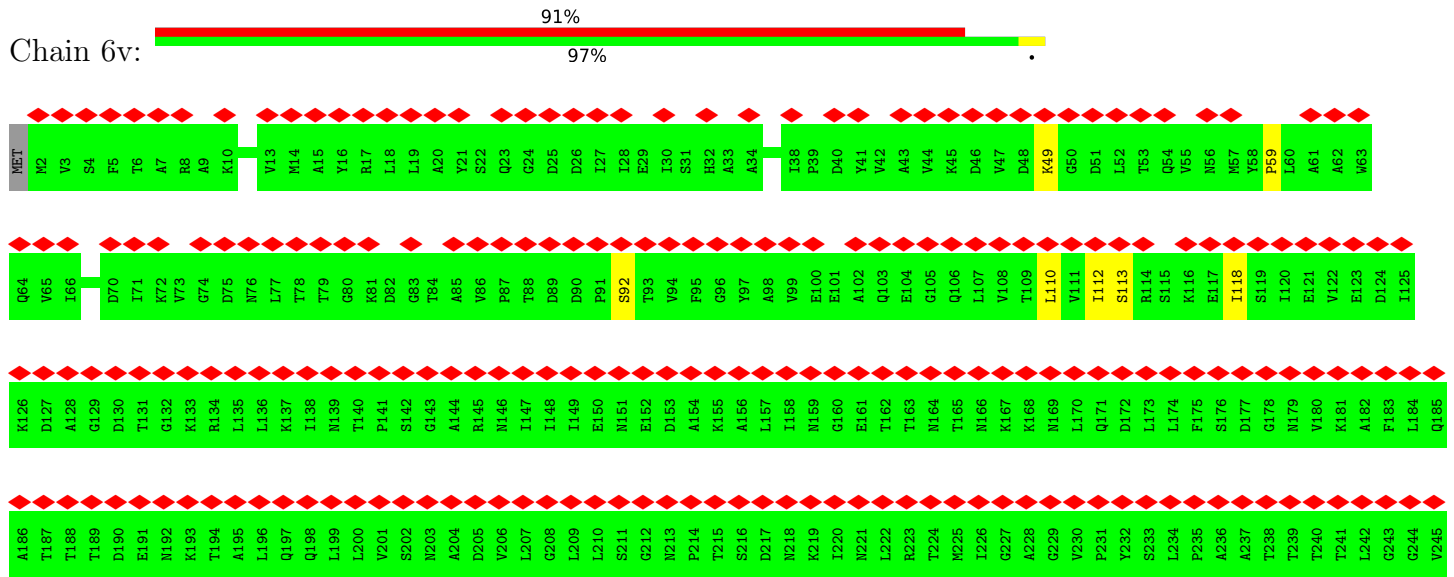


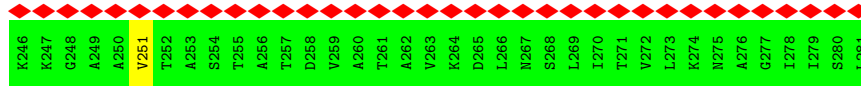


• Molecule 2: Capsid fiber protein

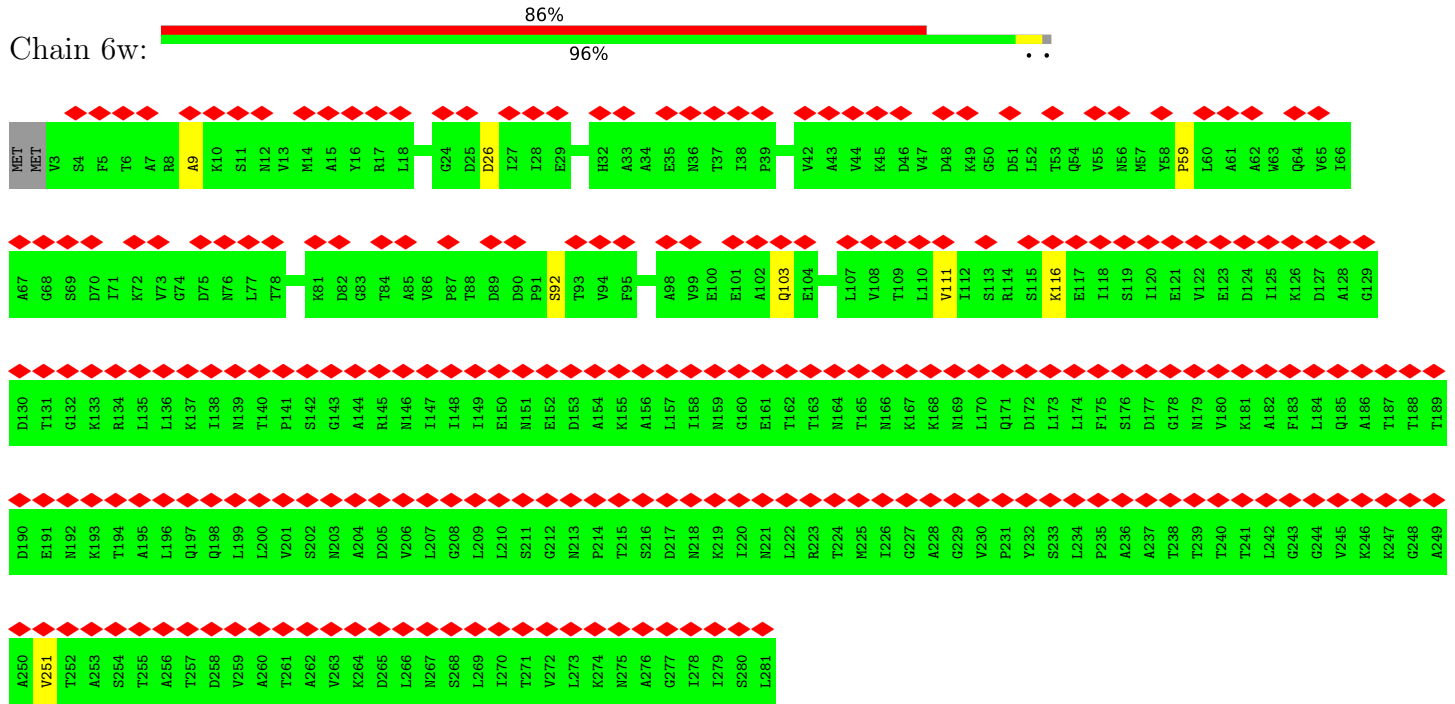


• Molecule 2: Capsid fiber protein

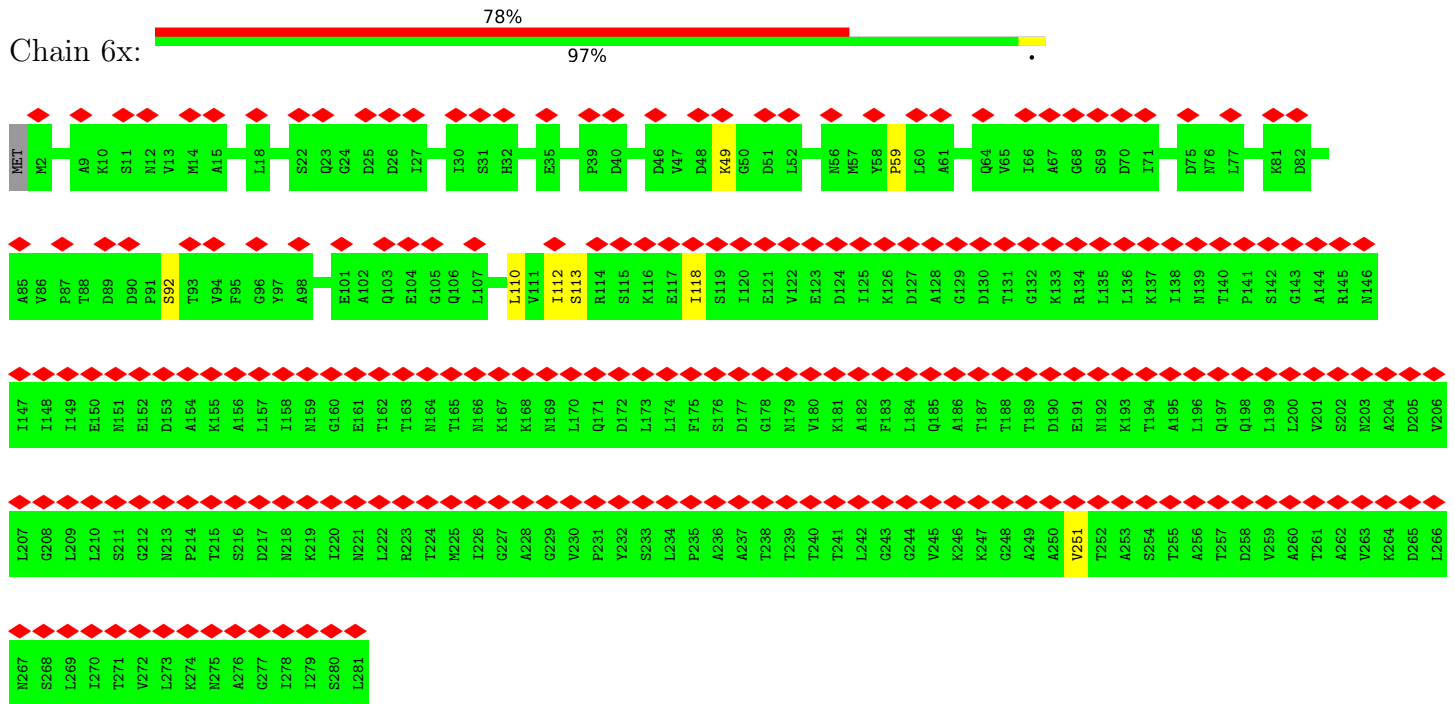




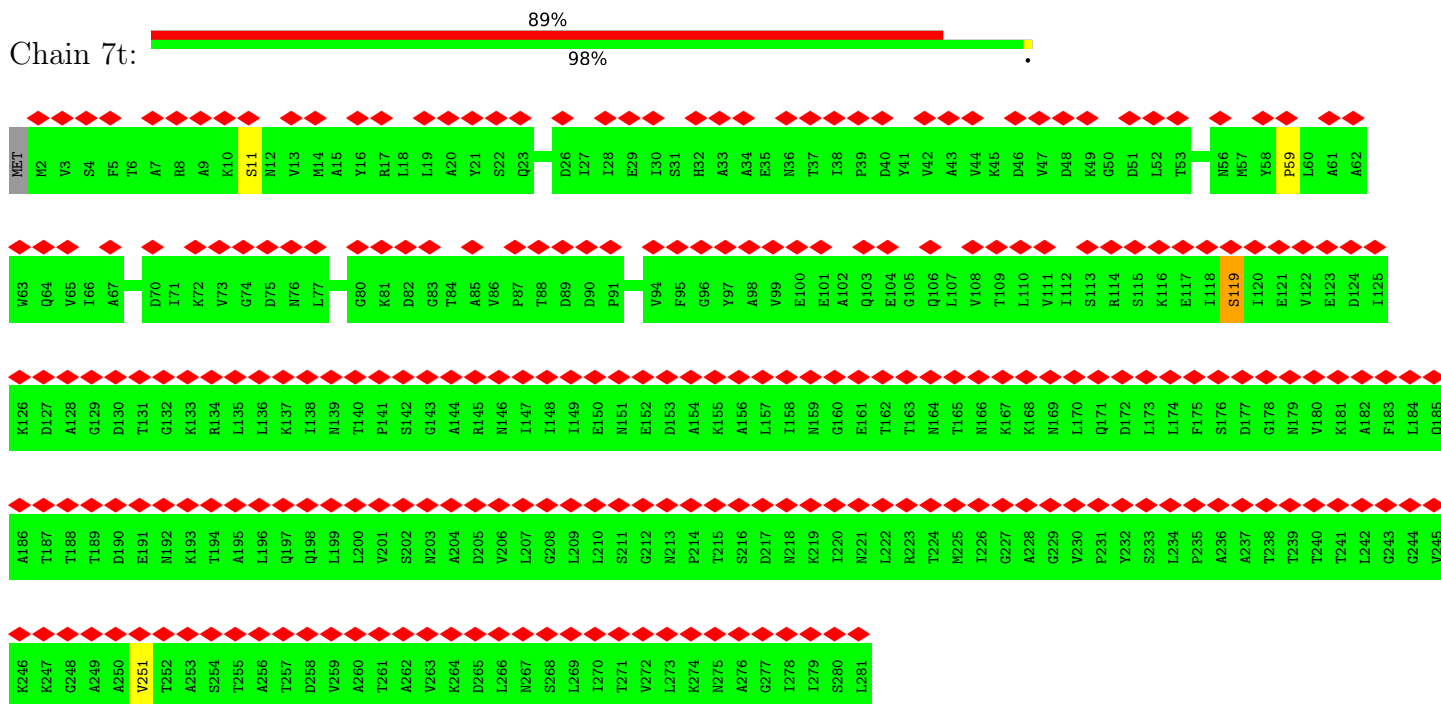
• Molecule 2: Capsid fiber protein



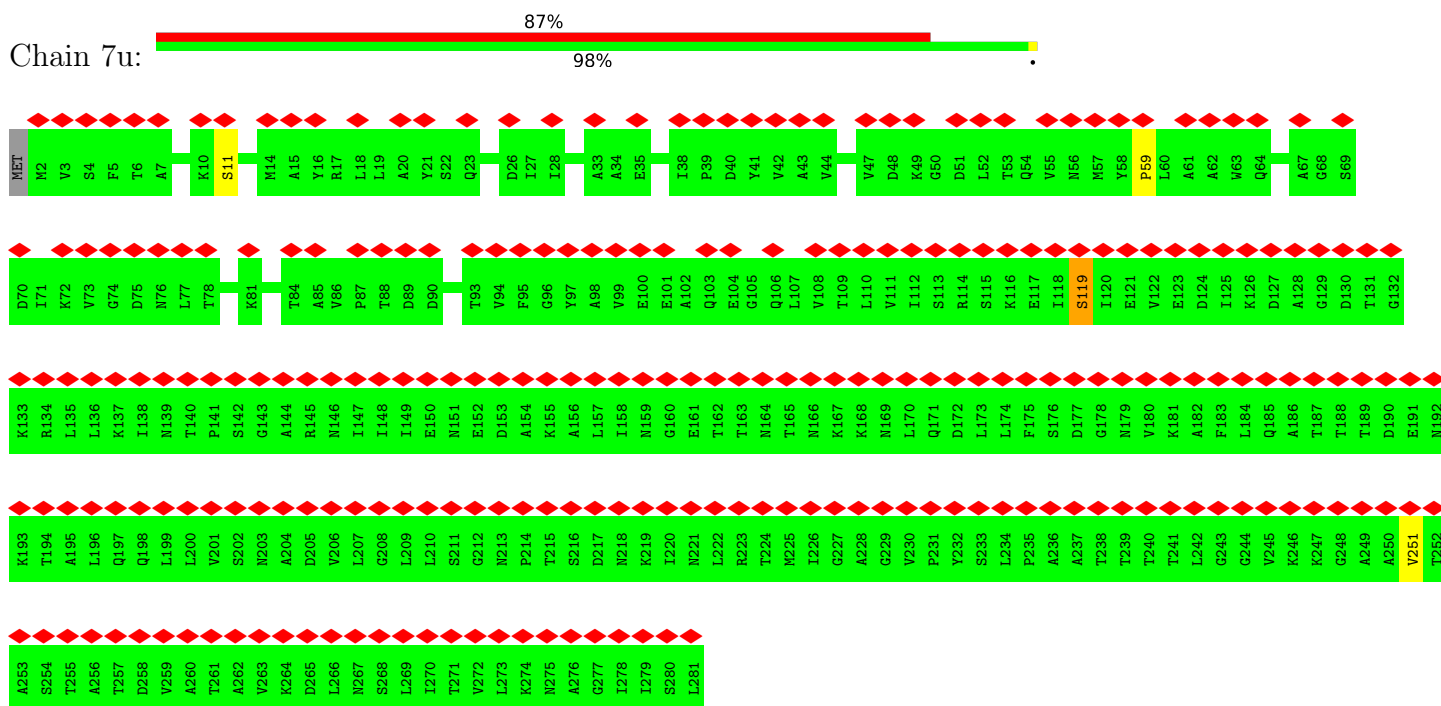
• Molecule 2: Capsid fiber protein



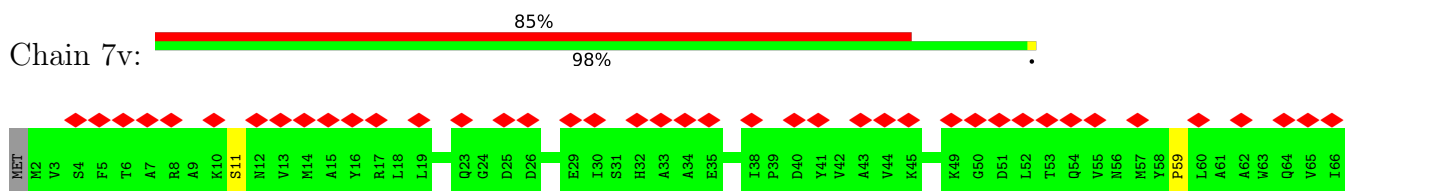
• Molecule 2: Capsid fiber protein

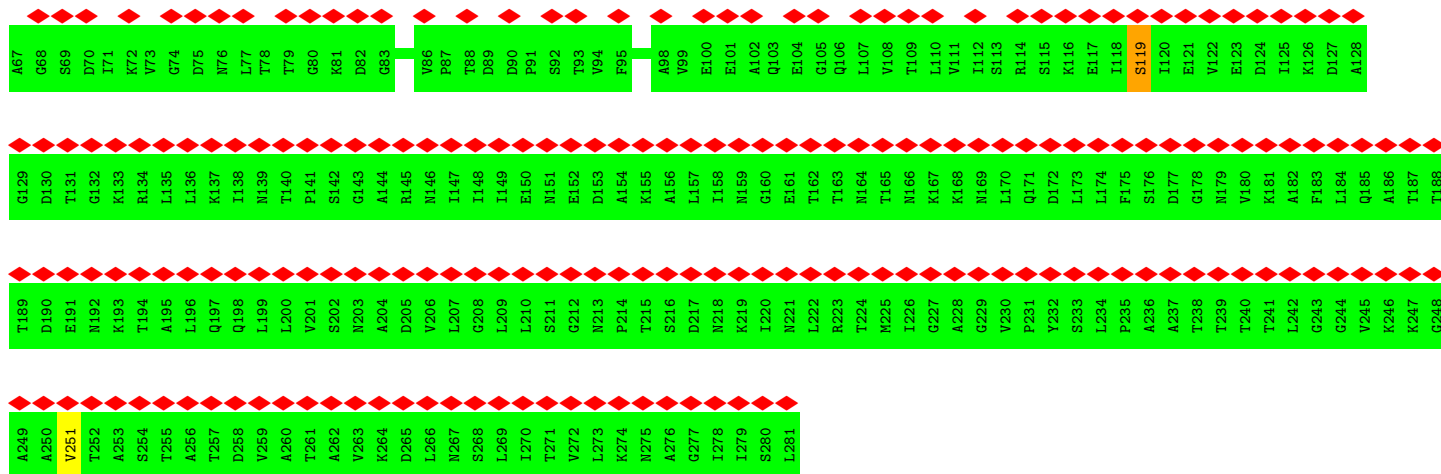


• Molecule 2: Capsid fiber protein

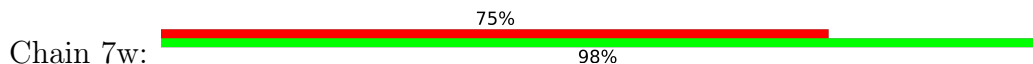


• Molecule 2: Capsid fiber protein

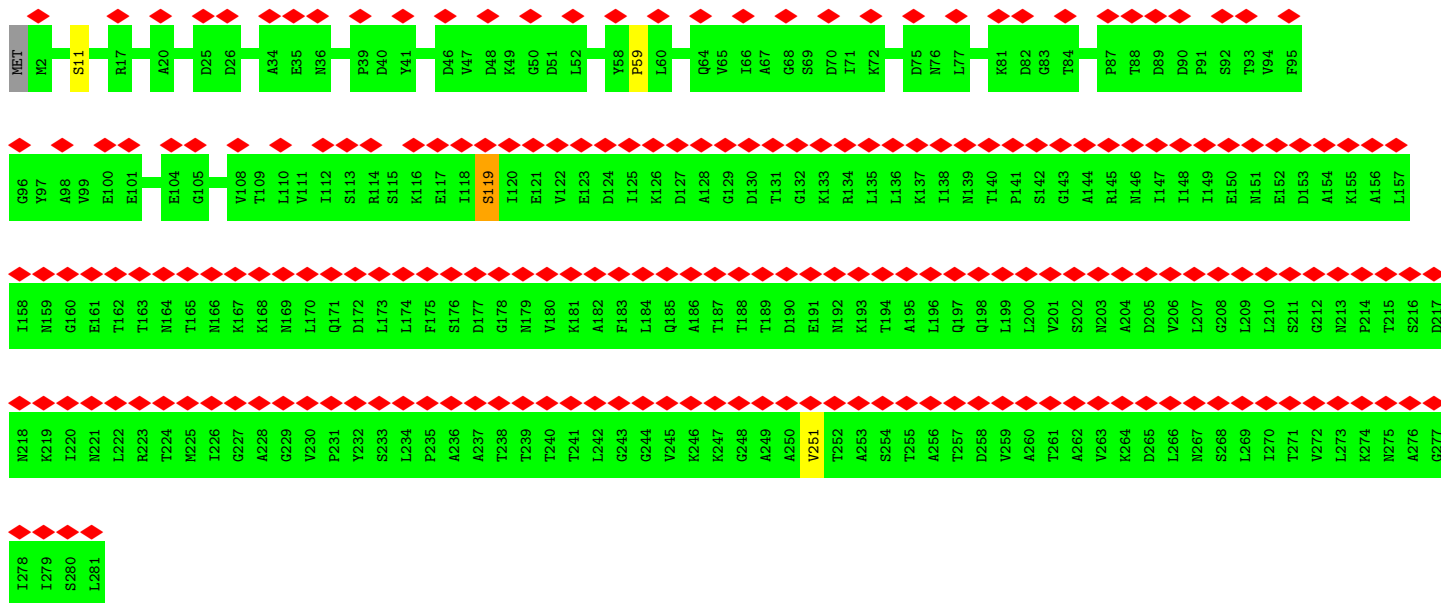




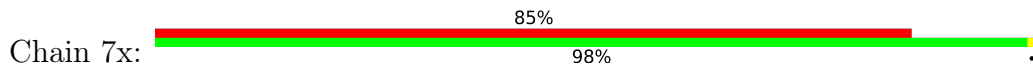
• Molecule 2: Capsid fiber protein



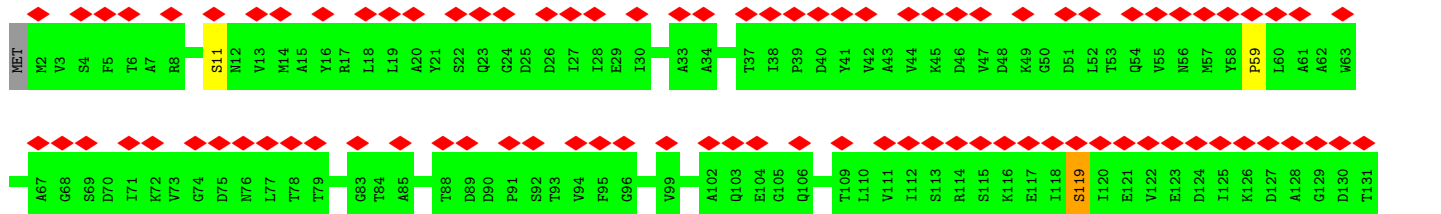
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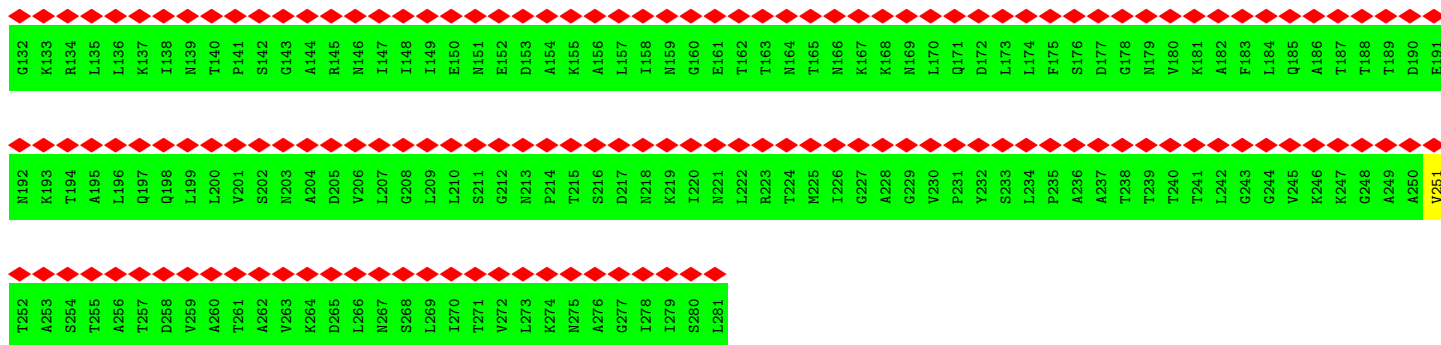


• Molecule 2: Capsid fiber protein

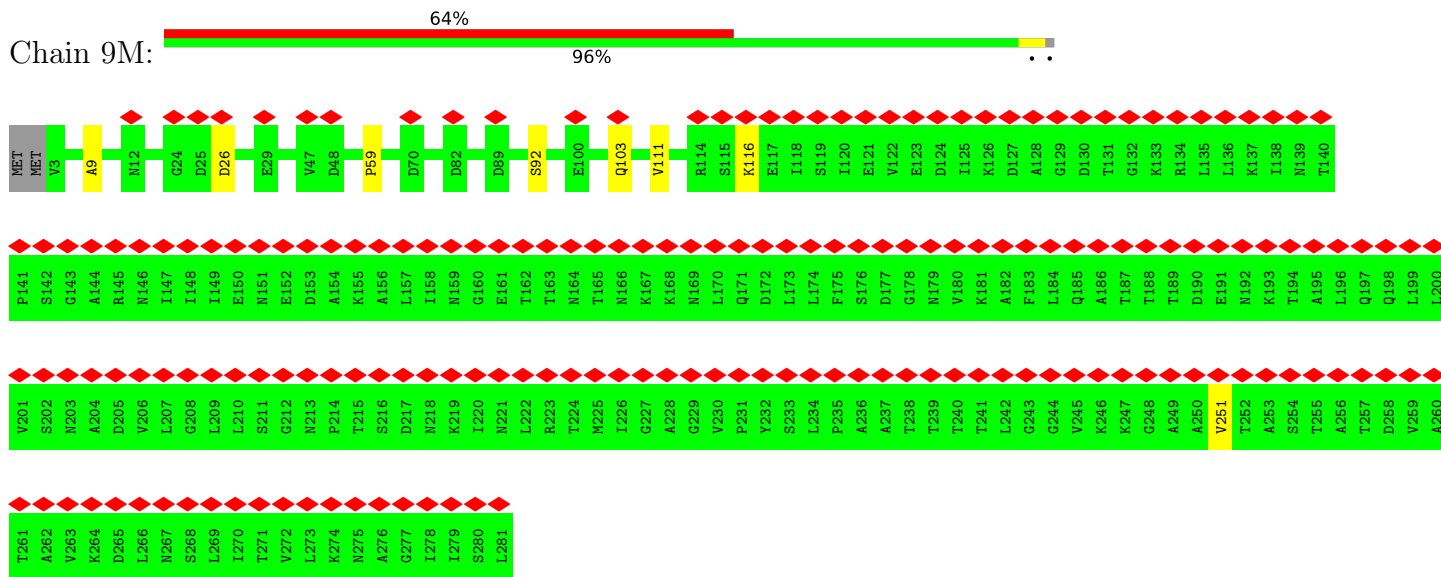


Chain 7x:

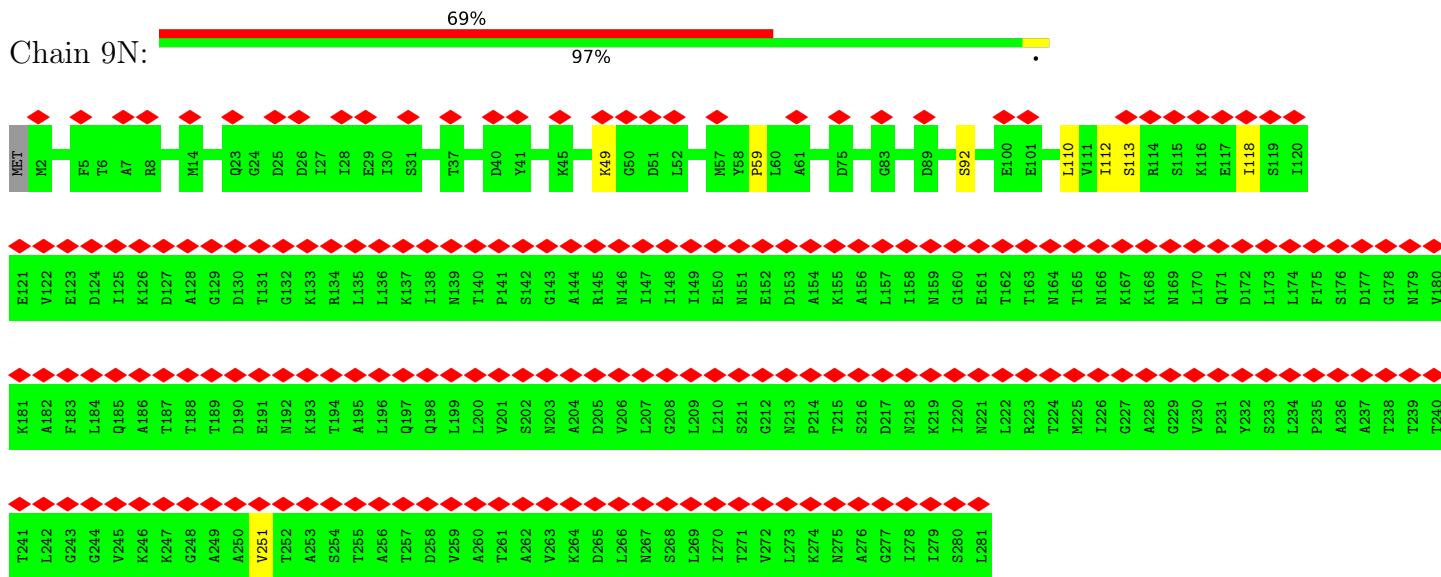




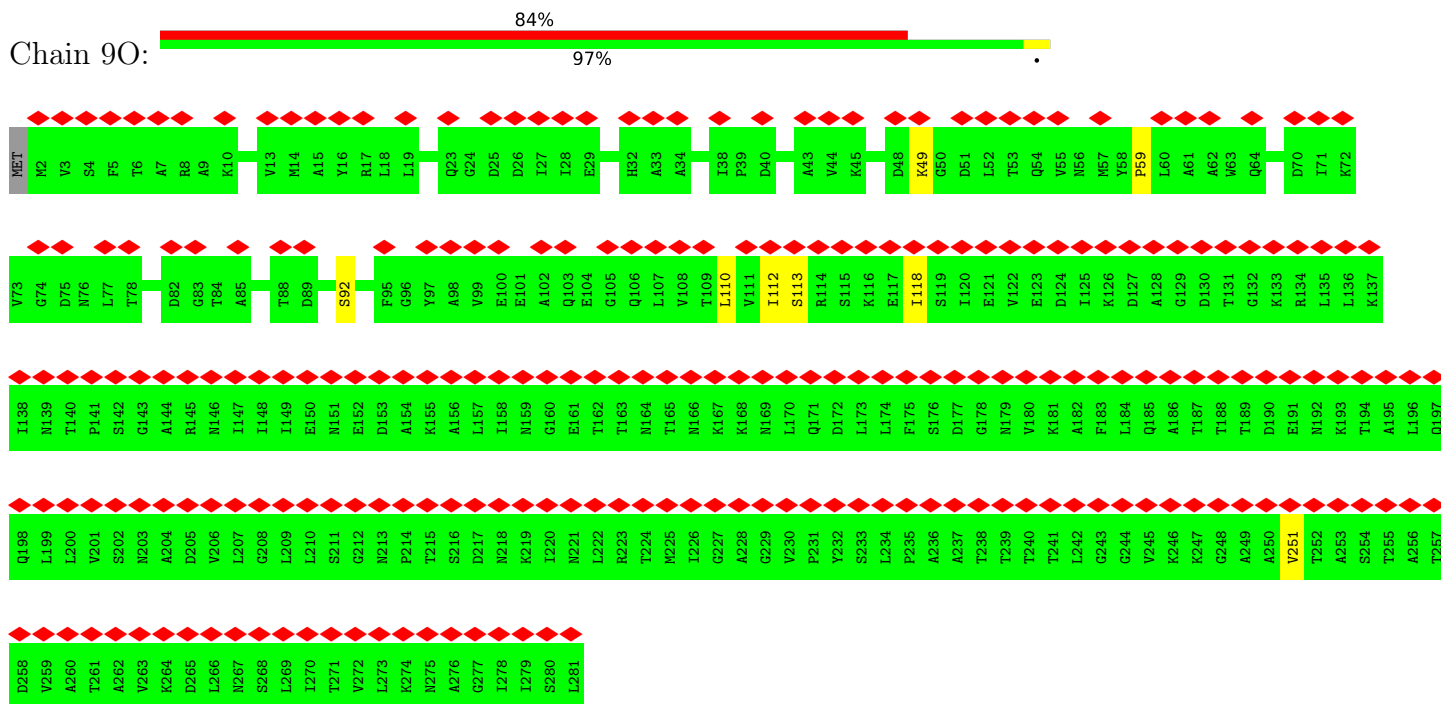
• Molecule 2: Capsid fiber protein



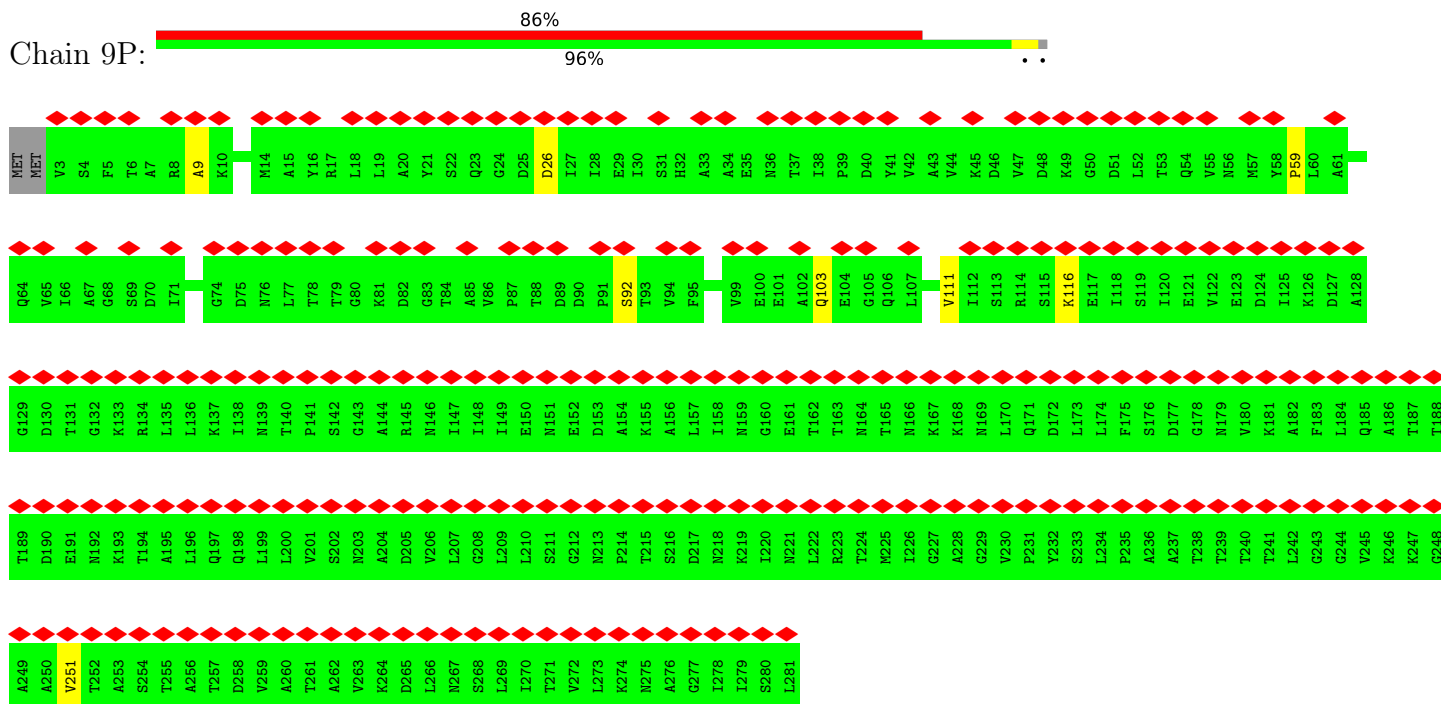
• Molecule 2: Capsid fiber protein



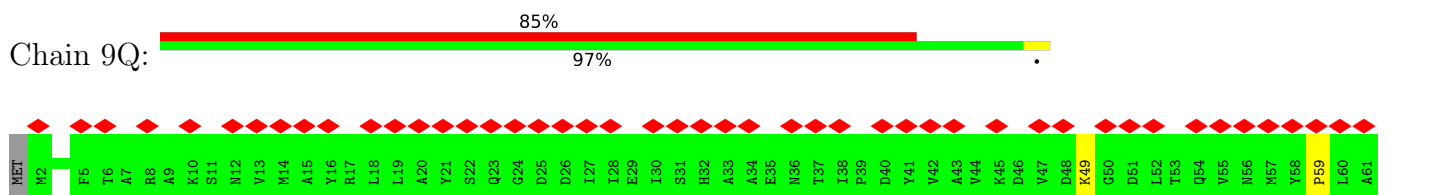
• Molecule 2: Capsid fiber protein

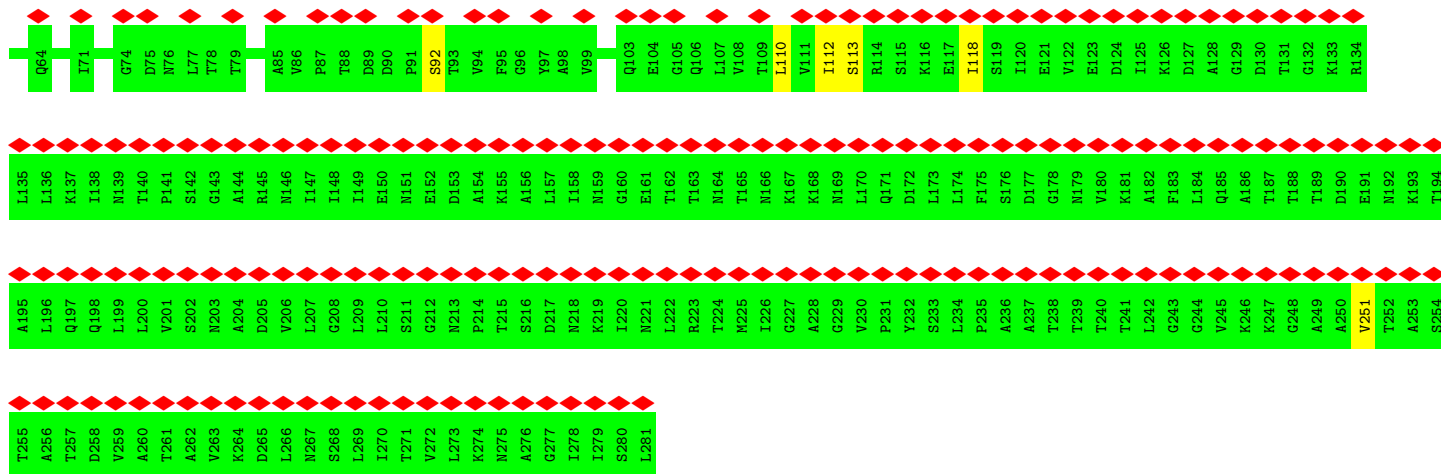


• Molecule 2: Capsid fiber protein

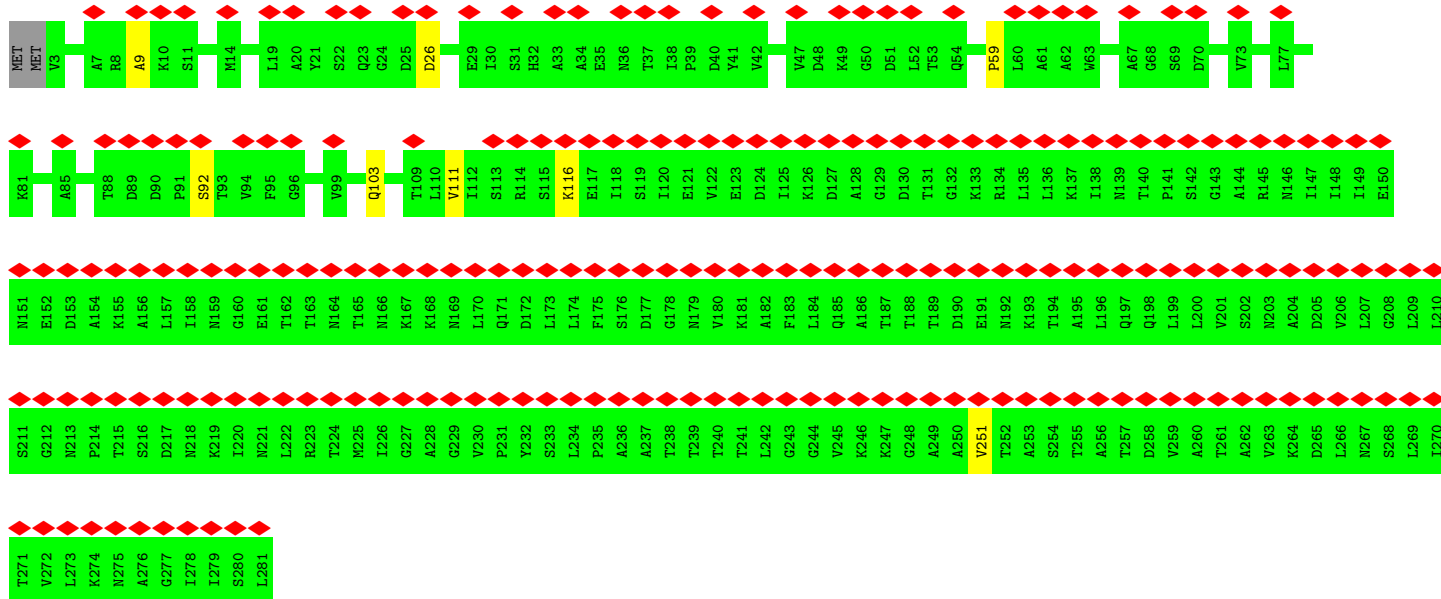
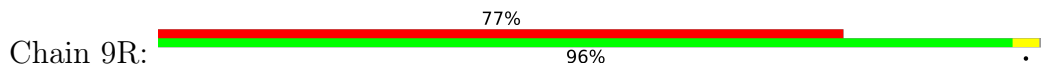


• Molecule 2: Capsid fiber protein

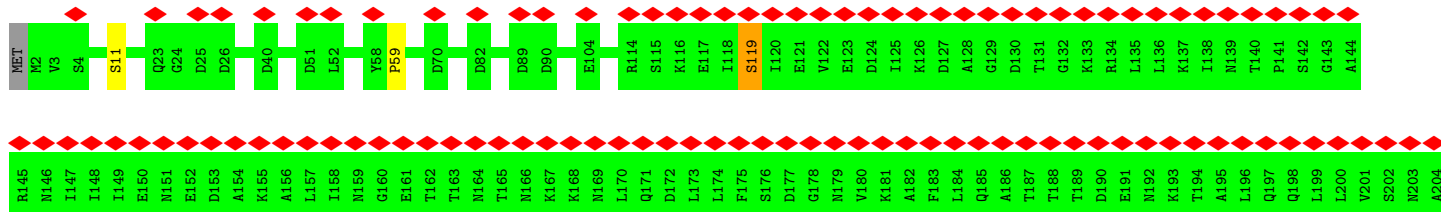




• Molecule 2: Capsid fiber protein



• Molecule 2: Capsid fiber protein



D205 V206 L207 G208 L209 L210 S211 G212 N213 P214 T215 S216 D217 N218 K219 I220 N221 L222 R223 T224 M225 I226 G227 A228 G229 V230 P231 Y232 S233 L234 P235 A236 A237 T238 T239 T240 T241 L242 G243 G244 V245 K246 K247 G248 A249 A250 V251 T252 A253 S254 T255 A256 T257 D258 V259 A260 T261 V263 K264

D265 L266 N267 S268 L269 I270 T271 V272 L273 K274 N275 A276 G277 I278 I279 S280 L281

4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	36730	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	GATAN K2 SUMMIT (4k x 4k)	Depositor
Maximum map value	22.084	Depositor
Minimum map value	-0.418	Depositor
Average map value	0.103	Depositor
Map value standard deviation	0.764	Depositor
Recommended contour level	3.0	Depositor
Map size (\AA)	740.8544, 740.8544, 740.8544	wwPDB
Map dimensions	572, 572, 572	wwPDB
Map angles ($^\circ$)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (\AA)	1.2952, 1.2952, 1.2952	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	0/3456	0.60	1/4693 (0.0%)
1	1B	0.61	0/3551	0.66	0/4822
1	1C	0.58	0/3547	0.62	0/4817
1	1D	0.60	0/3551	0.66	2/4822 (0.0%)
1	1E	0.57	0/3485	0.59	0/4732
1	1F	0.54	0/3513	0.64	2/4771 (0.0%)
1	1G	0.53	0/3456	0.60	1/4693 (0.0%)
1	1H	0.61	0/3551	0.66	0/4822
1	1I	0.58	0/3547	0.62	0/4817
1	1J	0.60	0/3551	0.66	2/4822 (0.0%)
1	1K	0.57	0/3485	0.59	0/4732
1	1L	0.54	0/3513	0.64	2/4771 (0.0%)
1	1M	0.53	0/3456	0.60	1/4693 (0.0%)
1	1N	0.61	0/3551	0.66	0/4822
1	1O	0.58	0/3547	0.62	0/4817
1	1P	0.60	0/3551	0.66	2/4822 (0.0%)
1	1Q	0.57	0/3485	0.59	0/4732
1	1R	0.54	0/3513	0.64	2/4771 (0.0%)
1	1S	0.53	0/3456	0.60	1/4693 (0.0%)
1	1T	0.61	0/3551	0.66	0/4822
1	1U	0.58	0/3547	0.62	0/4817
1	1V	0.60	0/3551	0.66	2/4822 (0.0%)
1	1W	0.57	0/3485	0.59	0/4732
1	1X	0.54	0/3513	0.64	2/4771 (0.0%)
1	1Y	0.53	0/3456	0.60	1/4693 (0.0%)
1	1Z	0.61	0/3551	0.66	0/4822
1	1a	0.58	0/3547	0.62	0/4817
1	1b	0.60	0/3551	0.66	2/4822 (0.0%)
1	1c	0.57	0/3485	0.59	0/4732
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	0.61	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	0/3547	0.62	0/4817
1	3F	0.61	0/3551	0.63	1/4822 (0.0%)
1	3G	0.63	0/3485	0.64	1/4732 (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	0/3547	0.62	0/4817
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	0/3547	0.62	0/4817
1	3R	0.61	0/3551	0.63	1/4822 (0.0%)
1	3S	0.63	0/3485	0.64	2/4732 (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	0/3547	0.62	0/4817
1	3X	0.61	0/3551	0.63	1/4822 (0.0%)
1	3Y	0.63	0/3485	0.64	2/4732 (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	0/3547	0.62	0/4817
1	3d	0.61	0/3551	0.63	1/4822 (0.0%)
1	4A	0.63	0/3485	0.62	1/4732 (0.0%)
1	4B	0.61	0/3485	0.67	1/4732 (0.0%)
1	4C	0.65	0/3489	0.67	0/4737
1	4D	0.65	0/3485	0.63	0/4732
1	4E	0.63	0/3547	0.65	0/4817
1	4F	0.64	0/3551	0.67	0/4822
1	4G	0.64	0/3485	0.62	1/4732 (0.0%)
1	4H	0.61	0/3485	0.67	1/4732 (0.0%)
1	4I	0.65	0/3489	0.67	0/4737
1	4J	0.65	0/3485	0.64	0/4732
1	4K	0.63	0/3547	0.65	0/4817
1	4L	0.64	0/3551	0.67	0/4822
1	4M	0.63	0/3485	0.62	1/4732 (0.0%)
1	4N	0.61	0/3485	0.67	1/4732 (0.0%)
1	4O	0.65	0/3489	0.67	0/4737
1	4P	0.65	0/3485	0.64	0/4732
1	4Q	0.63	0/3547	0.65	0/4817
1	4R	0.64	0/3551	0.67	0/4822
1	4S	0.63	0/3485	0.62	1/4732 (0.0%)
1	4T	0.61	0/3485	0.67	1/4732 (0.0%)
1	4U	0.65	0/3489	0.67	0/4737
1	4V	0.65	0/3485	0.64	0/4732
1	4W	0.63	0/3547	0.65	0/4817
1	4X	0.64	0/3551	0.67	0/4822
1	4Y	0.63	0/3485	0.62	1/4732 (0.0%)
1	4Z	0.61	0/3485	0.67	1/4732 (0.0%)
1	4a	0.65	0/3489	0.67	0/4737
1	4b	0.65	0/3485	0.64	0/4732
1	4c	0.63	0/3547	0.65	0/4817
1	4d	0.64	0/3551	0.67	0/4822
1	5A	0.64	0/3485	0.64	1/4732 (0.0%)
1	5B	0.62	0/3485	0.69	1/4732 (0.0%)
1	5C	0.63	0/3489	0.68	3/4737 (0.1%)
1	5D	0.62	0/3485	0.62	0/4732
1	5E	0.60	0/3547	0.68	2/4817 (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	0/3485	0.64	1/4732 (0.0%)
1	5H	0.62	0/3485	0.69	1/4732 (0.0%)
1	5I	0.63	0/3489	0.68	3/4737 (0.1%)
1	5J	0.62	0/3485	0.62	0/4732
1	5K	0.60	0/3547	0.68	2/4817 (0.0%)
1	5L	0.65	0/3551	0.67	0/4822
1	5M	0.64	0/3485	0.64	1/4732 (0.0%)
1	5N	0.62	0/3485	0.69	1/4732 (0.0%)
1	5O	0.63	0/3489	0.68	3/4737 (0.1%)
1	5P	0.62	0/3485	0.62	0/4732
1	5Q	0.60	0/3547	0.68	2/4817 (0.0%)
1	5R	0.65	0/3551	0.67	0/4822
1	5S	0.64	0/3485	0.64	1/4732 (0.0%)
1	5T	0.62	0/3485	0.69	1/4732 (0.0%)
1	5U	0.63	0/3489	0.68	3/4737 (0.1%)
1	5V	0.62	0/3485	0.62	0/4732
1	5W	0.60	0/3547	0.68	2/4817 (0.0%)
1	5X	0.65	0/3551	0.67	0/4822
1	5Y	0.64	0/3485	0.64	1/4732 (0.0%)
1	5Z	0.62	0/3485	0.69	1/4732 (0.0%)
1	5a	0.63	0/3489	0.68	3/4737 (0.1%)
1	5b	0.62	0/3485	0.62	0/4732
1	5c	0.60	0/3547	0.68	2/4817 (0.0%)
1	5d	0.65	0/3551	0.67	0/4822
1	6A	0.62	0/3547	0.63	0/4817
1	6B	0.62	0/3551	0.63	0/4822
1	6C	0.62	0/3485	0.67	1/4732 (0.0%)
1	6D	0.63	1/3489 (0.0%)	0.67	1/4737 (0.0%)
1	6E	0.62	0/3547	0.63	0/4817
1	6F	0.62	0/3551	0.63	1/4822 (0.0%)
1	6G	0.62	0/3547	0.63	0/4817
1	6H	0.62	0/3551	0.63	0/4822
1	6I	0.62	0/3485	0.67	1/4732 (0.0%)
1	6J	0.63	1/3489 (0.0%)	0.67	1/4737 (0.0%)
1	6K	0.62	0/3547	0.63	0/4817
1	6L	0.63	0/3551	0.63	1/4822 (0.0%)
1	6M	0.62	0/3547	0.63	0/4817
1	6N	0.62	0/3551	0.63	0/4822
1	6O	0.62	0/3485	0.67	1/4732 (0.0%)
1	6P	0.63	1/3489 (0.0%)	0.67	1/4737 (0.0%)
1	6Q	0.62	0/3547	0.63	0/4817
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	0/3547	0.63	0/4817
1	6T	0.62	0/3551	0.63	0/4822
1	6U	0.62	0/3485	0.67	1/4732 (0.0%)
1	6V	0.63	1/3489 (0.0%)	0.67	1/4737 (0.0%)
1	6W	0.62	0/3547	0.63	0/4817
1	6X	0.63	0/3551	0.63	1/4822 (0.0%)
1	6Y	0.62	0/3547	0.64	0/4817
1	6Z	0.62	0/3551	0.63	0/4822
1	6a	0.62	0/3485	0.67	1/4732 (0.0%)
1	6b	0.63	1/3489 (0.0%)	0.67	1/4737 (0.0%)
1	6c	0.62	0/3547	0.63	0/4817
1	6d	0.62	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	0/3547	0.61	0/4817
1	8C	0.61	0/3551	0.62	1/4822 (0.0%)
1	8D	0.59	0/3547	0.59	1/4817 (0.0%)
1	8E	0.58	0/3551	0.61	0/4822
1	8F	0.60	0/3547	0.61	1/4817 (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	0/3547	0.61	0/4817
1	8I	0.61	0/3551	0.62	1/4822 (0.0%)
1	8J	0.59	0/3547	0.59	1/4817 (0.0%)
1	8K	0.58	0/3551	0.61	0/4822
1	8L	0.60	0/3547	0.61	1/4817 (0.0%)
1	8M	0.58	0/3551	0.62	0/4822
1	8N	0.59	0/3547	0.61	0/4817
1	8O	0.61	0/3551	0.62	1/4822 (0.0%)
1	8P	0.59	0/3547	0.59	1/4817 (0.0%)
1	8Q	0.58	0/3551	0.61	0/4822
1	8R	0.60	0/3547	0.61	1/4817 (0.0%)
1	8S	0.58	0/3551	0.62	0/4822
1	8T	0.59	0/3547	0.61	0/4817
1	8U	0.61	0/3551	0.62	1/4822 (0.0%)
1	8V	0.59	0/3547	0.59	1/4817 (0.0%)
1	8W	0.58	0/3551	0.61	0/4822
1	8X	0.60	0/3547	0.61	1/4817 (0.0%)
1	8Y	0.58	0/3551	0.62	0/4822
1	8Z	0.59	0/3547	0.61	0/4817
1	8a	0.61	0/3551	0.62	1/4822 (0.0%)
1	8b	0.59	0/3547	0.59	1/4817 (0.0%)
1	8c	0.58	0/3551	0.61	0/4822
1	8d	0.60	0/3547	0.61	1/4817 (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	85/1183430 (0.0%)	0.65	152/1607950 (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 (85) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	7T	137	GLN	CA-CB	-7.08	1.38	1.53
1	7J	137	GLN	CA-CB	-7.07	1.38	1.53
1	7E	137	GLN	CA-CB	-7.07	1.38	1.53
1	7O	137	GLN	CA-CB	-7.06	1.38	1.53
1	7Y	137	GLN	CA-CB	-7.03	1.38	1.53
2	8v	111	VAL	C-N	-5.68	1.21	1.34
2	9L	111	VAL	C-N	-5.67	1.21	1.34
2	9R	111	VAL	C-N	-5.67	1.21	1.34
2	8j	111	VAL	C-N	-5.67	1.21	1.34
2	9P	111	VAL	C-N	-5.67	1.21	1.34
2	8h	111	VAL	C-N	-5.67	1.21	1.34
2	1n	111	VAL	C-N	-5.67	1.21	1.34
2	5j	111	VAL	C-N	-5.66	1.21	1.34
2	5f	111	VAL	C-N	-5.66	1.21	1.34
2	8n	111	VAL	C-N	-5.66	1.21	1.34
2	8p	111	VAL	C-N	-5.66	1.21	1.34
2	8z	111	VAL	C-N	-5.66	1.21	1.34
2	1v	111	VAL	C-N	-5.66	1.21	1.34
2	4h	111	VAL	C-N	-5.66	1.21	1.34
2	6q	111	VAL	C-N	-5.66	1.21	1.34
2	1r	111	VAL	C-N	-5.65	1.21	1.34
2	8k	111	VAL	C-N	-5.65	1.21	1.34
2	8t	111	VAL	C-N	-5.65	1.21	1.34
2	3s	111	VAL	C-N	-5.65	1.21	1.34
2	5l	111	VAL	C-N	-5.65	1.21	1.34
2	1f	111	VAL	C-N	-5.65	1.21	1.34
2	6e	111	VAL	C-N	-5.65	1.21	1.34
2	4j	111	VAL	C-N	-5.65	1.21	1.34
2	5n	111	VAL	C-N	-5.65	1.21	1.34
2	9M	111	VAL	C-N	-5.65	1.21	1.34
2	8e	111	VAL	C-N	-5.64	1.21	1.34
1	2U	238	VAL	CB-CG1	-5.64	1.41	1.52
2	3k	111	VAL	C-N	-5.64	1.21	1.34
2	3q	111	VAL	C-N	-5.64	1.21	1.34
2	6i	111	VAL	C-N	-5.64	1.21	1.34
1	2K	238	VAL	CB-CG1	-5.64	1.41	1.52
2	3g	111	VAL	C-N	-5.64	1.21	1.34

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	8q	111	VAL	C-N	-5.64	1.21	1.34
2	1x	111	VAL	C-N	-5.64	1.21	1.34
2	6u	111	VAL	C-N	-5.64	1.21	1.34
2	4n	111	VAL	C-N	-5.63	1.21	1.34
2	1j	111	VAL	C-N	-5.63	1.21	1.34
2	6m	111	VAL	C-N	-5.63	1.21	1.34
2	8w	111	VAL	C-N	-5.63	1.21	1.34
2	3e	111	VAL	C-N	-5.63	1.21	1.34
2	3i	111	VAL	C-N	-5.63	1.21	1.34
2	4f	111	VAL	C-N	-5.62	1.21	1.34
2	5h	111	VAL	C-N	-5.62	1.21	1.34
2	3m	111	VAL	C-N	-5.62	1.21	1.34
2	4l	111	VAL	C-N	-5.62	1.21	1.34
2	6o	111	VAL	C-N	-5.62	1.21	1.34
2	6s	111	VAL	C-N	-5.62	1.21	1.34
2	6g	111	VAL	C-N	-5.62	1.21	1.34
2	6k	111	VAL	C-N	-5.62	1.21	1.34
1	2A	238	VAL	CB-CG1	-5.61	1.41	1.52
2	3o	111	VAL	C-N	-5.61	1.21	1.34
2	3w	111	VAL	C-N	-5.61	1.21	1.34
2	6w	111	VAL	C-N	-5.61	1.21	1.34
2	1h	111	VAL	C-N	-5.61	1.21	1.34
2	3u	111	VAL	C-N	-5.60	1.21	1.34
1	2P	238	VAL	CB-CG1	-5.59	1.41	1.52
2	1l	111	VAL	C-N	-5.59	1.21	1.34
1	2F	238	VAL	CB-CG1	-5.59	1.41	1.52
2	1t	111	VAL	C-N	-5.58	1.21	1.34
2	1p	111	VAL	C-N	-5.58	1.21	1.34
1	3D	319	TYR	CD2-CE2	-5.33	1.31	1.39
1	3J	319	TYR	CD2-CE2	-5.33	1.31	1.39
1	3P	319	TYR	CB-CG	-5.32	1.43	1.51
1	3b	319	TYR	CB-CG	-5.32	1.43	1.51
1	3V	319	TYR	CD2-CE2	-5.31	1.31	1.39
1	3P	319	TYR	CD2-CE2	-5.30	1.31	1.39
1	3b	319	TYR	CD2-CE2	-5.30	1.31	1.39
1	3V	319	TYR	CB-CG	-5.29	1.43	1.51
1	3D	319	TYR	CB-CG	-5.29	1.43	1.51
1	3J	319	TYR	CB-CG	-5.26	1.43	1.51
1	6b	332	VAL	CB-CG1	-5.16	1.42	1.52
1	6J	332	VAL	CB-CG1	-5.15	1.42	1.52
1	6D	332	VAL	CB-CG1	-5.13	1.42	1.52
1	6P	332	VAL	CB-CG1	-5.12	1.42	1.52

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	6V	332	VAL	CB-CG1	-5.12	1.42	1.52
1	7E	437	ILE	C-N	-5.11	1.22	1.34
1	7J	437	ILE	C-N	-5.11	1.22	1.34
1	7Y	437	ILE	C-N	-5.10	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

All (152) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	1R	355	SER	C-N-CD	-9.96	98.69	120.60
1	1d	355	SER	C-N-CD	-9.96	98.69	120.60
1	1X	355	SER	C-N-CD	-9.96	98.70	120.60
1	1L	355	SER	C-N-CD	-9.95	98.71	120.60
1	1F	355	SER	C-N-CD	-9.95	98.72	120.60
1	3T	354	VAL	C-N-CA	8.15	142.08	121.70
1	3N	354	VAL	C-N-CA	8.15	142.07	121.70
1	3B	354	VAL	C-N-CA	8.14	142.06	121.70
1	3H	354	VAL	C-N-CA	8.14	142.05	121.70
1	3Z	354	VAL	C-N-CA	8.14	142.04	121.70
1	7X	330	LEU	CA-CB-CG	7.60	132.77	115.30
1	7D	330	LEU	CA-CB-CG	7.58	132.74	115.30
1	7I	330	LEU	CA-CB-CG	7.58	132.74	115.30
1	7N	330	LEU	CA-CB-CG	7.58	132.73	115.30
1	7S	330	LEU	CA-CB-CG	7.58	132.72	115.30
1	2V	355	SER	C-N-CD	-7.07	105.05	120.60
1	2L	355	SER	C-N-CD	-7.06	105.07	120.60
1	2B	355	SER	C-N-CD	-7.06	105.07	120.60
1	2G	355	SER	C-N-CD	-7.06	105.08	120.60
1	2Q	355	SER	C-N-CD	-7.05	105.08	120.60
1	1b	330	LEU	CB-CG-CD1	-6.80	99.44	111.00
1	1V	330	LEU	CB-CG-CD1	-6.79	99.46	111.00
1	1D	330	LEU	CB-CG-CD1	-6.78	99.48	111.00
1	1J	330	LEU	CB-CG-CD1	-6.76	99.50	111.00
1	1P	330	LEU	CB-CG-CD1	-6.76	99.51	111.00
1	4N	203	PRO	C-N-CA	6.71	138.48	121.70
1	4T	203	PRO	C-N-CA	6.70	138.46	121.70
1	4B	203	PRO	C-N-CA	6.69	138.43	121.70
1	4Z	203	PRO	C-N-CA	6.69	138.43	121.70
1	4H	203	PRO	C-N-CA	6.68	138.40	121.70
1	5c	294	LEU	CA-CB-CG	6.47	130.18	115.30
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	5W	294	LEU	CA-CB-CG	6.46	130.15	115.30
1	5E	294	LEU	CA-CB-CG	6.46	130.15	115.30
1	5Q	294	LEU	CA-CB-CG	6.45	130.13	115.30
1	2F	354	VAL	C-N-CA	6.43	137.78	121.70
1	2A	354	VAL	C-N-CA	6.43	137.77	121.70
1	2P	354	VAL	C-N-CA	6.42	137.75	121.70
1	2U	354	VAL	C-N-CA	6.41	137.72	121.70
1	2K	354	VAL	C-N-CA	6.40	137.69	121.70
1	5U	155	SER	C-N-CA	6.39	137.67	121.70
1	5O	155	SER	C-N-CA	6.38	137.65	121.70
1	5C	155	SER	C-N-CA	6.37	137.63	121.70
1	5a	155	SER	C-N-CA	6.37	137.62	121.70
1	5I	155	SER	C-N-CA	6.35	137.58	121.70
1	5a	130	LEU	CB-CG-CD1	-6.32	100.26	111.00
1	5C	130	LEU	CB-CG-CD1	-6.30	100.28	111.00
1	5O	130	LEU	CB-CG-CD1	-6.30	100.29	111.00
1	5I	130	LEU	CB-CG-CD1	-6.29	100.31	111.00
1	5U	130	LEU	CB-CG-CD1	-6.28	100.32	111.00
1	6d	330	LEU	CA-CB-CG	6.22	129.62	115.30
1	6F	330	LEU	CA-CB-CG	6.21	129.58	115.30
1	6L	330	LEU	CA-CB-CG	6.21	129.58	115.30
1	6R	330	LEU	CA-CB-CG	6.20	129.56	115.30
1	6X	330	LEU	CA-CB-CG	6.20	129.56	115.30
1	3M	249	LEU	CB-CG-CD2	-6.00	100.79	111.00
1	3S	249	LEU	CB-CG-CD2	-6.00	100.80	111.00
1	3A	249	LEU	CB-CG-CD2	-5.99	100.81	111.00
1	3Y	249	LEU	CB-CG-CD2	-5.99	100.82	111.00
1	3G	249	LEU	CB-CG-CD2	-5.95	100.88	111.00
1	7Y	306	LEU	CA-CB-CG	5.95	128.98	115.30
1	7T	306	LEU	CA-CB-CG	5.94	128.97	115.30
1	7E	306	LEU	CA-CB-CG	5.94	128.96	115.30
1	7O	306	LEU	CA-CB-CG	5.94	128.96	115.30
1	7J	306	LEU	CA-CB-CG	5.93	128.95	115.30
1	7F	39	ALA	C-N-CA	5.90	136.45	121.70
1	7A	39	ALA	C-N-CA	5.89	136.43	121.70
1	7U	39	ALA	C-N-CA	5.89	136.42	121.70
1	7P	39	ALA	C-N-CA	5.89	136.42	121.70
1	7K	39	ALA	C-N-CA	5.88	136.40	121.70
1	8I	130	LEU	CA-CB-CG	5.76	128.56	115.30
1	8C	130	LEU	CA-CB-CG	5.74	128.50	115.30
1	8O	130	LEU	CA-CB-CG	5.74	128.50	115.30
1	8a	130	LEU	CA-CB-CG	5.74	128.49	115.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	8U	130	LEU	CA-CB-CG	5.73	128.49	115.30
1	1A	250	ILE	CG1-CB-CG2	-5.73	98.80	111.40
1	1M	250	ILE	CG1-CB-CG2	-5.73	98.80	111.40
1	1S	250	ILE	CG1-CB-CG2	-5.72	98.81	111.40
1	1G	250	ILE	CG1-CB-CG2	-5.72	98.82	111.40
1	1Y	250	ILE	CG1-CB-CG2	-5.72	98.82	111.40
1	6U	134	ARG	NE-CZ-NH1	-5.62	117.49	120.30
1	6a	134	ARG	NE-CZ-NH1	-5.61	117.49	120.30
1	6C	134	ARG	NE-CZ-NH1	-5.57	117.52	120.30
1	1R	330	LEU	CB-CG-CD2	-5.54	101.58	111.00
1	1J	354	VAL	C-N-CA	5.53	135.51	121.70
1	1V	354	VAL	C-N-CA	5.53	135.51	121.70
1	1X	330	LEU	CB-CG-CD2	-5.52	101.62	111.00
1	5G	250	ILE	CG1-CB-CG2	-5.51	99.27	111.40
1	6I	134	ARG	NE-CZ-NH1	-5.51	117.54	120.30
1	1F	330	LEU	CB-CG-CD2	-5.51	101.63	111.00
1	1L	330	LEU	CB-CG-CD2	-5.51	101.63	111.00
1	1D	354	VAL	C-N-CA	5.51	135.47	121.70
1	5A	250	ILE	CG1-CB-CG2	-5.51	99.28	111.40
1	1b	354	VAL	C-N-CA	5.50	135.46	121.70
1	5Y	250	ILE	CG1-CB-CG2	-5.50	99.29	111.40
1	5S	250	ILE	CG1-CB-CG2	-5.50	99.30	111.40
1	1P	354	VAL	C-N-CA	5.50	135.44	121.70
1	1d	330	LEU	CB-CG-CD2	-5.50	101.66	111.00
1	5M	250	ILE	CG1-CB-CG2	-5.49	99.31	111.40
1	6O	134	ARG	NE-CZ-NH1	-5.46	117.57	120.30
1	8J	93	LEU	CA-CB-CG	5.45	127.83	115.30
1	8V	93	LEU	CA-CB-CG	5.44	127.82	115.30
1	8P	93	LEU	CA-CB-CG	5.44	127.80	115.30
1	8D	93	LEU	CA-CB-CG	5.43	127.80	115.30
1	8b	93	LEU	CA-CB-CG	5.43	127.80	115.30
1	4S	250	ILE	CG1-CB-CG2	-5.42	99.47	111.40
1	5W	224	LEU	CA-CB-CG	5.42	127.77	115.30
1	4A	250	ILE	CG1-CB-CG2	-5.42	99.48	111.40
1	4G	250	ILE	CG1-CB-CG2	-5.41	99.49	111.40
1	4Y	250	ILE	CG1-CB-CG2	-5.41	99.49	111.40
1	5Q	224	LEU	CA-CB-CG	5.41	127.75	115.30
1	5E	224	LEU	CA-CB-CG	5.40	127.71	115.30
1	4M	250	ILE	CG1-CB-CG2	-5.39	99.53	111.40
1	5K	224	LEU	CA-CB-CG	5.39	127.70	115.30
1	5c	224	LEU	CA-CB-CG	5.39	127.69	115.30
1	7I	330	LEU	CB-CG-CD1	-5.34	101.93	111.00

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	7D	330	LEU	CB-CG-CD1	-5.33	101.94	111.00
1	7N	330	LEU	CB-CG-CD1	-5.33	101.94	111.00
1	7S	330	LEU	CB-CG-CD1	-5.32	101.95	111.00
1	7X	330	LEU	CB-CG-CD1	-5.32	101.96	111.00
1	5N	374	ARG	NE-CZ-NH1	-5.25	117.67	120.30
1	5I	32	PHE	CB-CG-CD1	5.24	124.47	120.80
1	5a	32	PHE	CB-CG-CD1	5.23	124.46	120.80
1	5O	32	PHE	CB-CG-CD1	5.22	124.45	120.80
1	5Z	374	ARG	NE-CZ-NH1	-5.21	117.70	120.30
1	5C	32	PHE	CB-CG-CD1	5.18	124.42	120.80
1	5B	374	ARG	NE-CZ-NH1	-5.17	117.72	120.30
1	3a	250	ILE	CG1-CB-CG2	-5.16	100.05	111.40
1	5U	32	PHE	CB-CG-CD1	5.14	124.40	120.80
1	3C	250	ILE	CG1-CB-CG2	-5.13	100.10	111.40
1	3U	250	ILE	CG1-CB-CG2	-5.13	100.11	111.40
1	3I	250	ILE	CG1-CB-CG2	-5.13	100.12	111.40
1	3O	250	ILE	CG1-CB-CG2	-5.12	100.13	111.40
1	5T	374	ARG	NE-CZ-NH1	-5.10	117.75	120.30
1	5H	374	ARG	NE-CZ-NH1	-5.09	117.75	120.30
1	8d	250	ILE	CG1-CB-CG2	-5.08	100.22	111.40
1	8L	250	ILE	CG1-CB-CG2	-5.08	100.23	111.40
1	8X	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	8R	250	ILE	CG1-CB-CG2	-5.06	100.28	111.40
1	6J	317	GLY	N-CA-C	-5.03	100.52	113.10
1	3L	249	LEU	CA-CB-CG	-5.03	103.74	115.30
1	3d	249	LEU	CA-CB-CG	-5.03	103.74	115.30
1	3X	249	LEU	CA-CB-CG	-5.02	103.75	115.30
1	3R	249	LEU	CA-CB-CG	-5.02	103.75	115.30
1	6b	317	GLY	N-CA-C	-5.02	100.55	113.10
1	6D	317	GLY	N-CA-C	-5.02	100.56	113.10
1	3F	249	LEU	CA-CB-CG	-5.01	103.77	115.30
1	6P	317	GLY	N-CA-C	-5.01	100.58	113.10
1	6V	317	GLY	N-CA-C	-5.01	100.58	113.10
1	3Y	412	LEU	CA-CB-CG	-5.01	103.79	115.30
1	3S	412	LEU	CA-CB-CG	-5.00	103.79	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%)	402 (93%)	29 (7%)	0	100	100
1	1B	443/448 (99%)	400 (90%)	41 (9%)	2 (0%)	29	67
1	1C	443/448 (99%)	401 (90%)	41 (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%)	400 (92%)	34 (8%)	2 (0%)	29	67

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	1G	431/448 (96%)	402 (93%)	29 (7%)	0	100	100
1	1H	443/448 (99%)	400 (90%)	41 (9%)	2 (0%)	29	67
1	1I	443/448 (99%)	401 (90%)	41 (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%)	400 (92%)	34 (8%)	2 (0%)	29	67
1	1M	431/448 (96%)	402 (93%)	29 (7%)	0	100	100
1	1N	443/448 (99%)	400 (90%)	41 (9%)	2 (0%)	29	67
1	1O	443/448 (99%)	401 (90%)	41 (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%)	402 (93%)	29 (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%)	399 (90%)	42 (10%)	2 (0%)	29	67
1	1W	433/448 (97%)	406 (94%)	27 (6%)	0	100	100
1	1X	436/448 (97%)	399 (92%)	35 (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%)	399 (90%)	42 (10%)	2 (0%)	29	67
1	1c	433/448 (97%)	406 (94%)	27 (6%)	0	100	100
1	1d	436/448 (97%)	400 (92%)	34 (8%)	2 (0%)	29	67
1	2A	436/448 (97%)	410 (94%)	24 (6%)	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%)	35 (8%)	1 (0%)	47	79
1	2E	443/448 (99%)	402 (91%)	38 (9%)	3 (1%)	22	61
1	2F	436/448 (97%)	410 (94%)	24 (6%)	2 (0%)	29	67
1	2G	443/448 (99%)	410 (93%)	30 (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%)	410 (94%)	24 (6%)	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%)	410 (94%)	24 (6%)	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%)	35 (8%)	1 (0%)	47	79
1	2T	443/448 (99%)	402 (91%)	38 (9%)	3 (1%)	22	61
1	2U	436/448 (97%)	411 (94%)	23 (5%)	2 (0%)	29	67
1	2V	443/448 (99%)	409 (92%)	31 (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%)	35 (8%)	1 (0%)	47	79
1	2Y	443/448 (99%)	403 (91%)	37 (8%)	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%)	404 (91%)	39 (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%)	400 (92%)	33 (8%)	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%)	400 (92%)	33 (8%)	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%)	403 (91%)	40 (9%)	0	100	100
1	4X	443/448 (99%)	383 (86%)	60 (14%)	0	100	100
1	4Y	433/448 (97%)	401 (93%)	32 (7%)	0	100	100
1	4Z	433/448 (97%)	379 (88%)	48 (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%)	370 (86%)	61 (14%)	2 (0%)	29	67
1	5C	433/448 (97%)	386 (89%)	44 (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%)	399 (92%)	34 (8%)	0	100	100
1	5H	433/448 (97%)	370 (86%)	61 (14%)	2 (0%)	29	67
1	5I	433/448 (97%)	386 (89%)	44 (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%)	399 (92%)	34 (8%)	0	100	100
1	5N	433/448 (97%)	370 (86%)	61 (14%)	2 (0%)	29	67
1	5O	433/448 (97%)	386 (89%)	44 (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%)	395 (89%)	47 (11%)	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%)	370 (86%)	61 (14%)	2 (0%)	29	67
1	5U	433/448 (97%)	386 (89%)	44 (10%)	3 (1%)	22	61
1	5V	433/448 (97%)	394 (91%)	38 (9%)	1 (0%)	47	79
1	5W	443/448 (99%)	395 (89%)	47 (11%)	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%)	370 (86%)	61 (14%)	2 (0%)	29	67
1	5a	433/448 (97%)	386 (89%)	44 (10%)	3 (1%)	22	61
1	5b	433/448 (97%)	394 (91%)	38 (9%)	1 (0%)	47	79
1	5c	443/448 (99%)	395 (89%)	47 (11%)	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%)	407 (92%)	33 (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%)	407 (92%)	30 (7%)	6 (1%)	11	46
1	6H	443/448 (99%)	408 (92%)	32 (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%)	407 (92%)	33 (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%)	399 (90%)	43 (10%)	1 (0%)	47	79
1	6Y	443/448 (99%)	408 (92%)	29 (6%)	6 (1%)	11	46
1	6Z	443/448 (99%)	407 (92%)	33 (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%)	406 (92%)	37 (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%)	406 (92%)	36 (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%)	408 (92%)	34 (8%)	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%)	405 (91%)	38 (9%)	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%)	414 (94%)	27 (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%)	413 (93%)	30 (7%)	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%)	414 (94%)	27 (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
2	1j	285/281 (101%)	268 (94%)	12 (4%)	5 (2%)	8	41
2	1k	286/281 (102%)	271 (95%)	9 (3%)	6 (2%)	7	37
2	1l	285/281 (101%)	268 (94%)	12 (4%)	5 (2%)	8	41
2	1m	286/281 (102%)	271 (95%)	9 (3%)	6 (2%)	7	37
2	1n	285/281 (101%)	268 (94%)	12 (4%)	5 (2%)	8	41
2	1o	286/281 (102%)	271 (95%)	9 (3%)	6 (2%)	7	37
2	1p	285/281 (101%)	268 (94%)	12 (4%)	5 (2%)	8	41
2	1q	286/281 (102%)	271 (95%)	9 (3%)	6 (2%)	7	37
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
2	2c	286/281 (102%)	267 (93%)	16 (6%)	3 (1%)	15	54
2	2d	286/281 (102%)	267 (93%)	16 (6%)	3 (1%)	15	54
2	2e	286/281 (102%)	267 (93%)	16 (6%)	3 (1%)	15	54
2	2f	286/281 (102%)	267 (93%)	16 (6%)	3 (1%)	15	54
2	2g	286/281 (102%)	267 (93%)	16 (6%)	3 (1%)	15	54
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
2	2n	286/281 (102%)	267 (93%)	16 (6%)	3 (1%)	15	54
2	2o	286/281 (102%)	267 (93%)	16 (6%)	3 (1%)	15	54
2	2p	286/281 (102%)	267 (93%)	16 (6%)	3 (1%)	15	54
2	2q	286/281 (102%)	267 (93%)	16 (6%)	3 (1%)	15	54
2	2r	286/281 (102%)	267 (93%)	16 (6%)	3 (1%)	15	54
2	2s	286/281 (102%)	267 (93%)	16 (6%)	3 (1%)	15	54
2	2t	286/281 (102%)	267 (93%)	16 (6%)	3 (1%)	15	54
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
2	3g	285/281 (101%)	268 (94%)	12 (4%)	5 (2%)	8	41
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
2	3l	286/281 (102%)	271 (95%)	9 (3%)	6 (2%)	7	37
2	3m	285/281 (101%)	268 (94%)	12 (4%)	5 (2%)	8	41
2	3n	286/281 (102%)	271 (95%)	9 (3%)	6 (2%)	7	37
2	3o	285/281 (101%)	268 (94%)	12 (4%)	5 (2%)	8	41
2	3p	286/281 (102%)	271 (95%)	9 (3%)	6 (2%)	7	37
2	3q	285/281 (101%)	268 (94%)	12 (4%)	5 (2%)	8	41
2	3r	286/281 (102%)	271 (95%)	9 (3%)	6 (2%)	7	37
2	3s	285/281 (101%)	268 (94%)	12 (4%)	5 (2%)	8	41
2	3t	286/281 (102%)	271 (95%)	9 (3%)	6 (2%)	7	37
2	3u	285/281 (101%)	268 (94%)	12 (4%)	5 (2%)	8	41
2	3v	286/281 (102%)	271 (95%)	9 (3%)	6 (2%)	7	37
2	3w	285/281 (101%)	268 (94%)	12 (4%)	5 (2%)	8	41
2	3x	286/281 (102%)	271 (95%)	9 (3%)	6 (2%)	7	37
2	4e	286/281 (102%)	271 (95%)	9 (3%)	6 (2%)	7	37
2	4f	285/281 (101%)	268 (94%)	12 (4%)	5 (2%)	8	41
2	4g	286/281 (102%)	271 (95%)	9 (3%)	6 (2%)	7	37
2	4h	285/281 (101%)	268 (94%)	12 (4%)	5 (2%)	8	41
2	4i	286/281 (102%)	271 (95%)	9 (3%)	6 (2%)	7	37
2	4j	285/281 (101%)	268 (94%)	12 (4%)	5 (2%)	8	41
2	4k	286/281 (102%)	271 (95%)	9 (3%)	6 (2%)	7	37
2	4l	285/281 (101%)	268 (94%)	12 (4%)	5 (2%)	8	41
2	4m	286/281 (102%)	271 (95%)	9 (3%)	6 (2%)	7	37
2	4n	285/281 (101%)	268 (94%)	12 (4%)	5 (2%)	8	41
2	5e	286/281 (102%)	271 (95%)	9 (3%)	6 (2%)	7	37
2	5f	285/281 (101%)	268 (94%)	12 (4%)	5 (2%)	8	41
2	5g	286/281 (102%)	271 (95%)	9 (3%)	6 (2%)	7	37
2	5h	285/281 (101%)	268 (94%)	12 (4%)	5 (2%)	8	41
2	5i	286/281 (102%)	271 (95%)	9 (3%)	6 (2%)	7	37
2	5j	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
2	5l	285/281 (101%)	268 (94%)	12 (4%)	5 (2%)	8	41
2	5m	286/281 (102%)	271 (95%)	9 (3%)	6 (2%)	7	37
2	5n	285/281 (101%)	268 (94%)	12 (4%)	5 (2%)	8	41
2	6e	285/281 (101%)	268 (94%)	12 (4%)	5 (2%)	8	41
2	6f	286/281 (102%)	271 (95%)	9 (3%)	6 (2%)	7	37
2	6g	285/281 (101%)	268 (94%)	12 (4%)	5 (2%)	8	41
2	6h	286/281 (102%)	271 (95%)	9 (3%)	6 (2%)	7	37
2	6i	285/281 (101%)	268 (94%)	12 (4%)	5 (2%)	8	41
2	6j	286/281 (102%)	271 (95%)	9 (3%)	6 (2%)	7	37
2	6k	285/281 (101%)	268 (94%)	12 (4%)	5 (2%)	8	41
2	6l	286/281 (102%)	271 (95%)	9 (3%)	6 (2%)	7	37
2	6m	285/281 (101%)	268 (94%)	12 (4%)	5 (2%)	8	41
2	6n	286/281 (102%)	271 (95%)	9 (3%)	6 (2%)	7	37
2	6o	285/281 (101%)	268 (94%)	12 (4%)	5 (2%)	8	41
2	6p	286/281 (102%)	271 (95%)	9 (3%)	6 (2%)	7	37
2	6q	285/281 (101%)	268 (94%)	12 (4%)	5 (2%)	8	41
2	6r	286/281 (102%)	271 (95%)	9 (3%)	6 (2%)	7	37
2	6s	285/281 (101%)	268 (94%)	12 (4%)	5 (2%)	8	41
2	6t	286/281 (102%)	271 (95%)	9 (3%)	6 (2%)	7	37
2	6u	285/281 (101%)	268 (94%)	12 (4%)	5 (2%)	8	41
2	6v	286/281 (102%)	271 (95%)	9 (3%)	6 (2%)	7	37
2	6w	285/281 (101%)	268 (94%)	12 (4%)	5 (2%)	8	41
2	6x	286/281 (102%)	271 (95%)	9 (3%)	6 (2%)	7	37
2	7Z	286/281 (102%)	267 (93%)	16 (6%)	3 (1%)	15	54
2	7a	286/281 (102%)	267 (93%)	16 (6%)	3 (1%)	15	54
2	7b	286/281 (102%)	267 (93%)	16 (6%)	3 (1%)	15	54
2	7c	286/281 (102%)	267 (93%)	16 (6%)	3 (1%)	15	54
2	7d	286/281 (102%)	267 (93%)	16 (6%)	3 (1%)	15	54
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
2	7i	286/281 (102%)	267 (93%)	16 (6%)	3 (1%)	15	54
2	7j	286/281 (102%)	267 (93%)	16 (6%)	3 (1%)	15	54
2	7k	286/281 (102%)	267 (93%)	16 (6%)	3 (1%)	15	54
2	7l	286/281 (102%)	267 (93%)	16 (6%)	3 (1%)	15	54
2	7m	286/281 (102%)	267 (93%)	16 (6%)	3 (1%)	15	54
2	7n	286/281 (102%)	267 (93%)	16 (6%)	3 (1%)	15	54
2	7o	286/281 (102%)	267 (93%)	16 (6%)	3 (1%)	15	54
2	7p	286/281 (102%)	267 (93%)	16 (6%)	3 (1%)	15	54
2	7q	286/281 (102%)	267 (93%)	16 (6%)	3 (1%)	15	54
2	7r	286/281 (102%)	267 (93%)	16 (6%)	3 (1%)	15	54
2	7s	286/281 (102%)	267 (93%)	16 (6%)	3 (1%)	15	54
2	7t	286/281 (102%)	267 (93%)	16 (6%)	3 (1%)	15	54
2	7u	286/281 (102%)	267 (93%)	16 (6%)	3 (1%)	15	54
2	7v	286/281 (102%)	267 (93%)	16 (6%)	3 (1%)	15	54
2	7w	286/281 (102%)	267 (93%)	16 (6%)	3 (1%)	15	54
2	7x	286/281 (102%)	267 (93%)	16 (6%)	3 (1%)	15	54
2	8e	285/281 (101%)	268 (94%)	12 (4%)	5 (2%)	8	41
2	8f	286/281 (102%)	271 (95%)	9 (3%)	6 (2%)	7	37
2	8g	286/281 (102%)	271 (95%)	9 (3%)	6 (2%)	7	37
2	8h	285/281 (101%)	268 (94%)	12 (4%)	5 (2%)	8	41
2	8i	286/281 (102%)	271 (95%)	9 (3%)	6 (2%)	7	37
2	8j	285/281 (101%)	268 (94%)	12 (4%)	5 (2%)	8	41
2	8k	285/281 (101%)	268 (94%)	12 (4%)	5 (2%)	8	41
2	8l	286/281 (102%)	271 (95%)	9 (3%)	6 (2%)	7	37
2	8m	286/281 (102%)	271 (95%)	9 (3%)	6 (2%)	7	37
2	8n	285/281 (101%)	268 (94%)	12 (4%)	5 (2%)	8	41
2	8o	286/281 (102%)	271 (95%)	9 (3%)	6 (2%)	7	37
2	8p	285/281 (101%)	268 (94%)	12 (4%)	5 (2%)	8	41
2	8q	285/281 (101%)	268 (94%)	12 (4%)	5 (2%)	8	41

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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
2	8t	285/281 (101%)	268 (94%)	12 (4%)	5 (2%)	8	41
2	8u	286/281 (102%)	271 (95%)	9 (3%)	6 (2%)	7	37
2	8v	285/281 (101%)	268 (94%)	12 (4%)	5 (2%)	8	41
2	8w	285/281 (101%)	268 (94%)	12 (4%)	5 (2%)	8	41
2	8x	286/281 (102%)	271 (95%)	9 (3%)	6 (2%)	7	37
2	8y	286/281 (102%)	271 (95%)	9 (3%)	6 (2%)	7	37
2	8z	285/281 (101%)	268 (94%)	12 (4%)	5 (2%)	8	41
2	9F	286/281 (102%)	267 (93%)	16 (6%)	3 (1%)	15	54
2	9G	286/281 (102%)	267 (93%)	16 (6%)	3 (1%)	15	54
2	9H	286/281 (102%)	267 (93%)	16 (6%)	3 (1%)	15	54
2	9I	286/281 (102%)	267 (93%)	16 (6%)	3 (1%)	15	54
2	9J	286/281 (102%)	267 (93%)	16 (6%)	3 (1%)	15	54
2	9K	286/281 (102%)	271 (95%)	9 (3%)	6 (2%)	7	37
2	9L	285/281 (101%)	268 (94%)	12 (4%)	5 (2%)	8	41
2	9M	285/281 (101%)	268 (94%)	12 (4%)	5 (2%)	8	41
2	9N	286/281 (102%)	271 (95%)	9 (3%)	6 (2%)	7	37
2	9O	286/281 (102%)	271 (95%)	9 (3%)	6 (2%)	7	37
2	9P	285/281 (101%)	268 (94%)	12 (4%)	5 (2%)	8	41
2	9Q	286/281 (102%)	271 (95%)	9 (3%)	6 (2%)	7	37
2	9R	285/281 (101%)	268 (94%)	12 (4%)	5 (2%)	8	41
All	All	150460/151645 (99%)	138708 (92%)	10633 (7%)	1119 (1%)	24	61

All (1119) Ramachandran outliers are listed below:

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

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Mol	Chain	Res	Type
1	5B	386	SER
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	2F	355	SER
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	2K	355	SER
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

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Mol	Chain	Res	Type
1	2U	276	LEU
1	2U	355	SER
1	2V	356	PRO
1	3Z	355	SER
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

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Mol	Chain	Res	Type
2	8u	112	ILE
2	1q	112	ILE
2	1s	112	ILE
2	3r	112	ILE
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	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	2J	356	PRO
1	3G	251	ILE
1	4H	67	ASP

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Mol	Chain	Res	Type
1	4H	68	ARG
1	4H	386	SER
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	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	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	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
1	1b	404	VAL

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Mol	Chain	Res	Type
1	2V	201	ASP
1	2Y	336	ALA
1	3Y	405	SER
1	3b	92	PRO
1	4Z	203	PRO
1	4Z	287	SER
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	2C	356	PRO
1	2E	335	PHE
1	4B	287	SER
1	5C	156	TRP
1	5F	157	GLY
1	5F	440	ASN

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Mol	Chain	Res	Type
1	6B	157	GLY
1	8A	31	ASN
1	1J	380	ASP
1	2H	356	PRO
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	2O	335	PHE
1	2O	336	ALA
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	2R	356	PRO
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	5a	156	TRP
1	5d	157	GLY
1	5d	440	ASN
1	6Z	157	GLY
1	8Y	31	ASN
2	1e	49	LYS
2	1e	59	PRO
2	1g	49	LYS
2	1g	59	PRO
2	2Z	11	SER

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Mol	Chain	Res	Type
2	2a	11	SER
2	2b	11	SER
2	2c	11	SER
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

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Mol	Chain	Res	Type
2	4g	59	PRO
2	5g	49	LYS
2	5g	59	PRO
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

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Mol	Chain	Res	Type
2	7l	11	SER
2	7m	11	SER
2	7n	11	SER
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

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Mol	Chain	Res	Type
2	9I	11	SER
2	1u	49	LYS
2	1u	59	PRO
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	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

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Mol	Chain	Res	Type
1	5I	61	PHE
1	6G	382	LYS
1	6H	156	TRP
1	6I	356	PRO
1	8G	356	PRO
1	1R	92	PRO
1	2M	356	PRO
1	5O	61	PHE
1	6M	382	LYS
1	6N	156	TRP
1	6O	356	PRO
1	7O	287	SER
1	8M	356	PRO
1	1X	92	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	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	2D	337	ASN
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	7J	287	SER
1	2L	37	PRO
1	3P	426	PRO
1	4N	204	THR
1	7M	68	ARG
1	2Q	37	PRO
1	2S	337	ASN
1	3V	426	PRO
1	4T	204	THR
1	7R	68	ARG
1	2V	37	PRO
1	2X	337	ASN
1	3b	426	PRO
1	4Z	204	THR
1	7W	68	ARG
1	3D	20	ILE
1	3D	356	PRO
1	6C	202	GLU
1	3J	20	ILE
1	3J	356	PRO
1	6I	202	GLU

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Mol	Chain	Res	Type
1	3P	20	ILE
1	3V	20	ILE
1	3V	356	PRO
1	3b	20	ILE
2	2Z	59	PRO
2	2a	59	PRO
2	2b	59	PRO
2	2c	59	PRO
2	2d	59	PRO
2	7Z	59	PRO
2	7b	59	PRO
2	7c	59	PRO
2	7d	59	PRO
2	9F	59	PRO
2	2e	59	PRO
2	2f	59	PRO
2	2g	59	PRO
2	2h	59	PRO
2	2i	59	PRO
2	7e	59	PRO
2	7g	59	PRO
2	7h	59	PRO
2	7i	59	PRO
2	2j	59	PRO
2	2m	59	PRO
2	2n	59	PRO
2	7j	59	PRO
2	9H	59	PRO
2	2o	59	PRO
2	2p	59	PRO
2	2r	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	9I	59	PRO
2	2t	59	PRO
2	2w	59	PRO
2	7t	59	PRO
2	7v	59	PRO

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Mol	Chain	Res	Type
2	7w	59	PRO
2	7x	59	PRO
1	6F	356	PRO
1	8E	356	PRO
1	6L	356	PRO
1	8K	356	PRO
1	3P	356	PRO
1	6O	202	GLU
1	6R	356	PRO
1	8Q	356	PRO
1	6U	202	GLU
1	6X	356	PRO
1	8W	356	PRO
1	3b	356	PRO
1	6a	202	GLU
1	6d	356	PRO
1	8c	356	PRO
2	7a	59	PRO
2	7f	59	PRO
2	9G	59	PRO
2	2k	59	PRO
2	2l	59	PRO
2	7k	59	PRO
2	7l	59	PRO
2	7m	59	PRO
2	7n	59	PRO
2	2q	59	PRO
2	2u	59	PRO
2	2v	59	PRO
2	2x	59	PRO
2	7u	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

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Mol	Chain	Res	Type
1	5X	425	LYS
1	6S	355	SER
1	3a	356	PRO
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	369/384 (96%)	367 (100%)	2 (0%)	88	95
1	1B	381/384 (99%)	379 (100%)	2 (0%)	88	95
1	1C	380/384 (99%)	380 (100%)	0	100	100
1	1D	381/384 (99%)	379 (100%)	2 (0%)	88	95
1	1E	375/384 (98%)	375 (100%)	0	100	100
1	1F	379/384 (99%)	378 (100%)	1 (0%)	92	96
1	1G	369/384 (96%)	367 (100%)	2 (0%)	88	95
1	1H	381/384 (99%)	379 (100%)	2 (0%)	88	95

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	1I	380/384 (99%)	380 (100%)	0	100	100
1	1J	381/384 (99%)	379 (100%)	2 (0%)	88	95
1	1K	375/384 (98%)	375 (100%)	0	100	100
1	1L	379/384 (99%)	378 (100%)	1 (0%)	92	96
1	1M	369/384 (96%)	367 (100%)	2 (0%)	88	95
1	1N	381/384 (99%)	379 (100%)	2 (0%)	88	95
1	1O	380/384 (99%)	380 (100%)	0	100	100
1	1P	381/384 (99%)	379 (100%)	2 (0%)	88	95
1	1Q	375/384 (98%)	375 (100%)	0	100	100
1	1R	379/384 (99%)	378 (100%)	1 (0%)	92	96
1	1S	369/384 (96%)	367 (100%)	2 (0%)	88	95
1	1T	381/384 (99%)	379 (100%)	2 (0%)	88	95
1	1U	380/384 (99%)	380 (100%)	0	100	100
1	1V	381/384 (99%)	379 (100%)	2 (0%)	88	95
1	1W	375/384 (98%)	375 (100%)	0	100	100
1	1X	379/384 (99%)	378 (100%)	1 (0%)	92	96
1	1Y	369/384 (96%)	367 (100%)	2 (0%)	88	95
1	1Z	381/384 (99%)	379 (100%)	2 (0%)	88	95
1	1a	380/384 (99%)	380 (100%)	0	100	100
1	1b	381/384 (99%)	379 (100%)	2 (0%)	88	95
1	1c	375/384 (98%)	375 (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

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
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
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	380/384 (99%)	380 (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	380/384 (99%)	380 (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

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	3P	381/384 (99%)	380 (100%)	1 (0%)	92	96
1	3Q	380/384 (99%)	380 (100%)	0	100	100
1	3R	381/384 (99%)	380 (100%)	1 (0%)	92	96
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	380/384 (99%)	380 (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	380/384 (99%)	380 (100%)	0	100	100
1	3d	381/384 (99%)	380 (100%)	1 (0%)	92	96
1	4A	375/384 (98%)	375 (100%)	0	100	100
1	4B	375/384 (98%)	374 (100%)	1 (0%)	92	96
1	4C	376/384 (98%)	376 (100%)	0	100	100
1	4D	375/384 (98%)	375 (100%)	0	100	100
1	4E	380/384 (99%)	379 (100%)	1 (0%)	92	96
1	4F	381/384 (99%)	380 (100%)	1 (0%)	92	96
1	4G	375/384 (98%)	375 (100%)	0	100	100
1	4H	375/384 (98%)	374 (100%)	1 (0%)	92	96
1	4I	376/384 (98%)	376 (100%)	0	100	100
1	4J	375/384 (98%)	375 (100%)	0	100	100
1	4K	380/384 (99%)	379 (100%)	1 (0%)	92	96
1	4L	381/384 (99%)	380 (100%)	1 (0%)	92	96
1	4M	375/384 (98%)	375 (100%)	0	100	100
1	4N	375/384 (98%)	374 (100%)	1 (0%)	92	96
1	4O	376/384 (98%)	376 (100%)	0	100	100
1	4P	375/384 (98%)	375 (100%)	0	100	100

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	4Q	380/384 (99%)	379 (100%)	1 (0%)	92	96
1	4R	381/384 (99%)	380 (100%)	1 (0%)	92	96
1	4S	375/384 (98%)	375 (100%)	0	100	100
1	4T	375/384 (98%)	374 (100%)	1 (0%)	92	96
1	4U	376/384 (98%)	376 (100%)	0	100	100
1	4V	375/384 (98%)	375 (100%)	0	100	100
1	4W	380/384 (99%)	379 (100%)	1 (0%)	92	96
1	4X	381/384 (99%)	380 (100%)	1 (0%)	92	96
1	4Y	375/384 (98%)	375 (100%)	0	100	100
1	4Z	375/384 (98%)	374 (100%)	1 (0%)	92	96
1	4a	376/384 (98%)	376 (100%)	0	100	100
1	4b	375/384 (98%)	375 (100%)	0	100	100
1	4c	380/384 (99%)	379 (100%)	1 (0%)	92	96
1	4d	381/384 (99%)	380 (100%)	1 (0%)	92	96
1	5A	375/384 (98%)	374 (100%)	1 (0%)	92	96
1	5B	375/384 (98%)	374 (100%)	1 (0%)	92	96
1	5C	376/384 (98%)	373 (99%)	3 (1%)	81	93
1	5D	375/384 (98%)	375 (100%)	0	100	100
1	5E	380/384 (99%)	380 (100%)	0	100	100
1	5F	381/384 (99%)	378 (99%)	3 (1%)	81	93
1	5G	375/384 (98%)	374 (100%)	1 (0%)	92	96
1	5H	375/384 (98%)	374 (100%)	1 (0%)	92	96
1	5I	376/384 (98%)	373 (99%)	3 (1%)	81	93
1	5J	375/384 (98%)	375 (100%)	0	100	100
1	5K	380/384 (99%)	380 (100%)	0	100	100
1	5L	381/384 (99%)	378 (99%)	3 (1%)	81	93
1	5M	375/384 (98%)	374 (100%)	1 (0%)	92	96
1	5N	375/384 (98%)	374 (100%)	1 (0%)	92	96
1	5O	376/384 (98%)	373 (99%)	3 (1%)	81	93
1	5P	375/384 (98%)	375 (100%)	0	100	100
1	5Q	380/384 (99%)	380 (100%)	0	100	100

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	5R	381/384 (99%)	378 (99%)	3 (1%)	81	93
1	5S	375/384 (98%)	374 (100%)	1 (0%)	92	96
1	5T	375/384 (98%)	374 (100%)	1 (0%)	92	96
1	5U	376/384 (98%)	373 (99%)	3 (1%)	81	93
1	5V	375/384 (98%)	375 (100%)	0	100	100
1	5W	380/384 (99%)	380 (100%)	0	100	100
1	5X	381/384 (99%)	378 (99%)	3 (1%)	81	93
1	5Y	375/384 (98%)	374 (100%)	1 (0%)	92	96
1	5Z	375/384 (98%)	374 (100%)	1 (0%)	92	96
1	5a	376/384 (98%)	373 (99%)	3 (1%)	81	93
1	5b	375/384 (98%)	375 (100%)	0	100	100
1	5c	380/384 (99%)	380 (100%)	0	100	100
1	5d	381/384 (99%)	378 (99%)	3 (1%)	81	93
1	6A	380/384 (99%)	379 (100%)	1 (0%)	92	96
1	6B	381/384 (99%)	381 (100%)	0	100	100
1	6C	375/384 (98%)	375 (100%)	0	100	100
1	6D	376/384 (98%)	375 (100%)	1 (0%)	92	96
1	6E	380/384 (99%)	380 (100%)	0	100	100
1	6F	381/384 (99%)	381 (100%)	0	100	100
1	6G	380/384 (99%)	379 (100%)	1 (0%)	92	96
1	6H	381/384 (99%)	381 (100%)	0	100	100
1	6I	375/384 (98%)	375 (100%)	0	100	100
1	6J	376/384 (98%)	375 (100%)	1 (0%)	92	96
1	6K	380/384 (99%)	380 (100%)	0	100	100
1	6L	381/384 (99%)	381 (100%)	0	100	100
1	6M	380/384 (99%)	379 (100%)	1 (0%)	92	96
1	6N	381/384 (99%)	381 (100%)	0	100	100
1	6O	375/384 (98%)	375 (100%)	0	100	100
1	6P	376/384 (98%)	375 (100%)	1 (0%)	92	96
1	6Q	380/384 (99%)	380 (100%)	0	100	100
1	6R	381/384 (99%)	381 (100%)	0	100	100

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	6S	380/384 (99%)	379 (100%)	1 (0%)	92	96
1	6T	381/384 (99%)	381 (100%)	0	100	100
1	6U	375/384 (98%)	375 (100%)	0	100	100
1	6V	376/384 (98%)	375 (100%)	1 (0%)	92	96
1	6W	380/384 (99%)	380 (100%)	0	100	100
1	6X	381/384 (99%)	381 (100%)	0	100	100
1	6Y	380/384 (99%)	379 (100%)	1 (0%)	92	96
1	6Z	381/384 (99%)	381 (100%)	0	100	100
1	6a	375/384 (98%)	375 (100%)	0	100	100
1	6b	376/384 (98%)	375 (100%)	1 (0%)	92	96
1	6c	380/384 (99%)	380 (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

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

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	8Z	380/384 (99%)	380 (100%)	0	100	100
1	8a	381/384 (99%)	379 (100%)	2 (0%)	88	95
1	8b	380/384 (99%)	380 (100%)	0	100	100
1	8c	381/384 (99%)	381 (100%)	0	100	100
1	8d	380/384 (99%)	379 (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

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
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
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

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
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
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

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
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
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

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
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
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

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
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
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	127895/128025 (100%)	127370 (100%)	525 (0%)	91	95

All (525) 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

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Mol	Chain	Res	Type
1	2C	312	VAL
1	2E	357	ASN
1	3A	397	THR
1	3B	275	PHE
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	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

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Mol	Chain	Res	Type
1	3H	275	PHE
1	3I	438	ARG
1	3J	260	ASP
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

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Mol	Chain	Res	Type
1	3R	241	ARG
1	4N	295	VAL
1	4Q	195	PHE
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	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

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Mol	Chain	Res	Type
1	4X	195	PHE
1	5S	295	VAL
1	5T	312	VAL
1	5U	188	ASN
1	5U	295	VAL
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	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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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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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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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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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 (1625) 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	1A	377	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	43	ASN
1	2A	305	ASN
1	2B	142	GLN
1	2B	278	ASN
1	2C	28	GLN
1	2C	135	ASN
1	2C	168	ASN
1	2C	278	ASN
1	2C	351	GLN

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Mol	Chain	Res	Type
1	2D	28	GLN
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

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Mol	Chain	Res	Type
1	4E	278	ASN
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

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Mol	Chain	Res	Type
1	7B	43	ASN
1	7B	321	ASN
1	7C	22	ASN
1	7C	28	GLN
1	7C	248	HIS
1	7D	28	GLN
1	7D	137	GLN
1	7D	168	ASN
1	7D	234	ASN
1	7D	278	ASN
1	7D	366	GLN
1	7D	447	GLN
1	8A	145	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	54	ASN
1	9A	59	ASN
1	9A	76	GLN
1	9A	142	GLN
1	9A	168	ASN
1	9A	269	ASN
1	1G	168	ASN
1	1G	234	ASN

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Mol	Chain	Res	Type
1	1G	328	GLN
1	1G	357	ASN
1	1H	55	GLN
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	1J	407	ASN
1	1K	328	GLN
1	1L	278	ASN
1	1L	351	GLN
1	1L	410	ASN
1	2F	43	ASN
1	2F	305	ASN
1	2F	366	GLN
1	2G	278	ASN
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	366	GLN
1	2J	447	GLN
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

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Mol	Chain	Res	Type
1	3L	22	ASN
1	3L	43	ASN
1	3L	337	ASN
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	4K	407	ASN
1	4K	447	GLN
1	4L	142	GLN
1	4L	447	GLN
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	5K	22	ASN
1	5K	26	ASN

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Mol	Chain	Res	Type
1	5K	76	GLN
1	5K	234	ASN
1	5K	269	ASN
1	5K	278	ASN
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	5L	407	ASN
1	6G	278	ASN
1	6G	328	GLN
1	6G	447	GLN
1	6H	305	ASN
1	6H	407	ASN
1	6I	135	ASN
1	6J	142	GLN
1	6K	278	ASN
1	6K	321	ASN
1	6K	447	GLN
1	7F	59	ASN
1	7F	76	GLN
1	7F	168	ASN
1	7F	328	GLN
1	7F	407	ASN
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	7H	447	GLN
1	7I	137	GLN
1	7I	168	ASN
1	7I	234	ASN
1	8G	55	GLN
1	8G	305	ASN
1	8G	337	ASN
1	8H	234	ASN
1	8H	278	ASN
1	8H	328	GLN

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Mol	Chain	Res	Type
1	8I	76	GLN
1	8I	337	ASN
1	8I	363	GLN
1	8J	22	ASN
1	8J	328	GLN
1	8K	168	ASN
1	8K	278	ASN
1	8K	325	HIS
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	54	ASN
1	9B	59	ASN
1	9B	76	GLN
1	9B	142	GLN
1	9B	168	ASN
1	9B	269	ASN
1	9B	411	GLN
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	1P	407	ASN
1	1Q	328	GLN
1	1R	278	ASN
1	1R	351	GLN
1	1R	410	ASN
1	2K	43	ASN

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Mol	Chain	Res	Type
1	2K	305	ASN
1	2K	366	GLN
1	2L	278	ASN
1	2M	135	ASN
1	2M	168	ASN
1	2M	278	ASN
1	2M	351	GLN
1	2N	28	GLN
1	2O	76	GLN
1	2O	168	ASN
1	2O	366	GLN
1	2O	410	ASN
1	2O	447	GLN
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	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

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Mol	Chain	Res	Type
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
1	4Q	407	ASN
1	4Q	447	GLN
1	4R	142	GLN
1	4R	447	GLN
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	5R	407	ASN
1	6M	278	ASN
1	6M	328	GLN
1	6M	447	GLN

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Mol	Chain	Res	Type
1	6N	305	ASN
1	6N	407	ASN
1	6O	135	ASN
1	6P	142	GLN
1	6Q	168	ASN
1	6Q	278	ASN
1	6Q	321	ASN
1	6Q	447	GLN
1	7K	59	ASN
1	7K	76	GLN
1	7K	168	ASN
1	7K	328	GLN
1	7K	407	ASN
1	7L	26	ASN
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	7M	447	GLN
1	7N	28	GLN
1	7N	137	GLN
1	7N	168	ASN
1	7N	234	ASN
1	8M	117	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	145	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

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Mol	Chain	Res	Type
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	168	ASN
1	9C	269	ASN
1	9C	411	GLN
1	1S	168	ASN
1	1S	234	ASN
1	1S	328	GLN
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	1V	407	ASN
1	1W	328	GLN
1	1X	278	ASN
1	1X	351	GLN
1	1X	410	ASN
1	2P	43	ASN
1	2P	305	ASN
1	2P	337	ASN
1	2P	366	GLN
1	2Q	278	ASN
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	366	GLN
1	2T	410	ASN

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Mol	Chain	Res	Type
1	2T	447	GLN
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
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	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	4W	407	ASN
1	4W	447	GLN
1	4X	142	GLN
1	4X	447	GLN
1	5S	145	GLN

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Mol	Chain	Res	Type
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	168	ASN
1	5V	278	ASN
1	5V	328	GLN
1	5W	22	ASN
1	5W	26	ASN
1	5W	76	GLN
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	5X	407	ASN
1	6S	278	ASN
1	6S	328	GLN
1	6S	447	GLN
1	6T	305	ASN
1	6T	407	ASN
1	6U	135	ASN
1	6V	142	GLN
1	6W	168	ASN
1	6W	278	ASN
1	6W	321	ASN
1	6W	447	GLN
1	7P	59	ASN
1	7P	76	GLN
1	7P	168	ASN
1	7P	328	GLN
1	7P	407	ASN

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Mol	Chain	Res	Type
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	7R	447	GLN
1	7S	28	GLN
1	7S	137	GLN
1	7S	168	ASN
1	7S	234	ASN
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	145	GLN
1	8U	337	ASN
1	8U	363	GLN
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	9D	411	GLN
1	1Y	168	ASN

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Mol	Chain	Res	Type
1	1Y	234	ASN
1	1Y	328	GLN
1	1Y	357	ASN
1	1Y	377	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	1b	407	ASN
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	2U	366	GLN
1	2V	278	ASN
1	2W	135	ASN
1	2W	278	ASN
1	2W	351	GLN
1	2X	28	GLN
1	2Y	76	GLN
1	2Y	168	ASN
1	2Y	366	GLN
1	2Y	410	ASN
1	2Y	447	GLN
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

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Mol	Chain	Res	Type
1	3b	305	ASN
1	3b	337	ASN
1	3c	269	ASN
1	3c	337	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
1	4c	135	ASN
1	4c	168	ASN
1	4c	278	ASN
1	4c	407	ASN
1	4c	447	GLN
1	4d	142	GLN
1	4d	447	GLN
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

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Mol	Chain	Res	Type
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	5d	407	ASN
1	6Y	278	ASN
1	6Y	328	GLN
1	6Y	447	GLN
1	6Z	305	ASN
1	6Z	407	ASN
1	6a	135	ASN
1	6b	142	GLN
1	6c	278	ASN
1	6c	321	ASN
1	6c	447	GLN
1	7U	59	ASN
1	7U	76	GLN
1	7U	168	ASN
1	7U	328	GLN
1	7U	407	ASN
1	7V	26	ASN
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	7W	447	GLN
1	7X	28	GLN
1	7X	137	GLN
1	7X	168	ASN
1	7X	234	ASN
1	8Y	145	GLN
1	8Y	305	ASN

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Mol	Chain	Res	Type
1	8Y	337	ASN
1	8Z	141	HIS
1	8Z	234	ASN
1	8Z	278	ASN
1	8Z	328	GLN
1	8a	76	GLN
1	8a	145	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
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

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Mol	Chain	Res	Type
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	103	GLN
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	23	GLN
2	2c	159	ASN
2	2c	166	ASN
2	2c	179	ASN
2	2c	197	GLN
2	2c	218	ASN
2	2d	159	ASN
2	2d	166	ASN
2	2d	179	ASN
2	2d	218	ASN
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

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Mol	Chain	Res	Type
2	3g	76	ASN
2	3g	159	ASN
2	3g	166	ASN
2	3g	179	ASN
2	3g	218	ASN
2	3h	23	GLN
2	3h	159	ASN
2	3h	166	ASN
2	3h	179	ASN
2	3h	218	ASN
2	3h	267	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	76	ASN
2	6e	159	ASN
2	6e	166	ASN
2	6e	179	ASN
2	6e	218	ASN
2	6f	159	ASN
2	6f	166	ASN
2	6f	171	GLN
2	6f	179	ASN
2	6f	185	GLN
2	6f	203	ASN
2	6f	218	ASN

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Mol	Chain	Res	Type
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	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	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	64	GLN
2	7d	159	ASN
2	7d	166	ASN
2	7d	179	ASN
2	7d	218	ASN
2	8e	76	ASN
2	8e	159	ASN
2	8e	166	ASN
2	8e	179	ASN
2	8e	218	ASN
2	8f	23	GLN
2	8f	159	ASN
2	8f	166	ASN
2	8f	179	ASN
2	8f	218	ASN

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Mol	Chain	Res	Type
2	8g	159	ASN
2	8g	166	ASN
2	8g	179	ASN
2	8g	197	GLN
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	197	GLN
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	56	ASN
2	1i	159	ASN
2	1i	166	ASN
2	1i	179	ASN
2	1i	218	ASN
2	1j	56	ASN
2	1j	76	ASN
2	1j	159	ASN
2	1j	166	ASN
2	1j	179	ASN
2	1j	218	ASN
2	1k	159	ASN
2	1k	166	ASN
2	1k	179	ASN
2	1k	197	GLN
2	1k	218	ASN

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Mol	Chain	Res	Type
2	1l	56	ASN
2	1l	76	ASN
2	1l	159	ASN
2	1l	166	ASN
2	1l	179	ASN
2	1l	197	GLN
2	1l	218	ASN
2	2e	64	GLN
2	2e	106	GLN
2	2e	159	ASN
2	2e	166	ASN
2	2e	179	ASN
2	2e	218	ASN
2	2f	54	GLN
2	2f	56	ASN
2	2f	64	GLN
2	2f	103	GLN
2	2f	159	ASN
2	2f	166	ASN
2	2f	179	ASN
2	2f	218	ASN
2	2g	23	GLN
2	2g	159	ASN
2	2g	166	ASN
2	2g	179	ASN
2	2g	218	ASN
2	2h	23	GLN
2	2h	64	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

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Mol	Chain	Res	Type
2	3j	159	ASN
2	3j	166	ASN
2	3j	179	ASN
2	3j	218	ASN
2	3k	23	GLN
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	171	GLN
2	3l	179	ASN
2	3l	185	GLN
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	56	ASN
2	5g	159	ASN
2	5g	166	ASN
2	5g	179	ASN
2	5g	218	ASN
2	5h	76	ASN
2	5h	159	ASN
2	5h	166	ASN
2	5h	179	ASN
2	5h	197	GLN
2	5h	218	ASN
2	6i	76	ASN
2	6i	159	ASN
2	6i	166	ASN
2	6i	179	ASN
2	6i	218	ASN
2	6j	23	GLN

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Mol	Chain	Res	Type
2	6j	56	ASN
2	6j	159	ASN
2	6j	166	ASN
2	6j	179	ASN
2	6j	218	ASN
2	6k	76	ASN
2	6k	159	ASN
2	6k	166	ASN
2	6k	179	ASN
2	6k	218	ASN
2	6l	159	ASN
2	6l	166	ASN
2	6l	179	ASN
2	6l	218	ASN
2	7e	23	GLN
2	7e	159	ASN
2	7e	166	ASN
2	7e	179	ASN
2	7e	218	ASN
2	7f	23	GLN
2	7f	56	ASN
2	7f	64	GLN
2	7f	103	GLN
2	7f	106	GLN
2	7f	159	ASN
2	7f	166	ASN
2	7f	171	GLN
2	7f	179	ASN
2	7f	185	GLN
2	7f	203	ASN
2	7f	218	ASN
2	7g	159	ASN
2	7g	166	ASN
2	7g	179	ASN
2	7g	218	ASN
2	7h	56	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

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Mol	Chain	Res	Type
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	23	GLN
2	8m	159	ASN
2	8m	166	ASN
2	8m	179	ASN
2	8m	218	ASN
2	8n	23	GLN
2	8n	76	ASN
2	8n	159	ASN
2	8n	166	ASN
2	8n	179	ASN
2	8n	218	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	9G	267	ASN
2	1m	56	ASN
2	1m	159	ASN
2	1m	166	ASN
2	1m	179	ASN
2	1m	218	ASN

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Mol	Chain	Res	Type
2	1n	56	ASN
2	1n	76	ASN
2	1n	159	ASN
2	1n	166	ASN
2	1n	179	ASN
2	1n	218	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	64	GLN
2	2j	106	GLN
2	2j	159	ASN
2	2j	166	ASN
2	2j	179	ASN
2	2j	218	ASN
2	2k	54	GLN
2	2k	56	ASN
2	2k	64	GLN
2	2k	103	GLN
2	2k	159	ASN
2	2k	166	ASN
2	2k	179	ASN
2	2k	218	ASN
2	2l	159	ASN
2	2l	166	ASN
2	2l	179	ASN
2	2l	218	ASN
2	2m	64	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

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Mol	Chain	Res	Type
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	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
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	56	ASN
2	5i	159	ASN
2	5i	166	ASN
2	5i	179	ASN
2	5i	218	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

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Mol	Chain	Res	Type
2	6m	166	ASN
2	6m	179	ASN
2	6m	218	ASN
2	6n	23	GLN
2	6n	56	ASN
2	6n	159	ASN
2	6n	166	ASN
2	6n	179	ASN
2	6n	218	ASN
2	6o	76	ASN
2	6o	159	ASN
2	6o	166	ASN
2	6o	179	ASN
2	6o	218	ASN
2	6p	159	ASN
2	6p	166	ASN
2	6p	179	ASN
2	6p	218	ASN
2	7j	159	ASN
2	7j	166	ASN
2	7j	179	ASN
2	7j	218	ASN
2	7k	56	ASN
2	7k	64	GLN
2	7k	103	GLN
2	7k	106	GLN
2	7k	159	ASN
2	7k	166	ASN
2	7k	179	ASN
2	7k	218	ASN
2	7l	159	ASN
2	7l	166	ASN
2	7l	179	ASN
2	7l	218	ASN
2	7m	56	ASN
2	7m	159	ASN
2	7m	166	ASN
2	7m	179	ASN
2	7m	197	GLN
2	7m	218	ASN
2	7n	159	ASN
2	7n	166	ASN

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Mol	Chain	Res	Type
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	23	GLN
2	8r	159	ASN
2	8r	166	ASN
2	8r	179	ASN
2	8r	218	ASN
2	8s	23	GLN
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	8t	267	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
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	56	ASN
2	1q	159	ASN
2	1q	166	ASN
2	1q	179	ASN
2	1q	218	ASN

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Mol	Chain	Res	Type
2	1r	56	ASN
2	1r	76	ASN
2	1r	159	ASN
2	1r	166	ASN
2	1r	179	ASN
2	1r	218	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	106	GLN
2	2o	159	ASN
2	2o	166	ASN
2	2o	179	ASN
2	2o	218	ASN
2	2p	54	GLN
2	2p	56	ASN
2	2p	64	GLN
2	2p	103	GLN
2	2p	159	ASN
2	2p	166	ASN
2	2p	179	ASN
2	2p	218	ASN
2	2q	159	ASN
2	2q	166	ASN
2	2q	179	ASN
2	2q	218	ASN
2	2r	23	GLN
2	2r	64	GLN
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

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Mol	Chain	Res	Type
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	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	56	ASN
2	5k	159	ASN
2	5k	166	ASN
2	5k	179	ASN
2	5k	218	ASN
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

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Mol	Chain	Res	Type
2	6q	166	ASN
2	6q	179	ASN
2	6q	218	ASN
2	6r	23	GLN
2	6r	56	ASN
2	6r	159	ASN
2	6r	166	ASN
2	6r	179	ASN
2	6r	218	ASN
2	6s	76	ASN
2	6s	159	ASN
2	6s	166	ASN
2	6s	179	ASN
2	6s	218	ASN
2	6t	159	ASN
2	6t	166	ASN
2	6t	179	ASN
2	6t	218	ASN
2	7o	159	ASN
2	7o	166	ASN
2	7o	179	ASN
2	7o	218	ASN
2	7p	23	GLN
2	7p	56	ASN
2	7p	64	GLN
2	7p	103	GLN
2	7p	106	GLN
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	56	ASN
2	7r	159	ASN
2	7r	166	ASN
2	7r	179	ASN
2	7r	197	GLN
2	7r	218	ASN
2	7s	159	ASN

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Mol	Chain	Res	Type
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	23	GLN
2	8x	159	ASN
2	8x	166	ASN
2	8x	179	ASN
2	8x	218	ASN
2	8y	23	GLN
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	8z	267	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	56	ASN
2	1u	159	ASN
2	1u	166	ASN
2	1u	179	ASN

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Mol	Chain	Res	Type
2	1u	218	ASN
2	1v	56	ASN
2	1v	76	ASN
2	1v	159	ASN
2	1v	166	ASN
2	1v	179	ASN
2	1v	218	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	106	GLN
2	2t	159	ASN
2	2t	166	ASN
2	2t	179	ASN
2	2t	218	ASN
2	2u	54	GLN
2	2u	56	ASN
2	2u	64	GLN
2	2u	103	GLN
2	2u	159	ASN
2	2u	166	ASN
2	2u	179	ASN
2	2u	218	ASN
2	2v	23	GLN
2	2v	159	ASN
2	2v	166	ASN
2	2v	179	ASN
2	2v	218	ASN
2	2w	23	GLN
2	2w	64	GLN
2	2w	159	ASN
2	2w	166	ASN
2	2w	179	ASN
2	2w	218	ASN
2	2x	76	ASN

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Mol	Chain	Res	Type
2	2x	159	ASN
2	2x	166	ASN
2	2x	171	GLN
2	2x	179	ASN
2	2x	185	GLN
2	2x	218	ASN
2	3u	56	ASN
2	3u	76	ASN
2	3u	159	ASN
2	3u	166	ASN
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	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	56	ASN
2	5m	159	ASN
2	5m	166	ASN
2	5m	179	ASN
2	5m	218	ASN
2	5n	76	ASN
2	5n	159	ASN
2	5n	166	ASN

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Mol	Chain	Res	Type
2	5n	179	ASN
2	5n	197	GLN
2	5n	218	ASN
2	6u	76	ASN
2	6u	159	ASN
2	6u	166	ASN
2	6u	179	ASN
2	6u	218	ASN
2	6v	23	GLN
2	6v	56	ASN
2	6v	159	ASN
2	6v	166	ASN
2	6v	179	ASN
2	6v	218	ASN
2	6w	76	ASN
2	6w	159	ASN
2	6w	166	ASN
2	6w	179	ASN
2	6w	218	ASN
2	6x	159	ASN
2	6x	166	ASN
2	6x	179	ASN
2	6x	218	ASN
2	7t	159	ASN
2	7t	166	ASN
2	7t	179	ASN
2	7t	218	ASN
2	7u	23	GLN
2	7u	56	ASN
2	7u	64	GLN
2	7u	103	GLN
2	7u	106	GLN
2	7u	159	ASN
2	7u	166	ASN
2	7u	179	ASN
2	7u	218	ASN
2	7v	159	ASN
2	7v	166	ASN
2	7v	179	ASN
2	7v	218	ASN
2	7w	56	ASN
2	7w	159	ASN

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Mol	Chain	Res	Type
2	7w	166	ASN
2	7w	179	ASN
2	7w	197	GLN
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	23	GLN
2	9N	159	ASN
2	9N	166	ASN
2	9N	179	ASN
2	9N	218	ASN
2	9O	23	GLN
2	9O	159	ASN
2	9O	166	ASN
2	9O	179	ASN
2	9O	218	ASN
2	9P	76	ASN
2	9P	139	ASN
2	9P	159	ASN
2	9P	166	ASN
2	9P	179	ASN
2	9P	218	ASN
2	9Q	159	ASN
2	9Q	164	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

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Mol	Chain	Res	Type
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.

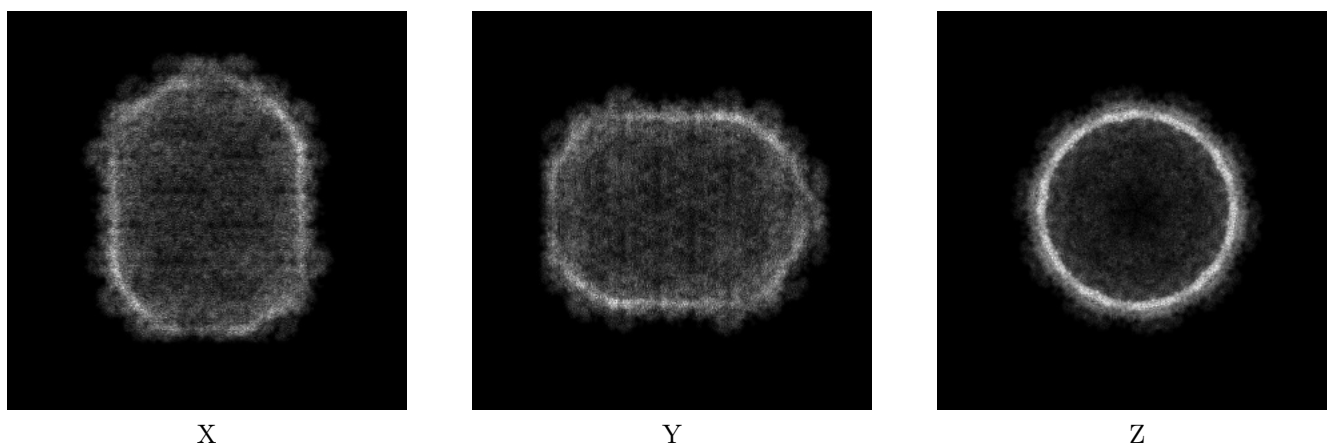
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-4677. 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](#)

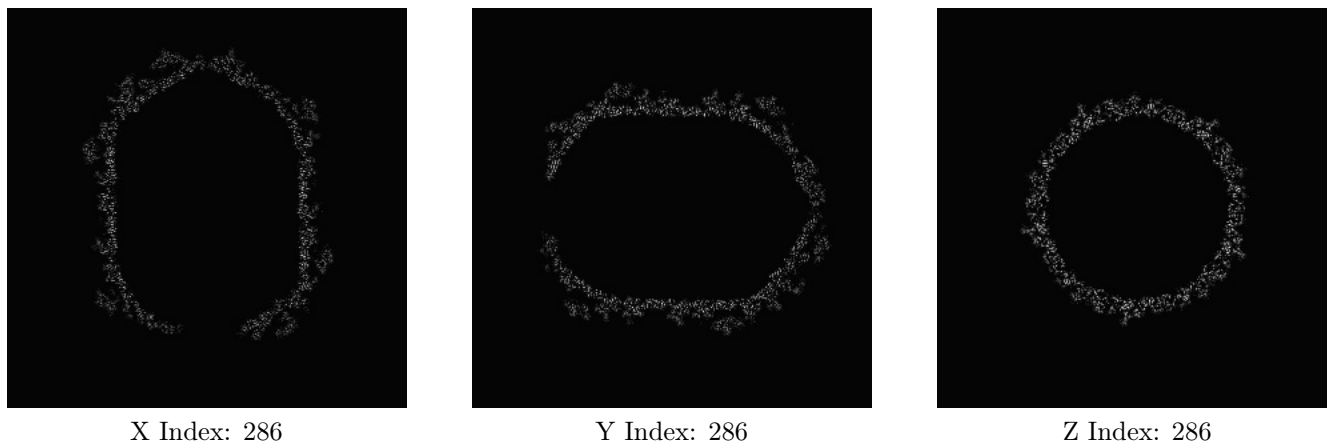
6.1.1 Primary map



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

6.2 Central slices [i](#)

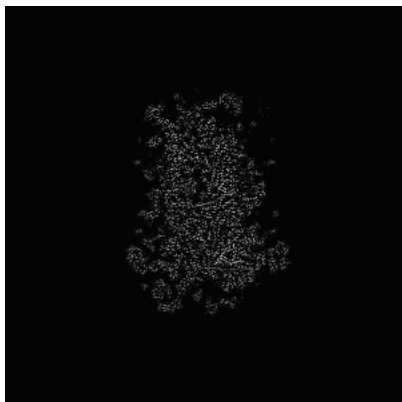
6.2.1 Primary map



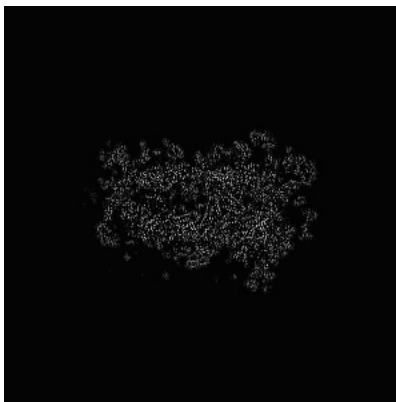
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

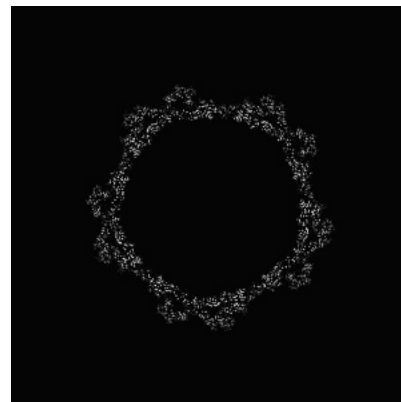
6.3.1 Primary map



X Index: 153



Y Index: 418

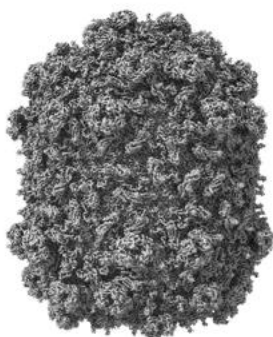


Z Index: 377

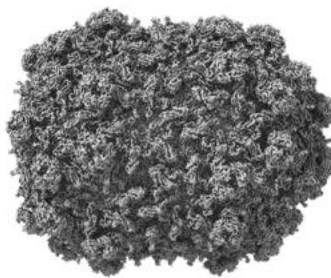
The images above show the largest variance slices of the map in three orthogonal directions.

6.4 Orthogonal surface views [i](#)

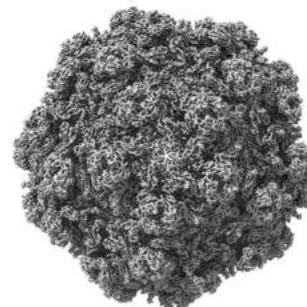
6.4.1 Primary map



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.

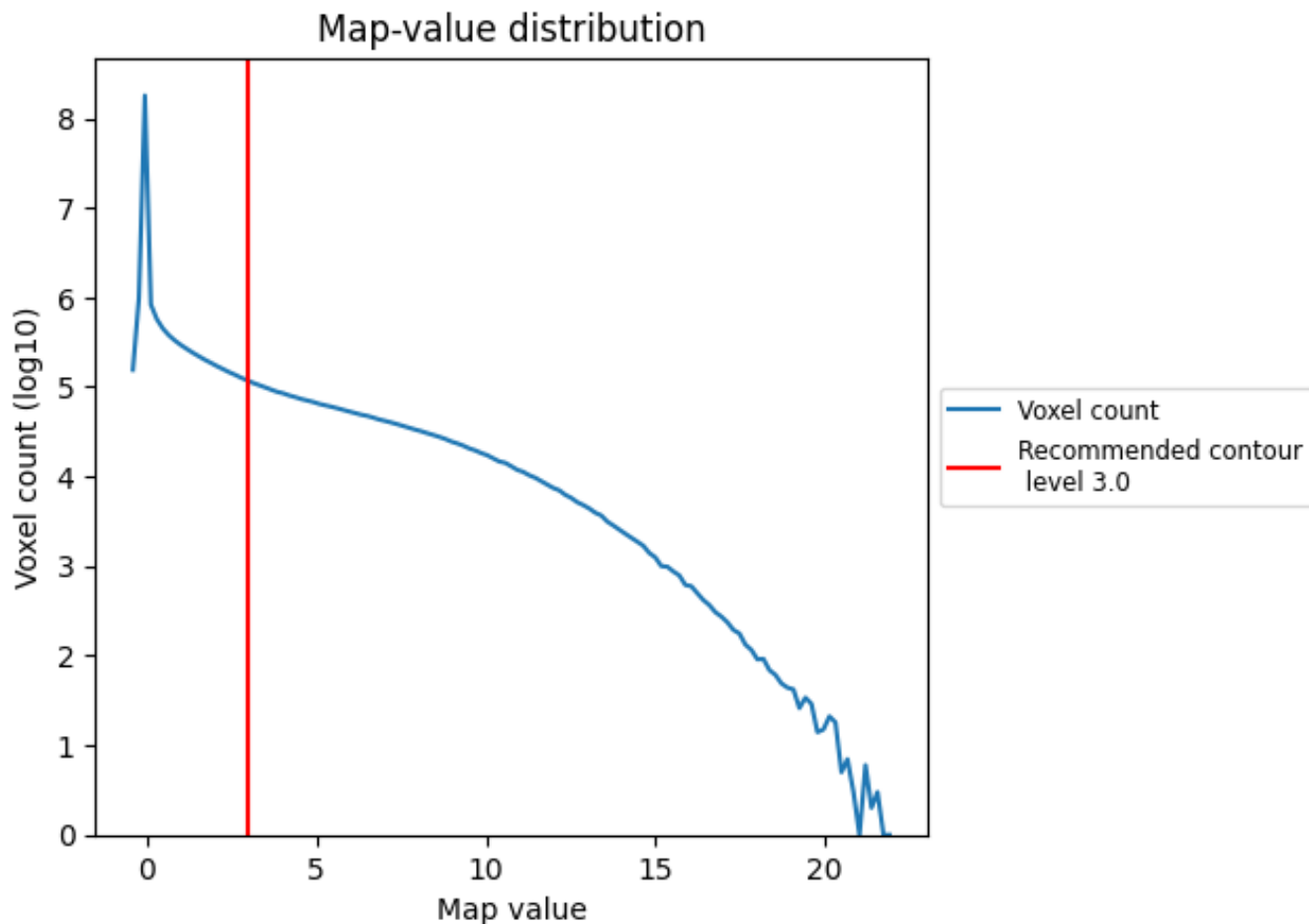
6.5 Mask visualisation

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

7 Map analysis [i](#)

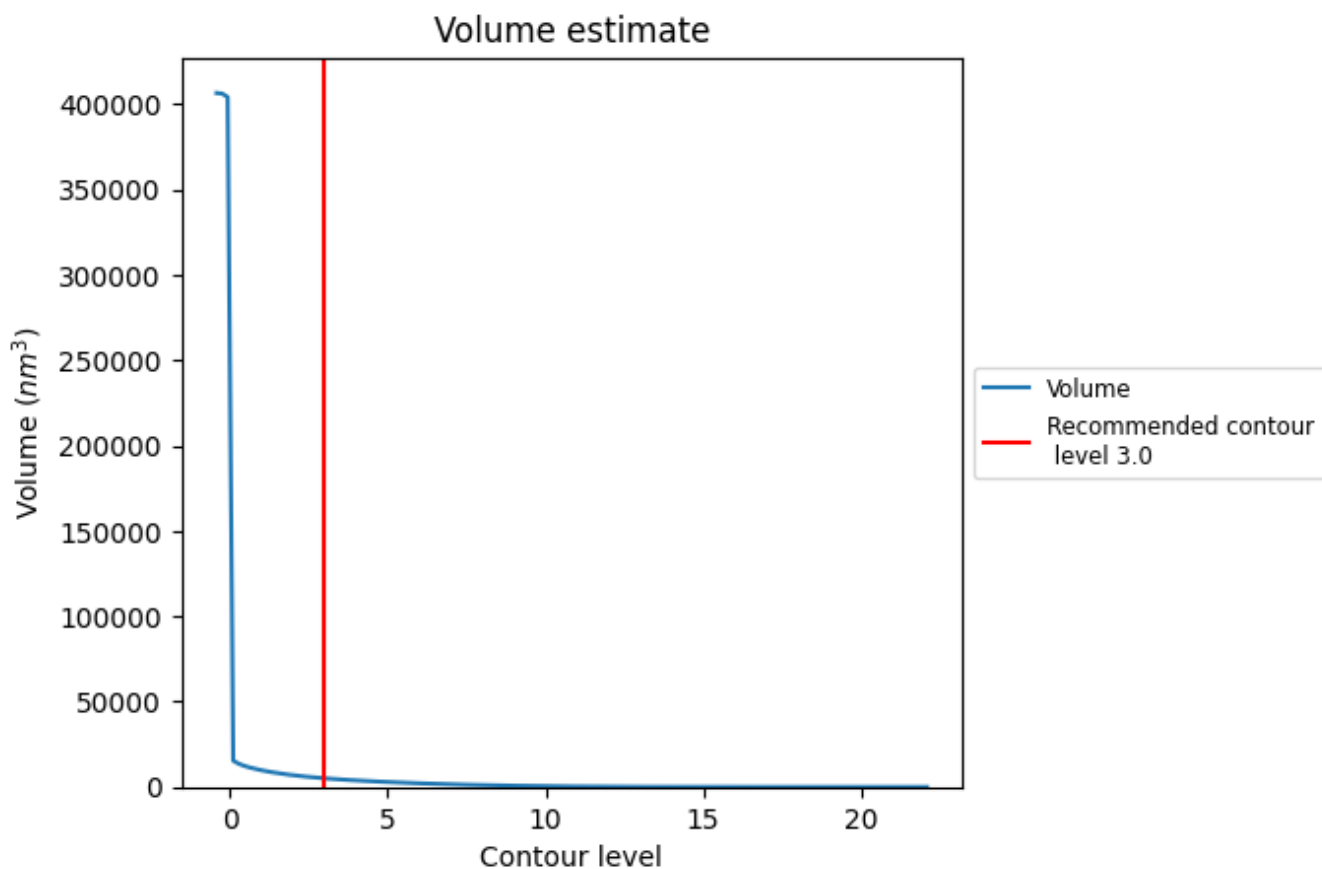
This section contains the results of statistical analysis of the map.

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.

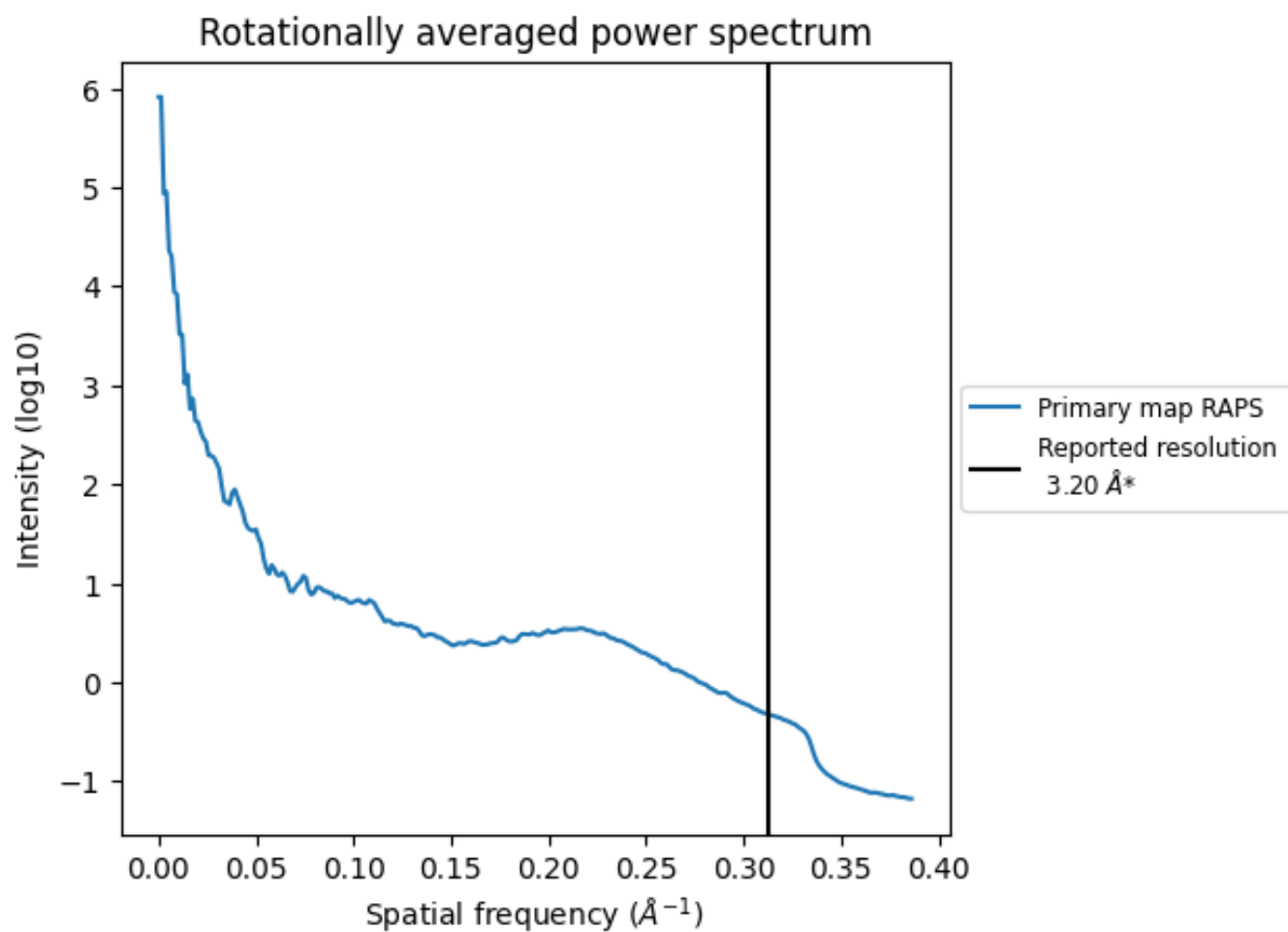
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 5075 nm³; this corresponds to an approximate mass of 4584 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

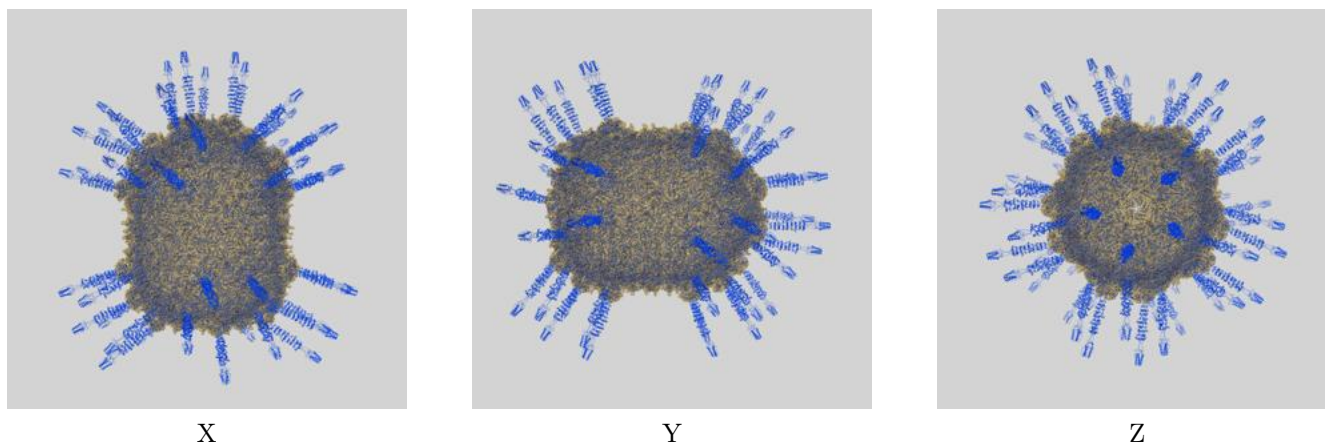
8 Fourier-Shell correlation

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

9 Map-model fit [i](#)

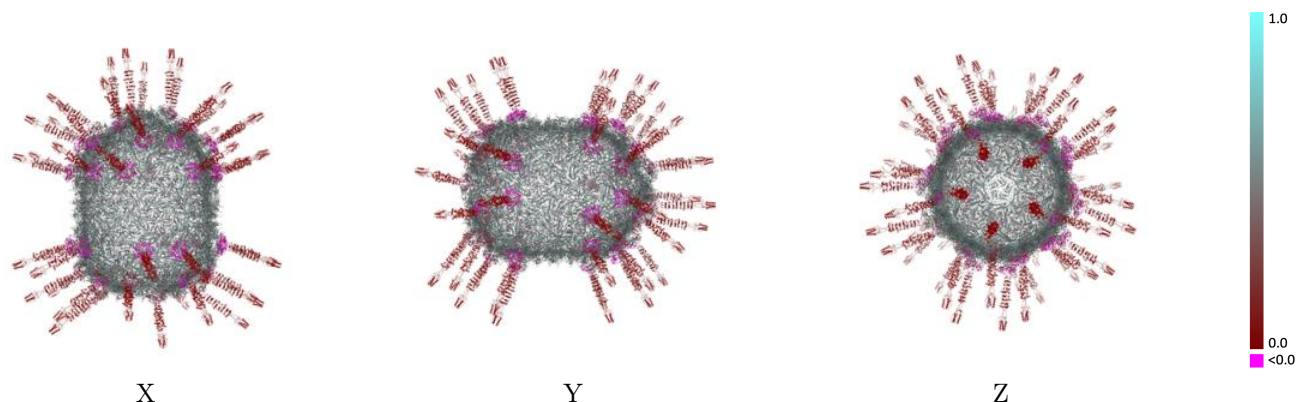
This section contains information regarding the fit between EMDB map EMD-4677 and PDB model 6QYD. Per-residue inclusion information can be found in section [3](#) on page [47](#).

9.1 Map-model overlay [i](#)



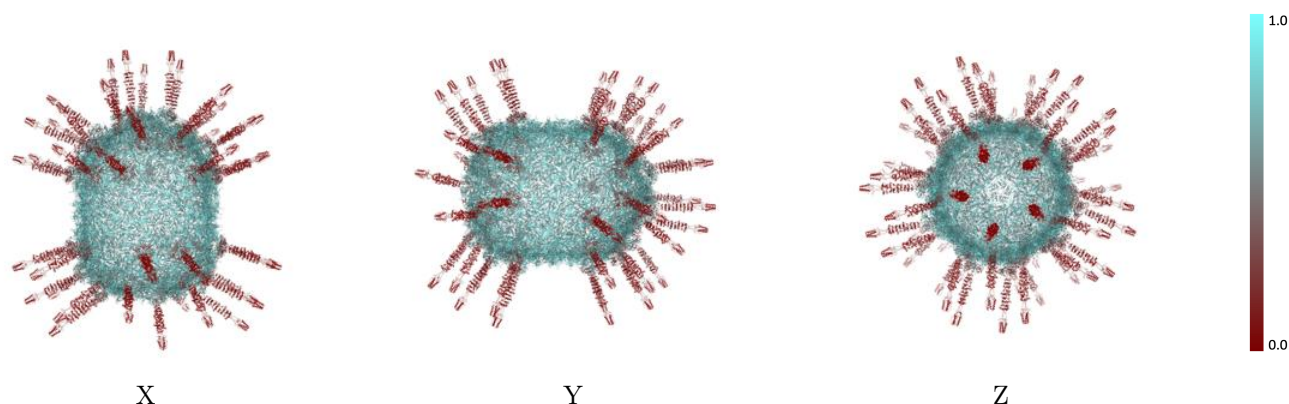
The images above show the 3D surface view of the map at the recommended contour level 3.0 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



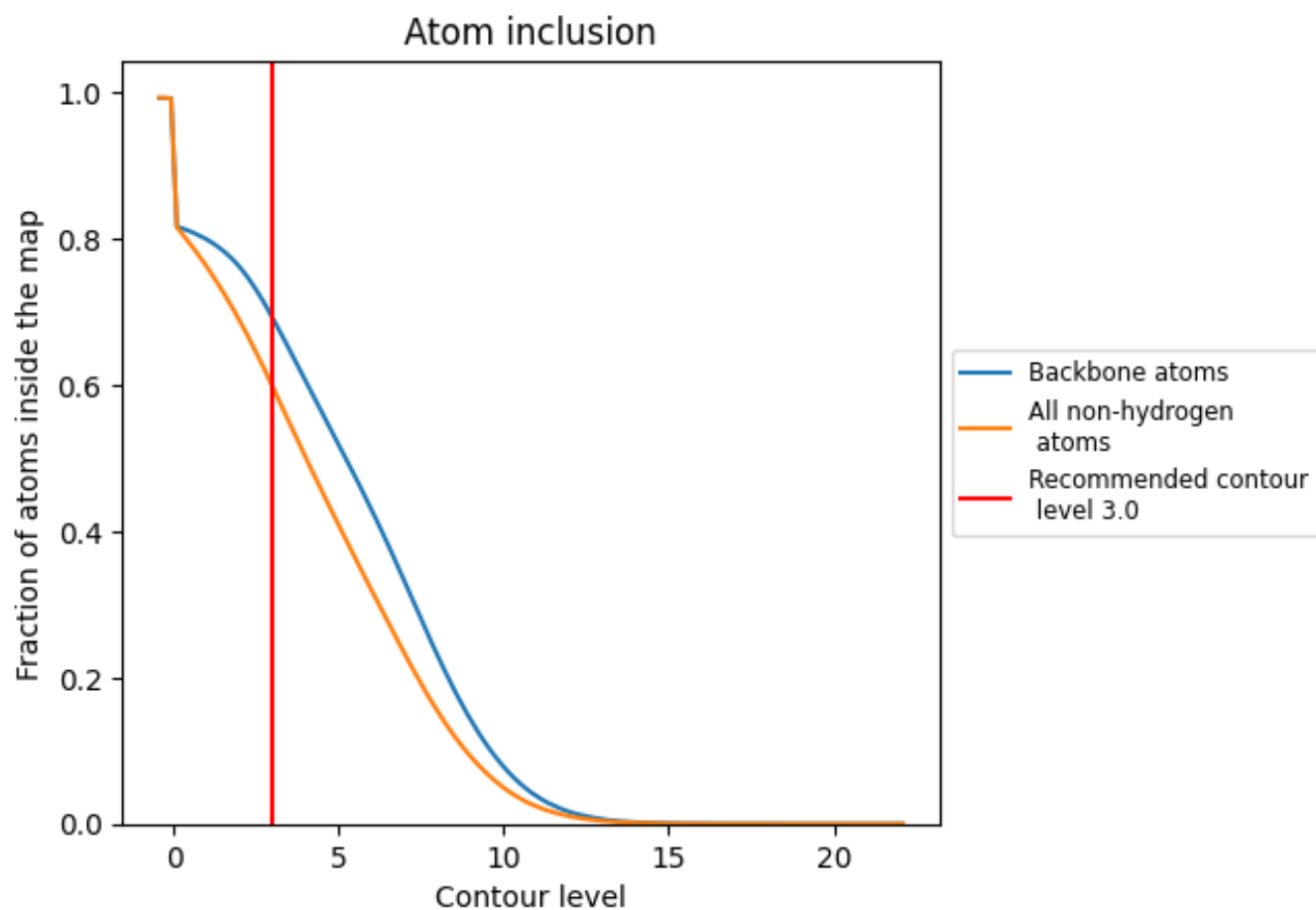
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions 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, 69% of all backbone atoms, 60% 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	 0.5988	 0.3850
1A	 0.6596	 0.4900
1B	 0.7655	 0.5290
1C	 0.7690	 0.5280
1D	 0.7628	 0.5220
1E	 0.7416	 0.5230
1F	 0.7124	 0.5030
1G	 0.6464	 0.4800
1H	 0.7640	 0.5230
1I	 0.7666	 0.5200
1J	 0.7585	 0.5120
1K	 0.7362	 0.5140
1L	 0.7071	 0.4960
1M	 0.6485	 0.4790
1N	 0.7590	 0.5220
1O	 0.7675	 0.5190
1P	 0.7602	 0.5150
1Q	 0.7336	 0.5150
1R	 0.7121	 0.4980
1S	 0.6500	 0.4800
1T	 0.7623	 0.5220
1U	 0.7640	 0.5200
1V	 0.7576	 0.5140
1W	 0.7383	 0.5140
1X	 0.7115	 0.4960
1Y	 0.6542	 0.4800
1Z	 0.7599	 0.5220
1a	 0.7643	 0.5200
1b	 0.7541	 0.5150
1c	 0.7351	 0.5150
1d	 0.7086	 0.4980
1e	 0.2639	 0.1710
1f	 0.2899	 0.1880
1g	 0.2663	 0.1670
1h	 0.2742	 0.1730























































































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Chain	Atom inclusion	Q-score
1i	0.1971	0.0850
1j	0.2150	0.0910
1k	0.2190	0.1000
1l	0.2165	0.0970
1m	0.1995	0.0870
1n	0.2125	0.0890
1o	0.2176	0.0990
1p	0.2150	0.0930
1q	0.1961	0.0840
1r	0.2101	0.0870
1s	0.2132	0.0930
1t	0.2032	0.0850
1u	0.1976	0.0850
1v	0.2169	0.0920
1w	0.2166	0.0990
1x	0.2106	0.0920
2A	0.7873	0.5360
2B	0.7964	0.5340
2C	0.8054	0.5380
2D	0.7733	0.5340
2E	0.7792	0.5320
2F	0.7814	0.5270
2G	0.7865	0.5250
2H	0.7943	0.5300
2I	0.7725	0.5260
2J	0.7730	0.5230
2K	0.7832	0.5260
2L	0.7853	0.5250
2M	0.7958	0.5280
2N	0.7713	0.5270
2O	0.7707	0.5200
2P	0.7787	0.5270
2Q	0.7847	0.5250
2R	0.7978	0.5280
2S	0.7710	0.5270
2T	0.7722	0.5210
2U	0.7781	0.5240
2V	0.7847	0.5210
2W	0.7943	0.5270
2X	0.7666	0.5270
2Y	0.7719	0.5200
2Z	0.2922	0.1950





















































































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Chain	Atom inclusion	Q-score
2a	 0.2902	 0.1830
2b	 0.2888	 0.1730
2c	 0.2722	 0.1730
2d	 0.2756	 0.1750
2e	 0.1898	 0.0700
2f	 0.1176	 -0.0060
2g	 0.0980	 -0.0180
2h	 0.1044	 -0.0180
2i	 0.2293	 0.1100
2j	 0.1907	 0.0680
2k	 0.1176	 -0.0050
2l	 0.0990	 -0.0180
2m	 0.1024	 -0.0190
2n	 0.2302	 0.1120
2o	 0.1805	 0.0640
2p	 0.1083	 -0.0090
2q	 0.0961	 -0.0190
2r	 0.1005	 -0.0210
2s	 0.2249	 0.1070
2t	 0.1907	 0.0730
2u	 0.1166	 -0.0010
2v	 0.1000	 -0.0190
2w	 0.1068	 -0.0180
2x	 0.2268	 0.1090
3A	 0.7960	 0.5220
3B	 0.7844	 0.5160
3C	 0.8011	 0.5290
3D	 0.7929	 0.5260
3E	 0.7830	 0.5260
3F	 0.7923	 0.5310
3G	 0.7874	 0.5110
3H	 0.7817	 0.5070
3I	 0.7891	 0.5190
3J	 0.7865	 0.5160
3K	 0.7777	 0.5180
3L	 0.7891	 0.5210
3M	 0.7850	 0.5090
3N	 0.7796	 0.5080
3O	 0.7918	 0.5200
3P	 0.7870	 0.5160
3Q	 0.7789	 0.5200
3R	 0.7873	 0.5210





















































































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Chain	Atom inclusion	Q-score
3S	 0.7883	 0.5120
3T	 0.7829	 0.5100
3U	 0.7947	 0.5220
3V	 0.7929	 0.5190
3W	 0.7821	 0.5190
3X	 0.7850	 0.5200
3Y	 0.7927	 0.5080
3Z	 0.7758	 0.5050
3a	 0.7903	 0.5170
3b	 0.7873	 0.5170
3c	 0.7772	 0.5180
3d	 0.7844	 0.5160
3e	 0.2782	 0.1720
3f	 0.2766	 0.1790
3g	 0.2566	 0.1360
3h	 0.2639	 0.1470
3i	 0.1239	 0.0080
3j	 0.2054	 0.0940
3k	 0.1817	 0.0530
3l	 0.1385	 0.0240
3m	 0.1249	 0.0060
3n	 0.2005	 0.0910
3o	 0.1734	 0.0480
3p	 0.1351	 0.0220
3q	 0.1219	 0.0030
3r	 0.1971	 0.0870
3s	 0.1636	 0.0390
3t	 0.1288	 0.0180
3u	 0.1268	 0.0110
3v	 0.2063	 0.0940
3w	 0.1680	 0.0400
3x	 0.1293	 0.0160
4A	 0.8046	 0.5330
4B	 0.7957	 0.5160
4C	 0.7948	 0.5200
4D	 0.8076	 0.5270
4E	 0.7883	 0.5240
4F	 0.7935	 0.5300
4G	 0.8017	 0.5240
4H	 0.7880	 0.5070
4I	 0.7900	 0.5110
4J	 0.8029	 0.5190





















































































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Chain	Atom inclusion	Q-score
4K	 0.7888	 0.5150
4L	 0.7885	 0.5220
4M	 0.8058	 0.5250
4N	 0.7880	 0.5080
4O	 0.7847	 0.5120
4P	 0.8005	 0.5190
4Q	 0.7897	 0.5150
4R	 0.7868	 0.5190
4S	 0.8032	 0.5240
4T	 0.7927	 0.5080
4U	 0.7897	 0.5130
4V	 0.8052	 0.5190
4W	 0.7853	 0.5160
4X	 0.7868	 0.5200
4Y	 0.7987	 0.5210
4Z	 0.7877	 0.5010
4a	 0.7850	 0.5090
4b	 0.7978	 0.5110
4c	 0.7839	 0.5120
4d	 0.7888	 0.5180
4e	 0.2751	 0.1520
4f	 0.2708	 0.1580
4g	 0.1298	 0.0090
4h	 0.1092	 -0.0200
4i	 0.1317	 0.0100
4j	 0.1117	 -0.0210
4k	 0.1234	 0.0070
4l	 0.1112	 -0.0240
4m	 0.1322	 0.0150
4n	 0.1141	 -0.0190
5A	 0.8043	 0.5280
5B	 0.7978	 0.5150
5C	 0.7954	 0.5220
5D	 0.8046	 0.5270
5E	 0.7880	 0.5160
5F	 0.7993	 0.5280
5G	 0.8020	 0.5170
5H	 0.7904	 0.5060
5I	 0.7906	 0.5100
5J	 0.7960	 0.5180
5K	 0.7789	 0.5060
5L	 0.7891	 0.5170





















































































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Chain	Atom inclusion	Q-score
5M	 0.7996	 0.5180
5N	 0.7936	 0.5060
5O	 0.7936	 0.5080
5P	 0.7942	 0.5170
5Q	 0.7772	 0.5050
5R	 0.7917	 0.5190
5S	 0.8032	 0.5210
5T	 0.7898	 0.5080
5U	 0.7924	 0.5110
5V	 0.7966	 0.5160
5W	 0.7789	 0.5060
5X	 0.7929	 0.5190
5Y	 0.7930	 0.5140
5Z	 0.7927	 0.5070
5a	 0.7903	 0.5090
5b	 0.8005	 0.5120
5c	 0.7754	 0.5010
5d	 0.7856	 0.5130
5e	 0.2644	 0.1560
5f	 0.2777	 0.1690
5g	 0.1307	 0.0140
5h	 0.1273	 0.0090
5i	 0.1341	 0.0150
5j	 0.1357	 0.0140
5k	 0.1337	 0.0150
5l	 0.1268	 0.0110
5m	 0.1429	 0.0250
5n	 0.1288	 0.0130
6A	 0.7956	 0.5320
6B	 0.7935	 0.5330
6C	 0.7921	 0.5210
6D	 0.7948	 0.5200
6E	 0.8020	 0.5250
6F	 0.7958	 0.5310
6G	 0.7909	 0.5240
6H	 0.7897	 0.5230
6I	 0.7865	 0.5100
6J	 0.7900	 0.5120
6K	 0.7967	 0.5160
6L	 0.7926	 0.5210
6M	 0.7848	 0.5250
6N	 0.7824	 0.5230





















































































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Chain	Atom inclusion	Q-score
6O	 0.7874	 0.5110
6P	 0.7894	 0.5130
6Q	 0.7982	 0.5180
6R	 0.7908	 0.5220
6S	 0.7850	 0.5260
6T	 0.7891	 0.5250
6U	 0.7898	 0.5120
6V	 0.7882	 0.5140
6W	 0.7923	 0.5190
6X	 0.7935	 0.5220
6Y	 0.7772	 0.5130
6Z	 0.7771	 0.5130
6a	 0.7820	 0.5050
6b	 0.7933	 0.5060
6c	 0.7915	 0.5090
6d	 0.7847	 0.5100
6e	 0.2483	 0.1420
6f	 0.2727	 0.1550
6g	 0.2640	 0.1590
6h	 0.2741	 0.1640
6i	 0.0896	 -0.0180
6j	 0.0907	 -0.0200
6k	 0.1278	 0.0090
6l	 0.1424	 0.0360
6m	 0.0955	 -0.0210
6n	 0.0932	 -0.0240
6o	 0.1386	 0.0170
6p	 0.1527	 0.0400
6q	 0.0921	 -0.0210
6r	 0.0917	 -0.0240
6s	 0.1278	 0.0120
6t	 0.1507	 0.0420
6u	 0.1043	 -0.0100
6v	 0.0956	 -0.0190
6w	 0.1347	 0.0200
6x	 0.1717	 0.0580
7A	 0.7943	 0.5430
7B	 0.7780	 0.5380
7C	 0.7900	 0.5390
7D	 0.7897	 0.5390
7E	 0.7961	 0.5350
7F	 0.7830	 0.5340





















































































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Chain	Atom inclusion	Q-score
7G	 0.7739	 0.5260
7H	 0.7850	 0.5240
7I	 0.7850	 0.5260
7J	 0.7862	 0.5250
7K	 0.7806	 0.5330
7L	 0.7684	 0.5270
7M	 0.7850	 0.5260
7N	 0.7798	 0.5260
7O	 0.7920	 0.5250
7P	 0.7844	 0.5360
7Q	 0.7693	 0.5300
7R	 0.7897	 0.5310
7S	 0.7833	 0.5280
7T	 0.7943	 0.5270
7U	 0.7815	 0.5250
7V	 0.7695	 0.5200
7W	 0.7786	 0.5250
7X	 0.7733	 0.5200
7Y	 0.7795	 0.5190
7Z	 0.2873	 0.1750
7a	 0.2654	 0.1630
7b	 0.2688	 0.1560
7c	 0.2756	 0.1740
7d	 0.2844	 0.1690
7e	 0.1215	 -0.0060
7f	 0.1459	 0.0350
7g	 0.1166	 0.0020
7h	 0.1863	 0.0710
7i	 0.1249	 0.0080
7j	 0.1268	 0.0050
7k	 0.1620	 0.0460
7l	 0.1307	 0.0130
7m	 0.2059	 0.0850
7n	 0.1278	 0.0110
7o	 0.1220	 -0.0050
7p	 0.1468	 0.0350
7q	 0.1268	 0.0070
7r	 0.2059	 0.0830
7s	 0.1259	 0.0080
7t	 0.1210	 -0.0050
7u	 0.1288	 0.0220
7v	 0.1351	 0.0170

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Chain	Atom inclusion	Q-score
7w	 0.2005	 0.0880
7x	 0.1361	 0.0190
8A	 0.7526	 0.5280
8B	 0.7585	 0.5340
8C	 0.7754	 0.5280
8D	 0.7731	 0.5330
8E	 0.7768	 0.5360
8F	 0.7593	 0.5290
8G	 0.7436	 0.5100
8H	 0.7579	 0.5170
8I	 0.7681	 0.5170
8J	 0.7614	 0.5210
8K	 0.7628	 0.5200
8L	 0.7515	 0.5130
8M	 0.7485	 0.5180
8N	 0.7570	 0.5220
8O	 0.7713	 0.5180
8P	 0.7669	 0.5230
8Q	 0.7652	 0.5260
8R	 0.7509	 0.5200
8S	 0.7480	 0.5200
8T	 0.7593	 0.5230
8U	 0.7693	 0.5200
8V	 0.7690	 0.5240
8W	 0.7675	 0.5240
8X	 0.7503	 0.5200
8Y	 0.7348	 0.5080
8Z	 0.7424	 0.5140
8a	 0.7573	 0.5100
8b	 0.7591	 0.5100
8c	 0.7620	 0.5130
8d	 0.7436	 0.5060
8e	 0.2542	 0.1630
8f	 0.2444	 0.1410
8g	 0.2527	 0.1600
8h	 0.2547	 0.1470
8i	 0.2415	 0.1380
8j	 0.2620	 0.1550
8k	 0.2512	 0.1600
8l	 0.2161	 0.1160
8m	 0.1390	 0.0430
8n	 0.0960	 -0.0200

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Chain	Atom inclusion	Q-score
8o	0.1102	-0.0000
8p	0.1371	0.0300
8q	0.2522	0.1610
8r	0.2302	0.1280
8s	0.1293	0.0310
8t	0.0975	-0.0200
8u	0.1102	0.0010
8v	0.1567	0.0420
8w	0.2502	0.1640
8x	0.2249	0.1250
8y	0.1327	0.0330
8z	0.0984	-0.0190
9A	0.7468	0.5330
9B	0.7299	0.5090
9C	0.7392	0.5170
9D	0.7430	0.5220
9E	0.7293	0.5140
9F	0.2473	0.1510
9G	0.2571	0.1640
9H	0.2610	0.1670
9I	0.2585	0.1720
9J	0.2571	0.1760
9K	0.1093	0.0020
9L	0.1513	0.0370
9M	0.2522	0.1630
9N	0.2137	0.1100
9O	0.1537	0.0640
9P	0.1210	0.0080
9Q	0.1288	0.0220
9R	0.1680	0.0500